Cairo University
Institute of Statistical Studies and Research
Department of Operations Research

A Comparative Study for Approximation Techniques to Nonlinear Optimization Problems

By

Gamal El-Dean Abdel Hakim Mohamed El-Emam

A Thesis Submitted to the Institute of Statistical Studies & Research

Cairo University

In Partial Fulfillment of the Requirements for the Degree of

Master of Science
In

Operations Research

Under the Supervision of

Prof. Mohamed Hassan Gadallah
Professor & Head
Department of Operations Research, Institute of Statistical Studies & Research,
Cairo University, Egypt

Dr. Ramadan Zein el Dean
Associate Professor
Department of Operations Research, Institute of Statistical Studies & Research,
Cairo University, Egypt

2010

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

Page #

LIST OF APPENDICES

Acknowledgements

I would like to thank my great supervisor Professor Mohamed Hassan Gadallah, Professor & Department Head of Operations Research, Institute of Statistical Studies & Research, Cairo University, for his expert advice and excellent guidance. I would also like to thank Dr. Ramadan A. Zein El-Dean Associate Professor, Department of Operations Research, Institute of Statistical Studies & Research, Cairo University, for his support along the past few years.

ABSTRACT

Constrained nonlinear programming problems often arise in many engineering applications and much of today's engineering analysis consists of running complex computer codes. Despite a steady increase in computing power, the complexity of engineering analyses seems to advance at the same rate. The use of statistical techniques to build approximations of expensive computer analysis codes pervades much of today's engineering design. These statistical approximations, or meta-models, are used to replace the actual expensive computer analyses, facilitating multidisciplinary and concept exploration. In this thesis, we review some of these techniques, especially Response Surface Methodology (RSM) and Kriging. Both methods are applied to thirty widely used classes' of single objective optimization problems. We compare the results of both Response Surface Methodology and Kriging model with the solutions of the original nonlinear optimization solutions. Generally speaking, Kriging method is able to return almost the same solution as the original model optimum for the majority of problems. Response Surface Methodology comes next to Kriging is finding the optimum to the original model. As a remedy, a new approach is proposed to split the model into several smaller sub-models. The problem is transformed into a number of sub-problems with an impact on increased model CPU processing time. A set of test bed problems is verified using both approximation methods. When Splitting is employed prior to approximation, both techniques are able to capture system optima consistently. Monotonicity and continuity are still important and valid concerns in any approximation.

CHAPTER I

INTRODUCTION

CHAPTER I

INTRODUCTION

Much of today's engineering analysis consists of running complex computer codes. Despite a steady increase in computing power, the complexity of engineering analyses seems to advance at the same rate. Traditional parametric design analysis is inadequate for the analysis of large-scale engineering systems because of its computational inefficiency, therefore, a departure from the traditional parametric design approach is required. In this thesis, we propose two approximation techniques, namely Response Surface Methodology and Kriging to non-random, deterministic computer analyses. After reviewing the Response Surface Method for constructing polynomial approximations, Kriging is presented as an alternative approximation method. Both methods are applied to thirty tested problems.

These approximations are then used in place of the actual analysis codes, offering the following benefits:

- They yield insight into the relationship between output responses, **y** and input design variables, **x**.
- They provide fast analysis tools for optimization and design space exploration since the inexpensive-to-run approximations are used in lieu of the expensive-to run computer analyses.
- They facilitate the integration of discipline dependent analysis codes.

We compare and contrast the use of Response Surface Models and Kriging models for approximating non-random, deterministic computer analyses. The primary focus of this thesis is a thorough research into both methods. They are applied to the different classes of nonlinear single objective problems with constraints equality and inequality. Approximation techniques may be applied to build computationally inexpensive models. Response-Surface Models are frequently utilized to construct surrogate approximations; however, they may be inefficient for systems having large number of design variables. Kriging is an alternative method for creating surrogate models. We present a comparative study that is performed on thirty different classes of test problems selected from the literature.

There are many applications in various branches of engineering field (e.g., mechanical engineering, chemical engineering, electrical engineering, aerospace engineering, etc.) that can be formulated as constrained nonlinear problems. The primary focus of this work is a thorough research into the approximation techniques for solving nonlinear single objective problems with and without constraints, whereby numerical algorithms are used to solve problems of the form:

$$\begin{aligned} &\text{Min} && f(x) \\ &\text{Subject to:} && g(x) \le 0 \\ &&& h(x) = 0 \\ &&& x_l \le x \le x_u \end{aligned} \tag{1.1}$$

The designer is to choose values for the vector of design variables, x, that minimizes the objective function, f(x), while satisfying the inequality constraints g(x), and the equality constraints, h(x), x_l and x_u denote the lower and upper bounds of the variables x, respectively. The functions in form (1.1) are nonlinear, problems of this form are referred to as nonlinear programming. In most of the nonlinear programming problems f(x), h(x), and g(x) are nonconvex and the problems have multiple locally optimal solutions. In the only case where the f(x) is convex, every h(x) is linear and every g(x) is convex, constrained local minimum is also constrained global minimum.

The general nature of nonlinear programming has led to specialized fields within optimization.

One field has focused on solving structural optimization problems which have a characteristically large number of design variables and constraints. Another field, Multidisciplinary Design Optimization (MDO) has focused on how to solve problems involving a variety of engineering fields effectively by solving the large problem as a collection of smaller sub- problems.

Simulation-based optimization addresses problems where the objective and/or constraint functions are not expressed with closed-form analytical equations, but with so-called “black box” computer simulations. Typically, the functions (a) are noisy or discontinuous (non-smooth) and/or (b) require a long time to compute. Each of these features causes specific difficulties that must be addressed in simulation-based optimization.

1.1 Classification of Approximations

There are many types of meta-models. These are Response Surface Methodology (RSM), Kriging Methodology, Surrogate Approximation, Taylor series expansion, Non-Uniform Rational B-Spline (NURBS) etc. Most popular ones are low-order polynomial regression models. Kriging is applied frequently in deterministic simulation. In this thesis, we focus on Kriging Methodology and Response Surface Methodology.

1.1.1. Response Surface Methodology (RSM)

Response Surface Methodology (RSM) is not an algorithm, it is a set of tools grouped together to analyze a problem. RSM is a collection of statistical and mathematical techniques useful for developing, improving and optimizing processes. It also has important applications in the design, development, and formulation of new products as well as in the improvement of existing product designs.

There are five major steps in the application of Response Surface Methodology:

1) Identify design space:

The designer identifies the area of interest and selects the design factors to study. Often, if there is numerous design variables, experiments are performed to "screen out" the less important effects.

2) Select an experimental design:

Sample points are chosen in the design space to investigate the relationship between the design factors and the responses and generate a predictive model.

3) Sample design space:

The computer analysis or simulation code being approximated is performed at each of the sample points identified in step 2.

4) Build predictive model:

Using the data gathered in step 3, a predictive model is constructed using a number of methods (e.g. response surfaces, Kriging, neural networks, splines, etc.).

5) Explore the design space:

The design space can then be explored to find regions of good design or optimized to improve the performance of the system. This is done using approximation models instead of the computationally expensive analysis codes and result in large computational savings.

Response surface modeling techniques are originally developed to analyze the results of physical experiments and create empirically-based models of the observed response values. Response surface modeling postulates a model of the form:

$$y(\mathbf{x}) = f(\mathbf{x}) + \varepsilon \tag{1.2}$$

where $y(\mathbf{x})$ is the unknown function of interest, $f(\mathbf{x})$ is a known polynomial function of $\mathbf{x}$, and ε is random error which is assumed to be normally distributed with mean zero and variance σ^2. The individual errors, ε_i, at each observation are also assumed to be independent and identically distributed. The polynomial function, $f(\mathbf{x})$, used to approximate $y(\mathbf{x})$ is typically a low order polynomial which is assumed to be either linear, Eqn. (1.3), or quadratic, Eqn. (1.4). Given a response y and a vector of independent factors **x** influencing y, the relationship between y and **x** is:

$$\hat{y}(\mathrm{x}) = \beta_0 + \sum_{i=1}^{k} \beta_i x_i \qquad (1.3)$$

$$\hat{y}(\mathrm{x}) = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x^2_i + \sum_{i=1}^{k} \sum_{j=,i<j}^{k} \beta_{ji} x_i x_j \qquad (1.4)$$

The parameters β_0, β_i, β_{ii}, and β_{ji}, of the polynomials in Eqns. (1.3) and (1.4) are determined through least squares regression which minimizes the sum of the squares of the deviations of predicted values $\hat{y}(\mathbf{x})$, from the actual values y(**x**). The coefficients of Eqns. (1.3) and (1.4) are used to fit the model and can be found using least squares regression given by the following Eqn.:

$$\beta = [\mathbf{X'X}]^{-1}\mathbf{X'y} \qquad (1.5)$$

where **X** is an *n x p* the design matrix of sample data points, **X**' is its transpose, and **y** is a column vector an *n x 1,* containing the values of the response at each sample point. It is to see that **X'X** is a *p x p* symmetric matrix and **X'y** is a *p x 1* column vector**.**

1.1.2. Kriging Methodology

Kriging Models have their origins in mining and geostatistical applications that deal with spatially and inter-correlated data. Many computer analysis codes are deterministic and therefore are not subject to measurement error. Based on this observation, some statisticians develop Design and Analysis of Computer Experiments (DACE) for deterministic computer-generated data based on the Kriging method. An optimization method using Kriging approximation is applied to a structural optimization problem. The