University of Alberta

PERFORMANCE CHARACTERIZATION AND REGULATORY FEEDBACK CONTROL DESIGN FOR TIME-INVARIANT DISCRETE-TIME STOCHASTIC PROCESSES

by

Michael Gregory Forbes

A thesis submitted to the Faculty of Graduate Studies and Research in partial fulfillment of the requirements for the degree of **Doctor of Philosophy**.

in

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"He knew nothing of the fogbound, ice-choked channels
he was proposing to enter."

- Pierre Berton, *The Arctic Grail*

University of Alberta

Faculty of Graduate Studies and Research

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research for acceptance, a thesis entitled **Performance Characterization and Regulatory Feedback Control Design for Time-Invariant Discrete-Time Stochastic Processes** submitted by Michael Gregory Forbes in partial fulfillment of the requirements for the degree of **Doctor of Philosophy** in *Process Control.*

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This thesis is dedicated to my late father,
David A. Forbes.

Abstract

With motivations from the processing and manufacturing industries, this thesis investigates the relationship between the dynamics and stationary probability density function (PDF) for a class of time-invariant discrete-time stochastic nonlinear process models. For stationary stochastic processes, long-term behaviour is concisely summarized by the stationary PDF and quantities derived from the PDF, such as mean and variance, are often key targets for process control or measures of operational performance and product quality.

In dealing with processes subject to random disturbances, the vast majority of results published in the process control literature take a standard approach, which includes linear processes, quadratic objective functions, and Gaussian disturbances. This linear-quadratic-Gaussian (LQG) framework facilitates theoretical developments in systems science. Unfortunately, in many industrial situations, any of the three tenets of the LQG paradigm do not hold, leading to inaccuracies. A framework that recognizes the practical realities of the process industries includes nonlinear processes, non-Gaussian disturbances, and nonquadratic performance measures. In this framework, an exact implicit relationship between process dynamics and stationary PDF is given by an integral equation for which no general, and very few specific, closed-form solutions are known. Explicit knowledge of the PDF is required for evaluating performance measures; thus intractability of the dynamics-PDF relationship presents a barrier to design and analysis in non-LQG situations. The proposed approximate solution develops relationships between the moments of the PDF and the coefficients in a parameterization of the process dynamics, reducing the integral equation to a set of algebraic equations.

This dynamics-PDF approximation technique is applied to two different regulatory controller synthesis problems. In the first problem, the design target is a pre-selected PDF

for the closed-loop (CL) process. An appropriate PDF is chosen based on engineering or economic concerns and the problem is then to find the control law that will result in the required CL dynamics. The second problem considers control design with respect to nonsymmetric, nonquadratic performance measures.

The mechanics and results of the dynamics-PDF approximation and controller synthesis techniques are demonstrated through example process applications with numerical simulations.

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There are many fine persons who have provided support and great friendship to me since I moved to Edmonton to begin my graduate studies. While I thank all of you for helping to make my time here a wonderful experience, if I were to mention everyone these acknowledgements might end up filling more pages than the technical details of my research. So, I am going to name only those who have had a direct influence on this thesis and hope that the rest will forgive me.

First and foremost, I would like to thank my two advisors, Dr. J. Fraser Forbes and Dr. Martin Guay, for all of their advice, encouragement and patience over the course of this research project. Both of them took the time to provide numerous valuable criticisms and suggestions and to help me sort my good ideas from my bad ones. While they gave me the latitude to explore many interesting tangents, they also ensured that my focus always returned to the main project.

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I don't want to violate my criteria of only mentioning 'those who have had a direct influence on this thesis' by listing all of my friends from back in Scarborough, but I will mention Sonia Lawrence, a professor at Osgoode Hall Law School. Last summer I was asking her about how she dealt with the pressure to achieve good research results. To summarize her response, she said that your best research is the work that you accomplish and not the work that you think you can accomplish. This wasn't implying that whatever you produce is fine, but that when you've worked hard to accomplish something, you should take pride in it. That simple statement of confidence, so well-phrased, has helped me to gain satisfaction from my own results.

Robin Naidoo, a good friend and fellow student at the U of A, showed me the possibilities that exist when one has the independence of thought to take established knowledge and look for new applications. He also introduced me to the fun of collaborating in inter-disciplinary research. Maybe we'll get that paper written someday, Robin.

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"The magician's underwear has just been found in a cardboard suitcase floating in a stagnant pond on the outskirts of Miami. However significant that discovery may be – and there is the possibility that it could alter the destiny of each and every one of us – it is not the incident with which to begin this report."

– Tom Robbins, *Another Roadside Attraction*

1 Introduction

In the processing and manufacturing industries, processes are subject to random disturbances such as non-uniform feedstocks, sensor inaccuracies, fluctuating ambient conditions, etc. Often there is no practical way to measure these disturbances and so even with very good mathematical models and numerous, high-accuracy sensors, it is impossible to predict the behaviour of any process with complete certainty. As a result, techniques for process analysis and controller design that account for random behaviour have been developed. Minimum variance controllers (Astrom, 1970), Kalman filtering (Davis, 2002), and multivariate statistical process monitoring (Kresta *et al.*, 1991) are some well known examples. A common element in all of these techniques is the use of stochastic process models, *i.e.*, dynamic models that include a random component. These frequently prove to be adequate for control engineering purposes. For stochastic processes, the mean process trajectory is often the key characteristic of interest, but the dispersion around the mean is also very important.

This thesis investigates the relationship between the dynamics and the stationary probability density function (PDF) for a class of time-invariant discrete-time stochastic nonlinear process models. For stationary stochastic processes, long-term behaviour is concisely summarized by the stationary PDF and quantities derived from the PDF, such as mean and variance, are often key targets for process control or measures of operational performance and product quality (Desborough and Harris, 1992). In some situations, such as plant operation near an operational or product quality constraint the tail behaviour of the PDF is very important.

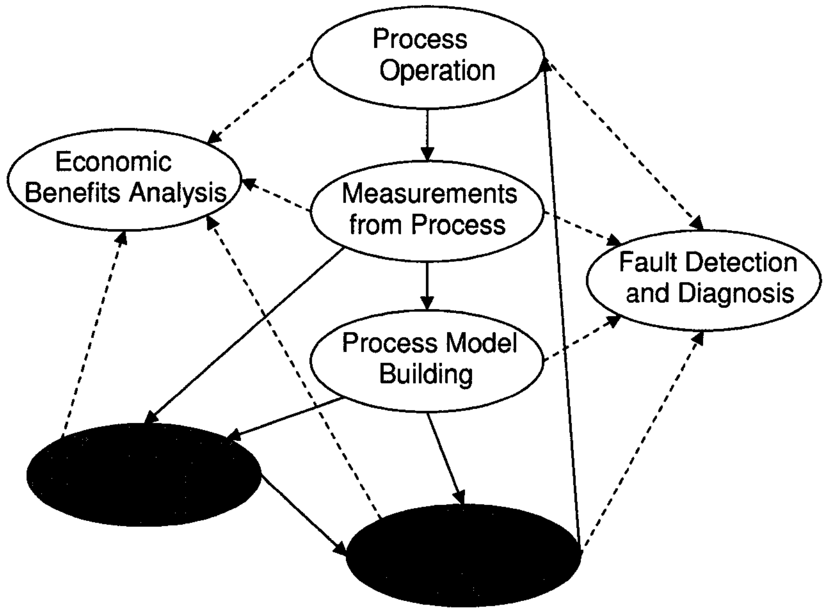


Figure 1.1: Diagram illustrating the interconnections between the many components in a broad process and control system framework.

In Figure 1.1, a broad overview of control engineering activities is given. The components of the figure form a web of interconnected activities. Process operation, at the top of the figure, is the physical basis and purpose for the other activities. Measurements of key process variables are taken using strategically placed sensors and the data is analyzed for building process models, in analyzing the performance of the process, in detecting and diagnosing faults and in determining the potential or realized benefits from implementing new process operating strategies. Using the process model, control systems are designed with the goal of improving process performance. The focus of this thesis is on the two areas shaded in the figure, performance analysis and control law design. For stochastic processes, both performance analysis and controller synthesis must account for the random behaviour of the process. In assessing the performance of a stochastic process, the data or process model can be analyzed to determine whether the behaviour, including the level of variability, is acceptable. Regulatory control laws designed for this situation have, either implicitly or explicitly, the goal of managing the random behaviour of the key process variables. These two topics are of great importance in influencing overall process operations. If a process is well-regulated, safe and profitable operation can be expected. As well, the task of fault detection becomes simpler as significant deviations from normal operation will be easier to identify. Proper characterization of a process leads to enhanced process knowledge and improved understanding of the process behaviour can be applied to better model building, better placement and selection of sensors, more accurate accounting of process economics and improved controller syntheses.

One representation of the behaviour of a random process is the stationary PDF. This function can be used as a key characterization of process performance. It can be set as a goal for some control law designs and as a key quantity that is manipulated in other designs. For the nonlinear and non-Gaussian processes discussed in this thesis, an exact implicit relationship between process dynamics and stationary PDF is given by an integral equation for which no general, and very few specific, closed-form analytical solutions are known. Explicit knowledge of the PDF is required for evaluating process performance metrics; thus the intractability of the dynamics-PDF relationship represents a significant barrier to the design and analysis in situations where nonlinear or non-Gaussian processes are being investigated. Since closed-form solution to this problem cannot be obtained, an approximate solution is proposed that can be applied to a wide class of processes. The approximation technique developed here takes advantage of the fact that a PDF can be described by its moments. Important features of the PDF, such as tail behaviour, are a consequence of the moments. By developing relationships between the moments of the PDF and the coefficients in a parameterization of the process dynamics, the integral equation is reduced to a set of algebraic equations in the two parameter sets. By choosing values for either parameter set, the other set of values can be obtained. In addition to the general approximation derivation, the special case of PDF parameterization using multivariate Gram-Charlier basis functions, which provide a practical and flexible representation of PDFs, is presented.

This dynamics-PDF approximation technique is applied in designing feedback control laws to regulate the long-term behaviour of discrete-time stochastic processes. Two regulatory controller synthesis problems are considered.

In the first design problem, the target for the design is a pre-selected PDF for the closed-loop (CL) process. An appropriate shape for the PDF is chosen, or designed, based on engineering or economic concerns and the problem is then to find the control law that results in the required CL dynamics. The proposed solution to this problem involves application of the dynamics-PDF approximation to find the parameterized CL process dynamics and control law. This synthesis technique is referred to as *PDF-shaping*.

The second controller synthesis problem considers performance objectives specified as the expected value of a nonsymmetric, nonquadratic loss functional. Solution to this general optimal control problem requires knowledge of the stationary PDF of the CL process. Application of the dynamics-PDF approximation technique in the optimal control framework results in a regulatory control law that is suboptimal with respect to design objective.

The mechanics of the dynamics-PDF approximation technique are demonstrated through example process applications. Results of the novel approaches to controller synthesis are illustrated with numerical process simulations.

The main motivation behind this research effort is the idea that the PDF is essential to the visualization of process behaviour and to the calculation of various measures of process performance. The PDF is therefore also essential to key areas of control engineering such as benefits analysis, performance assessment and controller design. For this reason the PDF should be a central focus in any effort to characterize process behaviour or to design control laws for stochastic processes.

It is emphasized here that the limitation of the research to stationary stochastic processes refers to the CL process. Open-loop processes with non-stationary characteristics, such as integrators or unstable processes, that can be made stationary through an appropriate feedback control design are therefore included in the discussion.

1.1 Standard Characterization and Control Methods

In dealing with stochastic processes, the vast majority of results published in the chemical process control literature take a standard approach, which is focussed on linear process models, quadratic performance functions, and disturbances with Gaussian distributions. This linear-quadratic-Gaussian (LQG) framework has the important advantage of facilitating theoretical developments in systems science.

There are two major optimal control design techniques for this framework: the linear quadratic regulator / Kalman filtering approach (Davis, 2002), which is referred to as LQ or LQG control; and the minimum variance control approach (Astrom, 1970; Harris, 1985). In both of these cases, the PDF of the CL process is Gaussian and so only the process variance is required to derive the control laws. Also, in both cases the result of the controller synthesis is a linear feedback control law.

Often, before control laws can be developed or other process control activities performed, it is necessary to analyze data obtained from historical process records or designed experiments. One of the more familiar types of analysis is the creation of dynamic process models from the data. However, there are many other types of data analysis that are valuable in a process control framework. Several papers serve to reinforce the importance of empirically estimated PDF's to benefits analysis studies. In (Latour, 1992) and (Latour, 1996), the need to estimate the PDF's of process variables from plant data is specifically addressed. In (Bao *et al.*, 2000), additional rigour is added to Latour's method. As well as requiring an estimate of the PDF, the identification of a linear dynamic model from plant data is demanded.

In designing, monitoring and maintaining control systems, the goal is performance. Performance may be defined in numerous different ways, both qualitative and/or quantitative. In some parts of this thesis, performance will be defined quantitatively in terms of a cost, or loss, function. This is a common technique used in industry and throughout the literature. Costs often include the consumption of energy and raw materials, and profit losses due to violation of operational constraints and production of off-specification products. Loss functionals should be carefully specified in the tradition of Taguchi's 'quality-loss', where quality is defined to account for broader societal demands on products (such as safety and environmental concerns) and not just engineering concerns (Ealey, 1988). The Taguchi approach makes a quadratic approximation of the true loss functional and, in doing so, is consistent with well known optimal control designs such as LQG control (Davis, 2002), minimum variance control (Astrom, 1970) and many model predictive control (MPC) designs (Seborg *et al.*, 1989). The quadratic, or variance, loss function is the well-accepted standard for objective function specification.

Techniques of stabilization for certain classes of stochastic processes are well-developed. One good reference is (Krstic and Deng, 1998). This reference discusses inverse optimal backstepping procedures for stabilization in probability of continuous time processes where the noise does not destabilize the process equilibrium. (Krstic and Deng, 1998) also discusses the disturbance attenuation problem, again for continuous time processes, where the noise will move the process away from what would otherwise be an equilibrium point. For this case, the concept of noise-to-state stability is introduced as an extension of the well-known input to state stability. Again, for the noise-to-state stabilization technique, the inverse optimality is discussed. Throughout this work there is no mention of the stationary PDF for the resulting CL processes. Additionally, because of the continuous-time focus of the book, the techniques cannot be applied in this thesis. At this time there do not seem to be references to any direct discrete-time extensions.

1.1.1 Limitations of Established Methods

The problem of regulatory control design for stochastic processes is typically considered from the perspectives of stability and optimality with respect to a cost function. Existing design techniques are mainly concerned with linear process models, quadratic objectives and Gaussian disturbances. This approach is used in the vast majority of results published in the chemical process control literature. An important advantage of this LQG framework is that theoretical developments can be made without explicit reference to the PDF of the system variables. Unfortunately, in industrial systems, any of the three tenets of the LQG framework do not hold, leading to inaccurate process analyses, unstable control designs, etc.

Justification for the Gaussian random disturbance assumption is often made with reference to the central limit theorem; however, some authors have suggested that, in practice, the assumption is not accurate. In (Orlov, 1991), it is argued that there is actually no theoretical justification for this assumption. While the assumption is valid if the disturbance results from the joint action of many small additive factors, it is rarely possible to prove that the action is not multiplicative or otherwise non-additive. Numerous experimental data sets are reviewed and shown to be predominantly non-Gaussian. It is concluded that data is generally non-Gaussian and in cases where a Gaussian PDF may be used as an approximation, the fit is never perfect.

(Viggers and Allen, 1994) asserts that although the data used in control practice is often assumed to be Gaussian, other distributions are common. The impact of noise distribution on controller performance is investigated through simulation of a number of controllers for an example process. It is concluded that control law performance could be strongly influenced by noise distribution. Additionally, it is observed that the effect of the disturbance distribution can be altered by the feedback control action.

In the LQG framework, the PDFs of the system state and output are Gaussian and therefore can be parameterized simply by the first two moments. In cases where the process is nonlinear or the disturbance non-Gaussian, the PDFs of the system will be non-Gaussian. Broadly applicable techniques to handle non-Gaussian PDFs have not been well developed. Consequently, this topic has not received much attention in the process control literature despite the existence of a number of results from the field of applied probability theory (Tong, 1990). For example, techniques of nonlinear time series analysis tend to focus on theoretical results for systems that have random inputs, but not inputs that may be manipulated, while the practicing control engineer requires results for processes with manipulatable inputs.

In many of the regulatory control design techniques found in the process control literature the focus is on the reduction of the process variance about a set operating point. While such techniques can be mathematically elegant in their derivation and often lead to practical control designs, they may fail to account for a number of additional concerns. For example, when a plant operates near a safety or performance specification, the tail behaviour of the process PDF becomes of critical importance. For example, the Taguchi approach to quality control takes advantage of a quadratic loss function (Ealey, 1988). However, there are numerous situations where such an approximation is misleading. For example, if the main influence on the cost function is associated with a product quality specification, the loss function can be highly nonsymmetric as it represents the large losses associated with low-quality production and the smaller losses associated with (unnecessarily) high-quality production. For this reason, other forms of loss functions are used in this thesis.

When working with general expectation-type loss functions, it should be noted that the integrand in these measures is the product of two functions: a loss functional, and the stationary PDF of the process. The loss functional is dictated by engineering concerns or process economics, and thus is pre-specified in a design context. In contrast, the PDF is a consequence of process dynamics, the form of the feedback control law and the PDF of the process disturbance. It is no surprise that this PDF can be extremely difficult to obtain. Consequently, the manipulation of the expectation-type loss functional is challenging since changes in the PDF and feedback control law are interdependent. General optimal control designs with respect to expectation-type loss functions are not available; however, a number of specific solutions have been achieved. If the process is linear and the disturbance is Gaussian, then solutions for the quadratic cost functionals are available (Astrom, 1970; Harris, 1985). In this case the control law is linear and the CL process generates a Gaussian PDF. Solutions for problems involving linear processes and with a general, nonsymmetric, nonquadratic cost functional in the process state have also been developed (Harris, 1992; Cain and Jansen, 1997). Again, the resulting control law is linear, so that the PDF of the CL process may be parameterized by the mean and the variance. A very different case is addressed in (Lee, 1990) where results for the general minimum variance cost functional are extended to a class of nonlinear processes. In this case, the control design procedure does not cover general nonsymmetric, nonquadratic cost functionals, nor does it consider the PDF of the CL process. While these three different control design techniques provide solutions to a number of related control problems, they do not solve the important case of design for a linear or nonlinear process with a nonsymmetric cost functional which includes the cost of control energy.

In the development of the design techniques given above, direct minimization of the cost function with respect to the manipulated variable is performed. Unfortunately, when working with more general cost functions direct minimization is not possible. The reason for this is that when the manipulated variable is used for feedback control, it becomes a function of the process state and cannot be extracted from the expectation operator. Additionally, it is unlikely that the CL process will be linear. In justifying this statement there are two cases to consider. First, if the open-loop process exhibits nonlinearities, which most industrial processes do (Shinskey, 2002), there is no reason to expect that the optimum control law will cause the CL process to behave linearly. Second, even if the open-loop process is linear, there is no reason to expect the optimum control law (with respect to a nonquadratic, nonsymmetric performance measure) to be linear. If a CL process is nonlinear, its stationary PDF will generally be non-Gaussian. Not only does this complicate evaluation and manipulation of the performance objectives, but it introduces an auxiliary equation to relate the dynamics of the CL process to the PDF of the CL process.

It is noted that the major barriers (lack of simple and reliable model identification techniques, complicated controller syntheses, absence of performance assessment and fault detection/diagnosis algorithms, etc.) to widespread adoption of a more flexible non-LQG framework can all be shown to have a common root cause: for nonlinear or non-Gaussian processes the relationship between process dynamics and the stationary PDF of the process variables is given by an integral equation for which no general and very few specific solutions are known. Since explicit knowledge of the PDF is required for evaluating process performance metrics, the intractability of the dynamics-PDF relationship represents a significant barrier to design and analysis in non-LQG situations.

1.1.2 Motivations for a New Approach

For most processes, there are safety, environmental or quality constraints on the operations. Frequently, processes operate near their constraints and an important goal for control design is to limit, if not eliminate, constraint violation. In the case of a process operating at a quality constraint, the consequences of constraint violation can be costly. The product may need to be reprocessed or reblended before it can be sold. If off-specification product is shipped to clients, it can lead to a loss of client confidence or even lost business. If off-specification product cannot be reprocessed, or sold at a lower price, it may be discarded outright. On the other hand, a product that consistently exceeds quality specifications may add to operational costs due to use of additional raw materials, energy, or processing time. A representation of the type of cost functional that may be associated with this type of process is given in Figure 1.2. The standard, quadratic loss functional around a chosen setpoint is shown, as well as a more realistic nonsymmetric loss functional. For such processes, the best operating strategy is to operate as close to the constraint as possible while keeping violations below some maximum tolerance. Of course, for many processes the loss functional will be dependent on the manipulated variable(s) as well as the state, or output.

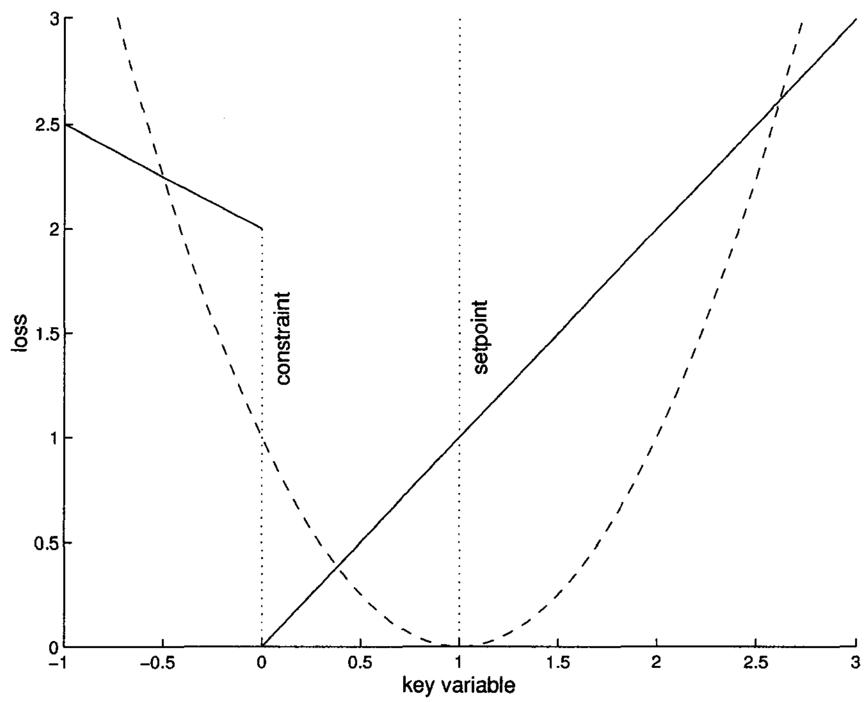
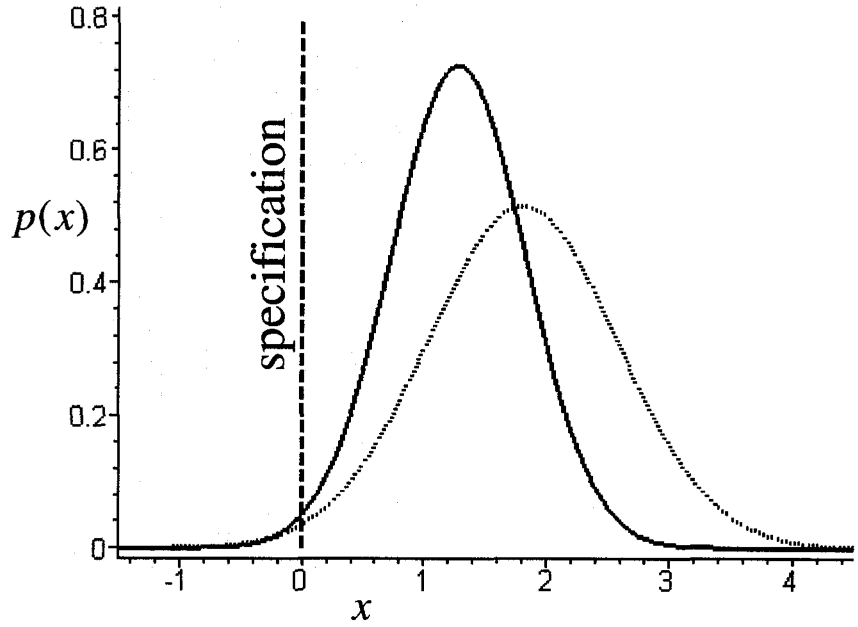


Figure 1.2: Illustration of a nonsymmetric, nonquadratic cost functional relating to a quality specification (solid line) and the well established quadratic cost functional about a setpoint (dotted line).

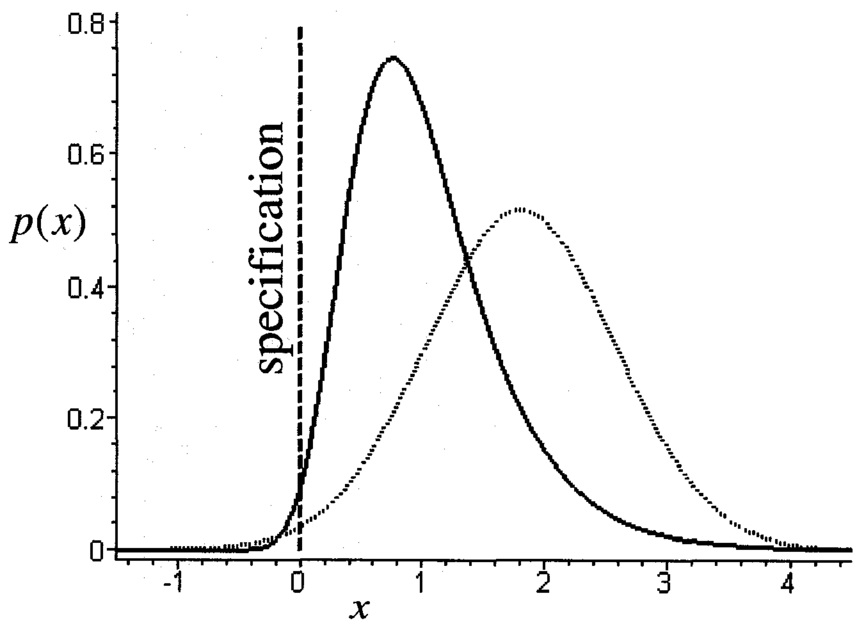
This type of situation is typical within a number of processing and manufacturing industries. In particular, drying processes, such as the one described in (Forbes *et al.*, 1984), provide straightforward examples. In (Forbes *et al.*, 1984), grain is being sent through a dryer. The main objective of the process is to ensure that moisture content is reduced below 15.5 percent wet basis. Over-moist grain cannot be safely stored and thus may not be sold, resulting in significant loss of profit. However, grain is sold by weight so as moisture is removed from the grain, profits are reduced. This trade-off between maximum acceptable moisture content and weight of product provides a nonsymmetric loss function in the process variable of interest. At the same time, the loss function for this process will include a term for the input, fuel flow to the dryer, reflective of the following considerations. To keep operating costs low, fuel flow should be kept to a low value; as well, for smooth operation, fluctuations in fuel flow should be kept to a minimum. This is by no means a singular example. There are many processes where economic and operational concerns lead to nonsymmetric cost functions. It has also been established that the loss functions for most processes are nonquadratic (Shinskey, 2002).

The usual approach to control design or redesign for a process at a quality constraint is to reduce process variance. A representative loss functional for this approach is given in Figure 1.2. The mean of the product quality may then be moved closer to the constraint without increasing the frequency of constraint violations. This approach to control (re-)design is illustrated in Figure 1.3(a). As discussed in (Latour, 1992) and (Latour, 1996), profits result not only from the change in setpoint, but also from the reduction in variance alone.

While this technique has proven to be successful, it does not account for a number of important issues. Focussing attention on mean and variance only often leads to the notion that the PDF is Gaussian. While it is true that for linear processes with Gaussian noise the PDF of the process is also Gaussian, this does not hold in general. Mean and variance do not capture features of non-Gaussian PDF's that may reflect significant process behaviour near a constraint. Also, even if the open-loop process has a Gaussian PDF, this does not necessarily mean that for the CL process a Gaussian PDF is desirable. Indeed, it may be useful to emphasize some non-Gaussian features of a PDF, such as reducing one of the tails. For these reasons, for analysis and design purposes, it is best to consider not just the first two moments of process PDF's but the entire PDF. Figure 1.3(b) illustrates this approach.



(a) Reduction in variance allowing a shift in mean.



(b) Complete re-shaping involving changes in mean, variance, and higher moments.

Figure 1.3: Illustrations of improved regulatory control through changes in PDF.

Clearly an approach that accounts for non-symmetric loss functions, nonlinear processes and non-Gaussian PDFs is needed to address these types of important industrial problems.

1.2 Building a New Approach

As discussed in the previous sections, techniques built around the standard LQG framework, while well-accepted and successful in many industrial situations, do have some limitations and shortcomings that can sometimes prove significant.

As a remedy to these shortcomings, a framework that recognizes the practical realities of industrial processes is proposed. This includes nonlinear process models, nonquadratic performance objectives, and non-Gaussian PDFs, *i.e.*, a non-LQG framework. While some results for this framework are available in the literature, this thesis takes a different perspective to add additional insight. Process behaviour is examined with a focus on the relationship between the CL process dynamics and the PDF of the CL process.

The main ideas motivating this research are as follows. Disturbances are an unavoidable fact in real-world process operations. Similarly, nonlinearity and nonquadratic objectives are practical realities. Efforts to circumvent these using standard techniques result inevitably in incomplete analyses and inaccurate techniques. Process characterization and control design techniques that can be applied without unjustified simplifications of the true situation should be developed. A key element linking all the process engineering activities in the non-LQG framework is the stationary process PDF. The focus of the work in this thesis is on the stationary PDF. It is viewed as a means of summarizing concisely the behaviour of the process and the target for controller design. While control engineers usually manage process behaviour by reducing process variance, more advantageous designs may be achieved by focussing on the entire PDF instead of just the second moment.

It is the goal of this research to develop techniques of process analysis, data analysis and control law design applicable to processes with non-Gaussian PDF's. Topics that will be addressed include: explicit determination of process PDFs from the process model or data; controller design for stochastic processes that enables control engineers to shape the process PDF; and control law design with respect to general objective functions. In the latter case the optimal control problem is re-formulated to highlight the barrier to solution presented by the dynamics-PDF relationship.

Figure 1.4 provides an illustration of the CL process as a PDF-altering operator. The long-term behaviour of a stationary random disturbance is best summarized by its PDF, which is treated as the argument. The process, over the long-term and in a very general sense, filters the disturbance. The filtered disturbance, assuming stationarity is preserved, may then also be summarized by its PDF, which is treated as the result of the operation. Therefore, process behaviour, when observed over a long time period, can be viewed as the re-shaping of the disturbance PDF.

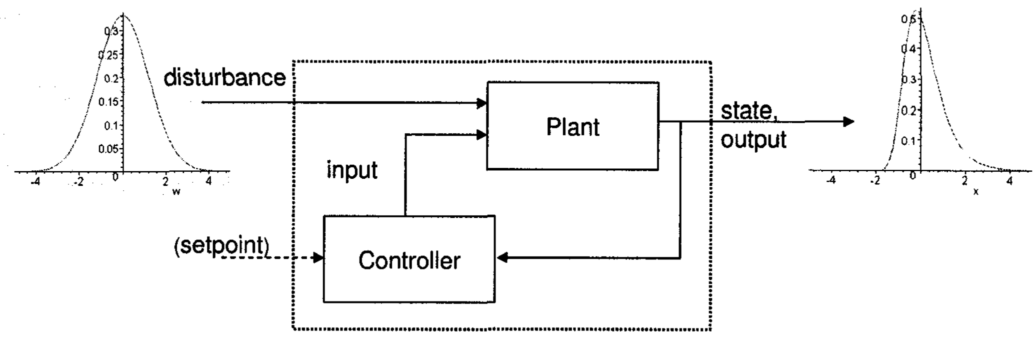


Figure 1.4: Diagram illustrating the notion of a regulated process as an operator to warp and re-shape distributions.

This idea relates to the investigation in (Viggers and Allen, 1994) where the influence of noise distribution on control performance is investigated. It is noted that feedback control action can alter the distribution of the process output. Instead of using probabilistic techniques, (Viggers and Allen, 1994) uses simulations for the investigation. While filter design for different types of noise distributions is considered, actual distribution oriented control design is not the focus of the article.

The use of probabilistic techniques to formulate the relationship between the stationary process PDF and process dynamics results in an integral equation for which few specific solutions are known. A number of approximation techniques for solution to this equation are given in (Tong, 1990) for the case of processes without manipulated variables. These focus on polynomial expansions of the nonlinear difference equation and make use of generating functions. One special case of these types of approximation methods is the common practice of linearizing and centering the system model, so that only the covariance matrix must be calculated. In this thesis, manipulated variables are included explicitly. Generating functions and approximation of open-loop process dynamics are not required. By parameterizing the CL process dynamics and the stationary PDF, the integral equation is reduced to a set of algebraic equations in the two parameter sets. By choosing values for either parameter set, the equations can be solved to give values for the other set.

The problem of designing a feedback control law to regulate the long-term behaviour of a discrete-time stochastic process is considered. Two different approaches to controller synthesis are investigated with the approximation of the dynamics-PDF relationship applied to both.

The first synthesis technique, referred to as PDF-shaping, considers control design for a target stationary process PDF. The framework developed here takes advantage of the fact that a PDF can be described by its moments; other features of the PDF, such as tail behaviour, are a consequence of the moments. By developing relationships between the moments, or coefficients of the PDF and the coefficients in a control law parameterization, an approximate control law is developed to shape the process PDF as desired. It is up to the process engineer to choose an appropriate shape for the process PDF based on economic or engineering concerns. This pre-selected distribution then becomes the target of the design. The feedback control law that will result in the CL process having the target PDF could then be derived.

To date, this approach to stochastic control design has received very little attention in the process control literature. The most closely related work may be (Karny, 1996) where a finite horizon control law formulation is derived by selecting a target PDF for the joint distribution of the process states and inputs over the time horizon. The result is a framework where time-evolving control laws can be created that include a random component. The focus of this paper is on finite control horizons and the goal of the design is to minimize the distance between target and actual process PDFs.

Another related work is (Wang, 1999), where a control strategy is developed for a distributed parameter system. In this case, there is a PDF associated with the quality of the process variable of interest at each instant of time. Wang reformulates the optimal stochastic control problem so that the goal of the design is to bring, over time, the distribution of the process variable to some target PDF. The result is an adaptive control law that attempts to match a univariate target PDF at each time step. In this approach, a model relating the inputs to the output PDF is developed using a spline network to represent the output PDF, so that the PDF may be shaped by the process inputs. It is the parameters of the PDF that are adjusted to match the target PDF as closely as possible, in the sense of minimizing the integral squared difference between the PDFs. The control actions are then back-calculated from the PDF parameters.

There are also a number of other, related works by Wang (Wang, 2000; Wang and Zhang, 2001; Wang, 2002). In (Wang, 2000), the novel B-spline model of the dynamic process PDF is applied to a number of additional problems, including mean and variance control, and fault diagnosis applications. This reference provides a comprehensive guide to the use of this unique approach for many different applications in both discrete and continuous time. This approach is further extended in (Wang and Zhang, 2001) and (Wang, 2002). In the former, a B-spline technique is used to model ARMAX type processes with arbitrary bounded disturbances and the goal of the control design is for the process PDF to evolve over time in a pre-specified manner. In the latter, no pre-specified PDF trajectory is given. Instead, the entropy concept is used to create an objective function for the control design. Control laws are designed to minimize the entropy-based objective and this causes the process PDF to evolve in an optimal manner. The types of processes modelled in this case are similar to those in the present work; however, there are major differences in the types of process model employed and in the way in which PDF is manipulated in the controller designs.

The technique developed here differs from the approaches of Karny and of Wang by focusing on the stationary state PDF and not the joint PDF or time-evolving PDF; also, a static feedback control law results. The difference between the two approaches can be best explained with reference to control of the process mean. In (Wang, 2000), the process mean is a measured or estimated quantity at each time step and the trajectory of this quantity is controlled. In the present work, there is only the scalar value of the process variable at each time step and the mean of the process may only be calculated by time averaging the value of the process variable. The same difference exists for the PDFs. In Wang's works, the PDF exists and evolves at each instant of time, while in the present work, the PDF is a summary of process behaviour over a long period of time. Additionally, in the proposed approach, a standard state-space model is used to represent the process dynamics.

The second synthesis technique investigated is performance-oriented controller design where the objective for design is specified as the expected value of a nonsymmetric, nonquadratic loss functional. There have been only a few results for this research area published in the literature. These were given in the preceding sections. In this thesis, it is shown that to properly address the general problem, it is necessary to relate CL process dynamics to the stationary PDF. Since explicit relationships are available for only a few special cases, solution of the general optimal control problem is not possible. Application of the approximation technique in the optimal control framework results in regulatory control laws suboptimal with respect to design objective.

As a part of the framework that this thesis outlines, the multivariate Gram-Charlier basis is presented as a flexible tool for PDF parameterization. The GC PDF is used in the proposed dynamics-PDF approximation technique and in the two controller synthesis techniques. It is both a mathematically rich structure, and a practical analysis and design tool.

1.3 Scope of the Thesis

This thesis examines performance characterization and controller synthesis for a class of time-invariant, discrete-time, stochastic, nonlinear processes, specifically those represented by a Markov ('state-space') process model, nonlinear in the dynamics, and additive in the random term. Discrete-time models were chosen as the focus of the research work because of their great relevance to the processing and manufacturing industries. With digital computers dominating the information and control systems of industrial plants, process variables are manipulated and sampled only at discrete instants of time, making discrete-time models an attractive way of representing process behaviour. Additionally, these systems are one of the obvious extensions of the time-invariant, discrete-time linear system models which have been studied extensively in the literature. The restriction of the investigation to the class of process models that have additive disturbance terms allows for some progress to be made in this challenging research area. While the models are simple enough to allow for a thorough investigation of the research topics, they are also rich enough to yield useful, broadly applicable results.

Perhaps a more realistic approach to modelling and analysis of industrial processes would be to use sampled-data techniques. The underlying idea of the sampled-data approach is that the real processes underlying data evolve continuously, while measurements are made only at discrete time intervals. It cannot be denied that this approach seems to be more in line with the true situation in industrial plants; however, the basic ideas and framework developed in this thesis can be applied to any number of process model classes. It is more convenient in the current study to use discrete-time processes as a basis for the introduction of the framework and its development.

The proposed work on regulatory feedback control law design focusses almost exclusively on state feedback control. This restriction is necessary so that CL processes can be formulated without the complications associated with observer design for nonlinear processes. Nonlinear observer design is an extremely challenging area that remains largely unsolved.

Wherever possible, the most general results are given. In most cases these generalities are followed with specialized results which either help to clarify the general result, or can be viewed independently as a valuable contribution to the thesis. For example, in developing an approximate solution to the dynamics-PDF relationship, the framework is first introduced for general parameterizations. The Gram-Charlier PDF parameterization is then introduced as a design tool with a number of advantages and to further develop some aspects of the technique. Similarly, the PDF-shaping control design technique is developed for general random process disturbances. However, the technique is specialized to the case of Gaussian disturbances to better illustrate the key points.

1.3.1 Major Contributions of the Thesis

Three main ideas are developed in this thesis. First, it is argued that key aspects of process behaviour are fully characterized only by the stationary PDF of the process. While standard techniques focus obliquely on the PDF through quadratic performance objectives, the approach taken here directly considers the full PDF for the description of process performance. Second, a novel regulatory controller synthesis technique, PDF-shaping, is introduced. This concept makes the achievement of a desirable target PDF (and thus achievement of desirable process behaviour) the objective of the control design. Third, the optimal control design problem for stochastic processes is re-examined from the perspective that knowledge of the stationary PDF is necessary to properly characterize process behaviour. In considering an expectation-type objective function, it is shown that the cost functional and the process PDF may be altered by process dynamics and that both influence the value of the cost function. The relationship between control law, process PDF, and objective is examined and a technique allowing the approximate solution of general cases is developed.

The results presented in this thesis lay down a framework for process characterization and control design on which future research initiatives can be built. As additional results are added to those given in this thesis, the overall approach forms a basis for an alternative paradigm in process control. The bulk of this thesis focuses on development of three ideas. While these ideas and results are illustrated using appropriate example process analyses and simulations, the practical implementation issues are left to future projects.

1.3.2 Outline of the Thesis

The remainder of this thesis is organized as follows. Chapter 2 reviews some topics from mathematics and statistics that are used throughout later chapters. In particular some concepts from applied probability theory are essential to the research topics. Chapter 3 discusses process characterization via the stationary PDF. Two different characterization techniques are given. The first characterization technique is developed as a process analysis tool. By considering the probabilistic properties of the process model, an approximation of the stationary process PDF is derived. The second technique is data-driven, using non-Gaussian data to recover an approximate PDF for the stationary process. Chapter 4 introduces the concept of PDF-shaping controller synthesis for stochastic first-order processes. Focusing on these simple processes allows for the technique to be clearly developed without the distractions of peripheral details. As well as deriving the general technique, the application of Gram-Charlier PDFs as a special case is given, as well as accuracy and stability analyses. A nine-step algorithm integrating the PDF-shaping technique into a complete controller (re-)design procedure concludes this chapter. The additional details needed to extend the PDF-shaping design to higher-order processes are given in Chapter 5. Process features such as delay and coloured noise are viewed as inherent limitations on the possible stationary PDFs that the process can achieve. Additionally, in the more general multidimensional framework, a second method for parameterizing the control structure is introduced. In Chapter 6 the role of the stationary PDF in optimal regulatory control designs is examined. First, complete problem formulations are given for the general and specific optimal control problems and it is shown how the dynamics-PDF relationship creates a barrier to the solution of these problems. The approximate solution to the equation governing the dynamics-PDF relationship is then applied to the specific optimal control problem. This results in a suboptimal but effective design technique. Finally, Chapter 7 briefly summarizes the work completed and suggests a number of potentially fruitful directions for future research endeavors. The importance of the latter should not be underestimated. Research into the analysis and synthesis of stochastic nonlinear processes is very much an open area in systems science. The approach taken in this thesis, by focusing on the stationary PDF, links elements from a number of different topics, that constitutes a new perspective on controlled process behaviour. The work completed in this thesis should be viewed as only the first steps along the path of fully developing a PDF-oriented perspective, while each of the stated future research directions represents several additional steps. Taken all together, and with many additional research initiatives, the sum has the potential to be a fruitful paradigm in systems science which focusses on the direct concerns of the process industries.

"Karma Police arrest this man he talks in maths."

– Radiohead

2 Preliminaries

It is useful to review some concepts from mathematics and statistics that will be used later in this thesis. Only the main ideas of the key concepts are given here while references are provided for those who require or desire additional information. Some additional concepts that enter the discussion, but are not repeatedly called upon, are included in Appendix B.

2.1 Probability

2.1.1 Basics

A fundamental aspect of the modelling of many physical phenomena is the concept of a distribution function. The (cumulative) distribution function, $P(\cdot)$, is a real-valued function on $\Re^n$ defined as: $P(\mathbf{z}) = Pr(\zeta \in (-\infty, \mathbf{z}])$. Consequently, $P(\cdot)$ has the following properties (Resnick, 1999):

1. $P(\mathbf{z})$ is right continuous,
2. $P(\mathbf{z})$ is monotone non-decreasing,
3. $P(\mathbf{z})$ has limits at $\pm\infty$ such that $\lim_{\mathbf{z}\to\infty} P(\mathbf{z}) = 1$ and $\lim_{\mathbf{z}\to-\infty} P(\mathbf{z}) = 0$

The distribution function provides all the information required to compute the probabilities of events. At times it can be cumbersome to perform mathematical manipulations with the distribution function; and often the closely related probability density function (PDF) is used instead.

Probability Density Functions

In this thesis, PDFs will be defined as real-valued functions, $p(\cdot)$, on $\Re^n$ with the following properties (Devore, 1995):

1. Non-negativity: $p(\mathbf{z}) \geq 0 \quad \forall \mathbf{z} \in \Re^n$
2. Unit measure: $\int_{\Re^n} p(\mathbf{z})\, \mathbf{dz} = 1$
3. Relation to distribution:
   $Pr(\mathbf{z} \in \Omega) = \int_{\Omega} p(\mathbf{z})\, \mathbf{dz}$, *i.e.* the probability that $\mathbf{z}$ is within some region Ω equals the integral of the PDF over that region.

From the third part of the definition, it can be seen that distribution functions and PDF's are related by differentiation / integration.

The Gaussian PDF

One of the most frequently used PDFs in mathematics, statistics, engineering and the sciences is the Gaussian PDF. The multivariate case is parameterized by a mean vector μ and covariance matrix $\mathbf{\Sigma}$ and is denoted $N_{\mu,\mathbf{\Sigma}}(\cdot)$.

$$N_{\mu,\mathbf{\Sigma}}(\mathbf{z}) = \frac{1}{\left(\sqrt{2\pi}\right)^n} \frac{1}{(\det(\Sigma))^{\frac{1}{2}}} \exp\left(-\frac{(\mathbf{z}-\mu)^T \Sigma^{-1} (\mathbf{z}-\mu)}{2}\right) \tag{2.1}$$

This simplifies to the univariate Gaussian PDF with mean μ and variance σ^2.

$$N_{\mu,\sigma}(z) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(z-\mu)^2}{2\sigma^2}\right) \tag{2.2}$$

Moments

The following notation is used is defining multivariate moments. A multivariate moment, $m^{\mathbf{i}}$, is defined as follows:

$$m^{i_1,i_2,\ldots,i_n} = E\left[\mathbf{z}^{i_1,i_2,\ldots,i_n}\right] = E\left[{z_1}^{i_1}{z_2}^{i_2}\ldots{z_n}^{i_n}\right] = \int\limits_{\Re^n} {z_1}^{i_1}{z_2}^{i_2}\ldots{z_n}^{i_n} p(\mathbf{z})\,\mathbf{dz} \quad (2.3)$$

where $E[\cdot]$ is the expectation operator. The subscripts refer to the corresponding element of the vector $\mathbf{z}$. This notation allows the moments to be indexed by ascending total degree with ties broken by lexicographical order (Cox *et al.*, 1997). Thus a vector of moments is:

$$\mathbf{m}_p = \int_{\Re^n} \begin{bmatrix} \mathbf{z}^{1,0,0,0,\ldots} \\ \mathbf{z}^{0,1,0,0,\ldots} \\ \vdots \end{bmatrix} p(\mathbf{z})\,\mathbf{dz} \quad (2.4)$$

For an n-variate PDF the number of moments of r^{th}-order is given by combination with replacement, $\binom{n+r-1}{r}$.

Transformation of Random Variables

The following theorem for computing the PDF of an n-dimensional random vector, ζ, from the PDF of the functionally related n-vector, $\mathbf{z}$, is taken from (Jazwinski, 1970). Let $\zeta = \mathbf{f}(\mathbf{z})$. If $\mathbf{f}^{-1}$ exists and both $\mathbf{f}$ and its inverse are continuously differentiable, then:

$$p_\zeta(\zeta) = p_z\left(\mathbf{f}^{-1}(\zeta)\right)\left\|\frac{\partial \mathbf{f}^{-1}(\zeta)}{\partial \zeta}\right\| \quad (2.5)$$

where $\left\|\frac{\partial \mathbf{f}^{-1}(\zeta)}{\partial \zeta}\right\|$ is the absolute value of the Jacobian determinant.

Addition of Random Variables

Take a sum of independent random variables:

$$\mathbf{z} = \zeta + \xi \quad (2.6)$$

where the PDFs for the variables on the right-hand side are, respectively: $p_\zeta(\zeta)$ and $p_\xi(\xi)$. The PDF of $\mathbf{z}$ can be derived from these PDFs using the equation (Zwillinger, 1996):

$$p_z(\mathbf{z}) = \int_\Omega p^*(\mathbf{z}|\xi)\, p_\xi(\xi)\mathbf{d}\xi \quad (2.7a)$$

$$= \int_\Omega p_\zeta(\mathbf{z}-\xi)\, p_\xi(\xi)\mathbf{d}\xi \quad (2.7b)$$

where Ω is the domain of ξ and $p^*(\mathbf{z}|\xi)$ represents the 'transition PDF from ξ to $\mathbf{z}$', or the PDF for $\mathbf{z}$ given ξ.

2.1.2 Deducing the PDF

In many situations a set of data is available and it is desired to know whether the data is consistent with a certain type of distribution. A number of statistical tests are available to resolve this question of distributional agreement. Here, two tests, one qualitative and one quantitative, are summarized briefly.

Probability Plots

Here we describe probability, or quantile-quantile, plots following the exposition given in (Devore, 1995). For a set of (univariate) data, $z_1, z_2, \ldots, z_N$, it is often desired to know whether the given sample is taken from a certain type of population distribution (e.g. Gaussian). Probability plots provide an effective way to check distributional assumptions. The basic idea of these plots is that if the distribution used to create the plot is correct, then the points on the plot fall on a straight line. If the actual distribution is different "the points should depart substantially from a linear pattern" (Devore, 1995).

Constructing a probability plot involves comparing the percentiles of the sample data and the corresponding percentiles of the candidate distribution. The first step is to determine the sample percentiles by placing the N observations in ascending order. The i^{th} smallest observation then represents the $\left(100\frac{(i-0.5)}{N}\right)^{th}$ sample percentile. Population percentiles are then calculated from the candidate distribution for each percentage, $100\frac{(i-0.5)}{N}$. Denoting the $\left(100\frac{(i-0.5)}{N}\right)^{th}$ population percentile as $\eta\left(\frac{(i-0.5)}{N}\right)$, the percentiles are calculated from:

$$P\left(\eta\left(\frac{(i-0.5)}{N}\right)\right) = \frac{(i-0.5)}{N} \tag{2.8}$$

where $P(\cdot)$ is the candidate distribution function. The probability plot is then created by plotting the coordinate pairs ($\eta\left(\frac{(i-0.5)}{N}\right)$, i^{th} smallest sample observation). For plots created by this procedure, the points should fall close to a 45° line when the candidate distribution is correct.

An example probability plot, generated by the MATLAB computer software package,

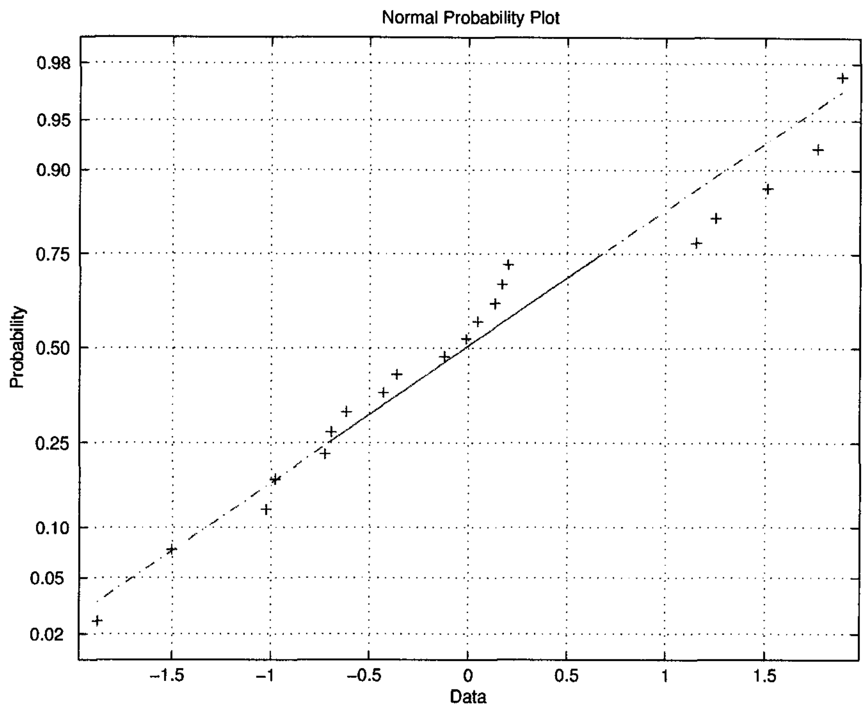


Figure 2.1: A normal probability plot, indicating Gaussian data.

is given by Figure 2.1. The data set here is actually Gaussian, and it can be seen that the points fall roughly along a straight line.

This concept may be extended to allow for comparison of sampled data to an entire family of distributions (instead of a single specific distribution); in particular, Gaussian probability plots are frequently used to assess whether any Gaussian distribution (with some unspecified mean and variance) can plausibly model the data. The details of such extensions may be found in (Devore, 1995).

The Goodness of Fit Test

While probability plots provide a good qualitative test of distributional agreement, sometimes a quantitative test is preferred. The goodness of fit test assesses whether a null hypothesis that the data agree with a given distribution is acceptable. Again, the description given here follows (Devore, 1995).

Given a set of data, $z_1, z_2, \ldots, z_N$, and a PDF, $p(\cdot)$, representing a candidate distribution for the data, it is desired to know whether the two are plausibly consistent. The test proceeds by dividing the domain of the data and PDF into a number of intervals or bins, as is done in creating a histogram. By comparing the number of observations in each bin to the expected number calculated from the PDF, a chi-squared test of distributional agreement is developed. The domain is divided into n bins $[a_0, a_1), [a_1, a_2), \ldots, [a_{n-1}, a_n)$. The number of observations in the bin $[a_{i-1}, a_i)$ is denoted N_i and the expected number of observations, o_i, is given by:

$$o_i = N \int_{a_{i-1}}^{a_i} p(z)dz \tag{2.9}$$

The bins should be selected so that $o_i \geq 5 \quad \forall i$. The sum of squares of differences between number of observed and expected observations is used to create the test statistic:

$$\chi^2 = \sum_{i=1}^{n} \frac{(N_i - o_i)^2}{o_i} \tag{2.10}$$

If $\chi^2 \geq \chi^2_{\alpha,n-1}$, where $\chi^2_{\alpha,n-1}$ is the critical value from the chi-squared distribution with $n-1$ degrees of freedom, then, with a level of significance of α, agreement of the candidate distribution with the data is rejected.

This goodness of fit test may be extended to situations where a family of distributions is being considered and maximum likelihood estimates of the parameters are made from the data. Details are given in (Devore, 1995).

2.2 Discrete-Time Stochastic Processes

Examination of the PDF for the state of a dynamic system leads to many important concepts. A few of the key concepts are discussed here.

2.2.1 Process Models

This thesis examines time-invariant discrete-time stochastic nonlinear processes. The most general model for these processes is (Jazwinski, 1970):

$$\mathbf{x}(t+1) = \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t), \mathbf{w}(t)) \tag{2.11}$$

where: $\mathbf{x}(t)$ is the process 'state' vector of dimension n_x; $\mathbf{u}(t)$ is the manipulated variable, or input, vector of dimension n_u; $\mathbf{w}(t)$ is an independent and identically distributed (iid) random disturbance sequence of dimension n_w, with PDF $p_w(\mathbf{w})$; and t is an integer-valued time index. This form of dynamic equation may also be referred to as a stochastic vector difference equation (Jazwinski, 1970).

In some situations, the state of the process may not be measured directly; instead, the available measurement is related to the process state through an output equation, such as:

$$\mathbf{y}(t) = \mathbf{f}_y(\mathbf{x}(t)) \tag{2.12}$$

Here the n_y-dimensional output $\mathbf{y}(t)$ is not necessarily of the same dimension as the state. Although the majority of this work focusses on characterization of the process state and state feedback control methods, there are times where extension to include the output equation (2.12) is possible.

Equation (2.11), while the most general time invariant model available, is beyond the scope of this thesis. Few general results are available without restricting attention to a sub-class of models. In this thesis, a simpler process model is considered:

$$\mathbf{x}(t+1) = \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t)) + \mathbf{B}\mathbf{w}(t) \tag{2.13}$$

where $\mathbf{x}(t) \in \Re^{n_x}$, $\mathbf{u}(t) \in \Re^{n_u}$ and the disturbance, $\mathbf{w}(t) \in \Re^{n_w}$, is included in an additive term on the right-hand side. The vector function $\mathbf{f}(\cdot,\cdot) \in \Re^{n_x}$ is a smooth mapping in its arguments. The $n_x \times n_w$ matrix $\mathbf{B}$ can prove cumbersome in process analysis. Fortunately, by reordering the states, and possibly with a linear changes of variables, it is possible to rewrite the process model to eliminate $\mathbf{B}$. There are a number of cases to consider.

First, when $n_x = n_w$ and the matrix $\mathbf{B}$ is full rank, a new disturbance variable, $\omega = \mathbf{B}\mathbf{w}$, may be created with a derived PDF given by the transformation of random variables theorem of the previous section.

If $n_x > n_w$ then a linear change of variables can be used to create a new matrix of the form $\begin{bmatrix} \tilde{\mathbf{B}} \\ 0 \end{bmatrix}$ where $\tilde{\mathbf{B}}$ is square. If it is also full rank, then a new disturbance variable can be created as in the previous case.

If $n_x < n_w$ then, possibly with a change of variables, the disturbance term should be written as $\omega = \tilde{\mathbf{B}}_1\mathbf{w}_1 + \tilde{\mathbf{B}}_2\mathbf{w}_2$ where the disturbance is partitioned so that $\mathbf{w}_1$ is n_x-dimensional and $\tilde{\mathbf{B}}_1$ is full rank. The following modified version of the transformation of random variables theorem may then be used to derive a PDF for ω.

Let $\omega = \tilde{\mathbf{B}}_1\mathbf{w}_1 + \tilde{\mathbf{B}}_2\mathbf{w}_2$ where the dimensions of ω and $\mathbf{w}_1$ are equal and $\tilde{\mathbf{B}}_1$ is full rank. When the (joint) PDF for w is $p_w(\mathbf{w}_1, \mathbf{w}_2)$ the derived PDF, $p_\omega(\omega)$, for ω is given by:

$$p_\omega(\omega) = \int_{-\infty}^{\infty} p_w\left(\tilde{\mathbf{B}}_1^{-1}\left(\omega - \tilde{\mathbf{B}}_2\mathbf{w}_2\right), \mathbf{w}_2\right)\left\|\det \tilde{\mathbf{B}}_1^{-1}\right\| \mathbf{dw}_2 \tag{2.14}$$

This is a special, extended case of the transformation of random variables theorem.

In the cases listed above, there are requirements of square, invertible matrices; while sometimes for the relationship $\omega = \mathbf{Bw}$ the dimensions of ω and $\mathbf{w}$ are equal but $\mathbf{B}$ is not invertible. In this case, a linear transformation should be used to get a matrix with the form $\begin{bmatrix} \tilde{\mathbf{B}} \\ 0 \end{bmatrix}$ where the matrix $\tilde{\mathbf{B}}$ is full rank. The technique of the previous case can then be applied.

Using these techniques, process models with the form of equation (2.13) can always be written in the form:

$$\mathbf{x}^{(1)}(t+1) = \mathbf{f}^{(1)}(\mathbf{x}(t), \mathbf{u}(t)) + \mathbf{w}(t) \tag{2.15a}$$

$$\mathbf{x}^{(2)}(t+1) = \mathbf{f}^{(2)}(\mathbf{x}(t), \mathbf{u}(t)) \tag{2.15b}$$

Throughout this thesis, we will refer almost exclusively to processes with the form of equation (2.15a), *i.e.* assuming that $n_x = n_w$, with the understanding that the results apply *mutatis mutandis* to the broader model (2.15). When the extensions are not straightforward, the salient details are given.

This state-space model (2.15) can be broadly applied. It can be used to represent input-output models of processes as well as those that recognize a true internal process state. Additionally, features such as delay, coloured noise, high-order dynamics, multiple inputs and multiple outputs can all be incorporated into the model structure.

Example 2.2.1 The realization of state-space forms of the ARIMA models commonly used in linear time series analysis is easily achieved. By creating a state vector consisting of an appropriate number of past and present outputs and inputs, the desired form is obtained. The same technique may also be applied to nonlinear ARIMA models. As an example of the flexibility of equation (2.15) consider the following model:

$$y(t+1) = f(y(t), u(t-1)) + d(t+1) \tag{2.16}$$

In keeping with the standard time series conventions, $y(t)$ is a process output of interest and $u(t)$ is a process input. The disturbance term, $d(t+1)$, is an integrated zero mean, unit variance Gaussian noise, i.e.

$$d(t+1) = \sum_{j=-\infty}^{t} w(j) \tag{2.17}$$

$$w(j) \sim N_{0,1}(w(j)) \quad \forall j \tag{2.18}$$

Making the transformations $x_1(t) = y(t)$, $x_2(t) = u(t-1)$, and $x_3(t) = d(t)$, this model may be rewritten as a third-order process with the form of equation (2.13).

$$\mathbf{x}(t+1) = \begin{bmatrix} f(x_1(t), x_2(t)) + x_3(t) + w(t) \\ u(t) \\ x_3(t) + w(t) \end{bmatrix} \tag{2.19}$$

Making the transformation $z_3(t) = x_3(t) - x_1(t)$ puts this model in the form of equation (2.15):

$$\begin{bmatrix} x_1(t+1) \\ x_2(t+1) \\ z_3(t+1) \end{bmatrix} = \begin{bmatrix} f(x_1(t), x_2(t)) + z_3(t) + x_1(t) + w(t) \\ u(t) \\ -f(x_1(t), x_2(t)) \end{bmatrix} \tag{2.20}$$

□

The time-invariant discrete-time stochastic nonlinear process model (2.15) provides a flexible mathematical tool for the design and analysis of industrial processes. It represents a natural extension of the linear state-space models used in 'modern control theory' and is capable of a level of sophistication exceeding that of completing model representations such as the Hammerstein models. When used in combination with the output equation (2.12) the model form also includes Wiener models as a subclass. These process models may be derived through discretization of a (fundamental) continuous-time model (Bequette, 1998), or from process data using identification techniques (Soderstrom and Stoica, 1989; Ljung, 1999).

2.2.2 The Markov Property

Equation (2.15) is a Markov process model, having the property that all available information (present and past states and inputs) relevant to future process behaviour is summarized by the present process state and input. This property is expressed as:

$$\begin{aligned} & Pr\left(\mathbf{x}\left(t+1\right) \leq \mathbf{z} | \mathbf{x}\left(\tau\right), \mathbf{u}\left(\tau\right) \quad \tau = 1, 2, \ldots, t\right) \\ = \; & Pr\left(\mathbf{x}\left(t+1\right) \leq \mathbf{z} | \mathbf{x}\left(t\right), \mathbf{u}\left(t\right)\right) \end{aligned} \tag{2.21}$$

for the real vector $\mathbf{z}$. In the case of the process (2.15), this implies that only $\mathbf{x}(t)$ and $\mathbf{u}(t)$ need to be known to make predictions about future states.

Analysis of process models with the Markov property can be considerably simpler than analysis of non-Markov models. In particular, analysis of the stationary PDF is made straightforward and control design is simplified.

2.2.3 Feedback Control

Automatic control strategies in the processing and manufacturing industries regularly make use of feedback control algorithms. In this thesis, the following state feedback control law is used to control processes in the form of equation (2.15).

$$\mathbf{u}(t) = \mathbf{k}(\mathbf{x}(t)) \tag{2.22}$$

Here, $\mathbf{k}(\cdot)$ is a smooth vector function of dimension n_u. This causal feedback control law takes advantage of the Markov property of the process (2.15). Since it is known that all relevant information about future process behaviour is given by the present state and input, the feedback control law is designed to make full use of the available information.

For completeness, it is noted here that some of the results in this work may also be extended to output feedback control, $\mathbf{u}(t) = \mathbf{k}_y(\mathbf{y}(t))$, when the output is given by equation (2.12).

The control law (2.22) is substituted into equation (2.15) to give the following model in closed-loop (CL) form:

$$\begin{aligned} \mathbf{x}(t+1) &= \mathbf{f}(\mathbf{x}(t), \mathbf{k}(\mathbf{x}(t))) + \mathbf{w}(t) \\ &= \tilde{\mathbf{f}}(\mathbf{x}(t)) + \mathbf{w}(t) \end{aligned} \tag{2.23}$$

The same closed-loop form may be written if output feedback is used, since $\mathbf{k}_y(\mathbf{y}(t)) = \mathbf{k}_y(f_y(\mathbf{x}(t)))$. Note that the CL process (2.23) retains the Markov property of the underlying open-loop process (2.15). Throughout this thesis, the CL process feedback, $\tilde{\mathbf{f}}(\mathbf{x}(t))$, will be referred to as CL feedback.

Typically in control design, the open-loop process model is known, while CL dynamics may be set as the result of design calculations. In such cases a feedback control law to achieve the desired CL dynamics may be obtained from:

$$\mathbf{f}(\mathbf{x}(t), \mathbf{u}(t)) = \tilde{\mathbf{f}}(\mathbf{x}(t)) \tag{2.24}$$

and solving for $\mathbf{u}(t)$:

$$\mathbf{u}(t) = \mathbf{k}(\mathbf{x}(t)) = \mathbf{f}_x^{-1}\left(\tilde{\mathbf{f}}(\mathbf{x}(t))\right) \tag{2.25}$$

where $\mathbf{f}_x^{-1}(\cdot)$ is the inverse of the function $\mathbf{f}(\mathbf{x}(t), \mathbf{u}(t))$ with respect to $\mathbf{u}(t)$, treating $\mathbf{x}(t)$ as a constant. This use of the inverse function theorem requires that $\mathbf{f}(\mathbf{x}, \mathbf{u})$ be uniformly C^∞ in $\mathbf{u}$.

2.2.4 Stationarity

Stationarity is an important property for a number of applications, including time series data analysis techniques. It plays a central role in the analysis of the transiency of stochastic processes. A stationary Markov process $\{\mathbf{x}(t)\}$ is defined as a stochastic process with the property that the distribution function of the process state does not vary with time (Tong, 1990), *i.e.*,

$$P_{x(t)}(\cdot) = P_{x(t+b)}(\cdot) \quad \forall b \in \mathbb{Z} \tag{2.26}$$

This implies that if a PDF exists for the distribution function, it too does not vary with time. For the CL process (2.23), if the process is stationary then the stationary PDF, $p(\cdot)$, is given implicitly by the integral equation (Tong, 1990):

$$p(\zeta) = \int_{\Re^{n_x}} p_w\left(\zeta - \tilde{\mathbf{f}}(\mathbf{z})\right) p(\mathbf{z}) d\mathbf{z} \tag{2.27}$$

This equation is sometimes referred to as the invariant equation. In this thesis, it is referred to as the *dynamics-PDF relationship*. While this equation gives an exact relationship between the CL process dynamics and the stationary PDF, in general, there is no closed-form analytical solution to this equation. Only a few specific solutions are known. This presents a significant barrier to process analysis and control design, even for relatively simple processes such as (2.15).

Equation (2.27) applies in the case $n_x = n_w$. For a closed-loop process with the form:

$$\mathbf{x}^{(1)}(t+1) = \tilde{\mathbf{f}}^{(1)}(\mathbf{x}(t)) + \mathbf{w}(t) \tag{2.28a}$$

$$\mathbf{x}^{(2)}(t+1) = \tilde{\mathbf{f}}^{(2)}(\mathbf{x}(t)) \tag{2.28b}$$

a slightly more complicated result exists. Using some techniques from (Jazwinski, 1970), the development of the dynamics-PDF relationship for the process (2.28) is given here.

Noting the $\mathbf{x}(t)$ and $\mathbf{w}(t)$ are independent, the addition of random variables rule (2.7) can be applied to the equations (2.28):

$$p_{x_{t+1}}(\mathbf{x}_{t+1}) = \int_{\Re^{n_x}} p^*(\mathbf{x}_{t+1}|\mathbf{x}_t)\, p_{x_t}(\mathbf{x}_t) d\mathbf{x}_t \tag{2.29}$$

where the modified notation $\mathbf{x}(t) = \mathbf{x}_t$ is used to reduce the length of the expression. Some care must be taken in specifying the transition PDF.

$$\begin{aligned} p^*(\mathbf{x}_{t+1}|\mathbf{x}_t) &= p^*\left(\mathbf{x}_{t+1}^{(1)}, \mathbf{x}_{t+1}^{(2)}|\mathbf{x}_t\right) \\ &= p^*\left(\mathbf{x}_{t+1}^{(1)}|\mathbf{x}_t\right) p^*\left(\mathbf{x}_{t+1}^{(2)}|\mathbf{x}_t\right) \\ &= p_w\left(\mathbf{x}_{t+1}^{(1)} - \tilde{\mathbf{f}}^{(1)}(\mathbf{x}_t)\right) \delta\left(\mathbf{x}_{t+1}^{(2)} - \tilde{\mathbf{f}}^{(2)}(\mathbf{x}_t)\right) \end{aligned} \tag{2.30}$$

Here $\delta(\cdot)$ is Dirac's delta function. Therefore equation (2.29) becomes:

$$p_{x_{t+1}}(\mathbf{x}_{t+1}) = \int_{\Re^{n_x}} p_w\left(\mathbf{x}_{t+1}^{(1)} - \tilde{\mathbf{f}}^{(1)}(\mathbf{x}_t)\right) \delta\left(\mathbf{x}_{t+1}^{(2)} - \tilde{\mathbf{f}}^{(2)}(\mathbf{x}_t)\right) p_{x_t}(\mathbf{x}_t) d\mathbf{x}_t \tag{2.31}$$

Since it is the stationary PDF that is being derived, $p_{x_{t+1}}(\cdot) = p_{x_t}(\cdot) = p(\cdot)$ and the final result is:

$$p(\zeta) = \int_{\Re^{n_x}} p_w\left(\zeta^{(1)} - \tilde{\mathbf{f}}^{(1)}(\mathbf{z})\right) \delta\left(\zeta^{(2)} - \tilde{\mathbf{f}}^{(2)}(\mathbf{z})\right) p(\mathbf{z}) d\mathbf{z} \tag{2.32}$$

where the dummy variables ζ and $\mathbf{z}$ are used to emphasize that this is the equation of a function, $p(\cdot)$.

The stationary PDF provides a concise summary of process behaviour. All of the dynamic process model (2.23) (both the CL feedback and the disturbance PDF) is incorporated into the right-hand side of equation (2.27). Even if the dynamic process model is unknown, estimates of the stationary PDF may be obtained if process data is available.

The following example illustrates the main points of this section and highlights the connection to more familiar linear processes.

Example 2.2.2 Consider a stationary first-order nonlinear process given by:

$$x(t+1) = f(x(t)) + w(t) \tag{2.33}$$

where $n_x = n_w = 1$ and $w(t)$ is iid with PDF $p_w(w(t))$. In this case equation (2.27) simplifies to:

$$p(\zeta) = \int_{-\infty}^{\infty} p_w(\zeta - f(z))\, p(z) dz \tag{2.34}$$

If the disturbance distribution is zero-mean Gaussian, *i.e.* $p_w(\cdot) = N_{0,\sigma_w}(\cdot)$, then equation (2.34) becomes:

$$p(\zeta) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma_w^2}} \exp\left(-\frac{(\zeta - f(z))^2}{2\sigma_w^2}\right) p(z) dz \tag{2.35}$$

Further, if equation (2.33) is linear, *i.e.* $f(x(t)) = \alpha x(t)$ for some constant α such that $|\alpha| < 1$, then equation (2.35) may be solved analytically (see Appendix B). For the purposes of this brief illustration, we use equation (2.35) to verify the well-known fact that a linear process subject to a Gaussian disturbance is a Gaussian process. The stationary PDF for the process (2.33) is assumed to be Gaussian with mean μ and standard deviation σ; thus equation (2.35) becomes:

$$\begin{aligned}
&\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(\zeta - \mu)^2}{2\sigma^2}\right) \\
=&\frac{1}{\sqrt{2\pi\sigma_w^2}} \int_{-\infty}^{\infty} \exp\left(-\frac{(\zeta - \alpha z)^2}{2\sigma_w^2}\right) \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(z-\mu)^2}{2\sigma^2}\right) dz \\
=&\frac{1}{\sqrt{2\pi\sigma_w^2}} \exp\left(-\frac{\zeta^2}{2\sigma_w^2} - \frac{\mu^2}{2\sigma^2}\right) \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \exp\left(\frac{\alpha\zeta\sigma^2 + \mu\sigma_w^2}{\sigma^2\sigma_w^2} z - \frac{\alpha^2\sigma^2 + \sigma_w^2}{2\sigma^2\sigma_w^2} z^2\right) dz
\end{aligned}$$

(completing the square, we obtain:)

$$
\begin{aligned}
&= \frac{1}{\sqrt{2\pi\sigma_w^2}} \exp\left(-\frac{\zeta^2}{2\sigma_w^2} - \frac{\mu^2}{2\sigma^2} + \frac{\left(\alpha\zeta\sigma^2 + \mu\sigma_w^2\right)^2}{\left(\alpha^2\sigma^2 + \sigma_w^2\right) 2\sigma^2\sigma_w^2}\right) \frac{1}{\sqrt{2\pi\sigma^2}} \\
&\int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}\left(\sqrt{\frac{\alpha^2\sigma^2 + \sigma_w^2}{\sigma^2\sigma_w^2}} z - \sqrt{\frac{\left(\alpha\zeta\sigma^2 + \mu\sigma_w^2\right)^2}{\left(\alpha^2\sigma^2 + \sigma_w^2\right)\sigma^2\sigma_w^2}}\right)^2\right) dz \\
&= \frac{1}{\sqrt{2\pi\sigma_w^2}} \exp\left(-\frac{1}{2}\frac{\left(\zeta - \alpha\mu\right)^2}{\alpha^2\sigma^2 + \sigma_w^2}\right) \frac{1}{\sqrt{2\pi\sigma^2}} \\
&\int_{-\infty}^{\infty} \exp\left(-\frac{1}{2\frac{\sigma^2\sigma_w^2}{\alpha^2\sigma^2+\sigma_w^2}}\left(z - \frac{\alpha\zeta\sigma^2 + \mu\sigma_w^2}{\alpha^2\sigma^2 + \sigma_w^2}\right)^2\right) dz \\
&= \frac{1}{\sqrt{2\pi\sigma_w^2}} \exp\left(-\frac{1}{2}\frac{\left(\zeta - \alpha\mu\right)^2}{\alpha^2\sigma^2 + \sigma_w^2}\right) \frac{1}{\sqrt{2\pi\sigma^2}} \sqrt{2\pi\frac{\sigma^2\sigma_w^2}{\alpha^2\sigma^2 + \sigma_w^2}} \\
&= \frac{1}{\sqrt{2\pi\left(\alpha^2\sigma^2 + \sigma_w^2\right)}} \exp\left(-\frac{1}{2}\frac{\left(\zeta - \alpha\mu\right)^2}{\alpha^2\sigma^2 + \sigma_w^2}\right) \qquad (2.36)
\end{aligned}
$$

Comparing the left and right-hand sides of the equation gives the two equalities $\mu = \alpha\mu$ and $\sigma^2 = \alpha^2\sigma^2 + \sigma_w^2$. These yield the solutions $\mu = 0$ and $\sigma^2 = \frac{\sigma_w^2}{1-\alpha^2}$. This result verifies the consistency of this approach to determining the stationary PDF with the well-known result for linear systems and Gaussian disturbances. Furthermore, the mean and variance found using this approach agree with those found using the standard expected value and long division approach (with B, the backshift operator):

$$
\begin{aligned}
x(t+1) &= \alpha B x(t+1) + w(t) = \frac{w(t)}{1 - \alpha B} \\
x(t+1) &= w(t) + \alpha w(t-1) + \alpha^2 w(t-2) + \ldots \qquad (2.37)
\end{aligned}
$$

$$
\mu = E\left[x(t+1)\right] = E\left[w(t) + \alpha w(t-1) + \alpha^2 w(t-2) + \ldots\right] = 0 \qquad (2.38)
$$

$$
\begin{aligned}
E\left[x^2(t+1)\right] &= E\left[\left(w(t) + \alpha w(t-1) + \alpha^2 w(t-2) + \ldots\right)^2\right] \\
\sigma^2 &= E\left[w^2(t)\right] + E\left[\alpha^2 w^2(t-1)\right] + E\left[\alpha^4 w^2(t-2)\right] \ldots \\
&= \sigma_w^2 + \alpha^2\sigma_w^2 + \alpha^4\sigma_w^2 + \ldots \\
&= \frac{\sigma_w^2}{1 - \alpha^2} \qquad (2.39)
\end{aligned}
$$

□

The example illustrates the fact that the invariant PDF equation (2.27) may be solved exactly for linear processes with Gaussian disturbances. The solutions for some other special cases are given in (Tong, 1990).

2.2.5 Ergodicity

The notion of ergodicity is related to, but much more powerful than, stationarity.

A stationary process $\{\mathbf{x}(t)\}$ is ergodic if normalized sums of functions of the time series converge to the expected value in the limit (Soderstrom and Stoica, 1989). For example, for a first order process, if:

$$\lim_{N\to\infty}\frac{1}{N}\sum_{t=1}^{N}\mathbf{x}(t)=E[\mathbf{x}(t)]=\mu \tag{2.40}$$

and

$$\lim_{N\to\infty}\frac{1}{N}\sum_{t=1}^{N}(\mathbf{x}(t+b)-\mu)(\mathbf{x}(t)-\mu)^T=E\left[(\mathbf{x}(t+b)-\mu)(\mathbf{x}(t)-\mu)^T\right] \tag{2.41}$$

then the process is ergodic with respect to the first two moments, or 'wide-sense' ergodic. A process is strictly ergodic if this is true for all functions $\nu(\mathbf{x}(t))\in\mathcal{L}^i(\mathbf{x}(t),p(\mathbf{x}(t)))$, $i=1,2$ (Hernandez-Lerma and Lasserre, 1996):

$$\lim_{N\to\infty}\frac{1}{N}\sum_{t=1}^{N}\nu(\mathbf{x}(t))=E[\nu(\mathbf{x}(t))] \tag{2.42}$$

Ergodicity is related to the law of large numbers (see Appendix B) and is often used in the analysis of identification techniques.

Another way of looking at ergodicity is to consider the evolution of the distribution of the state of a process. Consider the CL process (2.28a). Without the random input, $\mathbf{w}(t)$, it is just an ordinary difference equation with a solution $\mathbf{x}(t)$. In the stochastic case, a trajectory $\mathbf{x}(t)$ represents one of (infinitely) many possible realizations, and it is more appropriate to consider the behaviour of the distribution of $\mathbf{x}(t)$. Equation (2.31) gives the time evolution of the PDF and may be used for filtering and prediction applications, as is shown in (Sorenson and Stubberud, 1968) for first-order systems. If an initial PDF $p_{\mathbf{x}_0}(\mathbf{x}_0)$ (or a constant initial condition) is known then all subsequent PDFs may, in principle, be calculated recursively. If the system is ergodic, then the result of the recursive calculation will tend towards a steady-state PDF, $p(\cdot)$. This steady-state PDF is the stationary PDF. If $p_{\mathbf{x}_0}(\mathbf{x}_0) = p(\mathbf{x}_0)$, then the PDF remains unchanged for all time. In this case the process is said to be strictly stationary. This notion of time evolution of the PDF towards some sort of steady-state is reminiscent of deterministic stability notions.

For stochastic processes such as (2.28a), where the random disturbance is additive, one of the key concepts in the analysis and control design for processes, asymptotic stability, is not appropriate. The undisturbed process (setting $\mathbf{w}(t) = 0$) may have a stable equilibrium point; but this is destroyed by the disturbance. For such situations, ergodicity may be viewed as a stochastic analogue for deterministic asymptotic stability notions. In (Tong, 1990), relationships are developed between the ergodicity of a process such as (2.28a) and the stability of the associated process 'skeleton':

$$\mathbf{x}^{(1)}(t+1) = \tilde{\mathbf{f}}^{(1)}(\mathbf{x}(t)) \tag{2.43}$$

The stability of this ordinary difference equation may be analyzed in the sense of Lyapunov. In the stochastic case, it is the stability of the distribution of $\mathbf{x}(t)$ that should be analyzed with the stationary distribution as the analogue of an equilibrium point.

For further discussion of ergodicity and 'stochastic stability', see (Tong, 1990) and (Hernandez-Lerma and Lasserre, 1996).

2.3 Measures of Performance

In design and operation of controlled industrial processes, the goal is performance. While performance may be defined in a number of different ways, both qualitative and/or quantitative, this work focusses on quantitatively measuring performance in terms of objective functions, specifically, cost functions.

The general cost function on the trajectory of a process is:

$$J = \sum_{t=1}^{N} \ell(\mathbf{x}(t), \mathbf{u}(t)) \tag{2.44}$$

where the 'loss functional', $\ell(\mathbf{x}(t), \mathbf{u}(t))$, reflects the costs associated with both the state and the input. These costs often include the costs of consumption, such as energy and raw materials, as well as the profit losses due to violation of operational constraints and production of off-specification products. Loss functionals should be carefully specified in the tradition of Taguchi's 'quality-loss', where quality is defined to account for broader societal demands on products (such as safety and environmental concerns) and not just engineering concerns (Ealey, 1988). The Taguchi approach makes a quadratic approximation of the true loss functional and, in doing so, is consistent with well known optimal control designs such as LQG control, minimum variance control and many model predictive control (MPC) designs. However, there are numerous situations where such an approximation is misleading. For example, if the main influence on the cost function is associated with a product quality specification, the loss functional will be highly nonsymmetric as it represents the large losses associated with low-quality production and the smaller losses associated with (unnecessarily) high-quality production. For this reason, the general form of loss functional, $\ell(\mathbf{x}(t), \mathbf{u}(t))$, is used in this thesis.

Often it is assumed that the process will be operating in regulatory mode for a long time and so the infinite time loss function is used:

$$J = \sum_{t=1}^{\infty} \ell(\mathbf{x}(t), \mathbf{u}(t)) \tag{2.45}$$

While these types of loss functions are useful when working with deterministic processes, they prove cumbersome for stochastic processes. One problem is that equations (2.44) and (2.45) consider only one realization of a process path. For a stochastic system, there is no guarantee that different realizations give the same value of the objective function, especially in the finite time case. In the case of equation (2.45), the integral is not, in general, convergent. For quantifying the performance of stochastic systems, a different type of objective function is required. An alternative, but related, form of objective function measures performance in terms of the expected value of the loss functional.

2.3.1 Expected Value Objectives

Consider extending equation (2.44) to infinite time, while dividing by the number of time steps over which the objective is calculated:

$$J = \lim_{N \to \infty} \frac{1}{N} \sum_{t=1}^{N} \ell(\mathbf{x}(t), \mathbf{u}(t)) \tag{2.46}$$

The factor $\frac{1}{N}$ is just a constant and so, while it rescales the objective function, it does not change the overall shape of the objective and locations of minima, maxima, and other features of interest are preserved. However, by making this modification, the problem with convergence that exists for equation (2.45) is eliminated. Referring to equation (2.42), it is clear that if the processes $\mathbf{x}(t)$ and $\mathbf{u}(t)$ are ergodic then the cost function (2.46) is equivalent to:

$$J = E\left[\ell\left(\mathbf{x}(t), \mathbf{u}(t)\right)\right] \tag{2.47}$$

For processes operating under state feedback control, $\mathbf{u}(t)$ becomes a function of the state, *i.e.*, $\mathbf{u}(t) = \mathbf{k}(\mathbf{x}(t))$ and the definition of expected value can be applied:

$$J = \int_{\Re^{n_x}} \ell\left(\mathbf{x}, \mathbf{k}(\mathbf{x})\right) p(\mathbf{x})\, \mathbf{dx} \tag{2.48}$$

where the time index is omitted to reduce the length of the expression. The integrand in equation (2.48) is the product of two functions: the loss functional and the stationary PDF of the process state. The loss functional is dictated by engineering concerns or process economics and can therefore be specified by the control engineer. On the other hand, the stationary PDF is a consequence of process dynamics, the form of the feedback control law and the PDF of the process disturbance. Consequently, $p(\mathbf{x})$ can be difficult to obtain and so the real challenge in calculating the value of this objective function is in finding or estimating the system PDF.

Before continuing with the main discussion, it should be noted that the expectation type objective (2.48) can also be made to include costs associated with the process outputs, as given by equation (2.12), as follows:

$$J = E\left[\ell\left(\mathbf{x}, \mathbf{u}, \mathbf{y}\right)\right] \tag{2.49}$$

$$= E\left[\ell\left(\mathbf{x}, \mathbf{k}(\mathbf{x}), \mathbf{f}_y(\mathbf{x})\right)\right] \tag{2.50}$$

Expectation objectives in process variables consider what is likely to happen, or what, in the long run, will happen on average. In doing so they provide a measure of how process performance is sustained and thus are an excellent metric for regulatory control designs. The expectation objective is used in a number of well-established controller synthesis techniques, most notably minimum variance control (Astrom, 1970).

Again it is noted that the PDF $p(\cdot)$ in the integrand is the stationary PDF. This is an immediate consequence of the use of the ergodic theorem (2.42) in developing equation (2.47). From a practical point of view, if this type of cost function is to be useful as a metric in the context of long-term performance, it is necessary that a stationary PDF exist for the CL process. Discussion of non-stationary process models within this framework would be inappropriate since expected cost of operation would be forever changing and control strategies would need to be able to adapt to the changing process behaviour.

It is emphasized here that the processes discussed in this thesis have inputs that may be manipulated for control purposes, in particular using feedback control to create closed-loop processes. When referring to the stationarity of a process, it is the closed-loop process that is referred to. Processes that have open-loop non-stationary behaviour such as integrators or unstable processes are not necessarily excluded from the discussion and techniques in this thesis. Often the feedback control laws applied to these processes remove or negate non-stationary elements of the dynamics, so that the closed-loop process is stationary. In the feedback control designs of later chapters, control laws are designed with an implicit requirement that the closed-loop process be stationary. Therefore the resulting designs achieve both stationarity and performance.

One way of acquiring the stationary PDF is through equation (2.27), in which case $p(\cdot)$ is a function of the feedback control law through the CL feedback, $\tilde{f}(\mathbf{x}(t))$. Therefore, the feedback control law influences the expectation objective function through both the cost functional and the stationary PDF. The addition of the generally unsolvable dynamics-PDF relationship as an auxiliary equation to the expectation cost function can greatly impede nonlinear control design, even for a relatively simple process such as (2.15).

2.4 Gram-Charlier PDF's

A flexible and mathematically rich aid for process analysis and controller design is the Gram-Charlier (GC) basis of functions. This basis provides a structure well-suited to representation of weakly non-Gaussian PDFs. When a series of GC basis functions is assembled, forming a GC PDF, the coefficients in the series have statistical meaning; therefore, GC PDFs can be tailor-made to take on desirable statistical properties. On the other hand, the GC basis functions are orthogonal, and can be used as a generalized fourier series to create approximations of other PDFs.

Usually in the literature, a specific univariate GC basis is described that works best for creating PDFs with zero mean and a variance of either 1 or $\frac{1}{2}$ (Cramer, 1946; Stuart and Ord, 1994); however, in many situations (such as when analyzing dynamic processes) it is inconvenient to centre and normalize the variables of interest. For this reason a general univariate GC basis, that tailors the basis functions to work with PDFs of any mean and variance, is presented in this thesis. Once the GC PDFs have been introduced with the univariate case, the multivariate case is given.

2.4.1 The Univariate GC Basis

To fully illustrate the development and features of GC basis functions, the univariate case is described here. The univariate GC basis functions are generated by differentiating the Gaussian PDF, (2.2), as follows:

$$\phi_i(z) = (-1)^i \frac{\sigma^i}{\sqrt{i!}} \frac{d^i N_{\mu,\sigma}(z)}{dz^i} \tag{2.51}$$

The first five GC functions are:

$$\begin{aligned}
\phi_0(z) &= N_{\mu,\sigma}(z) \\
\phi_1(z) &= \frac{z-\mu}{\sigma} N_{\mu,\sigma}(z) \\
\phi_2(z) &= \frac{z^2 - 2\mu z + \mu^2 - \sigma^2}{\sqrt{2}\sigma^2} N_{\mu,\sigma}(z) \\
\phi_3(z) &= \frac{z^3 - 3\mu z^2 - 3\sigma^2 z + 3\mu^2 z + 3\mu\sigma^2 - \mu^3}{\sqrt{6}\sigma^3} N_{\mu,\sigma}(z) \\
\phi_4(z) &= \frac{z^4 - 4\mu z^3 + 6\mu^2 z^2 - 6\sigma^2 z^2 - 4\mu^3 z + 12\sigma^2\mu z + 3\sigma^4 - 6\sigma^2\mu^2 + \mu^4}{\sqrt{24}\sigma^4} N_{\mu,\sigma}(z)
\end{aligned} \tag{2.52}$$

These are plotted in Figure 2.2.

It should be noted that each GC basis function, $\phi_i(\cdot)$, is the product of a Hermite polynomial, $h_i(\cdot)$, and the Gaussian PDF, i.e.,

$$\phi_i(z) = h_i(z) N_{\mu,\sigma}(z) \tag{2.53}$$

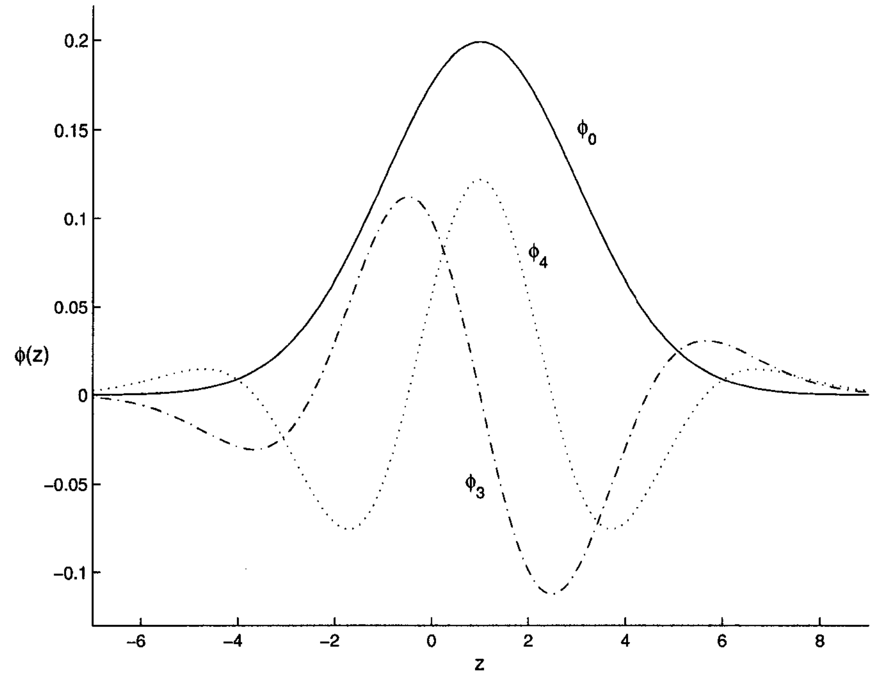


Figure 2.2: The zeroth, third and fourth GC functions based on a mean of one and a variance of four.

Therefore the GC basis functions inherit the orthogonality of Hermite polynomials with the inner product:

$$
\begin{aligned}
\langle \phi_i(z), \phi_j(z) \rangle &= \int_{-\infty}^{\infty} \frac{\phi_i(z)\,\phi_j(z)}{N_{\mu,\sigma}(z)} dz \\
&= \int_{-\infty}^{\infty} \frac{h_i(z)\,N_{\mu,\sigma}(z)\,h_j(z)\,N_{\mu,\sigma}(z)}{N_{\mu,\sigma}(z)} dz \\
&= \int_{-\infty}^{\infty} h_i(z)\,h_j(z)\,N_{\mu,\sigma}(z)\,dz = \delta_{ij} \qquad (2.54)
\end{aligned}
$$

where δ_{ij} is the Kronecker delta.

A full table of properties for Hermite polynomials (generated from $N_{0,\frac{1}{\sqrt{2}}}(z)$) is given in (Zwillinger, 1996). These may be generalized to the case of a general mean and variance and applied to Gram-Charlier basis functions.

Univariate GC PDFs

In figure 2.2 typical behaviour of the GC basis functions is illustrated. These functions are defined over all of $\Re$ and, as observed in the figure, they tend to zero as they move away from the location parameter, μ. Both of these properties make them especially useful for representation of PDFs.

A GC PDF, $p_{GC}(z)$, is formed from a weighted series of GC basis functions:

$$\begin{aligned} p_{GC}(z) &= c_0\phi_0(z) + c_1\phi_1(z) + \ldots + c_N\phi_N(z) \\ &= \mathbf{c}^T\phi(z) \end{aligned} \tag{2.55}$$

which can also be rewritten as a product of a series of Hermite polynomials and the Gaussian PDF:

$$\begin{aligned} p_{GC}(z) &= (c_0 + c_1h_1(z) + \ldots + c_Nh_N(z))\, N_{\mu,\sigma}(z) \\ &= \mathbf{c}^T\mathbf{h}(z)\, N_{\mu,\sigma}(z) \end{aligned} \tag{2.56}$$

For this to be a proper PDF, it must meet the defining requirements for a PDF, in particular, it must be non-negative everywhere. This means that the the polynomial, $\mathbf{c}^T\mathbf{h}(z)$, must be non-negative everywhere. This places constraints on the values of the coefficients, $\{c_i\}$, that may be used. Numerical techniques to ensure that the non-negativity constraint is satisfied are given by (Jondeau and Rockinger, 1999). The unit measure requirement for the PDF is always satisfied by setting $c_0 = 1$.

Equation (2.56) illustrates that GC PDFs are the product of a polynomial, $\mathbf{c}^T\mathbf{h}(z)$, and the Gaussian PDF. Therefore any PDF that is a product of a polynomial and a Gaussian PDF can be exactly parameterized by a GC PDF. GC PDFs are most often used for approximation of unimodal PDFs, although it is possible to obtain multimodal behaviour. The zeroth-order GC PDF is simply the Gaussian PDF and as a more non-Gaussian PDF is required, more terms are added to the series composing the GC PDF.

Equation (2.54) implies the following about the coefficients, $\{c_i\}$:

$$c_i = \int_{-\infty}^{\infty} h_i(z)\, p_{GC}(z)\, dz \tag{2.57}$$

Notice that this corresponds to the expected value of $h_i(z)$ with respect to the PDF $p_{GC}(z)$. Since $h_i(z)$ is just a polynomial, the expectation looks very much like the calculation of a moment. For this reason the coefficients $\{c_i\}$ in the GC PDFs are sometimes referred to as quasi-moments (Kuznetsov *et al.*, 1965). In fact, the following simple linear relationship between quasi-moments and moments exists:

$$\mathbf{c} = \begin{bmatrix} 1 & 0 & \cdots & & & \\ -\frac{\mu}{\sigma} & \frac{1}{\sigma} & 0 & \cdots & & \\ \frac{\mu^2-\sigma^2}{\sqrt{2\sigma^2}} & -\frac{2\mu}{\sqrt{2\sigma^2}} & \frac{1}{\sqrt{2\sigma^2}} & 0 & \cdots & \\ \frac{3\mu\sigma^2-\mu^3}{\sqrt{6\sigma^3}} & \frac{3\left(\mu^2-\sigma^2\right)}{\sqrt{6\sigma^3}} & -\frac{3\mu}{\sqrt{6\sigma^3}} & \frac{1}{\sqrt{6\sigma^3}} & 0 & \cdots \\ \frac{3\sigma^4-6\sigma^2\mu^2+\mu^4}{\sqrt{24\sigma^4}} & \frac{12\mu\sigma^2-4\mu^3}{\sqrt{24\sigma^4}} & \frac{6\left(\mu^2-\sigma^2\right)}{\sqrt{24\sigma^4}} & -\frac{4\mu}{\sqrt{24\sigma^4}} & \frac{1}{\sqrt{24\sigma^4}} & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} 1 \\ \mathbf{m}_{PGC} \end{bmatrix} \quad (2.58)$$

Note that if the transformation matrix is square it is then invertible.

Equation (2.57) may also be used to calculate coefficients for approximation of an arbitrary PDF, $p(\cdot)$:

$$c_i = \int_{-\infty}^{\infty} h_i(z)\, p(z)\, dz \quad (2.59)$$

Notice that for a distribution $p(z)$ with mean μ and variance σ:

$$\begin{aligned} c_1 &= \int_{-\infty}^{\infty} h_1(z)\, p(z)\, dz \\ &= \int_{-\infty}^{\infty} \frac{z}{\sigma} p(z)\, dz - \int_{-\infty}^{\infty} \frac{\mu}{\sigma} p(z)\, dz \\ &= \frac{\mu}{\sigma} - \frac{\mu}{\sigma} = 0 \end{aligned} \quad (2.60)$$

The constant c_2 also turns out to be zero but not the higher quasi-moments. This is because the zeroth-order GC approximation for any distribution is just $\phi_0(z) = N_{\mu,\sigma}(z)$ which takes into account the mean and variance of $p(z)$. Thus, the quasi-mean, c_1, and quasi-variance, c_2, are both zero. For non-normal PDF's, the higher quasi-moments will in general be non-zero.

In the literature, the fourth-order GC PDF is most commonly described:

$$p(z) = \left(1 + c_3 h_3(z) + c_4 h_4(z)\right) N_{\mu,\sigma}(z) \quad (2.61)$$

The constants c_3 and c_4 can be shown, using the quasi-moment property, to be directly related to the skewness and the kurtosis of the distribution, respectively. Thus when the fourth-order PDF is used as an approximation, it is accurate to the fourth moment.

GC PDFs are very closely related to the Edgeworth PDF approximation (Stuart and Ord, 1994). However, the Edgeworth PDF involves some additional structural restrictions and so the GC PDF is preferred as a more flexible modelling and analysis tool. In particular, it is noted in (Barton and Dennis, 1952) and (Jondeau and Rockinger, 1999) that the range of values of the PDF coefficients for which the PDF is non-negative is smaller for the Edgeworth PDF.

2.4.2 The Multivariate Case

The generation and properties of multivariate GC basis functions are very similar to the univariate case, with only a few differences. Instead of taking derivatives with respect to the individual elements of $\mathbf{z}$, to ensure orthogonality of the basis functions, derivatives are taken along the eigenvectors of the covariance matrix and, since there is more than one derivative of a given order, the indexing of the multivariate GC functions is more involved. Despite these minor complications, the extension of the GC basis functions to higher dimensions remains practically relevant.

The n-variate GC basis functions, $\phi^{\mathbf{i}}$, are generated from the n-variate Gaussian PDF, (2.1), by taking derivatives along the eigenvectors, $\{\mathbf{e}_j\}_{j=1,\ldots,n}$, of the covariance matrix. One way of representing this is to first create the vector ζ as follows:

$$\zeta = [\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n]\,\mathbf{z} \tag{2.62}$$

and then:

$$\phi^{i_1,i_2,\ldots,i_n} = b(\mathbf{i})\,\frac{\partial^r N_{\mu,\Sigma}(\mathbf{z})}{\partial \zeta^{\mathbf{i}}} \tag{2.63}$$

where $r = \sum_{j=1}^{n} i_j$ and the notation used for indexing is analogous to that used for moments. There are $\binom{n+r-1}{r}$ r^{th}-order GC basis functions. With the aid of equation (2.62) the differentiation can be performed using the chain rule. The normalizing factors, $b(\mathbf{i})$, are proportional to the eigenvalues, $\{\lambda_j\}$, of the covariance matrix:

$$b(\mathbf{i}) = \prod_{j=1}^{n} \frac{\sqrt{\lambda_j}^{\,i_j}}{\sqrt{i_j!}} \tag{2.64}$$

Figure 2.3 gives a representative illustration of a multivariate GC basis function. This particular function is a third-order bivariate GC basis function generated from the zero-mean Gaussian PDF with the covariance matrix:

$$\begin{bmatrix} 3 & 1 \\ 1 & 2 \end{bmatrix} \tag{2.65}$$

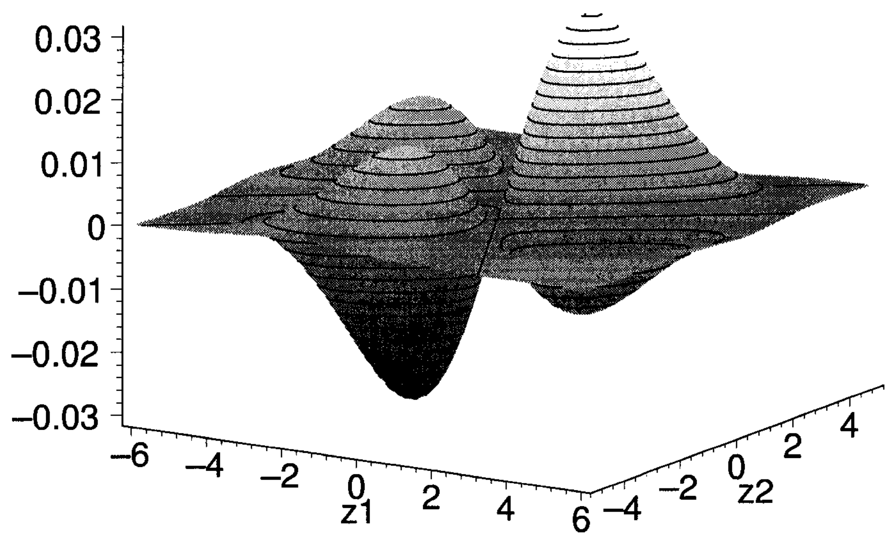


Figure 2.3: A third-order bivariate GC basis function derived from the zero-mean Gaussian PDF with covariance matrix (2.65).

Again, as in the univariate case, each GC basis function is the product of a Hermite polynomial, $h^{\mathbf{i}}(\mathbf{z})$, and the Gaussian PDF.

$$\phi^{\mathbf{i}}_{GC}(\mathbf{z}) = h^{\mathbf{i}}(\mathbf{z})\, N_{\mu,\Sigma}(\mathbf{z}) \tag{2.66}$$

Multivariate GC PDFs

Analogous to the univariate case, the multivariate GC PDF is:

$$\begin{aligned} p_{GC}(\mathbf{z}) &= \left(1 + c^{1,0,0,\ldots} h^{1,0,0,\ldots}(\mathbf{z}) + \ldots + c^{0,\ldots,0,N} h^{0,\ldots,0,N}(\mathbf{z})\right) N_{\mu,\Sigma}(\mathbf{z}) \\ &= \mathbf{c}^T \mathbf{h}(\mathbf{z})\, N_{\mu,\Sigma}(\mathbf{z}) \end{aligned} \tag{2.67}$$

All of the results for the univariate case also apply here. The multivariate GC PDF is the product of a series of multivariate Hermite polynomials and the multivariate Gaussian

PDF, and the polynomial factor must be non-negative everywhere for this to truly be a PDF. Also, when the mean and covariance matrix are appropriately chosen all of the first and second-order coefficients in the PDF expansion (2.67) are zero.

An inner product completely analogous to the univariate case is used to provide an orthogonality condition and the following equation governs the values of the coefficients, $\{c^{\mathbf{i}}\}$:

$$c^{\mathbf{i}} = \int_{\Re^n} h^{\mathbf{i}}(\mathbf{z})\, p_{GC}(\mathbf{z})\, d\mathbf{z} \tag{2.68}$$

This is the expected value of multivariate polynomial and so the coefficients may still be referred to as quasi-moments and a relationship analogous to (2.58) also exists.

2.5 Chapter Summary

A number of concepts from mathematics and statistics were reviewed in this chapter. These will be called upon repeatedly in future chapters as they apply to the process analysis and controller synthesis problems that form the main body of this thesis.

"You are here to learn the subtle science and exact art of potion-making."
– Professor Snape in *Harry Potter and the Philosopher's Stone*
by J.K. Rowling

3

Approximation of the Stationary PDF

With motivations from the processing and manufacturing industries, the relationship between dynamics and stationary probability density function (PDF) is investigated for discrete-time stochastic nonlinear system models. Since this relationship is given by an integral equation for which no general and few specific solutions are known, an approximate solution is developed. By parameterizing both the system dynamics and the PDF, the integral equation is reduced to a set of algebraic equations in the two parameter sets. By choosing values for either parameter set, the other set of values can be obtained. The proposed approach is applied to two controller synthesis problems.[1]

3.1 Introduction

The PDF of a stationary process provides a concise summary of long-term process behaviour. The equation governing the relationship between process dynamics and stationary PDF includes all the information about the dynamics of the process model and

[1]Parts of this chapter were presented at the 2000 Canadian Chemical Engineering Conference, at the Canadian Mathematical Society 2003 Summer Meeting and in (Forbes *et al.*, 2003*b*).

the distribution of the disturbance. Even if little is known about the process dynamics or the disturbances, if stationary data is available, a great deal about the PDF may be discovered.

The PDF, while useful in the calculation of measures of process performance, in developing optimal control strategies, in filtering and many other process control applications, can in itself be viewed as a process characteristic. Plots of PDFs, and their data-based analogue, the histogram, are easily interpreted as giving the relative frequency with which different events occur. As such they can provide powerful illustrations for presentations to management and explanations of various phenomena to non-technical personnel. A plot of a PDF immediately presents the region of operation, the mode - or main operating point, the spread of the process variables and the extent and frequency of large excursions from normal operation. This last feature, the tail behaviour, is often of critical importance in assessing process safety, environmental impacts, and product quality. The larger excursions from normal operation may represent violations of safety constraints, release of harmful process by-products, and production of sub-standard products. The tails of the PDF may be used to estimate the probability of such undesirable events.

In this chapter, the relationship between the dynamics and stationary PDF of a stationary process is examined. Two techniques for approximating the stationary PDF are developed. The first technique derives the PDF from the discrete-time stochastic nonlinear process model. By parameterizing both the closed-loop dynamics and the stationary PDF, the integral equation giving the dynamics-PDF relationship is reduced to a set of algebraic equations in the parameter sets. By choosing values for either parameter set, the other set of values can be obtained. This general result is applied here to the case where the dynamics are known and the PDF is sought.

A second technique is presented that finds an approximate form for the stationary PDF based on process data. Here, method of moments estimators are used to derive coefficients for a PDF composed of a series of GC basis functions. Even if very little is known about the dynamics and disturbances underlying the data, the information can be summarized and important indications of performance may be derived using the approximate PDF.

This chapter is organized as follows: §2 provides some context and background from the literature for the techniques proposed in this chapter. In §3 a very general approximation of the dynamics-PDF relationship is given. This relationship is then specialized in a number of ways. A data-based PDF approximation technique is given in §4. §5 illustrates the use of the proposed techniques through simulations of an example process. §6 concludes this study.

3.2 Background

A number of methods have been proposed to approximate the stationary PDF given by equation (2.27). In (Tong, 1990), a number of methods are outlined. The methods in Tong focus on polynomial expansions of the nonlinear difference equation and make use of generating functions. One special case of these types of approximation methods is the common practice of linearizing and centering the system model, so that only the covariance matrix must be calculated.

The use of univariate Gram-Charlier functions to approximate the densities in equation (2.27) for a filtering application is investigated in (Sorenson and Stubberud, 1968). While focussing on the univariate case, it is noted in (Sorenson and Stubberud, 1968) that the basic ideas of their work may be extended to the multivariate case; however, no details are given. Furthermore, the case of the steady-state or stationary PDF is never considered.

In another filtering application, (Gunther *et al.*, 1997) considers sampled-data systems, using complex exponential basis functions to yield the approximate evolution of the state PDF between samples. Again, this application does not consider the case of the steady-state distribution. Another limitation is that to use the complex exponential basis functions, it is necessary to select a region of interest for the state-space; however it is unclear how such a region is to be chosen.

Approximation of the conditional state PDF using Gaussian sums is investigated in (Sorenson and Alspach, 1971) and (Alspach and Sorenson, 1972). The approximation is performed in the context of a filtering application and the steady-state PDF is not considered. This technique has the advantage that any finite approximation of the true PDF will satisfy all the defining requirements of a PDF; however, no clear guidelines for choosing the variances and means of the Gaussian functions are provided. The Gaussian sum approximation technique was applied to linear systems with non-Gaussian input noise and to nonlinear systems. In the application to nonlinear systems, the technique made use of system linearizations about the mean of each Gaussian function in the sum. This technique, although promising, is somewhat complicated and does not appear to have received further attention in the literature.

In terms of data analysis techniques, there are an almost unlimited number of applications that make use of the mean and variance. For serially correlated data, seminal results for assessment of controlled processes were developed by Harris and co-workers, with (Desborough and Harris, 1992) being a representative publication. A key principle involved in these developments is the idea of a control invariant disturbance. Control invariant disturbances are the result of inherent limitations in the structure of the physical process and control system. The idea of inherent limitations is examined later in this chapter.

Stationary time series data is often serially and nonlinearly correlated. A number of works, such as (McLaughlin *et al.*, 1995) and (Hinich, 1982) examine measures of non-Gaussianity. The latter also includes a test for linearity of the underlying process. These techniques are useful complements to the data analysis technique developed in this section. If a process can be shown to be Gaussian, there is no need to attempt analysis involving statistics beyond the mean and covariance.

The need for an approximate PDF to represent long-term process behaviour becomes clear in benefits analysis studies, such as those described by (Latour, 1992; Latour, 1996). These articles provide a good discussion of the relationship between cost functional and PDF in measures of process performance. The PDF approximation techniques developed in this section, if applied in Latour's framework, can enhance the accuracy of any results.

The first approximation method proposed in this chapter is similar to that used in (Sorenson and Stubberud, 1968), extended to the multivariate case and the stationary PDF. One of the strengths of the proposed technique is that the original system equations are used to generate the PDF approximation, so that exact information about the system dynamics is built into the approximation.

3.3 Approximating the Relationship Between Dynamics and PDF

An approximate solution to equation (2.27) is developed by parameterization of both the system PDF and the CL feedback. These parameterizations allow for reduction of the integral equation to a set of algebraic equations in the two parameter sets. By choosing values for either set of parameters, the other set can then be obtained.

3.3.1 Formulation of the General Approximation Technique

The first step in approximating a solution to equation (2.27) is to parameterize the PDF, $p(\cdot)$, as follows:

$$p(\mathbf{z}) \simeq \hat{p}(\mathbf{z}; \mathbf{c}) \tag{3.1}$$

The PDF parameterization, consisting of either a PDF of known structure or a set of basis functions, must meet the defining requirements a PDF. In particular, it should be a nonegative function that integrates to a value of 1. For the purposes of the proposed technique, it is assumed that the parameters $\mathbf{c}$ are known functions of the moments, $\mathbf{m}_{\hat{p}}$, of the parameterizing PDF:

$$\mathbf{c} = \rho(\mathbf{m}_{\hat{p}}) \tag{3.2}$$

This is not a restrictive assumption as the parameters in many PDFs are known to be elementary functions the moments.

A second parameterization is now made, of the CL feedback, $\tilde{\mathbf{f}}(\cdot)$.

$$\tilde{\mathbf{f}}(\mathbf{z}) \simeq \mathbf{A}\theta(\mathbf{z}) \tag{3.3}$$

where $\theta(\mathbf{z})$ is a vector of basis functions in the process state and $\mathbf{A}$ is a matrix of coefficients. The two parameterizations, (3.1) and (3.3) are now substituted into equation (2.27).

$$\hat{p}(\zeta; \mathbf{c}) = \int_{\Re^n} p_{\mathbf{w}}(\zeta - \mathbf{A}\theta(\xi))\,\hat{p}(\xi; \mathbf{c})\,\mathrm{d}\xi \tag{3.4}$$

Next, the moments are calculated for each side of equation (3.4).

$$\int_{\Re^n} \begin{bmatrix} \zeta^{1,0,0,0,\ldots} \\ \zeta^{0,1,0,0,\ldots} \\ \vdots \end{bmatrix} \hat{p}(\zeta; \mathbf{c})\,\mathrm{d}\zeta = \int_{\Re^n} \begin{bmatrix} \zeta^{1,0,0,0,\ldots} \\ \zeta^{0,1,0,0,\ldots} \\ \vdots \end{bmatrix} \int_{\Re^n} p_{\mathbf{w}}(\zeta - \mathbf{A}\theta(\xi))\,\hat{p}(\xi; \mathbf{c})\,\mathrm{d}\xi\mathrm{d}\zeta \tag{3.5}$$

By making use of equation (2.4), and rearranging the right hand side, the following simplification may be made.

$$\mathbf{m}_{\hat{p}} = \int_{\Re^n} \left(\int_{\Re^n} \begin{bmatrix} \zeta^{1,0,0,0,\ldots} \\ \zeta^{0,1,0,0,\ldots} \\ \vdots \end{bmatrix} p_{\mathbf{w}} \left(\zeta - \mathbf{A}\theta\left(\xi\right)\right) \mathbf{d}\zeta \right) \hat{p}\left(\xi;\mathbf{c}\right) \mathbf{d}\xi \tag{3.6}$$

Making use of the change of variables $\mathbf{z} = \zeta - \mathbf{A}\theta\left(\xi\right)$ it becomes clear that the first integration results in translated moments of $p_{\mathbf{w}}$.

$$\mathbf{m}_{\hat{p}} = \int_{\Re^n} \left(\int_{\Re^n} \begin{bmatrix} \left(\mathbf{z} + \mathbf{A}\theta\left(\xi\right)\right)^{1,0,0,0,\ldots} \\ \left(\mathbf{z} + \mathbf{A}\theta\left(\xi\right)\right)^{0,1,0,0,\ldots} \\ \vdots \end{bmatrix} p_{\mathbf{w}} \left(\mathbf{z}\right) \mathbf{dz} \right) \hat{p}\left(\xi;\mathbf{c}\right) \mathbf{d}\xi \tag{3.7}$$

Therefore the result of the first integration is just a vector of multivariate polynomials in $\mathbf{m}_{p_{\mathbf{w}}}$ and $\mathbf{A}\theta\left(\xi\right)$ which is denoted by $\mathbf{q}$, such that

$$\mathbf{m}_{\hat{p}} = \int_{\Re^n} \mathbf{q}\left(\mathbf{m}_{p_{\mathbf{w}}}, \mathbf{A}\theta\left(\xi\right)\right) \hat{p}\left(\xi;\mathbf{c}\right) \mathbf{d}\xi \tag{3.8}$$

Performing the integration in the right hand side of equation (3.8) results in functions, $\tilde{\mathbf{q}}$, in the parameter sets $\mathbf{m}_{p_{\mathbf{w}}}$, $\mathbf{c}$, and $\mathbf{A}$.

$$\mathbf{m}_{\hat{p}} = \tilde{\mathbf{q}}\left(\mathbf{m}_{p_{\mathbf{w}}}, \mathbf{c}, \mathbf{A}\right) \tag{3.9}$$

Lastly, equation (3.2) is used to arrive at the final result.

$$\mathbf{c} = \rho\left(\tilde{\mathbf{q}}\left(\mathbf{m}_{p_{\mathbf{w}}}, \mathbf{c}, \mathbf{A}\right)\right) \tag{3.10}$$

This is a set of algebraic equations in the parameter sets representing the PDF of the disturbance, the stationary PDF, and the CL feedback.

Successful application of the proposed technique requires a few key elements. First, the basis functions for the CL feedback parameterization must be such that analytical solutions exist for integrals in the right hand side of (3.8). For this reason a series of polynomials may be a good choice, as polynomials are integrable in the same way that moments are calculated. A second issue is that there must be sufficient number of independent parameters available for solution of the equations (3.10). This implies that when making use of the approximation technique, the number of terms used for the two parameterizations should be carefully considered.

The possibility of multiple solutions to equation (3.10) exists and so some auxiliary conditions may be required to render a unique solution.

3.3.2 Application to PDF Approximation

When a closed-loop process model (2.23) is known, the technique given above can be used to derive an approximate PDF for the process model. There is no need to parameterize the closed-loop dynamics and so the technique becomes the problem of finding the PDF parameters based on the known process model.

Consider equation (3.4) with the true CL feedback instead of the parameterization:

$$\hat{p}(\zeta;\mathbf{c}) = \int_{\Re^n} p_{\mathbf{w}}\left(\zeta - \tilde{\mathbf{f}}(\xi)\right)\hat{p}(\xi;\mathbf{c})\,\mathbf{d}\xi \tag{3.11}$$

Again, calculating the moments for both sides of the equation leads to an equation similar to equation (3.7):

$$\mathbf{m}_{\hat{p}} = \int_{\Re^n}\left(\int_{\Re^n}\begin{bmatrix}\left(\mathbf{z}+\tilde{\mathbf{f}}(\xi)\right)^{1,0,0,0,\ldots}\\ \left(\mathbf{z}+\tilde{\mathbf{f}}(\xi)\right)^{0,1,0,0,\ldots}\\ \vdots\end{bmatrix}p_{\mathbf{w}}(\mathbf{z})\,\mathbf{dz}\right)\hat{p}(\xi;\mathbf{c})\,\mathbf{d}\xi \tag{3.12}$$

Invoking equation (3.2) leads to the following equation governing the calculation of approximate PDF parameters for a known time-invariant discrete-time stochastic nonlinear process model:

$$\mathbf{c} = \rho\left(\int_{\Re^n}\left(\int_{\Re^n}\begin{bmatrix}\left(\mathbf{z}+\tilde{\mathbf{f}}(\xi)\right)^{1,0,0,0,\ldots}\\ \left(\mathbf{z}+\tilde{\mathbf{f}}(\xi)\right)^{0,1,0,0,\ldots}\\ \vdots\end{bmatrix}p_{\mathbf{w}}(\mathbf{z})\,\mathbf{dz}\right)\hat{p}(\xi;\mathbf{c})\,\mathbf{d}\xi\right) \tag{3.13}$$

No further simplifications can be made for this general equation. For specific cases, depending on the form of the disturbance PDF, the CL feedback and the PDF parameterization, it may be possible to analytically perform one or both of the indicated integrations, or partial integrations for some elements of the state vectors. In other cases a successive substitution or other iterative approach, involving choosing the parameters, numerically integrating the right-hand side and then revising the choice of parameters based on the result, may be necessary. In the next section a very special approximation result is developed by making use of the GC basis functions.

3.3.3 Specialization for GC PDFs

Gram-Charlier basis functions may be used to approximate the stationary system PDF as follows. It is assumed that a finite series of GC basis functions will provide a satisfactory approximation of the PDF. Recalling equation (2.67), the approximate PDF takes the form:

$$\hat{p}(\mathbf{z}; \mathbf{c}) = \mathbf{c}^T \mathbf{h}(\mathbf{z}) N_{\mu,\Sigma}(\mathbf{z}) \tag{3.14}$$

This approximation is substituted into equation (2.27) as follows:

$$\mathbf{c}^T \mathbf{h}(\mathbf{z}) N_{\mu,\Sigma}(\mathbf{z}) = \int_{\Re^n} p_{\mathbf{w}}\left(\mathbf{z} - \tilde{\mathbf{f}}(\xi)\right) \mathbf{c}^T \mathbf{h}(\xi) N_{\mu,\Sigma}(\xi)\, \mathbf{d}\xi \tag{3.15}$$

Invoking the orthogonality condition, Equation (2.68), with some simplification and rearrangement, the following results:

$$\mathbf{c}^T = \mathbf{c}^T \underbrace{\int_{\Re^n} \int_{\Re^n} p_w\left(\mathbf{z} - \tilde{\mathbf{f}}(\xi)\right) N_{\mu,\Sigma}(\xi)\, \mathbf{h}(\xi)\, \mathbf{h}^T(\mathbf{z})\, dz d\xi}_{\Gamma} \tag{3.16}$$

In the right hand side of Equation (3.16), evaluation of the double integral results in an $N \times N$ matrix of real values, Γ. The final form of equation (3.16) is then:

$$\mathbf{c}^T = \mathbf{c}^T \Gamma \tag{3.17}$$

This implies an eigenvector/eigenvalue problem. The coefficient vector $\mathbf{c}$ is simply the left eigenvector of Γ corresponding to an eigenvalue of 1. The following example highlights the usefulness of this method.

Here it is assumed that a mean and (co)-variance have been selected so that the GC basis functions can be derived from the Gaussian PDF. Choosing a fixed mean and co-variance for the parameterization has the advantage of making the parameterization linear in the remaining coefficients. To ensure a good choice of mean and variance it is recommended that a quick Gaussian approximation of the stationary PDF be made. The mean and variance derived for the Gaussian approximation can then be used to derive the GC basis functions for the GC approximation. Errors in the mean and variance from the coarse approximation may then be corrected by the first and second order GC coefficients.

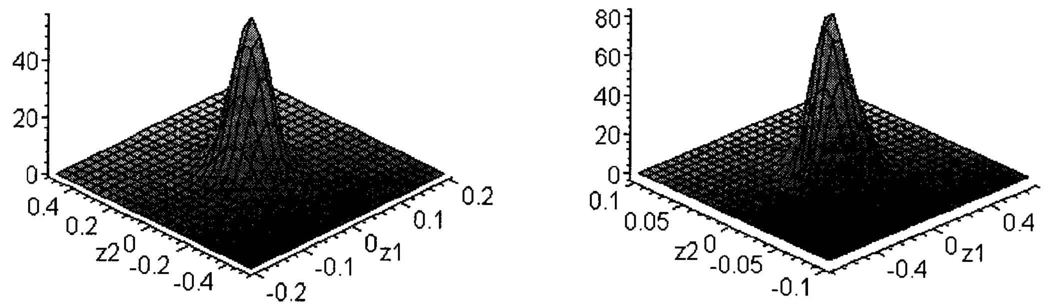
Example 3.3.1 A discrete-time model for a CSTR with a first-order irreversible reaction was developed:

$$\begin{aligned} c_A(k+1) &= g_1(T)\, c_A(k) + g_2(T)\, c_{A,in} \\ c_B(k+1) &= \alpha c_B(k) + g_3(T)\, c_A(k) + g_4(T)\, c_{A,in} \end{aligned} \tag{3.18}$$

where the factors $g_i(T)$ are functions of $\exp\left(-\frac{E}{RT}\right)$. c_A and c_B are, respectively, the concentrations of the reactant, A, and the product, B. $c_{A,in}$ is the concentration of the reactant A in the inlet flow to the reactor, and T is the reactor temperature. The complete development of this model is given in Appendix A. Here it is assumed that the temperature, T, is the manipulated variable, while the concentration of component B, c_B, is the controlled variable. $c_{A,in}$ is a disturbance variable, normally distributed with mean 10 and variance 0.25. The desired setpoint for c_B is 9.1. Under steady-state conditions with noise-free inlet concentration, the setpoint is achieved with a temperature of 380, and c_A becomes 0.9. These steady state values were subtracted from the system equations to put the equations in deviation variable form. Two control strategies were then developed for this reactor. The first strategy was to simply set the reactor temperature to 380 and to let the natural stability of the system reject disturbances. Under this control scheme, the system is linear and hence the PDF for the system states is Gaussian. Standard procedures to obtain the covariance matrix for the system were used. A plot of the state PDF for the first strategy is given by Figure 3.1(a). In Figures 3.1(a) and 3.1(b), for this example $z1$ represents the deviation variable transformation of c_A and $z2$ represents c_B.

The second control strategy was developed by designing an LQR for the linearized system, focussing on tight control of c_B. With temperature being a function of the states, under the LQ feedback control law the system becomes nonlinear. A plot of the state PDF for the second strategy is given by Figure 3.1(b).

In comparing the two figures, some interesting observations can be made. First, as



(a) No control (constant temperature).

(b) Linear, state-feedback control (LQR).

Figure 3.1: PDFs for the CSTR.

expected, the second strategy clearly does a better job in limiting the dispersion of c_B. It can be observed that, while in the first, open-loop, strategy there is relatively small dispersion of c_A and large dispersion of c_B, in the second, closed-loop, strategy the opposite situation arises. Since the second strategy was designed for tight control of c_B, the strategy shifts variability away from c_B and consequently c_A becomes more variable. It is interesting that for the second strategy, although it was designed with variance as a benchmark, the PDF is non-Gaussian and thus variance is an incomplete measure of system behaviour.

□

This type of analysis is insightful from an academic point of view, but it also has consequences in industrial applications. Often, variance is used along with the assumption of Gaussian distributions. The '6σ' region is used to assess quality and to define the normal operating region. When process behaviour is non-Gaussian, the 6σ region does not necessarily reflect the normal or 99% operating region. The mean may not be the centre of the operating region and variables may more (or less) frequently be outside of the assumed region.

3.3.4 An Alternate Interpretation of the Approximation

In this section, an interpretation of the $\boldsymbol{\Gamma}$ matrix developed in §3.3.3 as a multidimensional series expansion of the conditional PDF is described.

Take the conditional PDF, $p_c(\mathbf{x}(t+1)|\mathbf{x}(t))$ for the process (2.23). Holding $\mathbf{x}(t+1)$ constant, $p_c(\cdot)$ can be expanded as a series of Hermite polynomials in $\mathbf{x}(t)$, with coefficients that are functions of $\mathbf{x}(t+1)$, *i.e.*:

$$p_c(\mathbf{x}(t+1)|\mathbf{x}(t)) = p_w\left(\tilde{\mathbf{f}}(\mathbf{x}(t+1)) - \mathbf{x}(t)\right) = \mathbf{d}(\mathbf{x}(t+1))^T \mathbf{h}(\mathbf{x}(t)) \tag{3.19}$$

Invoking the orthogonality condition (2.68)to get the coefficients gives:

$$\mathbf{d}(\mathbf{x}(t+1)) = \int_{\Re^{n_x}} p_w\left(\tilde{\mathbf{f}}(\mathbf{x}(t+1)) - \mathbf{x}(t)\right) N_{\mu,\boldsymbol{\Sigma}}(\mathbf{x}(t))\,\mathbf{h}(\mathbf{x}(t))\,d\mathbf{x}(t) \tag{3.20}$$

Now, each element in the coefficient vector may be expanded as a series of GC functions, *i.e.* $\mathbf{d}(\mathbf{x}(t+1)) \approx \boldsymbol{\Gamma}\mathbf{h}(\mathbf{x}(t+1))\, N_{\mu,\boldsymbol{\Sigma}}(\mathbf{x}(t+1))$. Again, using the proper orthogonality condition to get the coefficients gives:

$$\begin{aligned}\boldsymbol{\Gamma} &= \int_{\Re^{n_x}} \mathbf{d}(\mathbf{x}(t+1))\,\mathbf{h}^T(\mathbf{x}(t+1))\,\mathbf{dx}(t+1) \\ &= \int_{\Re^{n_x}}\int_{\Re^{n_x}} p_w\left(\tilde{\mathbf{f}}(\mathbf{x}(t+1)) - \mathbf{x}(t)\right) \\ &\quad N_{\mu,\boldsymbol{\Sigma}}(\mathbf{x}(t))\,\mathbf{h}(\mathbf{x}(t))\,\mathbf{h}^T(\mathbf{x}(t+1))\,\mathbf{dx}(t)\,\mathbf{dx}(t+1)\end{aligned} \tag{3.21}$$

Making use of both approximations, the conditional PDF is:

$$p_c(\mathbf{x}_{k+1}|\mathbf{x}_k) \approx N_{\mu,\boldsymbol{\Sigma}}(\mathbf{x}(t+1))\,\mathbf{h}^T(\mathbf{x}(t))\,\boldsymbol{\Gamma}\mathbf{h}(\mathbf{x}(t+1)) \tag{3.22}$$

Comparing equation (3.21) with Equation (3.16) shows that the matrices developed for each case are identical. The conditional PDF is often used along with conditional expectation in analysis and controller designs for stochastic processes. The interpretation of the stationary PDF approximation as an approximation of the conditional PDF links these two approaches and provides a useful decomposition that can be used to manipulate the conditional PDF.

3.3.5 Features of the Approximations

While this technique shows a great deal of promise, there are still some issues to be resolved, both theoretical and practical. The $\boldsymbol{\Gamma}$ matrix in the GC approximation, results from a double integration over a large domain while the functions in the integrand tend to have the 'spiky' shape of PDF's. For this reason, numerical integration of the $\mathbf{\Gamma}$ matrix can be quite difficult. Gauss-Hermite quadrature works well for the univariate case while multivariate extensions are not well developed. Different numerical integration methods should be investigated and tested to create an accurate and efficient approximation technique for higher-order processes.

Another issue of practicality is a result of the Gram-Charlier functions themselves. Since they are a product of polynomials and Gaussian PDFs, there is no guarantee that the approximate PDF will meet the non-negativity requirement of PDF's. It should be noted that this issue has not been a problem in the examples investigated in this thesis. The approximation of very skewed PDFs yields approximate PDFs whose tails can oscillate about zero, leading to negative values and more than one mode. This behaviour is noted in (Stuart and Ord, 1994). For engineering purposes, this behaviour need not be a serious problem. (Jondeau and Rockinger, 1999) suggests a technique that may be used to guarantee positive definiteness of the approximate PDF, while (Barton and Dennis, 1952) presents regions of unimodality and positive definiteness for the forth-order univariate series. An alternative technique, consisting of averaging several high-order approximations, is suggested by (Robertson, 1967). Future research in this area could involve incorporation of these techniques into the PDF approximation. However, further investigation will be necessary to find extensions of some of these techniques to multivariate Gram-Charlier approximations.

Accuracy analysis of the approximate PDF is a challenging topic. Here, a sketch of the issues involved is made, while more detailed results are left to later chapters of the thesis. In assessing the accuracy of the proposed approximation, consider the case where the CL process model is known such that equation (3.3) can be made exact. A parameterization (3.1) is then made for the PDF of the CL system to approximate the true PDF, $p_{\mathbf{A}\theta}(\cdot)$, associated with system (2.23). This parameterized PDF does not, in general, provide an exact solution the the equations (3.10). An obvious basis for assessment of accuracy is then to compare $\hat{p}(\cdot;\mathbf{c})$ and $p_{\mathbf{A}\theta}(\cdot)$. Alternatively, the parameterized PDF, $\hat{p}(\cdot;\mathbf{c})$, has an exact corresponding CL feedback, $\tilde{f}_{\hat{p}}(\cdot)$. Comparison of the two feedbacks, $\mathbf{A}\theta(\mathbf{z})$ and

$$\begin{array}{|ccc|}\hat{p}(\cdot;\mathbf{c}) & \overset{\approx}{\longleftrightarrow} & p_{\mathbf{A}\theta}(\cdot) \\ \Updownarrow & & \Updownarrow \\ \tilde{f}_{\hat{p}}(\cdot) & \overset{\approx}{\longleftrightarrow} & \mathbf{A}\theta(\cdot)\end{array}$$

Figure 3.2: Diagram illustrating the challenge of accuracy analysis for the approximation technique.

$\tilde{f}_{\hat{p}}(\cdot)$ also provides a basis for assessing the accuracy of the approximation. The same arguments can be made for the case where the situation is reversed and the PDF is known, but the CL feedback is to be approximated.

The relationships between the exact and approximate functions are illustrated in Figure 3.2.

The problem is that neither $\tilde{f}_{\hat{p}}(\cdot)$ nor $p_{\mathbf{A}\theta}(\cdot)$ is available. This presents a major challenge to analysis of the accuracy of the proposed technique. When the technique is applied with specific forms of parameterization, a more extended analysis may be possible. (Forbes *et al.*, 2003*c*) gives an analysis of the case where Gram-Charlier basis functions are used to parameterize the PDF.

3.3.6 Inherent Process Limitations

Consider the following second-order process model:

$$\begin{aligned} x_1(t+1) &= 0.84x_1(t) + 0.75x_1(t)\,x_2(t) \\ &\quad -0.88x_2(t) + 0.32u(t) + w_1(t) \\ x_2(t+1) &= x_1(t) + w_2(t) \end{aligned} \tag{3.23}$$

where the disturbance variable is iid and Gaussian. For this process there is a major inherent limitation on the shapes of the stationary PDF that are possible. The dynamics of the second state are not directly influenced by the input, implying the following constraint on the marginal state PDFs:

$$p_{x_2}(\zeta) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{1.6\pi}} \exp\left(-\frac{(\zeta-\xi)^2}{1.6}\right) p_{x_1}(\xi)d\xi \tag{3.24}$$

In effect, this limits the number of parameter values that may be independently selected or approximated for the stationary PDF approximation.

Limitations such as these may be used to help reduce the number of parameters that must be calculated in developing approximate PDFs. Another common process limitation is that in many processes, no matter what form of feedback control is chosen, some minimum amount of noise filters through the process.

Example 3.3.2 For example, consider the process:

$$x(t+1) = \tilde{f}(x) + w(t) \tag{3.25}$$

and the objective function:

$$J = E\left[x^2(t+1)\right] \tag{3.26}$$

which is to be minimized with respect to the form of the CL feedback, $\tilde{f}(x(t))$. In such cases the minimization is equivalent to the minimization of the conditional expectation:

$$\begin{aligned} J &= E\left[x^2(t+1)\left|x(t)\right.\right] \\ &= \int_{-\infty}^{\infty} \left(\tilde{f}(x) + w(t)\right)^2 p_w(w(t))\, dw(t) \\ &= \tilde{f}^2(x(t)) + \sigma_w^2 \end{aligned} \tag{3.27}$$

By inspection, it can be seen for this process that the minimum possible variance is σ_w^2. In such cases, the structure of the PDF parameterization for a general process must allow for this constraint to be satisfied, *i.e.*, the variance of the approximate PDF has to be at least as great as the variance of the unremovable noise.

□

Inherent process limitations can be a nuisance in performance-based control design. In characterizing a process with the stationary PDF the inherent limitations are not necessarily a problem, they are just another feature of the process behaviour. In applying the approximation technique to a specific process, a careful analysis should be made to detect and incorporate the inherent limitations into the structure of the PDF parameterization.

3.3.7 Additional Applications

The general approximation technique given in §3.3.1 has a number of additional applications. In Chapters 4 and 5, the approximation is used in the context of PDF-shaping control design. This is in a sense the converse of the application presented above. Instead of having a known process model, and attempting to derive the PDF, in PDF-shaping control design, a target PDF is set and the challenge is to recover the corresponding closed-loop dynamics.

A second application is in controller design with respect to an expectation-type cost function. In such problems, neither the CL process dynamics nor the stationary process PDF are known and so the general approximation must be invoked. From another point of view, this can be interpreted as an approximate solution to the specific optimal control problem. In choosing a parameterization for the CL feedback, the problem is to find the parameters that optimize that cost functional. In this case, the CL feedback is known, at least structurally, and it is the PDF corresponding to this structure that must be approximated. Together the parameterized CL feedback and PDF are used to evaluate the objective and the parameters are varied to locate an approximate optimum.

3.4 Data-based PDF Approximation

Often in the chemical process industry, large amounts of process data are available, but not any sort of rigorous process model. In such cases, the control engineer attempts to recover knowledge about the process from the available data. Knowledge recovery may involve visualization, statistical tests, or model development. If the process data is rich enough in information, a dynamic model of the process may be empirically identified; however, this is not always necessary and often less extensive data analysis may be all that is desired.

In this section, a data analysis technique is presented that allows the data to be concisely summarized as an approximate PDF. The approximate PDF is then available for use in benefits analysis studies, performance evaluation, calculating probabilities of operational constraint violations, and so forth.

3.4.1 An Abundance of Data

Often, large amounts of data are available for an industrial process and the task of the control engineer is to analyze this data to extract useful information. The first step in any data analysis procedure should be visualization. Simple time series plots can be used to identify any unusual features in the data while plotting the coefficients of the FFT shows which frequencies are of greatest interest. Information obtained by visual inspection can often assist in the success of further analysis tools. For this reason, good visualization tools are very important. As an alternative or complement to time series data plots, histograms may be used to indicate the range and dispersion of the data. Sometimes it is desirable not only to visualize the distribution of the data but to develop a functional form for the PDF. (Scott, 1992) presents a number of techniques for estimating (multivariate) PDF's, including both parametric and nonparametric models. (Scott, 1992) does not consider multivariate Gram-Charlier expansions, nor does it provide many details for handling time-series data.

For many types of data, the next level of analysis after visualization is statistical testing. Such testing is especially important for time series data as tests can reveal much about the relationships between variables as they evolve through time. To identify and visualize non-Gaussian time series behaviour, (McLaughlin *et al.*, 1995) suggests using higher order statistics, such as the third-order and fourth-order moments, cumulants or frequency domain spectra. In particular, an estimate of the bispectrum (the Fourier transform of the third order cumulants) is used by (Hinich, 1982) to test for time series non-Gaussianity. (Hinich, 1982) also presents an additional test to determine whether non-Gaussian time series behaviour originates from a non-Gaussian innovations process or a nonlinear filtering operation, *i.e.* a nonlinear system. This work does not make any restrictions on the dimension of the system underlying the time series; however it is unclear how the test procedure relates to state space system models. Also, only the case of univariate noise is presented and multivariate time series are not considered. A number of additional techniques to test for linearity may be found in (Tong, 1990).

A different type of data analysis is needed in the field of signal processing. In (Wong and Blake, 1994) the problem of detecting a known constant signal in multivariate non-

Gaussian noise is described. While the statistical tests relating to this problem may be formally derived, they require the PDF of the test statistic. For non-Gaussian noise processes there is not, in general, a closed form representation for the PDF of the test statistic. Further, it is necessary to derive the PDF of the multivariate noise process in order to implement these tests. (Wong and Blake, 1994) develops 'approximately optimum' detectors by making use of Edgeworth approximations to represent the two required PDF's. While this type of analysis is not directly applicable to the process industries, (Wong and Blake, 1994) provides a useful contribution to the overall understanding of non-Gaussian data analysis by making an insightful connection between the Edgeworth coefficients, higher order statistics and nonlinear analysis.

Visualization and statistical testing can derive a great deal of information about a time series; however, for purposes of filtering, prediction and control, it is often necessary to know the functional form of the stationary PDF, or a dynamic process model.

A unique approach to recovering information about nonlinear processes is that of (Wang, 1999). Wang uses a network of spline functions to approximate the output PDF of the process as a function of the input. This technique allows for explicit shaping of the output PDF using the input variables. For control design, Wang suggests minimizing the difference between a reference PDF and the approximate output PDF but does not examine the relationship between the output PDF model and a nonlinear state-space model for the system itself.

In this section, an alternative idea is proposed for recovering knowledge and information from process data by focussing on fitting the data to a GC PDF.

3.4.2 Fitting Data to GC PDF's

The GC PDFs described in Chapter 2 may be used to derive an approximate PDF for stationary time series data. As discussed in §2.4.1, the coefficients in the approximation are quasi-moments of the PDF, linearly related to the moments by equation (2.58) or a multidimensional analogue. All of the parameters needed to form a GC PDF approximation may then be estimated by time averaging the given data if the process is ergodic. For simplicity the univariate case is presented here. There are no complications in extending the technique to the multidimensional case. Given a set of process data $\{x(1), x(2), \ldots, x(N)\}$, the mean and variance may be estimated from:

$$\hat{\mu} = \frac{1}{N}\sum_{j=1}^{N} x(j) \tag{3.28}$$

and

$$\hat{\sigma}^2 = \frac{1}{N}\sum_{j=1}^{N} (x(j) - \hat{\mu})^2 \tag{3.29}$$

These estimates may then be used to fill in the transformation matrix in equation (2.58). The remaining moments, with the i^{th} moment denoted $\mu^{(i)}$ are then estimated by:

$$\hat{\mu}^{(i)} = \frac{1}{N}\sum_{j=1}^{N} x^i(j) \tag{3.30}$$

Using these moment estimates to fill in the right hand side of equation (2.58) allows for the calculation of the quasi-moments estimates.

This is a simple, yet powerful technique. GC PDFs are a series of orthogonal basis functions. Therefore more detailed approximations of the PDF can be made by simply adding more GC basis functions. Thus without any knowledge of the underlying process dynamics or disturbance distribution, the behaviour of the process can be characterized through a single function that contains a rich amount of information.

The approximate PDF may be integrated against a cost functional to give estimates of process performance for control performance assessment of benefits analysis studies. The tails of the approximate PDF may be integrated to give estimates of critical values to help quantify the risk of large excursions from normal operation. It may also be possible to use the PDF approximation to help recover information about the process dynamics or disturbance distribution.

3.4.3 Accuracy Analysis

Once the approximate PDF has been developed, it is desirable to have a mean of assessing the validity of the approximation. For data that is univariate or bivariate, a quick qualitative method of assessing the fit of the PDF is to plot an appropriately scaled PDF on the same axes as a histogram. This allows for an easy visual inspection of whether the approximate

PDF captures the major features such as the mode, the spread of the data and the behaviour of the tails.

Another qualitative technique for univariate data is to use probability plots, as discussed in Chapter 2. Here quantiles of the data would be plotted against the corresponding quantiles calculated from the approximate PDF. If the plot shows a 45 degree line without any substantial deviations from the linear relationship, than the approximate PDF can be judged as correct.

A quantitative method to assess the agreement of data with a proposed PDF is to use a goodness of fit test, as described in Chapter 2 and in (Devore, 1995). Unfortunately, for this test to be applied, the estimates of any parameters must be maximum likelihood estimates. While the coefficients developed for the approximate PDF are obviously method of moments estimators, it cannot be ascertained whether they are maximum likelihood estimators. For stationary time series data, where the data are not independent, and the underlying process dynamics are unknown, there is no way to specify the joint PDF of the data. Therefore, maximum likelihood estimators cannot be easily developed. Further investigation of this challenging problem is beyond the scope of this thesis. The relationship between data, the underlying process dynamics, the stationary PDF and the joint PDF of data is well into the area of process identification. This may prove a fruitful area for future research initiatives.

3.4.4 Discussion

One issue relating to the data-based approximation is whether the approximate PDF is actually a stationary PDF. If the process order is not correctly identified the approximated PDF is either a marginal PDF (and therefore an incomplete summary of the process behaviour) or is of unnecessarily high order and partially redundant. The purpose of this section was to demonstrate how GC PDF parameters may be easily estimated. While the problem of process order estimation is easily handled for linear processes by correlation analysis or impulse response techniques, the problem is much more involved for nonlinear processes. This topic is beyond the scope of this thesis. For issues of process order determination, the reader is referred to the literature, such as (Ljung, 1999). Of course, for some applications, representation of a marginal PDF may be all that is desired. In these situations, order determination is not an issue and the coefficient estimates can be immediately made using the available process data.

If the stationary PDF of a process is known, then it may be possible to make use of the PDF to aid in dynamic model building. This would, in principle, require inversion of equation (2.27), which is not generally possible. However, it is possible to use relationships between parameterized process PDFs and parameterizations of the nonlinear CL feedback to develop an approximate inversion. For this to work, some structure must be imposed on the disturbance distribution to ensure well-posedness of the approximation problem. This topic is closely related to the results of Chapters 4 and 5 where for a known open-loop process model and disturbance distribution, the closed-loop process dynamics that correspond to a selected stationary process PDF are calculated. For process identification purposes, the open-loop process is unknown. If the closed-loop dynamics can be recovered, the open-loop dynamics can be back-calculated using knowledge of the feedback control law. This topic will be discussed in further detail in Chapter 7 where it is suggested as an area for future research investigations.

A related problem of potential interest to control engineers is the 'converse' problem discussed in (Tong, 1990). Assuming that the dynamics of the system are known and that the state PDF is known or can be estimated, the problem is to find the PDF of the process disturbance. While (Tong, 1990) presents a few results for this problem, it does not provide sufficient detail. The application of results in this area to process data could yield useful insights for industrial processes. For example, if a process model is available and the stationary PDF can be approximated from data, then an approximation of the PDF for the noise perturbing the system can be made. The approximate noise PDF can be useful as a tool for diagnosing sources of disturbances in industrial plant process. It may also be useful as a tool for verification of empirical system models.

To conclude this section, it has been shown how to use method of moments estimators to develop approximate GC PDFs from process data. Due to the nature of serially correlated process data, the standard goodness of fit test cannot be applied to this approximation, but some qualitative techniques are available. The proposed approximation has a large number of potential applications. Some of these, such as benefits analysis studies, can be realized using current frameworks, while others, such as process identification, are speculative and require further investigation.

3.5 Illustrative Example

This example demonstrates the effectiveness of the model-based and data-based PDF approximation techniques. The behaviour of the following first-order process is examined:

$$x(t+1) = \frac{2}{\sqrt{5}} |x(t)| + w(t) \tag{3.31}$$

The disturbance, $w(t)$ is iid with a PDF, $p_w(\cdot)$, that is zero-mean, unit-variance Gaussian. Note that the sign-change nonlinearity in this model at $x(t) = 0$ ensures that the stationary PDF is non-Gaussian.

3.5.1 Exact PDF

The process (3.31) is one of the rare cases where an exact stationary PDF may be solved for in equation (2.27). The solution, given in (Tong, 1990), is reproduced here. The stationary PDF is given by:

$$\begin{aligned} p(\zeta) &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\left(\zeta - \frac{2}{\sqrt{5}}|z|\right)^2}{2}\right) p(z)dz \\ &= \int_{-\infty}^{0} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\left(\zeta + \frac{2}{\sqrt{5}}z\right)^2}{2}\right) p(z)dz \\ &\quad + \int_{0}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\left(\zeta - \frac{2}{\sqrt{5}}z\right)^2}{2}\right) p(z)dz \end{aligned} \tag{3.32}$$

Using the symmetry of $p_w(\cdot)$:

$$\begin{aligned} p(-\zeta) &= \int_{-\infty}^{0} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\left(\zeta - \frac{2}{\sqrt{5}}z\right)^2}{2}\right) p(z)dz \\ &+ \int_{0}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\left(\zeta + \frac{2}{\sqrt{5}}z\right)^2}{2}\right) p(z)dz \end{aligned} \tag{3.33}$$

The two equations are added together to give:

$$\bar{p}(\zeta) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\left(\zeta - \frac{2}{\sqrt{5}}z\right)^2}{2}\right) \bar{p}(z)dz \tag{3.34}$$

where: $\bar{p}(\zeta) = \frac{p(\zeta)+p(-\zeta)}{2}$. If one recognizes that this is the equation for the stationary PDF of a first-order linear process (see example 2.2.2), then it is possible to deduce that the solution, $\bar{p}(\zeta)$, can be written as:

$$\bar{p}(\zeta) = \frac{1}{\sqrt{10\pi}} \exp\left(-\frac{\zeta^2}{10}\right) \tag{3.35}$$

Revisiting equation (3.32) allows the PDF, $p(\cdot)$, to be derived from $\bar{p}(\cdot)$ in the following way:

$$\begin{aligned} p(\zeta) &= \int_{0}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\left(\zeta - \frac{2}{\sqrt{5}}z\right)^2}{2}\right) 2\bar{p}(z)dz \\ &= \left(1 + \operatorname{erf}\left(\sqrt{\frac{2}{5}}\zeta\right)\right) \frac{1}{\sqrt{10\pi}} \exp\left(-\frac{\zeta^2}{10}\right) \end{aligned} \tag{3.36}$$

where $\operatorname{erf}(\cdot)$ is the error function. Since an exact non-Gaussian PDF is available for this process model, it can be used as a basis for assessing the accuracy of the proposed approximation techniques.

3.5.2 Approximate PDFs

For this PDF, three different approximations may be made. A GC approximation based on the exact PDF and approximations using the proposed model-based and data-based techniques.

Since the exact stationary process PDF is known, an easy means of validating the performance of the Gram-Charlier PDF as an approximating PDF is available. The mean and variance are calculated and used in the generation of a Gram-Charlier basis. Once the basis is calculated, equation (2.59) is used to calculate the coefficients for an eighth-order GC PDF approximation. The values of the coefficients are given in Table 3.1 and a plot of this approximate PDF is given is Figure 3.3(a).

Next, the proposed model-based approximation technique is applied. Note that no derivative exists for the process feedback $\frac{2}{\sqrt{5}}\|x\|$ at $x(t) = 0$. As a result, approximation techniques based on linearization near that point are difficult to use. Using the proposed model-based technique, the approximate PDF is developed. First, a Gaussian approximation is made to determine approximate mean and variance. Using the approximate Gaussian PDF, an eighth-order GC basis is created and used in the technique described in §3.3.1. The resulting coefficients are given in Table 3.1. Since, the GC basis is developed based on a Gaussian PDF approximation, the values for the first and second coefficients are not zero. To use the standard approach of automatically setting these to zero results in a less accurate PDF. The plot of this approximate PDF is given is Figure 3.3(b). It can be observed that this approximation is not as accurate as the approximation derived from the exact PDF. However, it remains nearly indistinguishable from the exact PDF.

The data-based approximation technique was also tested against the process (3.31). The process was simulated to generate ten thousand time steps of data. This data is plotted in Figure 3.3(c). Using the data, method of moments estimates of the mean, variance and GC coefficients up to eighth-order were made. Again, these are given in Table 3.1. The data used to generate a histogram, and the approximate PDF was appropriately scaled so that agreement of the data, the approximate PDF, and the exact PDF can be judged. This plot is given in Figure 3.3(d). It could be suggested that small errors in the approximate PDF generated from the data could be the result of an unusual data set. However, it is pointed out that even when the exact PDF is known, the analytical approximation is not exact. Additionally, the large size of the data set used suggests that better agreement with the true PDF cannot reasonably be expected from this approximation.

Table 3.1: Coefficients for the approximate PDFs

Parameter	Direct Calculation	Model-Based	Data-Based
μ	$\frac{2\sqrt{2}}{\sqrt{\pi}} \approx 1.60$	1.67	1.54
σ^2	$5 - \frac{8}{\pi} \approx 2.45$	2.22	2.35
c_0	1	1	1
c_1	0	-0.0475	0
c_2	0	0.0752	0
c_3	0.185	0.210	0.181
c_4	0.0623	0.0626	0.0823
c_5	-0.00136	0.0405	0.0354
c_6	0.0521	0.0887	0.0580
c_7	0.0478	0.0651	0.0122
c_8	0.0120	0.0359	-0.0358

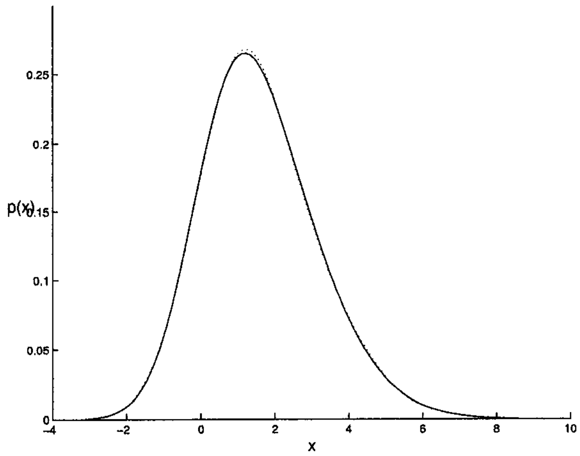
Three different PDF plots are given in the collection of Figures 3.3. In all of these plots, the approximate PDFs appear to be very comparable to the exact PDF. In all cases the mode is correctly positioned and the spread of the PDF is correct; in particular, the lengthy right tail of the PDF is well-represented. Probability plots are used to further assess the agreement of the three approximate PDFs with the true PDF. The 0.5% quantiles for the true distribution are plotted against the corresponding quantiles for the approximate distributions in Figures 3.4(a), 3.4(b) and 3.4(c). In all three cases the quantiles fall along a nearly perfect 45° line. It should be noted that the third plot, for the data-based approximate PDF shows some small deviation from the straight line. It is interesting to note that in this case the PDF approximation based directly on the model is more accurate than the approximation based on the simulated data, even though a very large amount of data is used.

3.6 Chapter Summary

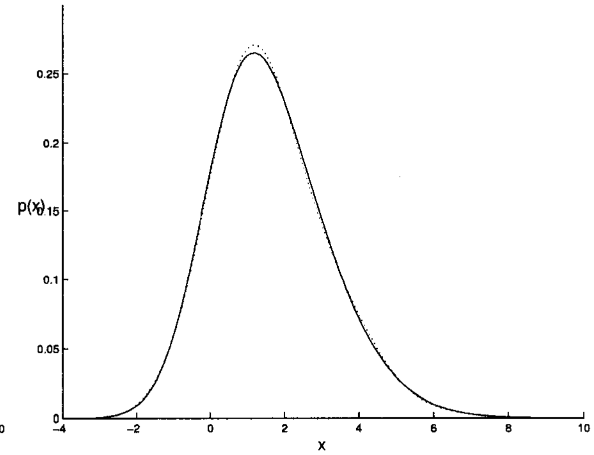
In this chapter, techniques to characterize stationary stochastic processes in terms of their PDFs are developed. Two different approaches are used. In the first case, an approximate representation of the PDF is derived from the process model. In general, solutions to the integral equation defining the relationship between process dynamics and the stationary PDF are not known. However, by carefully parameterizing the PDF the integral equation can be reduced to a set of algebraic equations. These are then solved using numerical techniques. The approximation is developed for the general case and then specialized to approximation using GC PDFs. The use of GC PDFs simplifies considerably the approximation technique.

In the second case, method of moments estimation is used to generate Gram-Charlier PDF parameters from process data. This is a simple technique that can always be applied to a given data set.

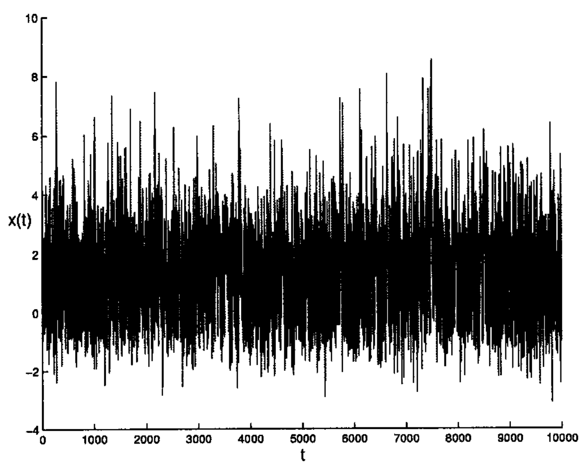
The two techniques are applied to an example process. The example process is one of the rare cases for which the stationary PDF can be obtained in closed-form and so approximate results are compared to the exact result. In both the cases, qualitative assessment of the approximations confirms the success of the techniques.



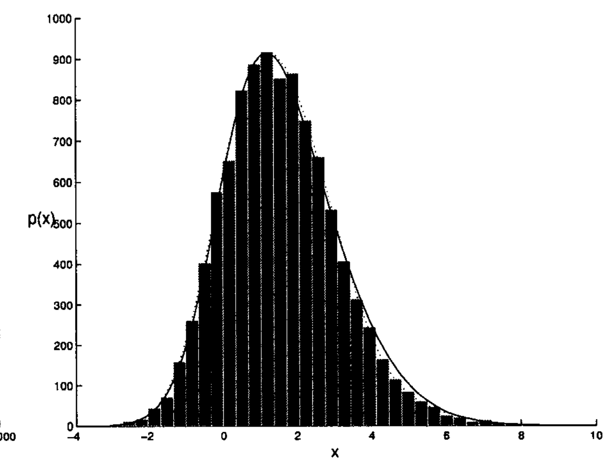
(a) Approximate PDF derived from the exact PDF.



(b) Approximate PDF derived from the process model.

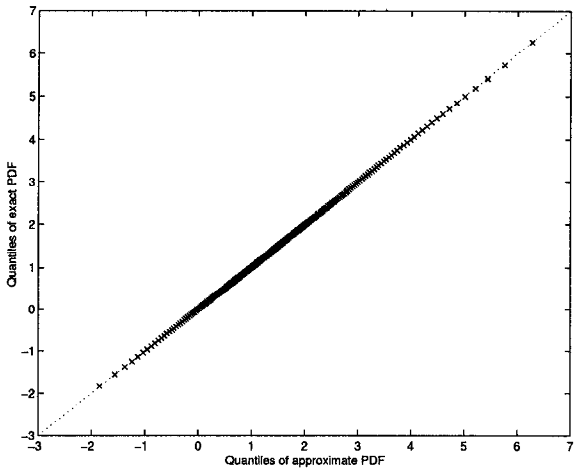


(c) Simulated time series data.

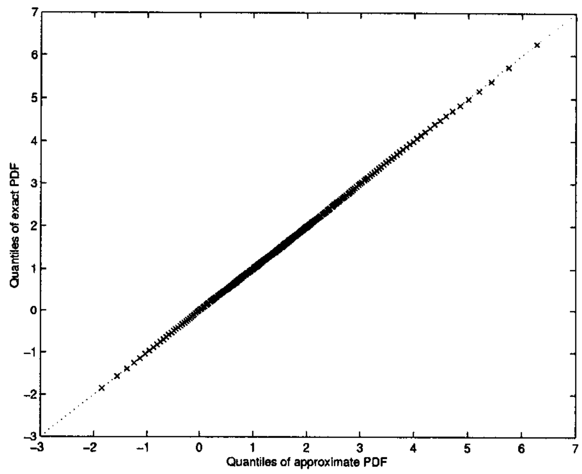


(d) Histogram and approximate PDF (scaled) for the process based on simulated data.

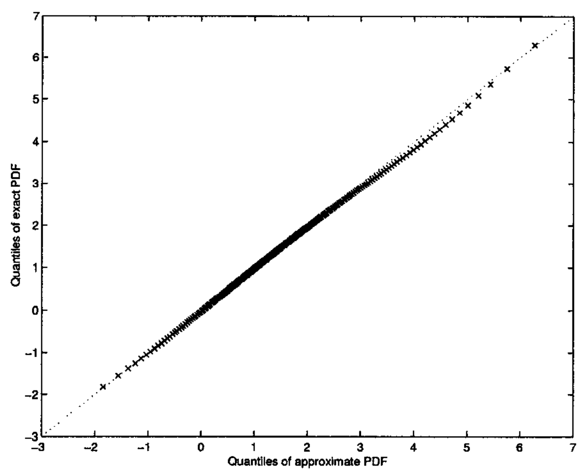
Figure 3.3: Plots associated with the example process (3.31) - in the PDF plots, the exact PDF is included, for comparison, as the solid line.



(a) Probability plot for the approximate PDF derived from the exact PDF.



(b) Probability plot for the approximate PDF derived from the process model.



(c) Probability plot for the approximate PDF derived from the simulated data .

Figure 3.4: Quantile-quantile plots (from 0.5% to 99.5% by 0.5%) to assess the accuracy of the 3 PDF approximations.

"Take all your problems
And rip 'em apart...
Be like the squirrel, girl
Be like the squirrel"
– The White Stripes

4

Introduction to PDF-Shaping Control Design

While the long-term behaviour of a stationary stochastic process is concisely summarized by the PDF, many well-established regulatory control techniques focus only on two quantities derived from the PDF, the mean and variance, as key design targets. This chapter presents a technique for the design of control laws that shape all aspects of the PDF of a first-order process. By developing relationships between the moments of the PDF and the coefficients in a control law parameterization, an approximate control law is developed to shape the process PDF as desired. The process engineer then chooses an appropriate shape for the process PDF based on economic, safety, or other engineering concerns.[1]

[1]Parts of this chapter were presented at the 2001 AIChE Annual Meeting and in (Forbes *et al.*, 2002*b*) and (Forbes *et al.*, 2002*a*).

4.1 Introduction

Random process behaviour means that even carefully controlled process variables, as they evolve over time, cannot be set at a single operating point; and even when control is introduced to reduce the variance of one variable, the result is increased variance of the manipulated variable or of closely integrated processes. Since stochastic behaviour is an unavoidable fact of industrial processes, it is unrealistic to task the control engineer with elimination of variability in key variables. Instead, random behaviour should be managed so that the process operates safely and with the greatest economy or profitably.

With this in mind, this chapter introduces the PDF-shaping regulatory control design concept. The long-term behaviour of a well-behaved stochastic process is summarized concisely by the stationary PDF, and quantities derived from the PDF, such as mean and variance, are often key targets for process control or measures of controller performance (Desborough and Harris, 1992) and (Astrom, 1970). In PDF-shaping control design, the entire shape of the PDF is set as the target for the design, and thus all of the moments are targeted and not just the first two.

For example, when a plant operates near a safety or performance specification, the tail behaviour of the process PDF becomes of critical importance. For this reason, the problem of control design to shape the process PDF is considered. The framework developed here takes advantage of the fact that a PDF can be described by its moments; other features of the PDF, such as tail behaviour, are a consequence of the moments. It is then up to the process engineer to choose an appropriate shape for the process PDF based on economic or engineering concerns.

By taking this approach, a number of important process considerations may be simultaneously built into the control design problem. For example, a target PDF with a small variance, a specific mean and only small tails extending past certain critical values may be selected.

PDF-shaping design to target a Gaussian PDF is one of the few cases for which an exact solution to the PDF-shaping design problem is available. This simple case is used in the following example.

Example 4.1.1 The PDF-shaping concept can be very quickly illustrated using the first-order linear process:

$$x(t+1) = \alpha x(t) + u(t) + w(t) \tag{4.1}$$

where $n_x = n_u = n_w = 1$ and $w(t)$ is an iid, zero-mean Gaussian disturbance with variance σ_w^2. The control law:

$$u(t) = a_0 + a_1 x(t) \tag{4.2}$$

is to be used. It is well known that this process is stationary and Gaussian, provided that $|\alpha + a_1| < 1$ (see example 3.3.1). Therefore the PDF of this controlled process has mean $\mu = \frac{a_0}{1-\alpha-a_1}$ and variance $\sigma^2 = \frac{\sigma_w^2}{1-(\alpha+a_1)^2}$. Taking advantage of these equalities allows the CL process to be written as:

$$\begin{aligned} x(t+1) =& \alpha x(t) + \mu\left(1 - \alpha - \left(\sqrt{1-\frac{\sigma_w^2}{\sigma^2}} - \alpha\right)\right) + \left(\sqrt{1-\frac{\sigma_w^2}{\sigma^2}} - \alpha\right) x(t) + w(t) \\ =& \mu + \sqrt{1-\frac{\sigma_w^2}{\sigma^2}}\,(x(t) - \mu) + w(t) \end{aligned} \tag{4.3}$$

This form of the CL process model shows that parameters in the process dynamics correspond to the parameters in the stationary PDF. Therefore the shape of the PDF can be altered by choosing different feedback control parameters. In this case, simple and exact relationships between the parameters are available. For more complex process-PDF combinations, exact relationships can be prohibitively complicated for control design applications, and so simplifying approximations are made.

□

Since only a handful of exact solutions to the stationary PDF equation (2.27) - and thus to the PDF-shaping problem - are known, an approximate PDF-shaping technique is proposed in this chapter. The design technique develops a set of algebraic equations giving an implicit relationship between the PDF parameters and the parameters in the state-space equation. By developing relationships between the moments of the PDF and the coefficients in a control law parameterization, an approximate control law is developed to shape the process PDF as desired. The result is a PDF-shaping control design technique that is useful both for control design as well as analysis of process behaviour.

Additionally, the special case of GC target PDFs is investigated in detail. The mathematical properties of this particular type of PDF make it extremely useful in simplifying and analyzing the approximation technique; as well, it can simplify the selection of a desirable PDF.

In this chapter, the concept of PDF-shaping control design is developed for single-input, first-order stochastic nonlinear processes. The focus is restricted to these simple processes in order to highlight the concept of PDF-shaping design without the distraction of too many technical details. The next chapter will deal with the more sophisticated multiple-input, multiple-output, higher-order processes, as well as the problems associated with coloured noise and delay.

This chapter is organized as follows: In §2, works from the literature related to the current topic are reviewed as well as some mathematical tools needed to develop the proposed technique. In §3 the PDF-shaping control design technique is introduced for the general case. The technique is then specialized and further developed for the case of Gram-Charlier PDFs in §4; as well, issues of stability and accuracy are discussed. §5 provides some linkages between the PDF-shaping control design and optimal control designs. The role of PDF-shaping design in the complete controller (re-)design strategy is given in §6. §7 provides an illustration of the mechanics and results of the proposed technique by designing a PDF-shaping control law for an example process and simulating the resulting closed-loop process. §8 concludes the chapter.

4.2 Background

The problem of regulatory control design for stochastic nonlinear processes is typically considered from the perspectives of stability and optimality with respect to a cost function. Existing design techniques are mainly concerned with linear processes and quadratic cost functions. In this chapter, an alternative perspective for control design is presented, where optimal cost considerations are replaced by a focus on the PDF as a performance criterion. A new design technique is introduced that designs controllers so that the long term behaviour of the closed-loop process matches a desired PDF.

Focussing attention on the shape of the process PDF has a number of advantages. As will be shown below, the equation describing the stationary distribution of a process includes complete information about both the process dynamics and the PDF of the noise. Thus, all information about the process is summarized in a single quantity that is sensitive to process nonlinearity and noise distribution. Traditional metrics such as mean and variance are easily calculated from the PDF, while plots of the PDF reveal a wealth of additional information. In particular, control engineers may be interested in the tails of the PDF and the presence of multiple modes. Such information is lost, or not considered, in established stochastic control design techniques.

For processes where a safety, environmental or quality constraint is present, PDF-shaping control design is well suited. Frequently, processes operate at their constraints and so an important goal for control design is to limit, if not eliminate, constraint violation. For ease of discussion, this chapter will focus on quality constraints; however, similar arguments can be made for other types of constraints. In the case of a process operating at a quality constraint, the consequences of constraint violation can be costly. The product may need to be reprocessed or reblended before it can be sold. If off-specification product is shipped to clients, it can lead to a loss of client confidence or even lost business. If off-specification product cannot be reprocessed, or sold at a lower price, it may be discarded outright. On the other hand, a product that consistently exceeds quality specifications will also result in added costs from the additional raw materials, energy costs or processing time used. For such processes, the best operating strategy is to operate as close to the constraint as possible while keeping violations below some maximum tolerance.

The usual approach to control design or redesign for a process at a quality constraint is to reduce process variance. The mean of the product quality may then be moved closer to the constraint without increasing the frequency of constraint violations. This approach to control (re-)design is illustrated in Figure 1.3(a) (§1.2). As discussed in (Latour, 1992) and (Latour, 1996), profits result not only from the change in setpoint, but also from the reduction in variance alone.

While this technique has proven to be successful, it does not account for a number of important issues. Focussing attention on mean and variance only often leads to the notion that the PDF is Gaussian. While it is true that for linear processes with Gaussian noise the

PDF of the process is also Gaussian, this does not hold in general. Mean and variance do not capture features of non-Gaussian PDF's that may reflect significant process behaviour near a constraint. Also, even if the open-loop process has a Gaussian PDF, this does not necessarily mean that for the closed-loop process a Gaussian PDF is desirable. Indeed, it may be useful to emphasize some non-Gaussian features of a PDF, such as reducing one of the tails. For these reasons, for analysis and design purposes, it is best to consider not just the first two moments of process PDF's but the entire PDF. PDF-shaping control design accounts for these considerations by selecting a certain shape for the process PDF as the goal of the control design procedure. This approach is illustrated in Figure 1.3(b) (§1.2).

To date, this approach to stochastic control design has received very little attention in the process control literature. The contributions made by (Karny, 1996) and in (Wang, 1999; Wang, 2000; Wang and Zhang, 2001; Wang, 2002) are discussed in Chapter 1 and the differences that exist between those works and the present topic are discussed.

It should be noted here that the PDF-shaping discussed in this thesis is a completely different problem from distribution shaping in the distributed parameter context, as is discussed in works such as (Rawlings *et al.*, 1993). This other notion of PDF-shaping involves quantities that are expressed as a distribution of values at each instant of time. The focus in such problems is on the evolution of the distribution over time, and possibly space, and the process models used are distributed parameter models. In contrast, here it is the stationary PDF of a lumped parameter system that is discussed.

4.2.1 Mathematics

Before proceeding with the development of the PDF-shaping technique, the relevant mathematics are briefly reviewed.

The discussion in this chapter is restricted to the first-order version of the process (2.15):

$$x(t+1) = f(x(t), u(t)) + w(t) \tag{4.4}$$

where the dimensions of the state, input and disturbance are $n_x = n_u = n_w = 1$. Again, a feedback control law is sought, which in this case is a scalar valued univariate function:

$$u(t) = k(x(t)) \tag{4.5}$$

The stationary PDF for this process is then:

$$\begin{aligned} p(\zeta) &= \int_{-\infty}^{\infty} p_w\left(\zeta - f\left(z, k\left(z\right)\right)\right) p\left(z\right) dz \\ &= \int_{-\infty}^{\infty} p_w\left(\zeta - \tilde{f}\left(z\right)\right) p\left(z\right) dz \end{aligned} \tag{4.6}$$

4.3 The PDF Shaping Control Design Problem

In this section the PDF-shaping control design technique is introduced. The proposed technique aims to find a control law that yields a stationary closed-loop process with a specified stationary PDF. An approximate technique is developed to overcome the intractability of the invariant integral equation governing the relationship between the CL process dynamics and the stationary PDF. By parameterizing both the CL dynamics and the stationary PDF, the integral equation is reduced to a set of algebraic equations in the parameters. Post-design stability analysis of the design is investigated, including a technique to eliminate any potential regions of instability in the state-space. For the type of process discussed in this chapter, there is one major restriction imposed on the shape of the PDF that may be chosen. This topic is addressed in §4.3.4. The analysis of the accuracy for the proposed approximate design technique is deferred to the next major section.

4.3.1 Formulation

The general PDF shaping design problem may be stated as follows.

For the process: $x(t+1) = f(x(t), u(t)) + w(t)$

find: $u(t) = k(x(t))$

such that: $p(x(t)) = p^*(x(t))$

The last part of the statement says that the stationary PDF, $p(\cdot)$, for the CL process should be equivalent to a target stationary PDF, $p^*(\cdot)$. This implies that the CL process should be stationary. An appropriate target PDF should be selected by the control engineer to reflect engineering concerns or the economics of the process. From previous discussions about the stationary PDF, it is apparent that the problem statement simplifies to the solution of the following equation for the feedback control law, $k\cdot$:

$$p^*(\zeta) = \int_{-\infty}^{\infty} p_w(\zeta - f(z, k(z)))\, p^*(z)\, dz \tag{4.7}$$

As stated above, few specific solutions to this problem are known. Therefore, the key design equation is also a major barrier to solving the PDF-shaping problem.

4.3.2 Approximate Solution

In order to find an approximate solution to the PDF shaping problem, the dynamics-PDF approximation technique from the previous chapter is applied here. Notice that this is the converse application to §3.3.2 where the CL process dynamics are known, but the PDF is not.

The chosen PDF, $p^*(\cdot)$, should be such that it has a few key parameters, *i.e.*,

$$p^*(z) = p^*(z; \mathbf{c}) \tag{4.8}$$

As in Chapter 3, it is assumed that the parameters $\mathbf{c}$ are known functions of the moments, $\mathbf{m}_{p^*}$, of the parameterizing PDF.

$$\mathbf{c} = \rho(\mathbf{m}_{p^*}) \tag{4.9}$$

The equation that must be solved is then:

$$\hat{p}(\zeta; \mathbf{c}) = \int_{\Re} p_{\mathrm{w}}\left(\zeta - \tilde{f}(\xi)\right) \hat{p}(\xi; \mathbf{c})\, \mathrm{d}\xi \tag{4.10}$$

Following the developments in Chapter 3, this equation is reduced to:

$$\mathbf{c} = \rho\left(\int_{\Re} \mathbf{q}\left(\mathbf{c}_w, \tilde{f}(\xi)\right) \hat{p}(\xi; \mathbf{c})\, \mathrm{d}\xi\right) \tag{4.11}$$

where $\mathbf{q}$ is a vector of multivariate polynomials in the parameters, $\mathbf{c}_w$, of the disturbance PDF and the closed-loop feedback, $\tilde{f}(z)$. To proceed, it is necessary to give a structure to the CL feedback, $\tilde{f}(\cdot)$. This is done with a parameterization of the following form:

$$\tilde{f}(z) \simeq \mathbf{a}^T \theta(z) \tag{4.12}$$

The parameterization, (4.12), is now substituted into equation (4.11).

$$\mathbf{c} = \rho\left(\int_{\Re} \mathbf{q}\left(\mathbf{c}_w, \mathbf{a}^T\theta\left(\xi\right)\right)\hat{p}\left(\xi;\mathbf{c}\right)d\xi\right) \tag{4.13}$$

Performing the integration in the right hand side of equation (4.13) will result in functions, $\tilde{\mathbf{q}}$, in the parameter sets $\mathbf{c}_w$, $\mathbf{c}$, and $\mathbf{a}$.

$$\mathbf{c} = \rho\left(\tilde{\mathbf{q}}\left(\mathbf{c}_w, \mathbf{c}, \mathbf{a}\right)\right) \tag{4.14}$$

This is a set of algebraic equations in the parameter sets representing the PDF of the disturbance, the stationary PDF, and the CL feedback.

Successful application of the proposed technique requires a few key elements. First, the basis functions for the CL feedback parameterization must be such that analytical solutions exist for integrals in the right hand side of (4.13). For this reason a series of polynomials may be a good choice, as polynomials are integrable in the same way that moments are calculated. A second issue is that there must be sufficient degrees of freedom for solution of the equations (4.14). This implies that when making use of the approximation technique, the relative orders of the parameterizations of the PDF and CL feedback should be balanced.

The possibility of multiple solutions to equation (4.14) exists and so some auxiliary conditions may be required to render a unique solution.

These equations may then be solved for the CL feedback parameters, $\mathbf{a}$. The closed-loop dynamics may then be inverted, as in equation (2.25), to give the feedback control law.

4.3.3 Stability of the Closed-Loop Process

PDF-shaping control design aims to create a control law that, when implemented, results in a closed-loop process that has a desired PDF. The corollary to this is that, if the control design is successful, the closed-loop process will be stationary, otherwise, there could not be a stationary PDF. While stationarity is useful in time series analysis and in most circumstances is a desirable process behaviour, related notions of stability are more commonly discussed in the process literature.

The relationship between stability, stationarity and ergodicity of stochastic processes is still an open area of research.

Techniques of stabilization for certain classes of stochastic processes are well-developed. One good reference is (Krstic and Deng, 1998). This reference discusses inverse optimal backstepping procedures for stabilization in probability of continuous time processes where the noise does not destabilize the process equilibrium. (Krstic and Deng, 1998) also discusses the disturbance attenuation problem, again for continuous time processes, where the noise will move the process away from what would otherwise be an equilibrium point. For this case, the concept of noise-to-state stability is introduced as an extension of the well-known input to state stability. Again, for the noise-to-state stabilization technique, the inverse optimality is discussed. Throughout this work there is no mention of the stationary PDF for the resulting closed-loop processes. Additionally, because of the continuous-time focus of the book, the techniques cannot be applied in this paper. At this time there do not seem to be references to any direct discrete-time extensions.

A theorem in (Tong, 1990) shows that for the closed-loop process (2.23) if the deterministic part of the process can be shown to be globally stable, then with some additional technical conditions, the process can be shown to be ergodic, and thus stationary. For the result of this chapter, the CL feedback depends, structurally, upon the set of basis functions chosen for the parameterization, so it is not possible to make any *a priori* guarantees about process stability. There is, however, a good likelihood that this technique will produce stable processes, at least locally.

Since the design goal is a stationary PDF, an indirect goal of creating a stationary process is built into the technique. No theorems are available stating that stationarity implies stability; however, it is hard to envision, an unstable, but stationary process. Similarly, as part of the PDF specification, the variance that the closed-loop process is to display is a specified finite value. Again, it is hard to envision a process that is unstable yet displays a finite variance. Therefore in specifying finite variance, it is likely that stability is also specified.

While, *a priori* stability guarantees cannot be made, an *a posteriori* stability analysis is easily performed. Once the CL feedback design has been completed, and the control law recovered, the stability of the deterministic portion of the process may be evaluated via a Lyapunov analysis. Heuristically, if a large region of stability (large relative to the variances of the process and noise PDF's) exists, the process should display a local type of ergodicity. The main problem in this situation is that occasional large disturbances may push the process outside of its stable region. To prevent this, a simple, stabilizing feedback control should be used outside of the designed control law's stable region. This stabilizing feedback may be designed using the Lyapunov analysis. The stability analysis and design work as follows. Taking the designed, closed-loop feedback, one locates the equilibrium point, x_e, of the deterministic process.

$$x_e - \mathbf{a}^T\theta(x_e) = 0 \tag{4.15}$$

Usually, but not necessarily, the equilibrium point will lie near the desired process mean. Using the standard Lyapunov function

$$V(x) = (x - x_e)^2 \tag{4.16}$$

one substitutes the designed CL feedback into the difference

$$\dot{V}(x_t) = V(x_{t+1}) - V(x_t) = \left(\mathbf{a}^T\theta(x_t) - x_e\right)^2 - (x_t - x_e)^2 \tag{4.17}$$

and then finds the region around the equilibrium:

$$[a, b] = \{x \mid V(x) \leq \alpha, \dot{V}(x) < 0 \,\forall\, x \neq x_e, \dot{V}(x_e) = 0\} \tag{4.18}$$

The designed CL feedback can then be used as a basis for control within some subregion of the stable region, $[a + \epsilon, b - \epsilon], \epsilon > 0$ and simple stabilizing CL feedback may then be designed for the regions, $[-\infty, a + \epsilon]$ and $[b - \epsilon, \infty]$. To ensure continuity of the CL feedback and the control law, the following simple closed-loop feedbacks are recommended.

$$\tilde{f}(x) = 0.7(x - z) + \mathbf{a}^T\theta(z) \tag{4.19}$$

where for the region to the left of the stable region $z = a + \epsilon$ and for the region to the right of the stable region $z = b - \epsilon$. Note that these modified feedbacks stabilize the equilibrium point, $x_e = \frac{-0.7z + \mathbf{a}^T\theta(z)}{0.3}$, of the closed-loop system and that these equilibrium points lie within the region of stability of the original designed feedback. Placing the process in deviation form, $\xi_t = x_t - \frac{-0.7z+\mathbf{a}^T\theta(z)}{0.3}$ gives:

$$\begin{aligned} \xi_{t+1} &= 0.7(\xi + \frac{-0.7z + \mathbf{a}^T\theta(z)}{0.3} - z) + \mathbf{a}^T\theta(z) - \frac{-0.7z + \mathbf{a}^T\theta(z)}{0.3} \\ &= 0.7\xi_t \end{aligned} \tag{4.20}$$

which shows the stability. Thus these stabilizing feedbacks steer the process back to the normal operating region.

The use of piecewise control ensures stability of the closed-loop process. The control law based on the designed CL feedback provides the desired performance while the simple stabilizing control laws ensure stability in the rare instances where the noise terms are exceedingly large.

4.3.4 Inherent Process Limitations

The first-order processes discussed in this chapter impose one inherent limitation on PDF-shaping control design.

From the result of example 3.3.2, it can be seen that the minimum variance for the process (4.1), under any control strategy is σ_w^2. In the feedback control law, and therefore in the CL process, if the process variance is set in violation of the minimum variance constraint, *i.e.*, $\sigma^2 < 1$ then the factor $\sqrt{1 - \frac{\sigma_w^2}{\sigma^2}}$ will not yield a real number. Therefore the structure (4.3), derived for the linear controlled process, prohibits violation of the inherent process limitations.

As will be seen in the next chapter, higher-order processes, can present a greater number of inherent limitations to PDF-shaping design.

4.4 Gram-Charlier PDF's and PDF-Shaping Design

For PDF-shaping control design, a desired stationary PDF for the closed-loop process is chosen. In order to simplify the selection of a desirable PDF, a Gram-Charlier PDF parameterization is introduced.

There are a number of practical reasons for the use of Gram-Charlier PDF's in this context. If one considers a linear process driven by Gaussian noise, under minimum variance control, the stationary PDF for the process will be Gaussian. Additionally, the same process, if open-loop stable, will have a Gaussian stationary PDF, with a larger variance under constant open-loop control. In fact any linear control law will result in a Gaussian PDF (see example 4.1.1 for an illustration).

The PDFs for the minimum variance and uncontrolled processes can be viewed as the extreme PDF's for linear processes, with Gaussian PDF's of any intermediate variance being possible depending on the chosen linear feedback control used. If small nonlinearities are introduced into the linear process, the resulting PDF will be non-Gaussian. If it is reasonable to assume that small nonlinearities in the process lead to small deviations from Gaussianity in the PDF, then the following connection can be made. First, the zeroth-order GC PDF is the Gaussian PDF. Therefore, only a zeroth-order GC PDF is required for linear CL processes. Now, as more terms are added in the series making up a GC PDF, the more non-Gaussian it can become. So, if the process nonlinearities are more extreme, more terms are needed to approximate the stationary PDF with a GC PDF. This is not an exact statement, but rather a useful heuristic. Further, in regulatory control situations, even for nonlinear processes, it is not often the case that the stationary PDF is multimodal, and if so, it is probably not desired. More likely, a unimodal, but somewhat skewed PDF would represent good performance. It is this type of PDF that GC PDF's are best represented by. For these reasons, GC PDF's are used to design target PDF's in this work.

Additionally, there are some cases for which the stationary PDF is exactly the product of a Gaussian PDF and another factor. Two cases are illustrated in the following example.

Example 4.4.1 Revisiting example 2.2.2, consider equation (2.35) for a process with a Gaussian disturbance:

$$p(\zeta) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma_w^2}} \exp\left(-\frac{(\zeta - f(z))^2}{2\sigma_w^2}\right) p(z)dz \tag{4.21}$$

With some elementary manipulations, the following form for this equation can be derived:

$$p(\zeta) = \underbrace{\frac{1}{\sqrt{2\pi\sigma_w^2}} \exp\left(-\frac{\zeta^2}{2\sigma_w^2}\right)}_{\text{Gaussian PDF}} \underbrace{\int_{-\infty}^{\infty} \exp\left(-\frac{-2\zeta f(z) + f^2(z)}{2\sigma_w^2}\right) p(z)dz}_{\text{warping factor}} \tag{4.22}$$

Similarly consider the exact PDF derived for the process (3.31) in §3.5:

$$p(\zeta) = \underbrace{\left(1 + \operatorname{erf}\left(\sqrt{\frac{2}{5}}\zeta\right)\right)}_{\text{warping factor}} \underbrace{\frac{1}{\sqrt{10\pi}} \exp\left(-\frac{\zeta^2}{10}\right)}_{\text{Gaussian PDF}} \tag{4.23}$$

□

The examples motivate the use of the GC PDF to represent stationary process PDFs.

4.4.1 Application of GC Basis Functions to the Problem

For design of PDF-shaping control laws, the desired stationary PDF for the process must be selected first. In this section a GC PDF (2.56), is selected. Additionally, to be able to further develop the result, it is assumed that the distribution of the disturbance will be Gaussian. Control design then proceeds by substitution of the target PDF into the stationary process equation (2.27).

$$\begin{aligned} &\mathbf{c}^T\mathbf{h}(x_{t+1})N_{\mu,\sigma}(x_{t+1}) \\ &= \int_{-\infty}^{\infty} N_{0,\sigma_w}(x_{t+1} - \tilde{f}(x_t))\mathbf{c}^T\mathbf{h}(x_t)N_{\mu,\sigma}(x_t)dx_t \end{aligned} \tag{4.24}$$

In an attempt to simplify this expression the orthogonality condition (2.54) is invoked:

$$\begin{aligned} c_0 &= 1 \\ 0 = c_1 &= \int_{-\infty}^{\infty} \left[\frac{\tilde{f}(x_t) - \mu}{\sigma}\right] \mathbf{c}^T\mathbf{h}(x_t) N_{\mu,\sigma}(x_t)\, dx_t \\ &= E\left[\frac{\tilde{f}(x_t) - \mu}{\sigma}\right] \\ 0 = c_2 &= E\left[\frac{\tilde{f}^2(x_t) - 2\mu\tilde{f}(x_t) + \sigma_w^2 - \sigma^2 + \mu^2}{\sqrt{2}\sigma^2}\right] \\ c_3 &= E\left[\frac{\tilde{f}^3(x_t) - 3\mu\tilde{f}^2(x_t) + 3\mu(\sigma^2 - {\sigma_w}^2) + 3({\sigma_w}^2 - \sigma^2 + \mu^2)\tilde{f}(x_t) - \mu^3}{\sqrt{6}\sigma^3}\right] \\ &\vdots \end{aligned} \tag{4.25}$$

Even with the parameterization of the PDF, the equations (4.25) cannot be solved for $\tilde{f}(\cdot)$. Therefore, the CL feedback is parameterized with a series of basis functions:

$$\tilde{f}(x_t) = a_0\theta_0(x_t) + a_1\theta_1(x_t) + a_2\theta_2(x_t) + \ldots \tag{4.26}$$

where $\{\theta_i(x_t)\}$ is a set of chosen basis functions and $\{a_i\}$ are the coefficients in the parameterization. Substituting this parameterization into equation (4.25) and performing the indicated integration yields

$$\begin{aligned} c_0 &= 1 \\ 0 &= q_1(\mathbf{a}, \mathbf{c}, \sigma, \mu) \\ 0 &= q_2(\mathbf{a}, \mathbf{c}, \sigma, \mu) \\ c_3 &= q_3(\mathbf{a}, \mathbf{c}, \sigma, \mu) \\ c_4 &= q_4(\mathbf{a}, \mathbf{c}, \sigma, \mu) \\ &\vdots \end{aligned} \tag{4.27}$$

where each $q_i(\mathbf{a}, \mathbf{c}, \sigma, \mu)$ is a different function of the parameters. These equations may then be solved for the CL feedback parameters, **a**. The ability to compute these parameters requires a few key elements. First, the basis functions for the CL feedback parameterization must be such that analytical solutions exist for integrals in (4.25). For this reason, a series of polynomials may be a good choice as polynomials are integrable against the Gaussian PDF. Second, once the integration has been performed, it must be possible to find real-valued solutions to the equations (4.27). This implies that there must be at least as many parameters in the CL feedback parameterization as in the PDF parameterization. Also, the possibility of multiple solutions to equation (4.27) exists and so some auxiliary conditions are required to render a unique solution. Since this approximation is for a simple first-order process, the correctness of the solution may be ascertained by inspection.

Once the CL feedback has been approximated, the feedback control law must be found by the back substitution

$$f(x_t, u_t) = \mathbf{a}^T \theta(x) \tag{4.28}$$

These equations may then be solved for the CL feedback parameters, **A**.The closed-loop dynamics may then be inverted, as in equation (2.25), to give the feedback control law.

4.4.2 Accuracy of the Approximate PDF-Shaping Design

As discussed in Chapter 3, accuracy analysis for the general PDF-dynamics approximation is a very difficult topic. However, for the special case of GC PDFs, some results are available.

The control design technique is approximate for the following reason. When a GC PDF of n^{th}-order is formed, the mean, variance and the first $n-2$ higher quasi-moments are selected; however, this implies that all remaining quasi-moments be zero. When the set of equations (4.27) is developed to design to CL process, only the selected GC parameters are considered. Therefore, while the design may satisfy the mean, variance and the chosen higher quasi-moments, there is no guarantee that the resultant PDF will be exactly as desired. Fortunately, the quasi-moments are somewhat like coefficients in a Taylor series in that as they get higher in order, they must be very large to have a large impact on the PDF. For this reason, some post-design analysis to check the higher-quasi moments as well as simulation studies is recommended. The use of statistical tests comparing target and realized PDFs is discussed in Chapter 2.

Alternatively there are two ways of reducing the likelihood of the higher quasi-moments causing difficulties. One way is to make a careful choice of the CL feedback parameterization. Ideally, a parameterization would be selected to create a one-to-one correspondence between CL feedback parameters and the quasi-moments. However, no such set of basis functions is currently known. A simpler way of eliminating the higher quasi-moments is to include more terms in the CL feedback parameterization. This allows for (4.27) to be augmented with additional equations to force some higher quasi-moments to zero.

Mathematical Accuracy Analysis

Mathematical accuracy analysis for the general design technique is an open problem; however, some *a posteriori* analysis may be performed for GC-based PDF-shaping. For brevity, the univariate case is described here. A higher-order GC PDF, $\tilde{\mathbf{c}}_{GC}^T\mathbf{h}(z)\,N_{\tilde{\mu},\tilde{\sigma}}(z)$, is calculated for the designed CL feedback and this is compared to the target PDF by integrating the square of the difference between the two:

$$I = \int_{\Re} \left(\mathbf{c}_{GC}^T\mathbf{h}(z)\,N_{\mu,\sigma}(z) - \tilde{\mathbf{c}}_{GC}^T\mathbf{h}(z)\,N_{\tilde{\mu},\tilde{\sigma}}(z)\right)^2 dz \tag{4.29}$$

Assuming that the target mean and variance are properly captured by the control design, the error measure (4.29) may be manipulated into the following form:

$$I = (\mathbf{c}_{GC} - \tilde{\mathbf{c}}_{GC})^T \mathbf{B} (\mathbf{c}_{GC} - \tilde{\mathbf{c}}_{GC}) \tag{4.30}$$

This is a weighted sum of squares of errors in the quasi-moments. The constant weighting matrix $\mathbf{B}$ has a recognizable pattern of elements and may be calculated independently of parameters in the GC PDF.

The analysis suggests that to improve overall accuracy, the design equations (4.27) should be augmented with additional equations to ensure that the higher (quasi-)moments of the target PDF will be correctly realized. This implies that additional parameters will be required in the CL feedback.

4.4.3 PDF-Shaping Design as an Optimal Design

The objective of PDF-shaping design is to find a control law so that closed-loop process behaviour, as described by the PDF, approximates a target PDF as closely as possible. This suggests a possible optimal control design approach for PDF-shaping control design. In fact, this is the approach taken by (Wang, 1999), where the objective function (based on output PDF's) is:

$$J = \int_{\Omega_y} (p(\mathbf{y}_k, \mathbf{u}_k) - p_d(\mathbf{y}_k))^2 \, d\mathbf{y}_k + \mathbf{u}_k^T \mathbf{R} \mathbf{u}_k \tag{4.31}$$

where $p_d(\cdot)$ is the fixed, target PDF. For a state-based approach to this problem the objective function becomes:

$$J = \int_{\Omega} (p(\mathbf{x}_k) - p_d(\mathbf{x}_k))^2 \, d\mathbf{x}_k \tag{4.32}$$

where the input cost is not neglected, but it is understood that the form of $p(\cdot)$ changes with the form of the feedback control law $\mathbf{u}_k$. The simplification of this type of metric for GC PDFs to a weighted sum or squares of errors in the quasi-moments was discussed in the previous section.

4.5 The Comprehensive PDF-Shaping Design Method

It is important to recognize that PDF-shaping control design requires an accurate process model. The intent is to develop high-performance control laws for situations where the variability of the process may have a large impact on profitability, safety or other concerns, but cannot be eliminated. In such cases, process noise should be managed to reduce impact. How PDF-shaping control design fits into the overall procedure of (re-)designing control for a high-performance situation is given in Table 4.1.

Table 4.1: The 9 Step PDF-Shaping Control Design Procedure

1. Review quality, safety and other specifications for the process.
2. Gather and review routine operating data. Plot the data as a histogram to benchmark process performance.
3. Using the routine operating data, develop an appropriate discrete time process model.
4. If possible, identify the minimum variance for the process and note any other inherent limitations of the process. The minimum variance provides a benchmark for elimination of process noise and thus places sets a constraint on potential target PDF's.
5. Set the target PDF, using the Gram-Charlier parameterization, focussing on the improvement of the current PDF (*e.g.* smaller tails, less variance).
6. Choose a parameterization for the closed-loop process and use the design equations to calculate values for the parameters.
7. Invert the closed-loop process dynamics to recover the feedback control law.
8. Perform appropriate post design evaluation (simulations, stability analysis, etc).
9. Implement, test and verify performance of the new control law.

4.6 Illustrative Example

The mechanics of the proposed control design technique is illustrated with a small case study. This example considers a decomposition reaction taking place in a CSTR. An inlet flow introduces reagent at a constant concentration of $c_{in} = 5\,mol/m^3$. The kinetics of the decomposition are 1^{st}-order (rate constant $k = 0.297\,m^3/s$) with an additive zero mean Gaussian random term, w_t (standard deviation of $0.0005\,mol/s$). The outlet flow, F_t, may be manipulated, but tank level is held constant via a well-tuned feedforward control strategy. Thus, the volume of liquid in the tank is assumed constant at $V = 3\,m^3$ for the purposes of this example. The goal of the process is to decompose as much of the reagent as possible while maintaining a nominal flowrate of $0.003\,m^3/s$. As a consequence of the tradeoff between decomposition and flow, the targeted stationary PDF for outlet reagent concentration is:

$$p(c_t) = (1 - 0.078h_3(c_t) + 0.048h_4(c_t))\, N_{0.05,0.00093}(T_t) \tag{4.33}$$

A plot of this fourth-order GC PDF is given by the solid line in Figure 4.1. The right tail of this PDF is light in reflection of the low desired reagent decomposition. To achieve this target, outlet flowrate will be adjusted based on outlet concentration measurements.

A discrete-time dynamic mole balance, for a time step of $\Delta t = 5\,s$, may be developed as follows. The reagent in the tank at the next time step, m_{t+1}, will be equal to the reagent currently in the tank, m_t, plus the sum of any additions and losses during the $5\,s$ control interval. The overall mole balance is then written as

$$m_{t+1} = m_t + m_{in} - m_{out} - m_{decomposed} \tag{4.34}$$

For the purpose of this example model, the reagent introduced and removed due to, respectively, the inlet and outlet flows is $m_{in} = c_{in}F_t\Delta t$ and $m_{out} = c_tF_t\Delta t$. Reagent lost to decomposition is $m_{decomposed} = (kc_t + w_t)\Delta t$. Reagent in the tank at time t is $m_t = c_tV$.

By applying the given assumptions and rearranging the mole balance, the following 1^{st}-order process for outlet reagent concentration is derived:

$$c_{t+1} = c_t + \frac{F_t}{V}(c_{in} - c_t)\Delta t - \frac{1}{V}(kc_t + w_t)\Delta t \tag{4.35}$$

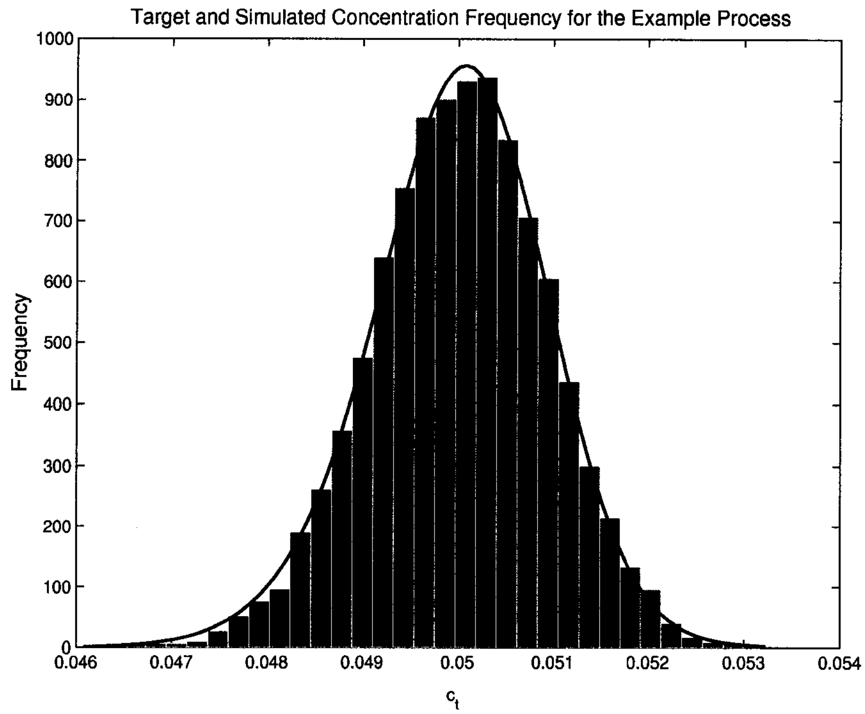


Figure 4.1: A histogram based on simulation of the example process is given by the bars while the target PDF (rescaled) is given by the solid line.

Substituting in the parameter values, the model

$$c_{t+1} = c_t + \frac{5}{3} F_t (5 - c_t) - 0.825 c_t - \frac{5}{3} w_t \tag{4.36}$$

is obtained, where $p_w(w_t) = N_{0,0.0005}(w_t)$.

As discussed in Section 4.3.1, it is not possible to find an exact control law to achieve the desired PDF (4.33). Instead, a fourth-order polynomial CL feedback parameterization is used:

$$\tilde{f}(c_t) = a_0 + a_1 c_t + a_2 c_t^2 + a_3 c_t^3 + a_4 c_t^4 \tag{4.37}$$

Substituting the target PDF (4.33) and the CL feedback parameterization (4.37), as well as the Gaussian PDF for the disturbance w_t into equation (4.24) and proceeding with the approximation technique yields a set of algebraic equations in the parameters $\mathbf{a}$. These equations are then solved numerically to yield the following parameter values for the CL feedback: $\{a_0 = 110.0,\ a_1 = -8883,\ a_2 = 268700,\ a_3 = -3609000,\ a_4 = 18160000\}$.

Making use of equation (2.25) gives the feedback control law:

$$F_t = \frac{3(a_0 + (a_1 - 0.505)c_t + a_2 c_t^2 + a_3 c_t^3 + a_4 c_t^4)}{25 - 5c_t} \tag{4.38}$$

An elementary Lyapunov-type stability analysis, based on the Lyapunov function $V = (c_t - 0.05)^2$, reveals that the deterministic portion of the CL process is locally asymptotically stable around $c_t = 0.05\, mol/m^3$. The region of stability is at least $[0.0442\, mol/m^3, 0.0541\, mol/m^3]$. This region of stability should be compared to the disturbances that may be encountered during operation. The controller is stable within ± 4.4 standard deviations of the mean concentration.

Dynamic simulations of the process (4.36) under this control strategy confirm that the realized PDF matches the design goal. A time series plot of this data is given in Figure 4.2. This reveals that the process in held in a region around the process mean with a moderate amount of control action. A histogram based on 10000 time steps of simulation data is given in Figure 4.1. The histogram takes a shape similar to that of the desired PDF. In particular, the tail behaviour of simulation histogram shows the desired negative skewness. This feature of the data is revealed clearly on a normal probability plot.

As further confirmation of the match between target and realized PDFs, goodness of fit tests were performed comparing the simulated data to Gaussian PDFs and the target PDF. The standard chi-square test was used with a 5% level of significance. The data was divided into 33 equally-sized bins (as in the histogram), with the first four bins combined so that all bins have a frequency of at least 5. Under this test, the chosen 4^{th}-order Gram-Charlier PDF cannot be rejected as the true PDF for the simulated data. On the other hand, the Gaussian PDF must be rejected as the underlying PDF. This shows that the process is significantly non-normal and does correctly match the target PDF within an acceptable margin of error.

4.7 Chapter Summary

A new regulatory control design technique for first-order discrete-time stochastic processes has been introduced. The technique is developed from the concept that long-term process behaviour, and thus performance, can be summarized by the process PDF. The technique may be summarized in four steps: choosing the desired process PDF, picking

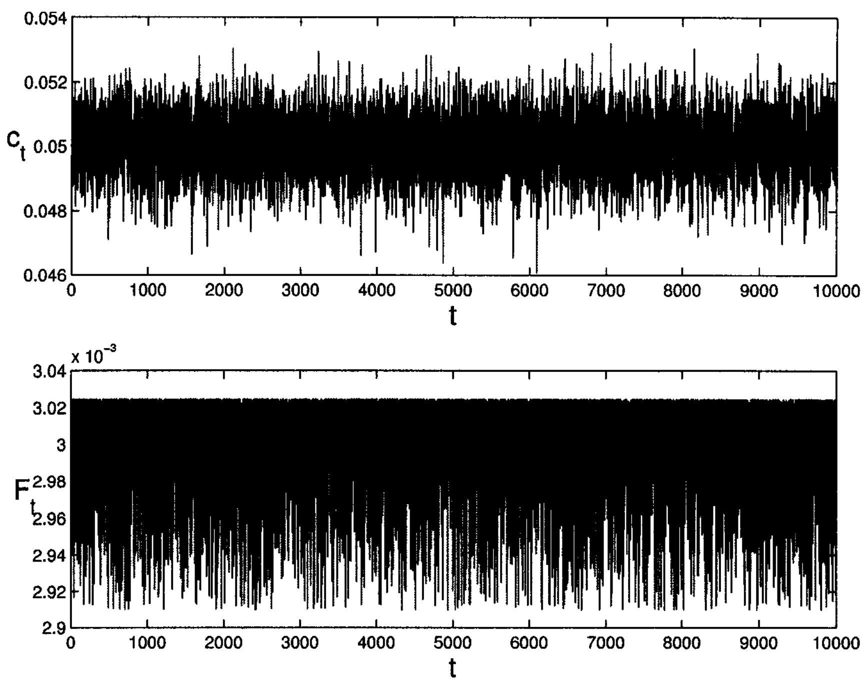


Figure 4.2: A plot of the time series data from simulation of the CL process.

an appropriate controlled process parameterization, equating the PDF parameters with the process parameters, and back-solving for the control law.

The design technique approximately solves the integral equation describing the stationary PDF of the closed-loop discrete-time process. The proposed technique allows for control design to cause the stationary PDF of the closed-loop process to be approximately a designer-selected PDF.

The GC PDF is proposed as a useful tool for control engineering. The main attraction of an nth-order GC PDF is that it incorporates information about the first n moments in a very simple manner. The standard, fourth-order, GC PDF thus includes parameters directly related to mean, variance, skewness and kurtosis. In this work, the GC PDF is used as a means of parameterizing the desired process PDF.

The main idea of the technique is to develop the relationship between the control law parameters and the parameters of the PDF. A short example demonstrates the mechanics and results of the technique. Additionally, analysis from the example suggests the closed-loop processes designed with this technique have a good domain of local stability.

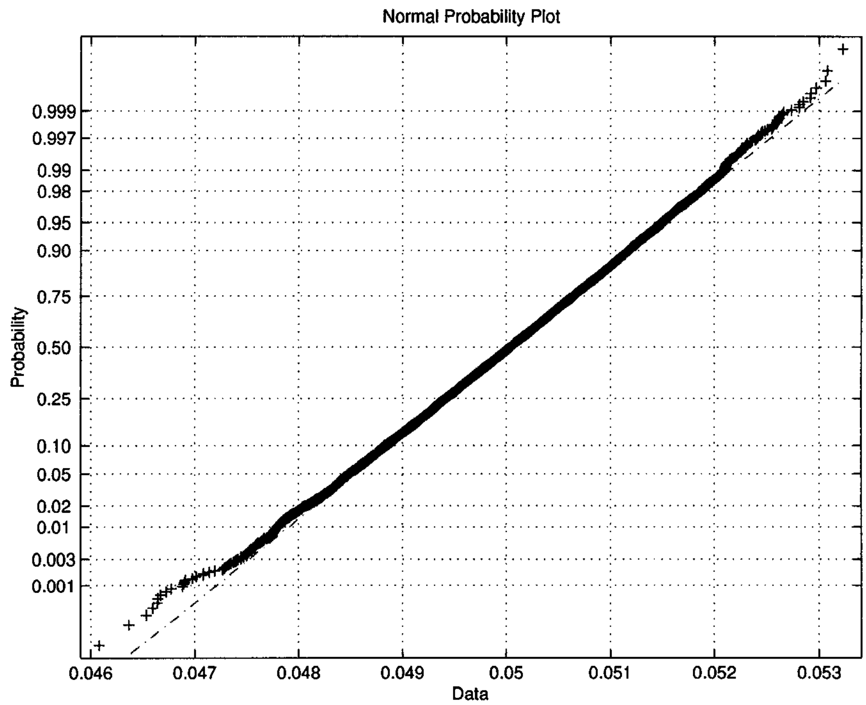


Figure 4.3: A normal probability plot, indicating non-Gaussian data.

"The Starpainters are taking over now,
their scaffolding is in its place."

– Gordon Downie

5

Advanced PDF-Shaping Control Design

This chapter extends the regulatory controller synthesis technique of the previous chapter from first-order processes to higher-order processes including those with delay and coloured noise. The target of the design is a pre-selected multivariate stationary PDF for the CL process. As for the previous case, multivariate PDF-shaping reduces the integral equation governing the PDF-dynamics relationship to a set of algebraic equations in the parameters representing the the CL process feedback. As well as extending this technique to higher-order processes, a second approach is presented where the control law itself is parameterized eliminating the need to invert CL process dynamics. Both the general multivariate PDF-shaping design procedure and the special case, where GC PDFs are used to design the PDF are presented, along with an example demonstrating application of the technique and illustrating the results with numerical simulations.[1]

[1]Parts of this chapter are presented in (Forbes *et al.*, 2003*c*).

5.1 Introduction

This PDF-shaping control concept was introduced for first-order processes in the previous chapter and the references cited therein. In this chapter more advanced versions of the PDF-shaping concept are presented.

For the most part, the first-order PDF-shaping technique may be extended *mutatis mutandis* to higher-order processes, including those with the complications of delay and coloured noise. Some additional care must be taken to handle the case where the dimensions of state and disturbance are unequal. For these cases the additional details are given.

To review, PDF-shaping is the problem of designing a feedback control law to regulate the long-term behaviour of a stochastic process. A target stationary distribution is selected based on engineering or economic concerns and a feedback control law is derived so that the correct closed-loop process dynamics are achieved. In general, exact solutions to this problem are not available and approximation is necessary. The approximation technique can be applied to a general class of processes.

In this chapter, two different methods of approximating the PDF-shaping feedback control are given. In the first, the CL dynamics are parameterized and the feedback control law is recovered through inversion of the open-loop dynamics. The second technique directly parameterizes the feedback control law. Again, the special case of PDF-shaping using Gram-Charlier PDFs is discussed.

This chapter is organized as follows: §2 gives some context and background from the related literature for the techniques proposed in this chapter. As well, the main mathematical concepts required from Chapter 2 are quickly reviewed. In §3 the general, multivariate PDF shaping technique is developed. Applications of this technique to special classes of processes, such as those with delay and those with coloured noise are also given. The issue of process stability and the effect of inherent process limitations are also examined. §4 develops the specific case of PDF-shaping when a GC PDF is used to specify the design target. For this special case, an accuracy analysis is developed. §5 demonstrates the mechanics of the proposed technique through application to a second-order example process. CL process behaviour resulting from implementation of the PDF-shaping control law is illustrated by a numerical simulation. §6 concludes the chapter.

5.2 Background

There is relatively little work on control of multivariate stationary PDFs in the literature. For the case of linear systems with Gaussian disturbances, the concept of covariance control (Huang *et al.*, 2003) may be viewed from this perspective. The goal of covariance control is to minimize the variance of the process inputs subject to constraints of the covariance of the process output or states. Although there is not a direct analogy, the idea is similar. A control law is being designed specifically to influence the PDF of the process. In this work, the goal of the controller design is to set not just the second-moment(s) of the PDF, but all aspects of the shape of the PDF. Since many PDFs may be completely parameterized by their moments, this is equivalent to controlling the covariance and all other moments.

Additional connections between the topic of PDF-shaping control design and works in the literature have been made in Chapters 1 and 5.

5.2.1 Mathematics

Here the key mathematical structures from Chapter 2 that are used in this chapter are briefly reviewed.

This chapter aims to develop regulatory control laws for the process:

$$\mathbf{x}^{(1)}(t+1) = \mathbf{f}^{(1)}(\mathbf{x}(t), \mathbf{u}(t)) + \mathbf{w}(t) \tag{5.1a}$$

$$\mathbf{x}^{(2)}(t+1) = \mathbf{f}^{(2)}(\mathbf{x}(t), \mathbf{u}(t)) \tag{5.1b}$$

where $n_w \leq n_x$ and if $n_w = n_x$ then only equation (5.1a) is used. As previously discussed, this model can represent a wide range of processes including those with nonlinear dynamics, delay, coloured noise, multiple inputs, high-order dynamics and input-output models. In this chapter the focus will be mainly on results for the case $n_x = n_w$. Extensions for a number of special cases where $n_w < n_x$ are then given.

The controller synthesis in this chapter creates feedback control laws of the form:

$$\mathbf{u}(t) = \mathbf{k}(\mathbf{x}(t)) \tag{5.2}$$

The process (5.1a), operating under the control strategy (5.2), takes the form:

$$\begin{aligned}\mathbf{x}(t+1) &= \mathbf{f}^{(1)}(\mathbf{x}(t), \mathbf{k}(\mathbf{x}(t))) + \mathbf{w}(t) \\ &= \tilde{\mathbf{f}}(\mathbf{x}(t)) + \mathbf{w}(t)\end{aligned} \quad (5.3)$$

The mapping $\tilde{\mathbf{f}}(\mathbf{x}(t))$ is referred to as the CL feedback.

In one version of the PDF-shaping design developed in this chapter, the desired CL feedback is approximated for a known open-loop process model and target stationary PDF. To recover the feedback control law in this situation, the open-loop process feedback is inverted as follows:

$$\mathbf{f}^{(1)}(\mathbf{x}(t), \mathbf{u}(t)) = \mathbf{f}^{(1)}(\mathbf{x}(t), \mathbf{k}(\mathbf{x}(t))) = \tilde{\mathbf{f}}(\mathbf{x}(t)) \quad (5.4)$$

$$\mathbf{u}(t) = \mathbf{k}(\mathbf{x}(t)) = \mathbf{f}_{\mathbf{x}(t)}^{(1)\,-1}\left(\tilde{\mathbf{f}}(\mathbf{x}(t))\right) \quad (5.5)$$

where $\mathbf{f}_{\mathbf{x}(t)}^{(1)\,-1}(\cdot)$ is the inverse of $\mathbf{f}^{(1)}(\mathbf{x}(t), \mathbf{u}(t))$ with respect to $\mathbf{u}(t)$, holding $\mathbf{x}(t)$ constant.

If the CL process (5.3) is stationary then its stationary PDF, $p(\cdot)$, is given by:

$$p(\zeta) = \int_{\Re^{n_x}} p_w\left(\zeta - \tilde{\mathbf{f}}(\xi)\right) p(\xi) \mathrm{d}\xi \quad (5.6)$$

Again, it is emphasized that this is true for the process (5.1a) where $n_w = n_x$. For the case where $n_w < n_x$, and the process model consists of both equations (5.1a) and (5.1b), there are some additional complications, as discussed in Chapter 2.

The previous chapter introduced the the special case of PDF-shaping control for first-order processes and univariate GC PDF's. Here, in dealing with higher-order processes and therefore with multivariate PDF's, the GC PDF case must be extended to multivariate GC PDF's. The reader is referred to Chapter 2 for the complete details of multivariate GC PDFs.

5.3 PDF-Shaping Feedback Control Design for n^{th}-Order Processes

Here the general PDF-shaping technique, presented in §4.3 for first-order processes is extended to higher-order processes.

The goal of PDF-shaping is to find a feedback control law so that the CL process will have the desired stationary PDF. The first step in PDF-shaping design is the selection of the target PDF, $p^*(\cdot)$. As previously discussed, a well known type of PDF may be selected, or a set of basis functions may be used to tailor a PDF to a desired shape. However the PDF parameterization is chosen, whether a PDF of known structure or a set of basis functions is used, it must meet the defining requirements of a PDF given in Chapter 2. The shape should take into account both engineering and economic concerns. The target PDF is then substituted into equation (5.6), which governs the relationship between the process dynamics and the stationary PDF:

$$p^*(\zeta) = \int_{\Re^{n_x}} p_w\left(\zeta - \tilde{\mathbf{f}}(\xi)\right) p^*(\xi)\mathbf{d}\xi \tag{5.7}$$

This equation should then be solved for the CL feedback, $\tilde{\mathbf{f}}(\cdot)$, which is then used in equation (5.5) to back-calculate the feedback control law. As discussed in Chapter 4, an approximate solution to the equation is developed.

There are two main ideas used in the approximation. The first idea is to take advantage of the simple relationships that often exist between the parameters and moments of a PDF. The second idea is to parameterize the CL feedback. This provides a structure which allows the integration on the right-hand side of equation (5.7) to be performed. The integral equation is then reduced to a set of algebraic equations which can be solved numerically for the CL feedback parameters.

5.3.1 Designing the Target PDF

The design of PDF-shaping control laws requires the selection of an appropriate shape for the target stationary PDF for the process. A good choice of PDF will be based on process economics, safety and other engineering concerns. In this work GC PDFs are recommended for use in designing a target PDF.

For a given process, the nature of the open-loop dynamics will impose inherent limitations on the shape of the stationary PDF that may be realized using feedback control. For the process model (2.15) considered in this thesis, the disturbance, $\mathbf{w}(t)$, is unmeasured and therefore there is no causal feedback control law that can prevent the disturbance from reaching the state at the next time step, $\mathbf{x}(t+1)$. Among other things, this means that the minimum variances of the states that can be realized for the stationary PDF are at least as great as those given by the covariance matrix of the disturbance, Σ_w. For this reason, care must be taken in choosing the target PDF. Selection of an infeasible target PDF will lead to the failure of the PDF-shaping technique. Although it cannot be guaranteed *a priori* that a given target PDF is achievable, careful selection of the target PDF can improve the chances of success.

While the selection of a GC target PDF will be different in each circumstance, some common criteria are enumerated in Table 5.1.

Table 5.1: Common Criteria for Selection of a Target PDF

1. In all cases, the variance(s) of the target PDF must be greater than, or equal to, the minimum achievable variances, *i.e.*, $\sigma_{x_i}^2 \geq \sigma_{x_{i_{min}}}^2$.
2. It is often desirable to reduce the dispersion of the output or state by minimizing variance(s): $\min\limits_{\{\mu,\sigma,\mathbf{c}\}} \sigma^2$, or $\min\limits_{\{\mu,\Sigma,\mathbf{c}\}} \text{trace}\Sigma$
3. The maximum acceptable chance of violating a constraint or specification may be imposed, *e.g.*, $\int\limits_{x_{max}}^{\infty} \mathbf{c}^T\mathbf{h}(x)\, N_{\mu,\sigma}(x)\, dx \leq 0.01$
4. The PDF may be designed with respect to some general objective function: $\min\limits_{\{\mu,\sigma,\mathbf{c}\}} \int\limits_{-\infty}^{\infty} \ell(x)\, \mathbf{c}^T\mathbf{h}(x)\, N_{\mu,\sigma}(x)\, dx$
5. The GC PDF may be designed to approximate another PDF, as in equation (2.67), using equation (2.68).

The PDF parameters can be chosen and adjusted by trial and error until the shape of the PDF is judged appropriate with respect to the given criteria, or more formal methods can be used. The fifth criterion can be handled in a straightforward manner, as long as the PDF being approximated is a reasonable choice, *i.e.*, not in violation of inherent process limitations such as the first criterion. If the PDF approximation displays some negative values, it will be necessary to use some non-negativity constraints, such as those given in (Jondeau and Rockinger, 1999). In the case of the first four criteria, one way the GC PDFs can be shaped is with the use of a semi-infinite optimization routine (Polak, 1997) where the second or fourth criterion is the objective function for the optimization. The first and third criteria are inequality constraints on the parameters. The non-negativity constraint on the GC PDF, $\mathbf{c}^T\mathbf{h}(x) \geq 0$, is a semi-infinite constraint for which an appropriate domain should be chosen.

Even with careful process analysis and PDF selection, there is still the possibility that an infeasible target PDF will be selected. In this case, the controller design algorithm will lead to a set of algebraic equations that cannot be solved for real-valued CL feedback parameters.

5.3.2 General Formulation

The chosen target PDF should be analyzed to find the relationship between the parameters of the PDF, $\mathbf{c}$, and a finite number of its moments, $\mathbf{m}_{p^*}$. It is assumed that an algebraic relationship can be found and will be represented as:

$$\mathbf{c} = \rho(\mathbf{m}_{p^*}) \tag{5.8}$$

As previously discussed, this is not a restrictive assumption as the parameters in many PDFs are known to be elementary functions of the moments. One of the most common examples of this feature is the Gaussian PDF, parameterized by the mean (first moment) and the covariance (second centred moment). For many other PDFs similar relationships exist; although they are not always obvious.

To begin the approximation of the solution to equation (5.7), the moments are calculated for each side of the equation:

$$\begin{aligned} &\int_{\Re^{n_x}} \begin{bmatrix} \zeta^{1,0,0,0,\ldots} \\ \zeta^{0,1,0,0,\ldots} \\ \vdots \end{bmatrix} p^*(\zeta)\,\mathbf{d}\zeta \\ = &\int_{\Re^{n_x}} \begin{bmatrix} \zeta^{1,0,0,0,\ldots} \\ \zeta^{0,1,0,0,\ldots} \\ \vdots \end{bmatrix} \int_{\Re^{n_x}} p_{\mathbf{w}}\left(\zeta - \tilde{\mathbf{f}}(\xi)\right) p^*(\xi)\,\mathbf{d}\xi\mathbf{d}\zeta \end{aligned} \tag{5.9}$$

Simplification is made by rearrangement and use of equation (2.4).

$$\mathbf{m}_{p^*} = \int_{\Re^{n_x}} \left(\int_{\Re^{n_x}} \begin{bmatrix} \zeta^{1,0,0,0,\ldots} \\ \zeta^{0,1,0,0,\ldots} \\ \vdots \end{bmatrix} p_{\mathbf{w}} \left(\zeta - \tilde{\mathbf{f}}(\xi) \right) \mathbf{d}\zeta \right) p^*(\xi)\, \mathbf{d}\xi \tag{5.10}$$

The change of variables $\mathbf{z} = \zeta - \tilde{\mathbf{f}}(\xi)$ makes it clear that the first integration yields translated moments of $p_{\mathbf{w}}$.

$$\mathbf{m}_{p^*} = \int_{\Re^{n_x}} \left(\int_{\Re^{n_x}} \begin{bmatrix} \left(\mathbf{z} + \tilde{\mathbf{f}}(\xi)\right)^{1,0,0,0,\ldots} \\ \left(\mathbf{z} + \tilde{\mathbf{f}}(\xi)\right)^{0,1,0,0,\ldots} \\ \vdots \end{bmatrix} p_{\mathbf{w}}(\mathbf{z})\, \mathbf{dz} \right) p^*(\xi)\, \mathbf{d}\xi \tag{5.11}$$

Therefore the result of the first integration is a vector of multivariate polynomials in $\mathbf{m}_{p_{\mathbf{w}}}$ and $\tilde{\mathbf{f}}(\xi)$ which will be denoted by $\mathbf{q}$.

$$\mathbf{m}_{p^*} = \int_{\Re^{n_x}} \mathbf{q}\left(\mathbf{m}_{p_{\mathbf{w}}}, \tilde{\mathbf{f}}(\xi)\right) p^*(\xi)\, \mathbf{d}\xi \tag{5.12}$$

Equation (3.2) is applied here.

$$\mathbf{c} = \rho\left(\int_{\Re^{n_x}} \mathbf{q}\left(\mathbf{m}_{p_{\mathbf{w}}}, \tilde{\mathbf{f}}(\xi)\right) p^*(\xi)\, \mathbf{d}\xi \right) \tag{5.13}$$

At this point, no further simplifications can be made and direct solution for $\tilde{\mathbf{f}}(\cdot)$ is not possible. Therefore the CL feedback is parameterized as a weighted sum of n_x-variate basis functions, $\{\theta_i(\cdot)\}_{i=0,1,\ldots,N}$, so that an approximate solution can be obtained.

$$\begin{aligned} \tilde{\mathbf{f}}(\cdot) &\simeq \mathbf{a}_0\theta_0(\cdot) + \mathbf{a}_1\theta_1(\cdot) + \ldots + \mathbf{a}_N\theta_N(\cdot) \\ &\simeq \begin{bmatrix} \mathbf{a}_0 & \mathbf{a}_1 & \ldots & \mathbf{a}_N \end{bmatrix} \begin{bmatrix} \theta_0(\cdot) \\ \theta_1(\cdot) \\ \vdots \\ \theta_N(\cdot) \end{bmatrix} \simeq \mathbf{A}\theta(\cdot) \end{aligned} \tag{5.14}$$

The parameterization is substituted into equation (5.13), allowing integration of the right hand side to be performed, to obtain the final result:

$$\mathbf{c} = \rho\left(\tilde{\mathbf{q}}\left(\mathbf{m}_{p_{\mathbf{w}}}, \mathbf{c}, \mathbf{A}\right)\right) \tag{5.15}$$

where $\tilde{\mathbf{q}}\left(\mathbf{m}_{p_{\mathbf{w}}}, \mathbf{c}, \mathbf{A}\right)$ is the vector function resulting from the integration. The result is a set of algebraic equations in: the known parameter sets associated with the PDF of the disturbance and the stationary PDF; and the unknown parameter set associated with the CL feedback. The equations (5.15) may be solved numerically for the parameter set $\mathbf{A}$, giving the approximate CL feedback.

Once the CL feedback has been approximated, the feedback control law must be found using equation (2.25)

$$\mathbf{u}(t) = \mathbf{k}(\mathbf{x}(t)) = \mathbf{f}_{\mathbf{x}(t)}^{(1)\,-1}\left(\mathbf{A}\theta(\mathbf{x}(t))\right) \tag{5.16}$$

There are a couple of key requirements for this technique to prove fruitful. First, the basis functions for the CL feedback parameterization must be such that analytical solutions exist for the integration in the right hand side of equation (5.11) or (5.38). For this reason a series of polynomials may be a good choice, as polynomials are integrable against many PDFs. Secondly, to find real-valued solutions to equation (5.15), at least as many independent parameters are required in the CL feedback parameterization as are included in the target PDF. The possibility exists of multiple solutions to these equations and so auxiliary conditions may be required to render a unique solution.

It is emphasized that this approximation results in an algebraic relationship between the parameters in the stationary PDF (which are directly related to the moments of the PDF) and those in the closed-loop feedback. Since many features of a PDF, such as tail behaviour, may be described with reference to the moments (and thus by the parameters of the PDF), the algebraic relationship given by equation (5.15) may be viewed as a relationship between the parameters in the closed-loop feedback and the shape of the PDF. It is for this reason that the technique is referred to as PDF-shaping control design. The 9-step algorithm, integrating PDF-shaping into a comprehensive control (re-)design procedure for high-performance situations, given in the §4.5, may also be applied in the case of multivariate PDF shaping. Similarly, just as there were inherent limitations on the possible shapes of PDFs for the first-order case, there are limitations in the multivariate case.

5.3.3 Limitations of the Technique

In the previous chapter, the main limitation of PDF-shaping was the portion of the disturbance that cannot be prevented from filtering through the process and reaching the state. The same limitation also exists in the multivariate case: no matter what the CL process dynamics are, the effect of the disturbance cannot be completely eliminated from the process state. This implies a restriction on the covariance matrix for the stationary process, including minimum variances for the process variables.

As well, there may exist additional restrictions on the form of the target PDF for the multivariate case, which depend on the structure of the process (5.1), there may be . There are many different restrictions that can arise. Common features and their impact on the design procedure are discussed in the following sections.

5.3.4 Special Higher-Order Process Features

The purpose of this section is to highlight some of the common features of the technique and how it can be adjusted. For simplicity, the adjustments are illustrated using second-order processes, with the understanding that extensions to higher-order processes are immediate.

Coloured Noise

A first-order process with a moving average disturbance may be represented by the process model:

$$y\left(t+1\right)=f\left(y\left(t\right),u\left(t\right)\right)+w\left(t\right)+\alpha w\left(t-1\right) \tag{5.17}$$

Making the transformations $x_1\left(t\right) = y\left(t\right)$ and $x_2\left(t\right) = w\left(t-1\right)$ this model may be rewritten in the form

$$\mathbf{x}\left(t+1\right)=\begin{bmatrix} f\left(x_1\left(t\right),u\left(t\right)\right)+w\left(t\right)+\alpha x_2\left(t\right) \\ w\left(t\right) \end{bmatrix} \tag{5.18}$$

The additional manipulations discussed in §2.2.1 may be used to put this model in the form of equation (5.1). For the purposes of this discussion it is unnecessary as the stationary PDF can be represented as:

$$p\left(\zeta\right)=\int_{\Re^2} p_w\left(\zeta_1-f\left(\xi_1,k\left(\xi\right)\right)\right)\delta\left(\zeta_2-\zeta_1+f\left(\xi_1,k(\xi)\right)+\alpha\xi_2\right)p\left(\xi\right)\mathbf{d}\xi \tag{5.19}$$

where the feedback control law $u\left(t\right) = k\left(\mathbf{x}\left(t\right)\right)$ is used. This means that by solving $\zeta_2-\zeta_1+f\left(\xi_1,k(\xi)\right)+\alpha\xi_2$ for ξ_2, *i.e.*, $\xi_2 = g(\xi_1,\zeta_1,\zeta_2)$, one part of the integration may be performed:

$$
\begin{aligned}
p(\zeta) = \int_{\Re} & p_w\left(\zeta_1 - f\left(\xi_1, k\left(\xi_1, g(\xi_1, \zeta_1, \zeta_2)\right)\right)\right) \\
& \cdot \delta\left(\zeta_2 - \zeta_1 + f\left(\xi_1, k(\xi_1, g(\xi_1, \zeta_1, \zeta_2))\right) + \alpha g(\xi_1, \zeta_1, \zeta_2)\right) \\
& \cdot p\left(\xi_1, g(\xi_1, \zeta_1, \zeta_2)\right) \mathbf{d}\xi_1
\end{aligned}
\tag{5.20}
$$

Without specifying anything about the stationary PDF, one part of the integration has been performed. This indicates that all aspects of the stationary PDF cannot be specified independently. In fact, for this situation the marginal PDF for one of the states can be directly derived from the other. In such a case, it might be best to shape one marginal PDF in a desirable fashion and then to check the joint stationary PDF to see if it is acceptable.

Non-Invertible Open-Loop Dynamics

Consider a second-order process:

$$x_1(t+1) = f_1(\mathbf{x}(t), u(t)) + w_1(t) \tag{5.21}$$

$$x_2(t+1) = f_2(\mathbf{x}(t)) + w_2(t) \tag{5.22}$$

If an arbitrary CL feedback, $\tilde{\mathbf{f}}(\mathbf{x}(t))$, is designed for this process, then it will not be possible to invert the open-loop dynamics to solve for $u(t)$. Observe that:

$$\tilde{f}_1(\mathbf{x}(t)) = f_1(\mathbf{x}(t), u(t)) \tag{5.23}$$

$$\tilde{f}_2(\mathbf{x}(t)) = f_2(\mathbf{x}(t)) \tag{5.24}$$

The CL feedback, $\tilde{\mathbf{f}}(\mathbf{x}(t))$, cannot be designed to satisfy equations (5.23) and (5.24) indenpendently. There is only freedom in the designing $\tilde{f}_1(\cdot)$, subject to the invertibility of $f_1(\cdot)$, uniformly in $\mathbf{u}(t)$. The implication of this on the stationary PDF-shaping is that only the CL feedback of the first state is parameterized and the feedback of the second state, $\mathbf{x}(t)$, remains $\mathbf{f}_2(\mathbf{x}(t))$. This implies a direct relationship between the marginal PDFs of the two states. Care must be taken in designing a target stationary PDF to avoid violation of this relationship.

Delay

A simple first-order process with a one time-step delay can be represented by the process model:

$$y(t+1) = f(y(t), u(t-1)) + w(t) \tag{5.25}$$

Transforming $x_1(t) = y(t)$ and $x_2(t) = u(t-1)$, this model can be rewritten in the form

$$\mathbf{x}(t+1) = \begin{bmatrix} f(x_1(t), x_2(t)) + w(t) \\ u(t) \end{bmatrix} \tag{5.26}$$

When a feedback control law $u(t) = k(\mathbf{x}(t))$ is used, the stationary PDF for this process is:

$$p(\zeta) = \int_{\Re^{n_x}} p_w(\zeta_1 - f(\xi_1, \xi_2))\,\delta(\zeta_2 - k(\xi))\,p(\xi)\mathrm{d}\xi \tag{5.27}$$

This is a special case of the non-invertible dynamics problem above. Nothing can be directly altered about the CL feedback of the first state. Once a parameterization is made for the CL feedback of the second state (in this case the CL feedback is the feedback control law) one of the integration on the right hand side can be performed using the technique given in the coloured noise section. This simplifies the stationary PDF equation, but it restricts what can be done in shaping the stationary PDF.

Alternatively, we can exploit the strict feedback structure of the process.

5.3.5 An Alternate Dynamics Parameterization

It is not always convenient to parameterize the entire closed-loop feedback, or to invert the open-loop process to recover the pdf-shaping feedback control law. In these situations it may be advantageous to parameterize the feedback control law instead of the CL feedback. In this case the approximation is:

$$\mathbf{u}(t) \approx \mathbf{A}\theta(\mathbf{x}(t)) \tag{5.28}$$

and the CL feedback is a mix of the exact open-loop feedback and the approximate feedback control law.

$$\tilde{\mathbf{f}}(\mathbf{x}(t)) = \mathbf{f}^{(1)}(\mathbf{x}(t), \mathbf{A}\theta(\mathbf{x}(t))) \tag{5.29}$$

Substituting this into equation (5.30) gives the following:

$$\mathbf{c} = \rho\left(\int_{\Re^{n_x}} \mathbf{q}\left(\mathbf{m}_{p_\mathbf{w}}, \mathbf{f}^{(1)}\left(\mathbf{x}\left(t\right), \mathbf{A}\theta\left(\mathbf{x}\left(t\right)\right)\right)\right) p^*\left(\xi\right) \mathrm{d}\xi\right) \tag{5.30}$$

If the indicated integration can be performed analytically, the final result is:

$$\mathbf{c} = \rho\left(\tilde{\mathbf{q}}\left(\mathbf{m}_{p_\mathbf{w}}, \mathbf{c}, \mathbf{A}\right)\right) \tag{5.31}$$

The form of this equation appears to be the same as equation (5.15); however the functions $\tilde{\mathbf{q}}\left(\mathbf{m}_{p_\mathbf{w}}, \mathbf{c}, \mathbf{A}\right)$ are different in each case. In the original case presented, the functions are products of the choice of CL feedback parameterization, while in this new case, the functions are products of both the open-loop dynamics and the feedback control law parameterization. In both cases the feedbacks must be chosen so that analytical integration is possible. In the second case, the interaction of the control law parameterization with the open-loop dynamics must be considered. This provides an opportunity to remove troublesome parts of the open-loop feedback with a judicious choice of control law parameterizations.

5.3.6 Stability of the Closed-Loop Process

In the previous chapter, the stability of the PDF-shaping control laws was discussed. To briefly summarize those comments, it is difficult to make any *a priori* statements about the stability of the PDF-shaping synthesis. *A posteriori* stability analysis of the process skeleton:

$$\mathbf{x}\left(t+1\right) = \tilde{\mathbf{f}}\left(\mathbf{x}\left(t\right)\right) \tag{5.32}$$

is recommended. A specific technique was given for assessing the process stability and for eliminating unstable regions. In this section, the technique is generalized and extended to higher-order processes.

To start, the equilibrium point(s) of the process should be identified from equation (5.32). They are obtained by solving the fixed-point equation:

$$\mathbf{x}_e = \tilde{\mathbf{f}}\left(\mathbf{x}_e\right) \tag{5.33}$$

If these cannot be identified by inspection and a search technique must be used, a reasonable approach is to consider an equilibrium point that is near the mean of the target PDF. This will be the equilibrium point around which it is suggested that process stability should be analyzed. A Lyapunov stability analysis can then be performed. In the absence of a natural choice of Lyapunov function, the standard quadratic function can be used:

$$V(\mathbf{x}) = (\mathbf{x} - \mathbf{x_e})^T (\mathbf{x} - \mathbf{x_e}) \tag{5.34}$$

The rate of change in this function over time is indicative of the process stability. For a discrete-time process the rate of change of the Lyapunov function is:

$$\dot{V}(\mathbf{x}) = V\left(\tilde{\mathbf{f}}(\mathbf{x})\right) - V(\mathbf{x}) \tag{5.35}$$

The process is asymptotically stable to the equilibrium point for the region (Davis, 2002):

$$\Omega_\alpha = \{\mathbf{x} \mid V(\mathbf{x}(t)) \leq \alpha, \dot{V}(\mathbf{x}) < 0 \; \forall \, \mathbf{x} \neq \mathbf{x}_e, \dot{V}(\mathbf{x}_e) = 0\} \tag{5.36}$$

Ideally, the region of stability is the entire domain of $\mathbf{x}$ ($\Re^{n_x}$ in the case of this thesis). For such globally asymptotically stable processes, it is reported in (Tong, 1990) for some special cases that, with some additional technical assumptions, the process is stationary. Unfortunately, it may not be possible to extend the region of stability to the entire domain. If the equilibrium point cannot be shown to have some acceptable region of stability then the process should be carefully analyzed and the control law re-designed. Assuming that there is some region of stability around the equilibrium point, a further analysis can be performed.

If the region of stability is large relative to the variance of the target PDF, then it can be assumed that the process almost always remains within the stable region. The 6σ rule is often sufficient to provide a reasonable assurance of long-term stability. It is recommended, as a heuristic, that the region of stability be at least $\pm 5\sigma$ about both the process mean and the equilibrium point. This corresponds to 99.9999% of the innovations arising from a Gaussian process.

In cases where the CL process is locally asymptotically stable, but only a small region of stability is obtained, it may be necessary to alter the PDF-shaping control law near the boundaries of and beyond the stable region. This approach was presented in the previous chapter. It is recommended that a simple stabilizing control law be used for these regions of possible instability to steer the process into the stable region. The idea is that the stable region is near the mean of the target PDF and is therefore the region for which the PDF-shaping control law is designed. This results in a piecewise control strategy consisting of the original PDF-shaping control law in the main operating region, near the process mean and equilibrium, and stabilizing control(s) for rare and extreme operations. The stabilizing control laws can be chosen in a number of ways and it can be tailored so that the piecewise control law has desirable properties, such as continuity, differentiability, smoothness, and so forth.

It should be noted that this is only one approach to analyze and to improve the stability properties of the PDF-shaping designs. In the general case, some different notions of stability may be required, leading to improved results. For further information on the connections between the deterministic notion of stability and the stochastic notion of ergodicity, the reader is referred to (Tong, 1990).

5.4 PDF-Shaping with GC PDFs

The PDF-shaping design technique developed above applies to processes with general noise PDF's, general target PDF's and general basis functions for approximation of the CL feedback, the specific case of processes driven by Gaussian noise, with Gram-Charlier target PDF's and with the closed-loop feedback approximated by polynomials has been considered in detail.

The previous chapter introduced the concept of PDF-shaping control design for simple first-order processes using univariate GC PDFs. The GC PDF can help to simplify selection of a target PDF and it also simplifies the mathematics of the technique. Here, in dealing with higher-order processes, the multivariate version is applied. Following the derivation of the technique from the previous section, the GC PDF (2.67) is substituted into equation (5.7).

$$p_{GC}(\zeta) = \int_{\Re^n} p_{\mathrm{w}}\left(\zeta - \tilde{\mathbf{f}}(\xi)\right) p_{GC}(\xi)\, \mathrm{d}\xi \tag{5.37}$$

Calculating moments from both sides of the equation, and taking advantage of equation

(2.58) produces the following result.

$$\mathbf{c}_{GC} = \int_{\Re^n} \left(\int_{\Re^n} \mathbf{h}(\zeta)\, p_{\mathbf{w}} \left(\zeta - \tilde{\mathbf{f}}(\xi) \right) \mathrm{d}\zeta \right) p_{GC}(\xi)\, \mathrm{d}\xi \tag{5.38}$$

The first integration again yields a vector of multivariate polynomials and the CL feedback is again parameterized as $\mathbf{A}\theta(\mathbf{z})$. Performing the second integration yields the following.

$$\mathbf{c}_{GC} = \tilde{\mathbf{q}}\left(\mathbf{m}_{p_{\mathbf{w}}}, \mu, \Sigma, \mathbf{c}_{GC}, \mathbf{A}\right) \tag{5.39}$$

If polynomial basis functions are used to parameterize the CL feedback, then the second integration can be performed analytically and polynomial vector functions, $\tilde{\mathbf{q}}$, are guaranteed to result. Additional simplifications result when the disturbance PDF, $p_{\mathbf{w}}(\cdot)$, is the Gaussian PDF, $N_{\mathbf{0},\Sigma_{\mathbf{w}}}(\cdot)$.

$$\mathbf{c}_{GC} = \tilde{\mathbf{q}}'\left(\Sigma_{\mathbf{w}}, \mu, \Sigma, \mathbf{c}_{GC}, \mathbf{A}\right) \tag{5.40}$$

The vector function $\tilde{\mathbf{q}}'$ may have a considerably simpler structure and instead of being dependent on a possibly large number of parameters, $\mathbf{m}_{p_{\mathbf{w}}}$, is dependent on $\Sigma_{\mathbf{w}}$.

Again, once the CL feedback has been approximated, by solution of equation (5.39) or (5.40), the feedback control law is recovered through use of equation (2.25).

While GC / polynomial PDF-shaping control design may seem somewhat restrictive, in light of the interpretation of GC PDFs as a weighted sum of basis functions and the property of polynomials being universal approximators, this special case can be applied in a broad range of circumstances. GC PDFs may be used to create infinite different PDF shapes while polynomials, as universal approximators, can provide good local approximations for process dynamics.

5.4.1 Accuracy of the Approximation

As discussed in both of the previous chapters the accuracy of the general PDF-shaping design technique is difficult to analyze. It is reiterated that the design technique is approximate and so it is reasonable to expect that the designed control law will not lead to a closed-loop process with the exact stationary PDF that was specified.

There are some simple techniques that can be used to help improve the overall accuracy of the approximation. First, by including extra basis functions in the closed-loop feedback parameterization, more of the true CL feedback can be captured by the approximation. Secondly, in coordination with the first technique, additional algebraic equations can be developed relating target PDF parameters to the CL feedback parameters. For each additional algebraic equation that is developed, an additional PDF parameter, or moment, may be satisfied. These cannot be added arbitrarily as there must be enough free parameters from the CL feedback so that there are sufficient degrees of freedom to simultaneously solve all the equations.

For the specific case of PDF-shaping with GC target PDFs, it was shown in the last chapter that a measure of the approximation accuracy may be developed by integrating the square of the difference between target and realized PDFs. The approximation metric was:

$$I = \left(\mathbf{c}_{GC} - \tilde{\mathbf{c}}_{GC}\right)^T \mathbf{B} \left(\mathbf{c}_{GC} - \tilde{\mathbf{c}}_{GC}\right) \tag{5.41}$$

which is a weighted sum of squares of errors in the quasi-moments and the matrix $\mathbf{B}$ had a recognizable pattern of elements and did not rely on the quasi-moments. For the case of GC PDFs the same type of metric can be derived; however, recognizing a clear pattern to the B matrix will not be simple, since there are several GC basis functions of a given order.

This type of metric does suggest an iterative approach to high-accuracy PDF-shaping design. Each time a PDF-shaping control law is designed, a high-order GC PDF can be used to approximate the exact PDF that the closed-loop process will display. The target and approximated PDFs may then be used to calculate the error measure. If the error measure is high, the PDF-shaping technique can be performed again, with additional basis functions added to the CL feedback parameterization. The procedure is repeated until the error measure is sufficiently low.

5.5 Illustrative Example

The proposed controller synthesis technique is applied to the following two-dimensional process model:

$$\begin{aligned} x_1(t+1) &= 0.84x_1(t) + 0.75x_1(t)\,x_2(t) \\ &\quad -0.88x_2(t) + 0.32u(t) + w_1(t) \\ x_2(t+1) &= x_1(t) + w_2(t) \end{aligned} \tag{5.42}$$

The disturbance variable, $\mathbf{w}(t)$, is iid with a zero-mean Gaussian distribution and covariance:

$$\Sigma_{\mathbf{w}} = \begin{bmatrix} \frac{6}{5} & \frac{1}{2} \\ \frac{1}{2} & \frac{4}{5} \end{bmatrix} \tag{5.43}$$

Before proceeding with the PDF-shaping control design, a major inherent limitation of the process should be noted. The dynamics of the second state are not directly influenced by the input, implying the following constraint on the marginal state PDFs:

$$p_{x_2}(\zeta) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{1.6\pi}} \exp\left(-\frac{(\zeta-\xi)^2}{1.6}\right) p_{x_1}(\xi) d\xi \tag{5.44}$$

In effect, this limits the number of parameters that can be independently selected in creating a viable target stationary PDF. The target PDF for the control design must be carefully chosen to ensure that it is consistent with the limitation.

5.5.1 Application of the Proposed Technique

It is desired to find the feedback control law $u(t) = k(x_1(t), x_2(t))$ so that the stationary PDF of the CL process is

$$p(x_1, x_2) = \mathbf{c}_{GC}^T \mathbf{h}(x_1, x_2) N_{\mu,\Sigma}(x_1, x_2) \tag{5.45}$$

where $\{c^0 = 1, c^{3,0} = 0.2, c^{4,0} = 0.2\}$,

$$\Sigma = \begin{bmatrix} 2 & \frac{77}{50} \\ \frac{77}{50} & \frac{14}{5} \end{bmatrix} \tag{5.46}$$

and all other parameters, including the mean vector are taken as zero. A plot of this 4^{th}-order bivariate GC PDF is given in Figure 5.1. The following parameterization for the CL feedback to the first process state is used:

$$\begin{aligned} \tilde{f}_1(x_1, x_2) &= a_0 + a_1 x_1(t) + a_2 x_1^2(t) \\ &+ a_3 x_1^3(t) + a_4 x_1^4(t) \end{aligned} \tag{5.47}$$

Taking advantage of the technique outlined in §5.4 yields $\{a_0 = 0.417, a_1 = 0.359, a_2 = -0.287, a_3 = 0.020, a_4 = 0.012\}$. Making use of equation (2.25) gives the feedback

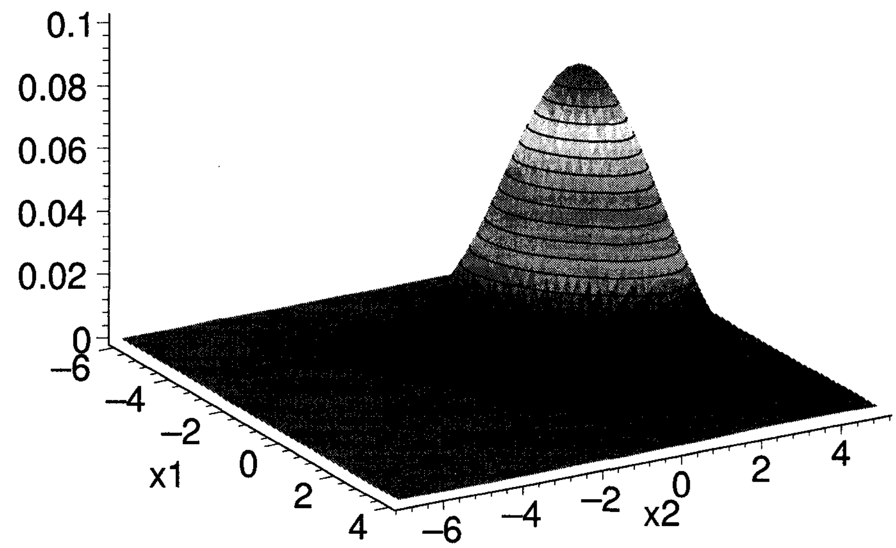


Figure 5.1: The desired stationary PDF, used as the target for controller design, for the example process (5.42).

control law:

$$u(t) = 1.30 - 1.50x_1(t) + 1.85x_1^2(t) + 0.0625x_1^3(t) + 0.0375x_1^4(t) - 2.34x_1(t)\,x_2(t) \tag{5.48}$$

An elementary stability analysis was performed for the CL process using the Lyapunov function $V(x) = (x_1 - 0.53)^2 + \frac{1}{20}(x_2 - 0.53)^2$. This reveals that the deterministic portion of the closed-loop process is asymptotically stable within the rectangle bounded by $x_1 \in [-7, 4.9]$ and $x_2 \in [-7, 7]$.

Simulations of the process, (5.42), under the designed control strategy, (5.48), confirm that the realized PDF matches the design goal. A histogram based on 10000 time steps of simulation data is given in Figure 5.2. The histogram takes a shape similar to that of Figure 5.1; in particular, the mode is in the correct area, the data is spread as expected, and the tail behaviour shows the desired 'negative' skewness. Additionally the stability of the CL process was validated over the 10000 time steps of the simulation. A plot of the time series data for the two states and the input for the example is given in Figure 5.3. The time series of the two states demonstrate reasonable dispersions about the process mean while the input signal takes occasional large negative values which are interpreted as being responsible for reproducing the heavy tail of the target PDF. It should be noted that the

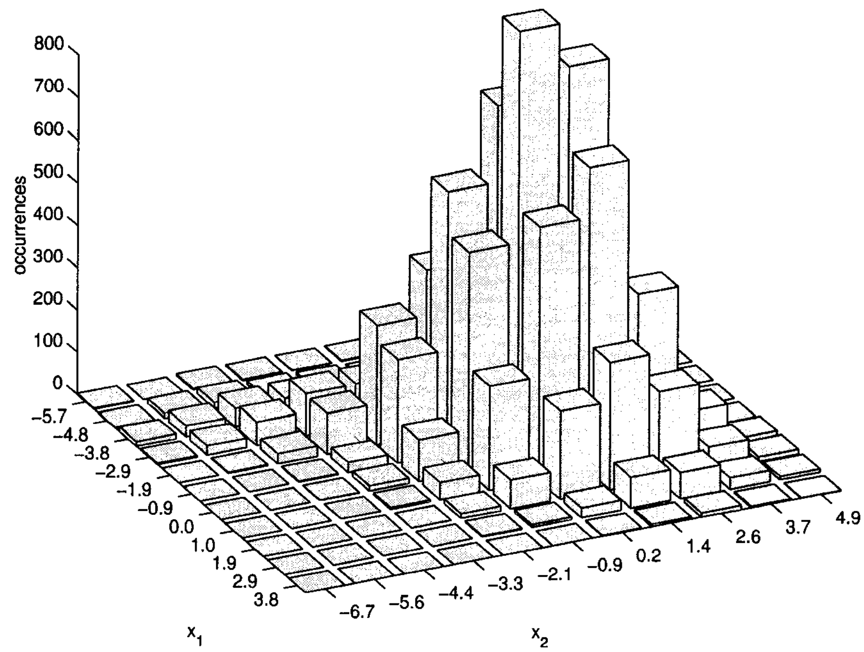


Figure 5.2: Histogram of data from simulation of example process (10000 time steps).

input values in general are large to compensate for the relatively small gain on the input in the process model.

5.6 Chapter Summary

For a general class of time-invariant discrete-time stochastic nonlinear processes, a new approach to controller synthesis is presented. The main idea behind the PDF-shaping concept is that the key factors in process operation and profitability of industrial processes may be represented by the stationary PDF of process. A PDF representing good performance should be chosen based on engineering and economic considerations. The control of the process should be exercised to meet the chosen PDF, thus ensuring safe, profitable and environmentally responsible operation. The PDF-shaping technique was introduced in the previous chapter for first-order processes, but is extended here to more complicated models, with different types of higher-order dynamics. Control design to shape the multivariate stationary PDF is approximately achieved by parameterizing the

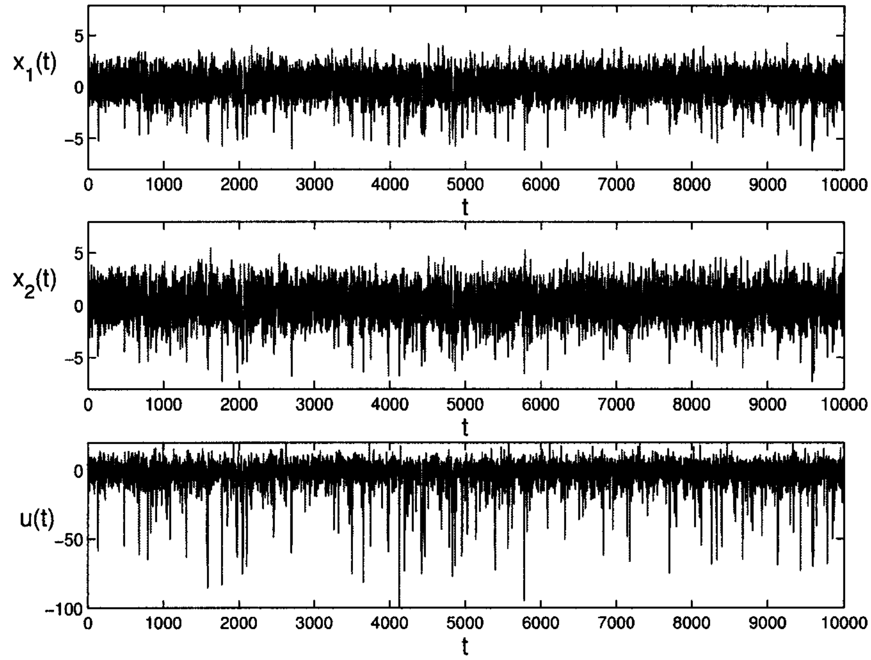


Figure 5.3: The time series data from the simulation.

closed-loop process dynamics and reducing the invariant equation to a set of algebraic equations. A second approach to the technique is given where the feedback control law is parameterized, instead of the CL feedback. The development of the technique is described for both the general case and the case where Gram-Charlier PDFs are used for the structure of the target PDF. An application of the technique to a second-order process is demonstrated through simulations.

"The ship in docking, inter-lockin
And up-rockin electro-shocking"
– The Beastie Boys

6

Optimal Control and the Stationary PDF

A performance-oriented controller synthesis technique for discrete-time stochastic nonlinear processes is proposed. When the objective for design is specified as the expected value of a nonsymmetric, nonquadratic loss functional, it is necessary to relate closed-loop process dynamics to the stationary PDF to properly address the problem. Since explicit relationships are available for only a few special cases, solution of the general optimal control problem is not possible. Application of the dynamics-PDF approximation technique in the optimal control framework results in regulatory control laws suboptimal with respect to design objective. Application of the technique to example processes is illustrated through simulations.[1]

6.1 Introduction

In this chapter the approximation of the dynamics-PDF relationship is applied to problem of regulatory control design with respect to a general (nonquadratic, nonsymmetric) objective

[1]Parts of this chapter were presented at the 2002 Canadian Chemical Engineering Conference and in (Forbes *et al.*, 2003*a*).

function. The result is a suboptimal but effective control design technique applicable to time-invariant discrete-time stochastic nonlinear processes. Motivation for the investigation of this problem comes from the processing and manufacturing industries, where not only are the costs of operation non-quadratic (Shinskey, 2002), but processes are often nonlinear and disturbances usually have non-Gaussian distributions. In this situation, when the objective is specified as the expected value of a nonsymmetric, nonquadratic loss functional, direct minimization of the cost functions is not possible as the (generally) non-Gaussian process PDF cannot be removed from the problem formulation. Therefore, it becomes necessary to relate the CL process dynamics to the stationary PDF in order to properly address the problem and this is an obstacle to control design. Since explicit relationships are available for only a few special cases, solution of the general optimal control problem is not possible.

The specific optimal control problem involves optimizing the parameters in a pre-selected control structure with respect to a given objective function. Again, for nonlinear processes and general objective functions, it is necessary to solve the dynamics-PDF relationship. Here the technique for approximating solution to the integral equation is applied in the specific optimal control framework to present a practical control design. This is a performance oriented approach to control design.

This chapter is organized as follows: §2 gives provides some context and background from the literature for the techniques proposed in this chapter. In §3 the general and specific optimal control design problems for stochastic processes are introduced and the barriers to their solution identified. Approximation techniques are proposed which result in suboptimal but effective control laws. §4 illustrates the use the the proposed techniques through simulations of an example process. §5 concludes this chapter.

6.2 Background

Often in the design of regulatory feedback control laws for industrial systems, performance is highly important. In such cases, controllers are designed to optimize some measure of system performance. In the case of stochastic systems, expectation cost functions are an appropriate choice. The optimal control problem discussed in this work shares the same basic formulation as those solved in (Harris, 1992), (Lee, 1990) and (Harris, 1985).

Controller synthesis for linear processes with quadratic objectives is well reported in the process control literature (Harris, 1985), but relatively few results are available for nonlinear processes with nonquadratic objectives. One of the best known results for the linear / quadratic case is the minimum variance control law (Astrom, 1970). Extensions to cover nonsymmetric and nonquadratic objectives have been presented in (Sandblom *et al.*, 1987), (Harris, 1992) and (Cain and Jansen, 1997), and for a class of nonlinear autoregressive moving average processes with quadratic objectives in (Lee, 1990). More recently some works have presented results where the objective for the control design is a pre-selected probability density function (Wang, 1999; Forbes *et al.*, 2002*a*).

For industrially well-established regulatory control design, typically a setpoint is chosen as a target for process operation and a quadratic cost functional expresses the loss in profit due to deviations from the setpoint. The cost functional, integrated against the relative likelihood of different operating conditions, is then used as an objective for control design. This cost functional is illustrated in Figure 1.2. In the development of optimal control designs for such cases, direct minimization of the cost function with respect to the manipulated variable is performed and explicit knowledge of the process PDF is not required.

This approach, while fruitful for some processes, is not appropriate when there is a safety constraint of quality specification to be met. In such cases, a cost functional that reflects the high costs of violating acceptable limits and the relatively low costs associated with exceeding minimum specifications. A representation of the type of cost functional that may be used in this situation is given in Figure 1.2. These types of objectives have been discussed in a number of works (Latour, 1992), (Latour, 1996) and (Marlin *et al.*, 1987).

In this chapter, it will be shown that there is no way to manipulate the cost function to achieve an analytical optimal control design. The relationship of the stationary PDF with the optimal control design problem is addressed and the dynamics-PDF approximation technique of Chapter 3 is invoked to derive suboptimal control laws. The following example gives some motivation to investigate nonlinear and nonquadratic control designs. In the example, analytical minimization of the cost objective is not possible and so the objective is changed to derive a suboptimal control law.

Example 6.2.1 The purpose of this example is to demonstrate that, even when the system under consideration is linear, the use of a nonsymmmetric and nonquadratic loss function with loss in the process input leads to a nonlinear control law. The controller design technique used here will closely follow that of (Harris, 1992). Consider the simple, first-order linear system:

$$x(t+1) = \alpha x(t) + \beta u(t) + w(t) \tag{6.1}$$

and the following objective function:

$$J = E\left[\ell\left(x(t+1)\right) + \lambda u^2(t)\right] \tag{6.2}$$

where the nonsymmetric, nonquadratic loss functional for the state is

$$\ell\left(x(t+1)\right) = \left\{ \begin{array}{ll} c_1 x(t+1) & x(t+1) < 0 \\ c_2 + c_3 x(t+1) & x(t+1) \geq 0 \end{array} \right\} \tag{6.3}$$

Unfortunately, there is no convenient way to apply the expectation operator to the entire loss functional, $\ell\left(x(t+1)\right)+\lambda u^2(t)$; however, a sub-optimal, but reasonable control design may be obtained by removing the control term from within the expectation operator and taking conditional expectation of the remaining term:

$$J = E\left[\ell\left(x(t+1)\right)|x(t)\right] + \lambda u^2(t) \tag{6.4}$$

This approach was originally proposed in (Clarke and Hastings-James, 1971). Controllers designed using the simplified loss function (6.4) are one-step ahead controllers. The control law makes a trade-off between the control energy used at each time step and the average value of losses associated with the state. The difference between (6.4) and (6.2) is discussed further in (MacGregor and Tidwell, 1977).

Inserting (6.1) and (6.3) into (6.4) and applying the definition of expectation gives:

$$\begin{aligned} J =& E\left[\ell\left(\alpha x(t) + \beta u(t)(\alpha x(t) + \beta u(t) + w(t)\right) p_w\left(w(t)\right) dw(t) \\ =& c_1 \int_{-\infty}^{-(\alpha x(t)+\beta u(t))} \left(\alpha x(t) + \beta u(t) + w(t)\right) p_w\left(w(t)\right) dw(t) \\ &+ \int_{-(\alpha x(t)+\beta u(t))}^{\infty} \left(c_2 + c_3\left(\alpha x(t) + \beta u(t) + w(t)\right)\right) p_w\left(w(t)\right) dw(t) + \lambda u^2(t) \end{aligned}$$

$$
\begin{aligned}
&= c_1 \int_{-\infty}^{-(\alpha x(t)+\beta u(t))} (\alpha x(t) + \beta u(t) + w(t))\, p_w(w(t))\, dw(t) \\
&+ c_2 \int_{-(\alpha x(t)+\beta u(t))}^{\infty} p_w(w(t))\, dw(t) \\
&+ c_3 \int_{-(\alpha x(t)+\beta u(t))}^{\infty} (\alpha x(t) + \beta u(t) + w(t))\, p_w(w(t))\, dw(t) + \lambda u^2(t) \qquad (6.5)
\end{aligned}
$$

To optimize this objective, it is necessary to differentiate with respect to $u(t)$ using Leibniz' Rule for differentiation of an integral (Appendix B) and set:

$$
\begin{aligned}
0 &= \frac{\partial J}{\partial u(t)} = c_1\beta \int_{-\infty}^{-(\alpha x(t)+\beta u(t))} p_w(w(t))\, dw(t) + \beta c_2 p_w(-(\alpha x(t) + \beta u(t))) \\
&\quad + c_3\beta \int_{-(\alpha x(t)+\beta u(t))}^{\infty} p_w(w(t))\, dw(t) + 2\lambda u(t) \qquad (6.6)
\end{aligned}
$$

Using $P_w(\cdot)$ to represent the cumulative distribution and integrating:

$$
\begin{aligned}
0 &= c_1\beta P_w(-\alpha x(t) - \beta u(t)) + c_2\beta p_w(-\alpha x(t) - \beta u(t)) \\
&\quad + c_3\beta (1 - P_w(-\alpha x(t) - \beta u(t))) + 2\lambda u(t) \qquad (6.7) \\
&= (c_1 - c_3)\beta P_w(-\alpha x(t) - \beta u(t)) + c_2\beta p_w(-\alpha x(t) - \beta u(t)) + c_3\beta + 2\lambda u(t)
\end{aligned}
$$

Equation (6.7) gives an implicit state feedback control law for the system (6.1) that is optimal with respect to Equation (6.3). The feedback control law is plotted in Figure 6.1 where the disturbance is zero-mean, unit-variance Gaussian and the following parameter values are chosen: $\alpha = \frac{1}{\sqrt{2}}$, $\beta = 1$, $c_1 = -1$, $c_2 = 3$, $c_3 = 1$, $\lambda = 2$. Clearly this is a nonlinear control law.

□

It is somewhat surprising that an unconstrained optimal controller design results in a nonlinear control law for a linear process. The representative plot of the control law given by Figure 6.1, as well as illustrating the nonlinearity of the control law, shows that the magnitude of the control action is absolutely bounded, regardless of the value of the state. The nonlinearity of the optimal control design prompts further investigation of optimal control designs for linear processes later in this chapter. While in the example, the objective is altered to enable derivation of a suboptimal control strategy, in the proposed technique, the objective function is not altered. It is the stationary PDF of the closed-loop process that is approximated to derive a suboptimal control design.

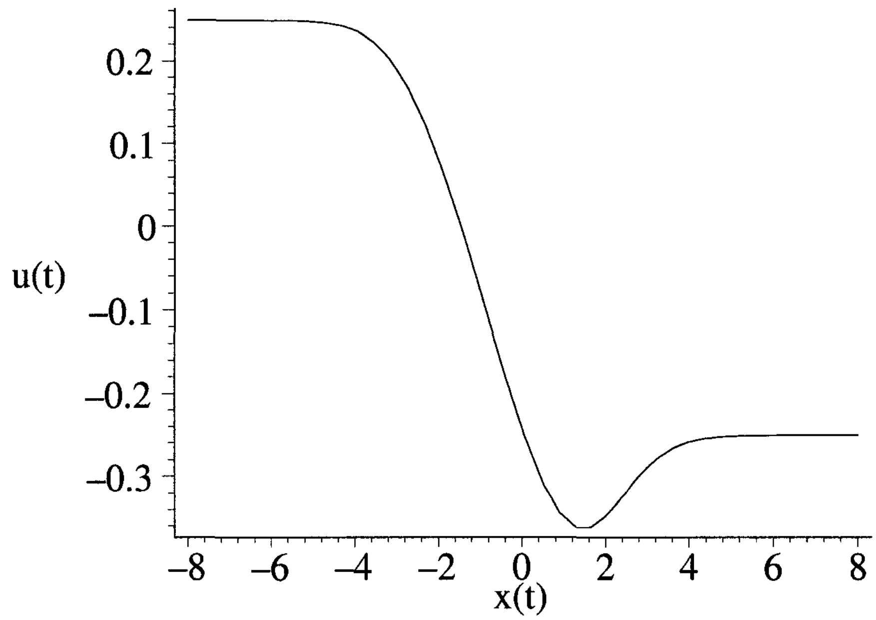


Figure 6.1: A representative Harris-type nonlinear feedback control law.

6.2.1 Expectation-Type Cost Functions

Expectation objectives in system variables consider what is likely to happen, or what, in the long run, will happen on average. In doing so, these objectives provide a measure of system performance. In the processing and manufacturing industries, a common objective is the minimization of costs associated with deviations from normal system operating points. This is expressed by the cost function:

$$J = E[\ell(\mathbf{x}_t, \mathbf{u}_t)] \tag{6.8}$$

where the functional $\ell(\mathbf{x}_t, \mathbf{u}_t)$ is relative to the cost of operation at the operating point $(\mathbf{x}_t, \mathbf{u}_t)$. To evaluate this cost function for the system (2.15) operating under a feedback control (2.22) the definition of expectation is used as follows.

$$J = \int_{\Re^n} \ell\left(\mathbf{x}_t, \mathbf{k}\left(\mathbf{x}_t\right)\right) p\left(\mathbf{x}_t\right) \mathbf{d}\mathbf{x}_t \tag{6.9}$$

For this type of cost function to be useful as a metric in the context of long-term performance, it is necessary that a stationary PDF exist for the CL system. It is inappropriate to discuss non-stationary system models within this framework because the expected cost of operation would be forever changing.

In the subsequent sections of this chapter, an approximation of the optimal controller design with respect to an expectation type objective function will be developed. The design technique will require that a set of parameters be found using numerical optimization.

6.2.2 Semi-Infinite Optimization

Semi-infinite optimization may be used to solve problems where there is a constraint on the decision variables, **a**, of the form:

$$\psi(\mathbf{a}, \mathbf{x}) \leq 0 \quad \forall \mathbf{x} \in \Omega \tag{6.10}$$

and Ω is a compact subset of $\Re^{n_x}$. In this chapter, the decision variables will be sets of parameters in a feedback control law parameterization and in a stationary PDF approximation. The general semi-infinitely constrained optimization problem formulation is:

$$\begin{aligned} \min_{\mathbf{a}} \quad J &= g_{obj}(\mathbf{a}) \\ \text{subject to :} & \\ \mathbf{g}_{eq}(\mathbf{a}) &= 0 \\ \mathbf{g}_{ineq}(\mathbf{a}) &\leq 0 \\ \psi(\mathbf{a}, \mathbf{x}) &\leq 0 \quad \forall \mathbf{x} \in \Omega \end{aligned} \tag{6.11}$$

A key aspect of the optimization algorithm is the discretization of the set Ω. This converts the semi-infinite inequality constraint to a finite set of inequality constraints. A complete discussion of semi-infinite optimization is given in (Polak, 1997).

6.3 Controller Design for Stochastic Processes

In standard control design techniques, feedback control laws are designed for a process such as the one given by equation (2.15) to optimize an objective function such as the one given by equation (6.8). In the more general case considered here the additional equation, (2.27), relating process dynamics to the stationary PDF enters the problem formulation.

6.3.1 General Optimal Control Problem Formulation

Regulatory control design for sustained system performance is formulated as follows. The feedback control law, equation (2.22), is to be found that minimizes the cost function, equation (6.9) subject to the dynamics of the system model, equation (2.15). It is assumed that the control law will result in a stationary CL system. Solution of this control problem is complicated because the stationary PDF is one term in the integrand on the right hand side of the cost function. As given by equation (2.27), the stationary PDF is a function of the CL system dynamics and it is therefore a function of the feedback control law. For this reason, equation (2.27) must be included in the problem formulation. The equation for the stationary PDF contains all information about the system model; therefore equation (2.27) is not an extra element of the problem formulation, but just a different way of incorporating the dynamic model (2.15). The general optimal regulatory control design problem formulation is:

$$\begin{aligned} \min_{k(\cdot)} \quad J &= \int_{\Re^n} \ell\left(\mathbf{x}, \mathbf{k}\left(\mathbf{x}\right)\right) p\left(\mathbf{x}\right) \mathbf{dx} \\ \text{subject to :} & \\ p\left(\zeta\right) &= \int_{\Re^n} p_{\mathbf{w}}\left(\zeta - \mathbf{f}\left(\xi, \mathbf{k}\left(\xi\right)\right)\right) p\left(\xi\right) \mathbf{d}\xi \end{aligned} \tag{6.12}$$

Exact solution to this regulatory control problem is, in most cases, intractable. The barrier is the lack of an explicit solution to the the stationary PDF equation.

6.3.2 Approximating the Relationship Between Dynamics and PDF

An approximate solution to the general regulatory optimal control design may be made by invoking the approximate solution to the dynamics-PDF relationship. Both the feedback control law and the stationary PDF resulting from the associated CL process are approximated. These parameterizations allow for reduction of the integral equation to a set of algebraic equations in the two parameter sets.

The first step in approximating a solution to equation (2.27) is to choose a feedback control law parameterization.

$$\mathbf{u}_t = \mathbf{k}(\mathbf{x}_t) \simeq \mathbf{A}\theta(\mathbf{x}_t) \tag{6.13}$$

This parameterization is now substituted into equation (2.27).

$$p(\zeta) = \int_{\Re^n} p_{\mathbf{w}}(\zeta - f(\xi, \mathbf{A}\theta(\xi)))\, p(\xi)\, \mathrm{d}\xi \tag{6.14}$$

As stated in Chapter 2 few exact solutions to this equation are known and parameterization of the control law does not, on its own, allow for explicit calculation of the PDF. A second parameterization is now made, using a GC PDF to approximate the stationary PDF.

$$p(\mathbf{z}) \simeq p_{GC}(\mathbf{z}) \tag{6.15}$$

So that equation (6.14) becomes:

$$p_{GC}(\zeta) = \int_{\Re^n} p_{\mathbf{w}}(\zeta - f(\xi, \mathbf{A}\theta(\xi)))\, p_{GC}(\xi)\, \mathrm{d}\xi \tag{6.16}$$

To both sides of this equation, condition (2.57) is applied and, with some rearrangement of factors in the integrand, the following results.

$$\mathbf{c}_{GC}^T = \int_{\Re^n} \left(\int_{\Re^n} p_{\mathbf{w}}(\zeta - f(\xi, \mathbf{A}\theta(\xi)))\, \mathbf{h}^T(\zeta)\, \mathrm{d}\zeta \right) p_{GC}(\xi)\, \mathrm{d}\xi \tag{6.17}$$

By making use of equation (2.58), and the change of variables $\mathbf{z} = \zeta - \tilde{\mathbf{f}}(\xi)$ a more insightful form is created.

$$\mathbf{c}_{GC}^T = \int_{\Re^n} \int_{\Re^n} p_{\mathbf{w}}(\mathbf{z}) \begin{bmatrix} 1 \\ \left(\mathbf{z} + \tilde{\mathbf{f}}(\xi)\right)^{1,0,0,0,\dots} \\ \left(\mathbf{z} + \tilde{\mathbf{f}}(\xi)\right)^{0,1,0,0,\dots} \\ \vdots \end{bmatrix}^T \mathbf{D}^T \mathrm{d}\mathbf{z}\, p_{GC}(\xi)\, \mathrm{d}\xi \tag{6.18}$$

The first integration results in linear combinations of the translated moments of $p_{\mathbf{w}}$. Therefore the first integration is a vector of multivariate polynomials in $\mathbf{m}_{p_{\mathbf{w}}}$ and $\tilde{\mathbf{f}}(\xi)$. These polynomials are denoted by $\mathbf{q}$. Equation (6.18) becomes:

$$\mathbf{c}_{GC} = \int_{\Re^n} \mathbf{q}\left(\mathbf{m}_{p_{\mathbf{w}}}, \tilde{\mathbf{f}}(\xi)\right) p_{GC}(\xi)\, \mathrm{d}\xi \tag{6.19}$$

Performing the integration in the right hand side of equation (6.19) will result in a vector of functions, $\tilde{\mathbf{q}}$, in the parameter sets $\mathbf{m}_{p_{\mathbf{w}}}$, $\mathbf{A}$, and $\mathbf{c}_{GC}$.

$$\mathbf{c}_{GC} = \tilde{\mathbf{q}}\left(\mathbf{m}_{p_{\mathbf{w}}}, \mathbf{A}, \mathbf{c}_{GC}\right) \tag{6.20}$$

This is a set of algebraic equations in the parameter sets representing the PDF of the disturbance, the feedback control law, and the stationary PDF.

6.3.3 Suboptimal Regulatory Control

Equation (6.20) provides the key component in finding an approximate solution to the specific optimal control problem. A judicious choice of parameterization for $\mathbf{k}(\cdot)$ is made and substituted into equation (6.20) and also, along with the GC PDF, into the objective (6.9). The control design problem (6.12) is then reduced to a parameter optimization problem as follows.

$$\begin{aligned} \min_{\mathbf{A},\mathbf{c}_{GC}} \quad J &= \int_{\Re^n} \ell\left(\mathbf{x}, \mathbf{A}\theta\left(\mathbf{x}\right)\right) p_{GC}\left(\mathbf{x}\right) \mathbf{dx} \\ \text{subject to :} & \\ \mathbf{c}_{GC} &= \tilde{\mathbf{q}}\left(\mathbf{m}_{p_{\mathbf{w}}}, \mathbf{A}, \mathbf{c}_{GC}\right) \end{aligned} \tag{6.21}$$

The problem is find the parameters $\mathbf{A}$ and $\mathbf{c}_{GC}$ that minimize the objective J. The dynamics-PDF approximation (6.20) adds a set of equality constraints in the parameters to the problem. As discussed previously, the coefficients in the GC parameterization must be chosen so that the expansion is a true PDF. This condition is added to the optimization problem (6.21) as:

$$p_{GC}\left(\mathbf{x}\right) \geq 0 \quad \forall \mathbf{x} \in \Re^n \tag{6.22}$$

This constrained optimization problem is in a form corresponding to a semi-infinite optimization problem. This type of problem can be solved numerically with using a mathematical software package.

Therefore, by first providing a parameterized structure for the optimal control law and then approximating the PDF associated with the CL process, there are two ways that this approximation of the general optimal control law may be suboptimal. Either parameterization, since they are finite series of basis functions, may be not provide sufficient detail to be good representations of the true feedback control law or stationary PDF. While a detailed accuracy analysis for this problem is beyond the scope of this work, the following approach could be coded for solution with a mathematical software package. An initial parameterization of the feedback control law is made. Repeated semi-infinite optimizations are performed with sequentially higher-order GC PDFs being used to approximate the stationary PDF. The semi-infinite optimizations are repeated until the value of the objective does not change more than some tolerance. A term is then added to the feedback control law parameterization and the repeated semi-infinite optimization is again performed. This overall algorithm is repeated until the value of the objective function meets a specified tolerance. Although crude, this algorithm should lead to better approximations of the optimal control law as more parameters are added to the feedback control law. The error from the approximation of the stationary PDF is managed at each level of feedback control law approximation by adding enough parameters in the PDF parameterization so that the addition of one more does not improve the PDF approximation.

6.3.4 Approximate Solution to the Specific Optimal Control Problem

Another way to view the technique described above is as an approximation of specific optimal control design. Specific optimal control design is the problem of finding the set of parameters for a fixed control structure that optimize the objective function for the design. In the general optimal control design, the entire structure of the controller must be determined, while in the specific optimal control design, only the parameters must be calculated. It has been stated in previous sections and chapters that even if the CL process dynamics are fully specified, an exact closed-form solution for the stationary PDF is not available. Therefore, for the specific optimal control problem, the formulation will be the same as for the approximation of the general optimal control problem:

$$\begin{aligned} \min_{\mathbf{A},\mathbf{c}} \quad J &= \int_{\Re^n} \ell\left(\mathbf{x}, \mathbf{A}\theta\left(\mathbf{x}\right)\right) \hat{p}\left(\mathbf{x};\mathbf{c}\right) d\mathbf{x} \\ \text{subject to}: & \\ \mathbf{c} &= \rho\left(\tilde{\mathbf{q}}\left(\mathbf{m}_{p_{\mathbf{w}}}, \mathbf{c}, \mathbf{A}\right)\right) \end{aligned} \tag{6.23}$$

The major difference between the approximate solutions of the general and specific optimal control laws is that there is only one source of error in the second case. In the first case, a parameterization of the feedback control law must be made before the parameters can be optimized, but for the specific optimal control problem, the structure of the feedback control law is predetermined, and only the accuracy of the PDF approximation is of concern. The crude algorithm of the previous section can be used to improve the accuracy of this approach, but for this case, the structure of the feedback control law does not change iteratively, as it is fixed. Only the parameterization of the feedback control law is altered until the value of the objective no longer changes.

The proposed synthesis techniques cannot guarantee global asymptotic stability of the CL process. For this reason an *a posteriori* stability analysis should be performed following the procedure outlined in §5.3.6.

6.4 Illustrative Examples

The following examples illustrate the application of the proposed design technique. In the first case, a number of different controller design techniques, including the proposed technique are are applied to a linear process. The performance of each of these techniques with respect to the given objective are compared. In the second objective, a control law is designed for a nonlinear process. In both examples, it is shown that the proposed control algorithm results in a feedback control law that performs well and can be easily implemented.

6.4.1 Optimal Control Design for Linear Processes

The first example considers control design for the linear process:

$$x(t+1) = \frac{4}{5}x(t) + u(t) + w(t) \tag{6.24}$$

where the disturbance has a Gaussian distribution with zero-mean and unit variance. This process is to be operated to minimize the objective function:

$$J = E\left[x^2 + u^2 + \frac{3}{4}u^3 + \frac{9}{32}u^4\right] \tag{6.25}$$

This loss functional is non-symmetric in the cost associated with the input. This type of loss functional may be appropriate for a process where the input is expensive and increases from the nominal input are costlier than decreases. A plot of the loss functional is given in Figure 6.2. Notice the egg-shaped contours.

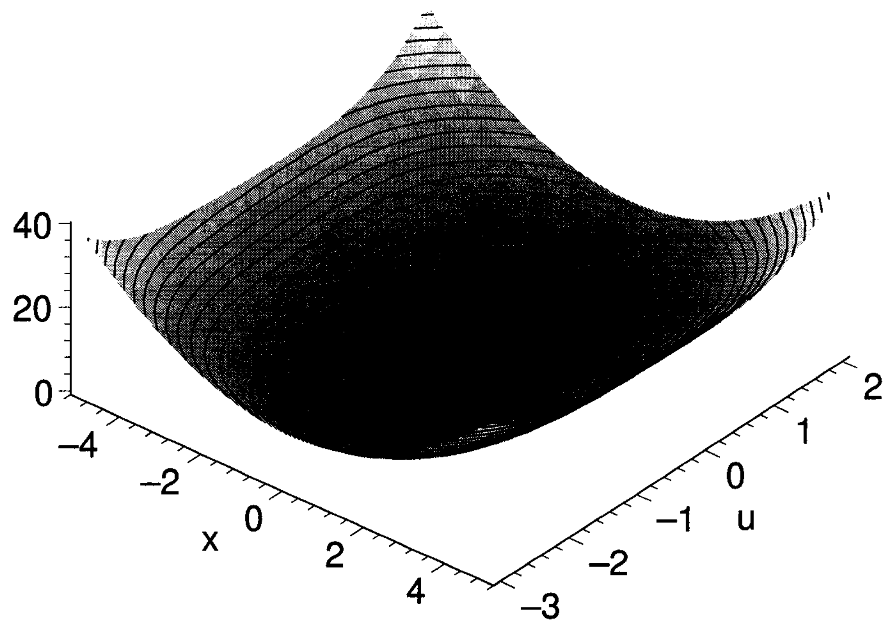


Figure 6.2: The loss functional.

Best Linear Control for the General Case

From the simple Markov structure of this model, it is inferred that all information known at time t about future process behaviour is given by $x(t)$. Therefore feedback control laws may be parameterized using functions of $x(t)$. For a linear feedback control law, the parameterization may be written as:

$$u(t) = a_0 + a_1 (x(t)) \tag{6.26}$$

With this feedback control law, the CL process becomes:

$$x(t+1) = a_0 + \left(\frac{4}{5} + a_1\right) x(t) + w(t) \tag{6.27}$$

and the loss function is:

$$J = E\left[x^2 + (a_0 + a_1 x)^2 + \frac{3}{4}(a_0 + a_1 x)^3 + \frac{9}{32}(a_0 + a_1 x)^4\right] \tag{6.28}$$

For a linear process with a Gaussian disturbance, and operating under linear feedback control, it is well known that the CL process will have a Gaussian stationary PDF. For the process (6.27), the stationary PDF may be parameterized by the mean $\mu = \frac{a_0}{1-\frac{4}{5}-a_1}$ and the variance $\sigma^2 = \frac{1}{1-\left(\frac{4}{5}+a_1\right)^2}$. These are substituted into the objective function 6.28 and the minimizing parameters a_0 and a_1, may be found by setting the partial derivatives of the objective to zero:

$$\begin{aligned} \frac{\partial J}{\partial a_0} &= 0 \\ \frac{\partial J}{\partial a_1} &= 0 \end{aligned} \tag{6.29}$$

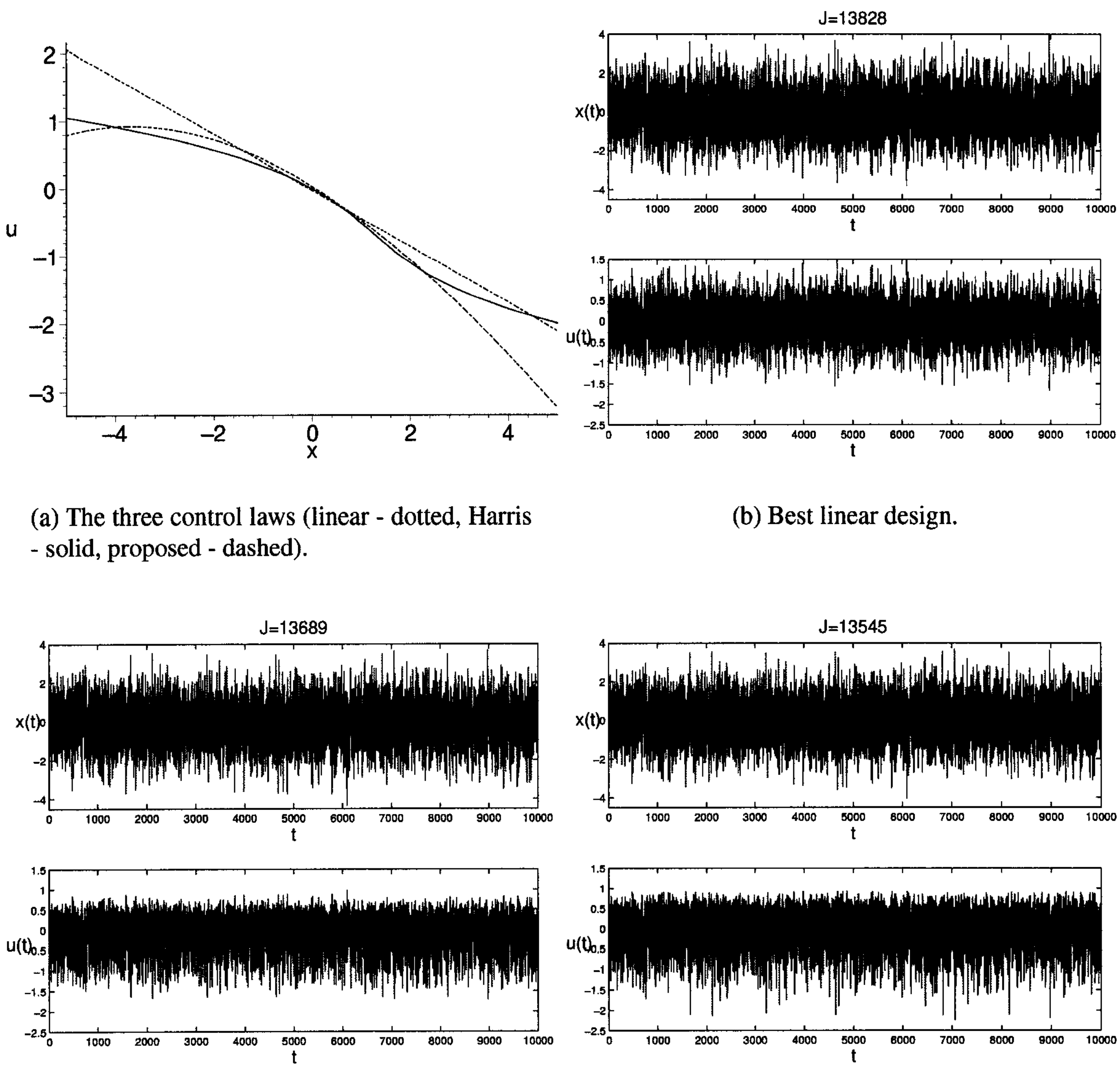
This produces a set of two equations in the two unknown parameters which are solved for the parameters. A plot of the optimal control law designed in this fashion is given in Figure 6.3(a) and a time series plot is given in Figure 6.3(b).

A Suboptimal Nonlinear Design

The technique proposed in (Harris, 1992) and illustrated in example 6.2.1 is used to develop a suboptimal control law for this process. Although an explicit closed-form control law cannot be obtained from this, it is possible to plot it, as in Figure 6.3(a). Clearly this is a nonlinear feedback. A plot of a simulated time series for the CL process operating with this control strategy is given in Figure 6.3(c). In all the plots, the value of the cost function is given. Note that the Harris suboptimal nonlinear control design results in a lower cost than the best linear control design.

Approximation of Specific Nonlinear Optimal Control Designs

The proposed design technique was also applied to develop a suboptimal control law for the example process (6.24) with respect to the objective function (6.25). The feedback control law was parameterized by a third-order polynomial and a fourth order GC PDF was used to approximate the PDF. Using the semi-infinite optimization function in MATLAB, an approximation of the optimal control law was derived. This is plotted in Figure 6.3(a) and a time series from the simulation is given in figure 6.3(d).



(a) The three control laws (linear - dotted, Harris - solid, proposed - dashed).

(b) Best linear design.

(c) Harris nonlinear design.

(d) Proposed nonlinear design.

Figure 6.3: Plots of the feedback control laws and time series for the three designs.

Remarks for the Linear Process Example

This example serves two purposes. First, it clearly demonstrates that for controlling linear processes for performance with respect to nonquadratic objectives, a nonlinear control law may be necessary to achieve optimum performance. For the specific process and objective in this example, the suboptimal nonlinear design outperformed the optimal linear design. The second purpose of the example is to demonstrate the effectiveness of the proposed technique. Even though the control law was parameterized with only a few polynomials, the suboptimal control law was superior to the exact optimum linear control law and related, exact optimal design technique. It is anticipated that improvements in performance would result from adding terms to the control law parameterization.

6.4.2 A Nonlinear Process

The proposed controller synthesis technique is demonstrated through application to the nonlinear process model:

$$y_{t+1} = \exp(\frac{y_t}{2}) - 1 + u_t + w_t \tag{6.30}$$

where y_t is a process output of interest and u_t is a process input. The disturbance term, w_t, is zero-mean, unit-variance Gaussian noise, *i.e.*,

$$w_t \sim N_{0,1}(w_t) \quad \forall t \tag{6.31}$$

A control law is to be designed to minimize the cost function

$$J = E\left[\ell(y_t) + 4u_t^2\right] \tag{6.32}$$

where

$$\ell(y_t) = \begin{cases} y_t & y_t \geq 0 \\ y_t^4 & y_t < 0 \end{cases} \tag{6.33}$$

A surface plot of the nonsymmetric, nonquadratic loss functional is given in Figure 6.4.

Application of Proposed Design Technique

The following feedback control parameterization is used,

$$\begin{aligned} u_t &= k(y_t) \\ &= a_0 + a_1 y_t + a_2 y_t^2 + a_3 y_t^3 \end{aligned} \tag{6.34}$$

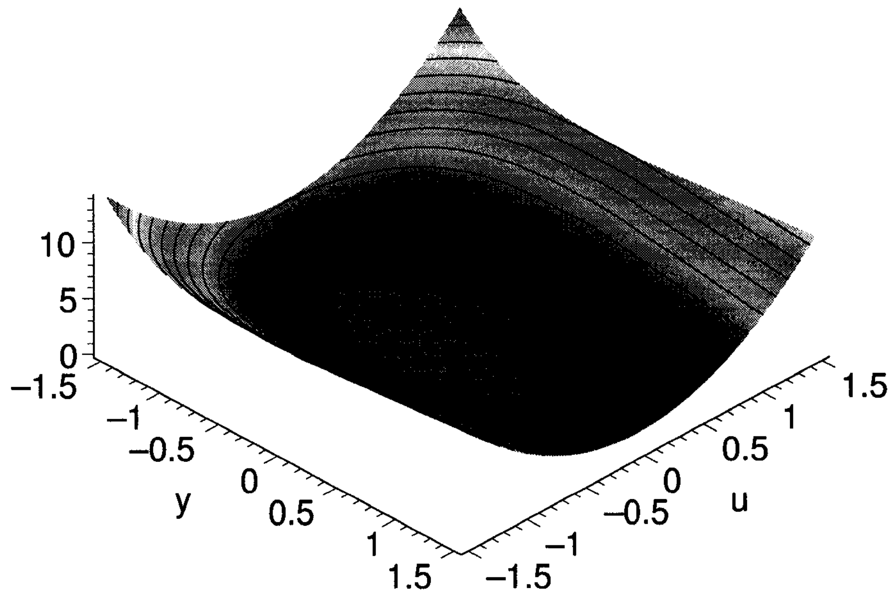


Figure 6.4: Nonsymmetric loss functional as given by equations (6.32) and (6.33).

and the stationary PDF of the CL process is approximated as a 4^{th}-order GC PDF:

$$p_{GC}(y) = (1 + c_3 h_3(y) + c_4 h_4(y)) N_{\mu,\sigma}(y) \tag{6.35}$$

Equations (6.9), (6.34) and (6.35) are applied to the cost function (6.32) as follows:

$$J = \int_{-\infty}^{\infty} \left(\ell(y) + 4(k(y))^2\right) p_{GC}(y)\, dy$$

The indicated integration is performed and the cost function becomes an algebraic function of the parameters. For the process (6.30) subject to the control law (6.34), the stationary PDF is:

$$p(\zeta) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\left(\zeta - \exp(\frac{\xi}{2}) + 1 - k(\xi)\right)^2}{2}\right) p(\xi)\, d\xi \tag{6.36}$$

Applying the GC PDF parameterization (6.35) and following the approximation technique of §6.3.4 yields equation (6.20). Solution of the problem using semi-infinite optimization yields the parameter set:

$$\{a_0 = 0.0238, a_1 = 0.1853, a_2 = 0.0150, a_3 = -0.0600,$$
$$\mu = 0.0802, \sigma = 1.0128, c_3 = 0.0001, c_4 = 0.0141\}$$

It can be shown by Lyapunov analysis that the designed control law stabilizes the CL process to an equilibrium point of zero in a region of at least $[-4, 5]$. Simple stabilizing control is used to handle the rare event of process deviations beyond the stable region.

A time series plot from the simulation of the closed-loop process is given by Figure 6.5. It can be seen that the control law does a good job in regulating the process near a

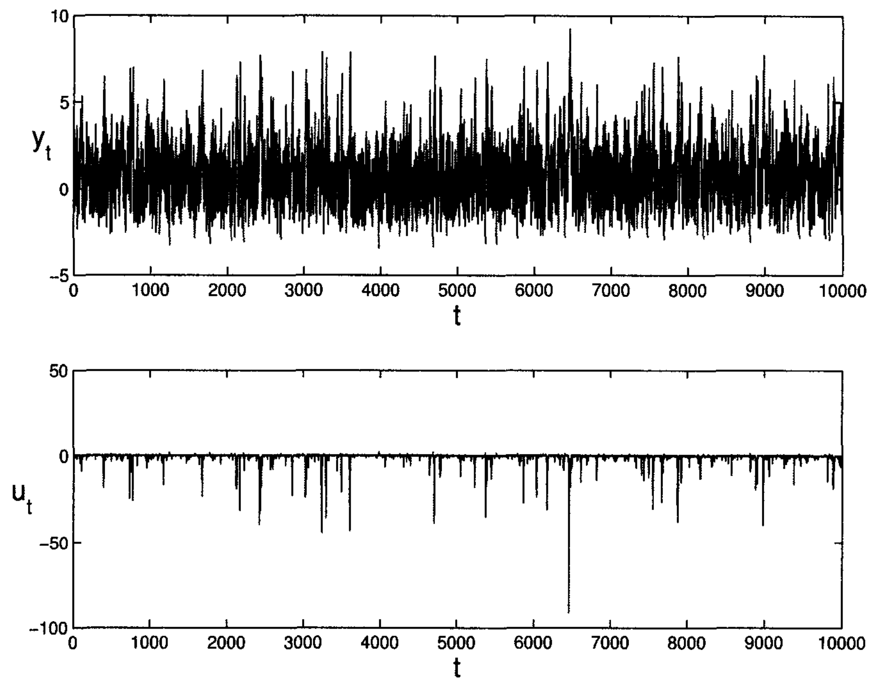


Figure 6.5: Time series plot for simulation of the nonlinear example process operating under the proposed control strategy.

mean value just above zero. Control action is generally small except when large actions may be taken to compensate for the exponential nonlinearity in the process. This example highlights the usefulness of the proposed technique in designing high-performance control laws for nonlinear processes with respect to non-quadratic objectives.

6.5 Chapter Summary

The problem of optimal control design for discrete-time stochastic processes with respect to a nonquadratic objective function has been investigated. It has been shown that the lack of an explicit relationship between the CL process dynamics and the stationary PDF presents a barrier to the solution of the optimal control problem. A technique of control law synthesis has been proposed that, while suboptimal with respect to the given objective, is an effective and practical approximation. This technique relies on a parameterization of the closed-loop process dynamics and an approximation of the corresponding stationary PDF. The special case of linear processes was investigated in a brief case study. Here two exact control designs were compared to the proposed approximate design. A second case study demonstrated the application of the technique to a process that included open-loop nonlinearity. The results of the case studies demonstrate that the proposed design techniques yields control laws that effectively regulate the process with respect to the objective. The study of the linear process demonstrated that the proposed technique is capable of outperforming exact optimal linear designs and an alternate suboptimal nonlinear design. A case study involving a nonlinear process, shows that the proposed technique develops control laws that are capable of compensating for significant and undesirable nonlinearities.

"You see, I've sort of succeeded beyond my level of ability."
– Bill Murray

7 Conclusions

7.1 Summary

With motivations from the processing and manufacturing industries, the long-term behaviour of stationary time-invariant, discrete-time stochastic processes has been investigated. For the specific class of processes examined, the long term behaviour may be concisely summarized by the stationary PDF. Typically in process analysis and controller synthesis, engineers focus on the process model and may consider quantities that can be derived from the stationary PDF, such as the process mean, or variance. However, the stationary PDF itself is rarely considered. It was pointed out in Chapters 2 and 6 that the stationary PDF is a key quantity in evaluating measures of process performance, which provides a wealth of information about process behaviour. For this reason the work in this thesis focussed on developing a framework that used both the dynamic process model and the stationary PDF for characterization of the process and designing control laws. This framework provides an alternative perspective for evaluating long-term performance of stochastic processes.

The first part of the research involved the use of the stationary PDF to characterize process performance. The stationary PDF can be used to calculate commonly used statistics such as mean and variance, and more general measures of performance. As well, visualization of the PDF provides additional information, such as the location and sharpness of the mode(s), tail behaviour and symmetry of the PDF. Critical values of the PDF may be calculated and used to evaluate the risk of violation of process constraints, such as quality specifications or safety and environmental limits. For analytical derivation of the stationary PDF, the relationship between the process dynamics, disturbance distribution and stationary process PDF cannot generally be solved to provide a closed-form solution. To overcome this problem, an approximation technique was proposed. The technique, by parameterizing both the closed-loop process dynamics and the stationary PDF, allows the integral equation giving the dynamics-PDF relationship to be reduced to a set of algebraic equations in the parameters. A second technique was proposed for approximating the PDF from process data. Methods of moments estimators for the parameters in a Gram-Charlier PDF are easily generated from process data. The approximated PDF may yield many insights into the process behaviour.

The second part of the research reformulated the analytical dynamics-PDF approximation technique for use in PDF-shaping control design. PDF-shaping control design takes the viewpoint that the stationary PDF incorporates all the process information relevant to the characterization of process performance. By carefully designing a stationary PDF as the target for control law design, the resulting controller regulates the process to perform reasonably within desired limitations on variance, near the target mean, or mode and with minimum violations of quality specifications and operating constraints. This part of the research work was split into two chapters. In Chapter 4 the PDF-shaping concept was introduced, using first-order processes as a simple basis to lead the discussion. In Chapter 5, PDF-shaping for higher-order processes is discussed. In both cases, the general PDF-shaping development was given along with the specific case of PDF-shaping for GC target PDFs.

The last part of the research approximated solution to the optimal control problem by making use of the dynamics-PDF approximation. By parameterizing the process dynamics and then using the approximation to relate the parameters of the dynamics to the parameters of a stationary PDF, the objective is reduced to a parameter optimization problem. This technique, while suboptimal, yields effective regulatory feedback control laws.

The work in this thesis may be viewed as some of the first small steps towards a broad non-LQG process analysis and controller synthesis paradigm. Linear process models, Gaussian disturbances and quadratic objectives may provide simple and reliable approximations for many industrial situations, but they are not always accurate and do not necessarily represent realistic performance objectives (Shinskey, 2002). As future work is done in the non-LQG area of stochastic process control research, a comprehensive set of techniques, including non-linear process identification, controller performance assessment with respect to non-quadratic performance measures, and fault detection and diagnosis will emerge as a new standard for analyzing and operating industrial processes. The literature has reported the tremendous economic value of even small improvements in process performance and so the value of more accurate and reliable process models, control laws and analysis techniques to the manufacturing and processing industries would be considerable.

7.2 Recommendations for Future Work

Here are a few of the possible areas for future work towards a comprehensive non-LQG paradigm.

7.2.1 Extensions of the Dynamics-PDF Approximation

There are a number of generalizations and specific applications of the approximate solution to the dynamics-PDF relationship that could be investigated.

Fully General Process Models

The focus of the research in this thesis was the general process model (2.15). Although this is a broadly applicable form of model, there are situations where the even more general process model given by equation (2.11) may be required to accurately represent the time evolution of the process variables.

If the feedback control law (2.22) is used for regulation the CL process is:

$$\begin{aligned} \mathbf{x}(t+1) &= \mathbf{f}\left(\mathbf{x}(t), \mathbf{k}\left(\mathbf{x}\left(t\right)\right), \mathbf{w}(t)\right) \\ &= \tilde{\mathbf{f}}\left(\mathbf{x}(t), \mathbf{w}(t)\right) \end{aligned} \tag{7.1}$$

and if this process is stationary, the stationary PDF, $p(\cdot)$, is given by:

$$p(\zeta) = \int_{\Re^{n_x}} p_w\left(\tilde{\mathbf{f}}^{-1}(\zeta, \xi)\right) \left\| \frac{\partial \tilde{\mathbf{f}}^{-1}(\zeta, \xi)}{\partial \zeta} \right\| p(\xi)\, d\xi \tag{7.2}$$

where $\tilde{\mathbf{f}}^{-1}(\zeta, \xi)$ is the inverse of $\tilde{\mathbf{f}}(\xi, \mathbf{w})$ with respect to $\mathbf{w}$, holding ξ constant; and $\left\| \frac{\partial \tilde{\mathbf{f}}^{-1}(\zeta,\xi)}{\partial \zeta} \right\|$ is the absolute value of the Jacobian determinant. The presence of this last function in the invariant equation complicates formulation of the analytical approximation of the dynamics-PDF relationship that was given in Chapter 3. In particular, work will need to be done to investigate how to handle the absolute value in the approximation of the CL dynamics.

Process Models with an Output Equation

Although there are instances in this thesis where it is suggested that the output equation (2.12) can be accommodated in the proposed techniques (control with an output feedback, in §2.2.3; expectation objectives, equation (2.50)), this topic has not been fully addressed. For the dynamic models discussed in this thesis, the dynamics-PDF approximation technique, PDF-shaping control design and the suboptimal control design of Chapter 6 can all be reworked for a dynamic output feedback control law, such as:

$$\zeta(t+1) = \alpha\left(\zeta(t), \mathbf{y}(t)\right) \tag{7.3}$$

$$\mathbf{u}(t) = \mathbf{k}_y\left(\zeta(t)\right) \tag{7.4}$$

Also, the suboptimal control design can be derived for situations where the objective function includes a cost relating to the process output. This type of objective is given by equation (2.50). Both of these situations can be examined with a focus on the state PDF to extend the applicability of the results of this thesis. They can also be investigated with a focus on the PDF of the output. This latter case adds significant complications. Current techniques can be readily applied to cases where the number of outputs and the number of states are the same, and where the functional relationship can be inverted. In that situation, the transformation of random variables result (2.5) can be used to derive the PDF of $\mathbf{y}$ from the PDF of $\mathbf{x}$. In the general case where there are less outputs than state variables, the relationship is more involved, and further analysis of the problem is required.

In many processes, a model in the form of process (2.15) and output equation (2.12) may not be appropriate. In many cases, the dynamics of the process may only be viewed through an output equation that is corrupted by noise. For example, the well known linear state-space version is:

$$\mathbf{x}(t+1) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) + \mathbf{w}(t) \tag{7.5}$$

$$\mathbf{y}(t) = \mathbf{C}\mathbf{x}(t) + \mathbf{v}(t) \tag{7.6}$$

The nonlinear equivalent is analogous. The techniques developed in this thesis are not general enough to cover this noisy output case. The techniques of this thesis should be extended and/or modified to handle this more general case. In particular, the PDF-shaping control design could be adapted to shape the output PDF, using output feedback. As a rule, output feedback control is required in industry. However, some state feedback controllers may be applied in industrial settings with careful use of an observer. Since exact PDF shaping is desired as the goal of PDF-shaping control design, it is doubtful that this approach will yield good results. A complete design approach that simultaneously considers control design and any required data filtering should be developed instead, *i.e.*, an approach that does not assume any sort of separation principle.

Wiener and Hammerstein Process Models

In contrast to the generalized techniques described above, in this section the specialization of the dynamics-PDF approximation and PDF-shaping to Wiener and Hammerstein process models is suggested. The purpose of specializing these techniques is the standard reason for specializing any technique. By making certain assumptions or limiting the scope of an investigation, more detailed results can often be developed. Some aspects of the adaptation of the work of this thesis to Wiener models are discussed in the previous section. However, when the dynamics are linear, and the disturbance is Gaussian, a simplification is available.

In this situation the stationary state PDF is Gaussian. Approximation and shaping of the output PDF is then only a problem of deriving the relationship between the output PDF and the mean and (co-)variance of the state PDF.

In the case of Hammerstein models, where the process is linear, except for a nonlinear input mapping, there are a number of techniques to be considered. First, if the input nonlinearity can be inverted, then the control design and PDF approximation can be performed exactly as if the process is linear. If the input nonlinearity cannot be inverted, then inversion the open-loop dynamics, equation (2.25), is not possible and direct parameterization of the feedback control law (as in §5.3.5) will need to be used. One possible advantage of looking at the Hammerstein model is that the input can be treated as a deviation from linearity and, in the case of a Gaussian disturbance, as a deviation from Gaussianity. When the input is constant, the process is linear, and as the input becomes more variable, the process becomes less linear.

7.2.2 Inverse Optimality of PDF-Shaping Control

PDF-shaping control design takes a different approach to regulatory control design than the standard cost function based approach. For the standard approach, the derivation of a minimizing control law for the given objective implicitly includes derivation of the 'optimum' PDF which will be associated with the optimally controlled process. For PDF-shaping controller design, the derived feedback control law will keep the process near a mean operating point with limited dispersion. For this reason, it seems that there should be some sort of optimality associated with the PDF-shaping control design. If controller design for a specific stationary PDF can be shown to be equivalent to the optimization of an expectation-type loss functional:

$$J = E\left[\ell\left(\mathbf{x}, \mathbf{u}\right)\right] \tag{7.7}$$

then the two types of regulatory controller synthesis are unified.

Clearly manipulation and substitution between the loss function (7.7), the stationary PDF equation (2.27) and the process dynamics (2.15) will be required to determine inverse optimality. However, no clear path from selection of the target PDF to back-calculation of the minimized objective presents itself. A preliminary result for the case of PDF-shaping with GC PDFs is available, but remains partial. In Chapter 4, the following measure of approximate PDF-shaping accuracy, based on integrating the square of the difference between the target and achieved PDF, was used:

$$I = \int_{\Re} \left(\mathbf{c}_{GC}^T \mathbf{h}(z) N_{\mu,\sigma}(z) - \tilde{\mathbf{c}}_{GC}^T \mathbf{h}(z) N_{\tilde{\mu},\tilde{\sigma}}(z) \right)^2 dz \tag{7.8}$$

where $\tilde{\mathbf{c}}_{GC}^T \mathbf{h}(z) N_{\tilde{\mu},\tilde{\sigma}}(z)$ is the PDF that is actually achieved by the control design. If the same mean and variance are used in the target and achieved GC PDF parameterizations, then the measure simplifies to:

$$I = (\mathbf{c}_{GC} - \tilde{\mathbf{c}}_{GC})^T \mathbf{B} (\mathbf{c}_{GC} - \tilde{\mathbf{c}}_{GC}) \tag{7.9}$$

where $\mathbf{B}$ is a constant symmetric weighting matrix. The measure is rearranged:

$$I = \mathbf{c}_{GC}^T \mathbf{B} \mathbf{c}_{GC} - 2\mathbf{c}_{GC}^T \mathbf{B} \tilde{\mathbf{c}}_{GC} + \tilde{\mathbf{c}}_{GC}^T \mathbf{B} \tilde{\mathbf{c}}_{GC} \tag{7.10}$$

Keeping in mind that $\mathbf{c}_{GC}$ is set by the control design and that the $\tilde{\mathbf{c}}_{GC}$ are quasi-moments, the following can be written:

$$I = \mathbf{c}_{GC}^T \mathbf{B} \mathbf{c}_{GC} - 2\mathbf{c}_{GC}^T \mathbf{B} E_{\tilde{p}}[\mathbf{h}(z)] + E_{\tilde{p}}[\mathbf{h}(z)]^T \mathbf{B} E_{\tilde{p}}[\mathbf{h}(z)] \tag{7.11}$$

This has a form similar to that of equation (7.7). However, the last term where there is a product of expectation operations causes problems. It is not possible to switch the order of the expectation and multiplication operations and so no further simplifications are apparent. Further investigation of this topic is required.

7.2.3 Existence of Solutions to the PDF-Shaping Equation

This is a challenging mathematical problem. In the PDF-shaping control design techniques proposed in this thesis, it was noted that not all stationary PDFs can be achieved for a given process, regardless of the control law that is used. For example, there were minimum possible variances that could be achieved. While many restrictions on the PDF can be recognized through careful process analysis and recognized in the design of the target PDF, this does not necessarily guarantee that the target PDF is achievable. It would be valuable to investigate the use of the invariant equation to find a set of conditions for existence of a solution the PDF-shaping problem. If it were known that a specific target PDF could be achieved, then the PDF-shaping approximation could be applied with the confidence that when enough basis functions are used in the CL feedback parameterization, an accurate approximation will result.

7.2.4 Tracking Control for Nonlinear Stochastic Processes

All of the research in this thesis was devoted to the study of stochastic processes under regulatory control. Control design for the more general tracking problem was not considered and there are some open research areas in design of tracking controllers within the stochastic process framework.

Trajectory control appears in the processing industries in the context of batch processes and process transitions. The characteristics of the batch evolve over a finite time horizon.

As a starting point for investigation of this topic, the following approach is suggested. Let the target process trajectory be given by $\mathbf{r}(t)$ and the tracking error be given by:

$$\mathbf{e}(t) = \mathbf{x}(t) - \mathbf{r}(t) \tag{7.12}$$

This implies that the error dynamics, for a process given by the model (2.15a), are:

$$\mathbf{e}(t+l) = \mathbf{f}(\mathbf{r}(t) + \mathbf{e}(t), \mathbf{u}(t)) + \mathbf{r}(t+1) + \mathbf{w}(t) \tag{7.13}$$

Again, as is the case for the state dynamics, there is nothing that can be done to prevent the disturbance $\mathbf{w}(t)$ from causing an error at the next time-step. Since the errors cannot be eliminated, one approach to tracking control design could be to manage the error distribution using PDF shaping. In choosing a stationary PDF for the errors, $p(e)$, it is implied that the error process (7.13) should be stationary. Since the process trajectory is a component of the error dynamics, the error dynamics are time-varying, adding complications to the PDF-dynamics relationship. A feedback control law for this process will need to be a function of the target trajectory, as well as the error, *i.e.*,

$$\mathbf{u}(t) = \mathbf{k}(\mathbf{e}(t), \mathbf{r}(t), \mathbf{r}(t+1)) \tag{7.14}$$

For this process, the PDF evolves according to:

$$p_{e_{t+1}}(\mathbf{e}_{t+1}) = \int_{\Re^{n_x}} p_w(\mathbf{e}_{t+1} - \mathbf{f}(\mathbf{r}_t + \mathbf{e}_t, \mathbf{k}(\mathbf{e}_t, \mathbf{r}_t, \mathbf{r}_{t+1})) - \mathbf{r}_{t+1}) p_{e_t}(\mathbf{e}_t) d\mathbf{e}_t \qquad (7.15)$$

If feedback control cannot make the process stationary, so that:

$$p_{e_{t+1}}(\cdot) = p_{e_t}(\cdot) \quad \forall t \qquad (7.16)$$

then a new approach will be required. A control law design that constrains the PDF as it evolves through time is one approach that could be taken. Iteration of equation (7.15) can be used to predict and reshape the PDF at the next time-step. Such an approach could be used to create a control law to adaptively correct the process trajectory as well as managing the dispersion about the trajectory.

7.2.5 Empirical Modelling for Discrete-Time Stochastic Nonlinear Processes

There are a number of ways that a focus on the distribution of process data could be used to improve existing techniques or possibly create new techniques of process identification. All of these suggestions are made with the viewpoint that process models should aggressively capture process behaviour for the normal operating region, *i.e.*, both the nonlinear dynamics and the nature of the random disturbance need to be modelled with high accuracy over the entire operating region. With an accurate process model available, high-performance control strategies, such as PDF-shaping can be designed.

For model building based on historical process data, the distribution of the data can have a direct influence over the accuracy of the process model. The PDF of the process data acts as a weighting term on the squared predication error objective for which minimizing model parameters are found. In situations where the distribution of historical data is not uniform, adjustments to the prediction error objective can be made so that the modelling objective enforces overall accuracy of the process model. Consider the process that can be represented by the discrete-time model:

$$\mathbf{x}_{t+1} = \mathbf{f}(\mathbf{x}_t, \mathbf{u}_t) + \mathbf{w}_t \qquad (7.17)$$

where $\mathbf{w}$ is a random disturbance with a Gaussian PDF, $p_w(\mathbf{w})$. For feedback control purposes, it is desired to find an approximate model for the one-step ahead prediction. One technique for identification of approximate process models is to choose a model structure parameterization. To recognize the dependence of the approximate model on the parameter set, $\{a_i\}$, the model is written as:

$$\hat{\mathbf{x}}_{t+1} = \hat{\mathbf{f}}\left(\mathbf{x}_t, \mathbf{u}_t; \mathbf{a}\right) \tag{7.18}$$

A standard approach in model identification for a data sequence of length N, is to calculate the minimizing parameter values for the sum of squares of the prediction errors (Ljung, 1999), *i.e.*,

$$\min_{\mathbf{a}} \quad J = \frac{1}{N-1}\sum_{t=1}^{N-1}\left(\mathbf{x}_{t+1} - \hat{\mathbf{f}}\left(\mathbf{x}_t, \mathbf{u}_t; \mathbf{a}\right)\right)^T\left(\mathbf{x}_{t+1} - \hat{\mathbf{f}}\left(\mathbf{x}_t, \mathbf{u}_t; \mathbf{a}\right)\right) \tag{7.19}$$

For ergodic processes and large N:

$$\begin{aligned} J &\approx E\left[\left(\mathbf{f}\left(\mathbf{x}_t, \mathbf{u}_t\right) - \hat{\mathbf{f}}\left(\mathbf{x}_t, \mathbf{u}_t; \mathbf{a}\right)\right)^T\left(\mathbf{f}\left(\mathbf{x}_t, \mathbf{u}_t\right) - \hat{\mathbf{f}}\left(\mathbf{x}_t, \mathbf{u}_t; \mathbf{a}\right)\right)\right] \qquad (7.20) \\ &\approx \int_{\Omega}\left(\mathbf{f}\left(\mathbf{x}_t, \mathbf{u}_t\right) - \hat{\mathbf{f}}\left(\mathbf{x}_t, \mathbf{u}_t; \mathbf{a}\right)\right)^T\left(\mathbf{f}\left(\mathbf{x}_t, \mathbf{u}_t\right) - \hat{\mathbf{f}}\left(\mathbf{x}_t, \mathbf{u}_t; \mathbf{a}\right)\right) p\left(\mathbf{x}_t, \mathbf{u}_t\right) d\mathbf{x}_t d\mathbf{u}_t \end{aligned}$$

This shows that in finding the function $\hat{\mathbf{f}}\left(\mathbf{x}_t, \mathbf{u}_t; \mathbf{a}\right)$ accuracy is weighted by the joint PDF of the state and input, $p\left(\mathbf{x}_t, \mathbf{u}_t\right)$. If the available data exhibits a PDF with a single mode near the centre of the operating region, as might be expected, the accuracy of the identified process model near the boundaries of the operating region may be poor. Adjustments of the prediction-error objective (7.19) should be investigated as means of assuring that the process model is accurate across the entire normal operating region.

The role of designed experimentation in this framework may also be investigated. Both mathematical analysis and numerical simulations have a role in evaluation of the impact of different identification input signals on the distribution of the generated data. The relationship between the dynamics of the process, as given by equation (7.17), and the stationary state PDF can be exploited to simplify process identification. For example, a process may be excited with a random dither signal, with a PDF $p_u(\mathbf{u})$. In this case, if: the process is stationary, and the input is independent of the state and random disturbance; then the stationary state PDF, $p(\cdot)$, is given by:

$$p(\mathbf{x}) = \int_{\Omega_{\mathbf{x}}} p_w\left(\mathbf{x} - \mathbf{f}\left(\mathbf{z}, \mathbf{u}\right)\right) p_u(\mathbf{u}) p(\mathbf{z}) d\mathbf{z} d\mathbf{u} \qquad (7.21)$$

Since this equation can be used for shaping the stationary state PDF of the identification data, a 7-step approach to process identification is proposed in Table 7.1.

Table 7.1: The Proposed 7-Step Process Modeling Procedure

1. Based on historical process data, determine process order, define the 'state' vector
2. Using the data, approximate the stationary PDF of the state, and use this to determine the region for which a reliable model can be identified.
3. Model structure selection (in this case, polynomial).
4. Parameter estimation, using the modified objective function. The parameters of the approximate (Gaussian) PDF model should also be determined.
5. If the region of model reliability, as determined in step 2, is unsatisfactory, then a dither signal should be designed, based on the results of step 4, so that more useful process data can be obtained.
6. Using the new data, verify that the process order and 'state' vector are correct and repeat steps 2-4.
7. Model validation.

Lastly, it might be possible to use the relationship between dynamics and PDF to gain insight into the process structure underlying the data. Given enough data from an ergodic process, and an estimate of the process order, an approximation of the stationary PDF can be made. Using this, along with the integral equation:

$$p(\zeta) = \int_{\Omega} p_u\left(\zeta - f_D\left(\xi\right)\right) p(\xi) d\xi \qquad (7.22)$$

gives the CL process dynamics, $\tilde{f}\left(\mathbf{x}_t\right)$, implicitly. If it can be shown that a reliable CL dynamic process model can be recovered from this equation then it should be possible to also determine the open loop dynamics, using the generally known control law.

7.2.6 Performance Assessment with Respect to Nonquadratic Objectives for Feedback Control of Nonlinear Processes

For industrial processes operating under regulatory feedback control it is useful to analyze the time-series data from these processes to evaluate how well the controller is regulating the process. For quadratic process objectives, this topic has been discussed by (Desborough and Harris, 1992) and (Huang and Shah, 1999). These works provide for assessment of control law performance against a minimum variance benchmark. This is done using the concept of invariant noise, which is closely related to the linear minimum variance control law. In keeping with the broader research goal of establishing a non-LQG paradigm, the framework developed in this thesis could be used to develop a controller performance assessment technique that explicitly recognizes nonlinear processes, non-quadratic performance measures and non-Gaussian disturbances. Chapter 6 of this thesis illustrates the difficulties of manipulating non-quadratic objectives in combination with nonlinear dynamics. The main barrier is the lack of solutions to the dynamics-PDF relationship. This is a very challenging topic that will need to build upon other results, such as process identification.

7.2.7 PDF-Shaping Control Design for Continuous Processes

In this thesis the topic of PDF-shaping control design for discrete-time processes is addressed. For continuous-time stochastic processes, described by the stochastic differential equation:

$$d\mathbf{x} = \mathbf{f}\left(\mathbf{x}, \mathbf{u}\right) dt + d\mathbf{w} \tag{7.23}$$

where $\mathbf{w}$ is a Wiener process, PDF-shaping should be investigated. It is known for these processes that the time evolution of the PDF is given by Kolmogorov's forward equation (Jazwinski, 1970). A steady-state solution to this equation can be set equal to a target PDF and the differential equation solved for the process feedback. If in the continuous-time framework, exact solutions can be found then issues such as inverse optimality and stability may addressed with fewer complications.

7.2.8 PDF-Shaping Control Design for Distributed Processes

For some processes, it is not the stationary PDF that is the probabilistic function of interest, but the distribution of a physical quantity at each time step. For example, there are a number of publications dealing with particle size distribution control, such as (Semino and Ray, 1995) and (Crowley *et al.*, 2000). In these types of processes, it is not the random behaviour of the process that leads to consideration of distributions, as opposed to trajectories, but the distributed nature of the process itself.

It is recommended that the adaptation of the probabilistic framework of this thesis, including the GC PDF parameterization, to apply to the problem of control of distributed processes be investigated. In particular the idea of the ergodicity-stability analogue may prove fruitful. In control design for distributed processes, it is desired that the distribution evolve as quickly as possible to a set target distribution. This target distribution may be viewed as a desired steady-state or equilibrium distribution. The control law should be designed to bring the distribution from an arbitrary initial distribution to the target distribution, in the same way that non-distributed processes move from an arbitrary initial condition to a desired equilibrium. The idea of distribution evolution is exactly the idea of ergodicity. The PDF of an ergodic process evolves over time from an arbitrary initial distribution to its stationary distribution.

7.2.9 Control Design with Manipulated Variable Saturation

The Harris suboptimal control design used as a motivating example for §6.2 resulted in a feedback control law that, as illustrated in Figure 6.1, tended to a constant, finite value near extremes of the domain. This suggests the possible application of this type of control design for processes with input constraints or saturations. The feedback control law (6.7) exhibits some interesting behaviour in the region near the origin. To simplify the discussion, let controller design for processes of the following form be considered:

$$x(t+1) = \alpha x(t) + u(t) + w(t) \tag{7.24}$$

where $|\alpha| \leq 1$, so that the open-loop process is stable, and the disturbance is zero-mean Gaussian with variance σ_w^2. A Harris-type suboptimal control design is developed for the objective:

$$J = E\left[\ell\left(x\left(t+1\right)\right) + \lambda u^2\left(t\right)\right] \tag{7.25}$$

where:

$$\ell\left(x_{t+1}\right) = \begin{cases} -b_1 x_{t+1} & x_{t+1} < 0 \\ b_2 x_{t+1} & x_{t+1} \geq 0 \end{cases} \quad b_1, b_2 > 0 \tag{7.26}$$

The design procedure is performed as follows (Harris, 1992). The input cost, $\lambda u^2\left(t\right)$ is moved outside of the expectation operator and conditional expectation is substituted for the remaining expectation term (with a simplifying change in notation):

$$J = E_c\left[\ell\left(x_{t+1}\right) \middle| x_t\right] + \lambda u_t^2 \tag{7.27}$$

Applying the definition of conditional expectation and differentiating with respect to Leibniz' Rule (Appendix B) yields:

$$\begin{aligned} \frac{\partial J}{\partial u_t} &= \int_{-\infty}^{-\alpha x_t - u_t} -\frac{b_1}{\sqrt{2\pi\sigma_w^2}} \exp\left(-\frac{w_t^2}{2\sigma_w^2}\right) dw_t \\ &+ \int_{-\alpha x_t - u_t}^{\infty} \frac{b_2}{\sqrt{2\pi\sigma_w^2}} \exp\left(-\frac{w_t^2}{2\sigma_w^2}\right) dw_t + 2\lambda u_t \end{aligned} \tag{7.28}$$

Performing the indicated integration implicitly gives the optimum feedback control law (with respect to the modified objective (7.27)):

$$\frac{b_1 + b_2}{2} \operatorname{erf}\left(\frac{\alpha x_t + u_t}{\sqrt{2}\sigma}\right) + \frac{b_2 - b_1}{2} + 2\lambda u_t \tag{7.29}$$

where erf $(\cdot)$ is the error function. This control law is plotted in Figure 7.1 for one set of parameter values.

Notice that:

- $\lim\limits_{x_t \to -\infty} u_t = \frac{b_1}{2\lambda}$
- $\lim\limits_{x_t \to \infty} u_t = \frac{-b_2}{2\lambda}$
- λ is actually a superfluous parameter and could be lumped into the parameters of $\ell\left(\cdot\right)$.
- The control law is approximately linear near the origin and the slope strongly depends on the value σ_w, *i.e.*, as σ_w becomes larger the slope is more relaxed.

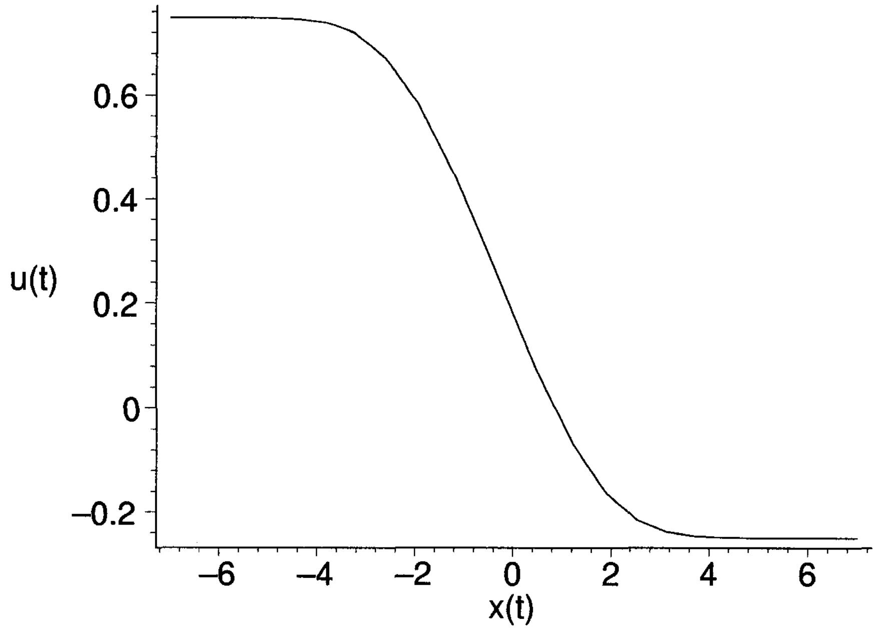


Figure 7.1: The Harris-type control law for parameter values $b_1 = \frac{3}{2}$, $b_2 = \frac{1}{2}$, $\sigma_w = 1$, $\alpha = \frac{4}{5}$ and $\lambda = 1$.

Therefore, for a process such as (7.24) a control law can be designed to respect hard constraints on the input. Additionally, by varying σ_w, the slope of the control law near the origin can be changed. The explicit adjustment of σ_w as a tuning parameter might be inappropriate for a process model identified from plant data, since the variance would also be fixed. However, if the process model is taken to represent the dynamics of the process with a Gaussian disturbance or arbitrary variance, then this type of controller design makes a statement about the size of disturbances that are expected. By taking the parameters b_1 and b_2 as tuning parameters, the meaning of the objective (7.27) is altered. This type of saturated-input control law clearly still has some sort of optimality, as it makes a trade off between an expected state cost and the current input cost at every time step. Research should be done to extend and clarify these ideas. Clearly there could be great latitude in the choice of cost functional, $\ell(\cdot)$ used in the objective (7.27).

The Last Word

The techniques for stochastic process analysis and control design developed in this thesis provide the first pieces of a comprehensive framework for engineering the efficient operation of a stochastic process. Of the future research directions suggested above, which are all additional components in the framework, a number of them are viewed as priorities.

Certainly, §7.2.5 demands attention. The techniques of this thesis are developed with the assumption that a model is already available for analysis or control law design. However, it is often the case that before analysis or design can occur a dynamic process model must be developed. The development of nonlinear continuous-time models from fundamental chemical and physical laws is well understood, as is the creation of linear discrete-time models from process data. In constrast, the creation of discrete-time nonlinear process models is still an open area of research. It is suggested that progress can be made towards a set of effective techniques for identification of stochastic nonlinear models by exploiting the relationship between process dynamics and the PDF of stationary processes.

Investigation of §7.2.7, the idea of PDF-shaping for continuous-time processes will help to more thoroughly establish the framework suggested in this thesis. Processes in the real world, including those in industry, generally evolve continuously over time. While discrete-time models often provide a good representation of process behaviour, there is some loss of detail. Once the continuous-time version of PDF-shaping has been developed, the necessary pieces will be in place to investigate PDF-shaping for continuous-time processes where the measurements and control adjustments are made discretely. Such a sampled-data approach most closely resembles the true situation for many industrial operations.

The research in this thesis was undertaken with the broad idea that improvements in the practice of process control are made when the techniques more accurately account for the true behaviour of processes. Whether it is process analysis, control design, or model identification, better results will come when nonlinear and non-Gaussian behaviour can be included and realistic process concerns, such as non-symmetric or nonquadratic objectives, can be addressed. It is hoped that the results of this thesis in combination with future research initiatives will, together, form a comprehensive framework that becomes an improved standard for process control.

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A

Discrete-Time CSTR Model Development

A discrete-time process model for a continuous stirred tank reactor (CSTR) is derived from the continuous-time model given in (Bequette, 1998). Consider the irreversible first-order reaction:

$$A \xrightarrow{K} B \tag{A.1}$$

with a temperature dependent rate constant K, taking place in a diabatic CSTR. A first-principles model governing this process consists of the following set of equations. First, the Arrhenius expression for the reaction rate constant is:

$$K(t) = k_0 \exp\left(-\frac{E}{RT(t)}\right) \tag{A.2}$$

where k_0 is the pre-exponential factor, E is the activation energy, R is the universal gas constant and $T(t)$ is temperature in the reactor at time t. For the purposes of developing a simple, second-order model, it will be assumed that temperature is a manipulated variable with no associated dynamics; tank volume, V, is held constant; and the inlet and outlet flow rates are held equal and constant at a value of F.

Mass balances on the reactant, A, and product, B, yield the following dynamic equations for the respective concentrations, c_A and c_B:

$$V\frac{dc_A}{dt} = Fc_{A,in}(t) - Fc_A(t) - k_0 \exp\left(-\frac{E}{RT(t)}\right) c_A(t) \tag{A.3}$$

$$V\frac{dc_B}{dt} = -Fc_B(t) + k_0 \exp\left(-\frac{E}{RT(t)}\right) c_A(t) \tag{A.4}$$

An exact discrete-time model of this process may be developed if the temperature and the inlet concentration are constant over the sampling interval Δ. Following the technique given in (Seborg *et al.*, 1989), the differential equations are integrated over the interval $[k\Delta, (k+1)\Delta)$. The values of the process states at the sampling times $\{\Delta, 2\Delta, 3\Delta, \ldots, k\Delta, (k+1)\Delta, \ldots\}$ are:

$$\begin{aligned} c_A(k+1) &= \exp\left(-\left(\tau + K(k)\right)\Delta\right) c_A(k) \\ &\quad + \frac{\tau\left(1 - \exp\left(-\left(\tau + K(k)\right)\Delta\right)\right)}{\tau + K(k)} c_{A,in}(k) \end{aligned} \tag{A.5}$$

$$\begin{aligned} c_B(k+1) &= \exp(-\tau\Delta) c_B(k) + \left(\exp(-\tau\Delta) - \exp\left(-\left(\tau + K(k)\right)\Delta\right)\right) c_A(k) \\ &\quad + \left(\frac{K(k) + \tau \exp\left(-\left(\tau + K(k)\right)\Delta\right)}{\tau + K(k)} - \exp(-\tau\Delta)\right) c_{A,in}(k) \end{aligned} \tag{A.6}$$

where the constant space time ratio $\frac{F}{V}$ is written as τ. The inlet reactant concentration, $c_{A,in}$ is a Gaussian disturbance variable with a mean value of 10 and a variance of 0.25. For simplicity of this example process, set $\tau = 1$ and $\Delta = 0.1$ and take the parameters in the Arrhenius rate constant as $k_0 = 65498400$, $E = 11843$ and $R = 1.987$.

For the equations with these values, a steady-state setpoint $c_B = 9.1$ can be achieved when inlet concentration is noise-free ($c_{A,in} = 10$) and the temperature is set to 380. Under these conditions, $c_A = 0.9$.

B
Additional Mathematics

B.1 Leibniz's Rule

Leibniz's rule gives the derivative of an integral as follows (Zwillinger, 1996):

$$\frac{d}{dx}\int_{f(x)}^{g(x)} h(x,t)dt = g'(x)h(x,g(x)) - f'(x)h(x,f(x)) + \int_{f(x)}^{g(x)} \frac{\partial h}{\partial x}(x,t)dt$$

B.2 The Central Limit Theorem

The central limit theorem states that for a random sample, $x_1, x_2, \ldots, x_N$, from a distribution with mean μ and standard deviation σ, then for a sufficiently large number of samples N, the sample mean, $\bar{x}$, will have approximately a Gaussian distribution with mean μ and standard deviation $\sigma/\sqrt{N}$. The approximation improves as N increases (Devore, 1995).

B.3 Stationary PDF of a Linear Process

B.3.1 Linear Combinations of Gaussian Random Variables

As stated in (Jazwinski, 1970), "linear operations on Gaussian random vectors produce Gaussian random vectors." The following proof is offered (Jazwinski, 1970). Take an n_z-dimensional random vector $\mathbf{z}$ from $N_{\mu_z,\Sigma_z}(\mathbf{z})$ and an n_ζ-dimensional random vector $\zeta = B_\zeta \mathbf{z} + \xi$ where B_ζ is an $n_\zeta \times n_z$ constant matrix and ξ is a constant n_ζ-vector. The characteristic function of ζ is:

$$\begin{aligned}
\phi_\zeta(\mathbf{y}) &= E\left[\exp\left(i\mathbf{y}^T\zeta\right)\right] = \exp\left(i\mathbf{y}^T\xi\right) E\left[\exp\left(i\mathbf{y}^T B_\zeta \mathbf{z}\right)\right] \\
&= \exp\left(i\mathbf{y}^T\xi\right)\exp\left(i\mathbf{y}^T B_\zeta \mu_z - \frac{1}{2}\mathbf{y}^T B_\zeta \Sigma_z B_\zeta^T \mathbf{y}\right) \\
&= \exp\left(i\mathbf{y}^T\left(B_\zeta \mu_z + \xi\right) - \frac{1}{2}\mathbf{y}^T B_\zeta \Sigma_z B_\zeta^T \mathbf{y}\right) \qquad \text{(B.1)}
\end{aligned}$$

This characteristic function is recognized as that of a Gaussian random variable. Therefore ζ is a Gaussian random variable with mean $B_\zeta \mu_z + \xi$ and variance $B_\zeta \Sigma_z B_\zeta^T$.

B.3.2 Linear Processes

Consider the following special case of the process (2.11):

$$\mathbf{x}(t+1) = A\mathbf{x}(t) + B\mathbf{w}(t) \qquad \text{(B.2)}$$

where A is an $n_x \times n_x$ constant matrix, B is an $n_x \times n_w$ constant matrix and $\mathbf{w}(t)$ is an iid, Gaussian disturbance vector. If this linear process has some initial condition, $x(0)$, that is independent of the disturbance sequence and is either a fixed constant or a Gaussian random variable, then, by the result of the previous section, the process (B.2) is a Gaussian process (Jazwinski, 1970).

B.4 The Law of Large Numbers

There are a number of versions of the law of large numbers with slightly different hypotheses and results. These are broadly divided into the weak and strong laws depending on the type of convergence in the result. Here, a strong law of large numbers is given for a sequence of iid random variables, $z_1, z_2, \ldots, z_N$ (Shiryaev, 1996). If the first absolute moment exists, *i.e.* $E[|z_i|] < \infty$, then the sample mean will approach the population mean as the length, N, of the sequence approaches infinity:

$$P\left(\lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} z_i = E[z_i]\right) = 1 \tag{B.3}$$

This type of convergence is referred to as 'convergence with probability one' or convergence 'almost surely'. To obtain a similar result for stationary time series data, a different hypothesis is required, since stationary time series data are identically distributed, but not independent. This leads to the notion of ergodicity.