OPTIMAL DESIGN OF MESOSTRUCTURED MATERIALS UNDER UNCERTAINTY

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Jiten Patel

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OPTIMAL DESIGN OF MESOSTRUCTURED MATERIALS UNDER UNCERTAINTY

Approved by:

Dr. Seung-Kyum Choi, Advisor
School of Mechanical Engineering
Georgia Institute of Technology

Dr. David Rosen
School of Mechanical Engineering
Georgia Institute of Technology

Dr. Rafi Muhanna
School of Civil Engineering
Georgia Institute of Technology

Date Approved: July 20, 2009

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LIST OF SYMBOLS AND ABBREVIATIONS

A_i = area of cross section of each truss element

d_i = distance from a sampling point

$f(b)$ = objective function

$g_j(.)$ = limit state function

K = stiffness matrix of the structure

L_i = length of each truss element

P = Internal pressure of the tank

r_i = domain influence factor

r = internal pressure of the tank

$u(.)$ = displacements of nodes

$V*$ = final volume of the structure

$W(.)$ = weight matrix

β_j = regression coefficient

e = error of the model equation

ξ_i = Gaussian random variable

SUMMARY

The main objective of the topology optimization is to fulfill the objective function with the minimum amount of material. This reduces the overall cost of the structure and at the same time reduces the assembly, manufacturing and maintenance costs because of the reduced number of parts in the final structure. The concept of reliability analysis can be incorporated into the deterministic topology optimization method; this incorporated scheme is referred to as Reliability-based Topology Optimization (RBTO). In RBTO, the statistical nature of constraints and design problems are defined in the objective function and probabilistic constraint. The probabilistic constraint can specify the required reliability level of the system.

In practical applications, however, finding global optimum in the presence of uncertainty is a difficult and computationally intensive task, since for every possible design a full stochastic analysis has to be performed for estimating various statistical parameters. Efficient methodologies are therefore required for the solution of the stochastic part and the optimization part of the design process.

This research will explore a reliability-based synthesis method which estimates all the statistical parameters and finds the optimum while being less computationally intensive. The efficiency of the proposed method is achieved with the combination of topology optimization and stochastic approximation which utilizes a sampling technique such as Latin Hypercube Sampling (LHS) and metamodeling techniques such as Local Regression and Classification using Artificial Neural Networks (ANN). Local regression is comparatively less computationally intensive and produces good results in case of low probability of failures whereas Classification is particularly useful in cases where the reliability of failure has to be estimated with disjoint failure domains. Because classification using ANN is comparatively more computationally demanding than Local regression, classification is only used when local regression fails to give the desired level

of goodness of fit. Nevertheless, classification is an indispensible tool in estimating the probability of failure when the failure domain is discontinuous.

Representative examples will be demonstrated where the method is used to design customized meso-scale truss structures and a macro-scale hydrogen storage tank. The final deliverable from this research will be a less computationally intensive and robust RBTO procedure that can be used for design of truss structures with variable design parameters and force and boundary conditions.

CHAPTER 1

INTRODUCTION

1.1 Mesostructured Materials

One of the most widespread trends in recent product development has been the copy of nature since nature has designed some of the most highly efficient systems for handling any condition in its environment. These natural systems utilize materials and structures capable of sensing the environment, processing data, responding, and adapting to the given condition. For instance, animal bones have been evolutionally optimized to support various loading conditions with minimum weight. The internal structure of bone can be considered a cellular structure which can be used to strength, stiffen, and even create light-weight parts. The pursuit of engineering cellular materials is biologically inspired as shown in Figure 1. 1. The key advantages offered by cellular materials are high strength, energy absorption characteristics, and improved thermal and acoustic insulation properties accompanied by a relatively low mass. However, the use of advanced novel materials as primary structural elements is still a rarity, particularly in the industrial vehicle arena due to the difficulty with comprehensive understanding of uncertainties in system behavior.

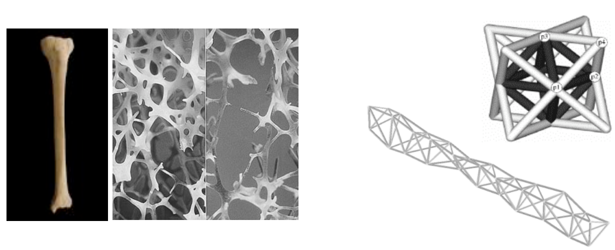

Figure 1. 1 Cellular material structures
(a) Natural (b) Artificial

Mesostructure materials are materials that have a characteristic cell length in the range of 0.1 to 10 mm. Small truss structures, honeycombs, and foams are examples of mesostructures [1]. The concept of mesostructured materials is motivated by the desire to put material only where it is needed for a specific application. Additive manufacturing processes are capable of fabricating the complex geometries inherent in cellular materials [2]. With the advancement of additive manufacturing technologies it is now possible to design custom mesostructures which have increased strength and low relative density when compared to the already available mesostructure materials [3]. For example Seepersad et al. [4] designed the topology of extruded cellular material to find the best compromise between heat transfer and part strength in a structural heat transfer application.

1.2 Topology Optimization

Topology optimization is often referred to as layout optimization or generalized shape optimization [5]. Topology optimization operates on a fixed mesh of finite elements and defines a design variable, which is associated with each element in the mesh. The stiffest structure problem [6] has been posed as a compliance minimization problem for the design of truss structures. Developments in the computational analysis of structures and components, especially by means of the Finite Element Method (FEM), have made the process of designing specialized truss structures using the topology optimization method possible. Bendsoe studied optimal shape design as a material distribution problem [7]. This method was adapted by various engineering fields for generating topologies for compliant mechanisms which have maximum displacement at a desired point [8, 9]. Many other applications of topology optimization are considered in the fields of material design for designing materials with prescribed macroscopic properties and recently in the field of biomechanics. In traditional topology optimization methods, it is assumed that the loading is prescribed and that a given amount of structural material is specified within a given 2D or 3D design domain with specified boundary conditions [10].

Research in the field of topology optimization of continuum structures began with the problem of generating optimal topologies in structural design in order to define the stiffest structures, which was explored by Bendsoe and Kikuchi [6]. Their strategy was to define the problem with a composite material represented by each element having material plus a void (hole) inside (Figure 1. 2). The building blocks can be rectangular in general and also be oriented at a certain angle θ to the horizontal as shown in Figure 1. 3. Here each building block is represented by five design variables namely, W1, W2, L1, L2 and θ. The material properties of each element are then dependent on the size and orientation of the void within the element according to a homogenization relationship. A sizing optimization is then performed to optimize the size/orientations of the voids of all the elements for a given objective function. Elements with large voids (low material density) will represent empty cells and the elements with small voids (high material density) indicate that material exists and hence that cell is a part of the structure. More details of this method can be found in [11].

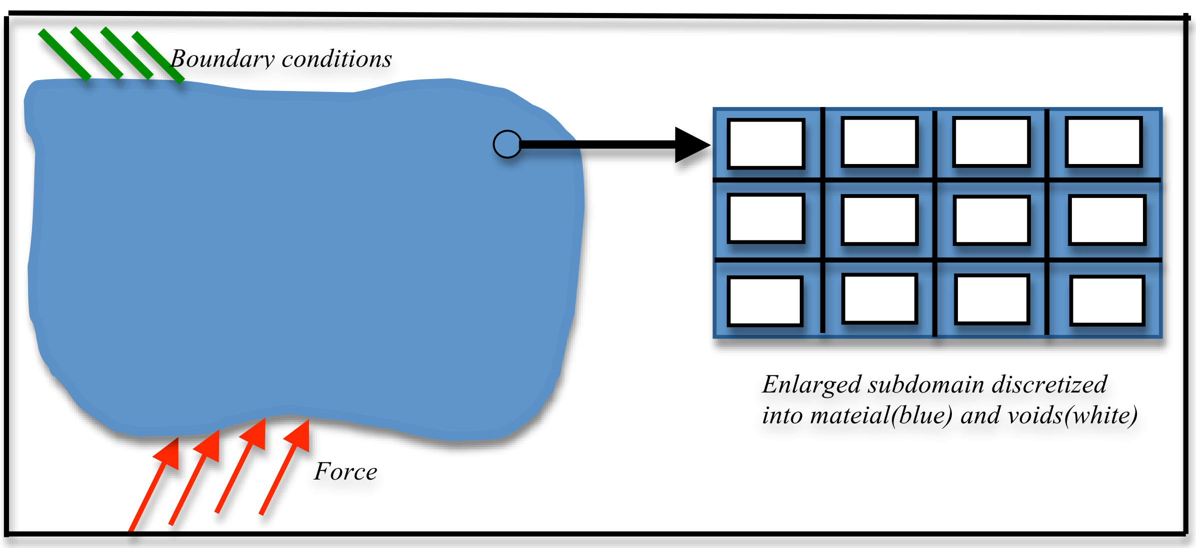

Figure 1. 2 Material structure as an arrangement of material and void

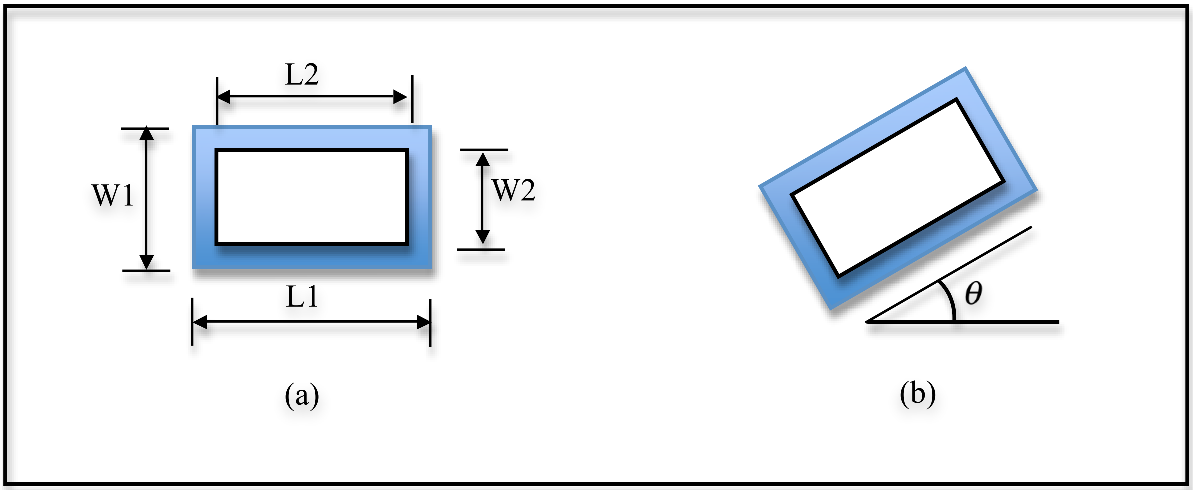

Figure 1. 3 Representation of building block with 5 design variables

An alternative but conceptually similar approach is to directly use the material density of each element (instead of voids) as the design variable. An empirical formula is required in this case instead of using the homogenization formulation. The topology optimization results from this formulation are reported to be similar to those obtained from the homogenization formulation [12].

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Strang and Kohn [13] recommended the use of composites in structural optimizatin problems because the existance/ non-existance of building blocks results in a ill-posed minimization problem, where the optimal solution might be difficult to obtain. To solve this problem they suggest a "relaxation" of the problem where the material in the design domain is modelled as a composite with continously varying density which transforms the original problem into one that has a solution. Hence by modeling the material as a composite and then using material homogenization techniques to determine the composite's structural properties, a minimization problem is created which can be solved by common optimization algorithms.

Optimality criteria methods are typically used to solve the minimization problem created by this "relaxation". Specifically, an iterative redesign procedure modifies the initial design values until the design satisfies a set of optimality criteria. Even though the optimality criteria values are satisfied, there is no guarantee that the design solution is a global optimum. It has been shown that an optimal component design's shape depends upon both the initial material density values and the material microstructure model when using homogenization-based techniques.

1.3 Uncertainty in Structural Design

Uncertainty is a acknowledged phenomenon in the process of structural design. During a design optimization process the designer looks for a safe design that has the ability to perform according to the design specifications while it is exposed to various uncertainties. Traditionally safety factors were used to account for the uncertainties. However, use of safety factor does not usually lead to minimum cost designs for a given level of safety because different structural members or different failure modes require different safety factors. Recently, probabilistic approaches have been used which can give a safer design at a certain computational cost. These methods give an alternative to the designers who use the traditional safety factor design approach. However, these kind of processes would require the statistical parameters for the design at hand which could be computationally expensive to obtain. Hence the probabilisic approaches require solving an expensive, complex optimization problem that needs robust formulations and efficient computational techniques for stable and accelerated convergence.

Probabilistic methods are used in reliability analysis by assuming that the amount of raw material available is sufficient to determine the probability density function and calculate other statistical inputs. However, in practical applications sufficient raw data might not be available due to restrictions in time, human and facility requirements and finances. It has been reported in Ref. [14] that probabilistic methods are not appropriate in cases where sufficient data is not available. To handle uncertainty with insufficient information, possibility-based (fuzzy set) methods have been recently introduced in the field of stochastic structural analysis and design optimization [15]. Additionally, Dempster- Shafer theory of evidence [16, 17], random set [18], probability bounds [19-21], imprecise probabilities [22] and convex model [23] are other methods that have been used to describe stochastic uncertainty well. All of these methods have a variety of mathematical description although all of them are based on interval analysis [24]. Although the theory of fuzzy sets was introduced by Zadeh [25], the application of interval analysis in structural analysis is very recent. An interval analysis approach utilizing the finite element method was introduced by Koyluoglu et al. [26] in order to deal with pattern loading and structural uncertainties. Recently, Muhanna and Mullen [27-29] formulated the development of interval based methods for fuzziness in continuum mechanics. These methods help to incorpporate uncertain loads in static structural problems using an interval-based fuzzy finite element in the analysis.

In cases when sufficient data is available Reliability based Design Optimization (RBDO) can be conducted using probabilistic methods. In case of RBDO the probability density function (PDF) should be known before starting the optimization process. The PDF is used to sample points using a Monte Carlo Simulation or Latin Hypercibe Sampling Scheme to simulate uncertain data on the design. The different methods for PDF estimation can be classified as *Parametric*, *Non-Parametric* and *Semi-Parametric*. In Parametric method the PDF is assumed to be of a standard form (gaussing, weibull, beta, etc.). The parameters of the assumed PDF can be estimated using Maximum

Likelihood estimation (MLE) or Bayesian Estimation. The Non-Parametric methods include histogram based methods and the K-nearest neighbor methods [30]. In Semi-Parametric methods the given density can be modeled as a combination of known densities. Mixture of Gaussians (MOG) is a well known method where a data set is assumed to come from different gaussian distributions. The parameters for MOG can then be estimated either by using gradient descent method or Expectation Maximization (EM) algorithm [30].

The behaviour of a structure in structural reliability analysis in probabilistic methods is measured by the performance function. The performance function is called the *limit state function* which is typically expressed as the difference between the capacity (e.g.,yield strength, displacement, allowable vibration level) and the response of the system (e.g., stress, maximum allowable displacement, actual vibration). Reliability analysis methods can be broadly classified into two categories- analytical methods and simulation methods. While analytical methods are easy to use and are mostly limited to single failure modes, the simulation methods can acess complex limit state functions and can also handle multiple limit states together. Simulation approaches like Monte Carlo Simulation (MCS) or Latin Hypercube Sampling (LHS) are computationally intensive but unlike analytical methods which can only handle only linear limit state functions, they can handle any kind of limit state functions. Most real life applications exhibit multiple limit state functions and multiple failure modes and most of the cases there is no prior information on the nonlinearity of the limit state function. Simulation based methods like MCS and LHS are the obvious choices in those scenarios. Since realibiality analysis is an iterative process and using crude MCS is computationally expensive, researchers develop variants of MCS or other methods like response surface and other function approximation techniques that can replace a part of the reliability analysis computational process and obviate the need to repeatedly access the expensive computer models viz. FEM in case of structural optimization.

1.4 Reliability based Design Optimization

In deterministic design optimization design solutions at the boundary of the design constraints are also considered leaving no latitude for variations in the design parameters. The resulting deterministic optimal solution is usually associated with a high chance of failure due to the influence of uncertainties inherently present during the modeling and manufacturing phases of the product and due to uncertainties in the external operating conditions of the product. Uncertainties in simulation-based design are inherently present and need to be accounted for in the design optimization process. Uncertainties may lead to high probability of failure, resulting from large variations in the performance characteristics of the system. Optimized deterministic designs determined without considering uncertainties can be unreliable and might lead to catastrophic failure of the product being designed. *Robust design optimization* and *reliability based design optimization* are methodologies that address these problems. The goal in robust design is to minimize the variations in the performance function. The goal in reliability-based design is to minimize the probability of failure. Hence in order to maintain high market share it is extremely important that designers consider variations in the design of new products and systems. This dissertation specifically focuses on reliability based design optimization problems in the context of topology optimization problems for the design of optimal truss structures. The goal in Reliability based Design Optimization (RBDO) is to minimize the probability of failure of a structural design. While using RBDO the designer has to make a tradeoff between making the design more reliable or minimizing cost. More reliable structures include more material than the corresponding deterministic optimization solution. The first step in RBDO is to characterize the important uncertain variables and the failure modes. In most engineering applications, the uncertainty is generally characterized using probability theory. Different statistical models can be used to describe the probability distribution function of the uncertain variables. While designing products with multiple failure modes it is important to justify the safety of the product with respect to each failure mode and also with respect to the overall system failure. In a RBDO formulation, the critical failure modes in deterministic optimization are replaced with constraints on probabilities of failure corresponding to each of the failure driven modes or with a single constraint on the system probability of failure. The reliability index, or the probability of failure corresponding to either a failure mode or the system, can be computed by performing a *probabilistic reliability analysis*. Some of the techniques used in reliability analysis are the first order reliability method (FORM), second order reliability method (SORM), and Monte Carlo simulation (MCS) techniques. FORM and SORM are based on the Taylor series expansion and MCS/LHS are simulation based methods that can be used alone or a solver substitution can be made using an appropriate surrogate modeling technique to reduce the computation. Figure 1. 4 represents the taxonomy of the different reliability assessment methods that can be used to evaluate the probability constraint. The methods within solver substitution can be further classified into function approximation based methods or classification based methods. Out of the many methods for classification neural networks using a back propagation method was used for this research because of their ease of use and effectiveness. In case of function approximation, Moving Least Squares local regression method was used because of their efficacy in approximating highly nonlinear responses and their ability to estimate low probability of failures.

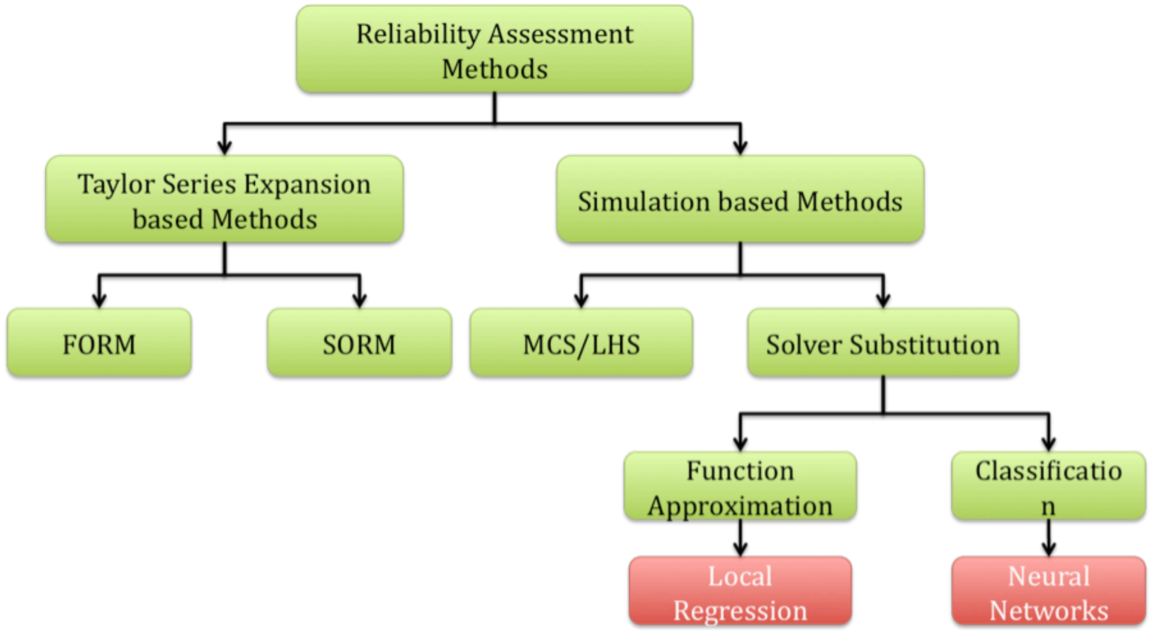


Figure 1. 4 Taxonomy of reliability assessment methods

1.5 Reliability-based Topology Optimization

Optimization algorithms traditionally have been solved using a deterministic approach where a design solution was obtained for specific force and boundary conditions. However, performing probabilistic analysis prior to the early stage of fabrication is critical to reduce cost, improve product quality, and provide a better understanding of failure mechanisms and sensitivity to process variation. With the high-powered digital computers, it has become feasible to find numerical solutions to realistic problems of large-scale, complex systems involving uncertainties in their behavior. This feasibility has sparked an interest in combining traditional optimization methods with uncertainty quantification measures. These new optimization techniques, which can consider randomness or uncertainty in the data, are known as *stochastic programming*, stochastic optimization, optimization under uncertainty, or reliability-based design optimization. These methods ensure robust designs that are insensitive to given uncertainties and provide the designer with a guarantee of satisfaction with respect to the uncertainties in the objective function, performance constraints, and design variables [31]

The use of integrated reliability analysis and topology optimization procedures, such as reliability-based topology optimization (RBTO) models as stated by Kharmanda et al. [32], yield structures that are more reliable than those produced by deterministic topology optimization methods. However, realistic representations of uncertainty and the improvement of the computational efficiency are still challenging in the existing methods [33, 34].

1.6 Discontinous Responses and Disjoint Failure Domains

The reliability analysis of complex structures is hindered by the implicit nature of the limit-state function. For their approximation use has been made of the Response Surface Method (RSM) and more recently of Artificial Neural Networks. Both these methods come into the broad category of Regression Approach.

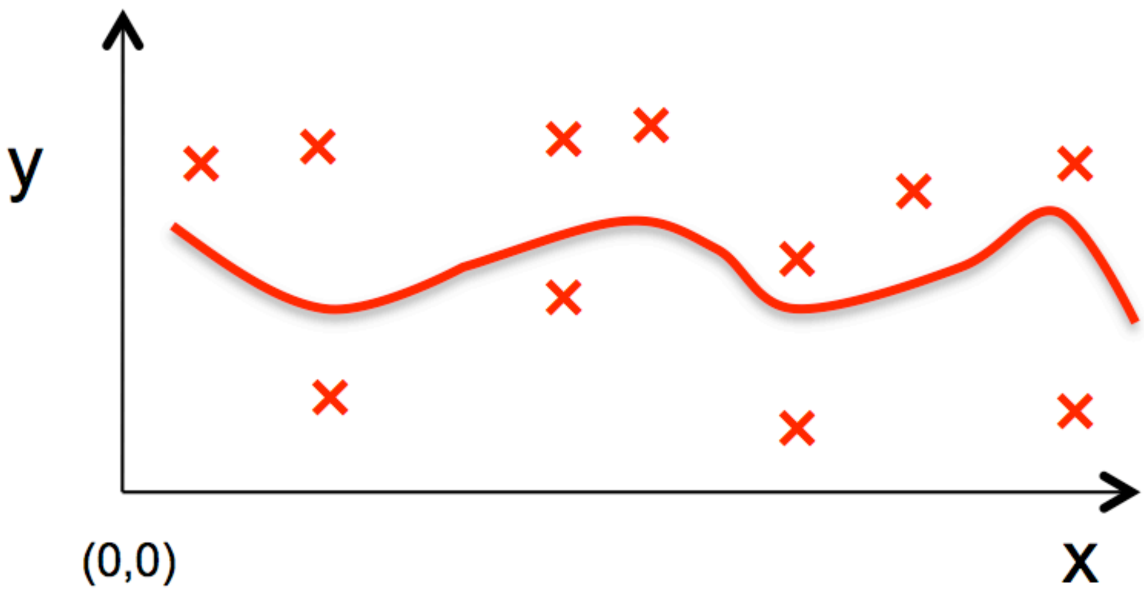


Figure 1. 5 Continuous failure domain example- suitable for regression approach

Figure 1. 5 shows design points in red, which belong to a continuous domain. Hence a single function can be used to approximate the failure behavior. Hence a regression-based approach is suitable for being used as a surrogate model in this case.

A common problem faced in case of approximation using the regression approach is the inability of regression based methods to approximate discontinous functions. A simple disjoint failure domain is represented in Figure 1. 6 where the red lines mark the boundary between the safe and unsafe regions in the design space. The red design points shown in the figure represent the unsafe designs and the green points represent the safe designs.

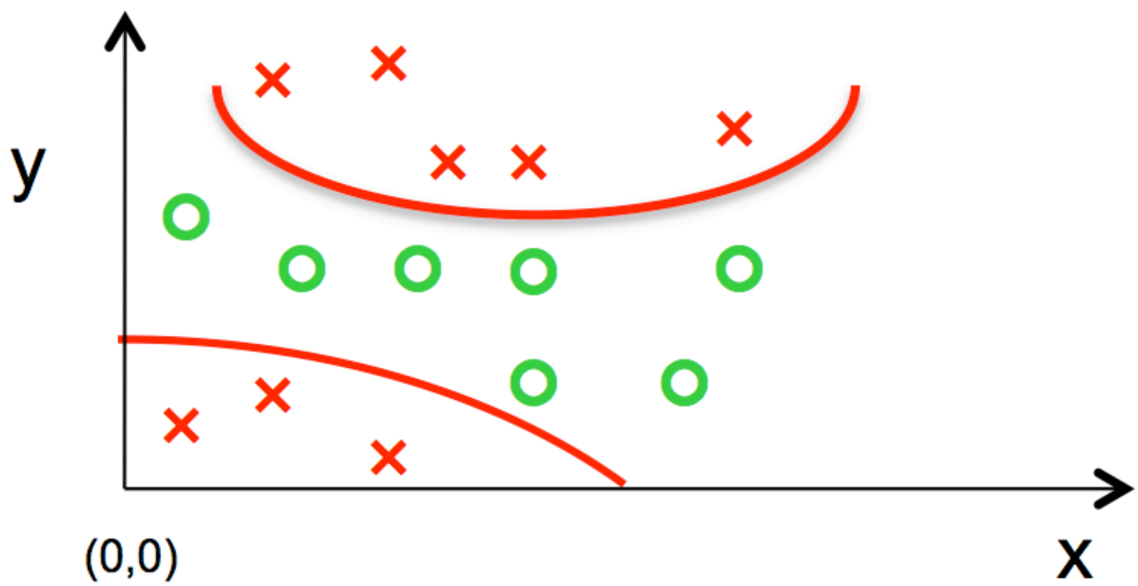


Figure 1. 6 Example of a disjoint failure domain limit state

Hence in cases where the failure domains are disjoint regression will not be suitable for estimating the failure behaviour of the design. A classification approach can be used in those cases for approximating the limit states and estimating the probability of failure.

1.7 Low Probability of Failures

In structural realiability analysis the designer would like to minimize the probabilty of failure as much as possible. Theoretically the probability value can't be zero hence a low value such as 10^{-4} or 10^{-6} is chosen by a majority of designers as the required probability of failure during a design optimization procedure. In order to reduce the computation cost in evaluating the reliability constraint during the optimization procedure a surrogate model is used by designers with the data obtained using a suitable experimental design procedure. Choi et. al. explored the application of response surface method[35] after Latin Hypercube Sampling (LHS) and Local Regression method[36] for the approximation of the limit state function during design optimization.

1.8 Research Questions and Hypothesis

The current thesis deals with the development of computationally efficient reliability based topology optimization procedure for the design of truss structures for different scales and applications in the presence of uncertainty. Traditional reliability based methods are not computationally efficient since they have to evaluate the limit state function during every iteration of the optimization algorithm. A surrogate modeling technique can be used in those cases for reducing the computational requirement of the RBTO procedure.

In cases where the failure domain is discontinuous a regression-based surrogate modeling technique will be invalid for use since regression can only approximate continuous domains. Another major concern in Reliability based designs is the need to deal with low probability of failures. The surrogate model should be able to estimate low values. Due to numerical stability issues many surrogate modeling techniques can't be used for estimating responses whose values range in different orders.

The factors discussed above raise the following research questions. Every research question is followed by the hypothesis. The following chapters validate these hypotheses.

Research Question 1

How can the Reliability based Topology optimization procedure be made computationally efficient for the design of truss structures?

Hypothesis:

The computational requirement of Reliability based Topology Optimization procedure can be reduced by approximating the reliability constraint with an appropriate surrogate modeling technique.

Research Question 2

How can the probability of failure be calculated in case of disjoint failure domains and low values of probability of failures?

Hypothesis:

Moving Least squares Local Regression procedure can be used for the efficient computation of the probability of failures. This method is efficient in estimating low probability of failures. In cases where the failure domain is not continuous a *classification*-based approach using Artificial Neural Networks can be used for estimating the probability of failure.

1.9 Current Research

The intent of the current research is to explore the synthesis of optimized truss-like mesostructured materials when the loading, boundary conditions and geometry vary according to assumed statistical properties. In this research, a reliability-based synthesis framework to develop risk-minimized cellular structures that satisfy the performance criteria while specific loading, displacement and shape conditions are imposed on them, is proposed. This is achieved by utilizing the stochastic *local regression* [36] procedure for approximating the failure behavior when the reliability constraint is linear in nature. In cases where the reliability constraints are nonlinear or discontinuous an *artificial neural network* based *classification* technique is proposed which can be used to approximate the failure behavior. Classification based reliability analysis divides the failure domain into safe and unsafe regions and evaluates and classifies the data into one of the two classifies hence eluding the need to evaluate the response.

The proposed algorithms include a simulation based risk estimation model that provides feedback to the design process and potentially improves the reliability of the mesoscale material structure. Thus, a reliability-based design technique will be integrated to mitigate the risk of structural failure via enhancements of conventional topology optimization techniques.

The following chapters describe important aspects of the algorithm and the solution principle for designing truss like material structure under uncertainty which will result in the design of more reliable mesostructured materials.

1.10 Thesis Organization

The thesis is organized as shown in Table 1. Chapter 1 introduces the concept of mesostructured materials and how they can be designed based on concepts from structural optimization. It also introduces basic ideas behind Topology Optimization, Uncertainty in design optimization and Relibility based Topology Optimization. The rest of the thesis introduces the research questions and the approach taken to validate the hypothesis for the research questions.

Table 1 Organization of the thesis

Chapter 1	Introduction
Chapter 2	Reliability-based Topology Optimization
Chapter 3	Efficient Reliability-based Topology Optimization
Chapter 4	Illustrative Examples
Chapter 5	Conclusion and Future Work

Chapter 2 introduces the concepts of reliability based topology optimization procedure. The basic concepts of Monte Carlo Simulation, Latin Hypercube Sampling, surrogate models and function approximation are described. Local regression and classification schemes are introduced and described in details. A brief description of artificial neural networks is also provided in this chapter since they are used for the classification procedure in this research. The concept of disjoint failure domains is then explained in this chapter with the help of an example.

Classification and Local regression are combined into the reliability based topology optimization framework in chapter 3. The overall framework that combines the efficacy of both Local regression procedure and the classification procedure is demonstrated.

Illustrative examples, which validate the efficacy of the proposed framework, are shown in chapter 4. The framework is also validated using the hydrogen tank design example.

Chapter 5 summarizes the main points outlined in the thesis along with the advantages of the proposed framework. The limitations of the current research are discussed along with the suggestions of future work that can improve this research.

CHAPTER 2

RELIABILITY-BASED TOPOLOGY OPTIMIZATION

With the advances in computer technology and the relative cheaply available computational resources, structural optimization has revolutionized the way structures are designed. This phenomenon has led designers to deviate from the traditional design-analysis-new design method of designing structures to the process of structural design through optimization [37].

2.1 Deterministic Optimization

2.1.1 Description of an Optimization Problem

An optimization problem seeks the maximum/minimum of a function $f(x)$ and the variable vector $X = (x_1, x_2, ..., x_n) \in R^n$ that it depends on. Here f is called the *objective function* and x_i, $i \in 1,.....,n$ are the variables that determine the objective function and are typically called *design variables*. Any vector X in the n dimensional design space represents a single design where n represents the number of design variables in the optimization problem. It is important to note that the design variables can be either continuous or discrete. For example, a structure might have to be made using truss elements for a machine component. If the areas of cross-sections are taken as the design variables and trusses with certain cross-sections can only be purchased then the design variables should be considered as discrete. Since we can purchase any length of these truss elements or cut the purchased truss elements to desired lengths, the lengths can be considered as continuous variables.

In many of the design scenarios the designer is posed with constraints in terms of geometry, performance, safety, cost and manufacturability. Some of these constraints might have an equality form. Owing to this the number of independent dimensions in the design space is reduced, from n, by the number of equality constraints. Along with this the strict inequality constraints reduce the design space to a subset of R^n.

In the most general form, an optimization problem can be represented as:

Minimize	$f(x)$		(2.1)
Subject to	$h_j(x) = 0,$	$j = 1,2,.......,n_h$	(2.2)
	$g_k(x) \leq 0,$	$k = 1,2,......,n_g$	(2.3)
	$x_i^l \leq x_i \leq x_i^u,$	$i = 1,2,.......,n$	(2.4)

where n_h, n_g and n are the number of equality constraints, inequality constraints and design variables, respectively. x_i^l and x_i^u are the lower and upper bounds on the design variable x_i. The implementation of a simple optimization procedure can be represented as shown in Figure 2. 1 below.

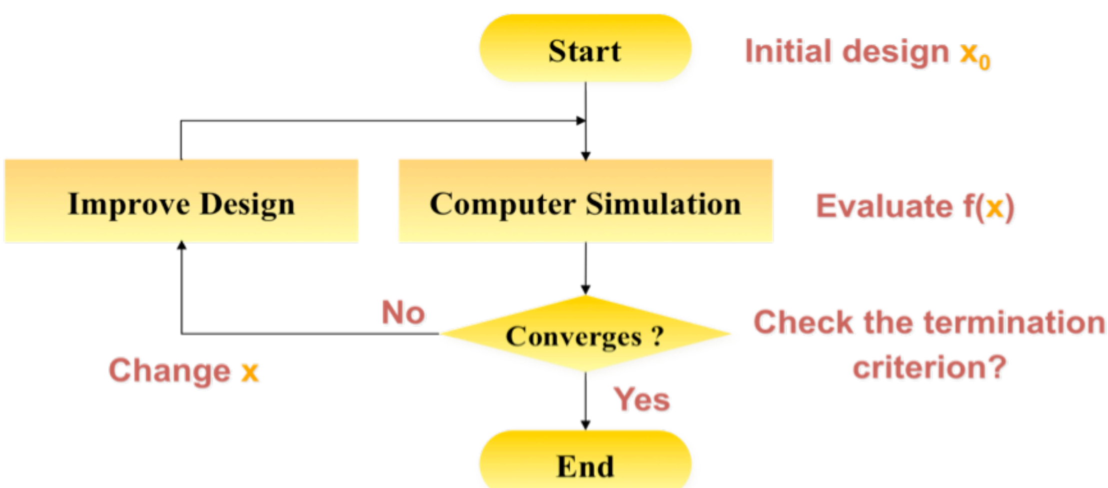


Figure 2. 1 The optimization procedure

If the objective function and all the constraints are linear functions of the design variables then the problem is termed *linear optimization* problem. In a *nonlinear optimization* problem, either the objective function or at least one of the constraints is nonlinear function of the design variables. In general structural optimization problems are non linear in nature. Further, design optimization can be classified into *size optimization*, *shape optimization* and *topology optimization*. A brief description of each type of optimization follows.

2.1.2 Size Optimization

In size optimization the domain is fixed and does not change during the optimization process. Hence most of the time size optimization is performed in the final stages of the product design process [38].

The basic idea behind size optimization is explained next with the help of Figure 2. 2. The figure shows a structure that can be discretized into six beam elements. For any given objective function the design can be optimized for a better performance by altering the thickness of the six beam elements. Hence the thicknesses of the beam elements are considered as the design variables in this case. An important thing to note here is that although the answer from this procedure might be "optimal", changes to the beam element's shapes and the overall topology could possibly give a better result.

Figure 2. 2 Size optimization of beam with six elements

2.1.3 Shape Optimization

Shape, or geometrical, optimization is somewhat more complex process. In case of shape optimization the topology[1] of the design is fixed whereas the shape is not fixed. The blue points shown in Figure 2. 3 can be used as control points to define the shape of the beam. The wider shape will mean more material usage in this case. Based on the designer's preference the eight variables can be changed that will define the location of the control points and the shape of the overall structure. Similarly, a collection of B-splines or Bezier curves [39] can be used for the shape optimization of a cross-sectional shape. Shape optimization is generally performed during the initial stages of the design process. In general shape optimization can lead to better results than size optimization but again changes to a beam's topology could possibly lead to better results.

Figure 2. 3 Shape optimization of beam with eight control points

[1] Mathematically, two geometrical figures are said to have the same topology if they can be transformed from one to another through continuous transformations. Continuous transformations means pulling, stretching, twisting, bending or squashing without tearing or gluing points together

2.1.4 Topology Optimization

Topology optimization has the complex features of both size and shape optimization. Topology optimization is often referred to as layout optimization or generalized shape optimization [5]. In this case, the design variables control the topology of the design. This is also the most general optimization procedure, as the size and shape of the structure are affected by the topology. The difficulty in implementing this procedure comes from its generality. Representing the topology of the structure is difficult and generally requires a large number of design variables. Topology optimization operates on a fixed mesh of finite elements and defines a design variable, which is associated with each element in the mesh. Common way of representing a topology optimization problem is to treat it as a configuration design problem where the design is treated as an assembly of a large number of “building blocks”. The procedure begins by discretizing the design space into all possible identical building blocks. As the optimization process proceeds, various “building blocks” are allowed to disappear or reappear, which in turn alters the topology of the structure. In some classical methods of topology optimization a design variable value of 1 means the corresponding building block is present whereas a value of 0 means that it is not. With some other optimization procedures the design variables can take intermediate values between 0 and 1, signifying that a material of low density is present in the corresponding block.

In Figure 2. 4 a topology optimization procedure with 72 design variables in shown. In order to design the stiffest beam for a given amount of material, the whole design domain is divided into 72 building blocks. Typically the target amount of material to be used in the final design is stated as a fraction of the total volume of the structure if all design variables were at their upper bound. As the optimization procedure proceeds the blocks in white are the ones that are removed from the final design. The final optimized design only constitutes of the building blocks in blue.

Figure 2. 4 Topology optimization of beam using density design variable

3.1.4.1 Topology optimization of truss structures

Topology optimization of trusses in the form of grid-like continua is a classical subject in structural design. Michell [33] pioneered the study of grid like continuum structures. The development of computationally efficient topology optimization methods is not only important for designing truss structures but also for the design of material structures. The optimization of the geometry and topology of trusses can be conveniently formulated with the so-called *ground structure* method [40]. The truss topology optimization problem is formulated so that the cross-sectional area of every possible truss element connecting the predefined nodes is a design variable. Each of these truss elements at the end of the optimization routine can either exist or vanish depending on the problem at hand. This is possible by defining the cross-sections as continously varrying, owing to which the problem can be viewed as a standard sizing problem. This sizing reformulation is possible because the truss as a continuum geometrically is described as one dimensional. Thus for both planer and space trusses there are extra dimensions in physical space that can describe the extension of the truss as a true physical element of space, simplifying the basic modeling for truss topology design as compared to topology design of three dimensional continuum structures [7]. Since area of cross-sections were formulated as continous design variables, a non-zero (small) lower bound on the cross-sectional areas has to be imposed in order to have a positive definite stiffness matrix. Two different types of preliminary structures are shown in Figure 2. 5.

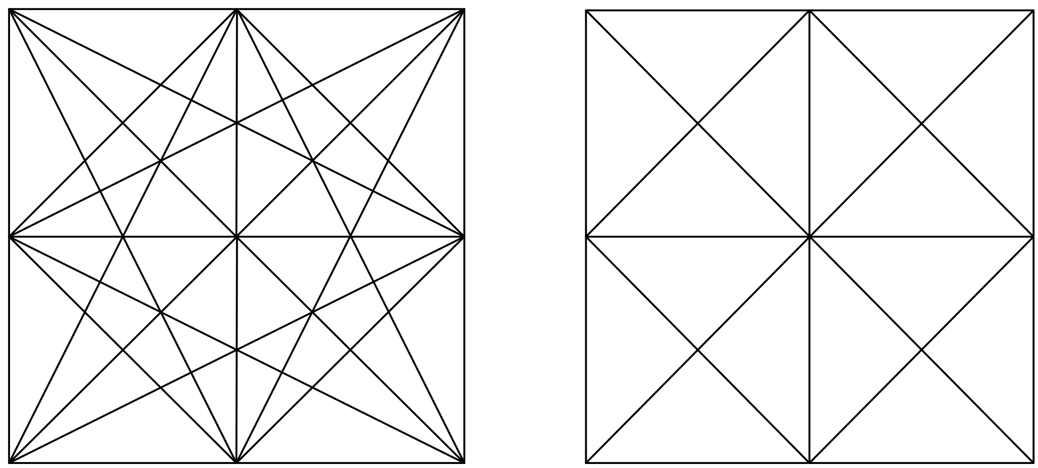


Figure 2. 5 Topological model for RBDO framework for (a) Ground structure and (b) Unit cell

Groundstructure in figure (a) consists of three nodes along the length and the height of the design space. In this case each node is connected to every other node. Practically trusses can cross each other in space since they can be bolted together to lie in different planes this kind of initial structure can be an effictive way to form the superset of all possible designs. In a ground structure if there are n nodes in total then the number of truss elements in the design space is m, which is represented by Equation 2.5 . The number of degrees of freedom equals $2n$ for a planer structure.

$$m = \frac{n(n-1)}{2} \tag{2.5}$$

In the unit cell each node is only connected to the most immediate neighbor making this kind of initial structure not as exhaustive as the ground structure. Nevertheless, these kind of initial structures are useful when the designer wants to keep the structure simple and easy to assemble from individual truss elements. These kind of structures can be advantageous while designing mesostructured materials. A simple formulation for topotlogy optimization with area of cross section A_i as the design variables for truss structures design for *stiffest structure* [41] objective can be represented as

Minimize: *Mean Compliance* (2.6)

Subject to: $\sum_{i=1}^{N} A_i L_i - V^* \leq 0$ (2.7)

$$A_l \leq A \leq A_u \tag{2.8}$$

$$Ku = F \tag{2.9}$$

Equation 2.6 represents the stiffest structure objective because a stiffest structure will have minimum mean compliance. Equation 2.7 represents the volume constraint where L_i represents the length of each truss element and V^* represents the target volume of the final optimized structure. A_l and A_u are the lower and upper bounds for the design variable. Equation 2.9 represents the finite element method that is used to evaluate the objective function and other constraints.

The following sections describe reliability based design. Reliability based design can easily be included in the formulation for topology optimization by including the *reliability constraint* into the formulation of topology optimization.

2. 2 Reliability Analysis

2.2.1 Structural Reliability Assessment

Reliability is the probability that a system will perform its function over a specified amount of time and under specified service conditions. Primarily, reliability-based design consists of minimizing an objective function while satisfying reliability constraints. The reliability constraints are based on the failure probability corresponding to each failure mode or a single failure mode decreasing the system failure. The estimation of failure probability is usually performed by reliability analysis. In case of structural optimization the structure is under the influence of loads and boundary conditions and the response also depends on the stiffness and mass properties. The responses that are critical for the reliability of the structure such as critical location stresses, resonant frequencies, displacements etc. are considered satisfactory when the design requirements imposed on the structural behavior are well within the degree of certainty. Each of these requirements is called *limit-state*. The probability of violation of the limit state is a metric for quantifying the reliability of the structure under consideration. Once the limit state has been violated the structure is believed to have undergone failure for the sake of calculations. By determining the number of times the structure failed out of the number of evaluations the probability of failure can be determined. Once the probability has been determined the next step will be to choose design alternatives that improve structural reliability and minimize the risk of failure.

Generally the limit state indicates the margin of safety between the resistance and the load of structures. The limit-state function, $g(.)$, and probability of failure, P_f, can be defined as

$$g(X) = R(X) - S(X) \tag{2.10}$$

$$P_f = P[g(.) < 0] \tag{2.11}$$

where R is the resistance and S is the loading of the system. Both $R(.)$ and $S(.)$ are functions of random variables X. Here $g(.) = 0$ represents the failure surface. $g(.) < 0$ and $g(.) > 0$ represent the failure region and safe region respectively.

The mean of the limit state $g(.)$ can be expressed as in Equations 2.8, where μ_R and μ_S represent the means of *R* and *S* respectively.

$$\mu_g = \mu_R - \mu_S \tag{2.12}$$

The standard deviation of *g(.)* is

$$\sigma_g = \sqrt{\sigma_R^2 + \sigma_S^2 - 2\rho_{RS}\sigma_R\sigma_S} \tag{2.13}$$

where, ρ_{RS} is the correlation coefficient between R and S, and σ_R and σ_S are the standard deviations of *R* and *S*, respectively. The *safety index* or *reliability index* is then defined as

$$\beta = \frac{\mu_g}{\sigma_g} = \frac{\mu_R - \mu_S}{\sqrt{\sigma_R^2 + \sigma_S^2 - 2\rho_{RS}\sigma_R\sigma_S}} \tag{2.14}$$

The safety index indicates the distance of the mean margin of safety from *g(.)=0*. The idea behind the safety index is that the design is more reliable if μ_g is farther to the limit state surface.

For a special case, if the resistance R and the loading S are assumed to be normally distributed and uncorrelated, then the probability density function of the limit-state function can be represented as

$$f_g(g) = \frac{1}{\sigma_g\sqrt{2\pi}}\exp\left[-\frac{1}{2}\left(\frac{g-\mu_g}{\sigma_g}\right)^2\right] \tag{2.15}$$

The *probability of failure* can then be represented as

$$P_f = \int_{-\infty}^{0} f_g(g)dg \qquad (2.16)$$

For a multidimensional case, the generalization of Equation 3.11 becomes

$$P_f = P[g(X) \leq 0] = \int ... \int f_X(x_1,...,x_n)dx_1..dx_n \qquad (2.17)$$

where *g(X)* is the *n*-dimensional limit-state function and $f_X(x_1,...,x_n)$ is the joint probability density function of all relevant random variables *X*.

Due to the curse of dimensionality in the probability of failure calculation in Equation 2.13 numerical methods can be used to simplify the numerical treatment of the integration process. The Taylor series expansion is often taken to make the limit state *g(X)=0,* linear. This is the basis of the First order reliability method (FORM) [42] and Second order reliability method (SORM) [43]. Other strategies have also been used in the past for probabilistic analysis for designing reliable structures. Stochastic Finite Element method [44, 45], sampling methods and stochastic expansions [46] are some of the most commonly used methods for conducting reliability analysis.

2.2.2 Sampling Methods

In this research the efficient use of sampling methods for design of reliable material structures is explored. The basic advantage of sampling methods is that the probabilistic information or mathematical solution of a problem can be obtained by direct use of experiments.

2.2.2.1 Monte Carlo Simulation

Monte Carlo methods were originally practiced under more generic names such as statistical sampling, and the name is a reference to the famous casino in Monaco. The methods use of randomness and iterative procedure is similar to a casino's activities. In Monte Carlo Sampling (MCS) [47] the *inverse transform method* is used to generate random variables with specified probability distributions. This method can be applied to variables for which the cumulative distribution function has been obtained from direct observation, or where an analytic expression for the inverse cumulative function, $F^{-1}(.)$, exists [31].

Let $F_X(x_i)$ be the Cumulative Distribution Function (CDF) of random variable xi. Since the value of CDF can only lie between 0 and 1, *F(.)* has a value between 0 and 1. If u is the uniformly distributed random variable that is generated using MCS then the inverse transfer method is used to equate u to $F_X(x_i)$ as follows:

$$F_X(x_i) = u \tag{2.18}$$

or

$$x_i = F_X^{-1}(u) \tag{2.19}$$

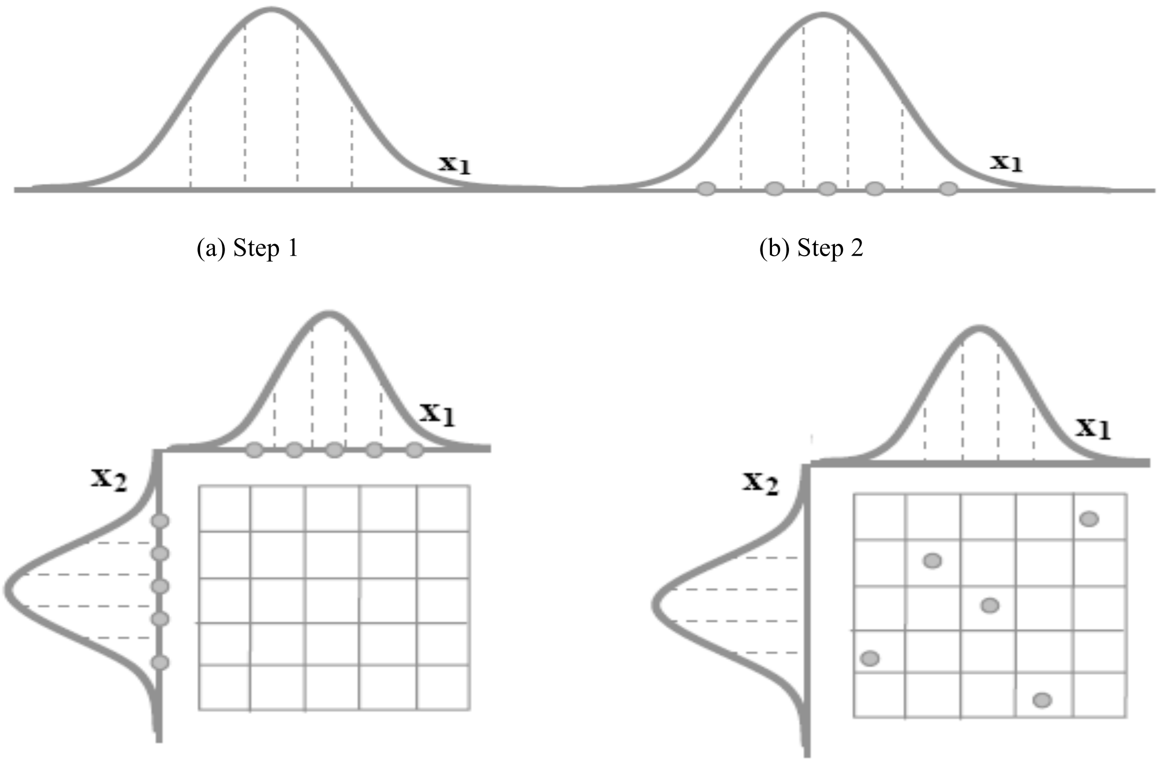
This method can be applied to variables for which a cumulative distribution function has been obtained from experiments or where an expression for the inverse cumulative function exists. The process starts with the random number generator producing random numbers between 0 and 1 based on randomly selected seed values. The corresponding CDF value of the uniform distribution and target distribution can easily be obtained using the random numbers that were generated. The final step is to obtain the random number for the target PDF using Equation 2.18.

Monte Carlo sampling can be very computationally expensive since they are random in nature. In order to make MCS less computationally expensive sometimes variance reduction techniques are integrated. Latin Hypercube Sampling is an excellent variance reduction technique that reduces the computational requirement for the simulation as well as increasing the accuracy with the same number of runs.

2.2.2.2 Latin Hypercube Sampling

In order to reduce the computational cost of the reliability assessment, a variance reduction sampling method, namely Latin Hypercube Sampling (LHS) [48], is introduced. LHS, also known as the stratified sampling technique, represents a multivariate sampling method that guarantees non-overlapping designs. In LHS, the distribution for each random variable can be subdivided into n equal probability intervals or bins. Each bin has one analysis point. There are n analysis points, randomly mixed, so each of the n bins has 1/n of the distribution probability. Figure 2. 6 shows the basic steps for the general LHS method, which are:

1. Divide the distribution for each variable into n non-overlapping intervals on the basis of equal probability.
2. Select one value at random from each interval with respect to its probability density.
3. Repeat steps (1) and (2) until you have selected values for all random variables, such as $x_1, x_2, \ldots, x_k$.
4. Associate the n values obtained for each x_i with the n values obtained for the other $x_{j \neq i}$ at random.



(a) Step 1 (b) Step 2

(c) Step 3 (d) Step 4

Figure 2. 6 Basic concept of LHS: two variables and five realizations [31]

The regularity of probability intervals on the probability distribution function ensures that each of the input variables has all portions of its range represented, resulting in relatively small variance in the response. At the same time, the analysis is much less computationally expensive to generate. The LHS method also provides flexible sample sizes while ensuring stratified sampling; i.e., each of the input variables is sampled at *n* levels.

<u>2.2.2.3 Probability of failure calculation</u>

The sampling methods can be used to calculate the probability of failure where the limit state function involves complex functions, and direct evaluation of the limit state is not possible. The following steps are taken to calculate the probability of failure P_f:

1. Generate a sampling set of random variables according to the corresponding probability density functions.
2. Set the mathematical model of the limit-state, which can determine failures for the drawing samples of the random variables.
3. The simulation is executed and for each run the limit state is evaluated.
4. If the limit-state function $g(.)$ is violated, the structure or the structural element has "failed".
5. The trial is repeated many times to guarantee convergence of the statistical results.
6. If N trials are conducted, the probability of failure is given approximately by

$$P_f = \frac{N_f}{N} \tag{2.20}$$

where N_f is the number of trials for which the limit state function is violated out of the N experiments conducted.

An example is illustrated in Figure 2. 7. Here 10 data points are generated using LHS procedure. For each of the data point *g(.)* is evaluated to check if the corresponding point belongs to the safe region or the unsafe region. The safe and the unsafe region are depicted in the figure. In this example, 3 points are assumed to be in the unsafe region. Hence the probability of failure for this case would be 0.3.

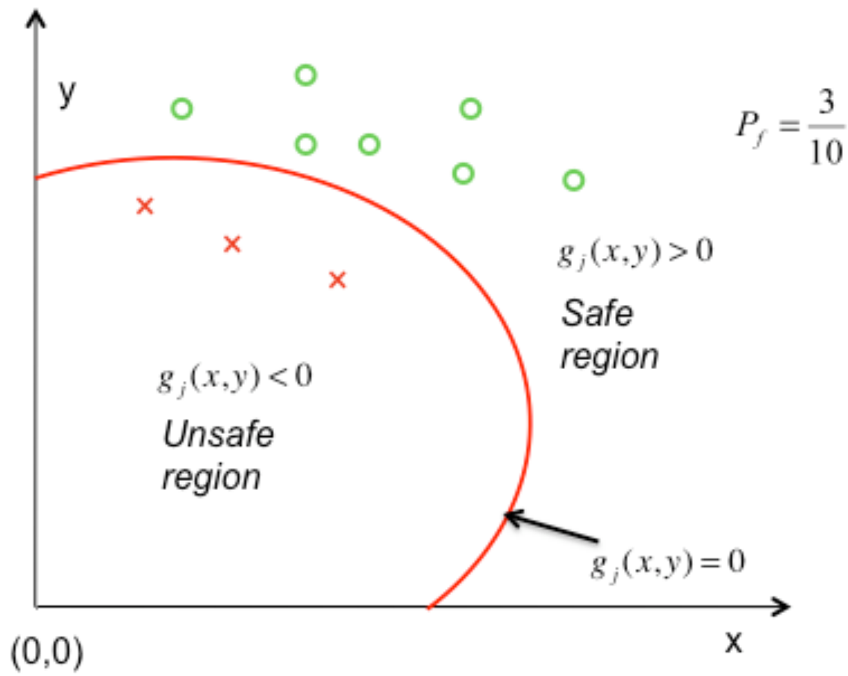


Figure 2. 7 Calculation of probability of failure using sampling procedure

2.3 Reliability - based Design Optimization

2.3.1 Formulation of RBDO

The formation of RBDO is similar to that of deterministic optimization:

Minimize: the objective function, $f(b, \mu_X)$ (2.21)

Subject to: $P_j[g_j(b,X) < 0] \leq P_{Rj}$ $\quad j = 1,.......,m$ (2.22)

or $P_j[g_j(b,X) \geq 0] \geq R_j$

where $g_j(.)$ represents the limit state function, b is the vector of deterministic design variables, and X is the random vector, which can be random design variables or random parameters of the system. P_{Rj} and R_j are the specified probability of failure level and the specified reliability level of the system, respectively.

Equation 2.16 can be expressed in terms of the safety index:

$$\beta_{g_j} \geq \beta_{Rj} \tag{2.23}$$

where β_{Rj} and β_{g_j} are the required safety index of the system and the safety index of the probabilistic constraint, respectively. This method for calculating the reliability of a structure is also referred to as the Reliability Index Approach (RIA) [49]. This method is used to calculate the probability of failure in this work.

An alternative approach for RBDO problems is the Performance Measure Approach (PMA), which can efficiently measure violations of the constraint. In PMA, the performance measure is determined after solving inverse reliability analysis problems. Details of PMA are available in [34] and [50].

Figure 2. 8 represents the Reliability-based design optimization procedure. Apart from the objective function and the constraints that are dealt with in the deterministic optimization procedure the evaluation of the reliability constraint is an important step in RBDO. The evaluation of the reliability constraint introduces randomness in the optimization procedure. Owing to the stochastic nature of this procedure this process can also be called *stochastic optimization* process. Consequently, evaluation of the reliability constraint increases the computational requirement of the procedure drastically. Hence a surrogate model can be used to estimate the value of the constraint. The surrogate model can be constructed after conducting a suitable *experimental design* such as Latin Hypercube Sampling method. This procedure will be explained in the next section.

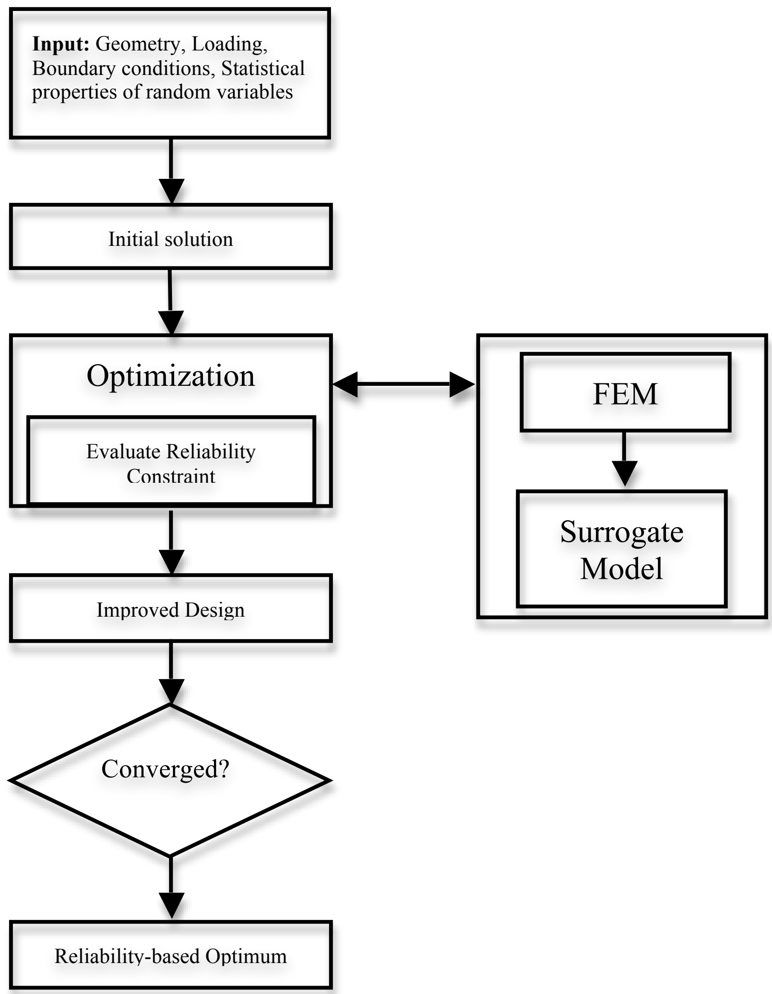


Figure 2. 8 Reliability-based design optimization

2.3.2 Stochastic Optimization

With the emergence of high power digital computers, it has become feasible to combine randomness or uncertainty in the optimization process and hence design large-scale complex systems. These methods are known as *stochastic programming* or *stochastic optimization* methods. These methods help the designer arrive at robust designs that are insensitive to given uncertainties and hence ensure a guarantee of satisfaction with respect to the uncertainty in the objective function, performance constraints and design variables.

Optimization under uncertainty, by its very nature is very expensive than solving deterministic problems, which alone may be computationally intensive. The computational cost of stochastic optimization problems turn out to be extremely high in many cases. This limitation has encouraged researchers to introduce and adapt efficient schemes to represent uncertainty in the optimization procedure. A common approach for treating the computationally expensive objective function and the constraints of the optimization problem is to build relatively inexpensive surrogate models using approximation techniques. The choice of surrogate-based optimization can be reasonable in typical engineering applications. Choi *et al.* [35] introduced a formulation that combines Polynomial Chaos Expansion (PCE) and Analysis of Variances (ANOVA) within the framework of LHS which can be effective in estimating the responses of large-scale uncertain structural problems. Specifically, to represent variability in stochastic constraints or objective functions, fluctuating components are introduced and approximated in this method. Many other function approximations techniques can be used in order to approximate the variability in the model that can help reduce the computational requirement of the optimization procedure drastically.

2.3.3 Function Approximation

Function approximations play a major role in iterative solutions and optimization of large-scale structures. For many structural optimization problems, evaluation of the objective function and constraints requires the execution of costly finite element analysis for displacements, stresses or other structural responses. The optimization process may require the evaluation of the objective function and the constraints hundreds or thousands of times. For example in case of the RBDO method, for every iteration of the optimization procedure the probability of failure has to be calculated using Equation 2.14, which can require the finite element analysis of the structure *N* number of times in order to evaluate the limit state function. In order to reduce the computational requirements of the procedure, an experimental design like LHS scheme is used to generate a small number of samples of input data and the response is obtained from the finite element analysis. This data is used to construct a surrogate model that can then be evaluated using *N* samples generated using any sampling scheme to evaluate the reliability constraint.

Some of these techniques can be used as a blackbox (viz. Neural Networks based methods), whereas for some of the methods (viz. Regression and Response surface techniques) it is important to have knowledge of the inherent physics of the problem. Furthermore, Artificial Neural Networks (ANN) has an added advantage that it can be used as either for function approximation or for *classification*. The following sections give a brief description of Moving Least Squares (MLS) and Artificial Neural Networks (ANN) methods.

2.3.3.1 Moving Least Squares

A primary challenge of stochastic analysis is to discover rigorous ways to forecast the low probability of failure, which is critical to reliability constraints. Simulation based methods evaluate the limit state function number of times in order to calculate the probability of failure. In case of reliability-based design the probability of failure has to be calculated every iteration making it a computationally- expensive procedure.

A common approach to the computationally expensive procedure of probabilistic methods is to approximate the system response using relatively inexpensive surrogate modeling techniques. To achieve a high quality surrogate model, the local regression model, namely Moving Least-Squares (MLS) method [51] can be used.

The main advantage of the MLS method is that the regression coefficients are not constant, but rather parameter dependent. This quality allows the data analysis to not be constrained to a specific global function in order to fit a model to the data. Instead, the fitting segments spawn a local-global approximation allowing the data to acclimate to the function over a wide range of parameters. The main idea of local regression is to fit curves and surfaces to localized subsets of the data by a multivariate smoothing procedure with moving processes.

The details of MLS process are shown in Figure 2. 9. In the first step we define the local domain based on the domain influence factor or the bandwidth, *r*. In the second step an approximation is estimated at the point x_i. This process can then be repeated at different calculation points by moving the local domain. Therefore, the regression coefficients of the MLS are not constant but a function of the calculation position or location.

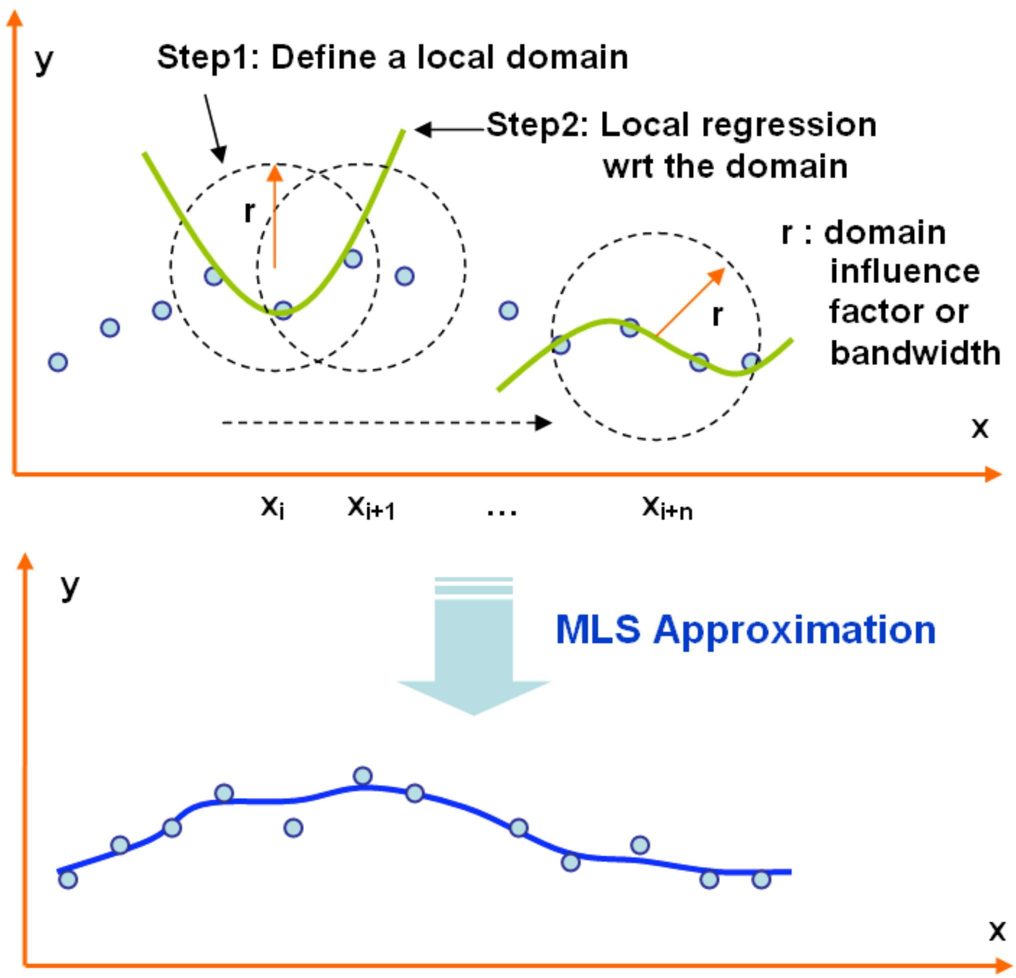


Figure 2. 9 Moving-least squares approximation [36]

A linear regression model can be written as

$$y(x) = \beta_0 + \beta_1 p_1(x) + ... + \beta_m p_m(x) + \varepsilon \tag{2.24}$$

where $p_j(x)$, j = 0,1,2,…,m, are the basis polynomial of order m, β_j are the regression coefficients, and ε, the error of the model equation, is assumed to be normally distributed with mean zero and variance σ_e^2. Equation 2.24 can be expressed in matrix notation for n sample values of x and y as

$$Y = X\hat{\beta} + e \tag{2.25}$$

where

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \quad X = \begin{bmatrix} 1 & p_1(x_1) & p_2(x_1) & . \; . & p_k(x_1) \\ 1 & p_1(x_2) & p_2(x_2) & . \; . & p_k(x_2) \\ \vdots & \vdots & \vdots & . \; . & \vdots \\ 1 & p_1(x_n) & p_2(x_n) & . \; . & p_k(x_n) \end{bmatrix} \quad \hat{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix} \quad \text{and} \quad e = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

Here, the simplest polynomial model is the monomials of x^m, i.e.,

$p^T(x) = [1, x, x^2, ..., x^m]$.

The coefficients can be calculated using a least square formulation. The regression coefficients can be represented as

$$\hat{\beta} = (X^T X)^{-1} X^T Y \tag{2.26}$$

The estimated target values and the errors are given by

$$\hat{Y} = X\hat{\beta} \text{ and } e = Y - \hat{Y} \tag{2.27}$$

The weight matrix *W(x)* is also present in the equation for coefficient matrix in case of Moving Least-Squares (MLS) approximation. The regression coefficient vector, $\hat{\beta}(x)$, can be calculated as

$$\hat{\beta}(x) = \left[X^T W(x) X\right]^{-1} X^T W(x) Y \tag{2.28}$$

where X is a n x p matrix of the levels of the regressor variables, Y is a n x 1 vector of the responses, and $W(x)$ is a none zero diagonal weight matrix which is given by

$$W(x) = \begin{bmatrix} w_1(x-x_1) & 0 & \dots & 0 \\ 0 & w_2(x-x_2) & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & w_n(x-x_n) \end{bmatrix} \tag{2.29}$$

A close examination of Equation 2.26 and Equation 2.28 Hence, the estimates for the MLS model $u^h(x)$ can be represented as follows

$$u^h(x) = \sum_{j=0}^{m} p_j(x)\hat{\beta}_j(x) = p^T(x)\hat{\beta}(x) \tag{2.30}$$

The weight matrix in Equation 2.29 is a function of the location or position of x and there are several types of weighting functions. The exponential, canonical and spline functions are widely used as weight functions and are represented as

Exponential weight function

$$w_i(x-x_i) = w(d_i) = \begin{cases} \exp(-(d_i/r_i)^2), & if \quad d_i/r_i \le 1 \\ 0, & if \quad d_i/r_i > 1 \end{cases} \tag{2.31}$$

Conical weight function

$$w(d_i) = \begin{cases} 1-(d_i/r_i)^2, & if \quad d_i/r_i \le 1 \\ 0, & if \quad d_i/r_i > 1 \end{cases} \tag{2.32}$$

Spline weight function

$$w(d_i) = \begin{cases} 1 - 6(d_i/r_i)^2 + 8(d_i/r_i)^3 - 3(d_i/r_i)^4, & if \quad d_i/r_i \le 1 \\ 0, & if \quad d_i/r_i > 1 \end{cases} \tag{2.33}$$

where $d_i = \|x - x_i\|$ is the distance from the sample point x_i to x, and r_i is the smoothening parameter or the bandwidth. The smoothening parameter is an important factor; depending on which the function approximation can widely vary.

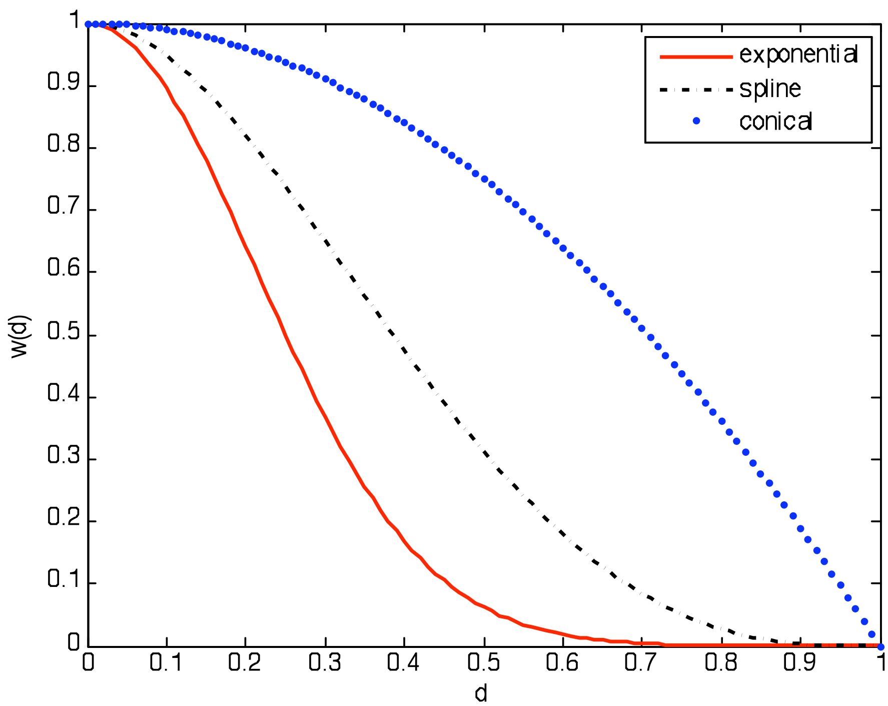


Figure 2. 10 Weight functions [36]

Figure 2. 10 depicts the three types of the weight functions discussed in this section. It is important to note that the shape of the fitted curve is not critically sensitive to the precise selection of the weight function. However, the careful adjustment of the domain influence factor of the weight function is critical so that the interval should contain enough data

points to obtain the regression coefficients. This is important in order to avoid the singularity of the weight matrix.

2.3.3.2 Artificial Neural Networks

2.3.3.2.1 Introduction and Applications

Artificial Neural Networks (ANNs) are processing devices (algorithms or actual hardware) that are loosely modeled after the neuronal structure of the mammalian cerebral cortex but on much smaller scales. A large ANN might have hundreds or thousands of processor units, whereas a mammalian brain has billions of neurons with a corresponding increase in magnitude of their overall interaction and emergent behavior. Neural networks have been used for a variety of applications in the past. Some of them are in Machine Learning [52] and data mining, which include:

- Having a computer program itself so that the programmer doesn't have to write the code by himself. This is achieved by **learning from a set of examples**.
- **Optimization**- Given an objective function and constraints, how do we find an optimal solution?
- **Classification**- How to group patterns of data into classes? For example the United States Postal Service uses a neural network based scanning system to recognize the zip code on addresses.
- **Associative memory**- Recalling a memory based on a partial match, which is analogous to case based reasoning.
- **Regression**- It has been proved that neural networks have an ability to approximate any function given the optimal number of *neurons* in the network.

Because of their robust nature and versatility, ANN's find application in a variety of fields [53]. They have been applied in

- Signal processing: suppress line noise, wit adaptive echo canceling, blind source separation
- Control: e.g. backing up a truck: cab position, rear position, and match with the dock get converted to steering instructions. Manufacturing plans for controlling automated machines.
- Robotics: navigation, vision control.
- Pattern recognition, i.e. recognizing handwritten characters
- Medicine: Storing medical records based on case information
- Speech recognition and production, which helps reading texts aloud.
- Vision based applications like face recognition, edge detection and visual search engines
- Business: Rules for mortgage decisions are made based on the old decisions that produced good results
- Financial applications: time series analysis, stock market prediction
- Data Compression: speech signal, image and faces.
- Game playing: chess, pacman etc.

The simplest computational element for a neural network is called a *neuron*. A neuron can receive inputs from other neurons or from external source. Each input to a neuron has an associated **weight** w, which can be modified to model synaptic learning. The weighted inputs are then summed to form the net input for the activation function f. A neuron computed some function f of the weighted sum of its inputs:

$$y = f\left(\sum x_i w_i\right) \tag{2.34}$$

The output from this neuron can be input into another neuron for making a network. There can be neurons in parallel or series making different layers of neurons that can make a complex network that is able to approximate any function. Most of the times the number of layers and the number of neurons in each layer has to be decided based on the problem at hand. A simple neuron model can be represented as shown in Figure 2. 11.

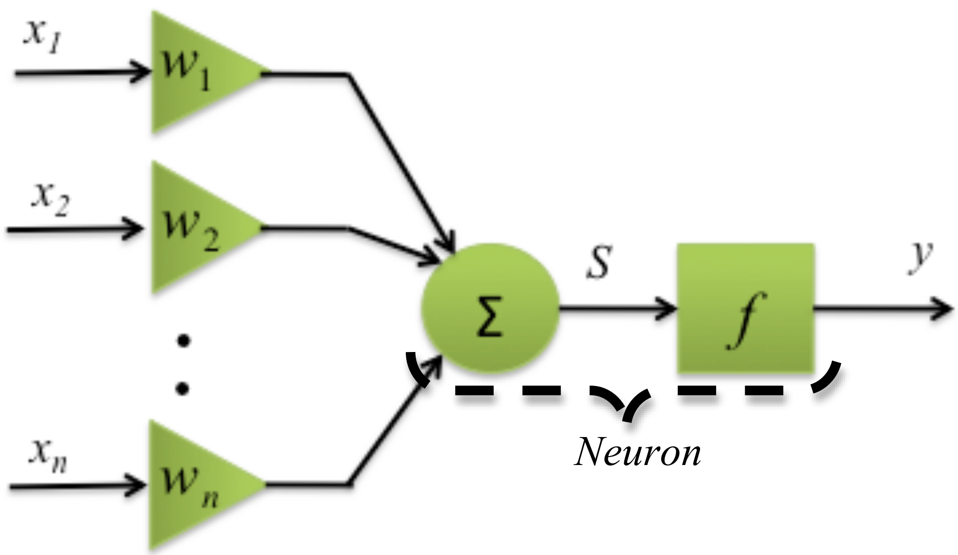


Figure 2. 11 A simple neuron model with n inputs

In Figure 2. 11 the weighted sum $\sum w_i x_i$ is called the net input to neuron unit *i* which is referred to as net_i or the sum *S*.

2.3.3.2.2 Transfer functions

The function *f* in Equation 2.32 is referred to as the unit's *activation function* or *transfer function*. For the simplest case, *f* is the identity function and the unit's output is just it's net input. The neuron in that case would be called a linear neuron. The *Hard-Limit transfer function* and the *Sigmoid transfer function* are the two other most used transfer functions. Each of these transfer functions are shown below with red color. The values of all the transfer functions range from -1 to +1.

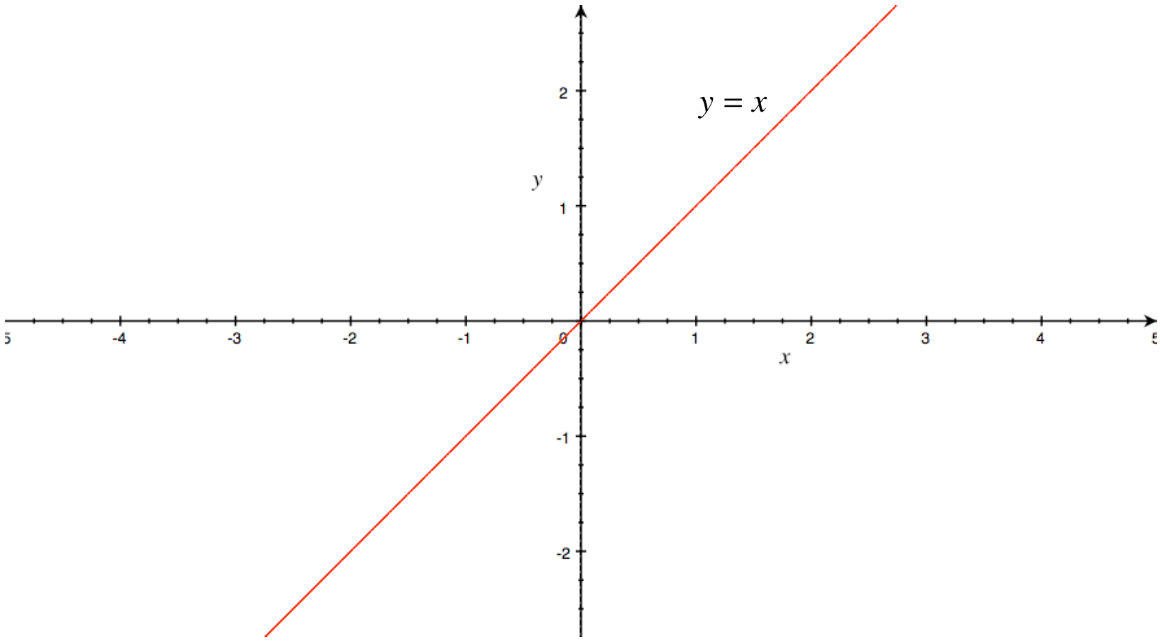


Figure 2. 12 Linear transfer function

The neurons of this type are used in linear filters as linear approximators.

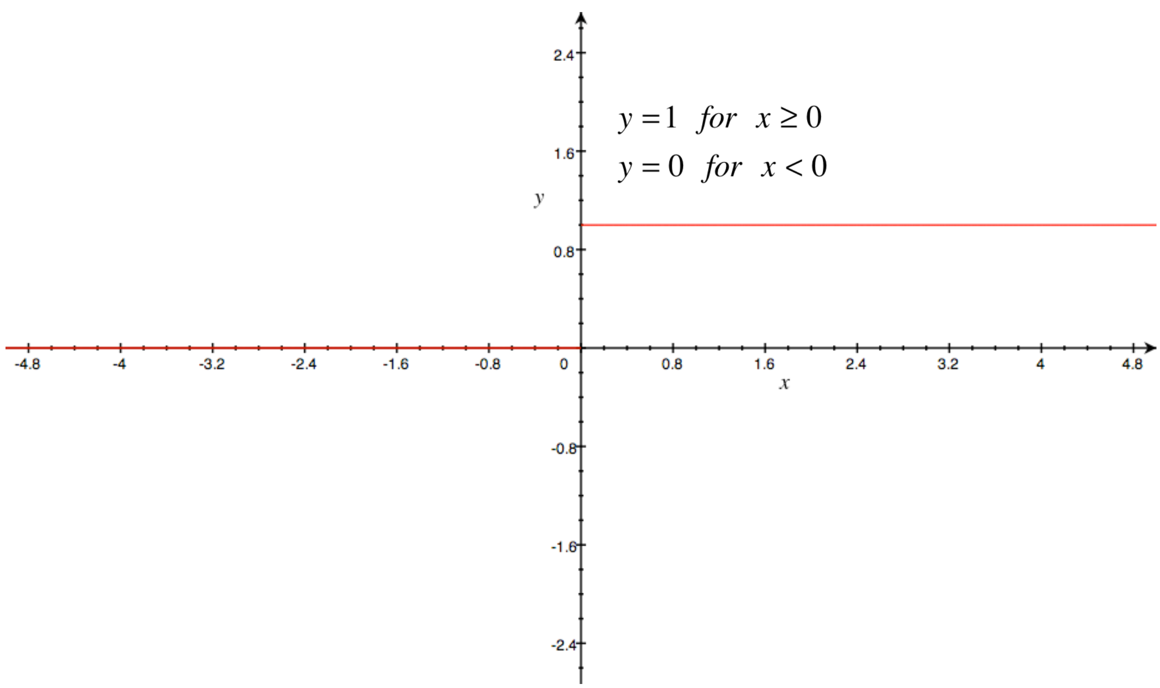


Figure 2. 13 Hard-limit transfer function

The Hard-limit transfer function shown in Figure 2. 13 limits the output of the neuron to either 0, if the net input argument x is less than 0, or 1, if x is greater than or equal to 0. This function is generally used in classification problems pertaining to perceptrons.

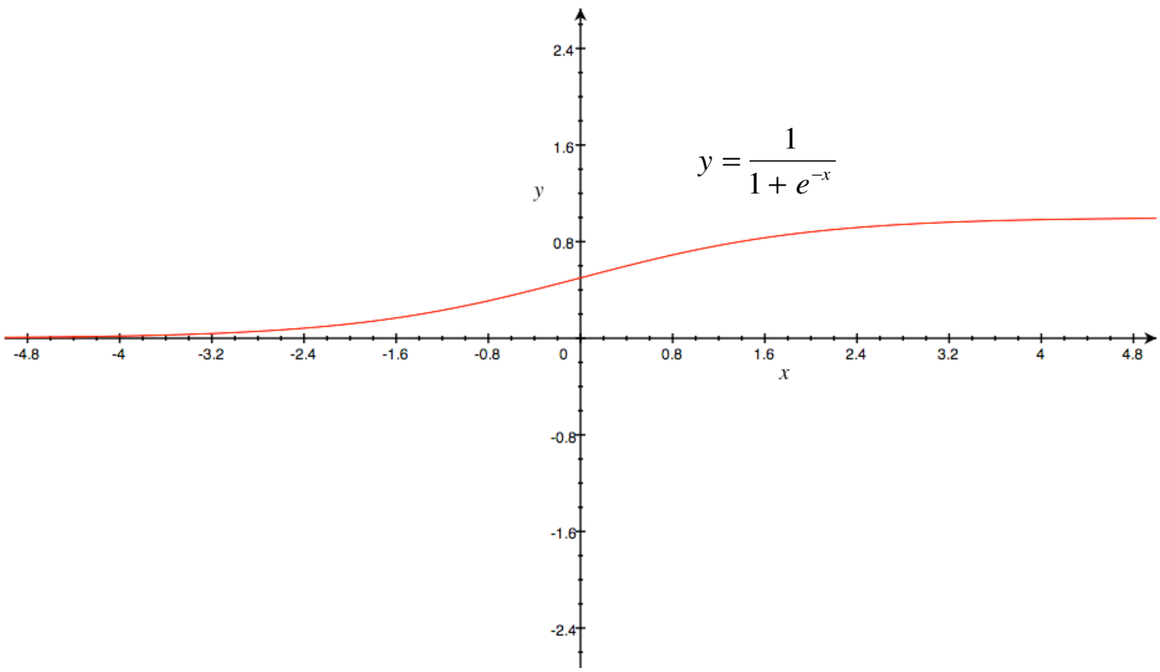


Figure 2. 14 Sigmoid transfer function

The Sigmoid transfer function is differentiable, which makes it suitable for use in backpropagation networks.

2.3.3.2.3 Back Propagation learning algorithm

In general there are many different types of ANNs and usually there is no single architecture that is suitable for all problems. The main types of ANN architectures widely used are *competitive learning*, the *Boltzmann machine*, the *Hopfield network* and the *back propagation network*. The back propagation network type is the most popular due to its simplicity and ease of use. Its name comes from the way it "back-propagates" the error that occurs during the training process. Back propagation network is used for the current research and only think kind of network will be discussed further.

A back propagating (BP) neural network consists of multiple interconnected processing elements belonging to different layers. In a BP algorithm learning is carried out using a set of input training patterns propagated through a network consisting of an input layer, one or more hidden layers and an output layer as shown in Figure 2. 15.

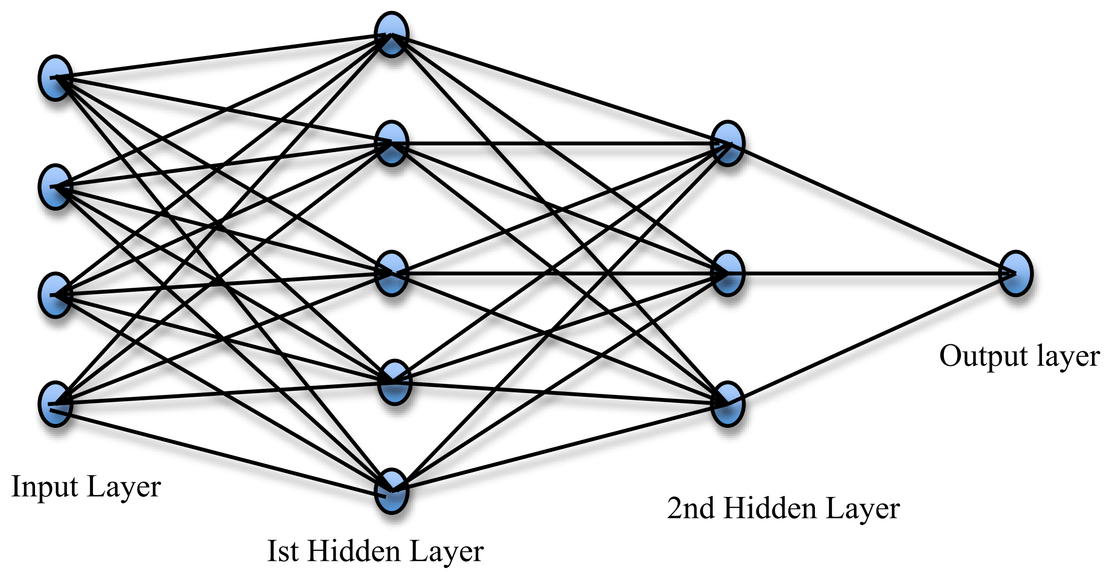


Figure 2. 15 A fully connected ANN configuration

The hidden layers represent complicated association between patterns and propagated data in a feed-forward manner from the input towards the output layer. The number of neurons and the number of hidden layers play an important factor in determining the ability of the network to model complex relationship between Inputs and outputs. In general, increasing the number of neurons and number of hidden layers increases the ability of the network to model nonlinear relationships, which also increases the training time for the network. The number of nodes in the hidden layer(s) is usually selected as the mean value of the number of the input and output nodes plus the input nodes [54]. More sophisticated networks use "dynamic node pruning" or "node growing" in intermediate layer(s).

Most of the neural networks use the gradient descent algorithms, such as least squares, in order to correct the values of the weight connections. This comes as an optimization problem where the difference between the computed and desired output values is minimized. The correction step of the weights mentioned above is generally called as the *delta rule.* Once the network has "learned", it produces different outputs for every set of different inputs it evaluates.

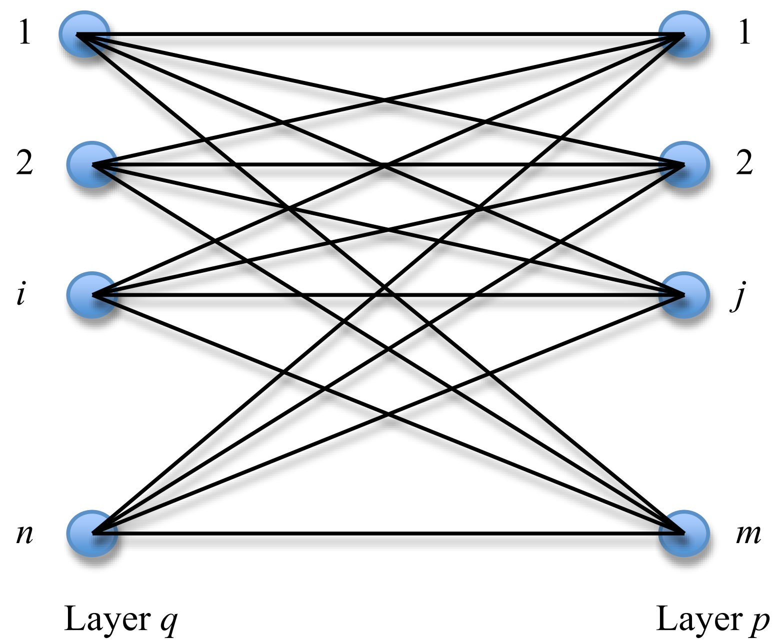


Figure 2. 16 Network layout between two layers with *n* and *m* neurons

Figure 2. 16 shows the connection between two layers of neurons. Let $w_{p,ij}$ be the connection weight between the i neuron in the q(source) layer and the j neuron in the p(target) layer. Let the input signal transmitted from the i neuron of the layer q to the nodes of the target layer p be called $net_{q,\,i}$, and the output produced at the j neuron of the layer p be $net_{p,\,j}$. The exterior inputs x_i corresponds to $net_{q,\,i}$ for the input layer.

In a typical neuron, the output signal is produced only if the incoming signal is strong enough to simulate the neuron. This output is simulated with NN by

$$Out_{p,\,j} = f(net_{p,\,j}) \tag{2.35}$$

where f is an activation function which produces the output at the j neuron of the p layer. The activation function used in this research is the commonly used sigmoid function

$$f(net_{p,j}) = \frac{1}{1+e^{-(net_{p,j}+b_{p,j})}} \quad (2.36)$$

where $b_{p,\ j}$ is a bias parameter which acts as a function shifting term that improves the overall network accuracy. Bias parameters can be learned during the training in the same manner as the other weights. Any random values can be assigned to the weights and bias and during the backpropagation and correction phase the values are improved as the procedure continues. One major advantage of the sigmoid function is that it can handle small as well as large input values. At the output the error can be calculated as the difference between the expected and the actual output value

$$err_{k,i} = tar_{k,i} - out_{k,i} \quad (2.37)$$

where $tar_{k,i}$ and $out_{k,i}$ are the target (expected) and the observed outputs for the node i of the output layer k respectively. The following relationship is used to evaluate the weight changes in the output layer that is related to the input signals.

$$\Delta w_{k,ji} = \eta \ \ \delta_{k,i} \ \ out_{p,j} \quad (2.38)$$

where η denotes the learning rate coefficient usually selected between 0.01 and 0.9 and out $_{p,\ j}$ denotes the output of the hidden layer p. Here, η is analogous to the step size parameter in gradient-based optimization algorithms.

The term $\delta_{k,i}$ is the result of the multiplication of the derivative of the activation function, for the neuron in question, with the error signal that is represented as in Equation 3.39.

$$\delta_{k,i} = df(net_{k,i}) \ \ err_{k,i} \tag{2.39}$$

The derivative of the sigmoid function is given by

$$df(net_{k,i}) = out_{k,i}(1 - out_{k,i}) \tag{2.40}$$

This method can be repeated until the desired error level is reached for the training set. This type of training mentioned above is called *supervised learning*. Only a brief description of backpropagation neural networks was given in the previous section. More detailed explanation of back propagation network and other kind of networks can be found in Ref. [30]

In order for the back propagation algorithm to give satisfactory results the training data has to be chosen carefully. A sufficient number of input data properly distributed in the design space together with the output data resulting from the undergone Finite element analysis is needed for producing satisfactory results in structural optimization problems.

The order to predict accurate structural analysis outputs the ANN has to be trained properly which encompasses three tasks:

1. Selecting the proper training set
2. Finding a suitable network architecture
3. Determining the appropriate values of the characteristic parameters such as the training rate

An important limitation of ANN is that there are no rules for determining the efficient training set, architecture or the training rate. Most of the times the designer has to rely on past experience to determine the appropriate characteristics for the data in hand. Most of the times a hit and trail approach is used.

In this research, in order to reduce the computational requirements of the procedure, backpropagation ANN is used for estimating the probability of failure with the classification approach in the reliability based topology optimization problem. The probability of failure will be estimated using two different approaches in this research:

1. **Regression approach-** In case randomness is introduced in a design variable x and the output from the FEA is y which is used to calculate the limit state, x is the input to the ANN and y is the expected output. A network is trained that can accurately estimate the response y for an input x. The output y can then be used to calculate the limit state and check if it satisfies the safety criteria. By counting the number of times the limit state has been violated, the probability of failure of the structure can be calculated.

   This method will be useful to approximate the limit state value in cases where the limit state is highly nonlinear. The disadvantage of this process lies in the fact that there is no set procedure to decide on the characteristics of the ANN such as the learning rate, number of neurons etc. Another major disadvantage of this procedure is that function approximation/regression gives unsatisfactory (wrong) results if the underlying limit state function is discontinuous. Even in such cases, the regression approach will give us a value for y for which the corresponding x value didn't exist in the *neighborhood* of the training dataset. The *classification* approach could be beneficial in this case.

2. **Classification approach-** Classification is used in case we have to classify the inputs into different classes. In order to determine the probability of failure we have to determine if for the inputs x the structure has failed or not. Then the ratio of the number of times the structure failed and the total number of input data gives us the probability of failure. Hence it should be sufficient to determine if the

structure has failed for the input xi. This implies that it would be sufficient to classify an input xi into either of two classes i.e., pass or fail.

This procedure starts with evaluating the limit state for each of the training data point xi and evaluating the limit state for each of them and checking if the structure has failed or not and assigning a corresponding class to it. This data is supplied to ANN and a network is created which classifies the test data into either of the two classes. By counting the number of elements in the fail class, the probability of failure can be calculated. This procedure is illustrated in the figure below.

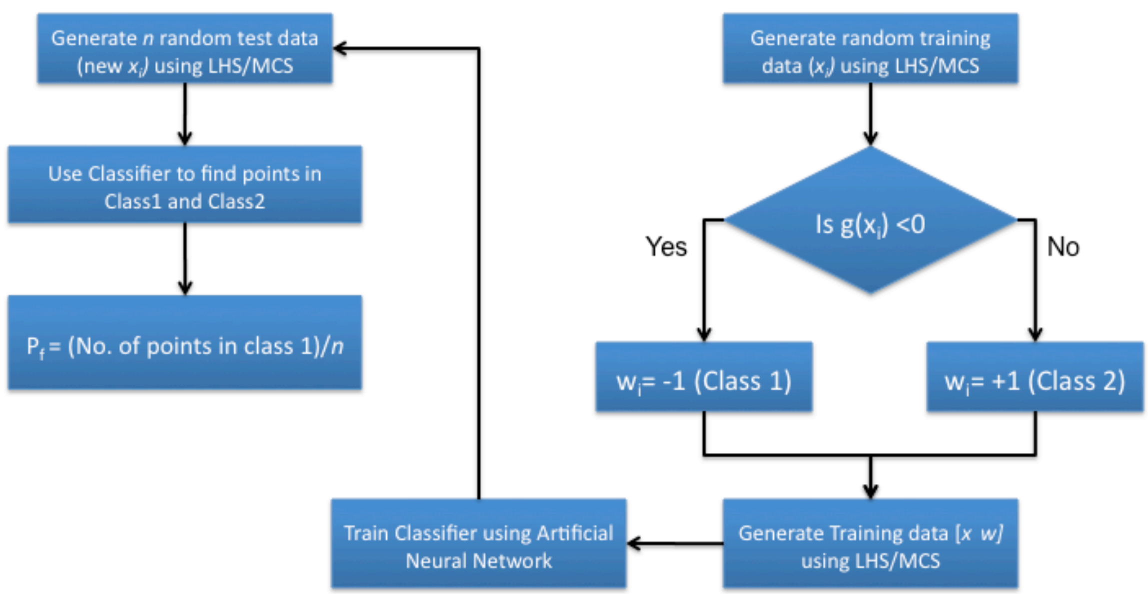


Figure 2. 17 Classification approach to probability of failure calculation

Both the regression approach and the classification approach can be used for estimating the probability of failure for structural reliability assessment. Specifically Artificial Neural Networks can be used for both the regression approach and the classification approach. The back propagation neural networks can be used for both the classification and well as the regression approach. In cases where the data is not linearly separable Probabilistic Neural Networks (PNN) can be used in order to classify the data.

The main differences between the regression approach and the classification approach of reliability analysis have been summarized in Table 2.

Table 2 Difference between the classification and regression approach to reliability analysis

Classification	*Function Approximation*
It is aimed at estimating the limit state function.	It is aimed at estimating the performance function.
Can be useful for estimating P_f even in case of disjoint failure domains.	Can be useful for calculating P_f in case of highly nonlinear functions.
Flexible and adaptive, hence less sensitive to the experimental plan used.	Sensitive to the experimental plan used for training.
May require more data points for training	Requires less data points

Classification can be used to calculate the probability of failure in case of disjoint failure domains. However, a classification process using artificial neural network might be computationally more expensive than the regression approach. Hence in case of large-scale problems function approximation using regression approach should be tried first in order to reduce the computation cost of the process.

CHAPTER 3

EFFICIENT RELIABILITY-BASED TOPOLOGY OPTIMIZATION

3.1 Reliability-based Topology Optimization of Truss Structures

3.1.1 Problem Formulation

In order to design reliable mesostructured materials a reliability based topology optimization procedure can be effective. In designing a structure using RBTO method it is wished that the new design were reliable enough to have acceptable performance in case the structure is exposed to expected uncertainty after it is manufactured and placed "*in the field*". "In the field" indicates the location for which the structure was designed. A simple reliability based topology optimization problem for minimizing mean compliance can be represented as

Minimize: *Mean Compliance* (3.1)

Subject to: $P_j[g_j(b,X)<0] \le P_{Rj} \qquad j=1,\ldots\ldots,m$ (3.2)

$$\sum_{i=1}^{N} A_i L_i - V^* \le 0 \tag{3.3}$$

$$A_l \le A \le A_u \tag{3.4}$$

$$Ku = F \tag{3.5}$$

where *g(.)* is the limit state function and P_{Rj} is the target probability of failure P_f of the structure after optimization. For practical applications this P_f value is set to 10^{-4}. A_i and L_i are the area of cross section and length of each truss element in the super structure respectively. Equation 3.4 represents the bounds on the design variables, which are areas of cross sections for this design problem. It is desirable to specify the lower limit on the design variable as a low number instead of 0 i.e., 10^{-3}~10^{-6}, in order to preserve the numerical stability of the optimization process. Equation 4.2 is commonly referred to as the *volume constraint*. Here V^* is the final target volume for the structure. A general rule of thumb is to specify the V^* as 30% of the initial volume of the structure before optimization i.e., the volume of the structure initially if all the elements had the maximum possible value for each of the design variable. In other words the required *volume fraction* could be specified as 0.3. Hence Equation 3.2 can also be specified in terms of the volume fraction and some designers prefer the volume fraction approach. Equation 3.5 represents the Finite Element Method, which is used to compute the objective function and the constraints. The objective function for this optimization problem is the minimization of mean compliance. Mean compliance is the total work done on the body by all external forces, which includes body forces, point forces and contact forces. According to Clayperon's theorem [55] the mean compliance of a body is half of the strain energy contained in the body. Hence, Equation 3.6 can further substitute Equation 3.1.

Minimize: $$SE = \frac{1}{2} u^T K u \tag{3.6}$$

In Equation 3.6 *SE* represents the Strain Energy of the structure, *u* represents the displacements of nodes in the structure and *K* is the global stiffness matrix of the structure. The displacement vector *u* is obtained after the finite element analysis of the structure.

3.1.2 Proposed framework using Local regression method

The proposed framework for designing optimal mesostructured materials is depicted in Figure 3. 1. First, the geometry of the super structure is specified with other input parameters such as material properties, loading and boundary conditions and corresponding statistical properties of the random variables. In this research two kinds of superstructures are used- *ground structure* and *unit cell*.

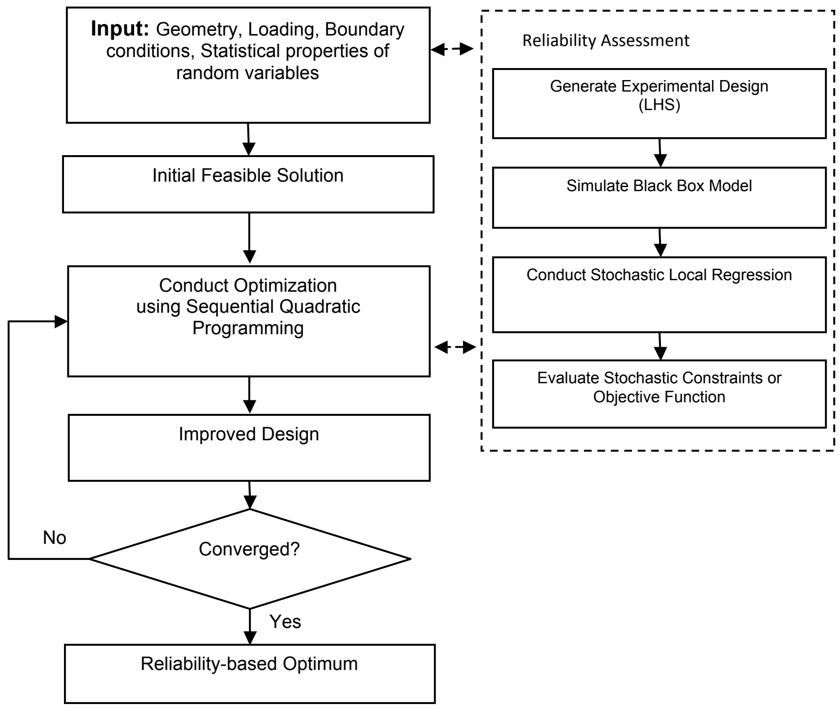


Figure 3. 1 Proposed framework using local regression for surrogate model

During the iterative optimization process, a nested loop computes the probabilistic constraints. The reliability constraint (Equation 3. 2) specifies the allowable probability of failure in the structure. In the nested loop, the uncertain input parameters are sampled using a stratified sampling technique such as Latin Hypercube Sampling (LHS). For each instance of the random variables, the FEA procedure is invoked. The results from the FEA procedure are used to evaluate the probabilistic constraint or specified limit state function. The limit state function is in turn predefined by the user and states if the structure has failed for that particular instance of random variables and other boundary conditions. In order to reduce the computational cost and improve the overall efficiency of the optimization procedure, the local linear regression method is utilized. Once the limit state function is modeled using the local regression procedure, the crude Monte Carlo Sampling (MCS) is applied to estimate the probability of failure of the constraints. This reliability assessment procedure can be readily integrated into the conventional optimization process. The final optimum design will be achieved when the required convergence criterion is satisfied.

3.1.3 Proposed framework using Classification-based ANN

The limit state function used in the previous section was a linear function of displacement of a single node. In practical applications it's rare to find a failure criteria, which is linear. Hence it is important to closely examine the function approximation methods that rely on simple curve fitting methods to estimate the probability of failure. One major complaint in case of function approximation techniques relying on regression based methods is the curse of dimensionality [30]. Hence it becomes necessary to investigate the use of other methods in order to estimate the response. In this research classification using neural networks is proposed as a useful alternative in determining the probabilities of failure in case when sampling methods are used for the estimation.

3.1.3.1 Classification

Statistical classification is a procedure in which individual data points are placed into groups based on quantitative information on one or more characteristics inherent in the data points and based on training set of previously labeled data points [56].

Formally, the problem can be stated as follows: given training data $\{(x_1, y_1), \ldots, (x_n, y_n)\}$ produce a classifier $h : X \rightarrow Y$ which maps an object $x \in X$ to its true classification label $y \in Y$ defined by some unknown mapping $g : X \rightarrow Y$ (ground truth). For example, if the problem is filtering spam, then x_i is some representation of an email and y is either "Spam" or "Non-Spam". Statistical classification algorithms are typically used in pattern recognition systems [57].

In analogy to the previous example, in case of Reliability-based Topology Optimization for estimation of the probability of failure, x_i is the random variable, which was assumed to have uncertainty. The values of x_i are generated from a probability density function (pdf) for which the designer provides the mean and variance to the optimization algorithms. The estimation in this case is w which has a value of -1 if the structure fails and has a value of +1 if the structure is safe for the generated x_i values. The points having a value of -1 for w can be considered to be from class 1 and those with value of +1 can be considered to be from class 2. Once w_i's are obtained for all x_i's the classifier is trained using artificial neural networks. n random numbers are generated using Latin Hypercube Sampling and new w is estimated for each of the new samples. The ratio of the number of points in class 1 and n gives the probability of failure P_f. This process is illustrated in Figure 3.2.

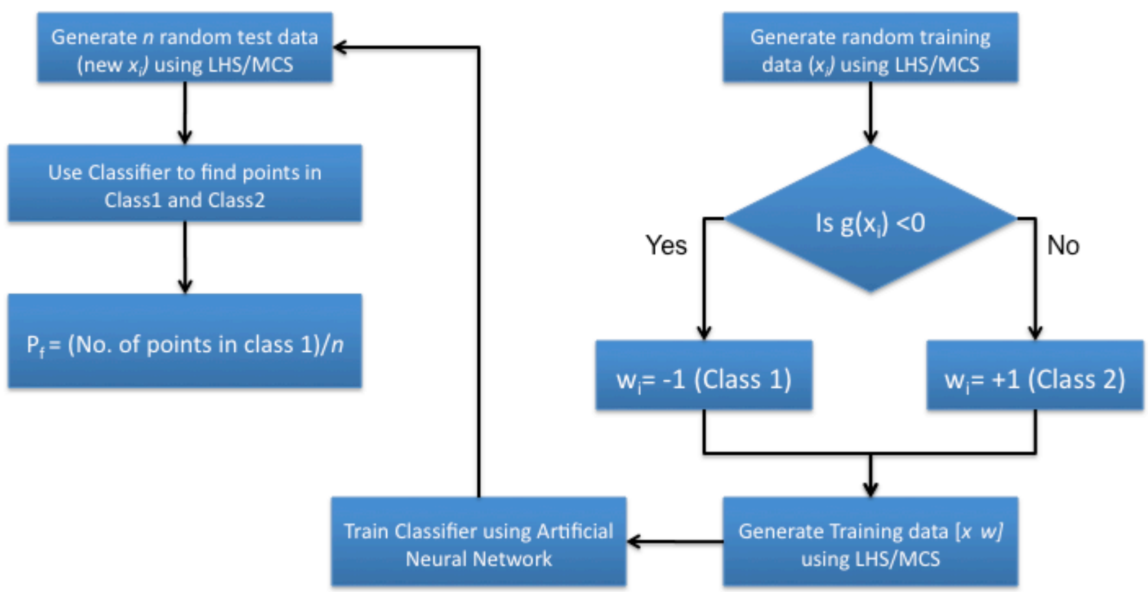


Figure 3. 2 Procedure for classification scheme

3.1.3.2 Classification using Artificial Neural Networks

Traditional statistical classification procedures such as discriminant analysis are built on the Bayesian decision theory [58]. In these methods, a probability model must be assumed in order to calculate the posterior probability upon which the classification decision is made [59]. Hence, the validity of the underlying assumptions is important for these methods to work properly. A good depth of knowledge in both data property and model capabilities is essential in order to use these methods properly.

Predictive learning is an important aspect of data mining. A wide variety of methods have been created for classification from which Artificial Neural Networks (ANN), Support Vector Machines (SVM), Decision Trees, Multivariate Adaptive Regression Splines (MARS), k- Nearest Neighbors and Kernel methods [30] have been used widely for varied applications. For each particular method there are situations for which it is particularly well suited, and others where it performs badly compared to the best that can be done with that data. Table 3 summarizes the characteristics of a number of classification techniques.

Table 3 Some characteristics of different learning methods, Key: 1=good, 2=fair, 3=poor [16]

Characteristic	**Neural Nets**	**SVM**	**Trees**	**MARS**	**k-NN, kernels**
Natural handling of data of "mixed" type	3	3	1	1	3
Handling of missing values	3	3	1	1	1
Robustness to outliers in input space	3	3	1	3	1
Insensitive to monotone transformations of inputs	3	3	1	3	3
Computational scalability	3	3	1	1	3
Ability to deal with irrelevant inputs	3	3	1	1	3
Ability to extract linear combinations of features	1	1	3	3	2
Interpretability	3	3	2	1	3
Predictive power	1	1	3	2	1

In general, the data obtained in industries or from commercial organizations are not complete and may also have missing values. In addition sometimes the data can be a mixture of categorical, quantitative and binary forms and hence difficult to interpret. Sometimes the data might also have a lot of outliers. In order to deal with these specific situations domain specific knowledge is required to filter out data that is not relevant to the problem at hand. But apart from the specific applications like pattern recognition, domain specific knowledge is difficult to obtain. In such cases "decision trees" have been suggested as an "off-the-shelf" technique that can be applied to the data without requiring a great deal of time consuming data preprocessing or careful tuning of the learning procedure [30]. Decision trees naturally deal with numerical and categorical data and also with missing predictor variables. They are also immune to predictor outliers and also immune to scaling and other general transformations. But Decision Trees suffer from inaccuracy in prediction (as can be seen in Table 3) making them inappropriate for many applications. On the other hand Neural Net, SVM and k-NN along with kernel methods perform well for prediction applications but don't perform well when dealing with data that is not preprocessed.

Neural networks have emerged as an important tool for classification. Various research have proved that ANN's [60] are a promising alternative to conventional classification techniques. Michie *et al.* [61] report a comparative study in which three general classification techniques of neural networks, statistical classifiers and machine learning using 23 techniques on 20 different real data sets. The general conclusion drawn from the study was that no single classifier is the best for all datasets. However, the feed forward and backpropagation ANN's have good performance over a wide range of problems. Artificial Neural Networks have also been compared to *decision trees* [60, 62], *discriminant analysis* [60, 63], *CART* [64, 65], *k-nearest–neighbor* [63, 66], and *linear programming* [63].

The advantages of neural networks above other methods are in the following theoretical aspects:

- Neural networks can be used as black box models since they are data driven and self-adaptive in nature. Hence they can adjust themselves to the data without any explicit specification of functional or distributional form for underlying model.
- Neural Networks have been proved to be able to approximate any function with arbitrary accuracy [67-69]. Since all classification procedures seek a functional relationship between the independent variable and the feature, this attribute is essential for the success of the classification procedure.
- Since Neural Networks are nonlinear in nature it makes it easier to model real world data complex relationship.
- Neural networks are able to estimate the posterior probabilities, which provides the basis for estimating classification rules like Bayes classification rule and perform statistical analysis [70].

Owing to above advantages, classification procedure using ANN’s have been used for bankruptcy prediction, bond rating, medical diagnosis, product recognition, handwritten character recognition and speech recognition applications. In case of reliability based design optimization problems the designer is faced with cases where the limit state function is nonlinear or discontinuous. In addition to discontinuities, nonlinear problems are characterized by disjoint failure regions, thus further limiting the use of classical approaches to assess the probabilities of failure [71]. Classification procedure can resolve all of these situations. Hence a classification based RBTO procedure using Artificial Neural Networks can be used for estimating the probability of failure.

3.1.3.3 Example of a two variable limit state function

Consider a limit state function with two random variables

$$g(u_1, u_2) = u_1 u_2 - 1 \tag{3.12}$$

where u_1 and u_2 can be any of the variables that are outputs of the finite element analysis. In case of this limit state function the structure is considered to be safe if $g(u_1, u_2) < 0$ and the structure is considered to have failed if $g(u_1, u_2) > 0$.

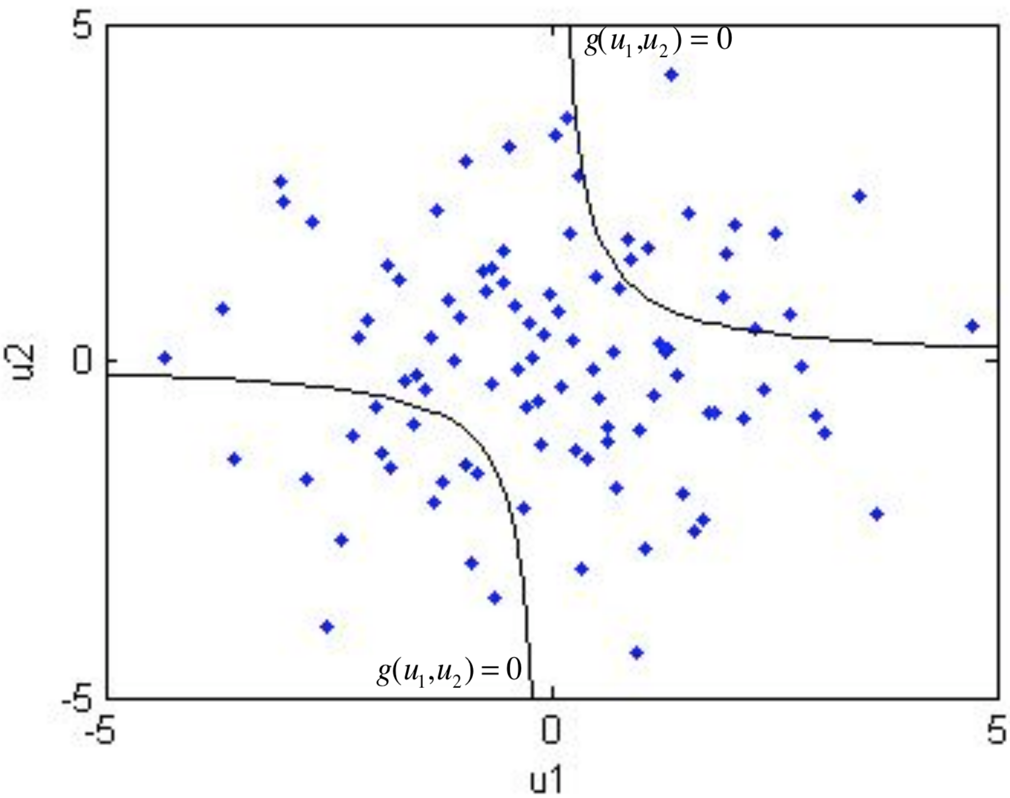


Figure 3. 3 Sampling space for evaluating the limit state function

Figure 3.3 shows the boundary of the limit state function $g(u_1, u_2)$ in black and the sampled data points in blue. The design variables u_1 and u_2 are sampled using Latin hypercube sampling method from a Gaussian distribution $\sim N(0,9)$. 100 points were sampled and classified according to their relative position in the *u1 vs. u2* space shown in Figure 3. 3.

A *probabilistic neural network* based ANN was used to classify the data points depending on whether they fall into the failure region or the safe region. Probabilistic neural networks (PNN) are a kind of radial basis network suitable for classification problems. This network has *radial basis* neurons for which weighted inputs are calculated using the Euclidean distance of the data point from the origin. Gaussian radial functions were used in this case which are given by

$$\varphi(r) = \exp\left(-\beta r^2\right) \text{ for } \beta > 0 \tag{3.13}$$

where $r = \|x - c_i\|$ and c_i is the center associated with this radial basis function. More information about radial basis networks and probabilistic neural networks can be found in Ref. [72].

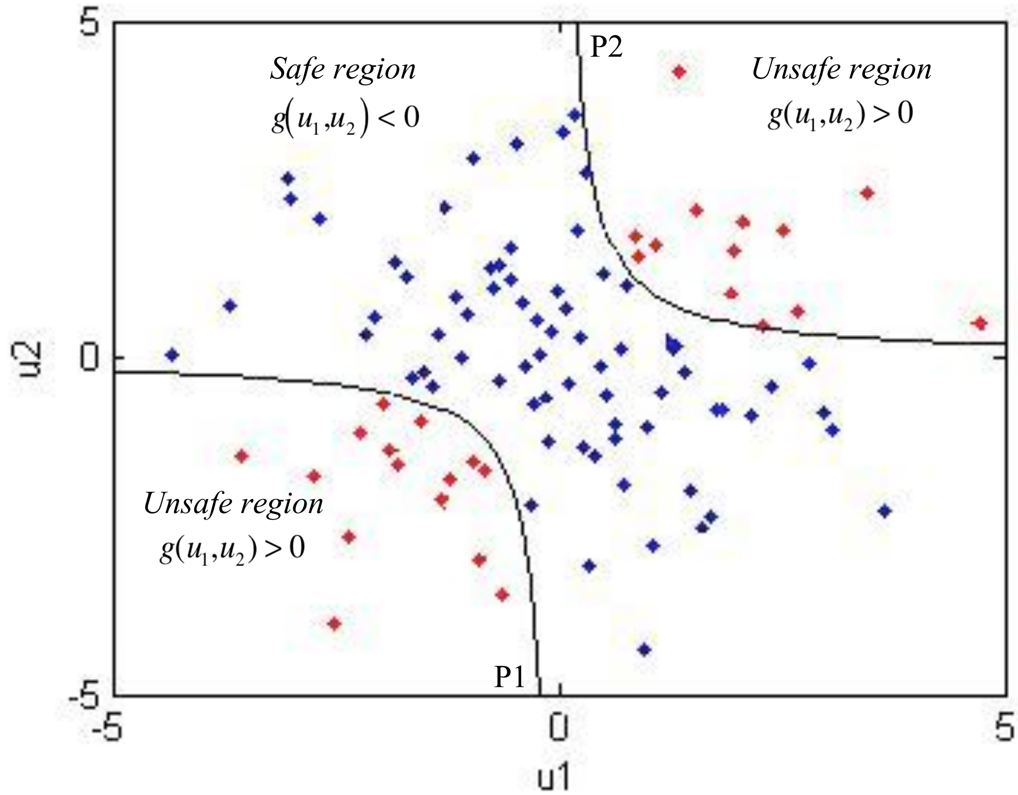


Figure 3. 4 Data points classified into *safe* and *unsafe* regions

This example problem was solved in MATLAB and the classification solution is shown in Figure 3. 4. The points in the safe region are in blue and those in the unsafe region are in red.

In order to validate the efficacy of the proposed method a Monte Carlo Simulation is conducted with 10,000 samples. The probability of failure is calculated from these 10,000 samples of MCS. This is done in order to validate the results obtained from the classification-based framework for calculation of probability of failure. The result obtained from the MCS is compared to the result obtained by both classification using ANN and local regression. The results are shown in Table 4.

Table 4 Results from the disjoint failure domain example

	Classification (200 Samples)	**Local Regression (200 Samples)**	**MCS (10,000 Samples)**
P_f	0.3452	0.5412	0.3566

The results confirm that classification gives close results in case of disjoint failure domains since the P_f value obtained from Classification is close to that obtained from MCS.

An important conclusion from the last example problem is that classification can be used to label points as fit/unfit better than estimating the function using a non-parametric techniques [30] and then calculating the probability of failure. Another advantage of using classification based approaches against the regression based methods is that regression based methods can't be used when the limit-state function is discontinuous. For example, if $g(u_1, u_2)$ were to be estimated using regression based methods, points P1 and P2 would have been joined since regression functions can't recognize the discontinuity pattern after point P1 and before point P2 in Figure 3.4.

3.1.3.4 Proposed framework for Classification based RBTO method

The previous section proved that classification could be an effective technique to calculate the probability of failure during the optimization procedure. Figure 3. 5 shows the framework for conducting Reliability-based Topology Optimization using an Artificial Neural Network for conducting classification.

As with the RBTO method using moving least squares local regression method that was discussed before, RBTO using artificial neural network has the same basic information flow. An initial geometry (ground truss or unit cell), force and boundary conditions, and statistical properties of the random variables have to be specified. Along with this a starting initial guess is required for the algorithm to proceed. The reliability constraint is then evaluated for a small number of samples generated using Latin Hypercube Sampling. Each of these data-points is then marked as safe/unsafe depending on whether the limit state function was satisfied. This data is the training data for the ANN. Once the network is trained data points are generated using Monte Carlo Sampling (MCS) method and these values are projected on the network to check whether a data point represents a safe design or a design that can fail when it is exposed to uncertainty. Hence, the network classifies the data into the two classes. The ratio of the number of data points in the fail class and total number of data points gives the probability of failure. Once the P_f value is calculated, the optimization algorithm updates the design and marches along the steepest gradient towards the optimum. The convergence criterion specifies if the required optimum is reached. If an optimum is reached then the final value of the design variables is the required solution. Figure 3. 5 shows a flowchart for the discussed framework.

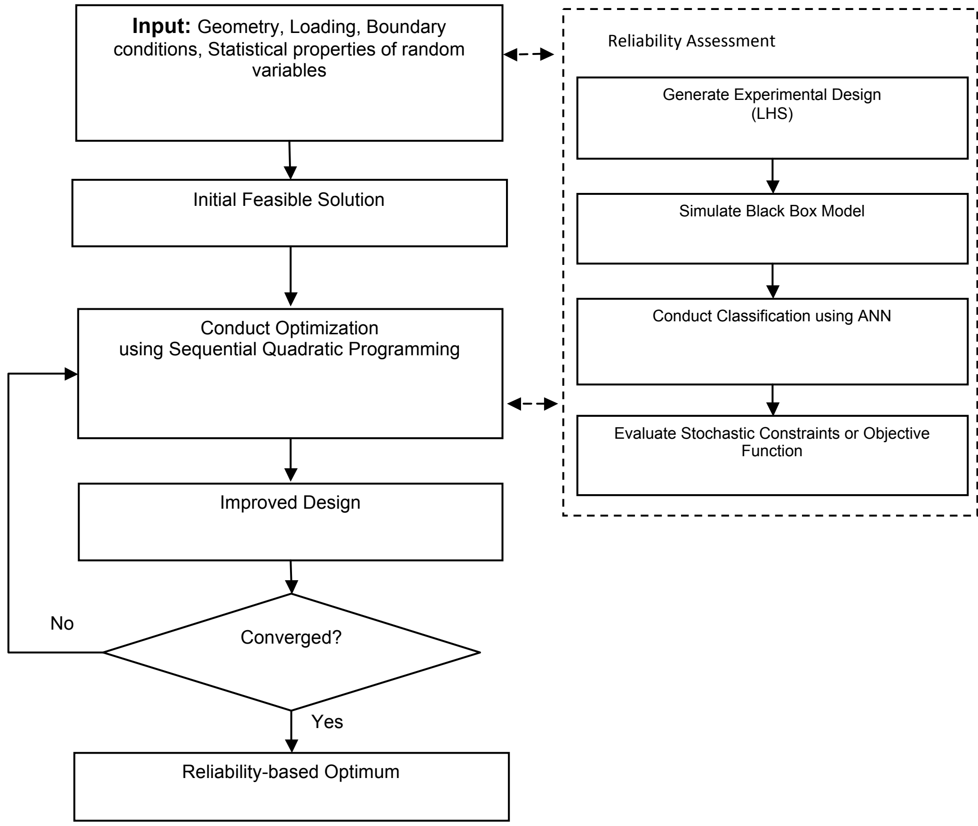


Figure 3. 5 Framework for RBTO using classification based RBTO

In case there is no prior knowledge of the limit state function it can be better to use the simulation based methods for reliability assessment since simulation based methods can handle discontinuous limit state functions as well as multiple limit state functions at the same time. To emphasis this feature of classification algorithms an example problem involving multiple limit state functions is solved next using probabilistic neural networks.

3.1.4 Overall Framework

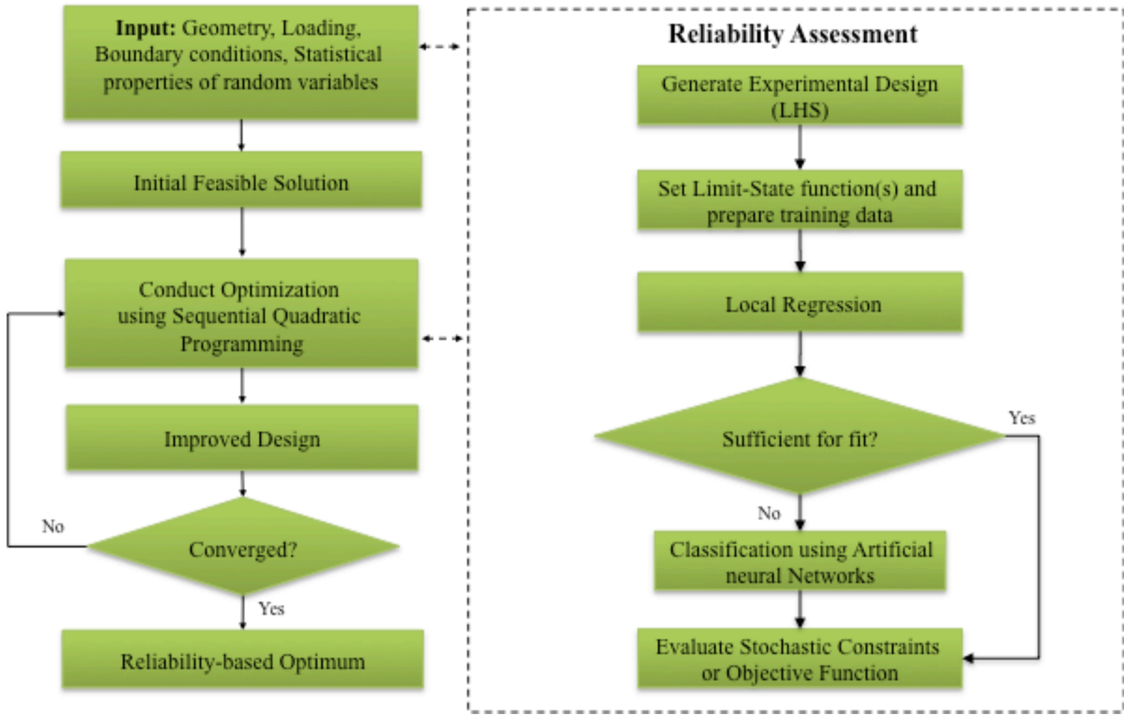


Figure 3. 6 Overall framework

The overall framework for Reliability based Topology Optimization can be represented as in Figure 3. 6. This framework combines the efficacy of Moving Least Squares Local Regression method and the Classification procedure using Artificial Neural Networks. In the reliability assessment part of the algorithm, after the evaluation of the limit state function and preparing training data Local regression is used for constructing the surrogate model for evaluating the reliability constraint. The fit of local regression is then checked using the R^2 statistic. If the value of R^2 is acceptable then the reliability constraint is evaluated using samples generated using MCS. In case the value is not acceptable classification using artificial neural network can be used. The classification procedure using artificial neural networks is relatively more computationally expensive than the local regression procedure. Hence it is used only if the local regression procedure fails to give satisfactory results.

One possible reason for not getting a good fit with local regression is in case of disjoint failure domain. The case of disjoint failure domain can be effectively encountered by classification approach as described in the previous sections. Hence this overall framework combines the effectiveness of both the local regression procedure and the classification based Artificial Neural Networks procedure.

This framework has been validated with the design of a hydrogen tank in the next section. The hydrogen tank is designed according to the design objectives for 2010.

CHAPTER 4

EXAMPLES

4.1 Stiffest Structure Design Problem

The stiffest structure problem, namely the minimization of compliance (maximization of stiffness) for a given total mass of the structure, is considered to show the efficacy and applicability of the developed framework. The objective function in this case is the minimization of strain energy for the structure when the cross-sectional areas are the design variables. A volume constraint specifies the maximum amount of material that can be used for the layout of the truss structure. The optimization statement for the ground structure example is represented as

Minimize: $$SE = \frac{1}{2} u^T K u \qquad (4.1)$$

Subject to: $$P_j \left[g_j(b,x) < 0 \right] \leq 0.0001 \qquad (4.2)$$

$$\sum_{i=1}^{N} A_i L_i - V^* \leq 0 \qquad (4.3)$$

$$A_l \leq A \leq A_u \qquad (4.4)$$

$$Ku = F \qquad (4.5)$$

Figure 4.1 represents a ground truss with three nodes on all four sides. The ground truss structure contains nine nodes in total and all nodes are pin-connected to each other with truss elements. The number of truss elements is 28. The boundary conditions of the nodes of the bottom part are fixed and a force of 100 N is applied at the top-right node. The length of each side of the square shaped ground structure is 100 mm and the Young's modulus of the material used for the structure is assumed as 2.1×10^5 N/mm^2 with a Poisson's ratio of 0.3. The upper bound on the cross-sectional area is taken as 10

mm^2 and the lower bound is taken as 10^{-4} mm^2. The cross sectional area is used as the design variable for this problem.

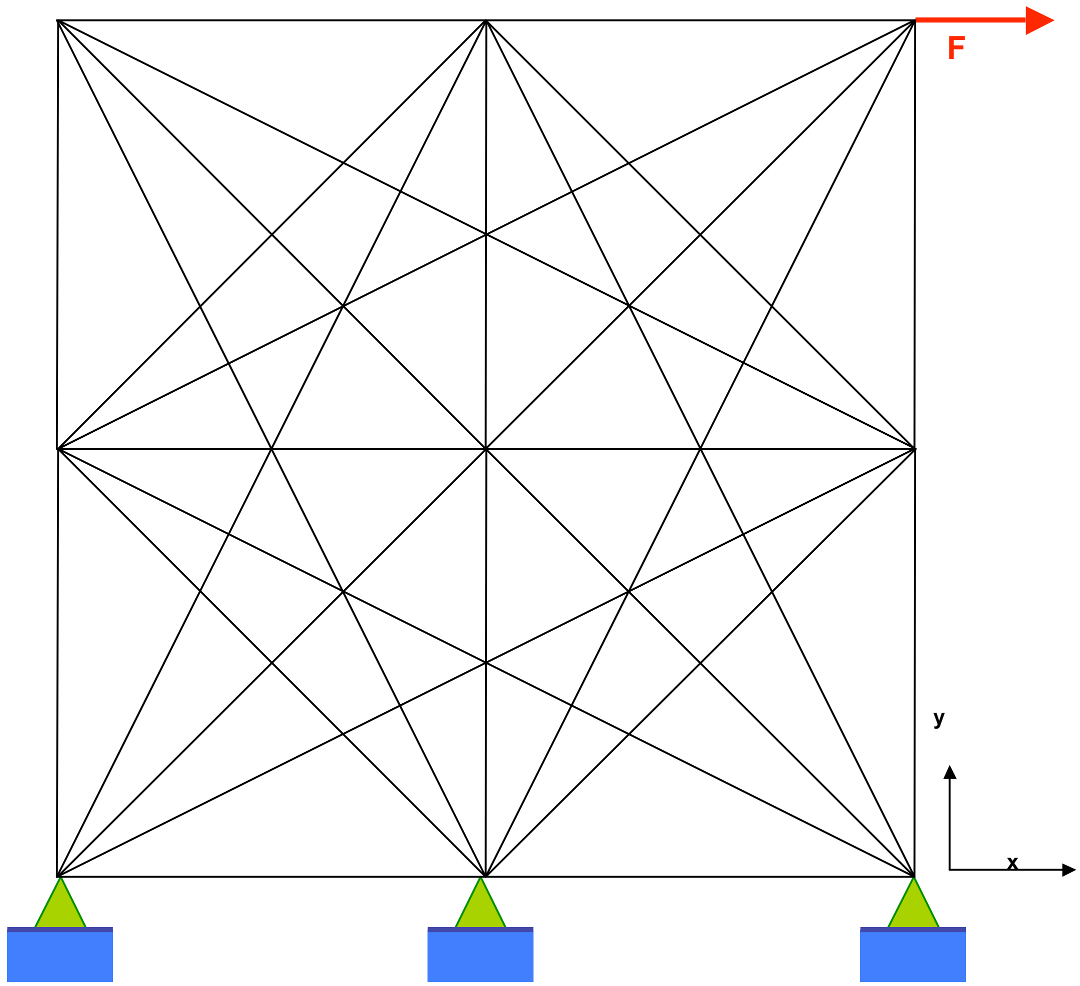
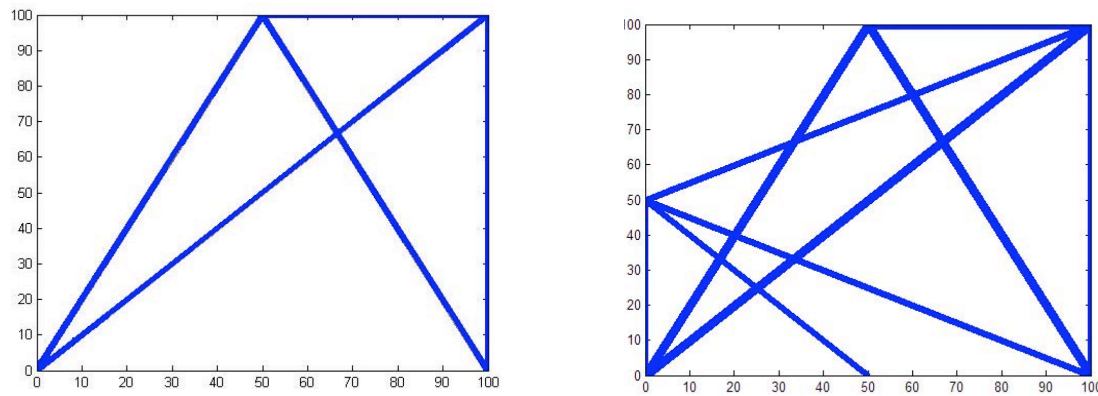


Figure 4. 1 Representation of a ground truss structure for solving stiffest structure problem

Figure 4. 2(a) shows the optimum truss structure for the deterministic case, which does not include the reliability constraint as shown in Equation 4.2. Five truss elements are retained in the final solution. All the truss elements have a cross-sectional area at the upper limit of 10 mm^2. The rest of the truss elements converged to the lower bound. This

optimization problem was solved using the Sequential Quadratic Programming (SQP) method. As the number of elements are increased corresponding to the increase in the number of nodes in the x- and y-axes the time taken for convergence increases exponentially. This structure does not guarantee to resist failure in the wake of uncertain boundary conditions and material properties. For a truss structure to resemble a material design, the material structure should be able to endure various boundary conditions in the wake of uncertainty.



(a) Deterministic optimum (b) Stochastic optimum

Figure 4. 2 Optimum solutions

For the stochastic optimization case, all the given conditions are the same as the deterministic problem except for the consideration of the reliability constraint (Equation 4.2). The applied force, *F*, is considered as the random variable. It is assumed to be normally distributed, *F~N* (100 N, 15 N). To consider the constraint of the probability of failure, the limit state function is taken as the displacement, *u*, in the positive *x*-direction at the top-right node; namely, *g(u)*= (*u* - 0.013) meters. The structure is said to have failed if *g(u)* > 0. The target probability of failure level is chosen as, $P_f = 10^{-4}$ in Equation 4.2. 200 samples were generated using LHS, which would represent variable force on the top right end node of the ground truss. The displacement at the top-right end node is calculated using the FEA for the 200 cases. In order to estimate the system response for subsequent cases a surrogate model is created using the local regression method. The probability of failure was calculated based on the number of displacement values for which $g(u) > 0$. The displacement values were calculated by projecting the 10,000 force values that were sampled using MCS on the local linear regression surface. The optimization problem was solved using SQP method and the optimized solution is shown in Figure 4. 2(b). The stochastic procedure distributed material in a wider space and contains more truss elements than the deterministic procedure. A higher number of truss elements connected to the point of application of the force helps to distribute the varying load more effectively. The obtained stochastic solution has a P_f value of 0.8×10^{-4} which represents a 53.6 % decrease in P_f value from the deterministic solution. This decrease in P_f value resulted in a 39.16 % increase in the volume of material compared to the volume used in the deterministic solution. Specifically, the deterministic solution resulted in a volume of $7.3\text{x}10^2$ mm^3 while the stochastic solution resulted in a volume of $1.203\text{x}10^3$ mm^3. Hence based on the design requirements, a more reliable structure can be designed using RBTO method while using some more material than that is required for the deterministic optimization method.

4.2 Hydrogen Storage Tank Design

With the depleting oil resources and the increasing concern for the environment, the focus for research in the automotive, marine, and aerospace industries has been on alternative fuels. A promising energy source that has had the attention of many researchers is hydrogen. Hydrogen has shown to be a high rated alternative to gasoline by providing lower emission levels, high efficiency, and it can be produced and consumed continuously. The two common methods for using hydrogen as an energy source is as a fuel cell to produce electricity, which is in turn, used to power an electric motor or as a hydrogen powered combustion engine similar to the traditional gasoline engine. For both methods, there exist technical difficulties in the use of hydrogen for commercial-level products. For instance, hydrogen has about three times greater energy content by weight than gasoline, but around four times less energy content by volume. For this reason, it is a difficult task to store hydrogen within the size and weight constraints for vehicular applications. One of the most technically difficult tasks impeding widespread use of hydrogen as an energy source is developing safe, reliable, compact, and cost-effective methods for storing hydrogen. Hydrogen-powered cars must be able to safely store sufficient amounts of hydrogen to travel more than 300 miles between fills in order to be competitive with conventional vehicles [73, 74]. This is a challenging task due to the significant amount of space required to store enough quantities of hydrogen. For light-duty vehicular applications the available compressed hydrogen tanks are larger and heavier than necessary. A higher amount of hydrogen is able to be stored in liquefied hydrogen tanks as compared to compressed hydrogen storage; however energy is required to liquefy hydrogen and the required tank insulation has large impact on the weight and allowable volume of hydrogen stored. As well as different methods for storing hydrogen, there is an urgent need to create concepts for conformable high-pressure hydrogen tanks to cope with the difficulties in packaging conventional cylindrical tanks.

A possible solution to the above mentioned problems with compressed hydrogen storage tanks is the design of a storage tank utilizing mesostructures within the tank wall as structural support. Since the tank is represented as a cylinder with constant radius with two hemispherical ends, analysis can be performed on half of the tank. In addition, given that the internal pressure, P, of the tank acts equally throughout the internal surface, the analysis will be reduced to the optimization of a single 3D unit cell as shown in Figure 4. 3.

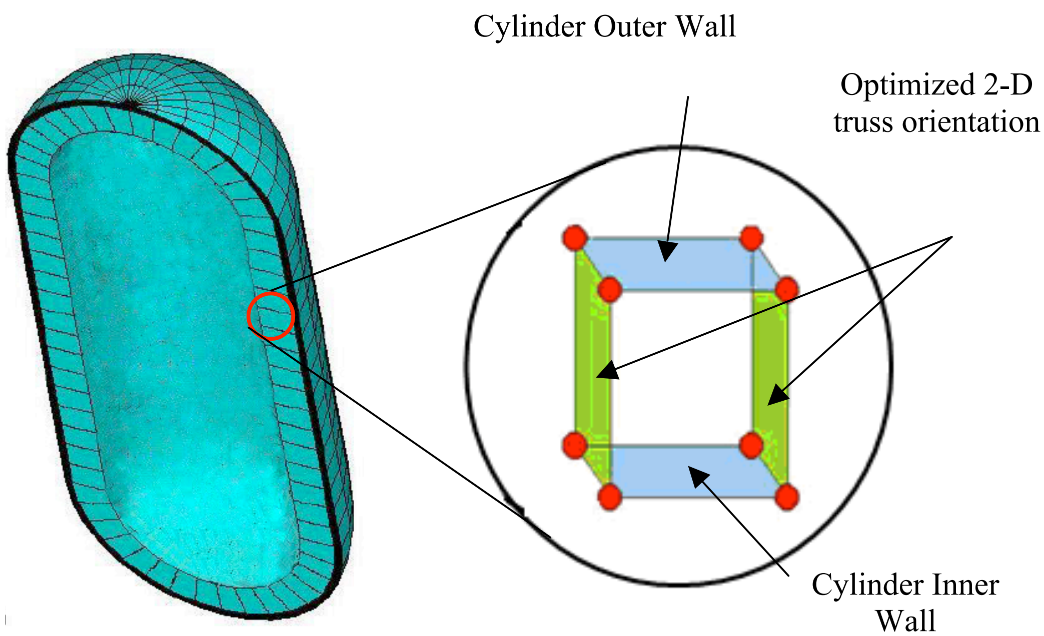


Figure 4. 3 Geometrical assumptions for designing the hydrogen tank

This assumption allows one to utilize the reliability based topology optimization model described previously. Since this model is used on a 2D unit cell, the optimized unit cell from the analysis is assumed to be the optimal cell, which is parallel to the cross-section of the cylindrical portion of the tank. This results in the creation of a 3D unit cell that is then copied throughout the surface of the tank resulting in the final design.

From the information gained from the solid wall analysis, the chosen size of the unit cell is a square with dimensions equal to that of the thickness of the tank. The stress on a thin walled pressure vessel with the geometry described above is broken up into the hoop stress, σ_h and radial stress σ_r which are determined as follows

$$\sigma_h = \frac{\Pr}{t} \tag{4.6}$$

$$\sigma_r = \frac{\Pr}{2t} \tag{4.7}$$

where P, r and t are obtained from the solid wall hydrogen tank optimization. Here P is the pressure inside the hydrogen tank, r is the internal radius of the cylindrical tank and t is the wall thickness of the tank. The various dimensions of the hydrogen tank are represented in Figure 4. 4.

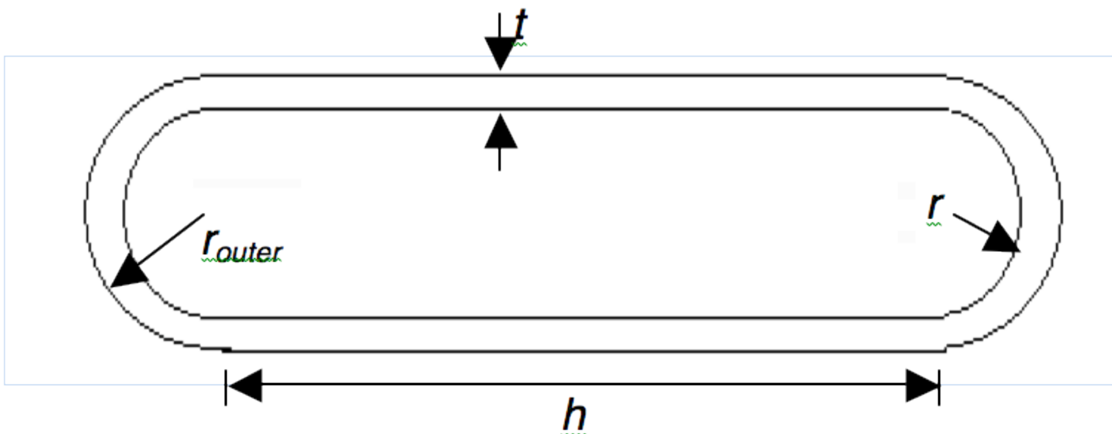


Figure 4. 4 Representation of various dimensions of the hydrogen tank

In addition to the hoop and radial stresses there is an axial stress applied as a results of the closed ends of the tank. The axial stress has been neglected in this analysis. In cases where the height of the tank is not too large compared to the other dimensions of the tank the axial stress cannot be neglected.

In order to design the hydrogen storage tank specific objectives and constraints must be defined. The objectives chosen for the design of the tank are to minimize the volume of the gas (*Volume*) and the tank material volume or weight of the tank material (*Weight*). The constraints chosen for these objectives are based on the goals for hydrogen storage for fuel cell applications. The main targets for fuel cell technology for the years 2010 and 2015 are shown in Table 5. For this thesis the goals for 2010 are chosen as the basis for the constraints.

Table 5: Targets for hydrogen storage for 2010 and 2015 [75]

	Targets for 2010	**Targets for 2015**
Gravimetric Density (wt%)	6	9
Volumetric Density (kg/m^3)	45	81
System Mass (kg)	83	55.6
System Volume (m^3)	0.111	0.062
Min Operating Temp. (°C)	-30	-30
Max Operating Temp. (°C)	85	85

Most hydrogen storage tanks are cylindrical in shape with spherical ends as shown in Figure 4. 4. The represented variables shown are the height, h, tank wall thickness, t, inner radius, r_{inner}, and outer radius, r_{outer}, which designate the main geometric design variables.

The volume of the gas is equal to the inner volume of the storage tank, shown in Figure 4. 4, and is calculated using Equation 4.8.

$$V_{gas} = \pi r_{inner}^2 h + \frac{4}{3}\pi r_{inner}^3 \tag{4.8}$$

The volume of the tank material can be calculated using a similar equation with the addition of the outer radius term. The equation for the tank material volume, V_{tank}, is shown in Equation 4.9.

$$V_{tank} = \pi(r_{outer}^2 - r_{inner}^2)h + \frac{4}{3}\pi(r_{outer}^3 - r_{inner}^3) \tag{4.9}$$

In addition to the volume calculations, a model equation is needed to calculate the mass of hydrogen for a given set of design variables. Since hydrogen is the lightest element, it needs to be compressed at high pressures to be able to store it. Increasing pressures cause gases, including hydrogen, to lose their compressibility. For situations such as this, the equation of state is given by

$$PV_{sgas}=zRT' \qquad (4.10)$$

where P is the pressure, V_{sgas} the specific volume of the gas, z the compressibility factor, R is the universal gas constant (8.314 m^3 Pa K^{-1} mol^{-1}) and T the temperature.

There are different methods for estimating the impact of increased pressure on the compressibility of gases. The Benedict-Webb-Rubin equation [76] has shown to be an accurate predictor of hydrogen state at high pressures which incorporates available compressibility. From this equation the compressibility factor can be expressed as follows.

$$z = 1 + (B_0 - \frac{A_0}{RT} - \frac{C_0}{T^3})\rho + (b - \frac{a}{RT})\rho^2 + \frac{a\alpha}{RT}\rho^5 + \frac{c\rho^2}{RT^3}(1+\gamma\rho^2).\exp(-\gamma\rho^2) \qquad (4.11)$$

where a, A_0, b, B_0, c, C_0, α, and γ are Benedict-Webb-Rubin constants defined in [76]. This equation combined with Equation 4.10 shows the relationship between the volumetric density and the pressure inside the tank. However, the equation is a 6th order polynomial making evaluation of the density of hydrogen difficult. A more simple equation to evaluate the compressibility accurately at high pressures is given in [77].

$$z = 0.99704 + 6.4149\times10^{-9} P \qquad (4.12)$$

Substituting this equation and the definition of specific volume into Equation 4.10 produces Equation 4.13.

$$m_{H_2} = \frac{0.002PV_{gas}}{RT(0.99704 + 6.4149\times10^{-9}P)} \tag{4.13}$$

The constant in the beginning of the equation represents the conversion from *mol* of hydrogen to *kg* of hydrogen based on the units of the universal gas constant, *R*. Equation 4.13 is used in this design problem to determine the mass of hydrogen in the tank for a specific set of design variables. Equation 4.13 relates the calculated volume of the tank, temperature, and pressure to the mass of hydrogen. To utilize this equation the pressure and temperature must be determined. For this evaluation the temperature is going to be taken as an uncertain variable that is normally distributed. The mean temperature is chosen to be 293.15 K with a standard deviation of 20 K based on the target specifications given in Table 5.

The following optimization problem is considered for the tank design.

Minimize: *Volume and Weight*

Subject to:

$$0.10 \le r \le 0.30 \text{ m} \tag{4.8}$$

$$0.0 \le h \le 1.0 \text{ m} \tag{4.9}$$

$$0.01 \le t \le 0.250 \text{ m} \tag{4.10}$$

$$H_{total} \le 1.35 \tag{4.11}$$

$$10 \le P \le 100 \text{ MPa} \tag{4.12}$$

$$g(u_{13}) = u_{13} - 0.015 \tag{4.13}$$

$$P_j[g(u_{13}) < 0] \le 10^{-4} \tag{4.14}$$

where h is the height of cylindrical portion of the tank and H_{total} is the total height of the tank. The objective in this optimization problem is to maximize the amount of hydrogen contained inside the hydrogen tank as well as

The given storage tank used for the RBTO procedure has a length of 1.35 m and an inner radius for the cylindrical portion of the tank of 0.3 m. The wall thickness is given as 8.29 mm. The internal pressure of the tank is given as 25.4 MPa. The storage tank is assumed to be made of a carbon composite with Young's Modulus of 379 GPa, and a Poisson's Ratio of 0.2. The target probability of failure for the mesoscale truss structure design is 10^{-4}.

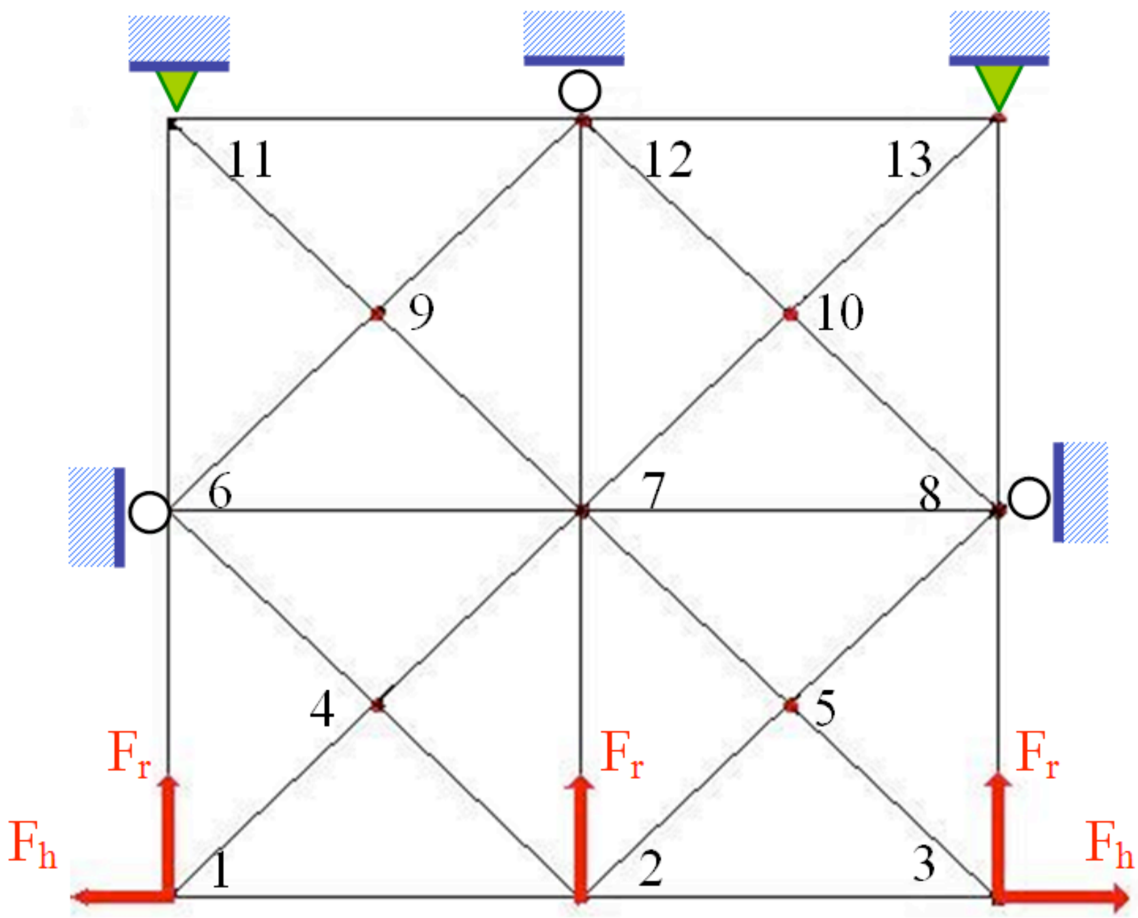
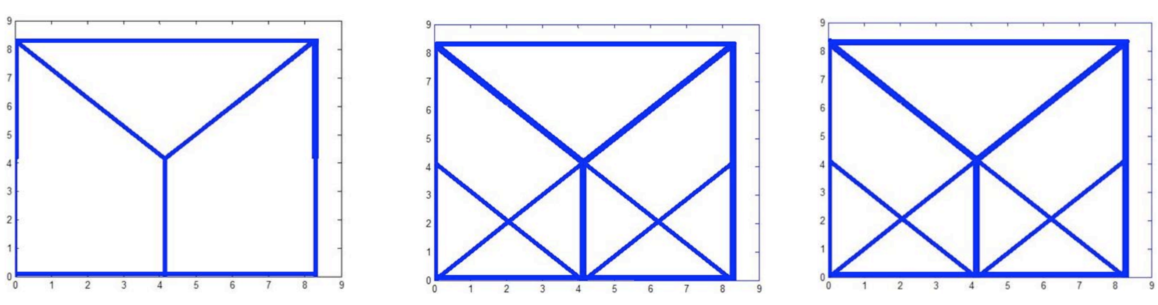


Figure 4. 5 Initial structural layout for the RBTO procedure

From the information gained from the solid wall analysis, the chosen size of the unit cell for both cases is a square with dimensions equal to that of the thickness of the tank which is 8.29 mm. From the given internal pressure, the hoop stress and radial stress are calculated using Eqs. (4.6) and (4.7). Since the devised RBTO algorithm only accepts forces acting at nodes these stresses are converted to point loads acting at the bottom nodes of the unit cell. The values of the forces due to these stresses are F_h=305072 N and F_r=152370 N. The radial force is applied in the vertical direction as shown in Figure 4. 5. The hoop force is applied to the bottom left node and the bottom right node in opposite directions which represents the tension applied to the bottom elements. The assumed manufacturing uncertainties are accounted for by varying the Young's Modulus. The variation is modeled as a PDF with mean value of the noted Young's Modulus of 3.78×10^8 N/mm^2 and a standard deviation of 10%.

The upper bound of the cross-sectional area for the analysis is chosen to be 7 mm^2. Variations in the volume fraction are used in order to determine an optimal truss orientation based on the RBTO method. By verifying a consistency in the results from variations in volume fraction a validation of the important cross members can be obtained. The chosen variation used in the analysis of the unit cell is 0.3, 0.4, and 0.5 for the volume fractions corresponding to a 70%, 60%, and 50% decrease in initial volume of the unit cell in Figure 4. 5. The results of the analysis process are shown in Figure 4. 6.

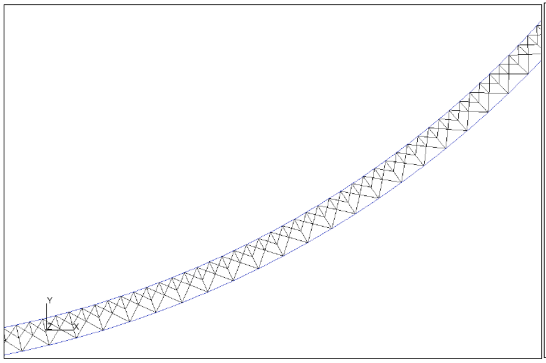


(a) V=0.3 (b) V=0.4 (c) V=0.5

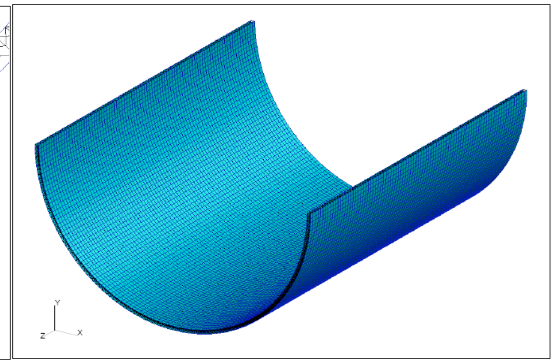
Figure 4. 6 Solutions for various volume fractions V

As can be seen from the results there are a number of elements that are not as important as others. There is also a trend showing that more truss members are needed near the inner wall where the applied load is to absorb the energy from the internal pressure. A very important observation can also be made from looking at these optimum designs as the volume fraction is decreased. It is shown in Figure 4. 6 that there is a convergence towards specific truss members representing an optimal topology. In Figure 4.6 (b) and Figure 4. 6(c) there is a constant overall orientation of truss members with only a change in cross-sectional area. Therefore it is deduced that this topology is optimal for the application of the hydrogen storage tank.

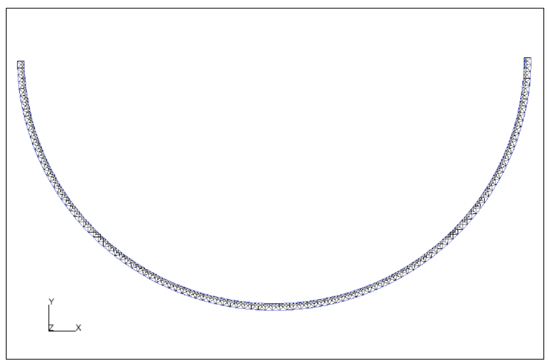
A finite element model of the cylindrical portion of the hydrogen storage tank is created using the above information as stated previously. The visualization of this portion of the tank is shown in Figure 4. 7. As can be seen from Figure 4. 7, the weight of the tank was reduced by 50% after this procedure while conserving the strength of the overall tank constant. An experimental design using Latin Hypercube Scheme was considered with 200 samples. Local regression process was used for creating the surrogate model during every iteration of the optimization process. After the surrogate model was created 10,000 samples were created using Monte Carlo scheme to evaluate the probability of failure. The probability of failure of the optimized mesostructure was 0.932×10^{-4}. This probability of failure value was calculated using the surrogate-based framework. A crude Monte Carlo sampling scheme with 100,000 samples was used for validating this result. The probability of failure value calculated using the Monte Carlo Sampling scheme was 0.966×10^{-4}.



(a) Iso-view



(b) Cross-section view



(c) Applied mesostructure

Figure 4. 7 Mesostructured hydrogen storage tank FEA model

As can be seen from Figure 4. 7, the weight of the tank will be significantly reduced compared to that of a solid wall tank from the use of cellular structures. In particular, the storage tank designed using cellular structures has 227 cells along the circumference and 88 cells along the length of the cylindrical section. This results in a total of 19,976 cell elements arranged together to form the cylindrical part of the storage tank. Since each cell consists of a volume of 338.224 mm^3 the total volume of the cylindrical section of the storage tank is 6,756.36 cm^3. In comparison the volume occupied by the cylindrical section of a metallic hydrogen storage tank is 21.386.95 cm^3. Therefore analyzing the above design and a tank comprising of a solid wall of the same dimensions and material that can endure the pressure of 25.4 MPa, the storage tank designed using cellular structures uses 68.41% less volume. Compared to a solid tank of the same dimensions as the mesostructured tank there is a significant improvement in the gravimetric density of the hydrogen storage tank. At a pressure of 25.4 Mpa the weight of hydrogen contained in the hydrogen tank is 9.492 kilograms for both the solid hydrogen tank and the mesostructured hydrogen tank. The gravimetric density, which is the ratio of mass of hydrogen in the tank to the mass of material of the tank, is 14.95% for a solid hydrogen tank whereas the gravimetric density for the mesostructured tank is 30.47%. Both of these values conform to the design requirements of 2010 and 2015. This design meets the goals of the optimization problem as well. In addition, the strength of the cellular structure tank can be compared to that of the solid wall tank through Finite Element Analysis. The purposes of topology optimization and the use of cellular structures are to reduce the overall volume of the material with little to no effect to the overall reliability of the system. Based on this statement it is hypothesized that further structural analysis of the cellular structure hydrogen storage tank will further validate this improved design.

CHAPTER 5

CONCLUSION

5.1 Contributions

The current research focuses on integrating reliability analysis in the topology optimization procedure in order to design reliable truss structures. In addition to this the current thesis answers the age-old problem of estimating probability of failure in case of disjoint failure domain and low probability of failure. The major contributions of this research are summed below:

- The topology optimization solutions obtained using the homogenization procedure has to go through post processing after running to optimization routine. Since the densities are not always 0 or 1 they have to be classified using an image processing application before they can be used. The ground structure based Topology optimization procedure used gives results that can be manufactured directly without the need of major post processing. Integrating reliability based optimization into the topology optimization procedure gives solutions that are not sensitive to fluctuating external and internal factors. Furthermore, since these results are obtained using the ground structure based topology optimization procedure they can be manufactured as they are obtained from the optimization procedure.

- Local regression method has been used as a surrogate modeling technique for estimating the probability of failure to reduce the computational requirement of the Reliability-based Topology Optimization procedure. The Local regression method is similar to the Moving Least squares method and it can be used when the failure domain is continuous.

- In cases where the failure domain is not continuous a classification approach instead of a regression approach can be used for the approximation of the reliability constraint. In classification the reliability assessment problem is framed as a decision problem where every design is labeled as either safe or unsafe. This underlies the reliability assessment as a simple problem of counting the number of design points in the unsafe region.

- It has been shown that Reliability based Topology Optimization provides design solutions with significantly lower probability of failure values. This reduction of probability of failure comes at a price. In case of topology optimization the low probability of failure underlies the use of more material than that is required by the Deterministic Topology Optimization solutions.

- Local regression procedure has been integrated with Topology optimization procedure for this first time in this research. Furthermore, the classification based approach for estimating the probability of failure has been used for the first used along with Topology optimization procedure. In this research Artificial Neural Networks have been used for the classification procedure. The main advantage of using Neural Network for classification is their ease of use and their applicability for use as a black box model. Hence, even with less knowledge of the data mining techniques the designers can use Neural Networks for the classification procedure for reliability assessment.

- A final framework was presented that uses the classification approach once the regression procedure using Local regression fails to achieve the desired accuracy. Correlation Coefficient R^2 is used as the parameter that determines the goodness of fit. In case R^2 has a low value a classification approach is then used. This proposed framework was validated using a design problem that involved the design of a hydrogen tank according to certain design constraints.

The following sections describe certain limitation of this research and further work that can improve the proposed framework and the design results.

5.2 Limitations

The research presents a novel application of classification based ANN and local regression within RBTO as surrogate modeling technique for approximating the limit state function. Nevertheless, it has the following limitations:

- The optimization results have not manufactured and the prototypes were not tested for the conditions they were made for. These mesostructures could possibly be made using additive manufacturing process where the prototyping process is divided into a layer based manufacturing process making it easier for prototyping even complex shapes.

- The overall framework switches from Local regression technique to Classification using ANN procedure based on the goodness of fit. The statistic that has been used for characterizing the goodness of fit is the R^2 value. While R^2 values are the easiest to compute and use they are not good indicators of goodness of fit [78]. Mallow's C_p, PRESS etc. could be better indicators of the goodness of fit for regression applications.

- The classification scheme using Artificial Neural Network is accurate but computationally inefficient compared to Support Vector Machines (SVM) which are better classification machines. But considering the ease of use which artificial neural networks provide, ANN was used for this research.

- The groundstruss used for the topology optimization process is in two dimensions. For optimizing complex products and structures the design process has to be extended to three dimensions that would increase the computational requirement of the process immensely. Using a commercially available FEM application like GENESIS, ANSYS, NASTRAN could increase the range of problems that can be handled using the proposed framework.

5.3 Future Work

The current research answers the research questions and hence gives a framework that can produce reliable truss structures in the face of disjoint failure domains and nonlinear failure behavior. This framework is also effective in dealing with low probability of failure values. The efficacy of the RBTO procedure has been shown with the help of a truss design example and a hydrogen storage tank design example. Nevertheless, the current work can be improved by the following:

- The optimization results can be prototyped and tested to check if they actually are insensitive to fluctuations of internal and external factors.

- The finite element and ground truss used for the examples are limited to two dimensions, which could be easily extended to three dimensions by using a commercial FEM application.

- In the proposed final framework the goodness of fit criteria can be switched from the correlation coefficient R^2 to a better goodness of fit parameter like PRESS which doesn't depend on the number of parameters used for the regression procedure and which are more global in nature.

- The hydrogen storage tank design shown in Figure 4. 7 should be validated using suitable FEA software such as NASTRAN, ANSYS, COMSOL etc. for it to be used in any real life application.

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