DISTRIBUTION OPTIMAL IMPORTANCE WEIGHTS FOR EFFICIENT UNCERTAINTY PROPAGATION THROUGH MODEL CHAINS

A Thesis

by

MEET NILESH SANGHVI

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Chair of Committee,	Douglas Allaire
Committee Members,	Astrid Layton
	Raymundo Arroyave
Head of Department,	Andreas A. Polycarpou

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ABSTRACT

This thesis proposes a least squares formulation to determine a set of empirical importance weights to achieve a change of probability measure. The objective of the thesis is to estimate statistics from a target distribution - distribution of interest using random samples generated from a different proposal distribution - cheap/available distribution. The approach taken here works directly with the probability measure of the proposal and target distributions, for which only samples from each are needed. The result is an approach more capable of achieving high dimensional probability measure change than current state-of-the-art methods. Such a method can enable efficient and accurate propagation of uncertainty through model chains of unknown input and output regularity, such as those often encountered in process-structure-property chains in materials science. The proposed approach is demonstrated on five benchmark problems of increasing dimension and also tested on a Gas Turbine System.

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All other work conducted for the thesis was completed independently.

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1. INTRODUCTION

1.1 Motivation

Uncertainty quantification and its propagation has been the subject of much recent interest due to the increasingly availability of parallel computing platforms, widespread advancement in numerical simulations and algorithms, and the development of complex simulation models. Usually, such models carry variability with them due to lots of factors which leads to uncertain model output/behaviour. When uncertainties are characterised, modeled and analyzed critically it can prove to be instrumental in the development of these computational models for the purpose of validation, confident decision-making and policy-making analysis. Therefore, UQ/ UP can be used to make predictions about the real world systems, to estimate risk probabilities and failure statistics associated with the model under assumptions, to identify critical components for the design optimization and/ or for performance enhancement. The demand and importance of UQ/UP has led to the introduction of uncertainty assessment tools in very diverse areas such as climate change, structural engineering, quality engineering, aerospace engineering and design, medicine, materials science, etc.

In the field of materials science, however, notions of UQ remain relatively unexplored even though it is of critical importance as the field progresses towards more predictive approaches to materials development. Indeed, UQ/UP across multi-scale model chains are key elements of decision-based [1, 2, 3] materials design in the framework of Integrated Computational Materials Engineering (ICME) [4, 5], where databases, multi-scale modeling, and experiments are integrated with the aim of time reduction in design and manufacturing of materials or products. In this context, the understanding and quantification of uncertainties can provide a confidence measure for the applicability of models for decision making in materials design. Although UQ/UP and overall uncertainty management have been recognized as essential components of simulation-assisted materials discovery/design efforts, relatively very few examples in computational materials science

exist [6, 7, 8, 9, 10]. UQ at the individual model stage has recently received much attention by the materials science community [11, 12, 13, 14]. Yet, to realize ICME, techniques are required for efficiently and accurately propagating uncertainty from the inputs of one model to its outputs and from lower level models to upper level models within a model chain.

The proposed approach tries to solve this problem by developing the state of the art efficient and accurate uncertainty propagation technique.

1.2 Science of Uncertainty Quantification

This thesis introduces one of the main applications of uncertainty quantification- uncertainty propagation and the necessary model framework to carry out complex UP and hence it is logical to start with defining what Uncertainty Quantification is, the science behind it and how it is relevant in the modern industry.

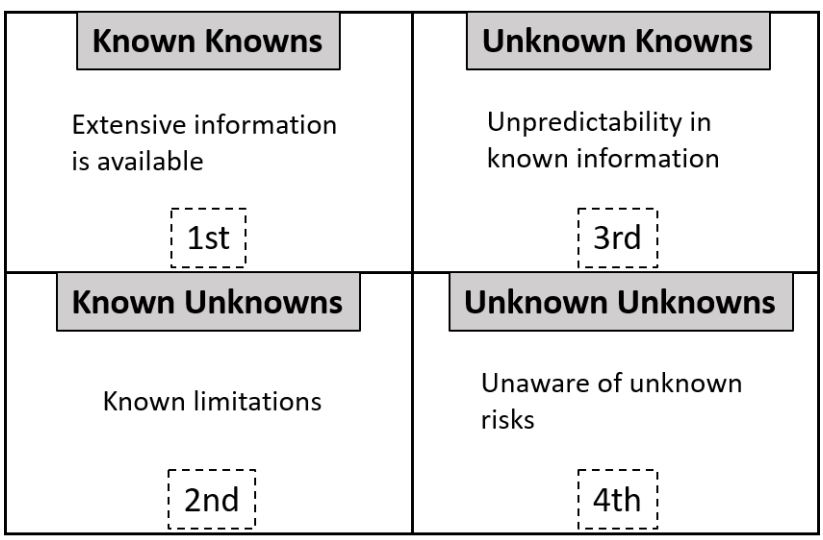

Figure 1.1: Matrix of knowledge with four quadrants.

Matrix of knowledge [15] is used to differentiate the various problems and challenges caused by uncertainty in engineering realm. As given in the Figure 1.1, first quadrant of known knowns are the things that are represented as the best practice in the industry. Typical engineering work

is done in this quadrant. The products are developed and validated using the known physics and simulation-based models. However, discrepancy in such models are also known and they come under the second quadrant of unknown knowns. For example, one might know factors that can improve the simulation model but within the certain error range. However, a little effort towards understanding such factors is what requires experience in modern-day engineering. The third quadrant is what is identified and addressed by scientific uncertainty quantification methodologies. This usually refers to the cases for which various parameters are known in which the data is either not robust/ reliable/ rigorous or misinterpreted. In other words, the data is known to predict the volatility in the operating system, but it is not systematically evaluated. In most of the cases, third sector is caused because of not having a systematic approach in the collection and analysis of data. However, in recent times, more responsible data collection practices have been advocated to deal with uncertainty. The fourth quadrant is the scariest one as usually no knowledge about it is evident. However, there are methods to address problems in this section such as the p-box approach. The general idea is to explore the parameter space in a systematic way to search for possible complications and quantify their risk. Particularly, important is the search for rare events with the disastrous consequences, so called Black Swans.

This work proposes methods for all three sectors devoting most of the work to the third quadrant: quantifying the variabilities of engineering predictions by efficiently propagating and incorporating experimental data.

1.3 Advantages in Industry

UQ methods are rapidly being adopted by engineers and modeling professionals across a wide range of industries because they can answer many questions that were previously unanswerable.

Multidisciplinary analysis is an extensive area of research, which helps in supporting today's modern engineering systems which are designed and developed by multiple teams (Figure 1.2). In addition to the difficulties associated with the design of such systems, the need to enhance performance and efficiency often drives the design to its physical limits. Modeling and simulation technologies have assisted in the analysis and development of many complex and integrated

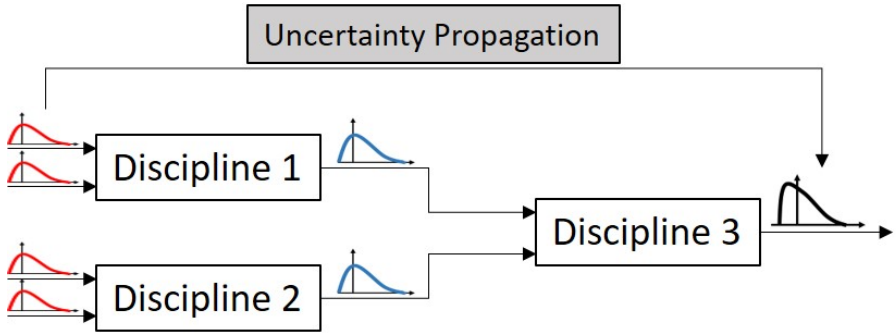

Figure 1.2: Uncertainty quantification and propagation can identify and predict the output variability in a multidisciplinary design model.

multidisciplinary systems. Virtual design through extensive modeling and simulation is extremely attractive for the engineering industry. Physical simulations help to improve product design, efficiency and competitiveness. They reduce the number of required real-life tests, to allow to design and test such products with minimal hardware prototyping, enhance speed to market and help to avoid costly production mistakes. However, the uncertainties in various parameters regarding the model can significantly affect the performance of the overall system. Hence, in order to assess the system robustness, reliability and for decision making, quantification of variabilities have become a practice in recent times.

UQ methods can be used to extend the capabilities of complex model further,

- UQ methods can be used to predict the system responses across uncertain and volatile inputs as shown in the Figure 1.3. They can be used to incorporate the effects of manufacturing errors and identify the probability of failure of a manufactured product through available data. Reliability predictions obtained through UQ are more accurate than pure statistical prediction because they complement the statistical data with high-fidelity physical information.

- UQ methods are also known to quantify the confidence in predictions. They can be used to calculate error bars (Figure 1.3) for experiments and computations which further can be employed to understand the robustness of the simulated model. However, as simulations are more deterministic and experiments contain uncertainties, it can also differentiate the

parameters causing discrepancy between simulation and experiments.

- Sensitivity analysis or parameter screening [16] is also a part of UQ methods. Generally, lowering the model order for the less sensitive parameter can aid to lowering costs without compromising efficiency (Figure 1.3). Conversely, increasing the safety margins that are too low helps to improve safety.

- Robust designing is the calculation of optima that are robust against the variations of the input parameters. Methods for uncertainty quantification lie at the heart of the robust design processes.

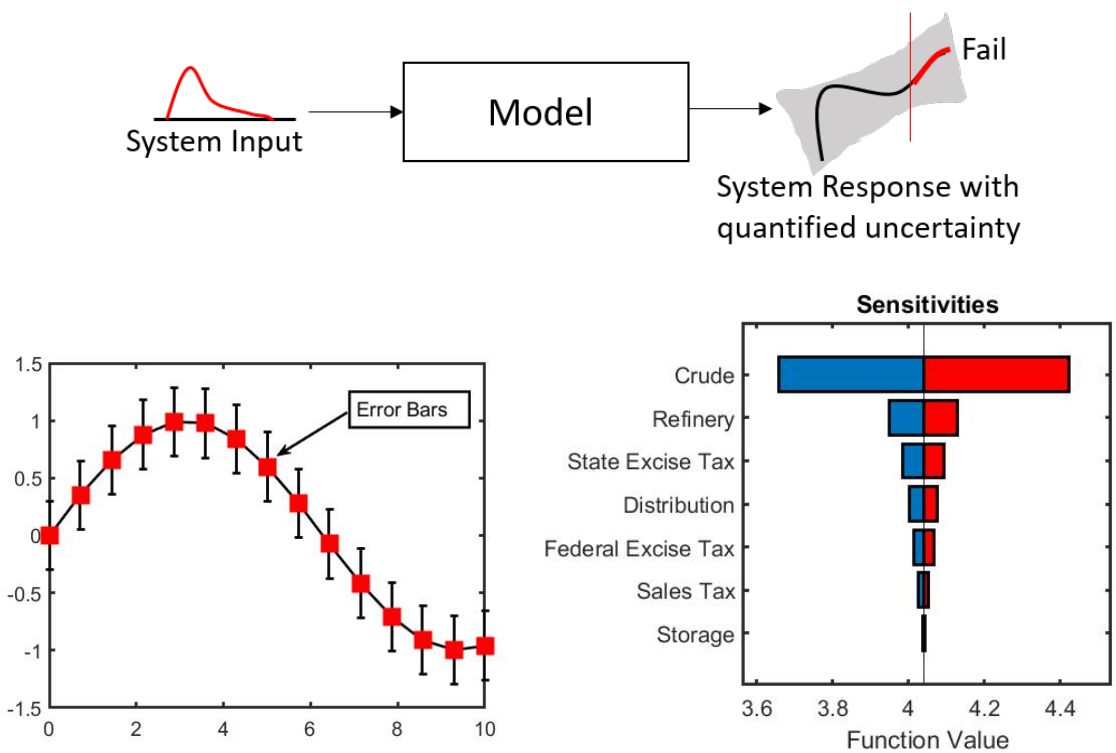

Figure 1.3: (top figure) Uncertainty propagation can help quantify uncertainty in system response when given a corresponding input. Grey area here represents the underlying uncertainty and the red region predicts failure probability (left bottom figure), Error bars (right bottom figure). Sensitivity analysis can identify the parameters sensitive to the response and help understand the model.

1.4 Types of Uncertainties

Uncertainty is an inherent part of the real world. No two physical experiments ever produce exactly the same output values and many relevant inputs may be unknown or not-measurable. Uncertainty effects almost all aspects of engineering modeling and design. Engineers have long dealt with measurement errors, uncertain material properties, and unknown design demand profiles by including factors of safety and extensively testing designs. By more deeply understanding and quantifying the sources of uncertainty [17], we can make better decisions with known levels of confidence.

1.4.1 Parameter uncertainty

This comes from the model parameters that are inputs to the computer model (mathematical model) but whose exact values are unknown and cannot be controlled in physical experiments, or whose values cannot be exactly inferred by statistical methods.

1.4.2 Parametric variability

This comes from the variability of input variables of the model. It is due to uncontrolled and/or unspecified input conditions. For example, uncertain loading of a material and the uncertain manufacturing process parameters can be examples of this type of uncertainty.

1.4.3 Structural uncertainty

Also known as model bias or model discrepancy, this comes from the lack of knowledge of the underlying missing physics, numerical approximations, inaccuracies of the computer model used to simulate real-life situation in the problem, considering they are the approximation of the reality. One example is when modeling the pendulum movement ignorance of air friction can be considered as a form of model discrepancy. This type of uncertainty is associated with the fact that no model is perfect and even though there is no unknown parameters in the model, a discrepancy is still expected.

1.4.4 Algorithmic uncertainty

Also known as numerical uncertainty, or discrete uncertainty. This type of uncertainty arises due to highly complicated models (most models are too complicated to solve exactly). This results from the surrgates used or numerical assumptions and approximation made to solve the given complex computational model. For example, the finite element method or finite difference method may be used to approximate the solution of a partial differential equation (which introduces numerical errors).

1.4.5 Residual Variability

This results from the uncertainty in intrinsic random variation in the process being modeled or in a lack of model detail which lead to different process values.

1.4.6 Experimental uncertainty

Also known as observation error, this comes from the variability of experimental measurements. The experimental uncertainty is inevitable and can be observed and mitigated by the repetition of the same experiment number of times methodically.

1.4.7 Interpolation uncertainty

This comes from a lack of available data collected from computer model simulations and/or experimental measurements. For other input settings that don't have simulation data or experimental measurements, interpolation becomes necessary which leads to uncertainty in the corresponding response. Even though the most accurate and efficient methods are used to interpolate the missing data, it is probabilistically impossible to interpolate each time correctly.

1.4.8 Aleatoric and Epistemic uncertainty

In broader terms uncertainty can be classified into two categories following [18, 19, 20, 21, 22],

1. Aleatoric uncertainty is also known as statistical uncertainty and is representative of unknowns that differ each time we run the same experiment. It arises through natural randomness in the system. This type of uncertainty is irreducible, in that there will always

be variability in the underlying variables and can be characterized by probability distribution. An example of aleatoric uncertainty is the randomness in the outcome of a fair coin flip. Without tossing the outcome can not be known, however it can be described by probabilities.

2. Epistemic uncertainty is also known as systematic uncertainty and is due to things one could in principle know but doesn't in practice. This may be because a measurement is not accurate, because the model neglects certain effects, or because particular data has been deliberately hidden. The parameter being measured is usually a characteristic of the material or the physical process. The uncertainty is related to the "lack of knowledge," about this parameter. It can be reduced by learning more about how things work. An example is distinguishing between a fair coin and a coin that lands heads 75 percent of the time; these correspond to two different models of reality, and you may have uncertainty over which of these models is correct.

In real life applications, both kinds of uncertainties are present. Uncertainty quantification intends to work toward reducing epistemic uncertainties to aleatoric uncertainties. The quantification for the aleatoric uncertainties can be relatively straightforward to perform, depending on the application. Techniques such as the Monte Carlo method are frequently used. To evaluate epistemic uncertainties, the efforts are made to gain better knowledge of the system, process or mechanism. Methods such as probability bounds analysis, fuzzy logic or evidence theory are used.

1.5 Challenges faced in Industry

While the mathematical theory of uncertainty quantification has been developed greatly in the last decade, many methodologies have been established and widely recognized. However, many techniques are still difficult to apply to actual engineering cases. These problems are: limited data and statistical assumptions, limited time, the curse of dimensionality, rare events and black swans, and model with discontinuity.

1.5.1 Limited Data

Obtaining measurement data is generally costly. The usual methods for the collection at higher level requires repeatability of measurements. While this is enough to estimate mean and variance, it is generally not enough to calculate statistical failure probabilities or perform a rare event analysis. Limited data generally leads to make assumptions about the behavior of the system. Here major simplifications as well as coarse assumptions are common. This can be problematic in statistics. The majority of the methods in the field of UQ assume that a sufficiently high number of samples are available. However, in most cases that is often not the case due to limited time and cost. Wrong assumptions about the parametric probability distribution is often underestimated.

Another problem is the wrong inputs, which lead to outputs in the region outside of defined space. As UQ heavily requires to identify the types of uncertainties in the system, if not known can cause undesirable effects to the solution. This conceptual error is only solved with the knowledge and experience regarding the subject. The method introduced in the subsequent chapter provides a single solution to the problems of how to deal with scarce data, and how to making avoid statistical assumptions.

1.5.2 Limited time and the curse of dimensionality

There is usually a time delay between the availability of results of a simulation and a complete UQ analysis. Receiving reliable UQ results on a standard workstation faster is only possible with a very efficient and intelligent UQ method and a reasonably fast model. However, the excess computational power at disposal for UQ is unfortunately not increasing nearly as rapidly as the total resources. The possible solution is of parallelizing the UQ methodologies with the access to high performance computing.

One of the major problems, is so called curse of dimensionality as suggested by M. Eldred and J. Burkardt in [**?**]. As the dimension increases the amount of data needed to obtain the reliable results grow exponentially increasing the computational expense. This is clearly shown in the Figure 1.4. Various surrogate modeling methodologies can be used to deal with the curse. Al-

though, such methods yield inefficient and unacceptable results. The result is a highly general new algorithm that can be parallelized easily to be used throughout any discipline.

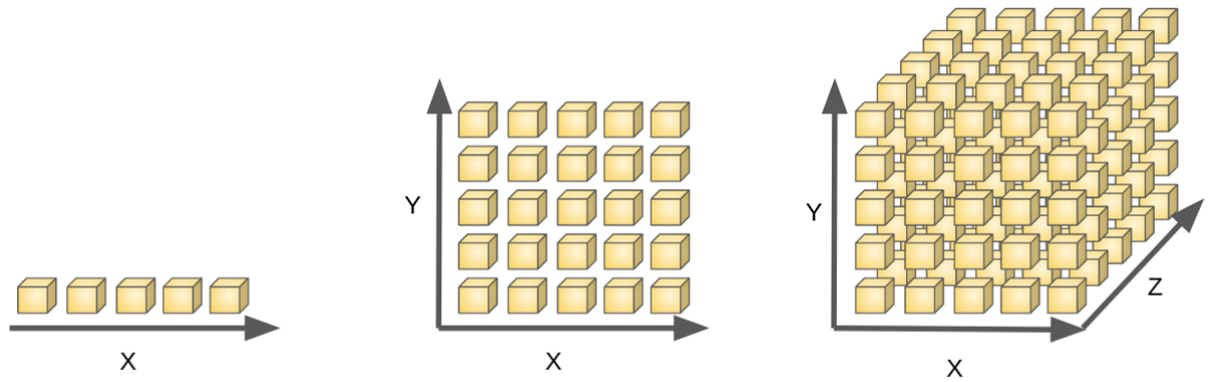

Figure 1.4: Illustration of curse of dimensionality. As the dimension increases the model evaluations rise quickly.

1.5.3 Rare Events and Black Swans

Uncertainty quantification can be used to perform risk analysis for a physical system using its virtual simulation model. Most popular in engineering is risk analysis using Gaussian distributions. However, they can give a false sense of security. The assumption of normality removes the possibility to account for rare events from the model. Events that are further away than five or more standard deviations from the mean are extremely unlikely for the normal distributions - more unlikely than they often are in reality. If such rare events have catastrophic consequences, they are called a Black Swan, as suggested by Taleb [23]. Black Swans have so far been studied mostly in mathematical finance to explain catastrophic market crashes. While physical laws and even aleotory input conditions can be discovered and incorporated into the simulation process, some unknown factors inevitably remain outside the scope of simulation. Hence, the fourth quadrant is considered to be the most unexplored region and most of the published literature deals with the third quadrant only. Especially for rare event analysis there is still lack of efficient uncertainty

propagation methods.

1.5.4 Models with discontinuity

Some computational models contain instabilities, bifurcations or sharp gradients [24] in their domain. Some discontinuities can be encountered if the uncertainties in that region is quantified. Overall, UQ for discontinuous models lacks behind methods for continuous problems.

1.6 Research Objectives

A large proportion of the research done in uncertainty quantification is on efficient uncertainty propagation methods. Having associated probability distributions to the parameters, we want to know what the probability distribution of the output or the quantities of interest look like, as in how the model converts the input probabilities to the output probabilities. Many methods in the field have appeared during the years, addressing different issues. Some of these methods will be presented in the coming Chapter 2. However, as it is often the case in numerical methods, the main issues encountered in the propagation are somewhat similar to the challenges mentioned before. Basically, they are related to the achievement of a good balance between accuracy and time consumed at higher dimensions. This research proposes a robust and reliable method to propagate and quantify uncertainties efficiently. The proposed methodology is developed keeping real-sized industrial problems in a non-intrusive way. This approach can also be used to handle chains of computational models via decomposition-based approaches [25, 20, 26, 27] that can enable rapid and accurate UP for materials analyses. To summarize, the high level objectives of this thesis are:

- **To develop a state of the art methodology to propagate uncertainties through complex model chain in a robust and efficient manner with the guarantees of analytical convergence**

  The proposed methodology is inspired by the change of probability measure approach. It formulates least square to determine importance weights in order to achieve the change of probability measure. It can provide more accurate statistical predictions for output quantities as it does not take any assumptions about the input probability distribution.

- **To perform system level uncertainty analysis by concurrently performing uncertainty analyses on individual disciplines followed by a synthesis of the discipline level analyses**

  We decompose the system uncertainty analysis into individual component level uncertainty analysis that are then assembled to achieve the desired system level uncertainty. This approach can be used to handle chains of computational models that can enable rapid and accurate UP for specifically materials analysis.

- **To develop a computationally efficient framework capable of handling higher dimensions**

  The developed approach utilizes matrices in order to solve the least square formulation. Such vector based approach can be parallelized easily and they are also relevantly easy to store when a very large input space is provided. Hence, the efficient computational framework can help solve higher dimensional problems. The proposed approach is also compatible with high performance computers which helps reduce the computational time significantly and increases the accuracy of the solution.

- **To demonstrate the developed approach on a real world application problem**

  The proposed approach is demonstrated on several benchmark test functions and a real world application problem to check the accuracy and efficiency of the results.

1.7 Thesis Content

For the aforementioned reasons the following building blocks are needed for a comprehensive UQ/ UP framework for industry: a method to deal with scarce experimental data to avoid statistical errors, a method capable of dealing with many input parameters to mitigate the curse of dimensionality, an efficient method to perform rare event analysis for complex computational models, a method to deal with discontinuous data, and a method to reduce high model-form uncertainty. Chapter 2 will go into different methodologies used in the current industry and their limitations. Chapter 3 introduces a state of the art strategy to solve the above stated problem and will go into

details about its functionality. Chapter 4 will cover different benchmark problems and will demonstrate how the developed approach compares with the approaches like kernel density estimation, L2O, Monte Carlo method, and Gaussian Processes. Chapter 5 demonstrates a complex gas turbine system problem and how the developed strategy can be employed to solve this problem and its results. Chapter 6 summarizes the importance, advantages and limitations of the approach and also talks about the future work.

2. BACKGROUND

Computational methods for uncertainty analysis of a single component can be classified into two groups: intrusive and non-intrusive approaches. The exploration of the reliability of a model using probabilistic methods is referred to as non-intrusive uncertainty quantification in the literature. The term non-intrusive means that the model is not modified but used as a black box. The basic procedure of a non-intrusive approach is demonstrated below.

Intrusive approaches, also known as embedded projection approaches, introduce a solution expansion into the formulation of the stochastic problem and projects the resulting equation into the expansion basis to yield a set of equations that the expansion co-efficient satisfy. This assembly and solution of the stochastic problem requires access and modification to the existing black box computational model. As it is limited to the models that can be modified, irreducible errors can not be propagated through such approaches [28, 29, 30, 31, 32]. Hence, it is not widely used in the industry.

Non-intrusive approaches on the other hand are also called as sampling-based methodologies due to the nature of non-invasiveness of the system formulation. This research focuses on non-intrusive approaches due to their broader applicability; that is, they can be applied to a wide range of models without requiring knowledge of or access to the underlying model information. In broader perspective we will show that these methods can be also be used to solve the issues lie within third and even fourth sector in the knowledge matrix.

We list here the common techniques used for a single component and will be used in the following chapters of the thesis for the benchmarking purpose.

2.1 Importance Sampling

Importance sampling is a commonly used technique to carry out efficient sampling from a proposal distribution [33]. Proposal distribution is a distribution from which the sampling has been done to match the target distribution. Surrogate model can be considered as a proposal distribution.

On the other hand, target distribution is a distribution from which drawing samples directly is either complicated, difficult or expensive [34]. Hence, proposal samples sampled from proposal distribution are then used to generate realization of the output response or target distribution.

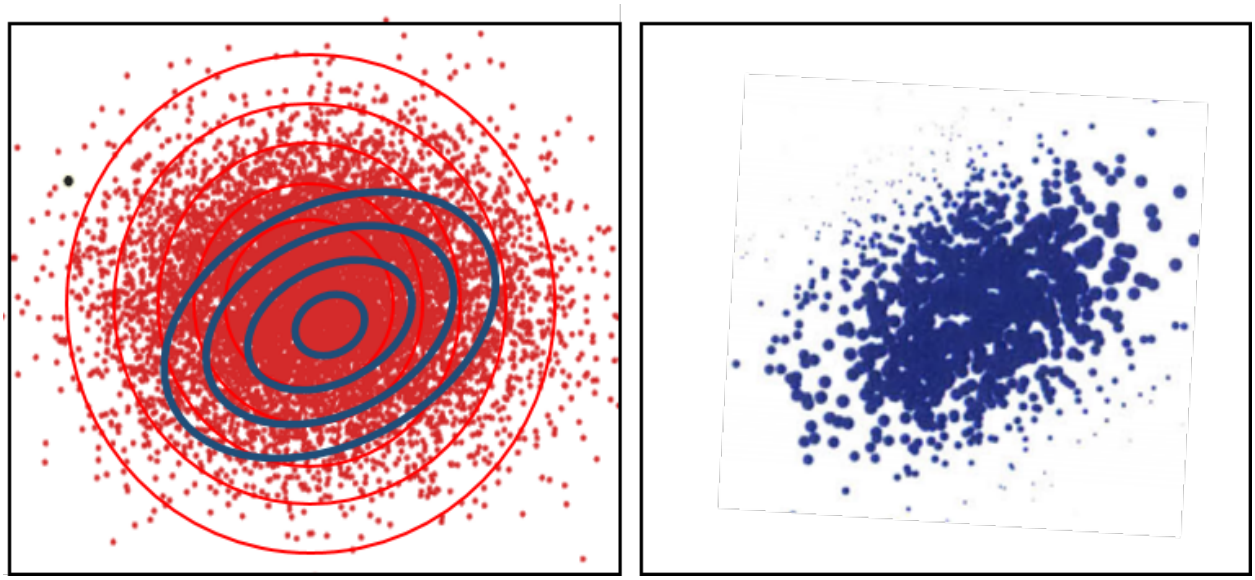

Figure 2.1: The importance sampling process uses the proposal samples generated (red dots on left figure) from a proposal distribution (red contours on left figure) to approximate a target distribution (blue contour on left figure), by weighing the proposal samples (blue dots on right figure).

As an example, we have available to us $x^1, x^2, ..., x^n$ drawn from rather unknown input proposal density f_μ. We also have available the corresponding model evaluations for each proposal sample $(g(x^1), g(x^2), ..., g(x^n))$. We consider the case where the inputs are now distributed according to a different target distribution. This refinement might happen because of the data getting available through updated upstream models or due to adopting a different input scenario during design process. If the model g is too expensive to evaluate which is the case for most of applications in engineering, then it becomes expensive to re-evaluate the model. Instead we use the importance sampling technique to estimate the target statistics (f_ν) from already generated samples from in-expensive proposal distribution.

In other words, as shown in Figure 2.1, instead of running the target samples over the com-

putational model, we use our proposal distribution to perform change of probability measure to approximate the statistics of interest.

The expectation of the target evaluations is:

$$\mathbb{E} = \mathbb{E}_{\nu}[g(\mathbf{t})] = \int g(\mathbf{t}) f_{\nu}(\mathbf{t}) dt \tag{2.1}$$

And through importance sampling this estimation can be approximated as

$$\mathbb{E}_{\ltimes} = \sum_{i=1}^{n} w^{i} g(\mathbf{x^{i}}) \tag{2.2}$$

Where, $w^{i} = f_{\nu}/f_{\mu}$, and $\mathbf{t}$ is the input samples

The importance weights w^{i} can be estimated using following techniques:

2.1.1 Monte Carlo Method

Monte Carlo method is the most common technique used for uncertainty quantification [35], due to its simplicity and good statistical results. However, its computational cost is extremely high, and, in many cases.

This technique generates random sampling to make numerical estimation of unknown parameters in our case that is unknown proposal distribution. All the data are combined through statistics to access the response under analysis. In other words, it is a method that is able to approximate a deterministic response of a function through many arbitrary inputs. However, this method needs large number of sample data to correctly identifying the target statistics accurately.

Other efficient sampling techniques which are faster and more methodical than generating random samples are latin hyper cube sampling [36], response surface method using central composite designs [37], advanced mean value with p-level iterations [38], etc.

2.1.2 Kernel Density Estimation

The kernel density estimation (KDE) is a method to compute the density statistics given the random samples [39]. Here, KDE approach is applied to approximate target density (f_{ν}) and

proposal density (f_μ) from their respective random. Then, we will compute the Radon-Nikodym importance weights by approximating the Radon-Nikodym derivative with $\frac{f_\nu}{f_\mu}$ [40].

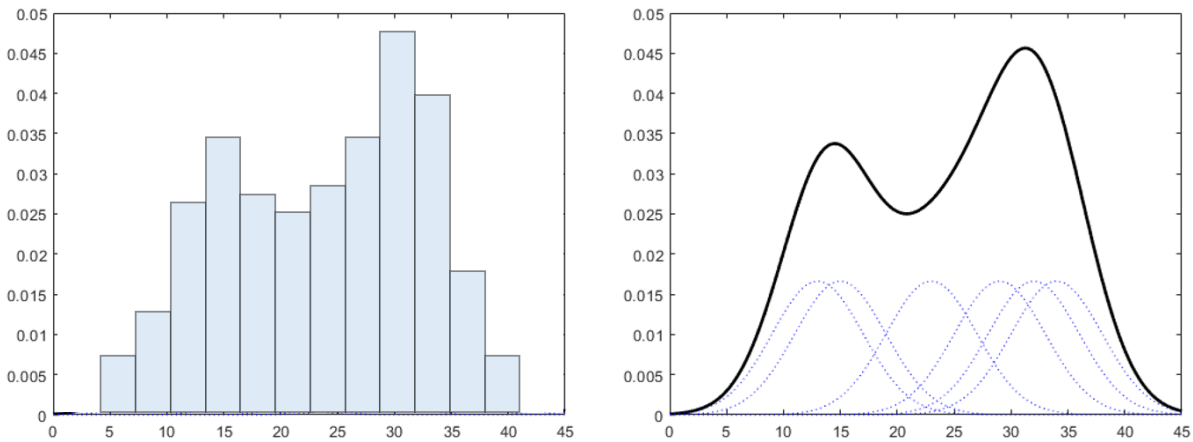

Figure 2.2: Histogram generated from the random samples can be approximated as a density function shown in the right figure using KDE. Kernel function (blue dotted line on right figure) is integrated over the sample size and the smooth density can be obtained (black continous line).

These estimators are defined by,

$$f(\mathbf{t}) = \left(\frac{1}{nh}\right) \sum_{i=1}^{n} K\left(\frac{\mathbf{t} - x^i}{h}\right) \tag{2.3}$$

Where, x^i are i.i.d random variables. h is called the bandwidth and K is a kernel function.

Intuitively, KDE uses the kernel function K to smooth out each data points into a smooth bump. Then, it sums over all these bumps to obtain density estimation. At regions with more data points, it will have many bumps yielding an overall large bump as shown in the Figure 2.2. On the other hand, regions with few observations, the density value from summing over the bumps will be low.

Usually the kernel is assumed to be non-negative and symmetric with integral 1. Here, the choice of bandwidth h is much more important than the choice of the kernel. Small values of h make the estimate wiggly and show spurious features, whereas big values of h lead to an estimate which is too smooth in the sense that it is too biased and may not reveal structural features. We

will be using the bandwidth chosen by minimal mean squared error (MMSE) principle and the Gaussian kernel as a kernel function.

Once the densities are computed, the Radon-Nikodym importance weights are approximated as below:

$$w^i = \frac{f_\nu}{f_\mu} \tag{2.4}$$

2.1.3 L_2 Optimized (L2O) Importance Weights

In L2O the optimal importance weights are obtained by solving the optimization statement using Frank Wolfe and Dai Fletcher Algorithms respectively for lower and higher dimensional problems [41]. Unlike density estimation techniques, this approach exploits the structure and optimizes the weights using optimization solvers. Intuitively, it minimizes the L_2 norm between weighted proposal empirical distribution function and empirical target distribution function finding the importance weights at each sample location (Figure 2.3).

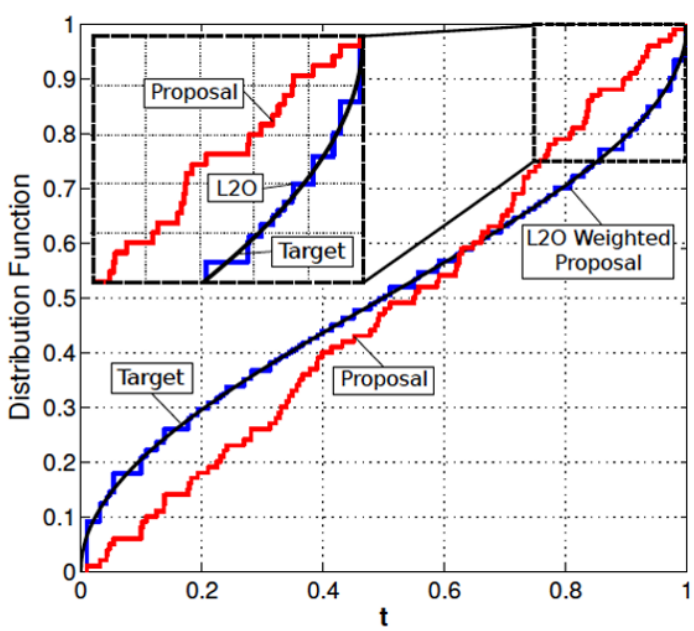

Figure 2.3: L2O approach minimizes, with respect to empirical importance weights associated with proposal samples, the L_2 -norm between the weighted and target distribution function.

The advantage of L2O over other approaches is that it solves itself without needing to tune any parameters. It also scales well handling a large number of samples. However, there are some numerical ill-conditioning when scaled for high dimensional distributions.

2.2 Gaussian Processes (GP)

The GP approach is a non-parametric Bayesian approach [42], in that it finds a distribution over the possible functions $g(\mathbf{t})$ that are consistent with the observed or here target random samples. As with all Bayesian methods it begins with a prior distribution and updates this as data points are observed, producing the posterior distribution.

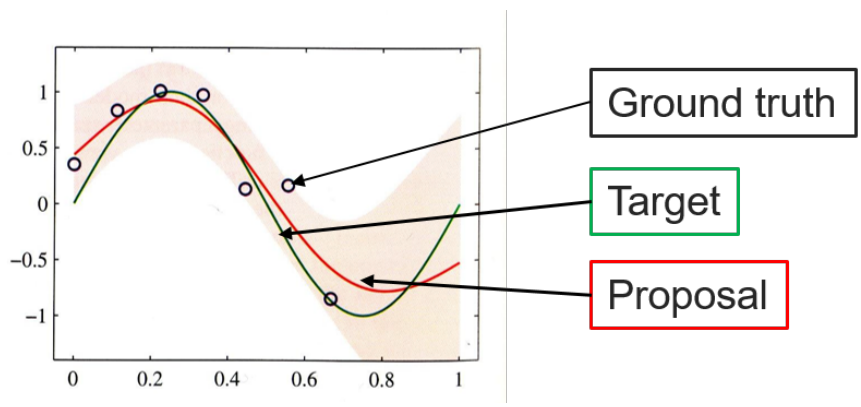

Figure 2.4: GP based on the target or ground truth corrects the distribution generated using joint Gaussian distribution.

In GP, it turns out we only need to be able to define a distribution over the function's value at a finite proposal random samples, arbitrarily, $x^1, x^2, ..., x^i$. As the name suggests GP assumes that probability density of $f_\nu(x^1), ..., f_\nu(x^i)$ is jointly Gaussian, with some mean and covariance.

$$f_\nu|\mathbf{X} \sim \mathbf{GP}(g(\mathbf{t})|\mathbf{m}(\mathbf{X}), \mathbf{k}(\mathbf{X}, \mathbf{X}')) \tag{2.5}$$

where $\mathbf{m}(\mathbf{X}) = (m(x^i))^i$, $\mathbf{k}(\mathbf{X}, \mathbf{X}') = (k(x^i, x^j))_{ij}$ and GP is the probability density function of a n-dimensional multivariate normal random variable with mean σ and covariance matrix $\sum$.

It then iteratively adds the data points ($\mathbf{X}'$) changing the joint distribution by updating the mean ($\mathbf{m}(\mathbf{X})$) and the covariance ($\mathbf{k}(\mathbf{X}, \mathbf{X}')$) according to an associated kernel function with each addition as shown in Figure 2.4. Here, the kernel function is created as a covariance matrix that restricts the set of functions under consideration. Once all the ground truth samples are sampled, the final distribution is formulated such that the error values are minimized resulting into accurate model of output distribution based on the target samples.

2.3 Current Practices

Previous work on uncertainty propagation via a change of probability measure that focuses on density estimation of unknown distributions summarized before can often fail to yield accurate results. If both proposal and target distributions are known and satisfy additional conditions, then the Radon-Nikodym theorem [40] provides a valid solution. This essentially states that the required importance weights can be computed via computation of the ratio of the target and proposal densities (Radon-Nikodym derivatives), hence the term density ratio. These approaches seek to change the measure from the given density ratio (proposal) to a specific target value. However estimating the unknown density function from the random samples in itself is a complicated task and especially challenging at higher dimensions. In the case of an unknown underlying probability distribution, even though the Radon-Nikodym theorem still applies, the density ratio is indeterminable and hence we cannot directly compute Radon-Nikodym derivatives for importance weight estimation.

For this situation, previous work has generally relied on attempts at estimating unknown probability density functions from random samples generated from unknown distributions using kernel density estimation [39]. However, similarly quite often density ratio based approaches that rely on estimated densities fail if the sample space is high-dimensional [43, 39, 44]. Thus, this method is used with dimensional reduction strategies like Principal Component Analysis (PCA), Generalized Discriminant Analysis (GDA), Projection Pursuit Density Estimation (PPDE), which can result in a significant loss of information and inaccurate UP results. In practice, this challenge can be overcome if the random samples are known to be generated from a parametric distribution family, in

which a parametric density estimation method can be employed.

Specifically, as input dimension increases, KDE requires significantly more samples to achieve the same accuracy, which eventually leads to numerical ill-conditioning that currently cannot be overcome. Other density and density ratio estimation approaches include the kernel mean matching approach that matches moments using a universal reproducing kernel Hilbert function [45]; the probabilistic classification approach, which computes the probability density ratio by applying Bayes' Theorem [46]; the importance estimation filtering approach, which minimizes the Kullback-Leibler divergence metric between the estimated and actual probability density ratios [47]; the unconstrained least squares importance filtering approach, which minimizes the L_2-norm between the estimated and actual probability density ratios [48]; and the direct density ratio estimation with dimension reduction, which solves the previous approach on a lower-dimensional space [49]. Each of these parametric approaches requires careful tuning to their respective parameters to ensure accurate results and can be challenging to employ in new problem domains. As a result, there has been a recent interest in developing approaches for importance weight estimation that avoid estimating the probability density function or density ratio.

One such recent approach is that of Ref. [50], which works only with determinable empirical distribution functions. The approach as discussed previously computes importance weights by minimizing the L_2-norm between a target distribution function and a weighted proposal empirical distribution function. This concept avoids using any basis function representations and regularization needs. Hence, this optimization approach can be implemented at large scale (both high dimensional and large sample size). However, eventually, numerical ill-conditioning enters owing to most samples occupying only the boundaries of high dimensional product spaces.

The work we present here extends the L2O approach of optimization of importance weights and introduces the novel approach of changing probability measure by computing importance weights directly with target and proposal measures. The resulting formulation is a linear system of equations that can be readily solved using least squares techniques. The appeal of using the probability measure rather than the cumulative distribution function of the L2O approach is that a user can

enforce where the probability measure is evaluated. Specifically, this allows for the inclusion of high probability areas on the boundaries of high dimensional input spaces.

3. APPROACH

In this section, we describe our model to propagate the uncertainty using a proposal and target probability measure via the importance weights computed in the process. We note here that, the importance weights and the probability density function need not be known explicitly and the proposed approach can be entirely sample based. By that we mean, given the incorrect input distribution or proposal random samples, this methodology can enable a rapid correction to uncertainty propagation results via target distribution measure or random samples. This correction is based on reweighting the previously executed model evaluations- which may have been computationally expensive or difficult to compute again- with importance weights formulated using the linear least square approach. Computed importance weights are such that the results converge to those results if the correct or target distribution had been used in the first place. Hence, being a non-intrusive method, no new model evaluations are needed for this approach, leading to rapid and efficient UP corrections.

In the example given below in Figure 3.1, the target and proposal random samples are generated from different normal distributions $\mathcal{N}(\mu = 1, \sigma^2 = 3)$ and $\mathcal{N}(\mu = 0, \sigma^4 = 4)$ respectively. The core idea of our methodology is to use the computed importance weights to transform the weighted proposal density shown as a green plot in the right image to the required target density function.

3.1 Framework

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space, where Ω is a sample space consisting of all the possible outcomes, $\mathcal{F}$ is a σ-field and $\mathbb{P}$ is probability measure on $(\Omega, \mathcal{F})$. $\mathcal{F}$ represents the collection of the subsets of possible outcomes Ω, which is used to define the probability measure $\mathbb{P}$ on the sample space. The random variable $Y : (\Omega, \mathcal{F}) \rightarrow (\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d))$, where d is the dimension of the input space, is such that the target measure, $\nu(A) = \mathbb{P}(Y^{-1}(A))$ for $A \subset \mathbb{R}^d$. The target measure $\nu(A)$ is the probability measure of all the target random samples. Likewise, the random variable $X : (\Omega, \mathcal{F}) \rightarrow (\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d))$ is associated with the proposal measure, μ on $\mathbb{R}^d$, such that

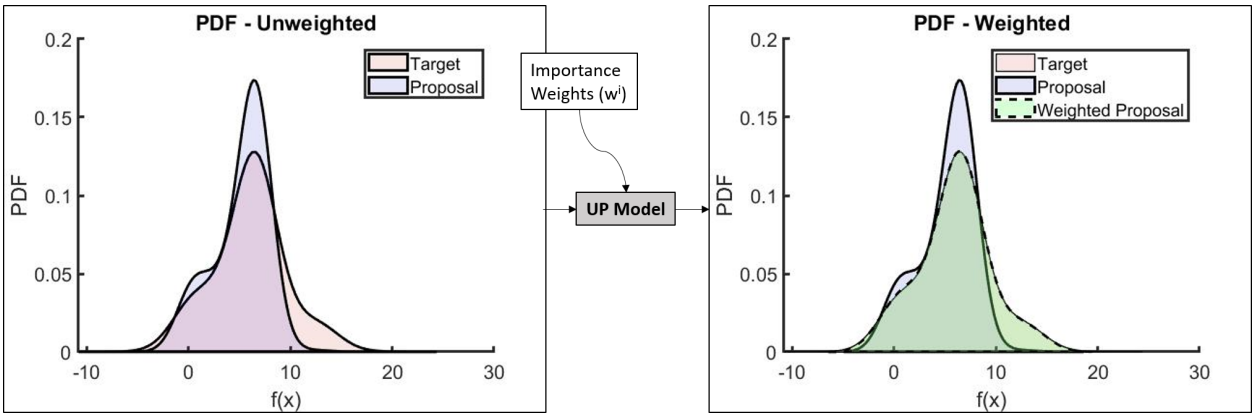

Figure 3.1: The proposed approach corrects the proposal distribution shown in the red (left figure) using importance weights and estimates the target distribution as a weighted proposal distribution (dotted plot on the right).

$\mu(A) = \mathbb{P}(X^{-1}(A))$ for $A \subset \mathbb{R}^d$. Similarly, $\mu(A)$ denotes for the probability measure on proposal random samples. Let $\mathcal{S}$ be a collection of closed subsets in $\mathbb{R}^d$ such that $\mathcal{S} = \{S_1, S_2, ..., S_m\}$. Here, topological space or Hausdorff space is given by, $S_j = I_1 \times I_2 \times ... \times I_d$ where I_k is the subset of the topological space in dimension k such that $I_k \in \mathcal{B}(\mathbb{R}^k)$. In our proposed approach, each of the S_j's can be represented as a hyper-sphere or n-sphere of dimension $\mathbb{R}^d$ in the measure space $\mathcal{B}(\mathbb{R}^d)$. For example, in one dimension an S_j simply represents an interval in the measure space with some radius R as shown in the Figure 3.2. Similarly, in two dimensions, an S_j can be considered as a disk in the measure space and in three dimensions it is a sphere.

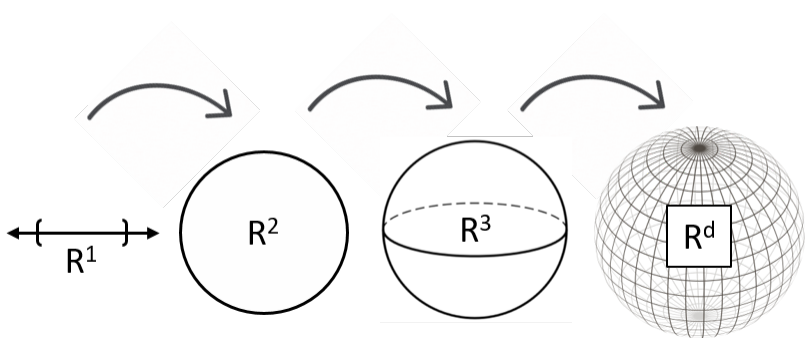

Figure 3.2: How the n-spheres look in one, two, three and d-dimensional space.

We then define the target probability measure as $\nu : \mathcal{S} \rightarrow [0, 1]$ of Y. Similarly, $\mu : \mathcal{S} \rightarrow [0, 1]$ is defined as the proposal probability measure of X. Target and proposal probability measures define the probability measure of a given hyper-sphere S_j conditioned to $S_j \in \mathcal{B}(R^d)$. In our problem formulation, the proposal measure μ is accessible to us only through sampling; that is, we are provided with random samples of the random variable X, but we can not evaluate μ explicitly. Let $\{x^1, x^2, ..., x^n\}$ be random samples of X, where n is the number of random samples. The objective of our work is to estimate statistics from the given or known target measure ν given random samples $\{x^1, x^2, ..., x^n\}$ generated from the proposal distribution μ.

To enable the change of measure on a set of samples, we compute the empirical measure of a given hyper-sphere as

$$\mu_i = \frac{1}{n} \sum_{j=1}^{n} \mathbb{I}_{S_i}(x^j), \tag{3.1}$$

where

$$\mathbb{I}_{S_i}(x^j) = \begin{cases} 1 & \text{if } x^j \in S_i, \\ 0 & \text{if } x^j \notin S_i. \end{cases}$$

Basically, it means that if a given random sample x^j lies in a hyper-spheres S_i, the indicator function will yield 1 for that particular hyper-sphere and it will produce 0 if it lies outside of that hyper-sphere. Hence, the proposal measure μ_i (Equation 3.1) will show normalized sum of all the points that lie within a particular hyper-sphere S_i. It can be proved that this a valid measure as it follows all the three axioms:

1. $\mu_i(S_i) \geqslant 0$ for every hyper-sphere S_i.

2. If a giant hyper-sphere enclosing the sample space is chosen, all the random samples are going to lie inside it, resulting to a measure with probability 1. $\mu(S) = 1$

3. If $S_i : i \in I$ is a countable, pairwise disjoint collection of hyper-spheres then,

$$\mu(\bigcup_{i \in I} S_i) = \sum_{i \in I} \mu(S_i)$$

Our goal is to change this empirical proposal measure to a weighted empirical proposal measure such that,

$$\mu_i = \sum_{j=1}^{n} w^j \mathbb{I}_{S_i}(x^j) \to \nu_i, \tag{3.2}$$

where convergence is in the L_2-norm sense to the target measure. The task is then to find the best set of weights, $\mathbf{w} = \{w^1, w^2, \ldots, w^n\}$ for accomplishing the measure change for each member of $\mathcal{S}$. For a given sample set, $\{x^1, x^2, \ldots, x^n\}$, a given set of hyper-sphere, $\mathcal{S}$, and a proposal measure μ, we denote the value taken by the indicator function for each sample point and each hyper-cube as

$$P_{ij}(\mu) = \mathbb{I}_{S_i}(x^j). \tag{3.3}$$

Given the P_{ij} for each point and each hyper-sphere, we can arrange this information in matrix form as

$$A = \begin{bmatrix} P_{11} & P_{12} & \cdots & P_{1n} \\ P_{21} & P_{22} & \cdots & P_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ P_{m1} & P_{m2} & \cdots & P_{mn} \end{bmatrix}, \tag{3.4}$$

where each row corresponds to a hyper-sphere in $\mathcal{S}$ and each column corresponds to a sample point, x^j. If we define $\mathbf{n} = (1/n, 1/n, \ldots, 1/n)^\top$ and $\mathbf{w} = (w^1, w^2, \ldots, w^n)^\top$, then we see that $A_i\mathbf{n}$ is Equation 3.1 and $A_i\mathbf{w}$ is the left side of Equation 3.2, where A_i is the ith row of A. Hence, a particular row in the matrix A corresponds to the respective member from the set of hyper-sphere S.

We can also assemble information regarding the desired target distribution. For this, we define measure of a given hyper-cube under the target measure as $T_i = \nu(S_i)$. Thus, for a given $\mathcal{S}$ we have the vector $\mathbf{t} = (T_1, T_2, \ldots, T_m)^\top$ representing the probability measure of each member of hyper-sphere S. Our goal then is to find a set of weights, $\mathbf{w}$, such that $A\mathbf{w} = \mathbf{t}$. In practice, we create A such that $m \gg n$ (number of hyper-spheres constructed are more than the number of available random samples) and compute an optimal set of weights via the normal equations,

$\mathbf{w} = (A^\top A)^{-1} A^\top \mathbf{t}$. It is our hypothesis that as $n \to \infty$, the sum of the computed weights via this procedure converges to unity, and that each individual weight is greater than zero. The study of these claims is a topic of future work.

To better understand the approach, we consider here also a graphical depiction provided in Figure 3.3. The left portion of Figure 3.3 shows 10000 normally distributed sample points from a given proposal measure. From this we will consider 4 points and 4 disks to clarify how the matrix (A) and vector ($\mathbf{t}$) is formed in our problem formulation.

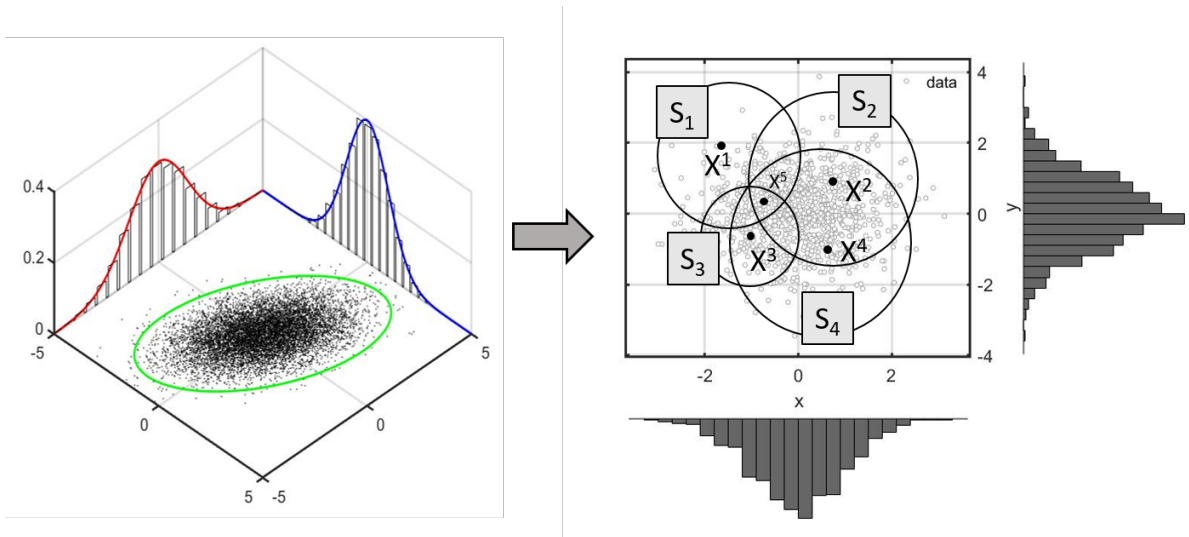

Figure 3.3: The construction of proposal measure matrix.

After determining the sample space (often from the problem definition itself) the hyper-spheres, S_i, which are disks here, are then constructed taking each random sample as a center and some specific value as a radius. This is done in such a way that each sample point lies inside at least one hyper-sphere. As illustrated in Figure 3.3, hyper-sphere S_1 has only one point lying inside it, point x^1 itself (note, there are clearly more points, but we are focusing only on the 4 highlighted points for clarity). Hence, the proposal measure of the first random sample x^1 lying inside the first disk S_1, $P_{11}(\mu)$ = 1. For the other three random samples, the measure for that particular disk S_1 is zero.

That is, the first row of A is

$$\begin{array}{cc} \begin{array}{cccc} x^1 & \mathrm{x}^2 & \mathrm{x}^3 & \mathrm{x}^4 \end{array} & \\ \begin{pmatrix} 1 & 0 & 0 & 0 \end{pmatrix} & S_1 \end{array}$$

where we are noting the column dependence on the samples and the row dependence on the given hyper-sphere.

Similarly, hyper-sphere S_2 encloses x^2 and x^4, resulting in 1's in the position of A_{22} and A_{24}. Just like S_1, hyper-sphere S_3 contains one point itself and hence following the same procedure it will take 1 in the space of A_{33}. Hyper-sphere S_4 contains three random samples and their respective rows are filled out in the same manner as the previous hyper-spheres. The result for this demonstration is

$$\begin{array}{cc} \begin{array}{cccc} x^1 & \mathrm{x}^2 & \mathrm{x}^3 & \mathrm{x}^4 \end{array} & \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 \end{pmatrix} & \begin{array}{l} S_1 \\ S_2 \\ S_3 \\ S_4 \end{array} \longrightarrow A \end{array}$$

The vector $\mathbf{t}$ can be formed in two ways. If the joint distribution of the target samples is known, the individual elements of the vector $\mathbf{t}$ will give the joint probability of that particular hyper-sphere. That is, $\mathbf{t} = \nu(S_i)$. If the underlying target measure is unknown but has been sampled (as in the case of a chain of models), the vector $\mathbf{t}$ can be formed empirically. This is similar to the construction of the matrix A, with the additional step of adding all the row elements and dividing by the total number of samples.

This is better explained by the following Equation. Let us consider the exact same space from the Figure 3.3 and call them target samples instead of proposal samples. The matrix $\mathbf{t}$ looks like this,

$$\left(\frac{1}{4}\right) \times \begin{pmatrix} 1+0+0+0 \\ 0+1+0+1 \\ 0+0+1+0 \\ 0+1+1+1 \end{pmatrix} \begin{matrix} S_1 \\ S_2 \\ S_3 \\ S_4 \end{matrix} \longrightarrow \begin{pmatrix} \frac{1}{4} \\ \frac{1}{2} \\ \frac{1}{4} \\ \frac{3}{4} \end{pmatrix} \begin{matrix} \mathrm{S}_1 \\ \mathrm{S}_2 \\ \mathrm{S}_3 \\ \mathrm{S}_4 \end{matrix} \longrightarrow \mathbf{t}$$

3.2 Algorithm

We conclude this section with a complete algorithm for implementing our methodology for measure based change of probability measure:

Algorithm 1 Change of measure via importance weights w^j's

Data : Proposal Sample Points X, Target Distribution ν, Number of Target Samples Points M
Number of Proposal Sample points N, and the termination criteria tol
Initialization: Find the domain of the sample space Ω
loop:
Start : Construct the hyper-spheres S with the initial radius rad at all the proposal sample points X
top : Update the existing hyper-spheres S by dividing the existing radius into half
Matrix A **Construction**:
j : *1:N*
$x^j =$ lies inside the hyper-sphere S_i
$P_{ij}(\mu) \leftarrow 1.$
$P_{ij}(\mu) \leftarrow 0.$
Vector t **Formulation**:
$\mathrm{T}_i(\nu) \leftarrow \nu(\mathrm{S}_i)$
end;
goto *top*.
End : The following condition has been achieved: $rad/2 \leqslant tol$ && $rad \geqslant tol$.
Find w $\leftarrow$ $(A^\top A)^{-1} A^\top \mathbf{t}$.

We note here that the generation of the set $\mathcal{S}$ proceeded by halving the radiuses successively. Empirically, we have found this to be superior to randomly choosing the radiuses for the hyper-spheres, though more analysis is needed to confirm this claim. This is a topic of future work. In our approach, the first set of hyper-spheres are generated with a specific radius such a way that

it contains the maximum number of sample points possible. The radius of the first set of hyper-spheres centered at the proposal sample points is halved resulting in a hierarchy of hyper-spheres. This hierarchy is grown until a user-specified required tolerance (radius) is achieved. By each iteration as the size of the hyper-spheres and the radius decreases the coverage of these hyper-spheres also reduces. Analytically it will be shown in the subsequent chapters that, smaller the radius higher the accuracy of the algorithm and ultimately more efficient UP method.

Our representation of the hyper-sphere generation process is shown in Figure 3.4. In two dimensions this set of hyper-spheres can be considered as a set of disks. Hence, with the specific radius first set of subsets from $S_1, ..., S_5$ will be formed. On the next step, radius will be divided into half and this division continues until tolerance requirements are met.

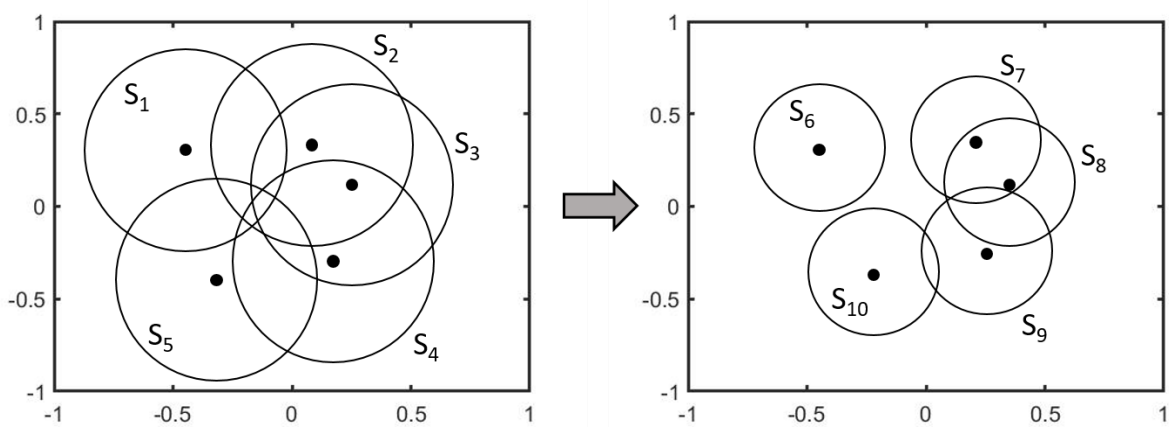

Figure 3.4: Hyper-sphere generation

3.3 Modified approach for high dimensional inputs

As explained earlier in the Chapter 1, the computational models and techniques available in the industry struggle at high dimensional inputs or when provided with large number of data samples. Surrogate models or dimensional reduction methods can prove to be useful in such cases. Generally these methods lack in efficiency or results in ill-conditioning of the model either way leading to in-accurate solutions. Recent advances in technology has led to wide availability of high-performing

computers. This aims to solve complex problems on large clusters of interconnected computers. To take the benefit of the high performance computing, it becomes necessary to mainly exploit the parallelization functionality.

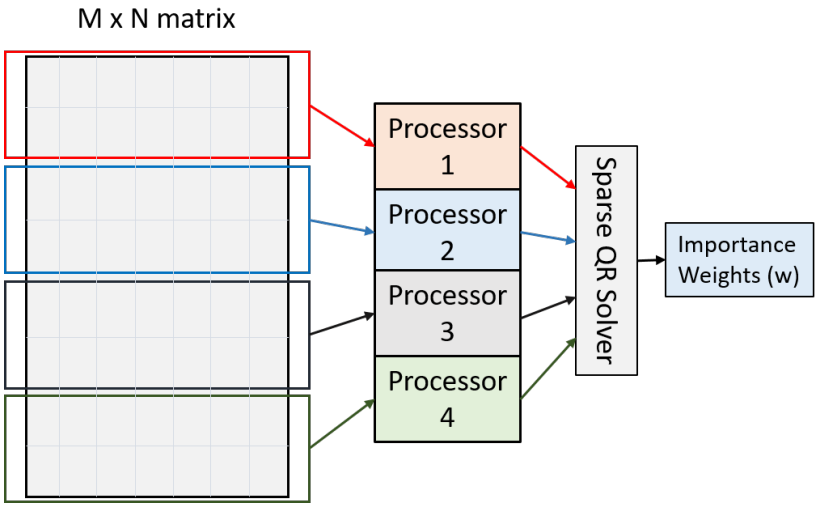

Figure 3.5: Basic layout of how the proposed algorithm distributes work among the available processors and solves the challenging least square problem in parallel.

The uncertainty propagation methodology adopted in this work require the construction of an ensemble of computations. Due to the high cost of each solution - as it is common in multi-disciplinary frameworks (i.e. aerodynamics, structure, control, etc.) - we have developed an environment for optimal resource allocation on a UNIX multiprocessor cluster. Its structure is based on a workflow managed via MATLAB through I/O that explicitly connects the software tools involved in the process. It is designed to run natively on any high-performance computing (HPC) system, by integrating with the job-submission/queuing system.

The vectorized matrix form used in our approach provides the accessibility to easy parallelization. Here, the subsets are vectorized and then used to generate the required matrix. This allows for the software platform to allocate the memory more efficiently. Even though it is vectorized, the allocation of proposal measure as an each individual element of the matrix requires intense for

loops, which is a necessary but quite an expensive step. In order to solve this problem, we are using the distributed arrays functionality.

As demonstrated in the Figure 3.5, the distributed array shares the work with the available processors in the system. It independently computes the decoupled matrix on each of its core without needing to exchange the data in between. The individual processors here store the matrices autonomously and hence will be able to compute all of them at the same time. We are using Sparse QR decomposition technique to compute least square for the solution, since it is already made possible to operate in parallel. This enables us to utilize the similar methodology without gathering the data at the end of the loops. Therefore, the already parallelized matrices can directly be solved saving computational time and storage space.

4. BENCHMARK RESULTS

In this section we consider 5 different numerical examples to benchmark the proposed approach and compare against the other change of measure techniques for the propagation of uncertainties. These methods are Kernel Density Estimation (KDE), Gaussian Process (GP), and Least Square Optimal (L2O). For this, we will assume that the measures, both proposal and target, are unknown. However, we have $x^1, x^2, ..., x^n$ drawn from according to the proposal μ and similarly, we have $y^1, y^2, ..., y^m$ drawn according to the target ν. We also have evaluations of each benchmark function associated with the proposal samples, which generically we can denote as $g(x^1), g(x^2), ..., g(x^n)$. The evaluation of each benchmark function associated with target samples $g(y^1), g(y^2), ..., g(y^m)$ is unavailable. Instead of evaluating the computational model over the target samples, we employ the change of measure to the proposal samples. The weighted proposal samples are then used to evaluate statistics of the weighted evaluation function $g_w(x^1), g_w(x^2), ..., g_w(x^n)$. The statistics of interest for this experiment are the mean and the variance of each benchmark under the target distribution, which is approximated by weighted proposal function evaluations. These approximations are given as

$$\mathbb{E}_w = \sum_{j=1}^{n} w^j g(x^j), \tag{4.1}$$

and

$$\text{Var}_w = \left(\frac{V_1}{V_1^2 - V_2}\right) \sum_{j=1}^{n} w^j (g(x^j) - \mathbb{E}(g(x))^2, \tag{4.2}$$

respectively, where $V_1 = \sum_{j=1}^{n} w^j$, V_2 is the squared sum of weights $V_2 = \sum_{j=1}^{n} (w^j)^2$. The importance weights, w^j, are obtained using KDE, GP and L2O for comparison approach.

The benchmark functions for which we test the change of measure approaches are:

1. Oakley and O'Hagan Function (d=1) [51]:

$$g_1 = 5 + t + \cos(t)$$

2. Short Column Function (d=3) [52]:

$$g_2 = 1 - \frac{4M}{bh^2Y} - \frac{P^2}{b^2h^2Y^2}$$

3. Borehole Function (d=8) [53]:

$$g_3 = \frac{2_u(H_u - H_l)}{\ln\frac{r}{r_w}\left(1 + \frac{2LT_u}{\ln\left(\frac{r}{r_w}\right){r_w}^2K_w} + \frac{T_u}{T_l}\right)}$$

4. Oakley and O'Hagan Multidimension Function (d=15) [51]:

$$g_4 = 5 + \Sigma_{i=1}^{15}(t^i + 2 * \cos t^i)$$

5. Discontinuous Integrand Family (d=1) [54]:

$$f(t) = \begin{cases} 0, & \text{if } t > 0.5 \\ exp(5 * t), & \text{otherwise} \end{cases}$$

For each benchmark, we describe the problem setup and present graphical results in terms of the probability density functions and cumulative distribution functions of the outputs of each benchmark. We then conclude this section with a table that provides quantitative information regarding the performance of each method on each benchmark.

Oakley and O'Hagan function. The Oakley and O'Hagan function [51] is a uni-dimensional problem. The target distribution follows $y \sim \mathcal{N}(0, 4)$ and the proposal distribution is selected to be uniformly distributed over the range of target samples as shown in Table 4.1. The numerical

experiment is conducted using 100 proposal random samples. The results of the experiment in terms of the output probability density function (PDF) and cumulative distribution function (CDF) for each method are shown in Figure 4.2. The results illustrate that the proposed approach produces accurate PDF and CDF estimates and appears to be superior to the KDE, GP and L2O methods.

For this benchmark problem we also studied the convergence behavior of both the weighted mean and weighted variance estimators for our proposed approach. The results of this study are shown in Figure 4.1. This figure reveals that the proposed approach is converging in both mean and variance to the target mean and variance. We note here again that the results of our method used only function evaluations taken from the proposal measure and reweighted those results to match the target. In the Figure 4.1, the blue lines represent Monte-Carlo convergence rates, which are essentially being followed here.

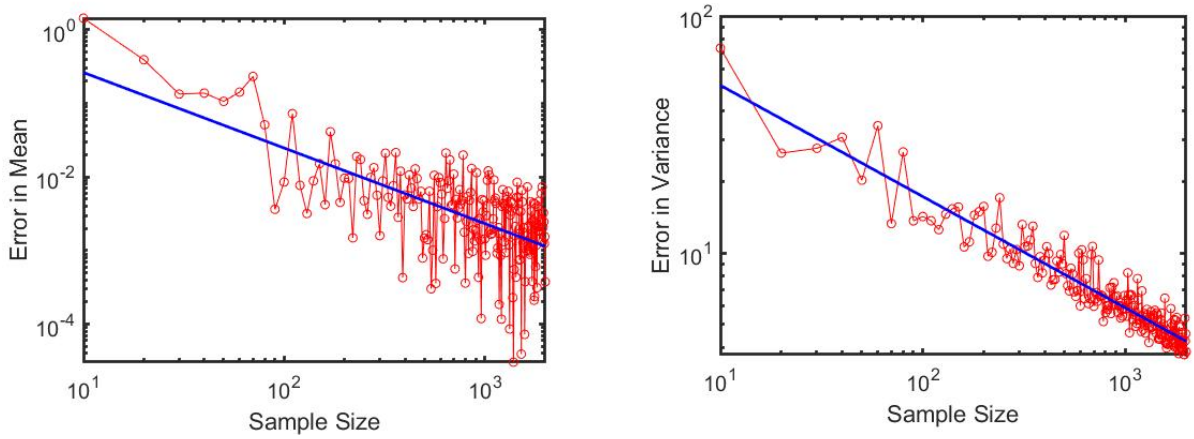

Figure 4.1: Convergence results for the weighted mean and weighted variance estimators using our proposed approach. The blue lines on each plot represent asymptotic brute force Monte Carlo simulation convergence rates.

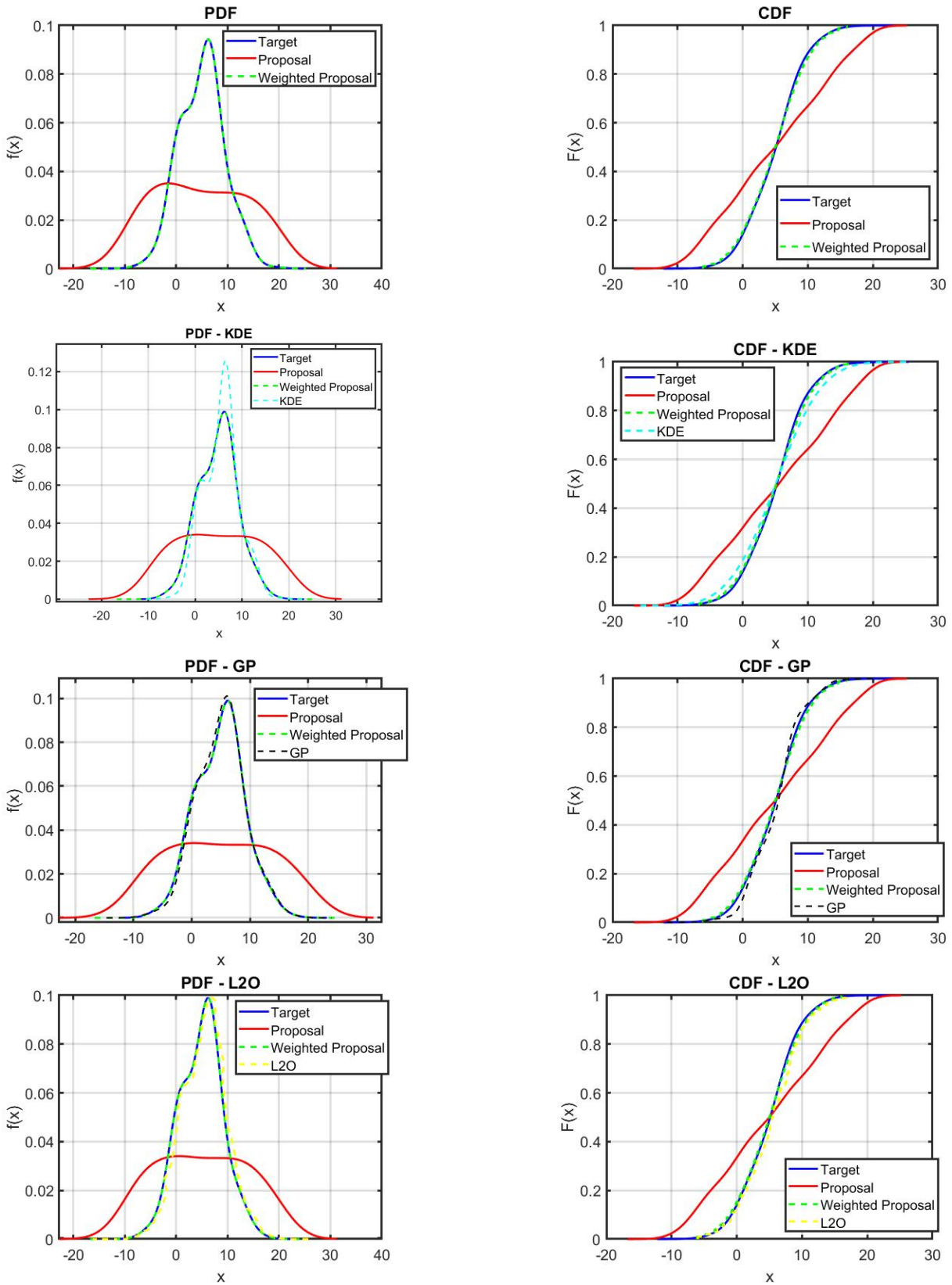

Figure 4.2: Results of applying our proposed approach, the KDE approach, the GP approach and the L2O approach to the Oakley & O'Hagan benchmark problem.

Short Column Function. The Short Column Function is a three-dimensional problem that takes Y as a lognormally distributed, M and P as normally distributed samples as target samples [53]. Proposal distribution are chosen on each dimension as shown below in Table 4.1. For this benchmark, 5,000 proposal samples were used for each method. The proposal samples were the same for each. The results of the experiment in terms of the output probability density function (PDF) and cumulative distribution function (CDF) are shown in Figure 4.3. The figure reveals that the our approach yields satisfactory results, however from the Table 4.2 GP and KDE performs poorly. However, L2O performs well in comparison to our proposed approach. We note here that the convergence rates of the mean and variance estimators for this problem showed similar trends to those of the previous benchmark, as was the case for the following benchmarks as well.

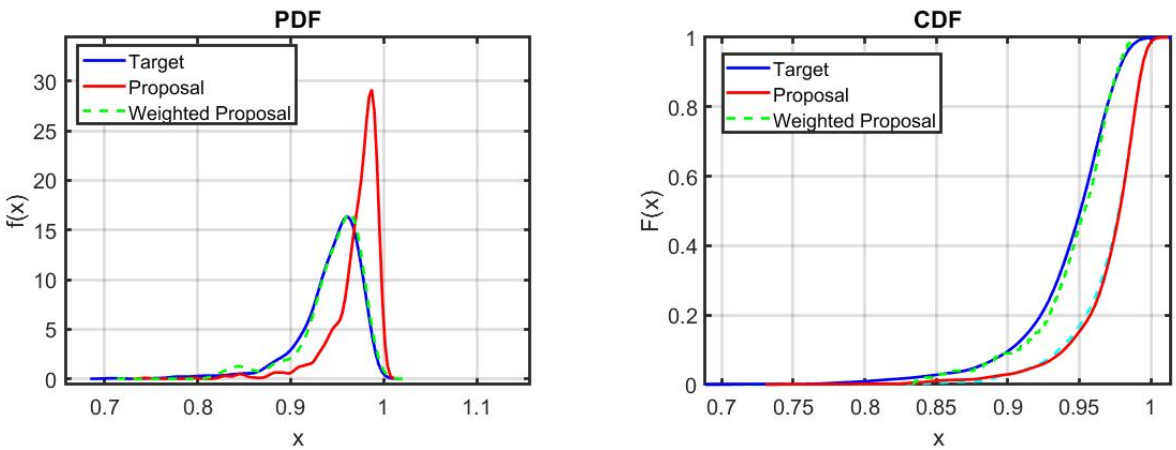

Figure 4.3: Results of applying the developed approach on Short Column Function.

Borehole Function. The borehole function is a model of water flowing through a borehole [53]. The radius of the borehole r_w, radius of the influence r, transmissivity of upper aquifer (m^2/yr), potentiometric head of upper aquifer H_u (m), transmissivity of lower aquifer T_l (m^2/year), potentiometric head of lower aquifer H_l (m), length of borehole L (m) and hydraulic conductivity of borehole K_w (m/yr) are problem constants. Thus, this benchmark is an eight-dimensional problem. For this problem, 50,000 proposal samples were used for each method. Proposal distribution

is chosen on each dimension as shown below in Table 4.1. The results of the experiment in terms of the output PDF and CDF for our proposed method are shown in the Figure 4.4. From the figure, it is clear that our proposed approach is able to accurately match the target PDF and CDF for this problem. We note that the GP, L2O and KDE methods were not able to produce satisfactory results for this benchmark in terms of the PDF and CDF.

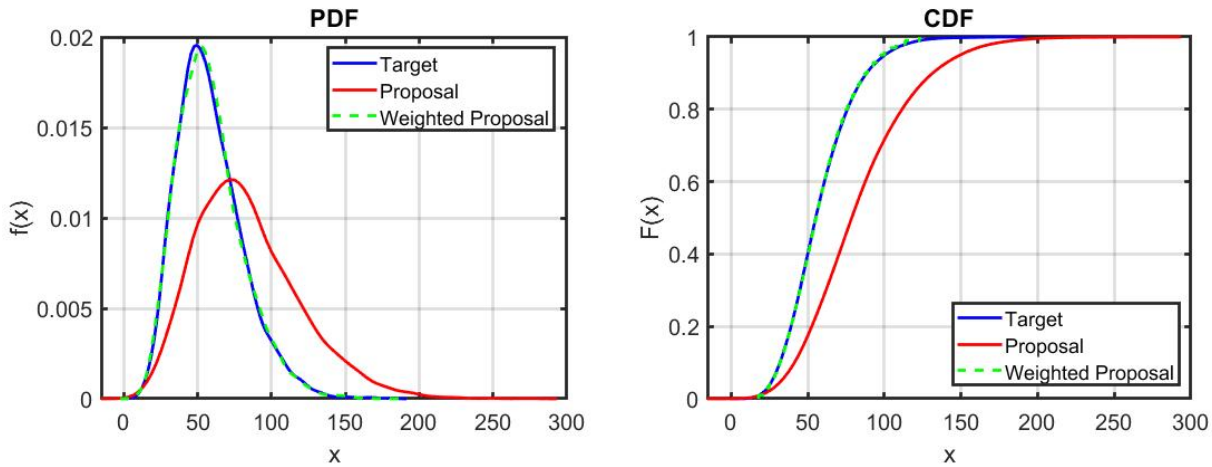

Figure 4.4: Results obtained from the developed approach as PDF and CDF of the Borehole Function.

Oakley and O'Hagan multi-dimensional Function. The Oakley and O'hagan multi-dimensional funtion [55] is a family of benchmark problems that can be evaluated with any dimension. For this demonstration, we use the fifteen-dimensional function to check our methods function-ability at higher dimension. Such a high dimensional input is often beyond the capability of traditional importance weighting methods. The target distribution follows the standard normal distribution for each input. Proposal distribution is chosen on each dimension as shown below in Table 4.1. The results of the experiment, which used 100,000 proposal samples, in terms of the PDF and CDF for our proposed method are shown in the bottom plots of Figure 4.5. Even for this challenging problem, it is clear that our approach is capable of matching the target. We note that for this problem

also, the GP, L2O and KDE methods were not able to produce satisfactory results in terms of the PDF and CDF.

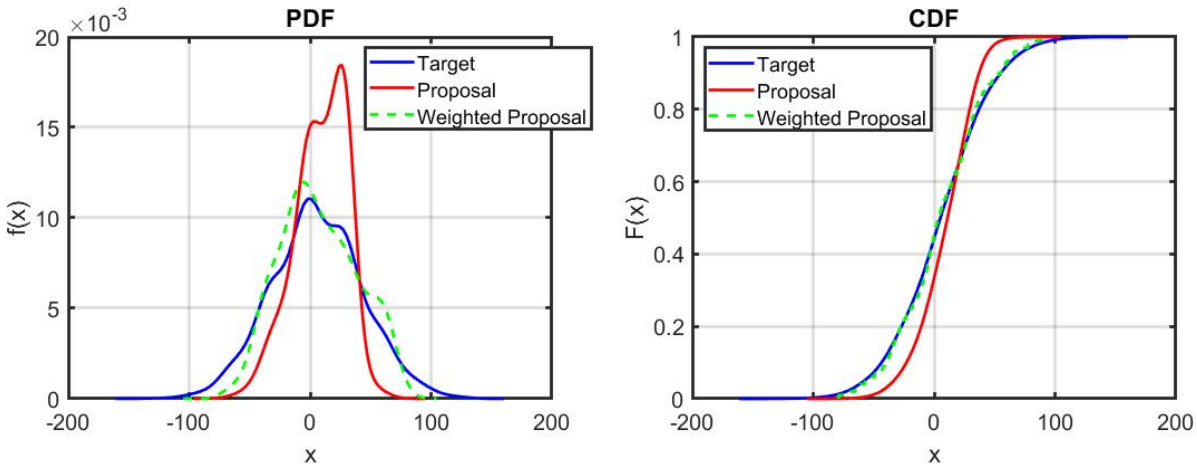

Figure 4.5: PDF and CDF of the weighted proposal, proposal and target random samples for Oakley & O'hagan multi-dimensional function.

Discontinous Integrand Family. This Discontinous family of funtions can be quickly integrated analytically and hence it can be used in multidimensional integration routine [24]. However, this family of functions generates discontinuous system response. For this reason we will be taking this test problem to demonstrate the effectiveness of our approach in discontinuous space. The results in terms of the CDF are shown in the Figure 4.6. Our proposed approach quickly estimated the target CDF. Once again, the other benchmark problems could not produce satisfying results.

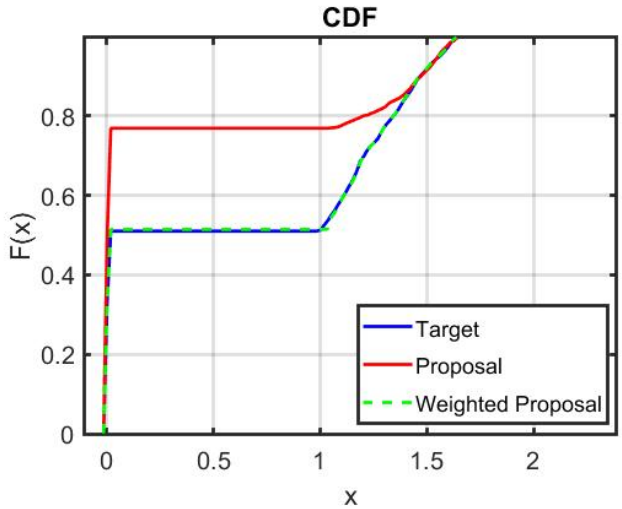

Figure 4.6: Results in terms of CDF of discontinuous integrand function when the proposed approach is employed.

Problem Functions	**Target Distribution**	**Proposal Distribution**
Oakley & O'Hagan (1-D)	$\mathcal{N}(\mu = 0, \sigma^2 = 4)$	$\mathcal{U}(-15, 15)$
Short Column Function	$Y \sim \mathcal{L}(a = 5, b = 0.5)$ $M \sim \mathcal{N}(\mu = 2000, \sigma^2 = 400)$ $P \sim \mathcal{N}(\mu = 500, \sigma^2 = 100)$	$Y \sim \mathcal{L}(a = 5.5, b = 0.7)$ $M \sim \mathcal{U}(500, 2500)$ $P \sim \mathcal{U}(-350, 1100)$
Borehole Function	$r_w \sim \mathcal{N}(\mu = 0.10, \sigma^2 = 0.017)$ $r \sim \mathcal{L}(a = 7.72, b = 1)$ $T_u \sim \mathcal{U}(63, 116)$ $H_u \sim \mathcal{U}(990, 1110)$ $T_l \sim \mathcal{U}(63.1, 116)$ $H_l \sim \mathcal{U}(700, 820)$ $L \sim \mathcal{U}(1120, 1680)$ $K_w \sim \mathcal{U}(9855, 12045)$	$r_w \sim \mathcal{N}(\mu = 0.9, \sigma^2 = 0.02)$ $r \sim \mathcal{N}(\mu = 6.5, \sigma^2 = 1)$ $T_u \sim \mathcal{N}(\mu = 75, \sigma^2 = 30)$ $H_u \sim \mathcal{N}(\mu = 1050, \sigma^2 = 100)$ $T_l \sim \mathcal{N}(\mu = 80, \sigma^2 = 30)$ $H_l \sim \mathcal{N}(\mu = 775, \sigma^2 = 40)$ $L \sim \mathcal{N}(\mu = 1400, \sigma^2 = 50)$ $K_w \sim \mathcal{N}(\mu = 11000, \sigma^2 = 500)$
Oakley & O'Hagan (15-D)	$\mathcal{N}(\mu = 0, \sigma^2 = 1)$	$\mathcal{U}(-3, 3)$
Discontinuous Integrand	$\mathcal{U}(0, 1)$	$\mathcal{B}(a = 2, b = 1)$

Table 4.1: The benchmark functions, target, and proposal distributions for comparison purpose.

To complete the comparative study, we present quantitative results regarding the performance of each method on each benchmark. For all five benchmarks, the results are quantified by the ab-

Problem Functions	Evaluation Statistics	Proposed Approach	L2O	GP	KDE
Oakley & O'Hagan (1-D)	$E_{\mathbb{E}}$	0.009	0.02	0.05	0.36
	$E_{\mathbb{V}}$	0.11	0.31	0.25	3.82
Short Column Function	$E_{\mathbb{E}}$	0.04	0.28	0.38	1.4
	$E_{\mathbb{V}}$	0.09	0.14	0.3	0.48
Borehole Function	$E_{\mathbb{E}}$	0.45	2.5	5.21	9.87
	$E_{\mathbb{V}}$	1.90	1.95	2.01	12.5
Oakley & O'Hagan (15-D)	$E_{\mathbb{E}}$	4.50	20.05	20.5	20.12
	$E_{\mathbb{V}}$	6.11	9.80	10.5	13.54
Discontinuous Integrand	$E_{\mathbb{E}}$	0.0012	0.35	0.84	0.89
	$E_{\mathbb{V}}$	0.01	0.21	0.65	0.67

Table 4.2: Tabulated results of the performance in terms of mean and variance estimation.

solute values of the difference between the mean of the target evaluation function and the weighted mean of the proposal evaluation function. In addition, the absolute value of the difference between the variances of the target and the weighted proposal evaluation function are compared. These are denoted as $E_{\mathbb{E}}$ and $E_{\mathbb{V}}$, respectively. The results from this numerical study are shown below in the Table 4.2. The estimates of $E_{\mathbb{E}}$ and $E_{\mathbb{V}}$ are averaged over 100 independent and identically conducted experiments. We note that our proposed approach, which computes importance weights using the proposal and target measures directly, outperforms the industry standard KDE method, GP method and the newly developed L2O approach.

5. APPLICATION

5.1 Problem Setup

In this section we present a demonstration of our proposed importance weighting methodology to a practical decomposition based uncertainty analysis problem. For this, we focus on a gas turbine blade application. Our application problem consists of four different components, each on their own represents disciplinary analysis: blade heat transfer, engine performance, turbine blade lifetime, and an economic model. The complete system model and the functional relationships between them is shown in the Figure 5.1.

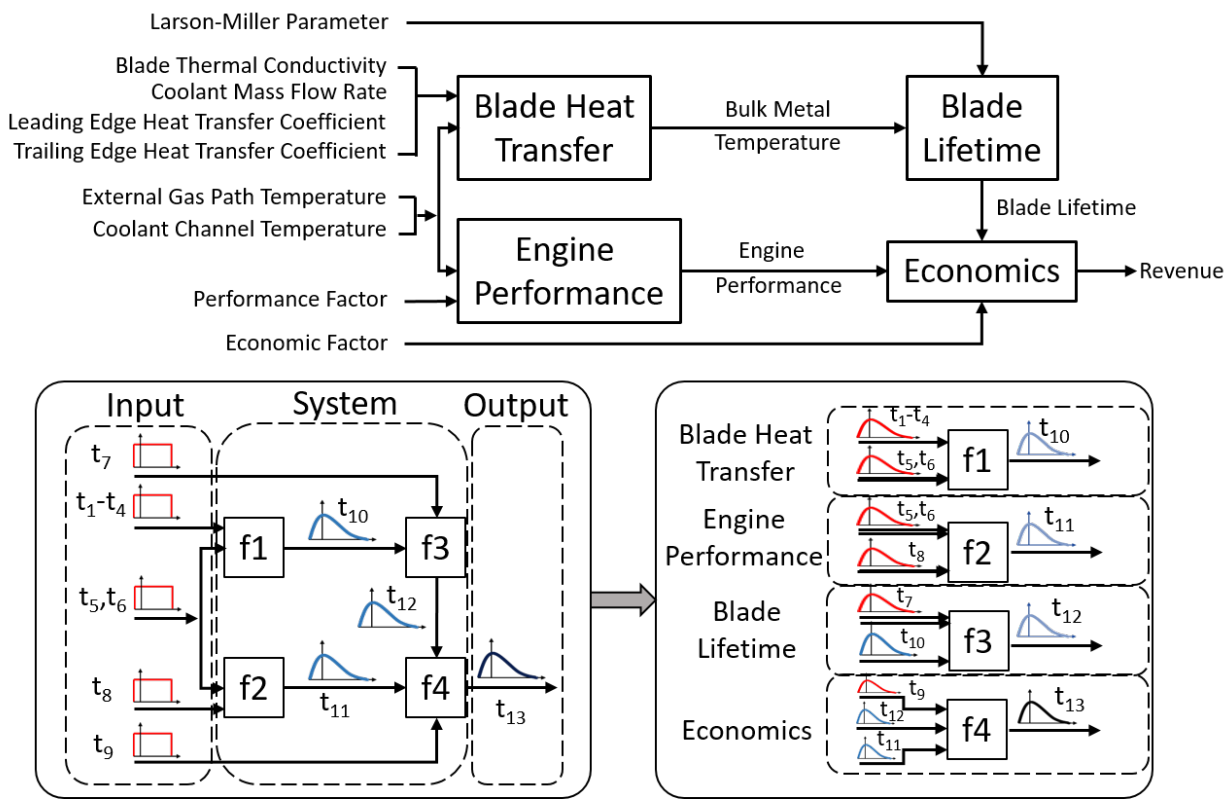

Figure 5.1: The gas turbine problem contains four subsystems, each representing a disciplinary analysis.

The gas turbine model represents an organizational multidisciplinary environment where each group is responsible for the assessment of different aspects of the problem. Hence, in order to quantify and propagate uncertainties through the entire system, the decoupled decomposition based assessment becomes useful. The specific objective of our analysis is to propagate the uncertainties from the decoupled model chain inputs to the output of interest, here the economics of turbine model. The uncertain input inputs, and their target distribution used for our analysis. These target distributions are considered unknown the local uncertainty analysis is carried out on each individual four components.

Variable	**Name**	**Description**	**Distribution**
t_1	T_{cool}	Coolant Temperature [K]	$\mathcal{U}(550, 650)$
t_2	k	Blade Thermal Conductivity [W/m/K]	$\mathcal{U}(29, 31)$
t_3	h_{LE}	Leading Edge Heat Transfer Coefficient [W/m^2/K]	$\mathcal{U}(1975, 2025)$
t_4	h_{TE}	Trailing Edge Heat Transfer [W/m^2]	$\mathcal{U}(975, 1025)$
t_5	$\dot{m}$	Coolant Mass Flow Rate [kg/sec]	$\mathcal{U}(0.108, 0.132)$
t_6	T_g	External Gas Path Temperature [K]	$\mathcal{U}(1225, 1275)$
t_7	LMP	Larson-Miller Parameter	$\mathcal{U}(2.45 * 10^4, 2.5 * 10^4)$
t_8	F_{perf}	Performance Factor	$\mathcal{U}(0.85, 0.95)$
t_9	F_{econ}	Economic Factor	$\mathcal{U}(0.9, 1.1)$

Table 5.1: Gas Turbine system input uncertainty distributions.

Heat Transfer Model The turbine blade heat transfer model with the help of finite element analysis simulates a cooled gas turbine blade in hot gas path flow. The uncertain inputs to this component is shown in Figure 5.1. The output of the heat transfer model is bulk metal temperature (T_{bulk}) [K]. The output variable is calculated using a finite element method solved for the heat equation.

Locally, this uncertainty propagation is carried out using the proposal random samples following their respective proposal distribution as shown in the Table 5.2.

Lifetime Model The lifetime model estimates the expected time until the blade fails assuming a Lason-Miller nickel super alloy stress-to-failure scenario. The inputs here are bulk metal temper-

Variable	Name	Description	Distribution
t_1	T_{cool}	Coolant Temperature [K]	$\mathcal{N}(595, 50)$
t_2	k	Blade Thermal Conductivity [W/m/K]	$\mathcal{N}(29, 1.5)$
t_3	h_{LE}	Leading Edge Heat Transfer Coefficient [W/m^2/K]	$\mathcal{N}(975, 1025)$
t_4	h_{TE}	Trailing Edge Heat Transfer [W/m^2]	$\mathcal{N}(1000, 100)$
t_5	$\dot{m}$	Coolant Mass Flow Rate [kg/sec]	$\mathcal{N}(0.12, 10^{-4})$
t_6	T_g	External Gas Path Temperature [K]	$\mathcal{N}(1250, 100)$

Table 5.2: Heat transfer model input proposal uncertainty distribution.

ature, which is the output of our first component, T_{bulk}, and Larson-Miller parameter, LMP [56]. The output of this subsystem is expected time until failure, $t_{fail}[hr]$. The model evaluation function is given by,

$$t_{fail} = exp(\text{LMP}/T_{bulk} - 20) \tag{5.1}$$

Similarly, the local proposal distribution and the sampled random variables are given in Table 5.3.

Variable	Name	Description	Distribution
t_7	LMP	Larson-Miller Parameter	$\mathcal{N}(2.48 * 1010^4, 200)$
t_{10}	T_{bulk}	Bulk Metal Temperature [K]	$\mathcal{N}(980, 20)$

Table 5.3: Blade lifetime model input proposal uncertainty distribution.

Performance Model Here, we consider rather, a simplified low-fidelity performance model to evaluate the maximum power output of the turbine system. It rewards high external hot gas oath temperatures and penalizes the coolant flow usage. The output engine performance, P_{eng} is defined as,

$$P_{eng} = F_{perf}(\dot{m}_o - N\dot{m})C_pT_o(T_g/T_o - 2\sqrt{T_g/To} + 1) \tag{5.2}$$

where, T_g is the external gas temperature, F_{perf} is the performance factor introduced to account

Variable	Name	Description	Distribution
t_5	$\dot{m}$	Coolant Mass Flow Rate [kg/sec]	$\mathcal{N}(0.115, 10^{-4})$
t_6	T_g	External Gas Path Temperature [K]	$\mathcal{N}(1240, 500)$
t_{11}	F_{perf}	Performance Factor	$\mathcal{N}(0.9, 0.02)$

Table 5.4: Performance model input proposal uncertainty distribution

for the effect on engine performance of randomness associated with the gas turbine components, $N(= 90)$ is the number of gas turbine blade, inlet compressor flow rate $\dot{m}_o(= 430$[kg/sec]), $C_p(= 1003.5$[J/kg/K]) being the specific heat at constant pressure, and inlet compressor temperature $T_o(= 300$[K]). The input proposal distribution assumed for the local analysis is given in Table 5.4.

Variable	Name	Description	Distribution
t_9	F_{econ}	Economic Factor	$\mathcal{N}(1.0, 0.01)$
t_{12}	t_{fail}	Blade Lifetime [year]	$\mathcal{N}(200, 100)$
t_{11}	P_{eng}	Engine Performance [MW]	$\mathcal{N}(120, 1)$

Table 5.5: Economics model input proposal uncertainty distribution

Economics Model This model simulates and estimates the revenue generated from the operating gas turbine system. The model evaluation rewards a high-performance gas turbine engine and penalizes a risky gas turbine engine. The inputs to this component are time until failure t_{fail}, engine performance factor P_{eng}, and economic factor F_{econ}. The output is defined as,

$$r_{econ} = F_{econ} t_{fail} P_{eng} c_o \tag{5.3}$$

where c_o is the cost of energy which is taken as 0.07 [$/kWh]. The input proposal distribution assumed are given below in the Table 5.5.

5.2 System analysis

In the system level analysis, the analysis is carried out following the target input distribution shown in Table 5.1. Global system analysis begins by evaluating the blade heat transfer model. Blade heat transfer model and the performance model both rely solely on system level input variables and thus both require no information from the upstream components for the analysis purpose. We obtain the target densities of the evaluated T_{bulk} and P_{eng}. The same procedure is applied to the lifetime model using the recently acquired input T_{bulk} to obtain the target density. Using the target density of t_{fail}, and system level inputs we acquire the desired target density of the output of interest generated from the economic model, revenue. Here, in order to generate the target densities, the system has to be in "online" phase, that is, the evaluation of the upstream components requires evaluation of the downstream components, hence needing the continuous data from the downstream.

5.3 Decomposition-based weighted uncertainty analysis

In the decomposition based approach, the importance weights calculated from individual components are used to update the proposal distribution based model evaluations. Hence, simultaneous corrections can be made without the need to couple the models. As shown in the Figure 5.2, the bulk metal temperature distribution is corrected employing the importance weights obtained from the proposal distribution of system inputs using the developed algorithm. The corrected distribution is then used to obtain the blade lifetime distribution. Similarly, the correct distribution of engine performance factor is constructed and together with the blade lifetime distribution as an input the output of interest in constructed. We note that, model evaluations are not needed here to estimate the required output distribution. The density of the output of interest Revenue from the decomposition based weighted approach is given in the Figure 5.1. For comparison, the proposal distribution and and the target monte-carlo analysis distribution from the system level assessment is also given for each model response. Results show how the proposed approach can be utilized to easier system level analysis. In particularly, the decomposition based approach several benefits

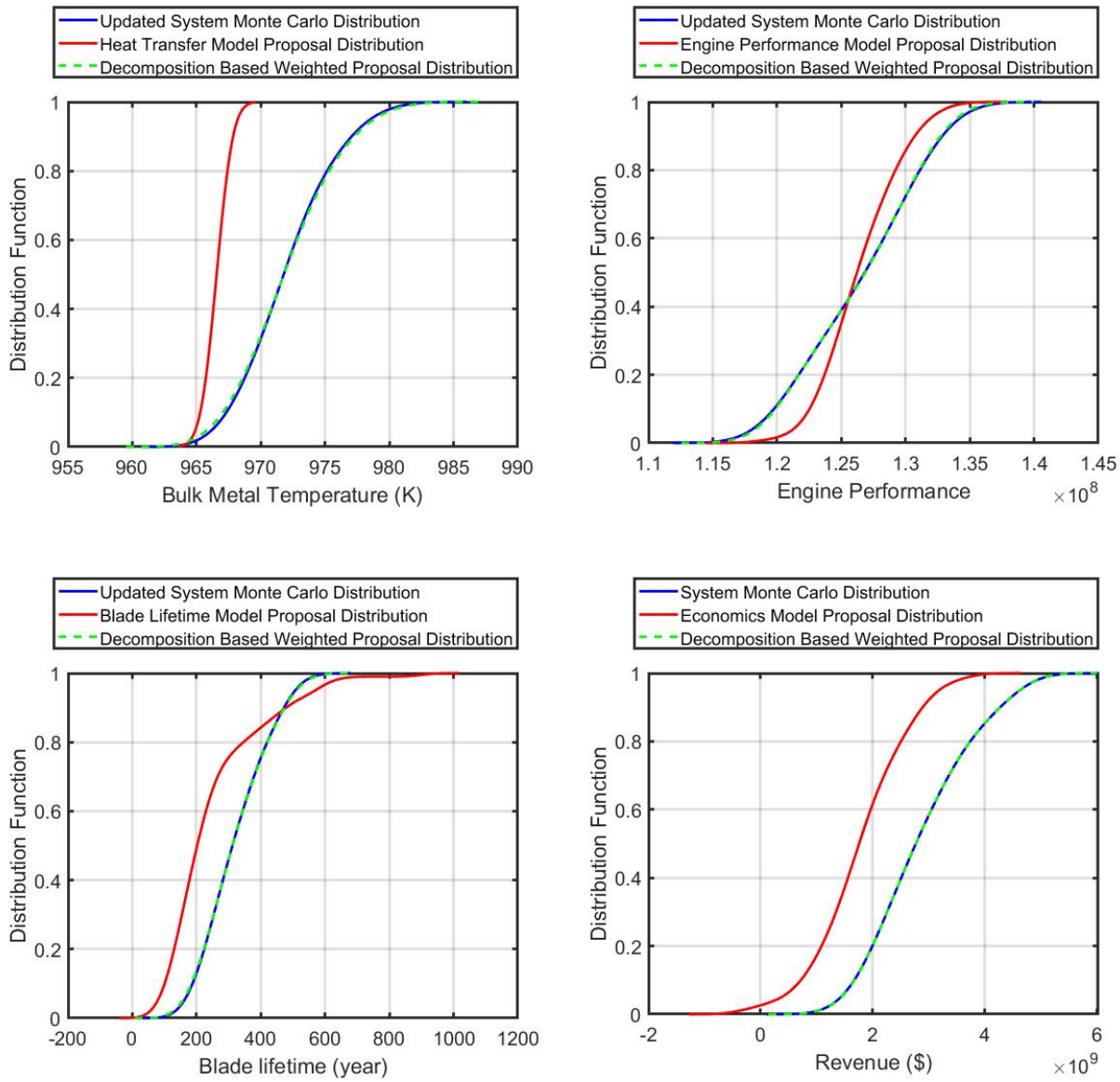

Figure 5.2: The top left figure shows the bulk metal temperature coming out from the heat transfer model, top right demonstrates the engine performance from the engine performance model, bottom left image is for blade life until failure coming out from the lifetime model, and bottom right is the final output of interest revenue generated from the economics model. Here, red line is the results obtained from the proposal sample evaluations, blue line is the system level or target Monte-Carlo simulations, and the dashed line is the result obtained from the decomposition-based multi-component uncertainty analysis.

over the system level analysis in terms of flexibility. If any system input distributions are modified, then the system output of interest can be recomputed without the additional need of component

analysis. However, in case of system uncertainty propagation approach, the samples associated with the modifications are to be reevaluated with respect to their associated component. In contrast, if the input distribution of the heat transfer model is changed, the recalculated importance weights are employed at the already evaluated bulk metal temperature distribution for the proposal samples and the updated target distribution can be estimated without the need of additional model evaluation.

6. CONCLUSION

In this chapter we provide the summary of the work done to meet the thesis objectives, the contribution made to the community, and discuss future research work that should be considered.

6.1 Summary

Uncertainty propagation and change of measure are important tools in estimating the system response under uncertainties. They are used wide-spread to support the confident decision making process and to estimate the . In traditional approaches, the change of measure generally fails or yields inaccurate results when used to estimate the response of a high dimensional input space. The method presented here in the thesis tries to solve that problem by making the formulation of importance weights a simple linear least square problem. Specifically, We have developed a probability measure based approach to estimate the importance weights. The primary application we have considered here is that of estimating statistics of a target distribution that has been propagated through a computational model using only samples from a proposal distribution that has been propagated through the same model. Natural need cases for such a capability include having available historical data that does not conform to a desired input distribution, running an incorrect input distribution in an uncertainty propagation analysis, or decomposing a model chain for uncertainty propagation with plans of updating samples as upstream information is generated.

It was shown how the developed method can be used to accurately and efficiently determine the target statistics on various test problems. Additionally, the advantage of the approach was also demonstrated for a decomposition based model chain application. The developed approach was shown to be particularly useful and seem to work better in high dimensions than literature counterparts such as density ratio methods based on kernel density estimation and the newly develop L_2-norm empirical cumulative distribution method, and regression methodology based gaussian process approach. These examples demonstrated that non-intrusive uncertainty propagation methods can indeed be applied to all kinds of computational models and that it provides a powerful tool

to predict the system volatility, reliability, failure under uncertain inputs.

The following contributions of this thesis are:

- A methodology that propagates uncertainties using change of measure which analytically proven to converge in distribution to the target distribution.
- An easily scalable approach demonstrated to perform well in high-dimensional distributions. A methodology enabling the system level uncertainty analysis using a decomposition based approach.
- A demonstration of the developed approach on a more realistic problem.

6.2 Future Work

The work in this thesis provides several potential future opportunities. The biggest opportunity is to formally understand the convergence behavior. The convergence behaviour would require the theoretical formulation of the developed approach. Further research is also required to extend the capability of our algorithm in highly complex and challenging model chains. Such examples and model chains are available especially in material science.

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