Mathematical Modelling of Bias and Uncertainty in Accident Risk Assessment

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0.1 Preface

This report is a summary of the results of an off-campus final project entitled "Mathematical modelling of bias and uncertainty in accident risk assessment" executed by the author at the National Aerospace Laboratory NLR, Amsterdam for a period of 28 weeks from December 2001 to June 2002. Execution of a final project is one of the necessary requirements for graduating with a Master of Science (M.Sc) degree in Engineering Mathematics at the Faculty of Mathematical Sciences, University of Twente, The Netherlands.

The report is divided into two parts. The first part, consisting of Chapters 1 through 5, contains mathematical background materials for uncertainty analysis of accident risk assessment while the second part, consisting of Chapters 6, 7, and 8, is devoted to a discussion of the simulation results and conclusions that can be drawn based on the work done during the 28 weeks.

The author would like to express his gratitude to the many people who have made contributions to this study. First of all the author would like to thank his supervisor Prof. Dr. Arunabha Bagchi at the University of Twente for his continuous support and for his insights and suggestions on various aspects of the problem being studied. Secondly the author is grateful to Dr. Henk A.P. Blom, for giving him the opportunity to execute a final project at the NLR , for reading the manuscript and providing feedback, and for the interesting ideas he had shared. The author is indebted to his supervisor at the NLR, ir. Mariken H.C. Everdij for the many fruitful discussions and the numerous feedback, for her careful reading of the manuscript and not too mention for being understanding and patient with the author during the duration of his stay at the NLR. A special thanks goes to ir. Bert Bakker for providing the author with some Matlab® m-files for simulation, for the many discussions, for reading sections of the manuscript related to his area of expertise and for looking carefully at some proofs proposed by the author. The author is also indebted to the head of the LL department, ir. Jan C. Terlouw, for swiftly taking care of a working permit problem way back in December 2001. Finally, the author thanks his room mate in Kamer 55.1.07 of the LL Building, ir. Marco van der Park, and all other members of NLR's ATM group (Margriet, Sybert, Edwin and newcomer Bart) for the relaxing chit chat while working or during lunch at the NLR canteen.

Amsterdam, June 6, 2002

Hendra I. Nurdin

Part I

Mathematical Preliminaries

Chapter 1

Introduction

1.1 Air Traffic Management Safety

In the design or selection of advanced air traffic management (ATM) concepts, safety is now recognized as a key factor even when capacity and efficiency are the drivers of development. The safety target is often described as 'equal or better' in comparison with existing practice, allowing a large freedom in the way to express safety[Blom01]. One may, for example, express it by the number of headlines in the news, or by assessing the availability of some vital aircraft systems, or by counting the number of collisions occurring.

In this final project report we will use accident risk as a measure for safety, where one collision counts as two accidents. Moreover, we consider the NLR developed methodology of assessing accident risk[Blom01]. According to this methodology, accident risk is assessed by evaluating the incrossing risk (i.e. integral of incrossing rate between two aircraft or more) for a particular scenario of an ATM operation. The Generalized Reich framework[Bakk93] is used to express the incrossing rate in terms of the joint probability density function of position and velocity of the separation process between two aircraft. In practice, it is usually very difficult or impossible to determine this joint probability density function from actual data. To overcome this problem, a stochastic dynamic model of the ATM operation is developed, incorporating aircraft evolution under all kinds of hazardous situations. Next, accident risk is decomposed into sums and factors, and Monte Carlo simulations on the stochastic dynamic model are used to evaluate these sums and factors. Finally, the incrossing rate and accident risk can be evaluated by combining these sums and factors and be compared with the required low levels.

1.2 Uncertainties in Accident Risk Assessment

Naturally there will be differences between a mathematical model and reality due to inherent uncertainties in the model. Below we mention some types of

uncertainties that can be encountered in mathematical modelling of a real life phenomenon:

1. Uncertainty due to assumptions adopted during the modelling process, etc. It can be the case that some assumptions made during a modelling process are not completely true.

2. Uncertainty of proper values for the parameters that are part of the mathematical model.

3. In some instances a mathematical model cannot be solved analytically in order to evaluate a desired quantity. In this case the solution has to be approximated numerically and this introduces uncertainty due to simulation numerical errors, e.g. discretization of continuous time systems, computer round-off etc.

For a complete uncertainty analysis, one should try to include the different types of uncertainties, although this may not always be possible. At NLR, Everdij and Blom in [Ever02] have proposed a framework for assessing uncertainties due to modelling assumptions and uncertainty of proper parameter values. Numerical errors in Everdij&Blom are treated by estimating their upper bounds. In another literature, Stern et al.[Ster01] have developed a framework for analyzing uncertainty for Computational Fluid Dynamics (CFD) simulations by so called *verification* and *validation* procedures. According to Stern et al, there is currently no known way to evaluate errors due to modelling assumptions, so in their approach errors from modelling assumptions are excluded from uncertainty analysis. However, they take into account errors due to use of previous data, such as fluid properties, and numerical errors. Everdij&Blom tries to evaluate uncertainty due to modelling assumptions by exploiting expert judgements. We summarize these two approaches in Figure 1.1. An important difference is that Stern et al.[Ster01] do not suggest to make use of operational expert judgement on the differences between truth and model while Everdij&Blom[Ever02] recommends to use this.

In this final project the scope of the study is limited to analyzing uncertainty in accident risk due to uncertainty in the proper parameter values. Our primary interest will be to investigate efficient techniques to carry out such analysis.

1.3 Organization of the Report

The report is divided into two main parts. The first part, consisting of Chapters 1, 2, 3, 4 and 5, is devoted to brief explanations of accident risk and methods for assessment of uncertainty in accident risk due to uncertainty in parameter values, while the second part, consisting of Chapters 6, 7 and 8, is for test results and conclusions. In Chapter 2, we will discuss the mathematical theory of incrossing risk developed in [Bakk93]. The next three chapters

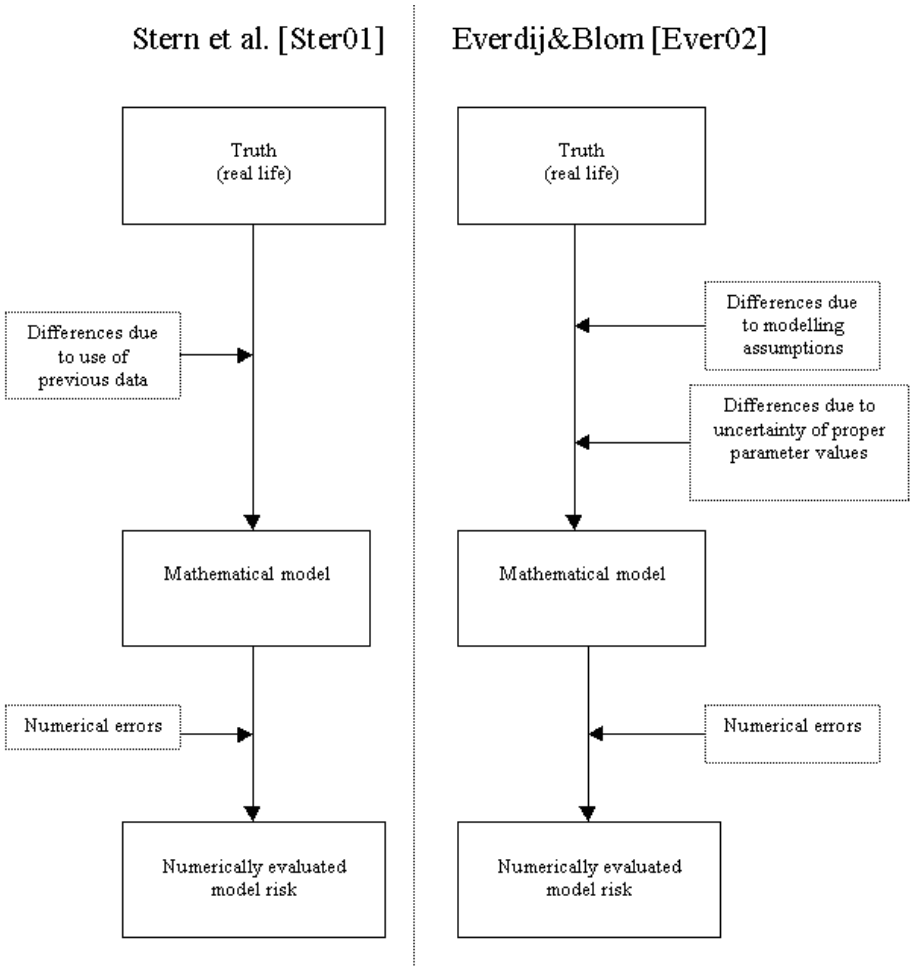

Figure 1.1: Different type of uncertainties that are analyzed by the uncertainty analysis approaches of Stern et al.[Ster01] and Everdij&Blom[Ever02]

deal with mathematical tools for uncertainty analysis. In Chapter 3, we will provide a problem description for this thesis and give a short description of the Everdij&Blom[Ever02] approach to uncertainty analysis. In Chapters 4 and 5 other methods of uncertainty analysis from the literature are discussed. Chapters 6 and 7 present the results of two simulations. Finally, in Chapter 8 conclusions that can be drawn from this final project are given along with some suggestions for efficient steps in performing uncertainty analysis and ideas for future research.

Chapter 2

Mathematical Theory of Incrossing Risk

In this chapter, we give a brief introduction to the mathematical theory of incrossing risk for a pair of aircraft, following [Bakk93]. We first consider the theory of the (first) hitting of an absorbing boundary by a Markov process. Since the characterization of (first) hitting is expressed in terms of a partial differential equation with boundary conditions, its numerical evaluation is too complex for the situation of many aircraft. In view of this, we next consider the incrossing of a transient boundary to evaluate the collision probability and the incrossing rate of a pair of aircraft. Finally, the relation between incrossing and collision risk is discussed.

2.1 Absorbing Boundary Approach

To evaluate the probability of a collision between a pair of aircraft, we assume their behaviour can be described by a stochastic differential equation for the joint state: (e.g $\xi_t = col\{\xi_t^1, \xi_t^2\}$ where ξ_t^i denotes the state of aircraft i at time t)

$$d\xi_t = f(\xi_t, t)dt + g(\xi_t, t)dw_t,\ \xi_t \in \mathbb{R}^N$$

where$\{w_t\}$ is a multi dimensional standard Brownian motion independent of ξ_0. Let the $\mathbb{R}^n$-valued separation process, $n < N$, satisfy

$$x_t = \mathfrak{s}(\xi_t),\ x_t \in \mathbb{R}^n \tag{2.1}$$

where $\mathfrak{s}$ is continuous mapping of $\mathbb{R}^N$ to $\mathbb{R}^n$.

Next we introduce the collision area of $\{x_t\}$ and $\{\xi_t\}$. Let $D{=}S^c$ denote the collision area of $\{x_t\}$ where $S \subset \mathbb{R}^n$ is some open set with boundary $\partial S \subset S^c$ and S^c is the complement of S. If $\mathbf{D}$ denotes the collision area of $\{\xi_t\}$ then it is obvious that $\mathbf{D} = \mathfrak{s}^{-1}(D)$.

Define the hitting time τ as

$$\tau \triangleq \inf_t \{t > 0; x_t \in D\}$$

where $\inf\{\} \triangleq \infty$. Then we also know that

$$\tau \triangleq \inf_t \{t > 0; \xi_t \in \mathbf{D}\}$$

The time τ is called the first hitting time of $\mathbf{D}$. The sets $\mathbf{D}^c$ and $\mathbf{D}$ are now referred to as the continuation and collision areas of $\{\xi_t\}$, respectively. Furthermore, define the absorbed process

$$\psi_t \triangleq \begin{cases} \xi_t \text{ if } t < \tau \\ \xi_\tau \text{ if } t \geq \tau \end{cases}$$

Notice that ξ_t can be called the transient boundary process. For clarity, Figure 2.1 illustrates one case of a transient boundary process ξ_t and the corresponding absorbed process ψ_t. We can see from the figure that the difference between these two processes is that after some time, i.e. τ, the absorbed process ψ_t enters the area $\mathbf{D}$ where it remains at the value ξ_τ while the transient process does not.

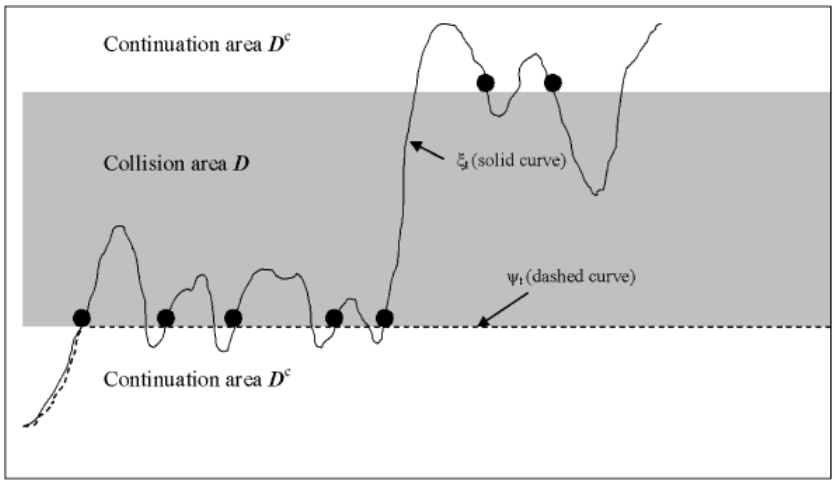

Figure 2.1: Transient and boundary absorption process (the black dots represent the points of in-crossing)

2.2 The Collision Rate

In this section we evaluate the probability of a collision between a pair of aircraft in a certain time period $(t_1, t_2]$ which corresponds to the probability of the

absorbed process having entered the collision area, following [Bakk93]. This can be written mathematically as follows:

$$P(\psi_{t_2} \in \mathbf{D}, \psi_{t_1} \in \mathbf{D}^c),\ t_2 \geq t_1 \geq 0$$

Hence, using the property of ψ_t, we have

$$\begin{aligned} P(\psi_{t_2} \in \mathbf{D}, \psi_{t_1} \in \mathbf{D}^c) =& P(\psi_{t_2} \in \mathbf{D}) - P(\psi_{t_2} \in \mathbf{D}, \psi_{t_1} \in \mathbf{D}) \\ =& P(\psi_{t_2} \in \mathbf{D}) - P(\psi_{t_1} \in \mathbf{D}) \end{aligned} \tag{2.2}$$

By further evaluation of equation (2.2) under the assumption that ξ_0 admits a density vanishing outside $\mathbf{D}$ and that $\frac{\partial P(\psi_t \in \mathbf{D} | \xi_0 = \xi)}{\partial t}$ exists, it can be shown [Bakk93] that

$$P(\psi_{t_2} \in \mathbf{D}, \psi_{t_1} \in \mathbf{D}^c) = \int_{t_1}^{t_2} \mu(t) dt \tag{2.3}$$

where $\mu(t)$ is called the collision rate at time t and is defined as:

$$\mu(t) \triangleq \int_D \frac{\partial P(\psi_t \in \mathbf{D} | \xi_0 = \xi)}{\partial t} p_{\xi_0}(\xi) d\xi \tag{2.4}$$

with $P(\psi_t \in \mathbf{D} | \xi_0 = \xi)$ satisfying a parabolic partial differential equation (PDE) with Dirichlet type boundary condition.

With the evaluation of equations (2.3) and (2.4), it is obvious that the complexity of a numerical evaluation of such a boundary valued PDE prohibits its application to the evaluation of probability of collision and collision rate between two aircraft. Hence, in order to avoid the boundary-valued PDE, the only alternative seems to be to extend the classical crossing theory for a transient boundary.

2.3 Transient Boundary Approach and the Generalized Reich Model

In this section, we evaluate the incrossing rate for the transient boundary situation following [Bakk93]. Let us go back to Figure 2.1. The incrossings of the transient boundary process ξ_t are represented by the black dots. From that figure, we see that incrossing can happen many times. We also notice that the absorbed process at time τ is the first incrossing.

We reconsider the separation process $\{x_t\}$ for aircraft which is given in equation (2.1). For the separation process $\{x_t\}$, every time a path enters D is called an incrossing. The incrossing rate represents the expected number of incrossings at time t per unit time and it is denoted by $\varphi(t)$. In [Bakk93] it is defined as:

$$\varphi(t) \triangleq \lim_{\Delta \downarrow 0} \frac{P(x_t \in D, x_{t-\Delta} \in D^c)}{\Delta} \tag{2.5}$$

assuming that the limit in equation (2.5) exists. In order for the incrossing rate to be well defined (see assumption A.1 below), [Bakk93] strictly assumes that $\{x_t\}$ has no Brownian motion component, i.e

$$dx_t = v_t dt \tag{2.6}$$

with $\{v_t\}$ is a right continuous stochastic process with left limit or càdlàg (continue à droite avec des limites à gauche). It is also assumed the separation process $\{x_t\}$ satisfies the following assumptions:

Assumption A.1

$$P(\{x_t \in D, (x_t - \Delta v_t) \in D^c, x_{t-\Delta} \in D\}) - P(\{x_t \in D^c, (x_t - \Delta v_t) \in D, x_{t-\Delta} \in D^c\}) = o(\Delta)$$

Assumption A.2

$$D = D_1 \times D_2 \times ... \times D_n$$

Assumption A.3

$$D_i = [-s_i, s_i],\ s_i > 0\ \forall i$$

Assumption A.4
For any i, t there is a constant L_i such that:

$$Ev_{i,t}^2 \leq L_i$$

$$E[v_{i,t}^2 | x_{i,t} = x_i] \leq L_i, \text{ for all } i,\ x_i \in [-s_i, s_i]$$

Assumption A.5
For any t, the pair (x_t, v_t) admits a density function $p_{x_t,v_t}(\cdot)$ such that for all $i \in \{1, 2, ..., n\}$:

$$(i) \int_{D^{i-1}} \int_{R^{i-1}} \prod_{j=1}^{i-1} 1_{[-s_j,s_j]}(x_j - \Delta v_j) \int_0^{2s_i/\Delta} \int_{-s_i}^{-s_i+\Delta v_i} p_{x_t,v_t}(x,v) dx_i dv_i d\widehat{v}_{i-1} d\widehat{x}_{i-1}$$

$$= \int_{D^{i-1}} \int_{R^{i-1}} \int_0^{2s_i/\Delta} \Delta v_i p_{x_t,v_t}(x_1, \ldots, -s_i, \ldots, x_n, v) dv_i d\widehat{v}_{i-1} d\widehat{x}_{i-1} + o(\triangle)$$

and

$$(ii) \int_{D^{i-1}} \int_{R^{i-1}} \prod_{j=1}^{i-1} 1_{[-s_j,s_j]}(x_j - \Delta v_j) \int_{-2s_i/\Delta}^{0} \int_{s_i+\Delta v_i}^{s_i} p_{x_t,v_t}(x,v) dx_i dv_i d\widehat{v}_{i-1} d\widehat{x}_{i-1}$$

$$= \int_{D^{i-1}} \int_{R^{i-1}} \int_{-2s_i/\Delta}^{0} -\Delta v_i p_{x_t,v_t}(x_1, \ldots, -s_i, \ldots, x_n, v) dv_i d\widehat{v}_{i-1} d\widehat{x}_{i-1} + o(\triangle)$$

where

$$\begin{aligned}\int\limits_{D^{i-1}}(\ldots)d\widehat{x}_{i-1} &= \int\limits_{-s_1}^{s_1}\ldots\int\limits_{-s_{i-1}}^{s_{i-1}}(\ldots)dx_{i-1}\ldots dx_1\\ \int\limits_{R^{i-1}}(\ldots)d\widehat{v}_{i-1} &= \int\limits_{-\infty}^{\infty}\ldots\int\limits_{-\infty}^{\infty}(\ldots)dv_{i-1}\ldots dv_1\end{aligned}$$

and

$$\lim_{\triangle\downarrow 0}\frac{o(\triangle)}{\triangle}=0$$

The dynamic model (2.6) in which v_t is càdlàg and the process $\{x_t, v_t\}$ satisfies assumptions A.1 through A.5 constitutes NLR's Generalized Reich model. Under all of the above assumptions the following Theorem holds (Theorem 1 in [Bakk93]):

Theorem 2.1 *Under assumptions A.1 through A.5 the incrossing rate satisfies*

$$\varphi(t)=\sum_{i=1}^{n}\int\limits_{\underline{D}_i}\left[\int\limits_0^{\infty}v_i p_{\underline{x}_{i,t},x_{i,t},v_{i,t}}(\underline{x}_i,-s_i,v_i)dv_i+\int\limits_{-\infty}^{0}-v_i p_{\underline{x}_{i,t},x_{i,t},v_{i,t}}(\underline{x}_i,s_i,v_i)dv_i\right]d\underline{x}_i$$

with $\underline{D}_i \triangleq D_1\times\ldots\times D_{i-1}\times D_{i+1}\times\ldots\times D_n$ *(*$\underline{D}_i=\{\}$ *if* $n=1$*)*
and $\underline{x}_i \triangleq (x_1,\ldots,x_{i-1},x_{i+1},\ldots,x_n)$.

If all assumptions are satisfied then Theorem 2.1 provides us with a nice formula to characterize the incrossing rate. The quantity that we are actually interested in is not the incrossing rate but rather the incrossing risk or the probability that an incrossing occurs in a certain time frame, say $[T_1,T_2]$, with $0\le T_1\le T_2$. Let us denote the probability of incrossing in $[T_1,T_2]$ by $\mathcal{R}_{[T_1,T_2]}$, then

$$\mathcal{R}_{[T_1,T_2]}=P(x_{T_2}\in D, x_{T_1}\in D^c)=\int\limits_{T_1}^{T_2}\varphi(t)dt$$

Note that $\mathcal{R}_{[T_1,T_2]}$ is a probability measure therefore it always satisfies the constraint:

$$0\le\mathcal{R}_{[T_1,T_2]}\le 1$$

Since the event of an incrossing is rare but not impossible, in practice we usually have that $0<\mathcal{R}_{[T_1,T_2]}<<1$. *In the following pages we will use the term incrossing risk to mean* $\mathcal{R}_{[\cdot,\cdot]}$ *on some specified interval.*

2.4 Relation Between Incrossing and Collision Risk

In reality a collision is the event of the first incrossing. Therefore the incrossing risk forms an upper bound for collision risk, i.e.

$$\text{Probability of collision in } [T_1, T_2] \leq \text{Probability of incrossing in } [T_1, T_2]$$

but this difference can be made arbitrarily small by appropriate modelling of the aircraft evolution[Blom02].

2.5 Contributions to the Generalized Reich Model

The remainder of this chapter presents some contributions to the Generalized Reich model, made as part of this study.

2.5.1 Sufficient Conditions for Assumption A.5 to Hold

Assumption A.1 in the previous section is an assumption made on the stochastic joint process $\{x_t, v_t\}$. It would probably be difficult to verify in practice, but at a glance it seems like a reasonably mild assumption. We will not try to derive sufficient conditions for Assumption A.1 here but it is an interesting question which should be given consideration in the near future. Assumptions A.2 to A.4 are clearly not restrictive, in fact the only assumption which is not intuitive and looks very complicated is Assumption A.5. A contribution of this work to the Generalized Reich model is in the derivation of sufficient conditions for $p_{x_t,v_t}(\cdot)$ under which Assumption A.5 is true. As we shall soon see, the sufficient conditions for A.5 are easy to understand and justifies the use of Theorem 2.1. For this purpose the following technical lemma is important:

Lemma 2.1 *Let $-\infty \leq a_k < b_k \leq \infty$ for $k = 1, \ldots, n$, and $x = (x_1, x_2, ..., x_n)$. Let H_i denote the set*

$$H_i = [a_1, b_1] \times \ldots \times [a_{i-1}, b_{i-1}] \times [\alpha_i - \epsilon, \alpha_i + \epsilon] \times [a_{i+1}, b_{i+1}] \times \ldots \times [a_n, b_n]$$

where $\alpha_i \in (a_i, b_i)$, ϵ is a small positive number and $[-\infty, \infty]$ is to be interpreted as $(-\infty, \infty)$. Suppose that $p : H_i \to \mathbb{R}$ is bounded on H_i and $p(\cdot)$ is continuous w.r.t. x_i at the points $\{x_i = \alpha_i\} \cap H_i$. Then there exists a function $O_i(\cdot) : [-\epsilon, \epsilon] \to [0, M]$ for some $M > 0$ with the following properties:
1. $|p(x_1, ..., x_{i-1}, \alpha_i + \Delta, x_{i+1}, ..., x_n) - p(x_1, ..., x_{i-1}, \alpha_i, x_{i+1}, ..., x_n)| \leq O_i(\Delta)$.
2. $O_i(\cdot)$ is a bounded, non-negative, even function that is non-decreasing in $[0, \epsilon]$.
3. $\lim_{\Delta \to 0} O_i(\Delta) = 0 = O_i(0)$.

Proof. The proof is by construction. Since p is bounded $\exists M > 0$ such that

$$|p(x_1, ..., x_{i-1}, \alpha_i + \Delta, x_{i+1}, ..., x_n) - p(x_1, ..., x_{i-1}, \alpha_i, x_{i+1}, ..., x_n)| \leq M$$

on H_i. Let $\underline{x}_i = (x_1, ..., x_{i-1}, x_{i+1}, ..., x_n)$ and keep it fixed for the time being. By the definition of continuity w.r.t. x_i at $x = (x_1, ..., x_{i-1}, \alpha_i, x_{i+1}, ..., x_n)$, for every $\varepsilon > 0$ there exists $\delta > 0$ depending on ε and the value taken by $\underline{x}_i$ such that

$$|p(x_1, ..., x_{i-1}, \alpha_i + \Delta, x_{i+1}, ..., x_n) - p(x_1, ..., x_{i-1}, \alpha_i, x_{i+1}, ..., x_n)| < \varepsilon$$

if $|\Delta| < \delta$.
Define the sequence $\{\varepsilon_k,\ k = 1, 2, ...\}$ where $\varepsilon_k = \frac{M}{2^{k-1}}$. Note that $\varepsilon_{k+1} < \varepsilon_k$. Since $\varepsilon_1 = M$ we may trivially set $\delta_1 = \epsilon$ and then in a sequential manner for $k = 2, 3, ...$ we can choose $\delta_k > 0$ such that

$$|p(x_1, ..., x_{i-1}, \alpha_i + \Delta, x_{i+1}, ..., x_n) - p(x_1, ..., x_{i-1}, \alpha_i, x_{i+1}, ..., x_n)| < \varepsilon_k$$

for $|\Delta| < \delta_k$ with $\lim_{k\to\infty} \delta_k = 0$ and $\delta_k < \delta_{k-1}$ (this is always possible since by definition we can always find $\delta_k \leq \delta_{k-1}$ if $\varepsilon_k < \varepsilon_{k-1}$. In the case $\delta_k = \delta_{k-1}$ then simply choose $\delta_k^{'} = \delta_{k-1} - h$ where $0 < h << \delta_{k-1}$ and then set $\delta_k = \delta_k^{'}$).

Define the set $\underline{H}_i$ as

$$\underline{H}_i = [a_1, b_1] \times \ldots \times [a_{i-1}, b_{i-1}] \times [a_{i+1}, b_{i+1}] \times \ldots \times [a_n, b_n]$$

and define the function

$$\widetilde{O}_i(\Delta; \underline{x}_i) = \begin{cases} 0 \text{ if } \Delta = 0 \\ \varepsilon_k \text{ if } \delta_{k+1} \leq |\Delta| < \delta_k,\ k = 1, 2, ... \\ M \text{ if } |\Delta| = \epsilon \end{cases}$$

on $[-\epsilon, \epsilon] \times \underline{H}_i$. Bear in mind that the $\delta_k's$ depend on $\underline{x}_i$. Hence we may write

$$|p(x_1, ..., x_{i-1}, \alpha_i + \Delta, x_{i+1}, ..., x_n) - p(x_1, ..., x_{i-1}, \alpha_i, x_{i+1}, ..., x_n)| \leq \widetilde{O}_i(\Delta; \underline{x}_i)$$

Since $\widetilde{O}_i(\Delta; \underline{x}_i)$ is a bounded function of $\underline{x}_i$ on $\underline{H}_i$ for any fixed value of Δ, $\sup_{\underline{H}_i} \widetilde{O}_i(\Delta; \underline{x}_i)$ exists for each Δ (note that if $\underline{H}_i$ is compact then $\sup_{\underline{H}_i} \widetilde{O}_i(\Delta; \underline{x}_i) = \max_{\underline{H}_i} \widetilde{O}_i(\Delta; \underline{x}_i)$). Now define the function

$$O_i(\Delta) = \sup_{\underline{H}_i} \widetilde{O}_i(\Delta; \underline{x}_i)$$

in particular $O_i(0) = \sup_{\underline{H}_i} \widetilde{O}_i(0; \underline{x}_i) = \sup_{\underline{H}_i} 0 = 0$. We may now write

$$|p(x_1, ..., x_{i-1}, \alpha_i + \Delta, x_{i+1}, ..., x_n) - p(x_1, ..., x_{i-1}, \alpha_i, x_{i+1}, ..., x_n)| \leq O_i(\Delta)$$

on H_i and by construction $O_i(\Delta)$ has properties 1, 2 and 3. ■

The following lemma provides sufficient conditions under which Assumption A.5 holds true:

Lemma 2.2 *Let $(x,v) \in \mathbb{R}^n \times \mathbb{R}^n$ where $x = (x_1, x_2, ..., x_n)$ and $v = (v_1, v_2, ..., v_n)$. For $i = 1, 2, ..., n$ let W_i^+ and $W_i^- \subset \mathbb{R}^n \times \mathbb{R}^n$ denote the sets*
$W_i^+ = \left[\overset{i-1}{\underset{j=1}{\otimes}}[-s_j, s_j]\right] \times [s_i - \epsilon_i, s_i + \epsilon_i] \times \left[\overset{n}{\underset{j=i+1}{\otimes}}(-\infty, \infty)\right] \times \left[\overset{n}{\underset{j=1}{\otimes}}(-\infty, \infty)\right]$
and
$W_i^- = \left[\overset{i-1}{\underset{j=1}{\otimes}}[-s_j, s_j]\right] \times [-s_i - \epsilon_i, -s_i + \epsilon_i] \times \left[\overset{n}{\underset{j=i+1}{\otimes}}(-\infty, \infty)\right] \times \left[\overset{n}{\underset{j=1}{\otimes}}(-\infty, \infty)\right]$
where $0 < \epsilon_i < s_i$.
Then assumption A.5 holds true if for all $i \in \{1, 2, .., n\}$ there exists $M_i > 0$ such that $p_{x_t,v_t}(x,v) = 0$ if $|v_i| > M_i$ (in other words $p_{x_t,v_t}(\cdot)$ has compact support in the $v_i's$) and there exists a choice of $\epsilon_1, \epsilon_2, ..., \epsilon_n$ such that
1. $p_{x_t,v_t}(\cdot)$ is bounded on W_i^+ and W_i^- for $i = 1, 2, ..., n$.
2. For each i, $p_{x_t,v_t}(x_1, ..., x_i, ..., x_n, v)$ is continuous w.r.t. the argument x_i at the points
$\{x_i = s_i\} \cap W_i^+$ and $\{x_i = -s_i\} \cap W_i^-$.

Proof. We will show the result for part (i) of Assumption A.5, the proof for part (ii) is similar. Furthermore, recall that $\Delta > 0$ ($\Delta \downarrow 0$) by the definition of incrossing rate.

We introduce the following notation:

$$\int\limits_{M^{j-1}} (\ldots) d\widehat{v}_{j-1} = \int\limits_{-M_1}^{M_1} \cdots \int\limits_{-M_{j-1}}^{M_{j-1}} (\ldots) dv_{j-1} \ldots dv_1$$

The proof follows four steps.
Step 1 Suppose that we have a plausible choice of $\epsilon_1, \epsilon_2, ..., \epsilon_n$. Let us choose real positive numbers Δ_k such that $\frac{\epsilon_k}{\Delta_k} \geq M_k$ for $k = 1, 2, ..., n$. For the following analysis let us take a fixed $i \in \{1, 2, ..., n\}$. By choosing Δ such that $0 < \Delta < \min\{\Delta_k\}$ we obtain

$$\int\limits_0^{2s_i/\Delta} \int\limits_{-s_i}^{-s_i+\Delta v_i} p_{x_t,v_t}(x,v) dx_i dv_i = \int\limits_0^{M_i} \int\limits_{-s_i}^{-s_i+\Delta v_i} p_{x_t,v_t}(x,v) dx_i dv_i$$

We write

$$p_{x_t,v_t}(x,v) = p_{x_t,v_t}(x_1, ..., -s_i + x_i + s_i, ..., x_n, v)$$

By virtue of our choice of Δ we also have $(x,v) \in W_i^-$ in the domain of integration and due to the hypothesis on $p_{x_t,v_t}(\cdot)$ by Lemma 2.1 we have that

$$\left| p_{x_t,v_t}(x,v) - p_{x_t,v_t}(x_1, ..., -s_i, ..., x_n, v) \right| \leq O_i(x_i + s_i) \leq O_i(\Delta v_i)$$

for some function $O_i(\cdot)$ having the properties stated in the lemma. In particular,

$$p_{x_t,v_t}(x,v) \leq p_{x_t,v_t}(x_1, \ldots, -s_i, \ldots, x_n, v) + O_i(\Delta v_i)$$

Since $v_i \in [0, M_i]$ it follows that $|\Delta v_i| \leq |\Delta M_i|$ and

$$p_{x_t,v_t}(x,v) \leq p_{x_t,v_t}(x_1,\ldots,-s_i,\ldots,x_n,v) + O_i(\Delta M_i)$$

Thus

$$\begin{aligned}\int_0^{M_i}\int_{-s_i}^{-s_i+\Delta v_i} p_{x_t,v_t}(x,v)dx_i dv_i &\leq \int_0^{M_i}\int_{-s_i}^{-s_i+\Delta v_i} \left[p_{x_t,v_t}(x_1,\ldots,-s_i,\ldots,x_n,v) + O_i(\Delta M_i)\right] dx_i dv_i \\ &= \int_0^{M_i} [p_{x_t,v_t}(x_1,\ldots,-s_i,\ldots,x_n,v) + O_i(\Delta M_i)]\Delta v_i dv_i \\ &= \int_0^{M_i} p_{x_t,v_t}(x_1,\ldots,-s_i,\ldots,x_n,v)\Delta v_i dv_i + \frac{1}{2}O_i(\Delta M_i)\Delta M_i^2\end{aligned}$$

In a similar fashion we can also show that

$$\int_0^{2s_i/\Delta}\int_{-s_i}^{-s_i+\Delta v_i} p_{x_t,v_t}(x,v)dx_i dv_i \geq \int_0^{M_i} p_{x_t,v_t}(x_1,\ldots,-s_i,\ldots,x_n,v)\Delta v_i dv_i - \frac{1}{2}O_i(\Delta M_i)\Delta M_i^2$$

hence

$$\begin{aligned}&\left| \int_{D^{i-1}}\int_{M^{i-1}} \prod_{j=1}^{i-1} 1_{[-s_j,s_j]}(x_j - \Delta v_j) \int_0^{2s_i/\Delta}\int_{-s_i}^{-s_i+\Delta v_i} p_{x_t,v_t}(x,v)dx_i dv_i d\widehat{v}_{i-1} d\widehat{x}_{i-1} \right. \\ &\left. - \int_{D^{i-1}}\int_{M^{i-1}} \prod_{j=1}^{i-1} 1_{[-s_j,s_j]}(x_j - \Delta v_j) \int_0^{M_i} p_{x_t,v_t}(x_1,\ldots,-s_i,\ldots,x_n,v)\Delta v_i dv_i d\widehat{v}_{i-1} d\widehat{x}_{i-1} \right| \\ &\leq \int_{D^{i-1}}\int_{M^{i-1}} \prod_{j=1}^{i-1} 1_{[-s_j,s_j]}(x_j - \Delta v_j)\frac{1}{2}O_i(\Delta M_i)\Delta M_i^2 d\widehat{v}_{i-1} d\widehat{x}_{i-1}\end{aligned}$$

Step 2 Observe that

$$\begin{aligned}&\int_{D^{i-1}}\int_{M^{i-1}} \prod_{j=1}^{i-1} \mathbf{1}_{[-s_j,s_j]}(x_j - \Delta v_j)\frac{1}{2}O_i(\Delta M_i)\Delta M_i^2 d\widehat{v}_{i-1} d\widehat{x}_{i-1} \\ &= \frac{1}{2}O_i(\Delta M_i)\Delta M_i^2 \prod_{j=1}^{i-1} \left[\int_{-s_j}^{s_j}\int_{-M_j}^{M_j} \mathbf{1}_{[-s_j,s_j]}(x_j - \Delta v_j) dv_j dx_j \right] \\ &= \frac{1}{2}O_i(\Delta M_i)\Delta M_i^2 K\end{aligned}$$

for some $0 < K < \infty$.

Hence, since

$$\begin{aligned}\lim_{\Delta\downarrow 0}\frac{1}{\Delta}\frac{1}{2}O_i(\Delta M_i)\Delta M_i^2 K \\ = \lim_{\Delta\downarrow 0}\frac{1}{2}O_i(\Delta M_i)M_i^2 K \\ = 0\end{aligned}$$

we have

$$\begin{aligned}&\int_{D^{i-1}}\int_{R^{i-1}}\prod_{j=1}^{i-1}1_{[-s_j,s_j]}(x_j-\Delta v_j)\int_0^{2s_i/\Delta}\int_{-s_i}^{-s_i+\Delta v_i}p_{x_t,v_t}(x,v)dx_i dv_i d\widehat{v}_{i-1}d\widehat{x}_{i-1} \\ &= \int_{D^{i-1}}\int_{R^{i-1}}\prod_{j=1}^{i-1}1_{[-s_j,s_j]}(x_j-\Delta v_j)\int_0^{2s_i/\Delta}\Delta v_i p_{x_t,v_t}(x_1,\ldots,-s_i,\ldots,x_n,v)dv_i d\widehat{v}_{i-1}d\widehat{x}_{i-1}+o_i(\Delta) \\ &= \int_{D^{i-1}}\int_{R^{i-1}}\prod_{j=1}^{i-1}1_{[-s_j,s_j]}(x_j-\Delta v_j)\int_0^{M_i}\Delta v_i p_{x_t,v_t}(x_1,\ldots,-s_i,\ldots,x_n,v) \\ &\qquad dv_i d\widehat{v}_{i-1}d\widehat{x}_{i-1}+o_i(\Delta) \quad (2.7)\end{aligned}$$

where

$$\lim_{\Delta\downarrow 0}\frac{o_i(\Delta)}{\Delta}=0$$

Step 3 Let $\underline{x}_i=(x_1,\ldots,x_{i-1},x_{i+1},\ldots,x_n)$ and $\underline{v}_i=(v_1,\ldots,v_{i-1},v_{i+1},\ldots,v_n)$ and define $g_i(\underline{x}_i,\underline{v}_i)=\int_0^{M_i}\Delta v_i p_{x_t,v_t}(x_1,\ldots,-s_i,\ldots,x_n,v)dv_i$. This integral exists since v_i is bounded and since $p_{x_t,v_t}(x_1,\ldots,-s_i,\ldots,x_n,v)$ is also bounded

by hypothesis. Let k be an integer, $1 \leq k \leq i-1$. We then have the following:

$$\begin{aligned}
&\int_{-s_k}^{s_k}\int_{-\infty}^{\infty} \mathbf{1}_{[-s_k,s_k]}(x_k-\Delta v_k)g_i(\underline{x}_i,\underline{v}_i)dv_k dx_k \\
&= \int_{-\infty}^{\infty}\int_{-s_k}^{s_k} \mathbf{1}_{[-s_k,s_k]}(x_k-\Delta v_k)g_i(\underline{x}_i,\underline{v}_i)dx_k dv_k \\
&= \int_{-M_k}^{M_k}\int_{-s_k}^{s_k} \mathbf{1}_{[-s_k,s_k]}(x_k-\Delta v_k)g_i(\underline{x}_i,\underline{v}_i)dx_k dv_k \\
&= \int_{-M_k}^{0}\int_{-s_k}^{s_k+\Delta v_k} g_i(\underline{x}_i,\underline{v}_i)dx_k dv_k + \int_{0}^{M_k}\int_{-s_k+\Delta v_k}^{s_k} g_i(\underline{x}_i,\underline{v}_i)dx_k dv_k \\
&= \int_{-M_k}^{0}\left[\int_{-s_k}^{s_k} g_i(\underline{x}_i,\underline{v}_i) + \int_{s_k}^{s_k+\Delta v_k} g_i(\underline{x}_i,\underline{v}_i)\right]dx_k dv_k \\
&\quad + \int_{0}^{M_k}\left[\int_{-s_k}^{s_k} g_i(\underline{x}_i,\underline{v}_i) - \int_{-s_k}^{-s_k+\Delta v_k} g_i(\underline{x}_i,\underline{v}_i)\right]dx_k dv_k \\
&= \int_{-M_k}^{0}\int_{-s_k}^{s_k} g_i(\underline{x}_i,\underline{v}_i)dx_k dv_k + \int_{0}^{M_k}\int_{-s_k}^{s_k} g_i(\underline{x}_i,\underline{v}_i)dx_k dv_k \\
&+ \int_{-M_k}^{0}\int_{s_k}^{s_k+\Delta v_k} g_i(\underline{x}_i,\underline{v}_i)dx_k dv_k - \int_{0}^{M_k}\int_{-s_k}^{-s_k+\Delta v_k} g_i(\underline{x}_i,\underline{v}_i)dx_k dv_k \\
&= \int_{-s_k}^{s_k}\int_{-M_k}^{M_k} g_i(\underline{x}_i,\underline{v}_i)dv_k dx_k + \int_{-M_k}^{0}\int_{s_k}^{s_k+\Delta v_k} g_i(\underline{x}_i,\underline{v}_i)dx_k dv \\
&\quad - \int_{0}^{M_k}\int_{-s_k}^{-s_k+\Delta v_k} g_i(\underline{x}_i,\underline{v}_i)dx_k dv_k
\end{aligned}$$

We note that

$$0 \leq \int_{s_k}^{s_k+\Delta v_k} \overbrace{\int_0^{M_i} \Delta v_i p_{x_t,v_t}(..., x_k, ..., -s_i, ..., v) dv_i dx_k}^{g_i(\underline{x}_i, \underline{v}_i)}$$

$$= \int_{s_k}^{s_k+\Delta v_k} \int_0^{M_i} \Delta v_i p_{x_t,v_t}(..., s_k + x_k - s_k, ..., -s_i, ..., v) dv_i dx_k$$

$$\overset{\text{Lemma 2.1}}{\leq} \int_{s_k}^{s_k+\Delta v_k} \int_0^{M_i} \Delta v_i [p_{x_t,v_t}(..., s_k, ..., -s_i, ..., v) + O_k(x_k - s_k)] dv_i dx_k$$

$$\leq \int_{s_k}^{s_k+\Delta v_k} \int_0^{M_i} \Delta v_i [p_{x_t,v_t}(..., s_k, ..., -s_i, ..., v) + O_k(\Delta v_k)] dv_i dx_k$$

$$\overset{v_k \in [-M_k, 0]}{\leq} \int_{s_k}^{s_k+\Delta v_k} \int_0^{M_i} \Delta v_i [p_{x_t,v_t}(..., s_k, ..., -s_i, ..., v) + O_k(\Delta M_k)] dv_i dx_k$$

$$= \Delta v_k \int_0^{M_i} \Delta v_i p_{x_t,v_t}(..., s_k, ..., -s_i, ..., v) dv_i + \frac{1}{2}(M_i)^2 O_k(\Delta M_k) \Delta^2 v_k \quad (2.8)$$

where $O_k(\cdot)$ is some function having the properties stated in Lemma 2.1. Now, using (2.8) and since $p_{x_t,v_t}(\cdot)$ is bounded, it is not hard to verify that

$$\lim_{\Delta \downarrow 0} \frac{1}{\Delta} \int_{-M_k}^{0} \int_{s_k}^{s_k+\Delta v_k} g_i(\underline{x}_i, \underline{v}_i) dx_k dv_k = 0 \quad (2.9)$$

Similarly we also have

$$\lim_{\Delta \downarrow 0} \frac{1}{\Delta} \int_{0}^{M_k} \int_{-s_k}^{-s_k+\Delta v_k} g_i(\underline{x}_i, \underline{v}_i) dx_k dv_k = 0 \quad (2.10)$$

Hence using (2.9) and (2.10) we get:

$$\int_{-s_k}^{s_k} \int_{-\infty}^{\infty} \mathbf{1}_{[-s_k, s_k]}(x_k - \Delta v_k) g_i(\underline{x}_i, \underline{v}_i) dv_k dx_k$$

$$= \int_{-s_k}^{s_k} \int_{-M_k}^{M_k} g_i(\underline{x}_i, \underline{v}_i) dv_k dx_k + o_k(\Delta) \quad (2.11)$$

$$= \int_{-s_k}^{s_k} \int_{-\infty}^{\infty} g_i(\underline{x}_i, \underline{v}_i) dv_k dx_k + o_k(\Delta)$$

where $o_k(\Delta)$ has the property $\lim_{\triangle \downarrow 0} \frac{o_k(\Delta)}{\Delta}$.

Step 4 Recall from (2.7) that

$$\int_{D^{i-1}} \int_{R^{i-1}} \prod_{j=1}^{i-1} 1_{[-s_j,s_j]}(x_j - \Delta v_j) \int_0^{2s_i/\Delta} \int_{-s_i}^{-s_i+\Delta v_i} p_{x_t,v_t}(x,v) dx_i dv_i d\widehat{v}_{i-1} d\widehat{x}_{i-1}$$

$$= \int_{D^{i-1}} \int_{R^{i-1}} \prod_{j=1}^{i-1} 1_{[-s_j,s_j]}(x_j - \Delta v_j) \int_0^{M_i} \Delta v_i p_{x_t,v_t}(x_1,\ldots,-s_i,\ldots,x_n,v) dv_i d\widehat{v}_{i-1} d\widehat{x}_{i-1} + o_i(\Delta)$$

$$= \int_{D^{i-1}} \int_{M^{i-1}} \prod_{j=1}^{i-1} 1_{[-s_j,s_j]}(x_j - \Delta v_j) \underbrace{\int_0^{M_i} \Delta v_i p_{x_t,v_t}(x_1,\ldots,-s_i,\ldots,x_n,v) dv_i}_{g_i(\underline{x}_i,\underline{v}_i)} d\widehat{v}_{i-1} d\widehat{x}_{i-1}$$

$$+ o_i(\Delta) \quad (2.12)$$

Substituting (2.11) into (2.12) consecutively for $k = i-1, i-2, ..., 1$ gives

$$\int_{D^{i-1}} \int_{R^{i-1}} \prod_{j=1}^{i-1} 1_{[-s_j,s_j]}(x_j - \Delta v_j) \int_0^{2s_i/\Delta} \int_{-s_i}^{-s_i+\Delta v_i} p_{x_t,v_t}(x,v) dx_i dv_i d\widehat{v}_{i-1} d\widehat{x}_{i-1}$$

$$= \int_{D^{i-1}} \int_{M^{i-1}} \left(\int_0^{M_i} \Delta v_i p_{x_t,v_t}(x,v) dx_i dv_i d\widehat{v}_{i-1} d\widehat{x}_{i-1} + \sum_{k=1}^{i-1} o_k(\Delta) \right) d\widehat{v}_{i-1} d\widehat{x}_{i-1} + o_i(\Delta)$$

$$= \int_{D^{i-1}} \int_{M^{i-1}} \int_0^{M_i} \Delta v_i p_{x_t,v_t}(x,v) dx_i dv_i d\widehat{v}_{i-1} d\widehat{x}_{i-1} + \int_{D^{i-1}} \int_{M^{i-1}} \left(\sum_{k=1}^{i-1} o_k(\Delta) \right) d\widehat{v}_{i-1} d\widehat{x}_{i-1} + o_i(\Delta)$$

$$= \int_{D^{i-1}} \int_{R^{i-1}} \int_0^{2s_i/\Delta} \Delta v_i p_{x_t,v_t}(x,v) dx_i dv_i d\widehat{v}_{i-1} d\widehat{x}_{i-1} + \left(\sum_{k=1}^{i-1} o_k(\Delta) \right) \int_{D^{i-1}} \int_{M^{i-1}} d\widehat{v}_{i-1} d\widehat{x}_{i-1} + o_i(\Delta)$$

$$= \int_{D^{i-1}} \int_{R^{i-1}} \int_0^{2s_i/\Delta} \Delta v_i p_{x_t,v_t}(x,v) dx_i dv_i d\widehat{v}_{i-1} d\widehat{x}_{i-1} + o(\Delta)$$

where

$$o(\Delta) = \left(\sum_{k=1}^{i-1} o_k(\Delta) \right) \int_{D^{i-1}} \int_{M^{i-1}} d\widehat{v}_{i-1} d\widehat{x}_{i-1} + o_i(\Delta)$$

Since

$$\int_{D^{i-1}} \int_{M^{i-1}} d\widehat{v}_{i-1} d\widehat{x}_{i-1} < \infty$$

$$\lim_{\Delta \downarrow 0} \frac{o_k(\Delta)}{\Delta} = 0 \text{ for } k = 1, 2, ..., i-1$$

$$\lim_{\Delta \downarrow 0} \frac{o_i(\Delta)}{\Delta} = 0$$

it follows that

$$\lim_{\Delta \downarrow 0} \frac{o(\Delta)}{\Delta} = 0$$

■

2.5.2 Implications of the Sufficient Conditions

In reality every joint density function of the position and velocity should have compact support in the $v_i's$ since the velocity range of any aircraft is always limited. However, in practice $p_{x_t,v_t}(\cdot)$ is usually fitted with some well known continuous distribution such as a multivariate Gaussian distribution or a Gaussian mixture which is continuous everywhere but does not have compact support in the $v_i's$. Therefore based on Lemma 2.2 we do not know whether the fitted distribution satisfies assumption A.5. Fortunately we do know that its value decreases to zero rapidly at points sufficiently far away from the mean. To be able to use Lemma 2.2 we simply assume that the fitted density function has values very close to the actual distribution for $\{|v_i| \leq M_i,\ i = 1, \ldots, n\}$ and then use it in Theorem 2.1 to obtain $\varphi(t)$ approximately. The approximation should be quite close to the true value of $\varphi(t)$. Note that this technique not only applies to multivariate Gaussian distributions but also to other well known distributions that go to zero fast enough for large values of $\{|v_i|\}$ and is close to the actual density function within the actual function's support.

From the previous discussion we see that Theorem 2.1 can be applied to a rather general class of density functions (e.g. is continuous and decreases to zero fast for large values of the velocity components) although it gives only an approximation of the value of the actual incrossing rate. However it is reasonable to expect that the value of the approximation will be close to the real value.

Chapter 3

Uncertainty Analysis of Model-Based Accident Risk

3.1 Background

As we had already discussed in the introduction, an accident risk model is very complex and is usually dependent on a large number of parameters (for an example of a mildly complex accident risk model see [Ever02]). Let us view the accident risk model as a system (with many interrelated components) and let us call the aforementioned parameters as system parameters. In general the values of these parameters are not precisely known; in one approach uncertainty is introduced by modelling each system parameter as a random variable[Ever02]. This kind of approach has also been taken by some researchers in chemical engineering (for example see [Isuk99] and [Webs96]). We can view accident risk, or incrossing risk (for example the probability of incrossing between two aircraft in a certain time frame) as the output of our system and the system parameters as inputs, see Figure 3.1.

Although the dynamics of the accident risk model are represented by a set of simultaneous mathematical equations, it is not always feasible to solve them analytically. Even for simple operations such a solution of the mathematical equations may not be obtainable. Therefore to evaluate the incrossing risk, Monte Carlo simulations of the model are executed and the value of the incrossing risk is numerically approximated. Consequently we might not have available an explicit functional relationship between incrossing risk and the parameters. In this case we may consider our model as a *black box*. In the sections to follow we will formalize some notations that will be used throughout the remaining parts of this document and give a concise description of the problem.

Next, we give an outline and some limitations of the approach developed in [Ever02] to accident risk uncertainty analysis. Finally, we make some contributions to this approach by developing some additional derivations.

3.2 Notations and Symbols

During the development of any model, usually several model assumptions are adopted. Let's say that we have n_a (n_a is a positive integer) possible assumptions which we may decide to keep or discard in our model. Following the notation in [Ever02], let b_i, $i = 1, ..., n_a$ be Boolean variables, i.e. $b_i = 0$ or 1 and let $B = (b_1, b_2, ..., b_{n_a})$. The $b_i's$ are to be interpreted as follows: if $b_i = 1$ then we are using assumption i in our model, on the other hand if $b_i = 0$ it means we are not using assumption i. If we take all assumptions to be true then $B = (1, 1, ..., 1)$. For short hand we will write $(1, 1, ..., 1)$ as $\mathbf{1}$. Let us also say that our model has n_p parameters which we represent by random variables denoted as $V_1, V_2, ..., V_{n_p}$ and let $V = (V_1, V_2, ..., V_{n_p})$.

The time interval that will be of interest to us here is $[0, \infty)$. For a particular ATM scenario, the incrossing risk value will depend on how we model the operation (B) and on the particular setting of the parameters (V)[Ever02], hence $\mathcal{R}_{[0,\infty)}$ is a function of B and V. For convenience we shall write $\mathcal{R}_{[0,\infty)}$ as $\mathcal{R}$. We will also adopt the convention that $\mathcal{R} = \rho(B, V)$ for some function $\rho(\cdot, \cdot)$. In this report we will only consider the case where all modelling assumptions hold true, i.e. $\mathcal{R} = \rho(\mathbf{1}, V)$. The case for general B, i.e. where uncertainty due to modelling assumptions are taken into account, is covered in [Ever02]. *Hereinafter $\rho(\mathbf{1}, V)$ will sometimes be written as $\rho(V)$ where it will not cause confusion.*

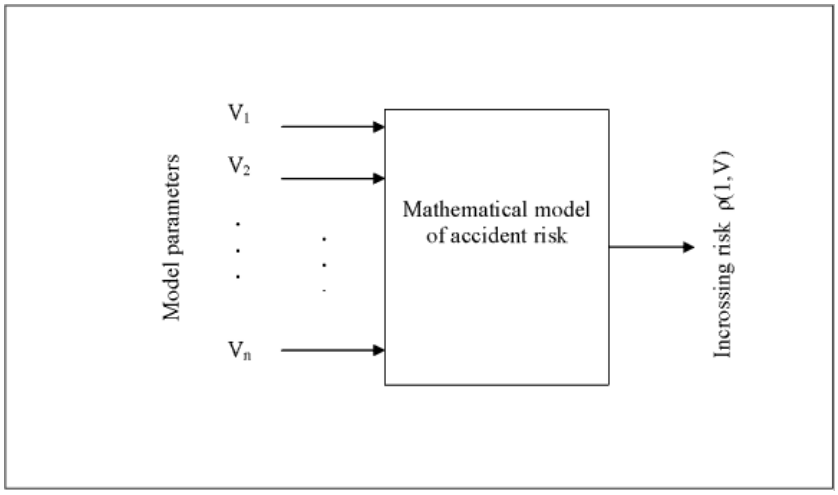

Figure 3.1: View of accident risk assessment as a black box

We will also need the following definition:

Definition 3.1 (Credibility Interval) *For $0 < \alpha < 1$ and a random variable X, an interval $[a, b]$, $b > a$, is called the $(1-\alpha) \times 100\%$ credibility interval (CrI)*

of X if a is the smallest real number such that $P(X < a) = \alpha/2$ and b is the largest real number such that $P(X > b) = \alpha/2$.

3.3 Statement of the Problem

Since $\rho(V)$ takes on very small values (near zero because collision is a rare event) and since $\rho(V)$ can change in orders of magnitude for small changes in some of the parameters (which we shall see later in Chapter 6), it is more suitable to express $\rho(V)$ as $\rho(V) = e^{g(V)}$ for some unknown function $g(\cdot)$. For this reason it will be more convenient for us to work with $g(V) = \ln \rho(V)$ instead of directly with $\rho(V)$. The problem that is to be considered during the execution of the final project is the following:

> Determine suitable methods to estimate the statistical properties of the random variable $\ln \rho(V)$, particularly the mean and 95% credibility interval, based on only a limited number of simulation runs (i.e. with only a small sample of $\ln \rho(V)$ available).

Note that out of these statistical properties the most important quantity seems to be the upper bound of the 95% CrI since it indicates how high $\ln \rho(V)$ can become 95% of the time under the prescribed uncertainty. If $[A, B]$ is the 95% CrI of $\ln \rho(V)$ then trivially the 95% CrI of $\rho(V)$ is $[e^A, e^B]$.

We should keep in mind that we also have *apriori* information about the problem at hand, i.e. in real scenarios we have

$$0 < \rho(V) < 1 \Leftrightarrow -\infty < \ln \rho(V) < 0$$

3.4 Everdij&Blom's Approach to Accident Risk Uncertainty Analysis

Everdij and Blom[Ever02] have developed an initial method to assess the bias and uncertainty in model based accident risk, due to bias and uncertainty in assumptions adopted and parameter values adopted. During the development of this method, several bias and uncertainty model assumptions are adopted, which are discussed on interpretation and practical use. We will now briefly review this method, restricting to the bias and uncertainty due to parameter value uncertainty.

3.4.1 Definitions and Assumptions

Let the nominal value for the parameters be $V_i = v_i$, $i = 1, 2, ..., n_p$ and $v = (v_1, v_2, ..., v_{n_p})$. Throughout this section we will assume that there is a basic probability space $(\Omega, \mathcal{F}, P)$ to which the stochastic variables $V_1, V_2, ..., V_{n_p}$

representing the parameters are measurable. Define the following:

$$\varphi_i(x_i) = \frac{\rho(\mathbf{1}, (v_1, \ldots, v_{i-1}, x_i, v_{i+1}, ..., v_{n_p}))}{\rho(\mathbf{1}, (v_1, \ldots, v_{i-1}, v_i, v_{i+1}, ..., v_{n_p}))}$$

$$\varphi_i'(x_i, x_{i+1}, \ldots, x_{n_p}) = \frac{\rho(\mathbf{1}, (v_1, \ldots, v_{i-1}, x_i, x_{i+1}, ..., x_{n_p}))}{\rho(\mathbf{1}, (v_1, \ldots, v_{i-1}, v_i, x_{i+1}, ..., x_{n_p}))}$$

$$\begin{aligned} H_i &= \ln \varphi_i(V_i) \\ \gamma_i &= E\{H_i\} \\ \theta_i^2 &= E\{(H_i - \gamma_i)^2\} \\ \omega_i^3 &= E\{|H_i - \gamma_i|^3\} \\ \Gamma &= \sum_{i=1}^{n_p} \gamma_i \\ \Theta^2 &= \sum_{i=1}^{n_p} \theta_i^2 \\ \Omega^3 &= \sum_{i=1}^{n_p} \omega_i^3 \end{aligned}$$

NLR's approach begins with the following assumptions:

Bias and Uncertainty Model Assumption 1
$V_1, V_2, \ldots, V_{n_p}$ are mutually independent.

Bias and Uncertainty Model Assumption 2
For any $i = 1, \ldots, n_p$ and $x_i, x_{i+1}, \ldots, x_{n_p}$, $\varphi_i'(x_i, x_{i+1}, \ldots, x_{n_p}) = \varphi_i(x_i)$

Bias and Uncertainty Model Assumption 3
For each $i = 1, 2, ..., n_p$ the expectation and variance of $\ln V_i$ exist and satisfy: $E\{\ln V_i\} = \mu_i$ and $Var\{\ln V_i\} = \sigma_i^2$.

Bias and Uncertainty Model Assumption 4
Each $V_i, i = 1, 2, ..., n_p$ is lognormally distributed.

Bias and Uncertainty Model Assumption 5
Each $\varphi_i(V_i), i = 1, 2, ..., n_p$ is lognormally distributed with parameters γ_i and θ_i^2. Notation: $\varphi_i(V_i) \sim \Lambda(\gamma_i, \theta_i^2)$.

Bias and Uncertainty Model Assumption 6
The inverse of $\varphi_i(\cdot)$, denoted by $\varphi_i^{inv}(\cdot)$ exists.

Bias and Uncertainty Model Assumption 7
For $i = 1, 2, ..., n_p$, there exists β_i such that

- $E\{\ln \varphi_i(V_i)\} = \beta_i(E\{\ln(V_i)\} - \ln v_i)$
- $E\{(\ln \varphi_i(V_i) - E\{\ln \varphi_i(V_i)\})^2\} = \beta_i^2 Var\{\ln(V_i)\}$

Bias and Uncertainty Model Assumption 8
$\lim_{n_p \to \infty} \frac{\Omega}{\Theta} = 0.$

Bias and Uncertainty Model Assumption 9
The number of parameters n_p goes to infinity: $n_p \to \infty$.

For the rest of this section we will refer to bias and uncertainty model assumption simply as "BUMA". We will see later that we can actually say more about BUMA 2 and relax BUMA 6.

3.4.2 Main Lemmas, Theorems and Corollaries

Based on BUMAs 1 to 9 the following inferences are made. Note that all proofs are omitted since they can be found in [Ever02].

Theorem 3.1 *If BUMA 2 holds true,* $\rho(\mathbf{1}, V) = \rho(\mathbf{1}, v) \prod_{i=1}^{n_p} \varphi_i(V_i)$

Lemma 3.1 *If BUMAs 1 and 6 hold true,* $\varphi_1(V_1), ..., \varphi_{n_p}(V_{n_p})$ *are independent stochastic variables.*

Lemma 3.2 *If BUMAs 3, 4, 5, 6 and 7 hold true,* $\varphi_i(V_i) = (\frac{V_i}{v_i})^{\beta_i}$, $i = 1, 2, ..., n_p$ *with* β_i *as in BUMA 7.*

Theorem 3.2 *If BUMAs 1, 3, 4, 5, 6 and 7 hold true,*

$$E\left\{\prod_{i=1}^{n_p} \varphi_i(V_i)\right\} = \exp\left(\sum_{i=1}^{n_p}\left(\beta_i(\mu_i - \ln v_i) + \beta_i^2 \frac{\sigma_i^2}{2}\right)\right)$$

Theorem 3.3 *Let*

$$\Delta^- = \sum_{i=1}^{n_p} \beta_i(\mu_i - \ln v_i) - 2\sqrt{\sum_{i=1}^{n_p} \beta_i^2 \sigma_i^2}$$

$$\Delta^+ = \sum_{i=1}^{n_p} \beta_i(\mu_i - \ln v_i) + 2\sqrt{\sum_{i=1}^{n_p} \beta_i^2 \sigma_i^2}$$

then if BUMAs 1, 3, 4, 5, 6 and 7 hold true,

$$P\left\{\prod_{i=1}^{n_p} \varphi_i(V_i) \in \left[\exp(\Delta^-), \exp(\Delta^+)\right]\right\} = 0.95$$

Corollary 3.1 *If BUMAs 1, 2, 3, 4, 5, 6 and 7 hold true*

$$E\{\rho(\mathbf{1},V)\} = \rho(\mathbf{1},v)\exp\left(\sum_{i=1}^{n_p}\left(\beta_i(\mu_i - \ln v_i) + \beta_i^2\frac{\sigma_i^2}{2}\right)\right)$$

and

$$P\left\{\rho(\mathbf{1},V) \in \left[\rho(\mathbf{1},v)\exp(\Delta^-), \rho(\mathbf{1},v)\exp(\Delta^+)\right]\right\} = 0.95$$

Lemma 3.3 *If BUMAs 1, 6, 8 and 9 hold true,* $\prod_{i=1}^{n_p}\varphi_i(V_i) \sim \Lambda(\Gamma,\Theta^2)$.

Theorem 3.4 *If BUMAs 1, 6, 8 and 9 hold true:*

$$E\left\{\prod_{i=1}^{n_p}\varphi_i(V_i)\right\} = \exp(\Gamma + \frac{\Theta^2}{2})$$

Theorem 3.5 *If BUMAs 1, 6, 8 and 9 hold true:*

$$P\left\{\prod_{i=1}^{n_p}\varphi_i(V_i) \in [\exp(\Gamma - 2\Theta), \exp(\Gamma + 2\Theta)]\right\} = 0.95$$

Corollary 3.2 *If BUMAs 1, 2, 6, 8 and 9 hold true:*

$$E\left\{\rho(\mathbf{1},V)\right\} = \rho(\mathbf{1},v)\exp\left(\Gamma + \frac{\Theta^2}{2}\right)$$

and

$$P\left\{\rho(\mathbf{1},V) \in [\rho(\mathbf{1},v)\exp(\Gamma - 2\Theta), \rho(\mathbf{1},v)\exp(\Gamma + 2\Theta)]\right\} = 0.95$$

Corollary 3.3 *If BUMAs 1, 2, 3, 6, 7, 8 and 9 hold true:*

$$E\left\{\rho(\mathbf{1},V)\right\} = \rho(\mathbf{1},v)\exp\left(\sum_{i=1}^{n_p}\left(\beta_i(\mu_i - \ln v_i) + \beta_i^2\frac{\sigma_i^2}{2}\right)\right)$$

and

$$P\left\{\rho(\mathbf{1},V) \in \left[\rho(\mathbf{1},v)\exp(\Delta^-), \rho(\mathbf{1},v)\exp(\Delta^+)\right]\right\} = 0.95$$

Note that in [Ever02] it is argued that Γ and Θ usually cannot be determined in practice, hence the most important result are Corollaries 3.1 and 3.3 which allow us to determine the $\beta_i's$ (this is not directly the case for Corrolary 3.3, a method to evaluate the $\beta_i's$ is proposed in Appendix IV of [Ever02]), evaluate $E\{\rho(\mathbf{1},V)\}$ and obtain a 95% credibility interval for $\rho(\mathbf{1},V)$.

3.5 Determining values for the $\beta_i's$

Everdij&Blom in [Ever02] have also proposed techniques to determine the values of $\beta_i's$. The $\beta_i's$ are evaluated according to one of the following formulas:

$$\beta_i^* = \frac{\ln(\frac{\rho(v_1,...,l_i v_i,...,v_{n_p})}{\rho(v_1,...,v_i,...,v_{n_p})})}{\ln l_i}$$

or

$$\beta_i^{**} = -\frac{\ln(\frac{\rho(v_1,...,v_i/l_i,...,v_{n_p})}{\rho(v_1,...,v_i,...,v_{n_p})})}{\ln l_i}$$

where $l_i = \exp(2\sigma_i)$ for $i = 1, 2, ..., n_p$ (for more details on $l_i's$ refer to Subsection 6.2.2). Everdij&Blom also propose that a safety conservative approach be taken by setting β_i to β_i^* or β_i^{**} for $i = 1, 2, ..., n_p$ such that the upper bound of the 95% CrI is as large as possible, but did not specify the exact method do it. An obvious way to do it is choosing $\{\beta_1, \beta_2, ..., \beta_{n_p}\}$, $\beta_i \in \{\beta_i^*, \beta_i^{**}\}$, such that the quantity

$$\sum_{i=1}^{n_p} \beta_i(\mu_i - \ln v_i) + 2\sqrt{\sum_{i=1}^{n_p} \beta_i^2 \sigma_i^2} \tag{3.1}$$

is maximized. However, this method is not feasible for large n_p because we have to search through 2^{n_p} possible combinations (because for each i, β_i can be set to either β_i^* or β_i^{**}) and then determining a combination which maximizes (3.1). In this report we propose a less expensive approximate method: choose $\{\beta_1, \beta_2, ..., \beta_{n_p}\}$, $\beta_i \in \{\beta_i^*, \beta_i^{**}\}$, such that the quantity

$$\beta_i(\mu_i - \ln v_i) + 2\,|\beta_i \sigma_i| \tag{3.2}$$

is maximized for each $i \in \{1, 2, ..., n_p\}$. The idea behind this approach is that for each i we set $\beta_j = 0$, $j \neq i$, and choose $\beta_i \in \{\beta_i^*, \beta_i^{**}\}$ which minimizes (3.1). Hence we have for $i = 1, 2, ..., n_p$

$$\beta_i^{\text{safety conservative}} = \begin{cases} \beta_i^* & \text{if } \beta_i^*(\mu_i - \ln v_i) + 2\,|\beta_i^* \sigma_i| \geq \beta_i^{**}(\mu_i - \ln v_i) + 2\,|\beta_i^{**} \sigma_i| \\ \beta_i^{**} & \text{otherwise} \end{cases}$$

3.6 Limitation of the Bias and Uncertainty Assessment Methodology

The remainder of this chapter presents some contributions to the Everdij&Blom approach, made as part of this study. First, we will summarize some limitations of the approach.

The crux of the described bias and uncertainty assessment methodology is that under the collection of BUMAs $\{2, 3, 4, 5, 6, 7\}$ we have the following special form for $\rho(V)$:

$$\rho(V) = \rho(v) \prod_{i=1}^{n_p} (\frac{V_i}{v_i})^{\beta_i} \tag{3.3}$$

from which the $\beta_i's$ are to be evaluated according to the techniques in Section 3.5.

The following issues deserve further attention (they have already been identified in [Ever02]):

- We should be careful when we have that β_i^* or β_i^{**} is very small. Intuitively we would presume that $\rho(V)$ is insensitive to paramater V_i but we should remember that this insensitivity arises on the condition that all other parameters V_j, $j \neq i$ are kept at their nominal values. If some of the $V_j's$ are not at their nominal values then it is possible that the insensitivity will no longer hold.

- Due to the special form that is assumed, $\rho(V)$ follows a lognormal distribution and $\ln \rho(V)$ follows a normal distribution. Consequently, since a normal distribution has infinite tails, it is possible that $P\{\ln \rho(V) > 0\}$ becomes significant which contradicts our apriori knowledge that theoretically $-\infty < \ln \rho(V) \leq 0$ (i.e. $P\{\ln \rho(V) > 0\} = 0$).

3.7 Some Additional Derivations

In this section we will

- Discuss BUMA 2 and show that it can be interpreted in a different way.

- Discuss BUMA 6 and show that in some of the results it can be relaxed.

3.7.1 Discussion on BUMA 2

We will show that BUMA 2 can be interpreted in a different way. For this purpose we introduce the following lemma and theorem:

Lemma 3.4 *BUMA 2 holds* ***if and only if*** $\rho(\mathbf{1}, (V_1, V_2, \ldots, V_{n_p})) = \prod_{i=1}^{n_p} \eta_i(V_i)$ *for some functions* $\eta_i(\cdot)$, $i = 1, 2, \ldots, n_p$.

Proof. The **if** part is easy to proof. It goes as follows:
Take any arbitrary i,

$$\begin{aligned}
\varphi_i'(x_i, x_{i+1}, \ldots, x_{n_p}) &= \frac{\rho(\mathbf{1}, (v_1, v_2, \ldots, x_i, x_{i+1}, \ldots, x_{n_p}))}{\rho(\mathbf{1}, (v_1, v_2, \ldots, v_i, x_{i+1}, \ldots, x_{n_p}))} \\
&= \frac{\prod_{j=1}^{i-1} \eta_j(v_j) \times \eta_i(x_i) \times \prod_{j=i+1}^{n_p} \eta_j(x_j)}{\prod_{j=1}^{i} \eta_j(v_j) \times \prod_{j=i+1}^{n_p} \eta_j(x_j)} \\
&= \frac{\eta_i(x_i)}{\eta_i(v_i)} \\
&= \frac{\rho(\mathbf{1}, (v_1, v_2, \ldots, x_i, v_{i+1}, \ldots, v_{n_p}))}{\rho(\mathbf{1}, (v_1, v_2, \ldots, v_i, v_{i+1}, \ldots, v_{n_p}))} \\
&= \varphi_i(x_i)
\end{aligned}$$

The **only if** part can also be shown easily. First we note the following for $i = 1$:

$$\varphi_1'(x_1, x_2, \ldots, x_{n_p}) = \frac{\rho(\mathbf{1}, (x_1, x_2 \ldots, x_{n_p}))}{\rho(\mathbf{1}, (v_1, x_2 \ldots, x_{n_p}))} = \varphi_1(x_1)$$

Note that $\varphi_i(v_i) = 1$. Since v_1 is fixed we can write $\rho(\mathbf{1}, (v_1, x_2 \ldots, x_{n_p})) = \phi_1(x_2, \ldots, x_{n_p})$ for some function $\phi_1(\cdot)$. Hence $\rho(\mathbf{1}, (x_1, x_2 \ldots, x_{n_p})) = \varphi_1(x_1) \times \phi_1(x_2, \ldots, x_{n_p})$. Repeating the previous procedure for $i = 2$ we have

$$\begin{aligned}
\varphi_2'(x_2, \ldots, x_{n_p}) &= \frac{\rho(\mathbf{1}, (v_1, x_2 \ldots, x_{n_p}))}{\rho(\mathbf{1}, (v_1, v_2 \ldots, x_{n_p}))} \\
&= \frac{\varphi_1(v_1) \times \phi_1(x_2, \ldots, x_{n_p})}{\varphi_1(v_1) \times \phi_1(v_2, \ldots, x_{n_p})} \\
&= \frac{\phi_1(x_2, \ldots, x_{n_p})}{\phi_1(v_2, \ldots, x_{n_p})} = \varphi_2(x_2)
\end{aligned}$$

Again since v_2 is constant we can again define $\phi_1(v_2, \ldots, x_{n_p}) = \phi_2(x_3, \ldots, x_{n_p})$ for some function $\phi_2(\cdot)$. We have $\phi_1(x_2, \ldots, x_{n_p}) = \varphi_2(x_2) \times \phi_2(x_3, \ldots, x_{n_p})$ hence $\rho(\mathbf{1}, (x_1, x_2 \ldots, x_{n_p})) = \varphi_1(x_1) \times \phi_1(x_2, \ldots, x_{n_p}) = \varphi_1(x_1) \times \varphi_2(x_2) \times \phi_2(x_3, \ldots, x_{n_p})$. Continuing for $i = 3, 4, \ldots, n_p - 1$ we obtain:

$$\rho(\mathbf{1}, (x_1, x_2, \ldots, x_{n_p})) = \prod_{i=1}^{n_p - 1} \varphi_i(x_i) \times \phi_{n_p - 1}(x_{n_p})$$

As in previous steps we know that $\frac{\phi_{n_p-1}(x_{n_p})}{\phi_{n_p-1}(v_{n_p})} = \varphi_{n_p}(x_{n_p})$ but since $\varphi_i(v_i) = 1$ it is clear that $\phi_{n_p-1}(v_{n_p}) = \rho(\mathbf{1}, (v_1, v_2, \ldots, v_{n_p}))$ hence $\phi_{n_p-1}(x_{n_p}) = \rho(\mathbf{1}, (v_1, v_2, \ldots, v_{n_p})) \times \varphi_{n_p}(x_{n_p})$ and

$$\rho(\mathbf{1}, (x_1, x_2, \ldots, x_{n_p})) = \rho(\mathbf{1}, (v_1, v_2, \ldots, v_{n_p})) \times \prod_{i=1}^{n_p} \varphi_i(x_i)$$

Now just define $\eta_1(x_1) = \rho(\mathbf{1}, (v_1, v_2, \ldots, v_{n_p})) \times \varphi_1(x_1)$ and $\eta_i(x_i) = \varphi_i(x_i)$ for $i = 2, \ldots, n_p$. We can rewrite the previous equality as:

$$\rho(\mathbf{1}, (x_1, x_2, \ldots, x_{n_p})) = \prod_{i=1}^{n_p} \eta_i(x_i)$$

It directly follows that

$$\rho(\mathbf{1}, (V_1, V_2, \ldots, V_{n_p})) = \prod_{i=1}^{n_p} \eta_i(V_i)$$

■

Theorem 3.6 $\rho(\mathbf{1}, (V_1, V_2, \ldots, V_{n_p})) = \rho(\mathbf{1}, (v_1, v_2, \ldots, v_{n_p})) \times \prod_{i=1}^{n_p} \varphi_i(V_i)$ ***if and only if*** *BUMA 2 holds true.*

Proof. The **if** part has been shown in [Ever02]. Hence we will only show the **only if** part: $\rho(\mathbf{1}, (V_1, V_2, \ldots, V_n)) = \rho(\mathbf{1}, (v_1, v_2, \ldots, v_n)) \times \prod_{i=1}^{n_p} \varphi_i(V_i) \Rightarrow$ for any $i = 1, \ldots, n_p$ and $x_i, x_{i+1}, \ldots, x_{n_p}$, $\varphi_i'(x_i, x_{i+1}, \ldots, x_{n_p}) = \varphi_i(x_i)$. Take any i, then

$$\begin{aligned}
\varphi_i'(x_i, x_{i+1}, \ldots, x_{n_p}) &= \frac{\rho(\mathbf{1}, (v_1, v_2, \ldots, x_i, x_{i+1}, \ldots, x_{n_p}))}{\rho(\mathbf{1}, (v_1, v_2, \ldots, v_i, x_{i+1}, \ldots, x_{n_p}))} \\
&= \frac{\rho(\mathbf{1}, (v_1, v_2, \ldots, v_{n_p})) \times \prod_{j=1}^{i-1} \varphi_j(v_j) \times \prod_{j=i}^{n_p} \varphi_j(x_j)}{\rho(\mathbf{1}, (v_1, v_2, \ldots, v_{n_p})) \times \prod_{j=1}^{i} \varphi_j(v_j) \times \prod_{j=i+1}^{n_p} \varphi_j(x_j)} \\
&= \frac{\rho(\mathbf{1}, (v_1, v_2, \ldots, v_{n_p})) \times \prod_{j=1}^{i-1} \varphi_j(v_j) \times \varphi_i(x_i)}{\rho(\mathbf{1}, (v_1, v_2, \ldots, v_{n_p})) \times \prod_{j=1}^{i} \varphi_j(v_j)} \\
&= \frac{\rho(\mathbf{1}, (v_1, v_2, \ldots, v_{n_p})) \times \prod_{j=1}^{i-1} \varphi_j(v_j) \times \varphi_i(x_i) \times \prod_{j=i+1}^{n_p} \varphi_j(v_j)}{\rho(\mathbf{1}, (v_1, v_2, \ldots, v_{n_p})) \times \prod_{j=1}^{i} \varphi_j(v_j) \times \prod_{j=i+1}^{n_p} \varphi_j(v_j)} \\
&= \frac{\rho(\mathbf{1}, (v_1, v_2, \ldots, x_i, v_{i+1}, \ldots, v_{n_p}))}{\rho(\mathbf{1}, (v_1, v_2, \ldots, v_{n_p}))} = \varphi_i(x_i)
\end{aligned}$$

■

Corollary 3.4 *$\rho(\mathbf{1}, (V_1, V_2, \ldots, V_{n_p})) = \rho(\mathbf{1}, (v_1, v_2, \ldots, v_{n_p})) \times \prod_{i=1}^{n_p} \varphi_i(V_i)$ if and only if ρ can be factored as $\rho(\mathbf{1}, (V_1, V_2, \ldots, V_{n_p})) = \prod_{i=1}^{n_p} \eta_i(V_i)$ for some functions $\eta_i(\cdot)$.*

Proof. This follows directly by combining the results of Lemma 3.4 and Theorem 3.6. ■

Remark 3.1 *The previous corollary shows that it is not possible to reduce BUMA 2 in order to obtain the special relation between $\rho(1, (v_1, v_2, \ldots, v_{n_p}))$ and $\rho(1, (V_1, V_2, \ldots, V_{n_p})$ as in Theorem 3.1. It turns out that the factorizability of $\rho(\mathbf{1}, (V_1, V_2, \ldots, V_{n_p}))$ is not only sufficient but also necessary for BUMA 2 to be true.*

Based on the preceeding arguments we can replace BUMA 2 with BUMA 2' (stated below) and discard Theorem 3.1 since it is no longer necessary.

Bias and Uncertainty Model Assumption 2'

The function $\rho(\mathbf{1}, V)$ satisfies $\rho(\mathbf{1}, (V_1, V_2, \ldots, V_{n_p})) = \prod_{i=1}^{n_p} \eta_i(V_i)$ for some functions $\eta_i(\cdot)$, $i = 1, 2, \ldots, n_p$.

3.7.2 Discussion on BUMA 6

In the proofs of Lemmas 3.1 and 3.3, Theorems 3.4 and 3.5, and Corollaries 3.2 and 3.3, BUMA 6 can be relaxed and replaced with BUMA 6'. It is then necessary that Lemma 3.1 be substituted by Lemma 3.5 below:

Bias and Uncertainty Model Assumption 6'

The functions φ_i, $i = 1, 2, \ldots, n_p$ are measurable with respect to the Borel σ-algebra $\Re$ of $\mathbb{R}$.

Lemma 3.5 *Under BUMAs 1 and 6', $\varphi_i(V_i)$, $i = 1, 2, \ldots, n_p$ are independent random variables.*

Proof. It is only necessary to prove the statement for two arbitrary measurable functions $f(\cdot)$ and $g(\cdot)$, i.e. V_1, V_2 are independent $\Longrightarrow$ $f(V_1)$, $g(V_2)$ are independent.

In probability theory, two sigma algebras $\mathcal{A}$, $\mathcal{B} \subset \mathcal{F}$ are said to be independent if for any set A $\in \mathcal{A}$ and B $\in \mathcal{B}$ we have that $P(A \cap B) = P(A)P(B)$. In a similar fashion two random variables X and Y are independent if the σ-algebras $\sigma(X)$ and $\sigma(Y)$ are independent.

Now $(fV_1)^{-1}(\Re) = V_1^{-1}(f^{-1}(\Re)) \subset \sigma(V_1)$ since $f^{-1}(\Re) \subset \Re$ and similarly $(fV_2)^{-1}(\Re) \subset \sigma(V_2)$. Since V_1 and V_2 are independent we have $\sigma(V_1)$ and $\sigma(V_2)$ are independent, hence so are $\sigma(fV_1) \equiv (fV_1)^{-1}(\Re) \subset \sigma(V_2)$ and $\sigma(fV_2) \equiv (fV_2)^{-1}(\Re) \subset \sigma(V_2)$. ■

3.8 An Alternative Approach to Yield the Result in Corollary 3.1

Let us introduce the following new BUMA:

Bias and Uncertainty Model Assumption 10
For all $i = 1, 2, ..., n_p$, $\varphi_i(V_i) = (\frac{V_i}{v_i})^{\beta_i}$ for some $\beta_i \in \mathbb{R}$

With the above BUMA in place we have the following result:

Theorem 3.7 *If BUMAs 1, 2, 3, 6', 8, 9 and 10 hold true then*

$$E\{\rho(\mathbf{1}, V)\} = \rho(\mathbf{1}, v) \exp\left(\sum_{i=1}^{n_p}\left(\beta_i(\mu_i - \ln v_i) + \beta_i^2 \frac{\sigma_i^2}{2}\right)\right)$$

and

$$P\left\{\rho(\mathbf{1}, V) \in \left[\rho(\mathbf{1}, v)\exp(\Delta^-), \rho(\mathbf{1}, v)\exp(\Delta^+)\right]\right\} = 0.95$$

Proof. From Corollary 3.2 we already have that if BUMAs $\{1, 2, 6', 8, 9\}$ hold true (note that although BUMA 6' is a relaxed version of BUMA 6 it can be easily checked that the result of the corollary still holds)

$$E\{\rho(\mathbf{1}, V)\} = \rho(\mathbf{1}, v) \exp\left(\Gamma + \frac{\Theta^2}{2}\right)$$

and

$$P\left\{\rho(\mathbf{1}, V) \in [\rho(\mathbf{1}, v)\exp(\Gamma - 2\Theta), \rho(\mathbf{1}, v)\exp(\Gamma + 2\Theta)]\right\} = 0.95$$

Hence we need to determine Γ and Θ. Recall that by definition

$$\Gamma = \sum_{i=1}^{n_p} E\{\ln \varphi_i(V_i)\}$$

and

$$\Theta^2 = \sum_{i=1}^{n_p} Var\{\ln \varphi_i(V_i)\}$$

By BUMA 10 we can readily evaluate $E\{\ln \varphi_i(V_i)\}$ and $Var\{\ln \varphi_i(V_i)\}$ for all $i \in \{1, 2, ..., n_p\}$. We do this as follows:

$$E\{\ln \varphi_i(V_i)\} = E\{\beta_i(\ln V_i - \ln v_i)\} = \beta_i(E\{\ln V_i\} - \ln v_i) = \beta_i(\mu_i - \ln v_i)$$

$$Var\{\ln \varphi_i(V_i)\} = Var\{\beta_i(\ln V_i - \ln v_i)\} = \beta_i^2 Var\{\ln V_i - \ln v_i\} = \beta_i^2 Var\{\ln V_i\} = \beta_i^2 \sigma_i^2$$

Therefore

$$\Gamma = \sum_{i=1}^{n_p} \beta_i(\mu_i - \ln v_i)$$

and

$$\Theta^2 = \sum_{i=1}^{n_p} \beta_i^2 \sigma_i^2$$

hence the result. ■

Chapter 4

Statistical Estimation with Polynomial Chaos Expansion

4.1 Introduction to the Approach

Recently, researchers in Chemical Engineering have also considered the problem of uncertainty analysis (see [Webs96][Isuk99] and the references therein). The setting of their problem is similar to the one considered here; the objective is to quantify the uncertainty in the output of a black-box model as a result of uncertainty in the model parameters based on a small number of simulation runs. The difference is that their black-box is the mathematical model of a chemical process while in our context the black-box is the mathematical model of an operation in ATM.

Both [Webs96] and [Isuk99] based their uncertainty analysis on polynomial chaos expansion (PCE). PCE was formulated by Norbert Wiener and is elaborated in [Ghan95]. The two methods of uncertainty analysis in the literature also differ:

1. [Webs96] uses PCE with the so called Probabilistic Collocation Method.

2. [Isuk99] uses PCE with the so called Regression Method with Improved Sampling.

This chapter first discusses the concept of PCE, and next discusses the two approaches mentioned above. Finally, we explain the relation between these PCE based uncertainty analysis approaches and the Everdij&Blom method of Chapter 3.

4.2 Motivation for Using Polynomial Chaos Expansion

In some situations obtaining a single output value of a black box model corresponding to a particular setting of the input may be very time consuming. Hence if the inputs are random with known distributions and we are interested in studying the statistical properties of the output, running a large number of Monte Carlo runs, say 10,000 or more, to estimate the output mean or variance is not practical. If one knows a simpler parametric model as a susbstitute for the black box model then it is much simpler to evaluate that black box. The polynomial chaos expansion can serve as such a substitute model. If the polynomial chaos expansion behaves closely to the actual model, the results of Monte Carlo runs on the expansion will be very close to the results that would be obtained if the Monte Carlo runs were executed on the actual model. The desired statistical estimates are then obtained from the polynomial chaos expansion instead of the actual model.

4.3 Definition of Polynomial Chaos

We will briefly discuss the theory of homogeneous polynomial chaos, for a more detailed exposition the reader is referred to [Ghan95] and [Scho00] upon which most of the discussion materials here are based.

Let us denote Θ as a space of square-integrable random variables w.r.t some probability triplet $(\Omega, \mathcal{F}, P)$, i.e. if Y is a random variable and $Y \in \Theta$ then $EY^2 < \infty$. Let $\{X_i\}_{i=1}^{\infty}$ be a set of mutually independent standard normal random variables. Consider the space $\widehat{\Psi}_p$ of all polynomials in $\{X_i\}_{i=1}^{\infty}$ of degree not exceeding p. The definition of polynomials in $\{X_i\}_{i=1}^{\infty}$ of order p is made clear in the following example:

Example 4.1 *A polynomial in* $\{X_i\}_{i=1}^{\infty}$ *of degree two has the form*

$$P(X_{i_1}, X_{i_2}) = a_0 + a_{i_1} X_{i_1} + a_{i_2} X_{i_2} + a_{i_1 i_2} X_{i_1} X_{i_2}$$

while a polynomial of degree three has the form

$$\begin{aligned} P(X_{i_1}, X_{i_2}, X_{i_3}) \quad = \quad & a_0 + a_{i_1} X_{i_1} + a_{i_2} X_{i_2} + a_{i_3} X_{i_3} + a_{i_1 i_2} X_{i_1} X_{i_2} + \\ & a_{i_1 i_3} X_{i_1} X_{i_3} + a_{i_2 i_3} X_{i_2} X_{i_3} + a_{i_1 i_2 i_3} X_{i_1} X_{i_2} X_{i_3} \end{aligned}$$

where $i_1, i_2, i_3 \in \{1, 2, ...\}$ *and* $a_0, a_{i_1}, a_{i_2}, ...$ *are arbitrary constants in* $\mathbb{R}$.

Let Ψ_p represent the set of all polynomials in $\widehat{\Psi}_p$ orthogonal to $\widehat{\Psi}_{p-1}$ and let us denote $\overline{\Psi}_p$ as the space spanned by Ψ_p. Define Ψ_0 to be the set containing the constant polynomial 1. Then we call the subspace $\overline{\Psi}_p$ of Θ the p^{th} homogeneous chaos, and Ψ_p is called a polynomial chaos of order p. Note that since random variables are actually functions, it is clear that polynomial chaoses are functions of functions returning a real number and hence are functionals.

The set of polynomial chaoses is a linear subspace of the space of square-integrable random variables Θ and is a ring with respect to the functional multiplication $\Psi_p\Psi_q(\varpi) = \Psi_p(\varpi)\Psi_q(\varpi)$, $\varpi \in \Omega$. Let the Hilbert space spanned by $\{X_i\}_{i=1}^{\infty}$ be denoted by $\Theta(X)$, then the resulting ring which we denote by $\Phi_{\Theta(X)}$ is called the ring of functions generated by $\Theta(X)$. It can be shown under some general conditions that the ring $\Phi_{\Theta(X)}$ is dense in Θ, hence any element of Θ can be approximated arbitrarily closely by elements from $\Phi_{\Theta(X)}$. The convergence of the approximation is taken to be in the mean square sense. Therefore any random variable $Y \in \Theta$ admits the representation:

$$Y = \sum_{p\geq 0} \sum_{n_1+n_2+\ldots+n_p=p} \sum_{r_1,r_2,\ldots,r_p} a_{r_1,r_2,\ldots,r_p}^{n_1,n_2,\ldots,n_p} \Gamma_p(X_{r_1}, X_{r_2}, ..., X_{r_p}) \tag{4.1}$$

where $\Gamma_p(X_{r_1}, X_{r_2}, ..., X_{r_p})$ is a polynomial in Ψ_p with arguments $X_{r_1}, X_{r_2}, ..., X_{r_p}$ and the superscript n_i denotes the number of times that X_{r_i} occurs in the argument list for Γ_p. Representation (4.1) can be easier understood if it is rewritten in the following equivalent form:

$$\begin{aligned} Y \quad = \quad & \underbrace{a_0\Gamma_0}_{\text{constant}} + \underbrace{\sum_{i_i=1}^{\infty} a_{i_1}\Gamma_1(X_{i_1})}_{1^{\text{st}} \text{ order terms}} \\ & + \underbrace{\sum_{i_i=1}^{\infty}\sum_{i_2=1}^{i_1} a_{i_1 i_2}\Gamma_2(X_{i_1}, X_{i_2})}_{2^{\text{nd}} \text{ order terms}} \\ & + \underbrace{\sum_{i_i=1}^{\infty}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2} a_{i_1 i_2 i_3}\Gamma_3(X_{i_1}, X_{i_2}, X_{i_3})}_{3^{\text{rd}} \text{ order terms}} \\ & + \underbrace{\sum_{i_i=1}^{\infty}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2}\sum_{i_4=1}^{i_3} a_{i_1 i_2 i_3 i_4}\Gamma_4(X_{i_1}, X_{i_2}, X_{i_3}, X_{i_4})}_{4^{\text{th}} \text{ order terms}} \\ & + \ldots \end{aligned} \tag{4.2}$$

Polynomial chaos terms of different order are orthogonal to each other as are polynomial chaos terms of the same order but with a different argument list. Note that for $k \geq 1$, there is an infinite number of k^{th} order terms in the expansion. Later we shall see the case where there are only a finite number of k^{th} order terms in the expansion. It can be shown that since the polynomial chaoses are orthogonal w.r.t the Gaussian probability measure, they are identical to the corresponding multidimensional Hermite polynomials. Hence $\Gamma_n(X_{i_1}, ..., X_{i_n})$ can be obtained as:

$$\Gamma_n(X_{i_1}, ..., X_{i_n}) = (-1)^n e^{-\frac{1}{2}X^T X} \frac{\partial^n}{\partial X_{i_1} ... \partial X_{i_n}} e^{-\frac{1}{2}X^T X}$$

where $X = (X_{i_1}, ..., X_{i_n})$. The expansion of a square-integrable random variable in terms of polynomial chaoses is called a *polynomial chaos expansion* (PCE).

Note that other types of polynomials other than multidimensional Hermite polynomial are also possible if the set of mutually independent variables $\{X_i\}_{i=1}^{\infty}$ follow some other distribution, for details see [Scho00].

4.4 Polynomial Chaos Expansion with a Finite Number of Terms

We saw in Section 4.3 that the number of k^{th} order terms, $k \geq 1$, in a PCE is infinite. Even if we decide to truncate the series using only terms up to the n^{th} order with $n < \infty$, we would still end up with an infinite series. This poses computational problems in practical applications. However, we will see that in our particular application (and in other applications of similar nature) we obtain an expansion where the number of k^{th} order terms are finite. We will explain this in the context of determining a PCE for the the natural logarithm of the incrossing risk $\ln \mathcal{R}$ (recall from Chapter 3 that we have defined $\mathcal{R} = \rho(V)$). Let us recall that $V = (V_1, ..., V_{n_p})$ where we assume (see BUMA 1, Chapter 3) that the $V_i's$ are mutually independent random variables. Suppose that we can generate the $V_i's$ by generating n_p mutually independent standard normal random variables $X_1, ..., X_{n_p}$, i.e. there exists for each $i \in \{1, 2, ..., n_p\}$ a measurable function G_i such that $V_i = G_i(X_i)$. Then we may write $\mathcal{R} = \rho(V) = \rho((V_1, ..., V_{n_p})) = \rho((G_1(X_1), ..., G_{n_p}(X_{n_p})) = \widetilde{\rho}(X_1, X_2, ..., X_{n_p})$ and regard $X_1, X_2, ..., X_{n_p}$ as our new random variables. Suppose now that we extend our set of standard normal variables by adding the set $\{X_k,\ k > n_p\}$ of mutually independent standard random variables which are independent of $X_1, ..., X_{n_p}$. Hence we now have the infinite set $\{X_i\}_{i=1}^{\infty}$. Assuming that $\ln \mathcal{R}$ is square integrable then by the theory in the previous section, $\ln \mathcal{R}$ has a PCE of the form:

$$
\begin{aligned}
\ln \mathcal{R} \quad = \quad & \underset{\text{constant}}{a_0 \Gamma_0} + \sum_{i_i=1}^{\infty} a_{i_1} \Gamma_1(X_{i_1}) \\
& + \sum_{i_i=1}^{\infty} \sum_{i_2=1}^{i_1} a_{i_1 i_2} \Gamma_2(X_{i_1}, X_{i_2}) \\
& + \sum_{i_i=1}^{\infty} \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} a_{i_1 i_2 i_3} \Gamma_3(X_{i_1}, X_{i_2}, X_{i_3}) \\
& + \sum_{i_i=1}^{\infty} \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} \sum_{i_4=1}^{i_3} a_{i_1 i_2 i_3 i_4} \Gamma_4(X_{i_1}, X_{i_2}, X_{i_3}, X_{i_4}) \\
& + \dots
\end{aligned}
$$

Remark 4.1 *We choose to identify the PCE of the log of the random variable of interest because of the nature of our application (discussed in Section 3.3). In*

[Webs96] and [Isuk99], it was the PCE of the random variable of interest that was identified.

However, we know apriori that $\ln \mathcal{R}$ is a function of $X_1, ..., X_{n_p}$. Since $X_1, ..., X_{n_p}$ are independent of $X_{n_p+1}, X_{n_p+2}, ...$ then $\ln \mathcal{R}$ is also independent of $X_{n_p+1}, X_{n_p+2}, ...$ implying that $a_{i_1 i_2 ... i_n} = 0$ if $i_k > n_p$ for some $1 \leq k \leq n$. Hence we may write

$$\begin{aligned} \ln \mathcal{R} &= \underset{\text{constant}}{a_0 \Gamma_0} + \sum_{i_i=1}^{n_p} a_{i_1} \Gamma_1(X_{i_1}) \\ &+ \sum_{i_i=1}^{n_p} \sum_{i_2=1}^{i_1} a_{i_1 i_2} \Gamma_2(X_{i_1}, X_{i_2}) \\ &+ \sum_{i_i=1}^{n_p} \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} a_{i_1 i_2 i_3} \Gamma_3(X_{i_1}, X_{i_2}, X_{i_3}) \\ &+ \sum_{i_i=1}^{n_p} \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} \sum_{i_4=1}^{i_3} a_{i_1 i_2 i_3 i_4} \Gamma_4(X_{i_1}, X_{i_2}, X_{i_3}, X_{i_4}) \\ &+ \dots \end{aligned} \tag{4.3}$$

Thus we have that the k^{th} order terms are finite although there is still an infinite sum to contend with. In order to approximate $\ln \mathcal{R}$ we may truncate this series to include only terms up to the n^{th} order, leaving a finite sum which is computable. *Note that we shall use the following terminology: if a PCE contains terms up to the n^{th} order we call this PCE an n^{th} order PCE.*

4.5 Summary of Assumptions for the PCE Method

Some assumptions were made in the previous sections so that the PCE method can be applied. We summarize them as follows:

1. $V_1, V_2, ..., V_{n_p}$ are mutually independent.
2. If our independent parameters $V_1, V_2, ..., V_{n_p}$ do not have standard normal distributions then we need to find transformations $G_1(.), G_2(.), ..., G_{n_p}(.)$ such that $V_i = G_i(X_i)$ for $i = 1, ..., n_p$ where $X_1, X_2, ..., X_{n_p}$ are mutually independent standard normal random variables (i.e., the $V_i's$ can be generated by the $X_i's$).
3. Some general conditions under which the ring $\Theta(X)$ is dense in Θ. These general conditions are not explicitly stated in [Ghan95] but references are provided therein.
4. The function $\ln \widetilde{\rho}(X_1, X_2, ..., X_{n_p})$ is square-integrable. We can expect this assumption to hold true because if it does not then $\ln \widetilde{\rho}(X_1, X_2, ..., X_{n_p})$ would have infinite variance.

4.6 Number of Terms in a PCE

The number of coefficients in a PCE depends on the number of variables (in our context, the number of uncertain parameters) and the order of the expansion. Figure 4.1 shows this relation.

		Order of polynomial chaos expansion					
		2	3	4	5	6	10
Number of uncertain parameters	2	6	10	15	21	28	66
	3	10	20	35	56	84	286
	4	15	35	70	126	210	1001
	5	21	56	126	252	462	3003
	6	28	84	210	462	924	8008
	10	66	286	1001	3003	8008	184756
	20	231	1771	10626	53130	230230	Huge
	30	496	5456	46376	324632	Huge	Huge
	80	3321	91881	1929501	32801517	Huge	Huge

Figure 4.1: Number of terms necessary in a polynomial chaos expansion

4.7 Determining the Coefficients of the PCE

If $\ln \mathcal{R} = \ln \widetilde{\rho}(X_1, X_2, ..., X_{n_p})$ satisfies the assumptions in the previous section then it has an expansion of the form (4.3). Now we need to determine the coefficients $a_0, a_1, a_2, ...$ efficiently. In the literature there are two methods proposed to do this:

1. The Probabilistic Collocation Method (PCM) [Webs96]
2. Regression Method with Improved Sampling [Isuk99]

Both methodologies use the principle of collocation. Let us expand $\ln \mathcal{R}$ in an n^{th} order PCE and let us denote this truncated expansion as $\ln \mathcal{R}_n = \ln \widetilde{\rho}_n(X_1, X_2, ..., X_{n_p})$. The principle of collocation imposes the requirement that $\ln \mathcal{R}_n$ is exact $(= \ln \mathcal{R})$ at a set of chosen collocation points, thus making the residual at those points equal to zero. The number of collocation points should be equal to the number of unknown coefficients to be found. Thus, for each output metric, a set of linear equations results with the coefficients as the unknowns; these equations can be solved using standard linear solvers. The two methods mentioned above differ in how the collocation points are chosen.

4.7.1 The Probabilistic Collocation Method (PCM)

In this method, the collocation points are chosen to correspond to the roots of the one-dimensional Hermite polynomial of a degree one higher than the order of the PCE. This method can be applied to multi-dimensional problems and

for one-dimensional problems it gives the same results as Galerkin's method , and hence is regarded as an "optimal method"[Isuk99]. For example, in order to solve for second order PCE in two variables , the roots of the third order Hermite polynomial $-4x(2x^2-3)$, i.e. $\frac{1}{2}\sqrt{6}$, $-\frac{1}{2}\sqrt{6}$ and 0, are used. Hence the possible collocation points are $(0,0)$, $(\frac{1}{2}\sqrt{6},0)$, $(0,\frac{1}{2}\sqrt{6})$, $(0,-\frac{1}{2}\sqrt{6})$, $(-\frac{1}{2}\sqrt{6},0)$, $(\frac{1}{2}\sqrt{6},\frac{1}{2}\sqrt{6})$, $(\frac{1}{2}\sqrt{6},-\frac{1}{2}\sqrt{6})$, $(-\frac{1}{2}\sqrt{6},\frac{1}{2}\sqrt{6})$ and $(-\frac{1}{2}\sqrt{6},-\frac{1}{2}\sqrt{6})$.

There are certain limitations in relation to selecting the collocation points. For example, for the two variables case described above, there are nine possible collocation points but with a second order PCE only six unknowns have to be determined. Similarly, for systems with more variables and for higher order approximations, the number of available collocation points is always greater than the number of points needed. In the absence of selection criteria, in the PCM method collocation points are selected at random from the set of available points; however, this may result in a poor approximation. Indeed, in [Isuk99] it is shown that in some cases the PCM cannot consistently guarantee convergence of the approximation to the true probability density with an increasing order of the PCE.

4.7.2 Regression Method with Improved Sampling (RMIS)

Due to the shortcoming of the PCM approach, an alternative approach of determining the collocation points was proposed in [Isuk99]. In this alternative approach, a set of points is selected from regions of high probability; this set forms a regression basis for calculating the unknown coefficients. These points are selected using a simple heuristic technique that is explained in the following. For each term of the series expansion, "corresponding" basis points are chosen. For example, the point corresponding to the constant term of a PCE is the origin, i.e. all variables $X_1, X_2, ..., X_{n_p}$ are set to value zero. For terms involving only one variable X_i, the regression basis points are chosen by setting all other parameters (X_j, $j \neq i$ and $1 \leq j \leq n_p$) to zero value and letting X_i take on values equal to the roots of the next order Hermite polynomial. For terms involving two or more variables, the values of the corresponding parameters are set to the values of the roots of the next order polynomial and all other variables are set to zero. If more points "corresponding" to a set of terms are available than needed, the points which are closer to the origin are preferred, as they typically fall in regions of higher probability. Further, when there is still an unresolved choice, the regression basis points are chosen so that the overall distribution of these points is more symmetric with respect to the origin. The advantage of this method is that the behavior of the model is captured reasonably well at points corresponding to regions of high probability. Further, if a higher number of points are selected than the minimum required this method leads to an estimation of parameter values and corresponding probability densities that is more robust compared to that obtained by other methods such as the PCM[Isuk99]. To make the concept more clear we provide the following example:

Example 4.2 *Let $Y = f(X_1, X_2)$ be an unknown function of two independent standard normal random variables X_1, X_2. Let us try to expand Y as a third order PCE. The roots of the fourth order Hermite polynomial $4(4x^4 - 12x^2 + 3)$ are -1.6507, -0.5246, 0.5246, and 1.6507. For this particular case there are 25 choices of possible collocation points:*

$(0, 0)$	$(-1.6507, 0)$	$(-0.5246, 0)$	$(0.5246, 0)$
$(1.6507, 0)$	$(0, -1.6507)$	$(0, -0.5246)$	$(0, 0.5246)$
$(0, 1.6507)$	$(-1.6507, -1.6507)$	$(-1.6507, -0.5246)$	$(-1.6507, 0.5246)$
$(-1.6507, 1.6507))$	$(-0.5246, -1.6507)$	$(-0.5246, -0.5246)$	$(-0.5246, 0.5246)$
$(-0.5246, 1.6507)$	$(0.5246, -1.6507)$	$(0.5246, -0.5246)$	$(0.5246, 0.5246)$
$(0.5246, 1.6507)$	$(1.6507, -1.6507)$	$(1.6507, -0.5246)$	$(1.6507, 0.5246)$
$(1.6507, 1.6507)$			

In order to determine the coefficients of the chaos expansion we only need to choose 10 collocation points (see Figure 4.1), however we may wish use to choose more points in which case the PCE coefficients can be determined by some least squares method. One possible choice of collocation points (it is not unique since it is a heuristical method) according to the RMIS principle is:

$(0, 0)$	$(-1.6507, 0)$
$(-0.5246, 0)$	$(0.5246, 0)$
$(1.6507, 0)$	$(0, -1.6507)$
$(0, -0.5246)$	$(0, 0.5246)$
$(0, 1.6507)$	$(0.5246, -0.5246)$

Since the input variables are all assumed to be standard normal random variables, 99% of the time each random variable would take a value in the interval $[-2.5, 2.5]$. From a practical point of view, it may be efficient not to use roots of the Hermite polynomials outside $[-2.5, 2.5]$ because it falls in a region of low probability.

To summarize, the basic idea of this method is to sample the unknown function at collocation points, including the origin, which are assumed to be "representative" of the function in the input region $\bigotimes_{i=1}^{n_p}[-2.5, 2.5]$. However, a problem which is not mentioned in [Isuk99] can arise in practice when choosing the collocation points, this is discussed in Subsection 4.9.1.

4.7.3 Additional Guidelines

Let the number of coefficients in a PCE be denoted by N and let the number of all possible collocation points be denoted by M. In practice, not any arbitrary collection of K collocation points, $K \geq N$, from the M possible collocation points is feasible for determining the PCE coefficients. The reason for this is the following:
Let $Y = g(X_1, X_2, ..., X_{n_p})$ where g is some unknown function and $X_1, X_2, ..., X_{n_p}$

are mutually independent standard normal random variables. We assume that $g(.)$ has a PCE. Let n be the order of the PCE and let $\widehat{Y}$ denote the PCE of Y. Denote $x^i = (x_1^i, x_2^i, ..., x_{n_p}^i)$ as some collocation point indexed by i, $i \in \{1, 2, ..., K\}$, and let

$$\widehat{Y}^i = g(x_1^i, x_2^i, ..., x_{n_p}^i) = h(x^i)a$$

where

$$a = \underbrace{(a_0, a_1, a_2, ...)}_{N \text{ terms}}^T$$

are the PCE coefficients and

$$h(x^i) = \underbrace{(1, x_1^i, ..., x_{n_p}^i, ...)}_{N \text{ terms}}$$

Note that $h(x^i)a$ is a compact way of writing the PCE of Y (refer to equation (4.3)) evaluated at the collocation point x^i. Since we have K collocation points we may write:

$$\widehat{\mathbf{Y}} = Ha \tag{4.4}$$

where H is a $K \times N$ matrix of the form:

$$H = \begin{bmatrix} h(x^1) \\ h(x^2) \\ . \\ . \\ h(x^K) \end{bmatrix}$$

and $\widehat{\mathbf{Y}}$ is a $K \times 1$ vector $\widehat{\mathbf{Y}} = (\widehat{Y}^1, \widehat{Y}^2, ..., \widehat{Y}^K)^T$. To be able to solve equation (4.4) to evaluate a, i.e. by solving a linear set of equations in the case $K = N$ or by a least squares method if $K \geq N$, we need that $rank(H) = N$.

Example 4.3 *Returning to Example 4.2, the number of the PCE coefficients in a third order expansion is 10. Out of the 25 possible collocation points the following 10 collocation points will make* $rank(H) = 10$:

$(0, 0)$	$(1.6507, 0)$
$(0, 1.6507)$	$(0.5246, 0)$
$(0, 0.5246)$	$(-0.5246, 0)$
$(0, -0.5246)$	$(-1.6507, -1.6507)$
$(1, 6507, 1.6507)$	$(1.6507, 0.5246)$

4.8 Assessing the Fit of the PCE

After the coefficients of the PCE have been determined, we need to assess how good the fit of the PCE is to the actual model. This can be done by collecting

a number of additional test points, different from the points which were used to determine the coefficients of the PCE, and then evaluating the average or weighted average of the square of the difference between the model-based value of incrossing risk at those test points and the value predicted by the PCE. We assume that the fit is good if the average or weighted average of the squared difference is small.

4.9 Limitations of the PCE Method

The PCE method is not without its limitations. First of all we will discuss the problem of determining collocation points and secondly the number of simulation runs.

4.9.1 Practical Problem in Choosing the Collocation Points

In Subsection 4.7.3 it was explained that not every arbitrary collection of K collocation points will make the matrix H satisfy the constraint $rank(H) = N$. For a function of many parameters and a high order PCE, the possible number of collocation points M is huge. Searching for a collection of K collocation points such that $rank(H) = N$ out of the M possible collocation points is a computationally demanding and time-consuming task. From our experience, this search seems to be practical only for PCEs which have up to around 600-700 coefficients.

4.9.2 Number of Simulation Runs

The number of simulation runs that have to be executed increases rapidly with increasing number of variables and increasing order of the PCE (Figure 4.1). If there are 30 parameters and one uses a PCE expansion of order 2 then there are already 496 terms in the expansion. If we know apriori, for example based on experience, that the actual model is insensitive to some specific parameters, or if we are interested in the sensitivities for a few parameters only, then we need not evaluate all these parameters.

In the next chapter we propose a small sample Monte Carlo simulation approach of estimating statistical properties.

4.10 Relation Between the Everdij&Blom Method and the PCE

In this section we will argue that under some conditions, certain Everdij&Blom results can be interpreted as a first order PCE. According to the Everdij&Blom

methodology we have that if BUMAs 2, 3, 4, 5 and 7 hold true,

$$\rho(V) = \rho(v)\prod_{i=1}^{n_p}(\frac{V_i}{v_i})^{\beta_i}$$

Taking the natural log of both sides of the previous equation we have

$$\ln\rho(V) = \ln\rho(v) + \sum_{i=1}^{n_p}\beta_i(\ln V_i - \ln v_i) \tag{4.5}$$

Assuming that the gradient of $\ln\rho(V)$ with respect to the natural log of the parameters exists, we may interpret this as a first order Taylor expansion of $\ln\rho(V)$ with respect to the variables $(\ln V_1, \ln V_2, ..., \ln V_{n_p})$ around the point $(\ln v_1, \ln v_2, ..., \ln v_{n_p})$ for appropriate values of the $\beta_i's$.

Since the $\beta_i's$ can be interpreted as the coefficients of the Taylor expansion of $\ln\rho(V)$ w.r.t $(\ln V_1, \ln V_2, ..., \ln V_{n_p})$ around $(\ln v_1, \ln v_2, ..., \ln v_{n_p})$ then ideally $\beta_i = \frac{\partial \ln\rho(V)}{\partial \ln V_i}\Big|_{\ln V_i = \ln v_i}$. In the Everdij&Blom method, β_i^* and β_i^{**} are essentially estimates of $\frac{\partial \ln\rho(V)}{\partial \ln V_i}\Big|_{\ln V_i = \ln v_i}$. This suggests that the method can be improved upon by evaluating

$$\beta_i^{avg} = \frac{\beta_i^* + \beta_i^{**}}{2}$$

or by more elaborate numerical schemes for derivative approximation proposed in the literature. This idea is illustrated in Figure 4.2.

We should note that due to its linear nature, a first order expansion will not be able to capture any sort of curvature in the function that is to be expanded.

We will now proceed to argue that in the unbiased case the Everdij&Blom method can be interpreted as a first order PCE. If the nominal values are unbiased we have $\ln v_i = \mu_i = E\{\ln V_i\}$ and $v_i = e^{\mu_i} = c_i$. Let us first rewrite equation (4.5) as follows:

$$\begin{aligned}\ln\rho(V) &= \ln\rho(v) + \sum_{i=1}^{n_p}\beta_i(\ln V_i - \ln v_i)\\ &= \ln\rho(c) + \sum_{i=1}^{n_p}\beta_i\sigma_i\frac{(\ln V_i - \mu_i)}{\sigma_i}\end{aligned}$$

where $c = (c_1, c_2, ..., c_{n_p})$ and $\sigma_i^2 = Var\{\ln V_i\}$. Denoting $X_i = \frac{(\ln V_i - \mu_i)}{\sigma_i}$, $X = (X_1, X_2, ..., X_{n_p})$ and $\widetilde{\rho}(X) = \rho(e^{\mu_1+\sigma_1 X_1}, ..., e^{\mu_{n_p}+\sigma_{n_p}X_{n_p}})$, we have that $X_i \sim N(0,1)$, hence

$$\begin{aligned}\ln\widetilde{\rho}(X) &= \ln\rho(c) + \sum_{i=1}^{n_p}\beta_i\sigma_i X_i\\ &= a_0 + \sum_{i=1}^{n_p}a_i X_i\end{aligned} \tag{4.6}$$

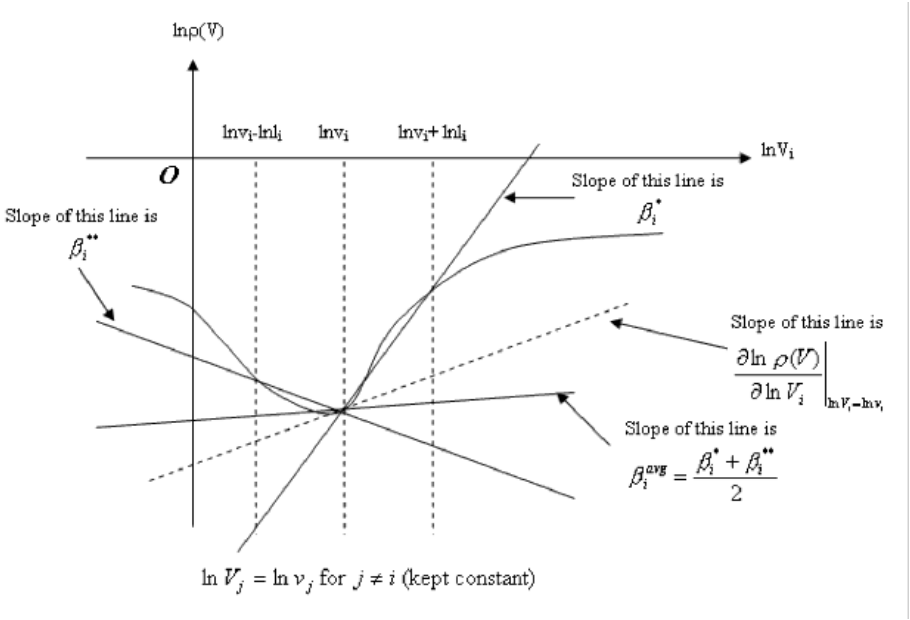

Figure 4.2: Interpreting β_i

where, $a_0 = \ln \rho(c)$ and $a_i = \beta_i \sigma_i$. We immediately recognize (4.6) as having the form of a first order PCE. Furthermore,

- The evaluation of β_i^* for $i = 1, 2, ..., n_p$ corresponds to the evaluation of the $a_i's$ based on the collocation points $x^0, x^1, ..., x^{n_p}$ where

$$x^i = \begin{cases} (0, ..., 0, ..., 0) & \text{for } i = 0 \\ (0, 0, ..., 2, ..., 0, 0) & \text{with the term 2 in the } i^{th} \text{ position for } i = 1, ..., n_p \end{cases}$$

- The evaluation of β_i^{**} for $i = 1, 2, ..., n_p$ corresponds to the evaluation of the $a_i's$ based on the collocation points $z^0, z^1, ..., z^{n_p}$ where

$$z^i = \begin{cases} (0, ..., 0, ..., 0) & \text{for } i = 0 \\ (0, 0, ..., -2, ..., 0, 0) & \text{with the term } -2 \text{ in the } i^{th} \text{ position } i = 1, ..., n_p \end{cases}$$

To see this result, we observe that $a_0 = \ln \widetilde{\rho}(x^0) = \ln \rho(c)$ and $\ln \widetilde{\rho}(x^i) = \ln \rho(c) + 2a_i$ for $i = 1, ..., n_p$. Hence a_i may be evaluated as $a_i^* = \frac{\ln \frac{\widetilde{\rho}(x^i)}{\rho(c)}}{2} = \sigma_i \frac{\ln \frac{\widetilde{\rho}(x^i)}{\rho(c)}}{\ln l_i} = \sigma_i \beta_i^*$ since by definition (see Section 3.5) $\frac{\ln l_i}{\sigma_i} = 2$ for $i = 1, ..., n_p$. Similarly, we can show that a_i may also be evaluated according to $a_i^{**} = \frac{\ln \frac{\widetilde{\rho}(z^i)}{\rho(c)}}{-2} = \sigma_i \left(-\frac{\ln \frac{\widetilde{\rho}(z^i)}{\rho(c)}}{\ln l_i} \right) = \sigma_i \beta_i^{**}$. Hence in the case of unbiased nominal values the Everdij&Blom method results in a first order PCE for $\ln \rho(V)$. We

should make note that in the unbiased case, $E\{\ln \rho(V)\}$ is always estimated as $a_0 = \ln \rho(c)$. This is another drawback of a first order expansion because it may not always be true that $E\{\ln \rho(V)\} \approx \ln \rho(c)$.

In the biased case where $\ln v_i \neq \mu_i$, X_i will not have zero mean, hence in this case (4.6) cannot be interpreted as a first order PCE. However, the reason why the estimates in the biased case are not satisfactory is that if $(\ln v_1, ..., \ln v_{n_p})$ is subtantially far from $(\mu_1, \mu_2, ..., \mu_{n_p})$ or if $\ln \rho(V)$ changes rapidly as we move $(\ln V_1, ..., \ln V_{n_p})$ away from $(\mu_1, \mu_2, ..., \mu_{n_p})$, the first order Taylor expansion of $\ln \rho(V)$ about $(\ln v_1, ..., \ln v_{n_p})$ may not give good approximation for values of $\ln \rho(V)$ about $(\mu_1, \mu_2, ..., \mu_{n_p})$. Since the region surrounding $(\mu_1, \mu_2, ..., \mu_{n_p})$ is a region of high probability, approximation errors will affect the statistical estimates significantly. Based on this we may expect that the Everdij&Blom approach may still tolerate relatively small bias. For simulation results on this, see Section 6.4.

Based on the interpretation of the Everdij&Blom method as a first order PCE, another alternative method of determining the $\beta_i's$ can be suggested: collect more than $n_p + 1$ collocation points (since at least $n_p + 1$ collocation points will be needed to evaluate the $\beta_i's$) and use a least squares method to determine the $\beta_i's$.

Chapter 5

Small Sample Monte Carlo Simulation Based Assessment

5.1 Introduction

In the previous chapter we discussed the PCE as an alternative approach in estimating the statistical properties of $\ln \mathcal{R}$. We also saw that a drawback of this method was the rapid increase in the number of coefficients of the PCE as the number of parameters and order of the PCE increased. This situation is due to the fact that in the PCE method we were trying to approximate a functional relationship between $\ln \mathcal{R}$ and V, i.e. we have to perform multivariate function approximation/interpolation. It is intuitively clear that multivariate function approximation or interpolation in many variables can be very expensive depending on the unknown relation between the variables. Therefore, if our goal is to estimate the mean and 95% CrI of $\ln \mathcal{R}$, perhaps we are doing too much. In the case where the PCE fails or is not feasible to provide a reasonable statistical estimate we should think of yet other alternative methods to estimate these statistical properties.

A further motivation for investigating alternative methods is that some simulations (to be discussed in Chapters 6 and 7) suggests that the distribution of $-\ln \mathcal{R}$ follows a lognormal distribution, i.e. $\ln(-\ln \mathcal{R}) \sim N(\mu, \sigma^2)$. If this property holds in general when the parameters are modelled as lognormal random variables and if the variance of $\ln(-\ln \mathcal{R})$ is not large then we may hope to obtain reasonably reliable estimates of μ and σ^2 and hence obtain a reasonable fit for the density of $-\ln \mathcal{R}$ even for small sample sizes. From the estimated density of $-\ln \mathcal{R}$ we may then derive other statistical estimates of interest

It seems more natural or intuitive that $-\ln \mathcal{R}$ follows a lognormal distribution rather than a normal distribution (as in the Everdij&Blom method) since

we automatically have the property

$$P(\mathcal{R} > 1) = P(\ln \mathcal{R} > 0) = P(-\ln \mathcal{R} < 0) = 0$$

Furthermore, the normal distribution can be considered as a special approximating case of the lognormal for small σ ($\sigma \downarrow 0$).

5.2 Small Sample Monte Carlo Based Estimation

Assume we have generated random samples of V, $\{V_1, V_2, ..., V_N\}$, and have used these to generate random samples of $\ln \mathcal{R}$, $\{x_1 = \ln \mathcal{R}_1, x_2 = \ln \mathcal{R}_2, ..., x_N = \ln \mathcal{R}_N\}$. Let us now view $\ln \mathcal{R}$ as a stand-alone random variable, ignoring its relationship with V. The idea is that we would like to obtain reasonable statistical estimates with only few samples of $\ln \mathcal{R}$ available (with N equal to, say, a few hundred samples). First of all we will review some basic and useful statistical tools.

5.2.1 Estimating the Mean and 95% CrI of $\ln \mathcal{R}$

Estimating the mean of $E\{\ln \mathcal{R}\}$ is straightforward, we simply average the samples of $\ln \mathcal{R}$ available, i.e. $x_1, x_2, ..., x_N$. Evaluating the 95% CI of the mean is also straightforward and a general method based on student's t-distribution is available[Rice95]. The $(1-\alpha) \times 100\%$ CI formula ($0 < \alpha < 1$) for the mean is as follows:

$$(1-\alpha) \times 100\%\ CI \text{ for mean} : [\overline{X} - \frac{S}{\sqrt{N}} t_{N-1}(\frac{\alpha}{2}), \overline{X} + \frac{S}{\sqrt{N}} t_{N-1}(\frac{\alpha}{2})] \quad (5.1)$$

where

$$\overline{X} = \frac{1}{N} \sum_{i=1}^{N} x_i$$

$$S = \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} (x_i - \overline{X})^2}$$

and $t_{N-1}(\frac{\alpha}{2})$ denotes the point beyond which the t-distribution with $N-1$ degrees of freedom has a probability $\frac{\alpha}{2}$.

Let the 95% CrI be denoted by $[A, B]$ and its estimate be denoted by $[\overline{A}, \overline{B}]$. Let $\alpha = 0.05$ and let the number of samples be N. Order the samples of $\ln \mathcal{R}$ in increasing value then let $N_l = N * \frac{\alpha}{2}$ and $N_u = N * (1 - \frac{\alpha}{2})$. Then $\overline{A}$ is evaluated as the value of sample number N_l while $\overline{B}$ is evaluated as the value of sample number N_u. Based on $[\overline{A}, \overline{B}]$, 95% CIs for both A and B can be estimated by *bootstrapping* (Section 5.4) or by a binomial distribution based method (Section 5.5).

Note that the estimate of the 95% CrI obtained by the above approach may not be reliable in the case of long-tailed distributions. For this reason, in the next subsection we explain a few approaches to improve on this situation.

5.2.2 Fitting a Continuous Density to Empirical Data

A second type of approach would be to use the samples $\{x_1, x_2, ..., x_N\}$ to estimate a density function for $\ln \mathcal{R}$ and to use this density function to determine $E\{\ln \mathcal{R}\}$ and the 95% CrI. For this purpose there seem to be three possible approaches of this type:

1. After collecting a number of samples of the random variable of interest, a histogram can be constructed. If the observed histogram suggests that the data (or the data after being transformed) can be fitted with some parametric density model (such as a normal distribution or lognormal distribution), fit a parametric density function to the observed data by first estimating the parameters of the parametric model by standard statistical techniques such as by maximum likelihood[Rice95].

2. Fit a continuous density $f_{\widehat{\ln \mathcal{R}}}$ as an estimate of the density $f_{\ln \mathcal{R}}$ of $\ln \mathcal{R}$ by the non-parametric method of kernel density estimation described in [Wand95] and employ $f_{\widehat{\ln \mathcal{R}}}$ to estimate the mean and 95% CrI.

3. Fit a continuous density f as an estimate of the density $f_{\ln \mathcal{R}}$ of $\ln \mathcal{R}$ by a newly introduced method of density estimation by support vector machines (SVMs) as explained in [Vapn98] and employ $f_{\widehat{\ln \mathcal{R}}}$ to estimate the mean and 95% CrI.

Method (1) is quite standard in statistics but depends on whether there is a suitable parametric model available to model the data. Method (3) is innovative and quite recent. It differs from (2) in that the continuous density estimate is obtained by viewing density estimation as a problem of solving an ill-posed integral equation. The ill-posedness of the problem is removed by employing a so called *regularizer* term [Vapn98]. However, to the best of our knowledge this method is not yet widely used and there are still many issues to be resolved. The density estimate obtained by method (3) is not guaranteed to be a density function (the estimate can take on negative values and may not integrate to one) and practical techniques to assess how well it can fit an unknown density function still need to be researched. The first problem with the SVM approach (3) does not appear in the kernel density estimation method of (2). However, in method (2) determining the optimal value of the so called bandwidth that achieves minimum fitting error is quite difficult unless the unknown density function is of some specific type such as a normal distribution. In cases where we have an idea of the specific density function, it is probably more convenient to employ a parametric fitting approach, i.e. method (1).

In the parts to follow in this chapter we will briefly discuss the basic ideas behind method (1), but because of the practical problems identified above we will not pursue methods (2) and (3).

5.3 Parametric Density Fitting

If a plot of the histogram of the data suggests that the data may follow a known parametric distribution then we could try fitting the parametric distribution to the data. In this section we will briefly discuss techniques to fit a normal or lognormal density to data.

In the special case where the random samples $x_1, x_2, ..., x_N$ were drawn from a normally distributed random variable, a formula for the $(1-\alpha)\times 100\%$ CI for the variance is:

$$(1-\alpha)\times 100\%\ CI \text{ for variance} : [\frac{N\widehat{\sigma}^2}{\chi^2_{N-1}(\alpha/2)}, \frac{N\widehat{\sigma}^2}{\chi^2_{N-1}(1-\alpha/2)}] \tag{5.2}$$

where

$$\widehat{\sigma}^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \overline{X})^2 \tag{5.3}$$

and $\chi^2_{N-1}(\alpha/2)$ denotes the point beyond which the chi squared distribution with $N-1$ degrees of freedom has a probability $\frac{\alpha}{2}$. Note that for large N (>120) we may use the approximation (Appendix B in [Rice95]):

$$\chi^2_N(\alpha) = \frac{1}{2}\left(z(\alpha) + \sqrt{2N-1}\right)^2$$

where $z(\alpha)$ denotes the point beyond which the standard normal distribution has a probability α.

If the distribution of a random variable Y can be modelled with a normal distribution $N(\mu, \sigma^2)$ or lognormal distribution $\Lambda(\mu, \sigma^2)$ which is parametrized by the mean, μ, and variance, σ^2, of some other random variable X which is related to Y, i.e. $X = Y$ in the case of a normal distribution and $X = \ln Y$ in the case of a lognormal distribution, then by maximum likelihood μ is estimated by $\widehat{\mu} = \overline{X}$ and σ^2 is estimated by $\widehat{\sigma}^2$[Rice95]. The estimates $\widehat{\mu}$ and $\widehat{\sigma}^2$ can be used to substitute for μ and σ^2 in the original parametric model.

5.4 Bootstrapping

The bootstrap, is a powerful and versatile computer-based method for assessing estimation variability. It is a well established and widely accepted technique in the statistics community. This section is devoted to an explanation of the ideas that motivated the development of the bootstrap method.

5.4.1 Plug-In Principle

Let $\mathbf{x} = (x_1, x_2, ..., x_N)$ be a sample of size N drawn from a scalar real valued random variable X with an unknown distribution function F. Let's say we are interested in some parameter of X. Formally, a parameter of X is defined as

a function of F. Denoting θ as a parameter, we write this functional relation as $\theta = t(F)$ where $t(F)$ means applying some numerical procedure $t(\cdot)$ to the distribution function F. Based on the sample $\mathbf{x}$ we can construct a so called *empirical distribution function* $\widehat{F}$ defined as:

$$\widehat{F}(x) = \frac{\#\{x_i \leq x\}}{N},\ x \in \mathbb{R}$$

where $\#\{x_i \leq x\}$ denotes the number of samples in $\mathbf{x}$ that have a value less than x. Note that $\widehat{F}$ assigns a probability of $\frac{1}{N}$ to each individual sample x_i and is a random function because it depends on the realization of the random sample. A *plug-in* estimate $\widehat{\theta}$ of θ is based on substituting $\widehat{F}$ for F in $t(\cdot)$, i.e. $\widehat{\theta} = t(\widehat{F})$. Note that $\widehat{\theta}$ is a statistic, i.e. it is a function of the sample $\mathbf{x}$, say $\widehat{\theta} = s(\mathbf{x})$. Statistics like $\widehat{\theta}$ which are used to estimate parameters are commonly called *summary statistics*, *estimates* or *estimators*.

5.4.2 Non-Parametric and Parametric Bootstrapping

Once we obtain an estimate $\widehat{\theta}$ we probably would also like to know how good our estimate is, for example we might wish to evaluate the standard error /deviation of $\widehat{\theta}$. Unfortunately, for a general statistic $\widehat{\theta}$ this is not always possible since to do this we need to know F, which we do not. The basic idea of *non-parametric bootstrapping* is to use $\widehat{F}$ instead of F in the estimation of the standard error, or any other appropriate measure of "goodness", of $\widehat{\theta}$.

Let $\widehat{\theta} = s(\mathbf{x})$. We generate B bootstrap samples $\mathbf{x}_1^*, \mathbf{x}_2^*, ..., \mathbf{x}_B^*$, ($\mathbf{x}_i^* \in \mathbb{R}^N$), by resampling from the sample vector $\mathbf{x} = (x_1,\ x_2, ..., x_N)$ according to $\widehat{F}$, i.e. putting uniform probability of $\frac{1}{N}$ for each x_i. Hence $\mathbf{x}_i^*$ could be $(x_1, x_2, x_2, ..., x_N)$, $(x_1, x_1, x_2, x_3, x_3, ..., x_{N-2})$, $(x_2, x_2, x_4, ..., x_N)$, et cetera. Based on these samples we obtain $\widehat{\theta}^* = (\widehat{\theta}_1^*, \widehat{\theta}_2^*, ..., \widehat{\theta}_N^*)$, where $\widehat{\theta}_i^* = s(\mathbf{x}_i^*)$ is called a bootstrap replication of $\widehat{\theta}$. With an appropriate estimator (this has to be treated case by case, depending on the parameter to be estimated), we may use $\widehat{\theta}^*$ to estimate quantities such as the standard error of $\widehat{\theta}$. Note that this approach can be applied to virtually any statistic, no matter how mathematically complicated $s(\cdot)$ might be.

The method explained above is called non-parametric since no special functional form was assumed for $\widehat{F}$, such as a normal or exponential distribution function. It is possible that we have knowledge that F follows some specific distribution with unknown parameters, in this case we may wish to model $\widehat{F}$ as having the specified distribution but using the estimated parameters instead of the true parameters. In this case we can again generate $\widehat{\theta}^*$ as above and the technique is called *parametric bootstrapping*.

5.4.3 Bootstrap Confidence Intervals

A problem which has been studied intensively by researchers in the area of bootstrapping is that of bootstrap estimation of the $(1-\alpha) \times 100\%$ confidence

interval (CI) of a parameter θ, where $0 < \alpha < 1$ (for a background on the concept of CIs the reader may consult [Rice95]). Several methods have been proposed to do this, among which are the bootstrap-t method, the bootstrap percentile method and the BC_a algorithm [Efro93]. The most sophisticated algorithm of the three is the BC_a algorithm. BC_a stands for *bias corrected and accelerated*, the mathematical motivation for this naming can be found in Chapter 22 of [Efro93]. We describe this algorithm below, for more detail refer to Chapter 14 and 22 of [Efro93].

As before let $\widehat{\theta} = s(\mathbf{x})$ be an estimate of θ, where $\mathbf{x}$ is a sample of size N. Based on $\mathbf{x}$ let us generate B bootstrap replications of $\widehat{\theta}$, i.e. $\widehat{\theta}^*_1, \widehat{\theta}^*_2, ..., \widehat{\theta}^*_N$. Define

$$\widehat{z}_0 = \Phi^{-1}\left(\frac{\#\{\widehat{\theta}^*_i < \widehat{\theta}\}}{B}\right) \text{ (called the } \textit{bias correction}\text{)}$$

where $\Phi^{-1}(\cdot)$ indicates the inverse of the standard normal cumulative distribution function, e.g. $\Phi^{-1}(0.95) = 1.645$. Let $\mathbf{x}_{(i)}$ denote $\mathbf{x}$ with the i^{th} point x_i removed and let $\widehat{\theta}_{(i)} = s(\mathbf{x}_{(i)})$. Define

$$\widehat{\theta}_{(\cdot)} = \frac{\sum_{i=1}^{N} \widehat{\theta}_{(i)}}{N}$$

and

$$\widehat{a} = \frac{\sum_{i=1}^{N} (\widehat{\theta}_{(\cdot)} - \widehat{\theta}_{(i)})^3}{6\{\sum_{i=1}^{N} (\widehat{\theta}_{(\cdot)} - \widehat{\theta}_{(i)})^2\}^{3/2}} \text{ (called the } \textit{acceleration}\text{)}$$

Let

$$\alpha_1 = \Phi\left(\widehat{z}_0 + \frac{\widehat{z}_0 + z^{(\alpha/2)}}{1 - \widehat{a}(\widehat{z}_0 + z^{(\alpha/2)})}\right)$$

$$\alpha_2 = \Phi\left(\widehat{z}_0 + \frac{\widehat{z}_0 + z^{(1-\alpha/2)}}{1 - \widehat{a}(\widehat{z}_0 + z^{(1-\alpha/2)})}\right)$$

where $z^{(\alpha)}$ denotes the 100α percentile point of a standard normal distribution, e.g. $z^{(0.95)} = 1.645$. Then the BCa estimate of the CI of θ is given by:

$$BC_a \text{ CI: } \left[\widehat{\theta}_{lo}, \widehat{\theta}_{up}\right] = \left[\widehat{\theta}^{*(\alpha_1)}, \widehat{\theta}^{*(\alpha_2)}\right]$$

where $\widehat{\theta}^{*(\alpha_1)}$ ($\widehat{\theta}^{*(\alpha_2)}$) denotes the $100\alpha_1$ ($100\alpha_2$) percentile point of the bootstrap replications.

The BC_a method has been shown to have two theoretical advantages:

1. The BC_a method is *transformation respecting*, meaning that BC_a endpoints transform correctly if we change the parameter of interest from θ to some monotonic function of θ.

2. If $\left[\widehat{\theta}_{lo}, \widehat{\theta}_{hi}\right]$ is a perfect estimate then we would have

$$P\{\theta < \widehat{\theta}_{lo}\} = \frac{\alpha}{2} \text{ and } P\{\theta > \widehat{\theta}_{hi}\} = \frac{\alpha}{2}$$

Unfortunately it is not a perfect estimate. However, it has been proven that it is *second order accurate*. This means that

$$P\{\theta < \widehat{\theta}_{lo}\} = \frac{\alpha}{2} + \frac{c_{lo}}{N} \text{ and } P\{\theta > \widehat{\theta}_{hi}\} = \frac{\alpha}{2} + \frac{c_{hi}}{N}$$

for two constants c_{lo} and c_{hi}. The other two methods mentioned earlier are only first order accurate, i.e.

$$P\{\theta < \widehat{\theta}_{lo}\} = \frac{\alpha}{2} + \frac{c_{lo}}{\sqrt{N}} \text{ and } P\{\theta > \widehat{\theta}_{hi}\} = \frac{\alpha}{2} + \frac{c_{hi}}{\sqrt{N}}$$

The second order accuracy of the BC_a algorithm suggests that it is a possible candidate for our purpose. A second order accuracy is more desirable than a first order since it has better convergence with respect to sample size.

5.5 A Simpler Technique for 95% CI Estimation

We should mention here that in fact for sufficiently large N it is not really necessary to employ the bootstrap to estimate the 95% CI of a percentile point such as A and B. To see this let's say that we would like to estimate the 100α percentile of a random variable X, let X^* denote the 100α percentile point of X and let $X_1, X_2, ..., X_N$ be N random samples of X. Note that $P(X_i \leq X^*) = \alpha$ for $i = 1, ..., N$. Let us first reorder $X_1, X_2, ..., X_N$ in ascending order and denote the ordered samples as $X'_1, X'_2, ..., X'_N$. Define Y_i as follows:

$$Y_i = \begin{cases} 0 & \text{if } X'_i > X^* \\ 1 & \text{if } X'_i \leq X^* \end{cases}$$

for $i = 1, 2, ..., N$. Clearly Y_i is a Bernoulli random variable with $P(Y_i = 1) = \alpha$ and $P(Y_i = 0) = 1 - \alpha$. Consider the random variable

$$Z = \sum_{i=1}^{N} Y_i$$

then Z follows a binomial distribution and Z can be interpreted as the number of samples in $\{X'_1, X'_2, ..., X'_N\}$ which fall below the point X^*. If $N\alpha > 5$ and $N(1-\alpha) > 5$ then the binomial distribution Z can be approximated reasonably well by a normal random variable with mean $N\alpha$ and variance $N\alpha(1-\alpha)$[Rice95]. Hence for sufficiently large N (> 200), the 95% CI for Z can be approximated as:

$$\left[N\alpha - 1.96\sqrt{N\alpha(1-\alpha)}, N\alpha + 1.96\sqrt{N\alpha(1-\alpha)}\right]$$

and the 95% CI for X^* is roughly

$$\left[X'_{\lceil N\alpha - 1.96\sqrt{N\alpha(1-\alpha)}\rceil}, X'_{\lceil N\alpha + 1.96\sqrt{N\alpha(1-\alpha)}\rceil}\right]$$

where $\lceil\cdot\rceil$ denotes the operation of rounding towards the nearest integer.

However, the above only applies in the special case of estimating the 95% CI of a quantile and is not for general purpose. On the other hand, the bootstrap can be employed to derive a CI estimate of almost any statistic. Thus it will very useful if we would later be interested in a quantity other than the 95% CrI. Furthermore the bootstrap does not make use of any "approximately normal" arguments.

Therefore we proceed to use the bootstrap anyway, to illustrate its usefulness and also because it might find further applications in future research.

5.6 Non-Parametric or Parametric Bootstrapping?

In the case of estimating a quantile CI, the choice of parametric or non-parametric bootstrap can be crucial. When we have a small sample of a random variable X we should first observe the histogram of X. If it seems that X has long tails, then the non-parametric bootstrapping method for quantile CI estimation will be likely to perform poorly due to the fact that the samples may not represent the tails adequately. In such cases it is imperative to use a parametric method where we fit some specific functional form $\widehat{F}_{parametric}$ for the observed distribution (assuming that such a functional exists). A parametric approach will allow the long tails to be modelled more adequately and tail samples can be generated by drawing a large number of samples from a random variable which has a distribution according to $\widehat{F}_{parametric}$.

Finally, we would like to conclude this chapter with the following remark:

Remark 5.1 *If no known parametric density function seem to fit the histogram of the random samples then we don't have much choice but to apply the small sample non-parametric bootstrap to evaluate standard error or confidence intervals even if it seems that the distribution has long tails. However, we should note that in most situations it is unlikely for* $\ln\mathcal{R}$ *to have long tails to the right (towards zero) since* $\ln\mathcal{R}$ *is bounded from above by zero. Hence we may still expect to obtain a reasonable estimate of the upper bound of the 95% CrI of* $\ln\mathcal{R}$.

Part II

Simulation and Analysis of Results

Chapter 6

First Test Case: Gaussian Lateral Deviations

In this chapter we implement the theories discussed in the preceeding chapters to evaluate the uncertainty of incrossing risk due to uncertainty in the parameter values, using a simple scenario involving a pair of jointly Gaussian aircraft.

6.1 Model of Evolution of Two Aircraft

First we give a description of the particular scenario that will be studied. The model was adopted from [Prib00]. Consider two aircraft flying at roughly the same altitude in parallel but opposite directions. Let the nominal distance of their parallel paths be S (see Figure 6.1).

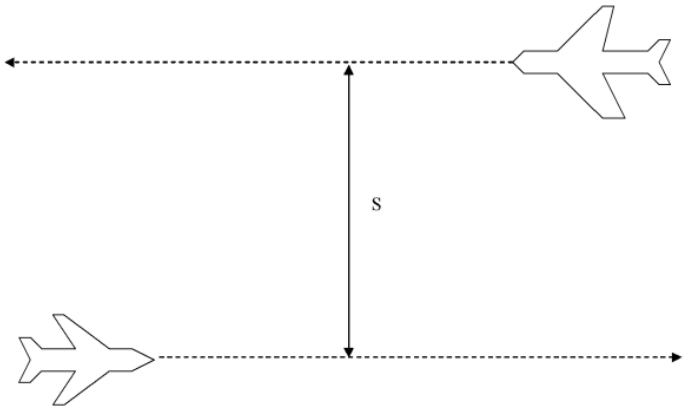

Figure 6.1: Two parallel aircraft flying in opposite directions

Let $x^i = (x_1^i, x_2^i, x_3^i)^T$ and $v^i = (v_1^i, v_2^i, v_3^i)^T$ denote the position and velocity

of aircraft i in the x, y, z direction (the subscripts 1, 2, 3 correspond to the motion component in the x, y and z direction, respectively). We model the aircraft motion based on the following hypothetical assumptions:

1. The motion of each aircraft in the x, y, z directions are independent of each other.
2. The motions of the two aircraft are independent of each other.

For each motion component of aircraft i we assume the following dynamical model:

$$x_j^i(t) = \overline{x}_j^i(t) + \widetilde{x}_j^i(t)$$
$$v_j^i(t) = \overline{v}_j^i(t) + \widetilde{v}_j^i(t)$$
$$d\widetilde{v}_j^i(t) = -a_j^i \widetilde{x}_j^i(t)dt - b_j^i \widetilde{v}_j^i(t)dt + c_j^i dw_j^i(t),\ \widetilde{v}_j^i(0) \sim N(0, (\alpha_j^i)^2), \alpha_j^i \geq 0$$
$$\overline{v}_j^i(t) = v_{j,nom}^i$$
$$\overline{x}_j^i(t) = x_{j,0}^i + v_{j,nom}^i t$$
$$d\widetilde{x}_j^i(t) = \widetilde{v}_j^i(t)dt,\ \widetilde{x}_j^i(0) \sim N(0, (\beta_j^i)^2), \beta_j^i \geq 0$$

where $a_j^i, b_j^i, c_j^i, v_{j,nom}^i, x_{j,0}^i$ are positive real constants for all i, j, $\widetilde{v}_j^i(0)$ and $\widetilde{x}_j^i(0)$ are independent real-valued random variables and $w_j^i(t)$ are mutually independent standard Brownian motions for all i, j. Let $\widetilde{z}^i(t) = (\widetilde{x}^i(t)^T, \widetilde{v}^i(t)^T)^T$, $\overline{z}^i(t) = (\overline{x}^i(t)^T, \overline{v}^i(t)^T)^T$ and $w^i(t) = (w_1^i(t), w_2^i(t), w_3^i(t))^T$. For notational convenience we shall sometimes write $z^i(t)$, $x^i(t)$, $w^i(t)$ etc as z_t^i, x_t^i, w_t^i etc. We can rewrite the previous dynamical model in a more compact form as follows:

$$\frac{d}{dt}\widetilde{z}^i(t) = \underbrace{\begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ -a_1^i & 0 & 0 & -b_1^i & 0 & 0 \\ 0 & -a_2^i & 0 & 0 & -b_2^i & 0 \\ 0 & 0 & -a_3^i & 0 & 0 & -b_3^i \end{bmatrix}}_{A^i} \widetilde{z}^i(t) + \underbrace{\begin{bmatrix} 0 \\ 0 \\ 0 \\ c_1^i \\ c_2^i \\ c_3^i \end{bmatrix}}_{B^i} N^i(t) \quad (6.1)$$

$$\widetilde{z}^i(0) = \begin{bmatrix} \widetilde{x}_1^i(0) \\ \widetilde{x}_2^i(0) \\ \widetilde{x}_3^i(0) \\ \widetilde{v}_1^i(0) \\ \widetilde{v}_2^i(0) \\ \widetilde{v}_3^i(0) \end{bmatrix}$$
$$z^i(t) = \overline{z}^i(t) + \widetilde{z}^i(t)$$

where $N^i(t) = \frac{dw^i(t)}{dt}$ (white noise). Since $z(t)$ is jointly Gaussian for $t \geq 0$, it is completely characterized by its mean vector, $\mu_t^i = E\{z_t^i\}$, and its covariance matrix, $P^i(t) = E\{(z_t^i - Ez_t^i)(z_t^i - Ez_t^i)^T\}$. It is easy to see that

$$\mu_t^i = \overline{z}^i(t)$$

According to [Bagc93], the symmetric positive definite matrix $P^i(t)$ satisfies the following matrix differential equation:

$$\frac{d}{dt}P^i(t) = A^iP^i(t) + P^i(t)(A^i)^T + B^i(B^i)^T$$

with

$$P^i(0) = P_0^i$$

which can be solved to obtain the entries for $P^i(t)$. However, we will be primarily interested in the steady state condition in which $\lim_{t\to\infty}\frac{d}{dt}P^i(t) = 0$, i.e. $P^i(t) = P_\infty^i$ where P_∞^i is a constant symmetric positive definite matrix. P_∞^i can be obtained by solving the algebraic Riccati equation (ARE):

$$A^iP_\infty^i + P_\infty^i(A^i)^T + B^i(B^i)^T = 0$$

Solving the ARE we obtain $P_\infty^i = \begin{bmatrix} P_1^i & P_2^i \\ P_2^i & P_3^i \end{bmatrix}$ where for $k, l = 1, 2, 3$

$$(P_1^i)_{kl} = \frac{(c_k^i)^2}{a_k^ib_k^i}\delta_{kl} = (\gamma_k^i)^2\delta_{kl}$$

$$(P_2^i)_{kl} = 0$$

$$(P_3^i)_{kl} = \frac{(c_k^i)^2}{2b_k^i} = (\omega_k^i)^2\delta_{kl}$$

where $\gamma_k^i = \frac{c_k^i}{\sqrt{a_k^ib_k^i}}$, $\omega_k^i = \frac{c_k^i}{\sqrt{2b_k^i}}$ and δ_{kl} is Kronecker's delta:

$$\delta_{kl} = \begin{cases} 1 \text{ if } k = l \\ 0 \text{ if } k \neq l \end{cases}$$

Let $x_t^s = x_t^1 - x_t^2$ and $v_t^s = v_t^1 - v_t^2$. Denote $s_t = ((x_t^s)^T, (v_t^s)^T)^T$ as the separation process $s_t = z_t^1 - z_t^2$. It is quite clear that since both aircraft are independent of each other that

$$E\{s_t\} = \mu_t^s = \overline{z}^1(t) - \overline{z}^2(t)$$

$$E\{(s_t - \mu_t^s)(s_t - \mu_t^s)^T\} = P_\infty^s = P_\infty^1 + P_\infty^2$$

hence the joint distribution of the position and velocity component of the separation process is:

$$p_{x_t^s, v_t^s}(x, v) = \frac{1}{\sqrt{2\pi\,|P_\infty^s|}}e^{-(s-\mu_t^s)^T(P_\infty^s)^{-1}(s-\mu_t^s)} \text{ where } s = (x^T, v^T)$$

After obtaining $p_{x_t^s, v_t^s}(x, v)$ we may evaluate the incrossing risk with Theorem 2.1. However, for the case of jointly Gaussian aircraft the evaluation of incrossing risk may be further simplified and is summarized in Theorem 1 of [Blom02]. As we shall see later on (Subsection 6.4.3), the evaluation of the incrossing risk may be simplified once again in the case of steady state jointly Gaussian aircraft.

6.2 Parameter Values

In this section we will discuss the nominal values taken for the parameters and how we model the uncertainty about the values of the parameters.

6.2.1 Nominal parameter values

Let the collision area surrounding aircraft one be a box of dimension $s_1 \times s_2 \times s_3$. In our scenario we take $S = 15,000$ m (corresponding to 15 km), $s_1 = 50$ m, $s_2 = 50$ m, $s_3 = 15$ m, $x^1_{1,0} = -20,000$ m, $x^2_{1,0} = 20,000$ m, $x^1_{2,0} = 0$ m, $x^2_{2,0} = S$, $x^1_{3,0} = x^2_{3,0} = 10,000$ m, and $v^i_{2,nom} = v^i_{3,nom} = 0$ m/s for $i = 1, 2$. Note that α^i_j and β^i_j can have any arbitrary value for $i = 1, 2$ and $j = 1, 2, 3$ since they do not effect the steady state distribution. We assume that the nominal values for the parameters ω^i_1, ω^i_2, ω^i_3, γ^i_1, γ^i_2, γ^i_3, $v^i_{1,nom}$ for $i = 1, 2$ are:

Parameter	Nominal value	Dimension
$v^1_{1,nom}$	v_1 =240	m/s
γ^1_1	v_2 =1000	m
γ^1_2	v_3 =900	m
γ^1_3	v_4 =20	m
ω^1_1	v_5 =10	m/s
ω^1_2	v_6 =10	m/s
ω^1_3	v_7 =1	m/s
$\lvert v^2_{1,nom} \rvert$	v_8 =240	m/s
γ^2_1	v_9 =1000	m
γ^2_2	v_{10} =900	m
γ^2_3	v_{11} =20	m
ω^2_1	v_{12} =10	m/s
ω^2_2	v_{13} =10	m/s
ω^2_3	v_{14} =1	m/s

Remark 6.1 *We do not consider the parameters a^i_j, b^i_j, c^i_j separately, but lump them into the parameters γ^i_j and ω^i_j ($i = 1, 2$, $j = 1, 2, 3$) since we have the relation $\gamma^i_j = \frac{c^i_j}{\sqrt{a^i_j b^i_j}}$ and $\omega^i_k = \frac{c^i_j}{\sqrt{2b^i_j}}$. Hence instead of modelling the uncertainty of a^i_j, b^i_j, c^i_j separately, we model the uncertainty of γ^i_j and ω^i_j.*

Hence $(v_1, v_2, ..., v_{14})$ is our set of nominal values. Note that the actual sign of $v^2_{1,nom}$ is negative since aircraft 2 is travelling a direction opposite to aircraft 1; this sign is incorporated in the simulations to follow but the value that is varied is that of $\lvert v^2_{1,nom} \rvert$.

6.2.2 Model of Uncertainty in the Parameter Values

We assume that the uncertainty about the value of a parameter V_i can be modelled as a random variable $\Lambda(\mu_i, \sigma^2_i)$ such that the 95% credibility interval

(CrI) of V_i (see Definition 3.1) is the interval $[\exp(\mu_i)/l_i, l_i \exp(\mu_i)]$ where $l_i = \exp(2\sigma_i)$. Conversely we could also have started by defining that 95% of the time V_i lies in $[c_i/l_i, c_i l_i]$ for some constants c_i and l_i, and to achieve this we assume that $V_i \sim \Lambda(\ln(c_i), \frac{1}{4}(\ln(l_i))^2)$. Note that it may occur that $c_i \neq v_i$. In such a case, according to [Ever02] we say that v_i is *biased*. In Figure 6.2 we summarize how the uncertainty in each parameter is modelled.

Parameter	c_i	l_i	95% CrI
$V_1 = \nu^1_{1,nom}$	228	1.14	[200,260]
$V_2 = \gamma^1_1$	1000	2.25	[444,2250]
$V_3 = \gamma^1_2$	760	1.1	[691,836]
$V_4 = \gamma^1_3$	20	1.5	[13.33,30]
$V_5 = \varpi^1_1$	10	2.25	[4.44,22.5]
$V_6 = \varpi^1_2$	10	2.25	[4.44,22.5]
$V_7 = \varpi^3_1$	1	2.25	[0.444,2.25]
$V_8 = \lvert\nu^2_{1,nom}\rvert$	228	1.14	[200,260]
$V_9 = \gamma^2_1$	1000	2.25	[444,2250]
$V_{10} = \gamma^2_2$	760	1.1	[691,836]
$V_{11} = \gamma^2_3$	20	1.5	[13.33,30]
$V_{12} = \varpi^2_1$	10	2.25	[4.44,22.5]
$V_{13} = \varpi^2_2$	10	2.25	[4.44,22.5]
$V_{14} = \varpi^2_3$	1	2.25	[0.444,2.25]

Figure 6.2: Modelling of uncertainty in the parameters

Figure 6.2 indicates that the list contains four nominal values that are biased, i.e. for which $c_i \neq v_i$. These are v_1, v_8, v_3 and v_{10}.

6.3 Results from Direct Monte Carlo Simulation

Given the fixed and random valued parameters in Section 6.2, we can use direct Monte Carlo simulations on the actual model to estimate $E\{\ln(\mathcal{R})\}$ and the 95% CrI of $\ln(\mathcal{R})$. Note that throughout the rest of this chapter an estimate of $E\{\ln(\mathcal{R})\}$ will be denoted by $\overline{\ln(\mathcal{R})}$

The results of 20,000 Monte Carlo runs are presented in Figure 6.3.

$\overline{\ln(\Re)}$	95% CI for $E\{\ln(\Re)\}$	$\overline{A}$	$\overline{B}$	Bootstrap 95% CI for A	Bootstrap 95% CI for B
-101.53	[-101.62, -101.44]	-114.79	-89.51	[-115.07, -114.56]	[-89.71, -89.37]

$\overline{\ln(\Re)}$ is an estimate of $E\{\ln(\Re)\}$ and $[\overline{A}, \overline{B}]$ is an estimate of the 95% CrI of $\ln(\Re)$ using 20,000 samples. Approximate CIs for A and B were obtained using 1000 bootstrap samples.

Figure 6.3: Statistical estimates obtained via direct Monte Carlo simulations

Since the bootstrap CI for A and B are relatively tight, we may assume that $[\overline{A}, \overline{B}]$ is a good estimate of the true 95% CrI.

6.4 Results from the Everdij&Blom Method

In this section we use the bias and uncertainty assessment method of [Ever02] to estimate $E\{\ln(\mathcal{R})\}$ and the 95% CrI of $\ln(\mathcal{R})$. Note that in the terminology of Chapter 3, according to the Everdij&Blom method

$$\begin{aligned}\overline{\ln \mathcal{R}} &= E\left\{\ln\left[\rho(\mathbf{1},v)\prod_{i=1}^{n_p}\left(\frac{V_i}{v_i}\right)^{\beta_i}\right]\right\} \\ &= E\left\{\ln\rho(\mathbf{1},v)+\sum_{i=1}^{n_p}\beta_i(\ln V_i-\ln v_i)\right\} \\ &= \ln\rho(\mathbf{1},v)+\sum_{i=1}^{n_p}\beta_i(\mu_i-\ln v_i)\end{aligned}$$

and the 95% CrI of $\overline{\ln \mathcal{R}}$ is evaluated by taking the natural logs of the Everdij & Blom 95% CrI (due to the monotonicity of $\ln(\cdot)$, if $P(a \le \mathcal{R} \le b) = \alpha$ then $P(\ln a \le \ln \mathcal{R} \le \ln b) = \alpha$).

6.4.1 Estimation using biased nominal parameter values

Note from Figure 6.2 that four of the parameter values used are biased; the nominal values were not in the centre of the 95% CrI, i.e. $v \neq c$. Instead of evaluating and using $\ln\rho(\mathbf{1}, c)$ to estimate $E\{\ln\rho(\mathbf{1}, V)\}$, the Everdij&Blom bias and uncertainty assessment method evaluates $\ln\rho(1, v)$ and next tries to compensate for the bias in parameter values by adding the term $\sum_{i=1}^{n_p}\beta_i(\mu_i - \ln v_i)$, with $\mu_i = \ln c_i$. In this subsection and Subsection 6.4.2 we try to evaluate if this compensation method works.

The values of the $\beta_i's$ are evaluated in three different ways, using β_i^*, β_i^{**} and $\beta_i^{\text{safety conservative}}$ as explained in Section 3.5.

First, the natural log of $\rho(\mathbf{1}, v)$ was determined:

$$\ln\rho(\mathbf{1},v) = -73.77$$

next a bias compensation term $\sum_{i=1}^{14} \beta_i(\mu_i - \ln v_i)$ was added to $\ln \rho(\mathbf{1},v)$. This term appeared to be equal to about -23.2, depending on the method used to evaluate β_i. Figures 6.4, 6.5 and 6.6 show the results of applying the Everdij&Blom method to estimate $E\{\ln(\mathcal{R})\}$ and the 95% CrI for $\ln(\mathcal{R})$ using the nominal values of the parameters in Section 6.2.

	$\overline{\ln(\Re)}$	95% CrI for $\ln(\Re)$	$\overline{e^2}$
Using β_i^{**}	-96.91	[-106.15, -87.68]	771.16
Using β_i^{*}	-97.07	[-106.36, -87.78]	771.49
Safety conservative	-96.91	[-106.15, -87.68]	771.58

$\overline{\ln(\Re)}$ and 95% CrI for $\ln(\Re)$ based on the Everdij/Blom methodology when the parameters of the nominal model are

$v_1 = v_8 = 240,\ v_2 = v_9 = 1000,\ v_3 = v_{10} = 900, v_4 = v_{11} = 20, v_5 = v_{12} = 10,$

$v_6 = v_{13} = 10, v_7 = v_{14} = 1$ (biased in v_1, v_8, v_3 and v_{10})

$\overline{e^2}$ denotes the average of the square of approximation errors over 20000 random samples of the parameters.

Figure 6.4: Results of applying the Everdij/Blom method when some of the v_is are biased

Parameters	Nominal value v_i	l_i	β_i^{*}	β_i^{**}	$\beta_i^{\text{safety conservative}}$
V_1, V_8	240	1.14	1.328×10^{-1}	-1.642×10^{-1}	-1.642×10^{-1}
V_2, V_9	1000	2.25	2.40×10^{-2}	-2.4×10^{-2}	-2.4×10^{-2}
V_3, V_{10}	900	1.1	68.86	68.49	68.49
V_4, V_{11}	20	1.5	-5.111×10^{-1}	-4.101×10^{-1}	-5.111×10^{-1}
V_5, V_{12}	10	2.25	2.40×10^{-2}	-2.40×10^{-2}	-2.40×10^{-2}
V_6, V_{13}	10	2.25	4.626×10^{-2}	-1.712×10^{-2}	4.626×10^{-2}
V_7, V_{14}	1	2.25	3.026×10^{-2}	-2.208×10^{-2}	3.026×10^{-2}

Figure 6.5: Values of the β_i's evaluated with the Everdij/Blom method

From Figures 6.4 and 6.6 we can observe that the mean of the Everdij&Blom estimate is biased to the right of the Monte Carlo estimate (compare the Everdij & Blom $\overline{\ln \mathcal{R}}$ estimate -96.91 with the Monte Carlo estimate -101.53) and so are the 95% CrI estimates (compare the Everdij & Blom 95% CrI estimate $[-106.15, -87.68]$ with the direct Monte Carlo estimate $[-114.79, -89.51]$). Furthermore, the Everdij&Blom estimate of the width of the 95% CrI (e.g. $106.15 - 87.68 = 18.47$) is considerably smaller than the direct Monte Carlo estimate of $114.79 - 89.51 = 25.28$.

We can also observe that the three methods of determining β_i give results which almost coincide with each other. The reason for this is because there are

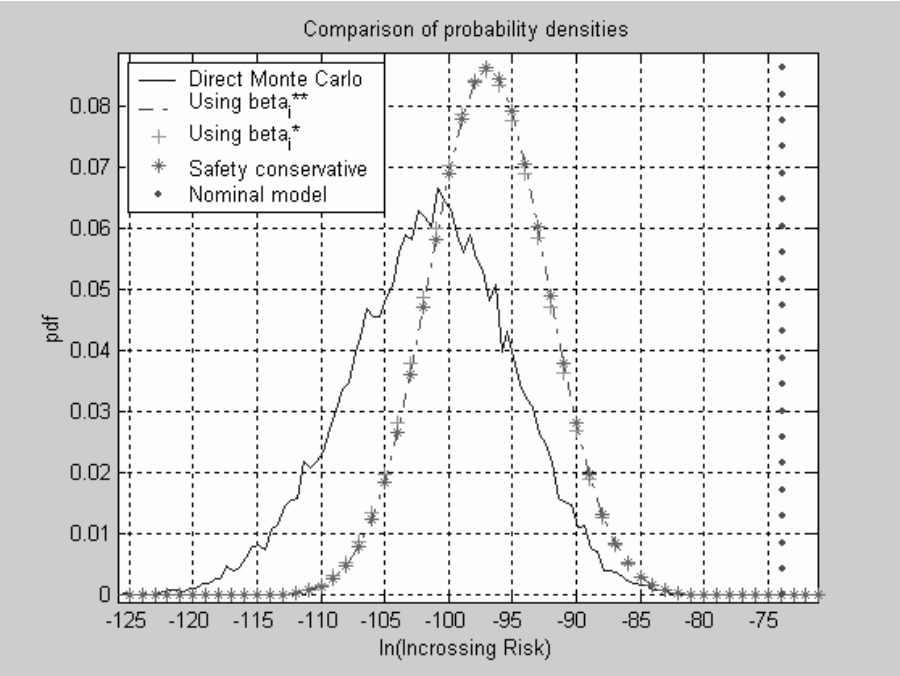

Figure 6.6: Comparison of direct Monte Carlo histogram with the Everdij/Blom density estimates when some of the $v_i's$ are biased

two dominant values of β_i, i.e. β_3 and β_{10}. All other $\beta_i's$ are much smaller than β_3 and β_{10} hence their effect becomes negligible. Because the three methods give more or less the same estimate for β_3 and β_{10}, different estimates for the other $\beta_i's$ do not really matter, hence the three methods seem to coincide. However, we should not make an inference from this particular example that the three methods will coincide in all cases.

6.4.2 Estimation using unbiased nominal parameter values

We now repeat the Everdij&Blom procedure for the case where the nominal values of the parameters take on the following unbiased values:

Parameter	Nominal value	Dimension
$v^1_{1,nom}$	$v_1 = c_1$ =228	m/s
γ^1_1	$v_2 = c_2$ =1000	m
γ^1_2	$v_3 = c_3$ =760	m
γ^1_3	$v_4 = c_4$ =20	m
ω^1_1	$v_5 = c_5$ =10	m/s
ω^1_2	$v_6 = c_6$ =10	m/s
ω^1_3	$v_7 = c_7$ =1	m/s
$v^2_{1,nom}$	$v_8 = c_8$ =228	m/s
γ^2_1	$v_9 = c_9$ =1000	m
γ^2_2	$v_{10} = c_{10}$ =760	m
γ^2_3	$v_{11} = c_{11}$ =20	m
ω^2_1	$v_{12} = c_{12}$ =10	m/s
ω^2_2	$v_{13} = c_{13}$ =10	m/s
ω^2_3	$v_{14} = c_{14}$ =1	m/s

The natural log of the nominal risk in this unbiased case is:

$$\ln(\rho(\mathbf{1}, v)) = \ln(\rho(\mathbf{1}, c)) = -101.51$$

Note that since all nominal values are unbiased we have that $\sum_{i=1}^{14} \beta_i(\mu_i - \ln v_i) = 0$, hence $\overline{\ln(\mathcal{R})} = \ln \rho(1, c)$. The results of the Everdij&Blom method are shown in Figures 6.7 and 6.8. It is clear that in this case the Everdij&Blom method gives a much better estimate of $E\{\ln(\mathcal{R})\}$ and its 95% CrI compared to the biased case.

	$\overline{\ln(\mathfrak{R})}$	95% CrI for $\ln(\mathfrak{R})$	$\overline{e^2}$
Using β_i^{**}	-101.51	[-114.49, -88.54]	0.1911
Using β_i^{*}	-101.51	[-114.55, -88.48]	0.1924
Safety conservative	-101.51	[-114.55 -88.48]	0.1919

$\overline{\ln(\mathfrak{R})}$ and 95% CrI for $\ln(\mathfrak{R})$ based on the Everdij/Blom methodology when the parameters of the nominal model are

$\nu_1 = \nu_8 = 228, \nu_2 = \nu_9 = 1000, \nu_3 = \nu_{10} = 760, \nu_4 = \nu_{11} = 20, \nu_5 = \nu_{12} = 10,$

$\nu_6 = \nu_{13} = 10, \nu_7 = \nu_{14} = 1$ (unbiased)

$\overline{e^2}$ denotes the average of the square of approximation errors over 20000 random samples of the parameters.

Figure 6.7: Results of applying the Everdij/Blom method when the v_i's are unbiased.

This confirms the Everdij&Blom suggestion that the method may perform better in the case where all nominal values are unbiased. However, their reasoning was that under the assumption that all parameter values are unbiased

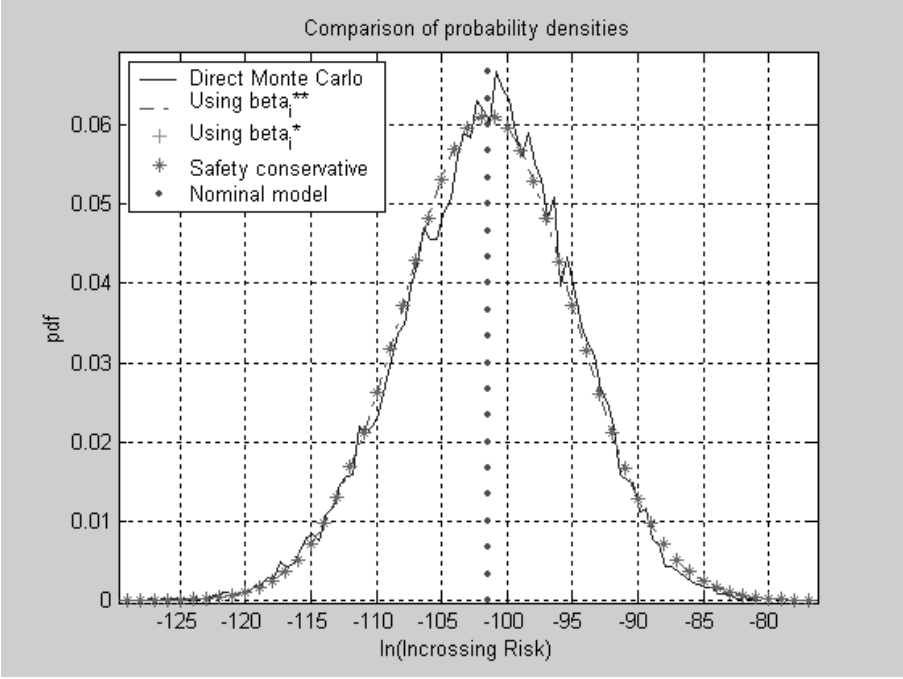

Figure 6.8: Comparison of the direct Monte Carlo histogram and the Everdij/Blom density estimates when the $v_i's$ are unbiased.

BUMA 7 (i.e. there exists β_i as a solution of two different equations, see Subsection 3.4.1) will hold because the first equation becomes zero and clearly there will always be some β_i which will satisfy the second equation. From our point of view, the method works better in the unbiased case because the effect of approximation errors due to a first order Taylor expansion is reduced (see Section 4.10 and Figure 4.2).

Again we see that the three methods of determining the $\beta_i's$ give results which almost coincide. The reason for this is the same as that given in the analysis of the case of biased nominal values.

Although Figure 6.8 indicates that the density of $\ln \mathcal{R}$ can be closely approximated by a Gaussian density, we can also observe that the histogram of $\ln \mathcal{R}$ has a slightly negative skew (longer tail to the left); this implies that $-\ln \mathcal{R}$ has a positive skew and suggests that $-\ln \mathcal{R}$ may have an approximately lognormal distribution (see also Figure 6.10).

6.4.3 Sensitivity of Incrossing Risk to the Parameters

From the values of the $\beta_i's$ in Figure 6.5 we observe two large ones: β_3, corresponding to $V_3 = \gamma_2^1$, and β_{10}, corresponding to $V_{10} = \gamma_2^2$. This indicates that $\mathcal{R}$ is very sensitive to these two parameters, $\mathcal{R}$ can change in orders for magnitude

for a small change in V_3 or V_{10} when the other parameters are kept at their nominal values.

This unusual insensitivity is not due to simulation coding error, but can be shown to be a property due to the jointly Gaussian model of the aircraft and due to the setup of the particular scenario. In the following we will argue why this sensitivity is true.

Let $x_t, v_t \in \mathbb{R}^3$ denote the position and velocity component of the separation process. Since we have a steady state scenario all covariance matrices are constant. Let Q_x, Q_v denote the covariance matrix of x_t, v_t, respectively, and let $Q_{x,v}$ be the cross-covariance matrix between x and v. For our scenario we have that:

$$Q_x = \begin{bmatrix} (\gamma_1^*)^2 & 0 & 0 \\ 0 & (\gamma_2^*)^2 & 0 \\ 0 & 0 & (\gamma_3^*)^2 \end{bmatrix}, Q_v = \begin{bmatrix} (\omega_1^*)^2 & 0 & 0 \\ 0 & (\omega_2^*)^2 & 0 \\ 0 & 0 & (\omega_3^*)^2 \end{bmatrix}$$

and

$$Q_{x,v} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \mu_v = [v_{1,0}, 0, 0]^T$$

where $\mu_v = E\{v_t\}$, $v_{1,0} = v_{1,nom}^1 - v_{1,nom}^2$, $(\gamma_k^*)^2 = (\gamma_k^1)^2 + (\gamma_k^2)^2$ and $(\omega_k^*)^2 = (\omega_k^1)^2 + (\omega_k^2)^2$ for $k = 1, 2, 3$.

Following the notation in [Blom02] define

$$\begin{aligned} a_k(t) &= \frac{1}{2}[Q_{v_k} - Q_{x,v_k}^T Q_s^{-1} Q_{x,v_k}]^{-1} \\ d_k(x,t) &= \mu_{v_k}(t) + Q_{x,v_k}^T Q_x^{-1}(x - \mu_x(t)) \\ v_k^+(x,t) &= \frac{e^{-a_k(t)d_k^2(x,t)}}{4\pi\,|a_k(t)|} + \frac{1}{2} d_k(x,t)[1 + \mathrm{erf}(d_k(x,t)\sqrt{a_k(t)}] \\ v_k^-(x,t) &= \frac{e^{-a_k(t)d_k^2(x,t)}}{4\pi\,|a_k(t)|} - \frac{1}{2} d_k(x,t)[1 - \mathrm{erf}(d_k(x,t)\sqrt{a_k(t)}] \end{aligned}$$

for $k = 1, 2, 3$, where $a(t), d(t) \in \mathbb{R}^3$, $a_k(t)$, $d_k(t)$, $\mu_{v_k}(t)$ are the k^{th} component of $a(t)$, $d(t)$, μ_v respectively, Q_{v_k}, Q_{x,v_k} are the k^{th} column of Q_v, $Q_{x,v}$, respectively, and $\mu_x(t) = E\{x_t\}$.

Note that due to the fact that $Q_{x,v_k} = [0, 0, 0]^T$ for $k = 1, 2, 3$, we have

$$a_k(t) = \tfrac{1}{2Q_{v_k}} = \tfrac{1}{2(\omega_k^*)^2}$$
$$d_k(x,t) = \begin{cases} v_{10} \text{ if } k = 1 \\ 0 \text{ if } k = 2 \\ 0 \text{ if } k = 3 \end{cases}$$

hence both $a_k(t)$ and $d_k(x,t)$ are constants independent of x and t. As a consequence, $v_k^+(x,t)$ and $v_k^-(x,t)$ are also constants. To simplify the notation let us write $v_k^\pm(x,t)$ simply as $v_k^\pm$. Then starting from Theorem 1 in [Blom02] we may further simplify the evaluation of the incrossing risk as follows:

$$\begin{aligned}\varphi(t) &= \sum_{k=1}^{3}\int\limits_{\underline{D}_k}\left[v_k^+(\underline{x}_k,-s_k,t)p_{\underline{x}_{k,t},x_{k,t}}(\underline{x}_k,-s_k)+v_k^-(\underline{x}_k,s_k,t)p_{\underline{x}_{k,t},x_{k,t}}(\underline{x}_k,s_k)\right]d\underline{x}_k \\ &= \sum_{k=1}^{3}\left[v_k^+\int\limits_{\underline{D}_k}p_{\underline{x}_{k,t},x_{k,t}}(\underline{x}_k,-s_k)d\underline{x}_k+v_k^-\int\limits_{\underline{D}_k}p_{\underline{x}_{k,t},x_{k,t}}(\underline{x}_k,s_k)d\underline{x}_k\right]\end{aligned}$$

Since x_1, x_2, x_3 are independent of each other we may also write:

$$p_{\underline{x}_{k,t},x_{k,t}}(\underline{x}_k,\pm s_k)=p_{x_{i,t}}(x_i)p_{x_{j,t}}(x_j)p_{x_{k,t}}(\pm s_k)$$

where $i,j\in\{1,2,3\}$ and $i\neq j\neq k$. Hence

$$\begin{aligned}\varphi(t) &= \sum_{k=1}^{3}\left[v_k^+p_{x_{k,t}}(-s_k)\int\limits_{\underline{D}_{i_k}}p_{x_{i_k,t}}(y)dy\int\limits_{\underline{D}_{j_k}}p_{x_{j_k,t}}(y)dy\right. \\ &\quad \left.+v_k^-p_{x_{k,t}}(s_k)\int\limits_{\underline{D}_{i_k}}p_{x_{i_k,t}}(y)dy\int\limits_{\underline{D}_{j_k}}p_{x_{j_k,t}}(y)dy\right] \\ &= \sum_{k=1}^{3}\left([v_k^+p_{x_{k,t}}(-s_k)+v_k^-p_{x_{k,t}}(s_k)]\int\limits_{\underline{D}_{i_k}}p_{x_{i_k,t}}(y)dy\right. \\ &\quad \left.\int\limits_{\underline{D}_{j_k}}p_{x_{j_k,t}}(y)dy\right) \qquad (6.2)\end{aligned}$$

where $i_k, j_k\in\{1,2,3\}$ and $i_k\neq j_k\neq k$ for each k,.

Now, we make the following observation:

$$\begin{aligned}\int\limits_{\underline{D}_2}p_{x_2}(y)dy &= \frac{1}{\sqrt{2\pi}\gamma_2^*}\int\limits_{-s_2}^{s_2}e^{-\frac{1}{2}\frac{(y-S)^2}{(\gamma_2^*)^2}}dy \\ &\approx \frac{1}{\sqrt{2\pi}\gamma_2^*}\int\limits_{-s_2}^{s_2}e^{-\frac{1}{2}\frac{S^2}{(\gamma_2^*)^2}}dy \\ &= \frac{2s_2}{\sqrt{2\pi}\gamma_2^*}e^{-\frac{1}{2}\frac{S^2}{(\gamma_2^*)^2}}\end{aligned}$$

because $S >> |s_2|$ (for example, in the simulation $S = 15000$ while $s_2 = 50$). We also observe that

$$p_{x_2}(s_2)=\frac{1}{\sqrt{2\pi}\gamma_2^*}e^{-\frac{1}{2}\frac{(s_2-S)^2}{(\gamma_2^*)^2}}\approx\frac{1}{\sqrt{2\pi}\gamma_2^*}e^{-\frac{1}{2}\frac{S^2}{(\gamma_2^*)^2}}$$

Finally, we note that for large S, the term $e^{-\frac{1}{2}\frac{S^2}{(\gamma_2^*)^2}}$ is very sensitive to changes in γ_2^* and hence also to γ_2^1 and γ_2^2. Since this term appears in every term on the right hand side of (6.2) it directly influences the incrossing risk. Next we provide a numerical example to show the claimed sensitivity.

Example 6.1 *Let $S = 15000$ m, $\gamma_2^1 = \gamma_2^2 = 1 \times 10^3$ m. In this case we have that $(\gamma_2^*)^2 = 2 \times 10^6$ m^2 and*

$$e^{-\frac{1}{2}\frac{S^2}{(\gamma_2^*)^2}} = 3.7234 \times 10^{-25}$$

Let us now change γ_2^1 to $\gamma_2^1 = 2 \times 10^3$ m and keep γ_2^2 as before. We then have $(\gamma_2^*)^2 = 5 \times 10^6$ m^2 and

$$e^{-\frac{1}{2}\frac{S^2}{(\gamma_2^*)^2}} = 1.6919 \times 10^{-10}$$

resulting in a change in the order of 10^{15}.

6.5 Results from PCE Method

Based on a number of collocation points (see Figure 4.1) selected with the Regression Method with Improved Sampling (Subsection 4.7.2), second and third order PCEs for the actual model were identified. Next, Monte Carlo simulations were performed using the PCEs to estimate $E\{\ln(\mathcal{R})\}$ and the 95% CrI of $\ln(\mathcal{R})$.

Figure 6.9 presents the results from running 20,000 Monte Carlo simulations on the second and third order PCEs (by drawing 20,000 samples of the parameters $(V_1, V_2, ..., V_{14})$ and then evaluating the incrossing risk for each sample).

Figure 6.10 compares the histograms of $\ln(\mathcal{R})$ obtained from this PCE approach with those of the direct Monte Carlo simulation approach of Section 6.3. One can clearly see that in this particular case study the histograms obtained from both approaches are almost indistinguishable. The estimates obtained from the direct Monte Carlo and the PCEs are very close as can be seen by comparing the results in Figure 6.9 with those in Figure 6.3. Based on the values of average error squared ($\overline{e^2}$) it is clear that the fits of the PCEs to the actual model are quite good; in this case a second order PCE is already sufficient. Bias that is attributed to approximation errors is also small since $\overline{e}$ is small. Furthermore, the second order PCE is also able to capture the presence of skewness in the distribution of $\ln \mathcal{R}$. On the other hand the Everdij&Blom method or first order PCE cannot do this since the estimated distribution will be normal, which is always symmetric about the mean.

Note the computational savings that can be made by using a second order PCE: with only 120 evaluations of the accident risk model we can obtain estimates which compare well with 20,000 runs of the accident risk model in a direct Monte Carlo simulation. Furthermore, this result indicates that a higher order PCE may not be necessary. An intuitive explanation as to why a higher

Order of PCE	No. of collocation points	$\overline{\ln(\Re)}$	95% CI for $E\{\ln(\Re)\}$	$\bar{e}$	$\overline{e^2}$
2	120	-101.58	[-101.66, -101.49]	0.0037	-0.045
3	680	-101.58	[-101.67, -101.49]	0.042	-0.048

$\bar{e} = \frac{1}{N}\sum_{i=1}^{N}(\ln(\Re_i) - \ln(\hat{\Re}_i))$, $\overline{e^2} = \frac{1}{N}\sum_{i=1}^{N}(\ln(\Re_i) - \ln(\hat{\Re}_i))^2$ where N=20000, $\ln(\Re_i)$=actual value of the natural log of incrossing risk for sample i, $\ln(\hat{\Re}_i)$=approximation of the natural log of incrossing risk by PCE for sample i.

Order of PCE	$\overline{A}$	$\overline{B}$	95% CI for A	95% CI for B
2	-114.77	-89.55	[-115.05, -114.55]	[-89.74, -89.39]
3	-114.84	-89.60	[-115.13, -114.60]	[-89.77, -89.42]

$[\overline{A}, \overline{B}]$ is an estimate of the 95% CrI of $\ln(\Re)$ using 20,000 samples. Approximate CIs for A and B were obtained using 1000 bootstrap samples.

Figure 6.9: Results of Monte Carlo simulation on 2^{nd} and 3^{rd} order PCEs

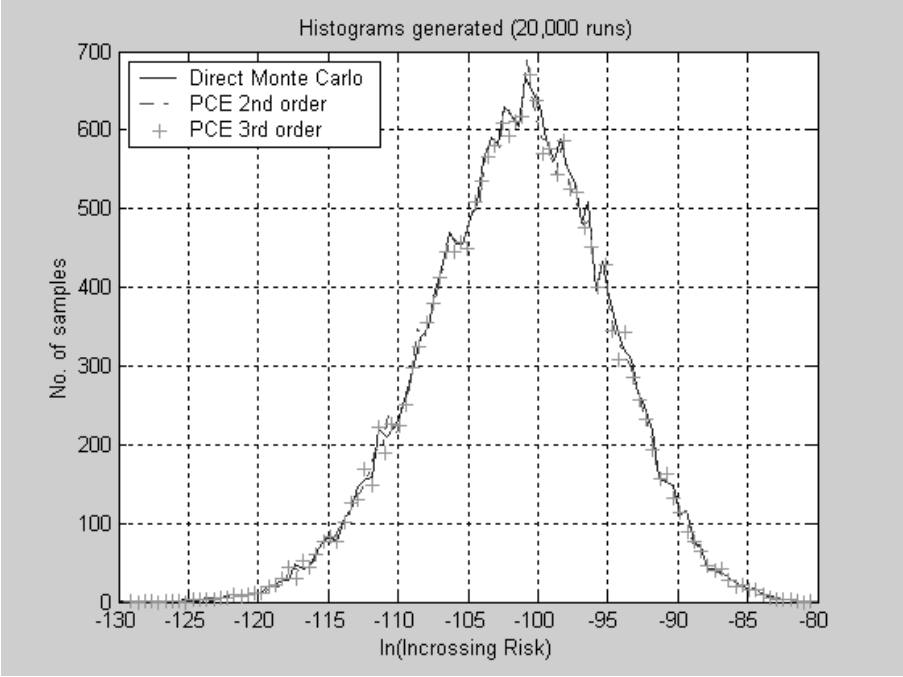

Figure 6.10: Comparison of histograms obtained from direct Monte Carlo simulation and Monte Carlo simulations of 2^{nd} and 3^{rd} order PCEs.

order PCE may not be necessary is that we are essentially approximating $\ln(\mathcal{R})$

as a function of $X_1, X_2, ..., X_{n_p}$ in a bounded region $\bigotimes_{i=1}^{n_p}[-2.5, 2.5]$ ($[-2.5, 2.5]$ is the 99% probability region of X_i since $X_i \sim N(0,1)$) and if $\ln(\mathcal{R})$ is sufficiently smooth and does not have too much curvature or fluctuations in that region then it is reasonable to expect that a low order expansion would suffice.

Figures 6.7 and 6.8 even indicates that a first order PCE (i.e. the Everdij&Blom method in the case of unbiased parameter values) can be considered sufficient.

6.6 Results of Fitting a Parametric Density

Figure 6.11 displays the histogram of 320 samples of $-\ln\mathcal{R}$ and Figure 6.12 displays the histogram of $\ln(-\ln\mathcal{R})$. One can notice that $-\ln\mathcal{R}$ has longer tails to the right while $\ln(-\ln\mathcal{R})$ looks more symmetic and normal. This suggests that $-\ln\mathcal{R}$ may have an approximately lognormal distribution. Also notice that the spread of $\ln(-\ln\mathcal{R})$ is quite narrow, thus it will have small variance.

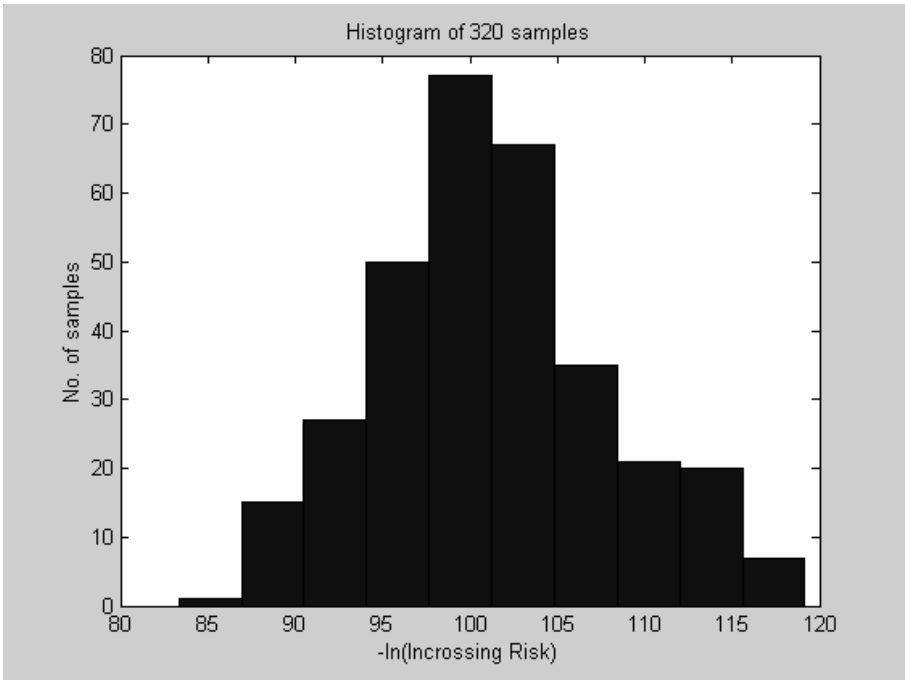

Figure 6.11: Histogram of 320 random samples of $-\ln\mathcal{R}$

Let $Y = -\ln\mathcal{R}$; we will try to fit a lognormal distribution to Y. In order to do this we must first estimate the mean and variance of $\ln Y = \ln(-\ln\mathcal{R})$ by using the formulas discussed in Section 5.3. Based on the 320 samples of $\ln Y$ we obtain the following estimates:

$$\widehat{\mu}_{\ln Y} = 4.6157,\ 95\%\ \text{CI for}\ \mu_{\ln Y} = [4.6086, 4.6228]$$

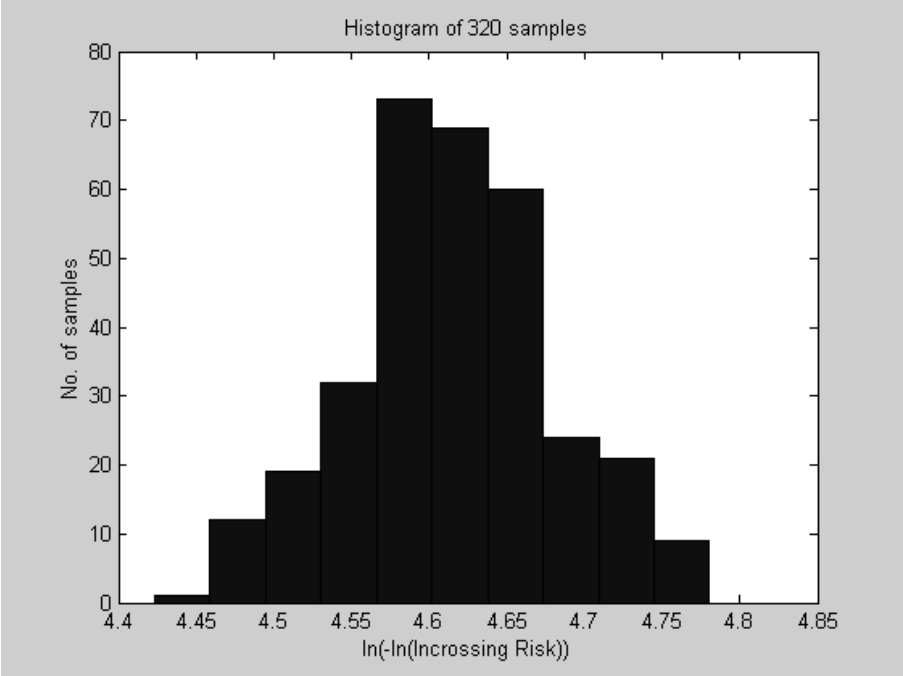

Figure 6.12: Histogram of 320 random samples of $\ln(-\ln \mathcal{R})$

$\widehat{\sigma}^2_{\ln Y} = 4.1750 \times 10^{-3}$, 95% CI for $\sigma^2_{\ln Y} = [3.6119 \times 10^{-3}, 4.9308 \times 10^{-3}]$

Based on $\widehat{\mu}_{\ln Y}$ and $\widehat{\sigma}^2_{\ln Y}$ and on the assumption that $\ln Y$ follows a normal distribution we find that the 95% CrI of $\ln Y$ is

$$[\widehat{\mu}_{\ln Y} - 1.96\widehat{\sigma}_{\ln Y}, \widehat{\mu}_{\ln Y} + 1.96\widehat{\sigma}_{\ln Y}] = [4.4891, 4.7423]$$

Hence the 95% CrI for $Y = [e^{4.4891}, e^{4.7423}] = [89.0374, 114.7027]$ and it directly follows that the 95% CrI for $\ln \mathcal{R} = [-114.7027, -89.0374]$. Notice how this estimate of the 95% CrI is not too different from the direct Monte Carlo estimate of $[-114.79, -89.51]$ of Section 6.3 which was based on 20,000 samples.

We may also estimate the mean of Y by the lognormal formula (see [Ever02])

$$\widehat{\mu}_Y = \exp(\widehat{\mu}_{\ln Y} + \frac{1}{2}\widehat{\sigma}^2_{\ln Y})$$

from which we get

$$\widehat{\mu}_Y = 101.27$$

hence

$$\widehat{\mu}_{\ln \mathcal{R}} = -101.27$$

Again note how the small sample estimate -101.27 is quite close to the direct Monte Carlo estimate of -101.53.

6.7 Results From Non-Parametric Bootstrapping Method

In this section we present the result of applying the plug-in principle and the bootstrap to estimate the mean and 95% CrI of $\ln(\mathcal{R})$ based on around 320-680 samples of $\ln(\mathcal{R})$. Figure 6.13 displays the results.

No. of samples	No. of bootstrap samples	$\overline{\ln(\mathcal{R})}$	95% CI for $E(\ln(\mathcal{R}))$	$\overline{A}$	$\overline{B}$	Bootstrap 95% CI for A	Bootstrap 95% CI for B
320	1000	-101.28	[-101.99, -100.55]	-115.50	-89.13	[-118.26, -114.52]	[-90.58, -88.47]
	2000					[-118.26, -114.52]	[-90.58, -88.56]
	5000					[-118.26, -114.52]	[-89.80, -88.56]
520	1000	-101.06	[-101.61, -100.50]	-114.70	-89.12	[-116.32, -113.39]	[-90.37, -88.56]
	2000					[-116.32, -114.27]	[-89.80, -88.48]
	5000					[-116.32, -113.39]	[-89.80 -88.48]
680	1000	-101.05	[-101.53, -100.57]	-114.81	-89.14	[-116.09, -113.39]	[-90.37, -88.48]
	2000					[-116.09, -114.27]	[-89.80 -88.48]
	5000					[-116.09, -113.39]	[-90.37, -88.48]

Figure 6.13: Results of non-parametric bootstrapping

We carry out the bootstrapping for different sample sizes of $\ln(\mathcal{R})$, i.e. sample sizes 320, 520, and 680. Compared with the direct Monte Carlo estimates shown in Figure 6.3, the estimate of the mean from all three sample sizes were quite good while the estimates of the 95% CrI were better for sample sizes of 520 and 680. A noticeable difference is that in the small sample case the width of the CI of the estimates are wider, which we would expect since the size of the data is small, and hence is more conservative. An important observation that we can make here is that although the CIs are more conservative, they do cover the CI obtained from the large sample Monte Carlo simulation in Section 6.3. In practice this is important since for the CI upper bound of B it is safety conservative to have an estimate which overestimates risk than one which underestimates the risk. The estimates from a data size of 680 samples do not differ very much from estimates obtained based on only 520 samples, suggesting that 520 could be sufficient for our purposes.

We may use the bootstrap results to obtain a safety conservative estimate of the 95% CrI by taking the upper bound of the CI of A and the upper bound of the CI of B. Hence for example, based on 520 samples and 2000 bootstraps we may take $[-113.39, -88.48]$ as our conservative estimate.

Chapter 7

Second Test Case: Double Exponential Lateral Deviations

7.1 Model of Evolution of Two Aircraft

In the previous chapter we discussed the modelling of a pair of aircraft as being jointly Gaussian. However, according to Civil Aviation Authority (CAA), based on actual flight data, the distribution of the lateral deviation of an aircraft (deviation in the y-direction) from its straight line course might better be modelled as double double exponential [CAA91]. A double double exponential distribution is a three parameter distribution with the following density function:

$$f(x) = \alpha \frac{1}{2\lambda_1} e^{-\frac{|x-\mu|}{\lambda_1}} + (1-\alpha)\frac{1}{2\lambda_2} e^{-\frac{|x-\mu|}{\lambda_2}}$$

where $\alpha, \lambda_1, \lambda_2$ are the parameters with $0 < \alpha < 1$, and $\lambda_1, \lambda_2 > 0$ (we do not consider $\mu \in \mathbb{R}$ as a parameter to conform with the standard definition of a double double exponential distribution as a three parameter distribution. In standard form μ is taken to be zero). If a random variable X follows a double double exponential distribution with parameters $\alpha, \lambda_1, \lambda_2$ (which we shall write as $X \sim DDE(\alpha, \lambda_1, \lambda_2)$) then

$$E\{X\} = \mu$$

$$Var\{X\} = 2\alpha\lambda_1^2 + 2(1-\alpha)\lambda_2^2$$

However, in this chapter we will consider the special case of the double double exponential where $\lambda_1 = \lambda_2 = \lambda$, called the double exponential distribution. Therefore the density in this special case is:

$$f(x) = \frac{1}{2\lambda} e^{-\frac{|x-\mu|}{\lambda}}$$

This distribution can be used to model an aircraft which only flies in one mode, e.g. the nominal mode, where it is assumed the aircraft never gets itself into a non-nominal mode. NLR has proposed a dynamic model for the motion of an aircraft such that in steady state the deviation in position in a particular direction has a double exponential distribution and the distribution of the deviation of the velocity in that direction is Gaussian [Daam99]. We will reuse the notation introduced in Subsection 6.1. For the dynamics in the x and z (x_1 and x_3, respectively) direction we use the equations already derived in the previous chapter. However, we now model the dynamics in the y direction as follows:

$$x_2^i(t) = \overline{x}_2^i(t) + \widetilde{x}_2^i(t)$$

$$v_2^i(t) = \overline{v}_2^i(t) + \widetilde{v}_2^i(t)$$

$$d\widetilde{v}_2^i(t) = -a_2^i sgn(\widetilde{x}_2^i(t))dt - b_2^i\widetilde{v}_2^i(t)dt + c_2^i dw_2^i(t),\ \widetilde{v}_2^i(0) \sim N(0,(\alpha_2^i)^2), \alpha_2^i \geq 0$$

$$\overline{v}_2^i(t) = v_{2,nom}^i$$

$$\overline{x}_2^i(t) = x_{2,0}^i + v_{2,nom}^i t$$

$$d\widetilde{x}_2^i(t) = \widetilde{v}_2^i(t)dt,\ \widetilde{x}_2^i(0) \text{ follows some initial distribution}$$

where

$$sgn(x) = \begin{cases} -1 \text{ if } x < 0 \\ 0 \text{ if } x = 0 \\ 1 \text{ if } x > 0 \end{cases}$$

It can be shown that by solving the associated Fokker Planck equation for the steady state case ($t \longrightarrow \infty$), $\widetilde{x}_2^i(t)$ and $\widetilde{v}_2^i(t)$ are independent of each other, $\widetilde{v}_2^i(t)$ follows a Gaussian distribution while $\widetilde{x}_2^i(t)$ follows a double exponential distribution (see Chapter 1 of [Risk89]). Consequently, $v_2^i(t)$ is Gaussian and $x_2^i(t)$ is double exponential as $t \longrightarrow \infty$.

In order for us to be able to use Theorem 1 of [Blom02] for the double exponential case, we exploit the fact that a double exponential density can be approximated by a sum of Gaussian density functions[Blom02]. We may write for some N_1, N_2:

$$p_{x_{2,t}^1}(x) \approx \sum_{j=1}^{N_1} \chi_j^1 p_{G_{j,t}}^1(x)$$

$$p_{-x_{2,t}^2}(x) \approx \sum_{j=1}^{N_2} \chi_j^2 p_{G_{j,t}}^2(x)$$

where

$$p_{G_{j,t}}^1(x) = \frac{1}{\sqrt{2\pi}\hat{\sigma}_{j,1}} \exp\left(-\frac{1}{2}\left(\frac{x - \overline{x}_2^1(t)}{\hat{\sigma}_{j,1}}\right)^2\right)$$

$$p_{G_{j,t}}^2(x) = \frac{1}{\sqrt{2\pi}\hat{\sigma}_{j,2}} \exp\left(-\frac{1}{2}\left(\frac{x + \overline{x}_2^2(t)}{\hat{\sigma}_{j,2}}\right)^2\right)$$

$\hat{\sigma}_{i,j} \geq 0$, $\chi^i_j \geq 0$ and $\sum_{j=1}^{N_i} \chi^i_j = 1$. Recall that $x^s_{2,t} = x^1_{2,t} - x^2_{2,t}$. Since $x^1_{2,t}$ and $-x^2_{2,t}$ are independent we have that

$$p_{x^s_{2,t}}(x) = (p_{x^1_{2,t}} * p_{-x^2_{2,t}})(x)$$

where $*$ denotes convolution. Hence

$$\begin{aligned} p_{x^s_{2,t}}(x) &\approx \int_R \left(\sum_{j=1}^{N_1} \chi^1_j p^1_{G_{j,t}}(z) \right) \left(\sum_{k=1}^{N_2} \chi^2_k p^2_{G_{k,t}}(z-x) \right) dz \\ &= \sum_{j=1}^{N_1} \sum_{k=1}^{N_2} \chi^1_j \chi^2_k \left(\int_R p^1_{G_{j,t}}(z) p^2_{G_{k,t}}(z-x) dz \right) \\ &= \sum_{j=1}^{N_1} \sum_{k=1}^{N_2} \chi^1_j \chi^2_k (p^1_{G_{j,t}} * p^2_{G_{k,t}})(x) \qquad (7.1) \\ &= \sum_{j=1}^{N_1} \sum_{k=1}^{N_2} \chi^1_j \chi^2_k p_{G_{jk}}(x) \qquad (7.2) \end{aligned}$$

where

$$p_{G_{jk,t}}(x) = \frac{1}{\sqrt{2\pi}\hat{\sigma}_{jk}} \exp\left(-\frac{1}{2} \left(\frac{x - \overline{x}^s_2(t)}{\hat{\sigma}_{jk}} \right)^2 \right)$$

$$\overline{x}^s_2(t) = \overline{x}^1_2(t) - \overline{x}^2_2(t)$$

$$\hat{\sigma}_{jk} = \sqrt{(\hat{\sigma}_{1,j})^2 + (\hat{\sigma}_{2,k})^2}$$

With the above knowledge we may evaluate the incrossing risk by replacing $p_{x^s_{2,t}}(x)$ with the double Gaussian sum (7.2), evaluate the incrossing risk for each Gaussian term by Theorem 1 of [Blom02] and then sum the incrossing risk associated with each Gaussian term.

7.2 Parameter Values

In this second simulation we will use the same nominal parameter values and the same model of uncertainty of the parameters as in the previous chapter.

7.3 Results from Direct Monte Carlo Simulation

Given the fixed and random valued parameters in Section 6.2, we can use direct Monte Carlo simulations on the actual model to estimate $E\{\ln(\mathcal{R})\}$ and the 95% CrI of $\ln(\mathcal{R})$. We proceed as in the previous chapter and the results of 10,000 Monte Carlo runs are presented in Figure 7.1. Only 10,000 samples were

$\overline{\ln(\Re)}$	95% CI for $E\{\ln(\Re)\}$	$\overline{A}$	$\overline{B}$	Bootstrap 95% CI for A	Bootstrap 95% CI for B
-28.34	[-28.35, -28.32]	-30.13	-26.63	[-30.20, -30.09]	[-26.68, -26.57]

$\overline{\ln(\Re)}$ is an estimate of $E\{\ln(\Re)\}$ and $[\overline{A}, \overline{B}]$ is an estimate of the 95% CrI of $\ln(\Re)$ using 10,000 samples. Approximate CIs for A and B were obtained using 1000 bootstrap samples.

Figure 7.1: Statistical estimates obtained via direct Monte Carlo simulation

evaluated, compared to 20,000 in the simulation in Chapter 6, because the time needed to evaluate the incrossing risk in this case was significantly longer. As in Chapter 6, $\overline{\ln(\mathcal{R})}$ denotes an estimate of $E\{\ln(\mathcal{R})\}$.

Since the bootstrap CI for A and B are relatively tight, we may assume that $[\overline{A}, \overline{B}]$ is a good estimate of the true 95% CrI.

7.4 Results from the Everdij&Blom Method

In this section we use the bias and model uncertainty assumption method of [Ever02] to evaluate $\overline{\ln(\mathcal{R})}$ and the 95% CrI of $\ln(\mathcal{R})$.

7.4.1 Estimation using biased nominal parameter values

Figures 7.2, 7.3 and 7.4 show the results of applying the Everdij&Blom method to estimate $E\{\ln(\mathcal{R})\}$ and a 95% CrI for $\ln(\mathcal{R})$ using the biased nominal value of the parameters in Section 6.2.

The natural log of the nominal risk in this biased case is:

$$\ln(\rho(\mathbf{1}, v)) = -24.40$$

The bias compensation term $\sum_{i=1}^{14} \beta_i(\mu_i - \ln v_i)$ that needs to be added to this nominal risk appeared to be around -4 depending on the method used to evaluate β_i.

The values of the $\beta_i's$ were calculated in three different ways, using β_i^* and β_i^{**} as explained in Section 3.6 and using a safety conservative approach. However, in addition we applied another method of estimating the $\beta_i's$ by

$$\beta_i^{avg} = \frac{\beta_i^* + \beta_i^{**}}{2}$$

From Figures 7.2 and 7.4 we can observe that the Everdij&Blom mean estimates are biased. Furthermore, estimates obtained based on β_i^{**} coincide with the safety conservative approach estimates. By studying Figure 7.4, we can also see that the safety conservative approach does actually yield a safety conservative estimate of the 95% CrI.

	$\overline{\ln(\Re)}$	95% CrI for $E\{\ln(\Re)\}$	$\overline{e^2}$
Using β_i^{**}	-27.42	[-28.65, -26.20]	15.62
Using β_i^{*}	-28.64	[-30.36, -26.92]	15.55
Safety conservative	-27.42	[-28.67, -26.18]	15.61
β_i^{avg}	-28.03	[-29.50, -26.56]	15.57

$\overline{\ln(\Re)}$ and 95% CrI for $E\{\ln(\Re)\}$ based on the Everdij/Blom methodology when the parameters of the nominal model are

$\nu_1 = \nu_8 = 240,\ \nu_2 = \nu_9 = 1000,\ \nu_3 = \nu_{10} = 900, \nu_4 = \nu_{11} = 20, \nu_5 = \nu_{12} = 10,$

$\nu_6 = \nu_{13} = 10, \nu_7 = \nu_{14} = 1$ (biased in ν_1, ν_8, ν_3 and ν_{10})

$\overline{e^2}$ denotes the average of the square of approximation errors over 10000 random samples of the parameters.

Figure 7.2: Results of applying the Everdij/Blom method when some of the v_i's are biased

Parameters	Nominal value v_i	l_i	β_i^{*}	β_i^{**}	$\beta_i^{\text{safety conservative}}$	β_i^{avg}
V_1, V_8	240	1.14	-1.487×10^{-2}	-1.484×10^{-2}	-1.487×10^{-2}	-1.486×10^{-2}
V_2, V_9	1000	2.25	0	0	0	0
V_3, V_{10}	900	1.1	12.54	8.95	8.95	10.74
V_4, V_{11}	20	1.5	-5.564×10^{-1}	-3.596×10^{-1}	-5.564×10^{-1}	-4.580×10^{-1}
V_5, V_{12}	10	2.25	0	0	0	0
V_6, V_{13}	10	2.25	2.071×10^{-2}	6.391×10^{-3}	2.071×10^{-2}	1.355×10^{-2}
V_7, V_{14}	1	2.25	6.293×10^{-3}	1.927×10^{-3}	6.293×10^{-3}	4.110×10^{-3}

Figure 7.3: Values of the β_i's evaluated with the Everdij/Blom method

7.4.2 Estimation using unbiased nominal parameter values

We now repeat the Everdij&Blom procedure for the case where the nominal values of the parameters take on unbiased values. The natural log of the nominal risk in this unbiased case is:

$$\ln(\rho(\mathbf{1}, v)) = \ln(\rho(\mathbf{1}, c)) = -28.33$$

Since in this case the bias compensation is equal to zero, we have that $\overline{\ln \mathcal{R}} = \ln \rho(1, c)$.

The results of the unbiased Everdij&Blom method are shown in Figures 7.5 and 7.6. As we have seen in Chapter 6, in this case the Everdij&Blom method gives a much better estimate of $E\{\ln(\mathcal{R})\}$ and its 95% CrI compared to the biased case. Note that the estimates based on β_i^* coincide with that of the safety conservative estimates.

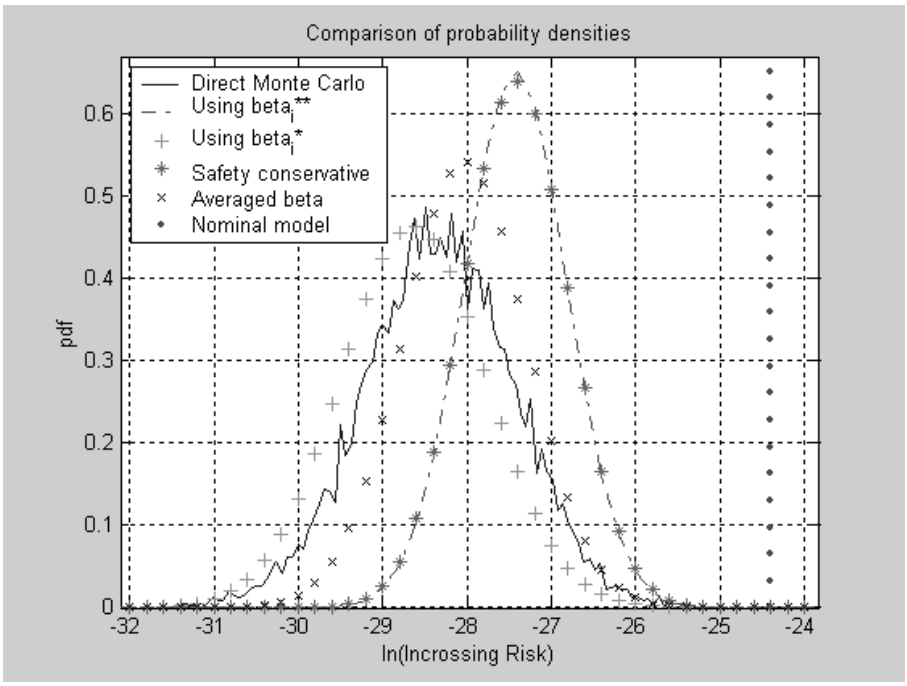

Figure 7.4: Comparison of a direct Monte Carlo histogram with the Everdij/Blom density estimates when some of the v_i's are biased

	$\overline{\ln(\Re)}$	95% CrI for $\ln(\Re)$	$\overline{e^2}$
Using β_i^{**}	- 28.33	[-29.75, -26.91]	6.475×10^{-2}
Using β_i^{*}	- 28.33	[-30.42, -26.24]	6.026×10^{-2}
Safety conservative	- 28.33	[-30.42, -26.24]	6.026×10^{-2}
β_i^{avg}	- 28.33	[-30.08, -26.58]	3.673×10^{-2}

$\overline{\ln(\Re)}$ and 95% CrI for $\ln(\Re)$ based on the Everdij/Blom methodology when the parameters of the nominal model are

$v_1 = v_8 = 228,\ v_2 = v_9 = 1000,\ v_3 = v_{10} = 760, v_4 = v_{11} = 20, v_5 = v_{12} = 10,$

$v_6 = v_{13} = 10, v_7 = v_{14} = 1$ (unbiased)

$\overline{e^2}$ denotes the average of the square of approximation errors over 10000 random samples of the parameters.

Figure 7.5: Results of applying the Everdij/Blom method when the v_i's are unbiased

Both figures indicate the improvement gained by using β_i^{avg}, i.e. the estimate

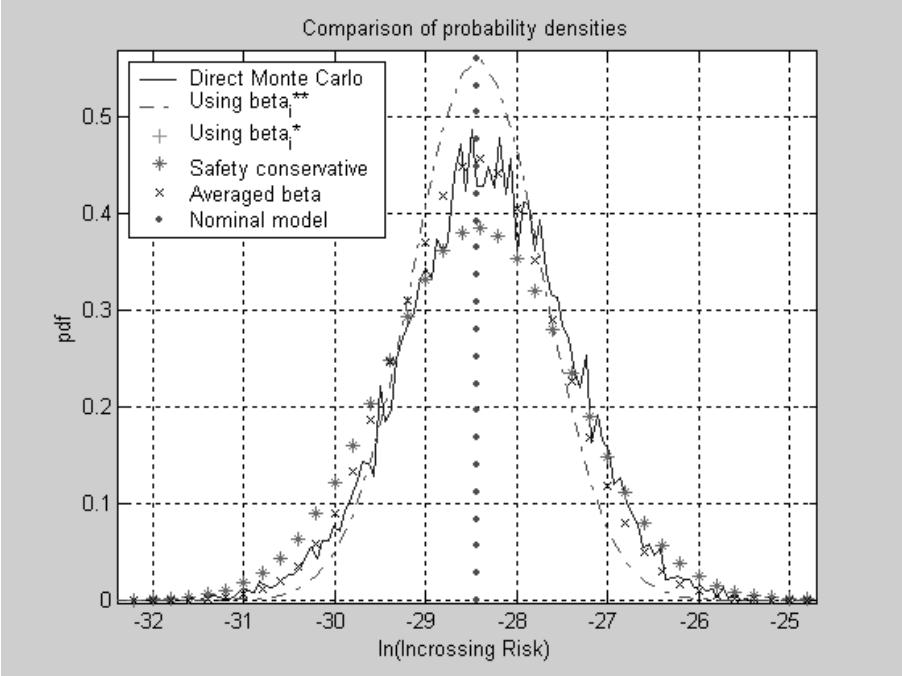

Figure 7.6: Comparison of the Monte Carlo histogram and the Everdij/Blom density estimates when the $v_i's$ are unbiased

of the 95% CrI estimate and the estimated density better matches the direct Monte Carlo results.

7.5 Results from PCE Method

Based on a number of collocation points (see Figure 4.1) selected with the Regression Method with Improved Sampling (Subsection 4.7.2), second and third order PCEs for the actual model were identified. Monte Carlo simulations were performed using the PCEs to estimate $E\{\ln(\mathcal{R})\}$ and the 95% CrI of $\ln(\mathcal{R})$.

Figure 7.7 presents the results from running 10,000 Monte Carlo simulations on the second and third order PCEs (by drawing 10,000 samples of the parameters $(V_1, V_2, ..., V_{14})$ and then evaluating the incrossing risk for each sample).

Figure 7.8 compares the histograms of $\ln(\mathcal{R})$ obtained from the direct Monte Carlo simulations of Sections 7.3 and PCE based Monte Carlo simulations. The histograms obtained from the actual model and its 2^{nd} order PCE are almost indistinguishable. Based on the values of average error squared ($\overline{e^2}$) it is clear that the fit of the 2^{nd} order PCE to the actual model is quite good. Once again we observe that the second order PCE is able to capture the skewness in the distribution of $\ln \mathcal{R}$. However, the 3^{rd} order PCE does not perform quite as

Order of PCE	No. of collocation points	$\overline{\ln(\Re)}$	95% CI for $E(\ln(\Re))$	$\bar{e}$	$\overline{e^2}$
2	120	-28.33	[-28.35, -28.31]	6.45×10^{-3}	5.95×10^{-4}
3	680	-28.325	[-28.35, -28.30]	1.26×10^{-2}	4.25×10^{-1}

$\bar{e} = \frac{1}{N}\sum_{i=1}^{N}(\ln(\Re_i) - \ln(\hat{\Re}_i))$, $\overline{e^2} = \frac{1}{N}\sum_{i=1}^{N}(\ln(\Re_i) - \ln(\hat{\Re}_i))^2$ where N=10000, $\ln(\Re_i)$=actual value of the natural log of incrossing risk for sample i, $\ln(\hat{\Re}_i)$=approximation of the natural log of incrossing risk by PCE for sample i.

Order of PCE	$\overline{A}$	$\overline{B}$	95% CI for A	95% CI for B
2	-30.12	-26.60	[-30.19, -30.08]	[-26.64, -26.54]
3	-30.57	-26.10	[-30.64, -30.49]	[-26.19, -25.99]

$[\overline{A}, \overline{B}]$ is an estimate of the 95% CrI of $\ln(\Re)$ using 10,000 samples. Approximate CIs for A and B were obtained using 1000 bootstrap samples.

Figure 7.7: Results of Monte Carlo Simulations on 2^{nd} and 3^{rd} order PCEs

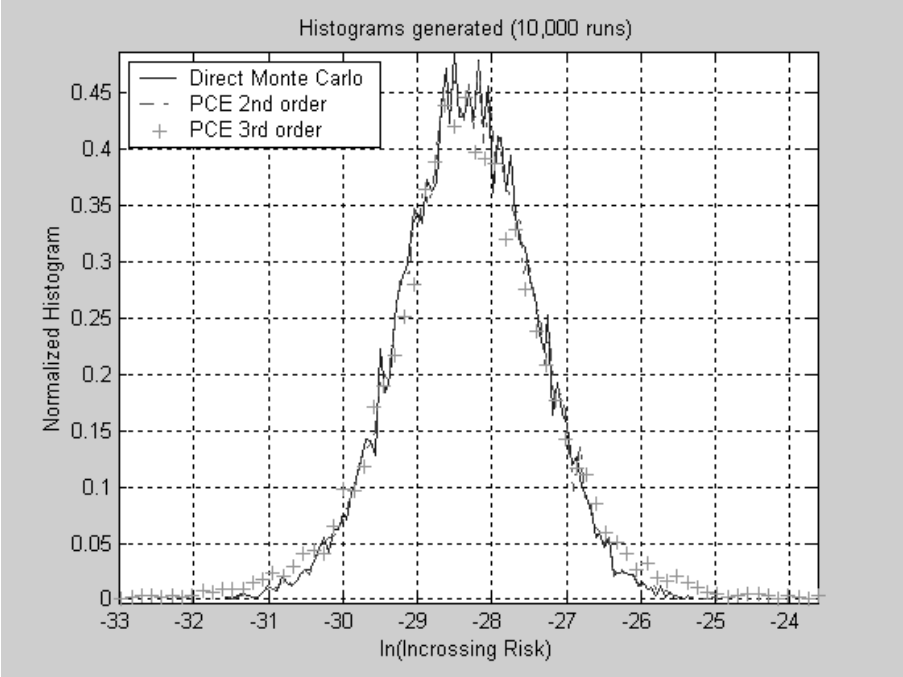

Figure 7.8: Comparison of histograms obtained from direct Monte Carlo simulation and Monte Carlo simulations of 2^{nd} and 3^{rd} order PCEs

well. There could be several reasons for this phenomenon, one possible one is that perhaps the choice of collocation points here is inadequate and maybe more

collocation points can be added to obtain a better fit. However, in the context of this project it is not really important since in practice we would not go to a 3^{rd} order PCE due to the large number of collocation points required.

7.6 Results of Fitting a Parametric Density

Figure 6.11 displays the histogram of 320 samples of $-\ln\mathcal{R}$ and Figure 6.12 displays the histogram of $\ln(-\ln\mathcal{R})$. In this case it is not so obvious that $-\ln\mathcal{R}$ follows a lognormal distribution. Both histograms in fact look as if they follow a normal distribution. However, in the following we assume that $-\ln\mathcal{R}$ can be adequately modelled by a lognormal distribution and observe the estimates that we get under this assumption. Once again note how the spread of $\ln(-\ln\mathcal{R})$ is quite narrow, thus it will have small variance.

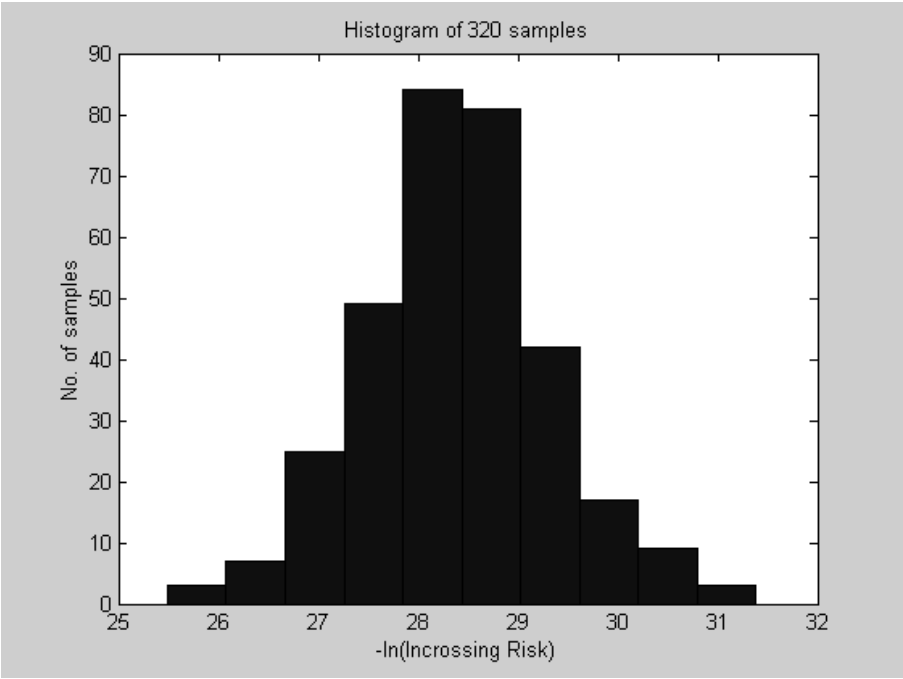

Figure 7.9: Histogram of 320 random samples of $-\ln\mathcal{R}$

Let $Y = -\ln\mathcal{R}$; we will try to fit a lognormal distribution to Y, in order to do this we must first estimate the mean and variance of $\ln Y = \ln(-\ln\mathcal{R})$ by using the formulas discussed in Section 5.3. Based on the 320 samples of $\ln Y$ we obtain the following estimates:

$$\widehat{\mu}_{\ln Y} = 3.3453,\ 95\%\ \text{CI for}\ \mu_{\ln Y} = [3.3417, 3.3489]$$

$$\widehat{\sigma}^2_{\ln Y} = 1.0791 \times 10^{-3},\ 95\%\ \text{CI for}\ \sigma^2_{\ln Y} = [9.3352 \times 10^{-4}, 1.2744 \times 10^{-3}]$$

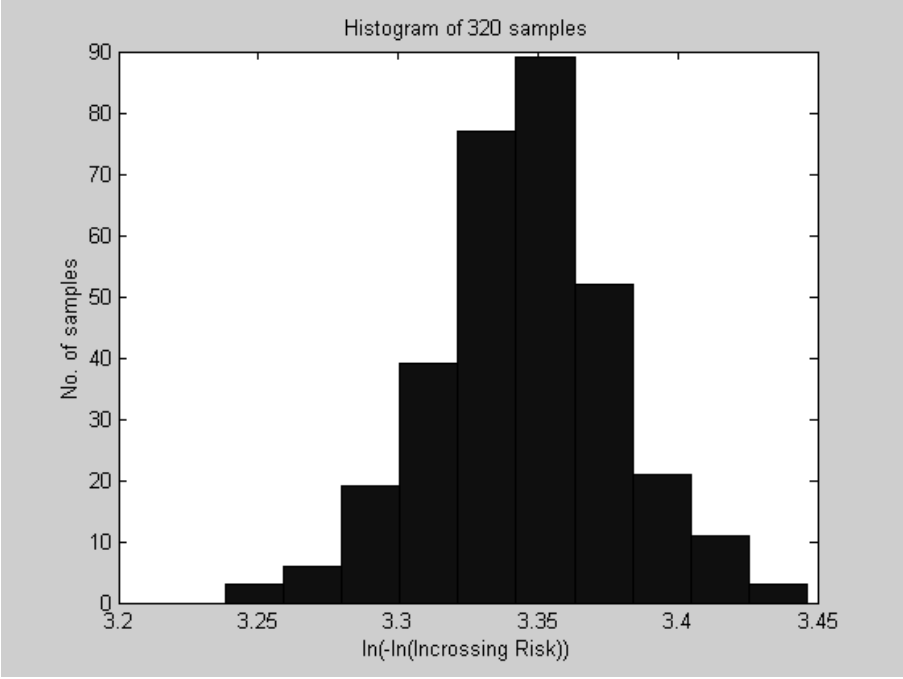

Figure 7.10: Histogram of 320 random samples of $\ln(-\ln(\mathcal{R}))$

Based on $\widehat{\mu}_{\ln Y}$ and $\widehat{\sigma}^2_{\ln Y}$ and on the assumption that $\ln Y$ follows a normal distribution we find that the 95% CrI of $\ln Y$ is

$$[\widehat{\mu}_{\ln Y} - 1.96\widehat{\sigma}_{\ln Y}, \widehat{\mu}_{\ln Y} + 1.96\widehat{\sigma}_{\ln Y}] = [3.2809, 3.4097]$$

Hence the 95% CrI for $Y = [e^{3.2809}, e^{3.4097}] = [26.5997, 30.2562]$ and it directly follows that the 95% CrI for $\ln \mathcal{R} = [-30.2562, -26.5997]$. Notice how this estimate of the 95% CrI is not too different from the direct Monte Carlo estimate of $[-30.13, -26.63]$ of Section 6.3 which was based on 10,000 samples.

We may also estimate the mean of Y by the lognormal formula (see [Ever02])

$$\widehat{\mu}_Y = \exp(\widehat{\mu}_{\ln Y} + \frac{1}{2}\widehat{\sigma}^2_{\ln Y})$$

from which we get

$$\widehat{\mu}_Y = 28.38$$

hence

$$\widehat{\mu}_{\ln \mathcal{R}} = -28.38$$

Again note how the small sample estimate -28.38 is quite close to the direct Monte Carlo estimate of -28.34. Based on the closeness of the small sample estimates to the direct Monte Carlo estimates it seems plausible that $-\ln \mathcal{R}$ may indeed follow a lognormal distribution.

7.7 Results From Non-Parametric Bootstrapping Method

In this section we present the result of applying the plug-in principle and the bootstrap to estimate the mean and 95% CrI of $\ln(\mathcal{R})$ based on 320 to 680 samples of $\ln(\mathcal{R})$. Figure 7.11 displays the results.

No. of samples	No. of bootstrap samples	$\overline{\ln(\mathcal{R})}$	95% CI for $E(\ln(\mathcal{R}))$	$\overline{A}$	$\overline{B}$	Bootstrap 95% CI for A	Bootstrap 95% CI for B
320	1000	-28.38	[-28.49, -28.28]	-30.32	-26.57	[-30.80, -30.22]	[-26.91, -26.09]
	2000					[-30.795, -30.22]	[-26.91, -26.09]
	5000					[-30.795, -30.22]	[-26.91, -26.09]
520	1000	-28.38	[-28.46, -28.30]	-30.29	-26.61	[-30.68,-30.15]	[-26.80, -26.41]
	2000					[-30.44,-30.15]	[-26.80, -26.41]
	5000					[-30.68, -30.15]	[-26.80, -26.42]
680	1000	-28.38	[-28.45, -28.31]	-30.29	-26.65	[-30.43, -30.10]	[-26.80, -26.52]
	2000					[-30.43, -30.10]	[-26.80, -26.52]
	5000					[-30.43, -30.10]	[-26.80, -26.52]

Figure 7.11: Results of non-parametric bootstrapping

Based on 520 samples we take $[-30.10, -26.52]$ as our conservative 95% CrI estimate. Comparing with the direct Monte Carlo conservative estimate of $[-30.09, -26.57]$, the bootstrap estimate seems quite acceptable.

Chapter 8

Conclusions and Suggestions

8.1 Conclusions

In this report we have studied possible methods to analyze uncertainty in ATM accident risk assessment due to uncertainty in the values of the model parameters. We analyzed the method proposed by Everdij&Blom in [Ever02] for $\ln \mathcal{R}$, studied and implemented for $\ln \mathcal{R}$ the PCE based approach proposed in [Webs96] and [Isuk99], and investigated the possibility of using small sample Monte Carlo based methods. We showed that the Everdij&Blom methodology can be reinterpreted in terms of a first order Taylor expansion of $\ln \mathcal{R}$ and as a first order PCE in the case of unbiased nominal values and suggested methods to improve determination of the $\beta_i's$. Furthermore, two simulations that were executed indicate that the method performs better when the nominal values of the parameters are unbiased. In the biased case it seems the Everdij&Blom method can still yield a reasonable but conservative estimate of the 95% CrI. A minor detail which should be taken into account when working with the Everdij&Blom method is that small values of a particular β_i^* or β_i^{**} may lead to the conclusion that $\rho(V)$ is insensitive to V_i. However, we should keep in mind that this insensitivity arises on the condition that all other parameters V_j, $j \neq i$ are kept at their nominal values. If some of the $V_j's$ are not at their nominal values then it is possible that the insensitivity will no longer hold (Section 3.6).

We implemented the PCE method on the two simulations mentioned above. The corresponding second order PCE performed well for both simulations, needing only 120 simulation runs to give statistical estimates which were very close to estimates obtained through 20,000 or 10,000 direct Monte Carlo runs of the accident risk model. However, the PCE is no longer efficient when the number of parameters becomes large and there is always the possibility that a second order PCE may not provide a good fit. Hence in this case other techniques have to be utilized. In such a situation we propose small sample Monte Carlo

based methods that use only few hundred samples of $\ln \mathcal{R}$. We propose carrying out parametric density fitting or application of the plug-in principle with the bootstrap method to assess the confidence interval of the statistical parameters of interest. The motivation for the parametric fitting method is the observation, based on the simulations, that $-\ln \mathcal{R}$ seems to follow a lognormal distribution while the main reason for proposing the bootstrap is that it can be implemented in a non-parametric fashion, this is particularly useful if our assertion that $-\ln \mathcal{R}$ follows a lognormal distribution does not hold true. The simulations results indicate that the parametric density fitting approach and bootstrapping can yield acceptable estimates of $E\{\ln \rho(V)\}$ and the 95% CrI.

We also made a contribution to the Generalized Reich model by deriving sufficients conditions for which Assumption A.5 of the model holds true and made some additional derivations for the Everdij&Blom framework.

8.2 Suggestions

Based on the study that has been carried out, in this section we suggest an outline of efficient steps in carrying out uncertainty analysis of ATM accident risk assessment due to uncertainty in the parameter values. The basic idea is given below:

- Model the parameters as lognormal random variables as in [Ever02].
- Apply the Everdij&Blom method with as low bias as possible based on β_i^{avg} (Chapter 4) or $\beta_i^{\text{safety conservative}}$ (Chapter 3) unless the number of parameters to be considered is too large to handle. If so, perform the small sample based Monte Carlo simulation (Chapter 5, for examples see the simulations in Chapters 6 and 7).
- Assess the approximation errors in the Everdij&Blom method. If the error level is not satisfactory and the number of parameters is large (say > 25), do the small sample Monte Carlo method and then stop. Otherwise implement the second order PCE (Chapter 4).
- Assess the approximation errors of the second order PCE. If error is satisfactory then stop. Otherwise attempt to refit the second order PCE or do a small sample Monte Carlo simulation.

Details on the steps suggested above are given in the Appendix.

8.3 Future Research

An observation that was made during this study is that when the parameters are modelled as lognormal random variables the distribution of $-\ln \mathcal{R}$ seems to approximately follow a lognormal distribution $\Lambda(\mu, \sigma^2)$ (note that this includes

the normal distribution as a special approximate case when the parameter σ is small. Refer to Chapters 6 and 7, particularly Figures 6.8, 6.11, 7.6 and 7.9). This is quite interesting and leads us to wonder under what conditions we may expect this property to hold. Further research on this could start by performing a small Monte Carlo simulation on a more complex system to observe whether this phenomenon still occurs. If it turns out that under some conditions this is a consistent property of $-\ln \mathcal{R}$ and if the variance of $\ln(-\ln \mathcal{R})$ is not large, then we can have some confidence that Monte Carlo based parametric methods (i.e. fitting of a lognormal distribution) can produce good estimates even when there are hundreds of uncertain parameters and only a few hundred samples of $\ln \mathcal{R}$ available.

In general, the incrossing risk is formulated as[Ever02]:

$$\mathcal{R}_{[T_1,T_2]} = \sum_{i=1}^{N} \mathcal{R}(K_i) \times P(K_i) \tag{8.1}$$

where $K_1, K_2, ..., K_N$ are specific events, $\mathcal{R}(K_i)$ is the K_i conditional accident risk and $P(K_i)$ is the probability of the occurence of event K_i. Future research can also be focused on how to carry out uncertainty analysis for such a general formulation of the incrossing risk.

Another topic that can be the theme of further research is the determination of collocation points for the second order PCE. The methods that are available in the literature at the moment and implemented in this study are based on heuristics, where the selection of collocation goes by the principle of sampling the unknown function at points which can be regarded as being "representative". However, it would be very helpful if we could determine if there does indeed exist some optimal choice of collocation points in cases where we want to approximate $\ln \mathcal{R}$ by using a second order PCE when in fact $\ln \mathcal{R}$ can be closely modelled by a d^{th} order PCE (for some $d > 2$). A similar question is the topic of research in the area of surface response methods and experiment designs[Khur96], it would be interesting to see if some of these methods can be extended to the case of the PCE. This direction may also involve exotic elements from approximation and interpolation theory.

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Appendix

In this appendix we provide more detail on the efficient steps for uncertainty analysis due to uncertainty in the parameter values suggested in Chapter 8. A flowchart of the scheme is provided in Figure 1.

The detailed explanation is as follows:

1. Define a lognormal distribution for the uncertainty of each parameter, i.e. $V_i \sim \Lambda(\mu_i, \sigma_i^2)$ (see Chapter 3).

2. If the number of parameters to be considered is too large to be handled by the Everdij&Blom method (Chapter 3) proceed to step 5, otherwise go to the next step. A large number of parameters means that many accident risk model evaluations will be needed to evaluate the $\beta_i's$, hence in such cases the Everdij&Blom method would be less efficient than a small sample Monte Carlo based approach.

3. Implement the Everdij&Blom method with as low bias as possible or with unbiased nominal parameter values (i.e., use $v_i = e^{\mu_i}$). We recommend that the $\beta_i's$ be determined by the averaging method (Chapter 4), i.e. $\beta_i^{avg} = \frac{\beta_i^* + \beta_i^{**}}{2}$, or by the safety conservative approach (Chapter 3).

   Let N denote the number of coefficients in a second order PCE expansion. Generate $K > N$ collocation points, $x^1, x^2, ..., x^K$, such that $rank(H) = N$ (see Subsection 4.9.1). Select a suitable number of M collocation points from the K collocation points and evaluate $\ln \mathcal{R}_i = \ln \widetilde{\rho}(x^i)$ and the Everdij&Blom approximation $\ln \widehat{\mathcal{R}}_{i,EB}$ at those points where

$$\ln \widehat{\mathcal{R}}_{i,EB} = \ln \rho(c) + \sum_{j=1}^{n_p} \beta_i \sigma_i z_j^i$$

   $z^i = (z_1^i, ..., z_{n_p}^i)$, $z^i \in \{x^1, x^2, ..., x^K\}$ for $i = 1, ..., M$ and $z^i \neq z^j$ for $i \neq j$. Finally evaluate the average squared approximation error:

$$\overline{e^2} = \sum_{i=1}^{M} w_i (\ln \mathcal{R}_i - \ln \widehat{\mathcal{R}}_{i,EB})^2$$

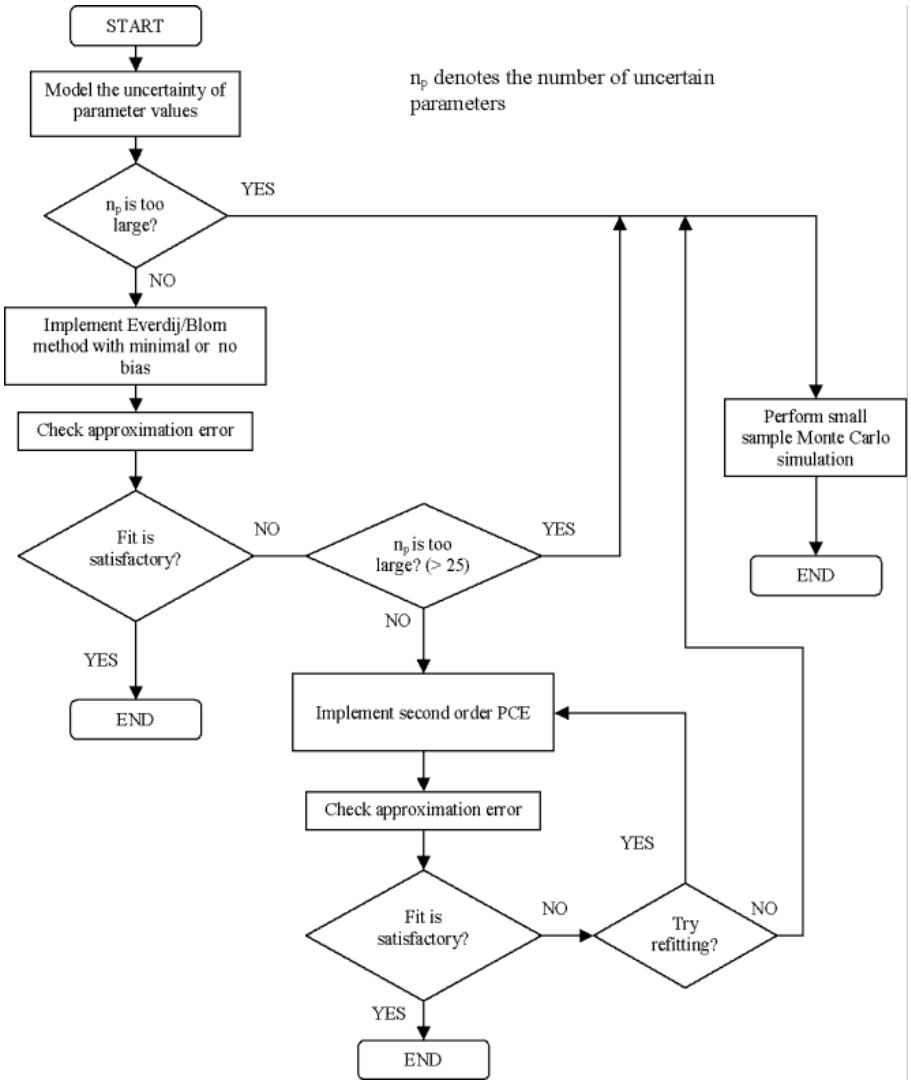

Figure 1: Flowchart of suggested efficient steps in uncertainty analysis

where $w_i \geq 0$ is some suitable weighing function, e.g. $w_i = \frac{f(x^i)}{\sum_{i=1}^{M} f(x^i)}$ where $f(x^i)$ is the density of $X = (X_1, X_2, ..., X_{n_p})$ at x^i or $w_i = \frac{1}{M}$. If $\overline{e^2}$ is deemed satisfactory (i.e. a reasonable fit is obtained) then we use the Everdij&Blom estimates as our estimates of the mean and 95% CrI, if not proceed to step 4. Determining how small $\overline{e^2}$ should be is depends on the goal of the uncertainty analysis: whether we want to get a rough estimate of the statistical parameters of interest or an accurate estimate.

The simulations show that in the case of the Everdij&Blom method with biased parameters, errors can be large yet the method was still able to provide a reasonable estimate of the upper bound of the 95% CrI. Based on the simulations, to get accurate estimates then $\overline{e^2} < 10^{-2}$ would be desirable while for a rough estimate then $\overline{e^2}$ in the range of 10^{-2} to 1 (or even > 1) seems acceptable.

4. Carry out this step only if the number of uncertain parameters is not large (say less than or equal to 25), if not go to step 5. Partition the K collocation points in step 3 into two parts: partition A containing K_1 collocation points to determine the coefficients of the PCE and partition B containing K_2 collocation points to assess the fit of the second order PCE (as in step 3), where $K_1 + K_2 = K$. Note that the collection of points in partition A should be such that $rank(H_A) = N$ (H_A denotes the matrix H corresponding to the K_1 collocation points in A, see Subsection 4.7.3). Evaluate $\ln \mathcal{R}_i = \ln \widetilde{\rho}(x^i)$ for the collocation points in A and determine the coefficients of the second order PCE by solving a linear equation (if $K_1 = N$) or by a least squares method (if $K_1 > N$). Evaluate $\ln \mathcal{R}_i$ and $\ln \widehat{\mathcal{R}}_{i,PCE}$ (to denote the PCE approximation to $\ln \mathcal{R}_i$) at the remaining collocation points in B. Check for the quantity $\overline{e^2}$ as in step 3. If $\overline{e^2}$ is satisfactory then use the second order PCE estimates as our estimate of the $E\{\ln \mathcal{R}\}$ and 95% CrI, if not then we may choose to repeat this step by adding points from partition B to partition A, reevaluating the PCE coefficients and recalculating $\overline{e^2}$ (note that the number of points in B becomes smaller), or we may choose to go to step 5.

5. Collect a small number of random samples of $\ln \mathcal{R}$, e.g. 320 or 520 samples. Observe the histogram of $\ln \mathcal{R}$; if the distribution seems to follow a normal or lognormal distribution then try to fit a normal or lognormal density (see Section 5.3), otherwise apply the non-parametric bootstrap (Section 5.4). Use the small sample Monte Carlo estimate of the mean and 95% CrI as the estimates which we will present (see for example Subsection 6.7 and 7.7).