Sensitivity analysis and section positioning for road design model

by

Soroor Sarafrazi

M.Sc., Shahid Bahonar University of Kerman, 2011

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF
THE REQUIREMENTS FOR THE DEGREE OF
MASTER OF SCIENCE

in
THE COLLEGE OF GRADUATE STUDIES
(Interdisciplinary Studies - Optimization)

THE UNIVERSITY OF BRITISH COLUMBIA
(Okanagan)
September 2016
© Soroor Sarafrazi, 2016
The undersigned certify that they have read, and recommend to the College of Graduate Studies for acceptance, a thesis entitled: **SENSITIVITY ANALYSIS AND SECTION POSITIONING FOR ROAD DESIGN MODEL** submitted by **SOROOR SARAFRAZI** in partial fulfillment of the requirements of the degree of Master of Science

Prof. Yves Lucet (Arts & Sciences, UBC Okanagan)
Supervisor, Professor (please print name and faculty/school above the line)

Dr. Jason Loeppky (Arts & Sciences, UBC Okanagan)
Co-Supervisor, Professor (please print name and faculty/school above the line)

Dr. Warren Hare (Arts & Sciences, UBC Okanagan)
Supervisory Committee Member, Professor (please print name and faculty/school above the line)

Dr. Kasun Hewage (School of Engineering, UBC Okanagan)
University Examiner, Professor (please print name and faculty/school above the line)

September 2016
(Date Submitted to Grad Studies)
Abstract

Economy is one of the most important factors to develop a country and roads are vital to expedite the economy growth. Although road networks lead to social and economic development, the road construction and maintenance are expensive activities. Therefore, there is a strong interest in minimizing the construction cost, while satisfying safety and environmental constraints. Different road design models have been proposed, but the sensitivity of these models to their input parameters has not yet been analyzed.

Sensitivity analysis of a road model before building the road is highly suggested because it helps to investigate the stability of the model and identify the parameters that have the most effect on the variability of the model output. In addition, sensitivity analysis helps to enhance the communication between modelers and decision makers (managers). Therefore, different sensitivity analysis methods are presented in this thesis and the sensitivity of a road model to its inputs is studied.

Moreover, in a road design model, the ground is discretized into sections and the number of sections is highly correlated with the optimization time. Designing roads that consider all sections is too time consuming to be practical. Thus, different methods are presented in this thesis to reduce the number of sections while keeping the accuracy of the ground profile.
Preface

A paper co-authored with Dr. Jason Loeppky and Dr. Yves Lucet is adapted from the second chapter of this thesis. This paper is submitted for publication to the journal of Reliability Engineering & System Safety [SLL16]. In addition, a presentation, joint work with Dr. Jason Loeppky and Dr. Yves Lucet, was adapted from the third chapter and given at the 58th Canadian Operational Research Society Annual Conference in Banff, Canada.
# Table of Contents

Abstract .......................................................... iii
Preface .............................................................. iv
Table of Contents ................................................ v
List of Tables ....................................................... vii
List of Figures ..................................................... ix
Acknowledgments .................................................. x
Dedication .......................................................... xi

Chapter 1: Introduction .......................................... 1

  2.1 Sensitivity analysis ........................................... 3
  2.2 Basic notation and definitions ............................... 6
  2.3 Linear and monotonic Sensitivity Analysis (SA) methods .. 8
  2.4 Nonlinear SA methods ....................................... 9
    2.4.1 Variance ................................................. 9
    2.4.2 Variance-mean ........................................... 17
    2.4.3 Factor screening methods .............................. 20
    2.4.4 Derivative-based method .............................. 21
    2.4.5 Distance between distributions ....................... 23
    2.4.6 Moment independence measures ...................... 24
  2.5 Surrogate-based methods for expensive function models ... 25
  2.6 Sensitivity indices for multivariate outputs ............. 26
    2.6.1 Multivariate Sobol sensitivity analysis ............. 27
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.6.2</td>
<td>2.6.2 Sequential sensitivity analysis</td>
<td>27</td>
</tr>
<tr>
<td>2.6.3</td>
<td>2.6.3 Principal Components Analysis (PCA)-based multivariate sensitivity analysis</td>
<td>28</td>
</tr>
<tr>
<td>2.6.4</td>
<td>2.6.4 Variance-based multivariate sensitivity analysis</td>
<td>28</td>
</tr>
<tr>
<td>2.7</td>
<td>2.7 Numerical examples and discussion</td>
<td>29</td>
</tr>
<tr>
<td>2.7.1</td>
<td>2.7.1 Study 1</td>
<td>29</td>
</tr>
<tr>
<td>2.7.2</td>
<td>2.7.2 Study 2</td>
<td>30</td>
</tr>
<tr>
<td>2.7.3</td>
<td>2.7.3 Study 3</td>
<td>34</td>
</tr>
<tr>
<td>2.8</td>
<td>2.8 Discussion</td>
<td>37</td>
</tr>
<tr>
<td>3</td>
<td>3 Chapter 3: Section positioning in the road design vertical alignment problem</td>
<td>40</td>
</tr>
<tr>
<td>3.1</td>
<td>3.1 The road design problem</td>
<td>40</td>
</tr>
<tr>
<td>3.2</td>
<td>3.2 The road design model</td>
<td>41</td>
</tr>
<tr>
<td>3.3</td>
<td>3.3 Section positioning methods</td>
<td>45</td>
</tr>
<tr>
<td>3.3.1</td>
<td>3.3.1 Method 1: The heuristic method</td>
<td>45</td>
</tr>
<tr>
<td>3.3.2</td>
<td>3.3.2 Method 2: The regression tree</td>
<td>45</td>
</tr>
<tr>
<td>3.3.3</td>
<td>3.3.3 Method 3: Piecewise constant approximation</td>
<td>46</td>
</tr>
<tr>
<td>3.4</td>
<td>3.4 Results and Discussion</td>
<td>48</td>
</tr>
<tr>
<td>3.4.1</td>
<td>3.4.1 Comparing the three methods</td>
<td>50</td>
</tr>
<tr>
<td>3.5</td>
<td>3.5 Summary of the section positioning methods</td>
<td>59</td>
</tr>
<tr>
<td>4</td>
<td>4 Chapter 4: Conclusion</td>
<td>60</td>
</tr>
<tr>
<td></td>
<td>4 Bibliography</td>
<td>62</td>
</tr>
</tbody>
</table>
## List of Tables

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Table 2.1</td>
<td>The Pearson, Spearman and the main Sobol sensitivity indices of four functions (2.27).</td>
<td>30</td>
</tr>
<tr>
<td>Table 2.2</td>
<td>The sensitivity indices of the linear and monotonic methods for the Ishigami function.</td>
<td>32</td>
</tr>
<tr>
<td>Table 2.3</td>
<td>The numerical values of the Mckay and Sobol indices obtained from symbolic integration in Maple for the Ishigami function.</td>
<td>32</td>
</tr>
<tr>
<td>Table 2.4</td>
<td>The average of sensitivity indices of different nonlinear methods for the Ishigami function.</td>
<td>33</td>
</tr>
<tr>
<td>Table 2.5</td>
<td>The Sobol and FAST indices for Moreb’s problem.</td>
<td>36</td>
</tr>
<tr>
<td>Table 3.1</td>
<td>Approximation of Cut volumes using side-slopes for a cut area.</td>
<td>45</td>
</tr>
<tr>
<td>Table 3.2</td>
<td>Four different grounds.</td>
<td>49</td>
</tr>
<tr>
<td>Table 3.3</td>
<td>The performance of the heuristic method on Ground A.</td>
<td>53</td>
</tr>
<tr>
<td>Table 3.4</td>
<td>The performance of the Regression tree on Ground A.</td>
<td>54</td>
</tr>
<tr>
<td>Table 3.5</td>
<td>The performance of the piecewise constant approximation method on Ground A.</td>
<td>55</td>
</tr>
<tr>
<td>Table 3.6</td>
<td>Comparing methods on Ground A according to two stopping criteria.</td>
<td>55</td>
</tr>
<tr>
<td>Table 3.7</td>
<td>Comparing methods on Ground B according to two stopping criteria.</td>
<td>55</td>
</tr>
<tr>
<td>Table 3.8</td>
<td>Comparing methods on Ground C according to two stopping criteria.</td>
<td>56</td>
</tr>
<tr>
<td>Table 3.9</td>
<td>Comparing methods on Ground D according to two stopping criteria.</td>
<td>56</td>
</tr>
<tr>
<td>Table 3.10</td>
<td>Comparing methods on Ground A based on the material volumes and according to two stopping criteria.</td>
<td>57</td>
</tr>
<tr>
<td>Table 3.11</td>
<td>Comparing methods on Ground B based on the material volumes and according to two stopping criteria.</td>
<td>58</td>
</tr>
</tbody>
</table>
Table 3.12 Comparing methods on Ground C based on the material volumes and according to two stopping criteria. 58
Table 3.13 Comparing methods on Ground D based on the material volumes and according to two stopping criteria. 58
# List of Figures

| Figure 2.1 | The CSM\(_i(q)\) for three inputs of the Ishigami function. | 18 |
| Figure 2.2 | The effect of the symmetric reducing of the range to \([q, 1 − q]\) on variance for the three inputs for the Ishigami function. | 19 |
| Figure 2.3 | The scatter plot of Ishigami function with \(N = 1000\). | 31 |
| Figure 2.4 | The road and ground profiles. | 34 |
| Figure 2.5 | Summary of SA methods for inexpensive models. | 38 |
| Figure 3.1 | The vertical alignment of the ground profile. | 41 |
| Figure 3.2 | The cross-section of a road with and without side-slopes. | 44 |
| Figure 3.3 | Approximation of side-slopes for a cut area. | 44 |
| Figure 3.4 | Three iterations of the heuristic method. | 46 |
| Figure 3.5 | Three iterations of the regression tree. | 47 |
| Figure 3.6 | The piecewise constant approximation. | 48 |
| Figure 3.7 | Four ground profiles. | 50 |
| Figure 3.8 | An example for Algorithm 2 which approximates the side-slopes of merged sections. | 51 |
Acknowledgments

I would like to express my deep sense of gratitude to my supervisors Dr. Yves Lucet and Dr. Jason Loeppky for their updated knowledge, continuous support, great guidance and patience during my research.

I also like to thank my committee members Dr. W. Hare, Dr. Yves Lucet and Dr. Jason Loeppky for their great advice and inspiration.

I truly appreciate the support of our industrial partner (Softree Technical Systems Inc.). In particular David Mills, Craig Speirs, and Alexis Guigue were always very supportive and their technical information is highly appreciated.

I owe my deepest gratitude to my parents, and family members for their support and encouragement throughout my life.

This research is partially funded by Natural Sciences and Engineering Research Council of Canada, Canada Foundation for Innovation, British Columbia Knowledge Development Fund, and Softree Technical Systems Inc.
Dedication

To my beloved parents and family members.
Chapter 1

Introduction

A high quality road network can increase the standards of living, facilitate trading and lead to social and economic development. However, a road network has some negative effects including damaging environment, accidents, air and noise pollution [FJM+01]. Therefore, designing a road implies trade-offs between safety, social, environmental and economic impacts; it is a complicated and challenging process [JSJ06]. The road design is usually split into three interconnected stages: horizontal alignment, vertical alignment, and earthwork [HKL11].

In the horizontal alignment, the road curve is examined from a satellite’s eye view and the primary objective in this stage is minimizing environmental issues and construction costs [EM07]. After the horizontal alignment is fixed, the starting and end points can be connected by a curve and the vertical ground profile can be examined along this curve. In other words, a road’s change in elevation can be studied in the vertical alignment stage. The primary objective in this stage is minimizing the construction cost [HKL11]. After the vertical alignment stage, the earth is rearranged with minimum cost in the earthwork optimization stage. In this stage, the ground profile changes to a desired smooth road profile [MS81].

In all stages of the road design model, there are several inputs and their uncertainties lead to uncertainty in the model output. SA studies how the model output uncertainty can be assigned to different sources of uncertainty in inputs [SAA+10]. SA indicates if the model is robust to small changes in inputs and determines the robustness of the model when one or some of the model parameters are varied simultaneously [STCR04]. In other words, SA can help to improve the road design model and test the robustness of a decision. Therefore, different SA methods are presented and compared in this thesis and the most appropriate SA methods are applied to a road design model.

In addition to the SA of the road design model, the optimization time of this model should also be considered. In the road design model, the ground profile is discretized into sections [HHLR14] and the optimization time is proportional to the number of sections. Optimizing long roads with a lot
of sections is too time consuming to be practical. Therefore, the number of sections should be reduced while considering a trade-off between time and accuracy of approximation. Consequently, different methods are presented and compared in this thesis for section positioning and reducing the number of sections.

This thesis is organized as follows. Chapter 2 is a survey paper on SA which is submitted for publication to the journal of Reliability Engineering & System Safety [SLL16]. This paper also includes SA on a road design model. Chapter 3 introduces and compares different methods for section positioning. Finally, conclusions with directions for future research are provided in Chapter 4.
Chapter 2

A Survey on the Sensitivity Analysis Methods for Understanding Complex Models

Mathematical models representing real world situations are now ubiquitous across science, engineering and the humanities. One major challenge with these models is in understanding and quantifying the effect of uncertain inputs on the output of the function. In this Chapter, we review fundamental sensitivity analysis methods and classify them to allow non-specialists to select the method most appropriate for their specific problem. The classification is based on the SA method and assumption. These SA methods for non-expensive models are summarized with a decision tree. We also consider the sensitivity analysis of expensive models, and models with multivariate outputs. The accuracy and computational costs of the methods are compared on three numerical examples and on a real-world application in road design.

2.1 Sensitivity analysis

Mathematical models widely used in natural sciences, engineering and network science are subject to different sources of uncertainty, e.g., inaccurate parameter values, uncertain model structure, and unknown parameter ranges [GMPS14]. Some of the biggest challenges for modelers are dealing with uncertainty in the input parameters and finding the parameters that have the largest effects on the model output. Different terms are used interchangeably for these parameters, such as “important”, “sensitive”, “most influential”, “effective”, “major contributor”, or “correlated (with output)” [Ham94, SCS+00]. Identifying the important parameters and under-
ing their contributions to the output is one goal of sensitivity analysis (SA) [STCR04, OO04] and this goal is called factor prioritization [BP16].

The other goals of the SA are factor fixing, model structure, direction of change and stability. Factor fixing is associated with finding the least important inputs that can be fixed anywhere in their variability ranges. The model structure applies in cases where the model inputs affect the output individually or the interactions between inputs have an important role in influencing the output. Direction of change studies whether an increase (decrease) in a model input causes an increase (decrease) in the model output. Stability determines the input space over which the optimal solution does not change [BP16].

SA gives insight into a model’s behavior by these five goals [Alv09, Ham94]. SA also helps validating a model by factor fixing and model structure goals [IL14, AIGMA05, CP02].

SA has seen applications in a diverse setting. For example, it is used to assess the risk caused by the uncertainty in the parameters of a CO$_2$ storage model [AON13]. Cannavo [Can12] implemented SA to validate and develop a model that can best describe the state of volcano. Sellers and Crompton [SC04] implemented SA on a biomechanical model and they strongly encourage the use of SA as a validation technique for modeling. Saint-Geours et al. [SGBG14] implemented a flood damage assessment model and the quality of the conclusions drawn from the model output are studied by SA. In [LMM14], SA is used to find the dependability of complex systems and helps to predict failures and schedule maintenance.

SA methods are based on producing a quantitative evaluation of the contribution of each parameter in the form of sensitivity indices. Using the values of these indices, one can rank the input parameters from most important to least important. SA methods with different assumptions may lead to different ranking of inputs that influence the model output. Therefore, SA methods should be chosen properly to find the ranking most appropriate for a given application [CHT00]. Using two or more methods with different mechanisms is recommended to identify the key inputs with more confidence [CP02].

SA methods are usually categorized into local and global methods. Local SA methods concentrate on the sensitivity of the output with respect to small perturbations around the input values. In local SA, the values of the input parameters of interest are perturbed, while the other parameters are fixed at their nominal values (all inputs are perturbed if the local sensitivity of output to all inputs is required). While local SA methods do not study the whole ranges of inputs, they can capture co-dependencies using higher
order derivatives or profile-based measures [SK11]. Global SA methods take one or a combination of input parameters and study the model output over the entire ranges of the input parameters [Sud08, SK11].

One can classify global SA methods as mathematical, statistical or graphical [CP02]. However, in this paper, we choose to focus on the methods assumptions and mechanisms. The global SA methods in this paper are classified according to linear, monotonic and nonlinear methods.

Linear SA methods assume a linear approximation of the model output with the variable of interest (where all others are ignored). If these methods find a highly important input, then the model has one active input and the model can be approximated by a linear function of the important input. Monotonic SA methods assume modeling a monotonic relationship between the model output with the variable of interest (where all others are ignored). Nonlinear SA methods do not assume any relationship between the model output and inputs.

In this paper, unlike the other review papers [IL14, Ham94, AIGMA05, Ham95], a wide range of global SA methods are studied and the presented framework helps to choose an appropriate method where appropriateness is based on the type of problems a method can solve and its computational cost.

When the evaluation of a function, provided as a black-box, is expensive in term of computation time, SA methods become too time consuming. In that situation, one needs to approximate the function using a surrogate. There are numerous methods to construct a surrogate model such as moving Least-Squares [Lev98], Polynomial Chaos Expansion [Sud08, Ale13, DNM+03], Gaussian Process (GP) [OO04], Artificial Neural Network [MCLH14], linear model [PPS09], Support Vector Machine [BM08], Chebyshev polynomials [WLZZ15], etc. In the present survey, we will focus on the GP methods since sensitivity indices are obtained while building the GP surrogate (applying a Bayesian approach to the GP). For other surrogate models, the sensitivity indices should be estimated after the surrogate is developed.

When a model is vector-valued (multivariate output), the model output is time dependent (dynamic) or not (static). According to the model output, different SA methods have been presented in this chapter.

For the static models with high dimensional outputs, Gamboa et al. [GJKL13] generalize the Sobol method. The sensitivity of dynamic models can be presented graphically or shown by indices. The sequential sensitivity analysis method introduced in [PCS+96] and the PCA based method used in [LMM11, LML+09, CMW06] present the sensitivity indices graphically.
2.2. Basic notation and definitions

The factor and time sensitivity indices introduced by Cao et al. [CDD13] are suggested for the sensitivity analysis of dynamic models. We discuss both static and dynamic multivariate sensitivity analysis in Section 2.6.

The paper is organized as follows. Section 2.2 is devoted to basic notations and definitions. Section 2.3 presents the linear and monotonic SA methods. The nonlinear SA methods are described in Section 2.4. Sections 2.3 and 2.4 consider SA methods for nonexpensive models that can be evaluated quickly, while the methods for expensive models are discussed in Section 2.5. Section 2.6 presents the SA methods for models with multivariate outputs. In Section 2.7, the SA methods are implemented on three numerical examples and also on an engineering model with a comparison of accuracy and computational costs. Finally, conclusions are provided in Section 2.8. These conclusions discuss how to pick a proper SA method according to the SA goal, the number of model inputs and the complexities of the model and the SA methods.

2.2 Basic notation and definitions

In what follows a bold capital letter (X) denotes a matrix, a bold lowercase letter (x) is a vector, a regular capital letter (X) is a random variable and a scalar is denoted by a regular lower-case letter (x).

The model input parameters are denoted by \( x = (x_1, ..., x_d) \) which has dimension \( d \). Let \( G(x) \) be the model function we wish to study; the possibly vector-valued output is denoted by \( y = (y_1, ..., y_l) = G(x) \).

The vector \( x_{-i} \) of dimension \( d - 1 \) denotes all the inputs of \( x \) except \( x_i \). A subset of inputs is denoted by \( x_R = (x_{i_1}, x_{i_2}, ..., x_{i_{d'}}) \) with \( R = \{i_1, ..., i_{d'}\} \) \((d' \leq d)\). The complementary set for this subset is given by \( x_{R^c} \) \((c \text{ denotes the set complement})\) and contains the remaining inputs such that \( R \cup R^c = \{1, ..., d\} \) and \( R \cap R^c = \emptyset \).

Let \( f_X(x) \) denote the joint distribution of a vector of random variables \((x = (X_1, ..., X_d))\), then \( f_{X_i}(x_i) = \int \frac{\partial}{\partial x_i} f_X(x) \prod_{t \neq i} dx_t \) is the marginal distribution and \( F_{X_i}(x_i) = \int_{-\infty}^{x_i} f_{X_i}(s) ds \) is the cumulative distribution function (CDF) of \( X_i \).

The expectation, the variance, the standard deviation and the covariance
2.2. Basic notation and definitions

of random variables \( X \) and \( Y \) are respectively

\[
E(X_i) = \int x_i f_{X_i}(x_i) dx_i, \\
V(X_i) = E[(X_i - E[X_i])^2], \\
\sigma_{X_i} = \sqrt{V(X_i)}, \\
\text{Cov}(X_i, Y) = E[X_i - E[X_i]]E[Y - E[Y]].
\]

When inputs are viewed as random variables, the output \( Y = G(X) \) is also a random variable and \( E(Y) = \int G(x) f_X(x) dx \) is the output mean. The mean of \( G(X) \) conditional on knowing \( X_R \) is given by

\[
E(Y|X_R) = \int G(x) f_{X_R}(x) dx_{R^c},
\]

where \( f_{X_R}(x) \) is the conditional distribution of \( X_{R^c} \).

To estimate the sensitivity indices, \( N \) samples for each random variable are used. The \( s^{th} \) sample of the input is indicated by \( x_s = (x_{1,s}, ..., x_{d,s}) \), which leads to the output \( y_s \). Further let \( \bar{x}_i \) and \( \sigma^2_{X_i} \) denote the usual sample mean and variance of the \( i^{th} \) coordinate.

Remark 2.1 (Dependent inputs). Most SA methods assume the inputs are independent. Consequently, these methods cannot be directly implemented on models with dependent inputs. For example, if \( x_1 \) is dependent on \( x_2 \), then the sensitivity index of \( x_1 \) indicates the contributions of both \( x_1 \) and \( x_2 \).

A procedure to define a set of independent parameters from a set of dependent inputs is suggested by Mara and Tarantola [MT12]. These transformed inputs are then used to study the sensitivities using the methods discussed in Sections 2.3 and 2.4. The new orthogonal input parameters \( x' = (X'_1, X'_2, ..., X'_d) \) can be obtained from the dependent normal inputs \( x = (X_1, X_2, ..., X_d) \) using the following procedure [MT12]

\[
\begin{cases}
X'_1 = X_1, \\
X'_i = X_i - E(X_i|X'_1, ..., X'_{i-1}), \forall i = 2, ..., d.
\end{cases}
\]

It is assumed that the conditional expectation distinguishes the dependency between the inputs. The new inputs \( x' = (X'_1, X'_2, ..., X'_d) \) are independent and orthogonal.

It should be noted that this procedure produces new independent inputs and the sensitivity indices of these independent inputs do not indicate the importance of the original inputs (the dependent inputs).
2.3. Linear and monotonic SA methods

Depending on the problem, a change of variable to obtain independent input followed by SA of output with respect to the new independent inputs may be acceptable. Otherwise, the methods in Remark 2.4 or Subsection 2.4.6 should be used.

Remark 2.2 (Monte Carlo integration). Numerical integration is a particular usage of Monte Carlo methods, which were named by Ulam and Metropolis [MU49].

Consider the integration \( I = \int_\Omega f(x)dx \) and let \( V = \int_\Omega dx \). Monte Carlo integration uses \( N \) samples of \( x \) to estimate

\[
I \approx I' = \frac{V}{N} \sum_{s=1}^{N} f(x_s).
\]

The error of Monte Carlo integration is independent of the number of dimensions and proportional to \( 1/\sqrt{N} \). Thus, the convergence of Monte Carlo integration can be slow but does not suffer from the “curse of dimensionality”. Techniques to improve the performance of Monte Carlo integration are discussed in [Wei00].

2.3 Linear and monotonic SA methods

In this section, SA methods that find the linear and monotonic effects of each input \( X_i \) on the output \( Y = G(x) \) are described. Because these methods are mainstream, only a brief sketch of the methods are provided. Both methods assume inputs are independent. Pearson’s method is a correlation-based SA method and is a linear SA method. An example of Monotonic SA method is Spearman’s method that is also correlation-based sensitivity analysis method. For finding the Pearson and Spearman coefficients, \( N \) samples for input \( x \), which lead to \( N \) samples for the output \( Y, (y_1, ..., y_N) \), are considered.

The concept of correlation was first introduced by Galton in 1888 [Gal88] and the Pearson (product-moment) correlation \( r \) was proposed by Pearson in the 1890s [Pea95]. The correlation between the input \( X_i \) and the output \( Y = G(x) \) that shows the sensitivity of \( X_i \) is given by

\[
r_i = \frac{\text{Cov}(X_i, Y)}{\sigma_{X_i} \sigma_Y} \approx \frac{\sum_s (x_{i,s} - \bar{x}_i)(y_s - \bar{y})}{\sqrt{\sum_s (x_{i,s} - \bar{x}_i)^2} \sqrt{\sum_s (y_s - \bar{y})^2}},
\]

where \( \text{cov}(X, Y) \) denotes the covariance of \( X \) and \( Y \).
The positive or negative value of cov(X, Y) shows the positive or negative slope of Y as a function of X. The correlation coefficient (−1 ≤ r_i ≤ 1) measures both the strength and direction of a linear relationship between X_i and Y. If r_i = ±1, it means input i is linearly important. If X_i and Y are independent, then the covariance and the correlation are zero, but the reverse is not always true. This method does not identify nonlinear relationships between the input and output [Con80].

The Spearman correlation is computed by replacing the data with their ranks in the Pearson correlation coefficient. In this situation, the Spearman correlation coefficient can be used to determine sensitivities of monotonic relationships between the model output with the variable of interest (where all others are ignored). SA methods that do not consider linear or monotonic relationships between model output and inputs are studied in the next section.

2.4 Nonlinear SA methods

In this section, nonlinear SA methods that do not assume any specific relationship between model output and inputs are presented. These methods are based on various mechanisms such as variance, metric distance and differentiation. In what follows we assume that the inputs are independent.

2.4.1 Variance

In this subsection, SA methods based on variance are introduced. They are classified into decomposing and classical approaches. In a decomposing approach, such as Sobol’s method, a “decomposition” of the original model is first computed. By this decomposition, the mapping factor between inputs and output and all the sensitivity indices can be obtained. In the classical family of methods, the Fourier Amplitude Sensitivity Test (FAST) estimates the variances directly to obtain the sensitivity indices [CFS+73, CLS78]. Higher order interactions can be computed using the Extended FAST method [STC99].

Sobol’s method

Sobol’s method is a global SA method for nonlinear models. It decomposes the output variance and then analyzes the variances decomposition [Sob01]. In other words, the Sobol’s method is an analysis of variances
2.4. Nonlinear SA methods

(ANOVA) decomposition. The Sobol sensitivity indices are obtained from the ANOVA decomposition of $G(x)$

$$G(x) = G_0 + \sum_i G_i(x_i) + \sum_{i<j} G_{ij}(x_i, x_j) + ... + G_{12...d}(x_1, x_2, ..., x_d). \quad (2.2)$$

In this method, $G(x)$ must be square-integrable and Equation (2.2) is unique only if the inputs are independent. The expectations of all orthogonal components in Equation (2.2) except $G_0$ are zero. These orthogonal components can be obtained by

$$G_0 = E[Y],$$
$$G_i(x_i) = E[Y|X_i] - G_0,$$
$$G_{ij}(x_i, x_j) = E[Y|X_i, X_j] - G_0 - G_i(x_i) - G_j(x_j).$$

The variance of $G(x)$ equals

$$V[G(x)] = V[G_0] + \sum_i V[G_i(x_i)] + \sum_{i<j} V[G_{ij}(x_i, x_j)] + ... + V[G_{12...d}(x_1, x_2, ..., x_d)].$$

Finally, the sensitivity of the $i$th input denoted by $(SI_i)$ is the contribution of the input $x_i$ to the output variability. This sensitivity index is defined as

$$SI_i = \frac{V[G_i(x_i)]}{V[G(x)]} \in [0, 1]. \quad (2.3)$$

Note that

$$SI_i + SI_{i,j} + ... + SI_{i,j,...,d} = 1.$$

**Fact 2.3. [JKLN13]** The following relation holds.

$$SI_i = \frac{V[G_i(x_i)]}{V[G(x)]} = \frac{\text{cov}(G_i(x_i), G(x))}{V[G(x)]}.$$  

**Proof.** Considering $E[G_i(x_i)] = 0$ and $E[G_i(x_i), G(x)] = E[G_i(x_i)^2]$ because of the orthogonal elements in Equation (2.2), $V[G_i(x_i)] = \text{cov}(G_i(x_i), G(x))$ since

$$V[G_i(x_i)] = E[G_i(x_i)^2] - (E[G_i(x_i)])^2 = E[G_i(x_i)^2],$$
$$\text{cov}(G_i(x_i), G(x)) = E[G_i(x_i), G(x)] - E[G_i(x_i)] E[G(x)] = E[G_i(x_i)^2],$$

the result follows. \qed
2.4. Nonlinear SA methods

The complete sensitivity information of input \( x_i \) is given by its main effect on the output variability \((SI_i)\) and its interactions with other inputs. The main effect of input \( x_i \) and its interactions are shown by its total sensitivity index \((SI^\text{tot}_i)\), which is computed as

\[
SI^\text{tot}_i = 1 - \frac{V(G_{-i})}{V(G)} = 1 - SI_{-i},
\]

where \( V(G_{-i}) \) denotes the variance of all the orthogonal elements in Equation (2.2) that do not have input \( x_i \). For example, \( SI^\text{tot}_1 \) for a model with 3 inputs is

\[
SI^\text{tot}_1 = SI_1 + SI_{1,2} + SI_{1,3} + SI_{1,2,3} = 1 - SI_2 - SI_3 - SI_{2,3}.
\]

The Sobol total sensitivity indices \( SI^\text{tot}_i \) help to find the inputs that can be fixed in their ranges of variability without influencing the output [SRTC05] (in this case, \( SI^\text{tot}_i \) is zero for input \( i \) while its \( SI_i \) is not zero [SRTC12]).

Sobol used the Monte Carlo method to estimate the sensitivity indices and suggested to use Sobol sequences for faster convergence [Sob01, SRA+08]. Equation (2.3) \((SI_i)\) and Equation (2.4) \((SI^\text{tot}_i)\) give a deep understanding of the model. Using Equation (2.4) and estimating it by the Monte Carlo method helps to eliminate the curse of dimensionality since there is no need to estimate all terms in Equation (2.2) (or for example the terms in Equation (2.5)) [SRTC05].

Janon et al. [JKLN13] presented the Homma [HS96] and Monod estimators [MNM06] to approximate the Sobol indices. Two independent samples with identical distributions \( x_s = (x_{R,s}, x_{R^c,s}) \), \( x'_s = (x'_{R,s}, x'_{R^c,s}) \) are considered \((s = 1, ..., N)\). In addition, two outputs \( y_s = G(x_s) \) and \( y'_s = G(x'_{R,s}, x'_{R^c,s}) \) are computed. The Sobol index estimators are

\[
H_{x_R} = \frac{1}{N} \sum y_s y'_s - \left( \frac{1}{N} \sum y_s \right) \left( \frac{1}{N} \sum y'_s \right) \approx \frac{\text{cov}(Y,Y^*)}{V(Y)},
\]

\[
M_{x_R} = \frac{1}{2N} \sum y_s y'_s - \left( \frac{1}{2N} \sum y_s + y'_s \right)^2,
\]

where \( H_{x_R} \) and \( M_{x_R} \) denote the Homma estimator and the Monod estimator, respectively. The asymptotic variance of the Monod estimator is less or equal to that of the Homma estimator [JKLN13]. Consequently, \( M_{x_R} \) is more accurate than \( H_{x_R} \) and should be used instead.

There are other Monte Carlo based estimators for the Sobol indices [GI12, Sal02, STG+07, Jan99, SAA+10, LT09]. The Glen formula [GI12]...
2.4. Nonlinear SA methods

estimates the Sobol indices with regard to the Pearson correlation. Consider
\[ y_s = G(x_s), \quad y_s' = G(x_{R,s}, x_{Rc,s}'), \quad y_s'' = G(x_{R,s}', x_{Rc,s}) \text{ and } \quad y_s' = G(x_s'). \]

The Glen equations for the first order sensitivity and the total sensitivity of \( x_R \) are denoted by \( G_{X_R} \) and \( G_{X_R}^{\text{tot}} \) and defined as

\[
G_{x_R} = \frac{1}{2} \left[ r(Y^*, Y) + r(Y', Y^*) - r(Y', Y) - r(Y'', Y^*) \right],
\]

\[
G_{x_R}^{\text{tot}} = 1 - \frac{1}{2} \left[ r(Y'', Y) + r(Y', Y^*) - r(Y', Y) - r(Y'', Y^*) \right],
\]

where \( r \) denotes the Pearson correlation. The term \(-r(Y', Y) - r(Y'', Y^*)\) improves the accuracy of the index estimation [GI12].

In [GI12], this estimator is implemented on a test function and compared with other Monte Carlo based estimation formulas such as Mauntz formulas [Sal02, STG07], Jansen formula [Jan99, SAA10], Lilburne and Tarantola formula [LT09] and eight other formulas. The comparison on this test function shows that the Glen formula [GI12], and the Lilburne and Tarantola formula [LT09] are more accurate than the other methods.

**Remark 2.4 (Dependent input parameters).** Chastaing et al. [CGP12] introduce new indices measuring the sensitivity of output to the dependent inputs as

\[
SI_i = \frac{V[G_i(X_i)] + \sum_{v \neq \emptyset, i \notin v} \text{Cov}(G_i(X_i), G_v(X_v))}{V[Y]},
\]

(2.7)

where \( G_v(X_v) \) is any component in Equation (2.2) that does not have input \( i \).

**Fourier Amplitude Sensitivity Test (FAST)**

The FAST method is also based on the ANOVA decomposition and the conditional variances are obtained by the Fourier coefficients. In other words, this method uses a periodic sampling and the Fourier transformation to find the output variance and the conditional variances [CFS73]. For obtaining the FAST indices, frequencies are assigned to the inputs by an arbitrary function \( g \)

\[
x_i(s') = g_i \left( \sin \left( w_i s' + \phi_i \right) \right),
\]

where the frequency, \( w_i \) \((i = 1, ..., d)\) is an integer [CLS78]. One of the transformations \( (g) \) suggested by Saltelli et al. [STC99] is \( x_i = \frac{1}{2} + \frac{1}{2} \arcsin(\sin w_i s + \phi_i) \), where \( \phi_i \) is a random phase-shift uniformly chosen \( \in [0, 2\pi) \). Cukier et al. [CFS73] explain how to select the set of integer frequencies. One
2.4. Nonlinear SA methods

frequency is assigned to each input parameter and each input is a function of \( w \) and \( s' \) \((-\infty < s' < \infty)\). The Weyl theorem [Wey38] gives

\[
\int_{0}^{1} G(x) \, dx_1 \ldots dx_d = \lim_{T \to \infty} \frac{1}{2T} \int_{-T}^{T} G(x(s')) \, ds',
\]

therefore, \( G_0 = \lim_{T \to \infty} \frac{1}{2T} \int_{-T}^{T} G(x(s')) \, ds' \). As the function \( G(x(s')) \) is periodic with period \( 2\pi \), then \( \lim_{T \to \infty} \frac{1}{2T} \int_{-T}^{T} G(x(s')) \, ds' = \frac{1}{2\pi} \int_{-\pi}^{\pi} G(x(s')) \, ds' \). Hence, the expectation and the variance of the output are approximated as

\[
G_0 = \frac{1}{2\pi} \int_{-\pi}^{\pi} G(x(s')) \, ds',
\]

\[
V(G(x)) = \frac{1}{2\pi} \int_{-\pi}^{\pi} G^2(x(s')) \, ds' - G_0^2.
\]

The application of Parseval’s theorem to Equation (2.8) leads to

\[
V(G(x)) = 2 \sum_{l=1}^{\infty} (A_l^2 + B_l^2),
\]

where, \( A_l \) and \( B_l \) are the cosine and the sine Fourier coefficients at harmonic \( l \) [SB98].

The conditional variance \( V(G_i(x_i)) \) is obtained by the cosine and the sine Fourier coefficients at frequency \( w_i \) and the higher harmonics (\( l \)). The cosine and the sine Fourier coefficients at frequency \( w_i \) and harmonic \( l \) are denoted \( A_{l,w_i} \) and \( B_{l,w_i} \), and given by

\[
A_{l,w_i} = \frac{1}{\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} G(x(s')) \cos(lw_is') \, ds',
\]

\[
B_{l,w_i} = \frac{1}{\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} G(x(s')) \sin(lw_is') \, ds'.
\]

The variances are estimated as

\[
V(G_i(x_i)) = 2 \sum_{l=1}^{\infty} (A_{l,w_i}^2 + B_{l,w_i}^2) \approx 2 \sum_{l=1}^{M} (A_{l,w_i}^2 + B_{l,w_i}^2),
\]

\[
V(G(x)) \approx 2 \sum_{i=1}^{d} \sum_{l=1}^{M} (A_{l,w_i}^2 + B_{l,w_i}^2),
\]
and the sensitivity index is computed as

\[ SI_i = \frac{V(G_i(x_i))}{V(G(x))} \approx \frac{\sum_{l=1}^{M} (A_{l,w_i}^2 + B_{l,w_i}^2)}{\sum_{i=1}^{d} \sum_{l=1}^{M} (A_{l,w_i}^2 + B_{l,w_i}^2)}, \]

(2.9)

where \( M \) is the interface factor (4 or higher) [STC99] and for estimating \( A_{l,w_i} \) and \( B_{l,w_i} \), \( N = 2Mw_{\max} + 1 \) samples are used \((s' = 1, ..., N)\) where \( w_{\max} \) is the maximum frequency among \( w_i(i = 1, ..., d) \).

**Extended Fourier Amplitude Sensitivity Test (EFAST)**

The FAST method above only allows for estimation of main effects [AIGMA05]. To improve the EFAST method, the extended FAST (EFAST) was introduced by Saltelli et al. [STC99]. The EFAST method is based on the FAST method and also finds the higher interactions. The EFAST sensitivity indices are computed as

\[ x_i = g(\sin(w_i s')) , \]

\[ V(G_i) = 2 \sum_{l=1}^{\infty} (A_{l,w_i}^2 + B_{l,w_i}^2) \approx 2 \sum_{l=1}^{M} (A_{l,w_i}^2 + B_{l,w_i}^2) , \]

\[ V(G) \approx 2 \sum_{i=1}^{d} \sum_{l=1}^{M} (A_{l,w_i}^2 + B_{l,w_i}^2) , \]

\[ SI_i = \frac{V(G_i)}{V(G)} , \]

\[ ST_i^{tot} = 1 - SI_{-i} . \]

(2.10)

For estimating \( V(G_i) \), \( N = 2Mw_{\max} + 1 \) samples are used \((s' = 1, ..., N)\) for \( x_i \) and the cosine and the sine Fourier coefficients [MTS82] can be estimated as

\[ A_j = \begin{cases} 0 & \text{when } l \text{ is odd}, \\ \frac{1}{N} \left[ y(N_0) + \sum_{k=1}^{q} CosS(k) \cos \left( \frac{\pi j k}{N} \right) \right] & \text{when } l \text{ is even}, \end{cases} \]

\[ B_j = \begin{cases} 0 & \text{when } l \text{ is even}, \\ \frac{1}{N} \left[ y(N_0) + \sum_{k=1}^{q} SinS(k) \sin \left( \frac{\pi j k}{N} \right) \right] & \text{when } l \text{ is odd}, \end{cases} \]

where \( CosS(k) = (y(N_0 + k) + y(N_0 - k)) \).
2.4. Nonlinear SA methods

where \( \sin S(k) = (y(N_0 + k) - y(N_0 - k)), q = \frac{N-1}{2} \) and \( N_0 = q + 1 \).

The EFAST method (like the FAST method) needs fewer samples than Sobol’s method, and (like Sobol’s method) is also able to find higher interactions \([\text{AIGMA05, STC99}]\).

First-order variance coefficient

The first-order variance coefficient is another interpretation for ANOVA and is defined \([\text{M}^+95, \text{MMM08}]\) as

\[
\theta_i = V[Y] - E[V[Y|X_i]], \\
\eta_i = \frac{\theta_i}{V[Y]},
\]

(2.11)

where \( \eta_i \) is equal to the Sobol sensitivity index \( SI_i \). For the Monte Carlo estimation of these sensitivity indices, Morris et al. \([\text{MMM08}]\) consider a sampling method for inputs that is called unbiased permuted column sample (UPCS) plans, and finds the precise estimation of the first-order sensitivity indices. As the UPCS plan can estimate the first-order sensitivity index precisely and this index just gives information about the main effects of inputs, this method can be used when the interactions between inputs are not required to be studied.

UPCS plan

The UPCS is generated as follows. Suppose matrix \( A^a \) \((a = 1, 2, \ldots, r)\) has \( N' \) rows and \( d \) columns and each column contains a random permutation of the integers from 1 to \( N' \). The random integer \( i \) in column \( j \) denotes the \( i^{th} \) sample in the sample set of input \( j \). The \( N' \) samples of \( d \) inputs are shown by matrix \( X^a \) which can be obtained by matrix \( A^a \) and input sample sets. Consequently, \( N = r \times N' \) samples for inputs are obtained by \( r \) matrices of \( X^a \) which lead to \( N \) samples of \( Y \).

For example, suppose \( d = 3, N' = 4 \) and all inputs have the same random sample set \( \{0.125, 0.375, 0.625, 0.875\} \). If the matrix \( A^a \) is equal to

\[
A^a = \begin{bmatrix}
2 & 1 & 4 \\
1 & 3 & 1 \\
3 & 4 & 3 \\
4 & 2 & 2 \\
\end{bmatrix},
\]
2.4. Nonlinear SA methods

then $Y^a$ becomes

$$X^a = \begin{bmatrix}
0.375 & 0.125 & 0.875 \\
0.125 & 0.625 & 0.125 \\
0.625 & 0.875 & 0.625 \\
0.875 & 0.375 & 0.375
\end{bmatrix}.$$  

Note that this permuted column sample is unbiased when $(A^{a}_{i,j}, A^{a'}_{i,j'})$ \neq $(A^{a'}_{i,j'}, A^{a}_{i,j'})$ for all $a = 1, 2, ..., r, a' = 1, 2, ..., r, i = 1, 2, ..., N', i' = 1, 2, ..., N', i \neq i', j = 1, 2, ..., d, j' = 1, 2, ..., d$ and $j \neq j'$.

The $\eta_i$ in Equation (2.11) is estimated by the Monte Carlo method and the UPCS in [MMM08].

Wei’s method

Wei et al. [WLS13] introduced a variance-based SA method, which provides different information than Sobol’s method. The ranking of the proposed indices indicates the influences of the parameters that reduce the output variance. The goal is to evaluate the impact of the range of input parameters on the output. Reducing the size of the interval of input parameters results in significant computation savings while providing the same information.

In this method, one input or a set of inputs ($x_R = (x_{i_1}, x_{i_2}, ..., x_{i_{d'}})$ with $d' \leq d$) is selected. For each selected input, two quantile values that are correlated and uniformly distributed are considered. Let $q_{i_k}(1)$ and $q_{i_k}(2)$ ($i_k \in \{i_1, ..., i_{d'}\}$) be the two quantile values for the $k^{th}$ member of the selected set of inputs such that $0 < q_{i_k}(1) < q_{i_k}(2) < 1$. The quantile values of different inputs should be independent since the inputs are supposed to be independent. These quantile values lead to values $u_{i_k}(1) = F^{-1}_{i_k}(q_{i_k}(1))$ and $u_{i_k}(2) = F^{-1}_{i_k}(q_{i_k}(2))$ that define the reduced range of the input $x_{i_k} \in [u_{i_k}(1), u_{i_k}(2)]$.

Consider the two matrices

$$Q_R = \begin{bmatrix}
q_{i_1}(1) & q_{i_2}(1) & ... & q_{i_{d'}}(1) \\
q_{i_1}(2) & q_{i_2}(2) & ... & q_{i_{d'}}(2)
\end{bmatrix}^T,$$

$$U_R = \begin{bmatrix}
u_{i_1}(1) & u_{i_2}(1) & ... & u_{i_{d'}}(1) \\
u_{i_1}(2) & u_{i_2}(2) & ... & u_{i_{d'}}(2)
\end{bmatrix}^T,$$

the main and the total sensitivity indices for the selected inputs are denoted
2.4. Nonlinear SA methods

by $W_R$ and $W_{TR}$ and they are defined [WLS13] as

\[
W_R = \frac{E_{Q_R} [V(Y) - V_X(Y|x_R \in U_R)]}{V(Y)} = 1 - \frac{E_{Q_R}([V_X(Y|x_R \in U_R)])}{V(Y)},
\]

\[
W_{TR} = \frac{E_{Q_{-R}} [V_X(Y|X_{-R} \in U_{-R})]}{V(Y)},
\]

where the output model is noted $Y$, and $V_X$ is the variance with respect to $x_R$ over the reduced ranges $U_R$ and with respect to $x_{-R}$ over the full ranges. The expectation with respect to all elements of $Q_R$ is noted $E_{Q_R}$ and these sensitivity indices are bounded in $[0, 1]$.

Sensitivity index $W_R$ studies the effect of reducing the selected inputs ranges (to matrix $U_R$) on the output variable. A small value of $W_R$ indicates that reducing the range (distribution) of $x_R$ has a small effect on the reduction of output variability. For example, if $W_R = 0$, then $E_{Q_R}([V_X(Y|x_R \in U_R)]) = V(Y)$, which means that when the ranges of $x_R$ are reduced to $U_R$, the variance of the output stays constant. In other words, reducing the range of $x_R$ has no effect to reduce output variability. If $W_R = 1$, then $E_{Q_R}([V_X(Y|x_R \in U_R)]) = 0$, which means that by reducing the range of $x_R$ ($x_R \in U_R$), the output variability becomes 0.

Sensitivity index $W_{TR}$ studies the effect of reducing the remaining inputs ranges on the output variable. If $W_{TR} = 1$, then $E_{Q_{-R}}([V_X(Y|x_{-R} \in U_{-R})]) = V(Y)$ which means if the ranges of the remaining inputs $x_{-R}$ are reduced, the output variance stays constant $V(Y)$. This reveals that the output variance is fully dependent on $x_R$. If $W_{TR} = 0$, then the output variance is fully dependent on $x_{-R}$ and no variance is caused by $x_R$.

Consequently, the information provided by Wei’s and Sobol’s methods are different. The high values of the Wei indices indicate the inputs that reduce output variability when these input ranges are reduced, whereas the high values of the Sobol indices indicate which inputs has the highest contribution to the output variability when the distribution of inputs are fixed.

2.4.2 Variance-mean

The contribution to the sample mean (CSM) plot and the contribution to the sample variance (CSV) plot are two graphical SA methods. The CSV is presented by Tarantola in [TKBL+12] who combined it with the CSM proposed by Sinclair [Sin93]. The CSV and the CSM for the input $X_i$ show
the influence of this input on the output $Y$. They are defined as

$$ E(Y) = \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} G(x) f_X(x) dx, $$

$$ CSM_{X_i}(q) = \frac{1}{E(Y)} \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} \int_{-\infty}^{F_{X_i}^{-1}(q)} G(x) \prod_{i=1}^{d} f_{X_i}(x_i) dx_i dx_1 \ldots dx_{i-1} dx_{i+1} \ldots dx_d, \quad (2.13) $$

$$ V(Y) = \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} f_X(x) (G(x) - E(G(x)))^2 dx, $$

$$ CSV_{X_i}(q) = \frac{1}{V(Y)} \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} \int_{-\infty}^{F_{X_i}^{-1}(q)} (G(x) - E(G(x)))^2 \prod_{i=1}^{d} f_{X_i}(x_i) dx_i $$

$$ \times dx_i dx_1 \ldots dx_{i-1} dx_{i+1} \ldots dx_d, \quad (2.14) $$

where $q \in [0, 1]$.

The $CSM_{X_i}$ values are plotted for different values of $q$ and the sensitivity of $X_i$ can be measured by how much the $CSM_{X_i}(q)$ curves deviates from the diagonal. As an example, the $CSM_{X_i}(q)$ for three inputs of the Ishigami function (2.28) shown in Figure 2.1 indicates the most important input is $x_1$.

![Figure 2.1: The $CSM_{X_i}(q)$ for three inputs of the Ishigami function.](image)

The $CSV_{X_i}(q)$ is used to study the reduction of output variability by reducing the ranges of inputs. Let us define $VarRatio_{X_i}(q_1, q_2)$ (which can
be bigger than 1) as

\[ VarRatio_{X_i}(q_1, q_2) = \frac{CSV_{X_i}(q_2) - CSV_{X_i}(q_1)}{q_2 - q_1}, \quad (0 \leq q_1 < q_2 \leq 1). \]

This function \( VarRatio_{X_i}(q_1, q_2) \) shows the ratio of the output variance when the range of input \( X_i \) is reduced ([\( q_1, q_2 \)]) to the output variance when the range of input \( X_i \) is not reduced ([0, 1]). By plotting \( VarRatio_{X_i}(q_1, q_2) \), the effect of reducing the range of input \( X_i \) to the output variance is shown. The effect of reducing the input ranges on the output variance of the Ishigami function is shown in Figure 2.2.

As Figure 2.2 shows, if \( q = 0.05 \) for \( X_3 \) (which means reducing the range of \( X_3 \) to [0.05,0.95] or reducing the range of \( X_3 \) by 10%), then the variance of the output reduces by 32% (100% - 68%) (the output variance ratio is 0.68 which indicates that the ratio of the output variance when the range of \( X_3 \) is reduced (by 10%) to the output variance with no input range reduction is 0.68). Figure 2.2 also shows that reducing the range of \( X_2 \) toward zeros (\( q = 0.5 \)) increases \( VarRatio_{X_i}(q_1, q_2) \). Consequently, an effective variance reduction can be obtained by reducing the range of \( X_3 \).

Plischke [Pli12] introduces the CUSUNORO approach that improves CSM for non-positive data or an output with mean of zero.
2.4. Nonlinear SA methods

2.4.3 Factor screening methods

In this section, two methods based on factor screening proposed by Morris [Mor91] and Saltelli et al. [SRTC12] are explained.

Morris method

Morris introduced a SA method for models that have a moderate-to-large number of inputs [Mor91]. This method can measure the nonlinear relationship between the input and the output. The important input parameters are identified and ranked efficiently using an One-At-a-Time (OAT) design. The OAT SA design changes the input parameters by the same relative amount. The input which makes the largest variation in the output is the most important input. The Elementary Effect ($EE$) is defined as

$$EE_i = \frac{y(x_1, ..., x_{i-1}, x_i + \Delta, ..., x_d) - y(x)}{\Delta}, \tag{2.15}$$

where $\Delta$ is a multiple of $1/(p - 1)$ and $p$ is the number of values (levels) an input can have in a range. The $EE$ evaluates the effect of changing an input by $\Delta$. For example, if $p = 4$, then the possible values for inputs are $\{0, 1/3, 2/3, 1\}$ and an input matrix for $d = 3$ ($d$ is the input dimension) and $\Delta = 1/3$ can be

$$X = \begin{bmatrix}
1 & \frac{1}{3} & 0 \\
1 & \frac{2}{3} & 0 \\
1 & \frac{2}{3} & \frac{1}{3} \\
\frac{2}{3} & \frac{2}{3} & \frac{1}{3}
\end{bmatrix},$$

where column $i$ shows 4 samples for input $X_i$; one of the inputs is changed by a positive or negative $\Delta$ in each input sample (row). By putting the outputs of the first and second rows of this matrix in Equation (2.15), $EE_2$ is obtained (because only $x_2$ is changed). $EE_3$ is obtained by putting the outputs of the second and third rows of this matrix in Equation (2.15) (as input $x_3$ is changed). While the outputs of the third and fourth rows give $EE_1$.

Morris sensitivity indices are calculated by the mean ($\mu_i$) and the standard deviation ($\sigma_i$) of $N$ values of $EE_i$. The biggest values of $\mu_i$ and $\sigma_i$ show the most important input parameter. In addition, $\sigma_i$ shows the interaction with other input and/or the nonlinear effect on the output. They are
computed as

\[ \mu_{EE_i} = \frac{\sum_{s=1}^{N} EE_{i,s}}{N}, \]

\[ \sigma_i = \sqrt{\frac{1}{N} \sum_{s=1}^{N} (EE_{i,s} - \mu_{EE_i})^2}. \] (2.16)

Saltelli et al. [STCR04] suggests to set \( N \) between 4 and 10 and Campolongo [CCS07] proposes to use \( \mu^*_{EE_i} = \frac{\sum_{s=1}^{N} |EE_{i,s}|}{N} \) instead of \( \mu_{EE_i} \) because \( \mu^*_{EE_i} \) prevents any cancellation of the effects that may happen in \( \mu_{EE_i} \).

**Radial screening measure**

Saltelli et al. introduce the following elementary effect

\[ EE_i = |\frac{G(X_{XX}^i) - G(X)}{X_{XX}^i - X}|, \] (2.17)

where matrices \( X \) and \( XX \) are two independent samples for inputs (matrices with \( N \) rows and \( d \) columns) and all the columns of matrix \( X_{XX}^i \) are the same as the columns in \( X \) except its \( i^{th} \) column is obtained from matrix \( XX \). Matrices \( X \) and \( X_{XX}^i \) span the input space since the \( N(d+2) \) samples of \( X \), \( XX \) and \( X_{XX}^i \) make a “radial” design. In other words, the samples from the first row of matrix \( X \) and the first rows of the \( d \) matrices \( X_{XX}^i \) can make a design. The core of this star is the sample from \( X \) while the \( d \) samples from \( d \) matrices \( X_{XX}^i \) make the rays of the star. As there are \( N \) samples, the number of stars is \( N \).

Finally, the radial screening measure for input \( i \) is the average of \( N(N \approx 4 - 8) \) elementary effects \( EE_i \). The advantage of this method is that it explores the input space more efficiently than the Morris method.

**2.4.4 Derivative-based method**

In what follows, two methods based on derivatives, namely derivative-based global sensitivity measures (DGSM) [K+09] and Wang’s methods [WLHZ14], are described. DGSM is just based on the partial derivatives while the partial derivatives and the ANOVA-like decomposition (described in Subsection 2.4.1) are used in Wang’s method.
2.4. Nonlinear SA methods

Derivative-based global sensitivity measures

Kucherenko et al. [K+09] use the local sensitivity measures based on partial derivatives \( \frac{\partial G}{\partial x_i} \) and define three measures as

\[
M_i^* = \int \left| \frac{\partial G}{\partial x_i} \right| \, dx,
\]

\[
\Sigma_i^* = \sqrt{\int \left( \left| \frac{\partial G}{\partial x_i} \right| - M_i^* \right)^2 \, dx},
\]

\[
\Gamma_i = \Sigma_i^* + M_i^*.
\]

The set of \( M_i^*, \Sigma_i^*, \Gamma_i \) are called derivative-based global sensitivity measures (DGSM) [K+09]. DGSM are compared with the Sobol and Morris methods in [K+09] and the results show this approach is faster and more accurate than the Morris method. In addition, there is a link between DGSM and the Sobol indices. However, the computational time for computing DGSM is lower than the computational time for the Sobol indices.

Wang’s method

The distribution parameters of inputs (such as the means and variances of input distributions) are not taken into account in the variance-based sensitivity indices [WLHZ14]. Thus, Wang et al. propose sensitivity indices based on derivative and ANOVA-like decomposition that indicate the influence of input distribution parameters [WLHZ14]. In other words, the proposed sensitivity indices are complementary to the variance-based sensitivity indices.

The proposed sensitivity indices are obtained by the partial derivative first-order variance contribution (FOVC) with respect to the distribution parameters. These indices are simplified by the kernel functions that are obtained analytically for different distributions. For example, the partial derivatives of \( V_i \) with respect to the distribution parameters \( \theta_{X_i} \) of input \( X_i \) and \( \theta_{X_j} \) of input \( X_j \) \( (X_j \in x_R) \) are derived as

\[
\frac{\partial V_i}{\partial \theta_{X_i}} = E \left( (E(Y|X_i) - E(Y))^2 \right) k_i,
\]

\[
\frac{\partial V_i}{\partial \theta_{X_j}} = 2E \left( (E(Y|X_i) - E(Y)) (E(Y|X_j) - E(Y|X_j)) \right),
\]

where \( k_i \) is the kernel function of \( \theta_{X_i} \) and equals \( \frac{\partial f(x_i)}{\partial x_i} \frac{1}{f(x_i)} \).
For example, assume the model is a quadratic polynomial without cross terms such as

\[ Y = a_0 + \sum_{i=1}^{d} a_i X_i + \sum_{i=1}^{d} b_i X_i^2, \]

where input \( X_i \) has normal distribution with mean \( \mu_i \) and variance \( \sigma_i^2 \). The kernel function of these normal distribution parameters \( \mu_i \) and \( \sigma_i^2 \) are found as

\[ k_{\mu_i} = \frac{X_i - \mu_i}{\sigma_i^2}, \]

\[ k_{\sigma_i} = \frac{1}{\sigma_i} \left( \frac{X_i - \mu_i}{\sigma_i} \right)^2 - 1. \]

Finally, the proposed sensitivity indices, which are the derivatives of FOVC with respect to \( \mu_i \) and \( \sigma_i \), are

\[ \frac{\partial V_i}{\partial \mu_i} = 4b_i \sigma_i^2 \left( a_i + 2b_i \mu_i \right), \]

\[ \frac{\partial V_i}{\partial \sigma_i} = 2\sigma_i \left( a_i^2 + 4a_i b_i \mu_i + 4b_i^2 (\mu_i^2 + \sigma_i^2) \right). \]

The FOVC \( V_i \) are independent of \( \mu_j \) and \( \sigma_j \) in a model without cross terms.

Since FOVC does not need additional computational cost during computing the variance-based sensitivity indices, this method should be used as a by-product of the Sobol method (or any variance-based method). In addition, FOVC and variance-based sensitivity indices may lead to different information and using the information of both methods leads to a better insight.

### 2.4.5 Distance between distributions

Chun [CHT00] examines the problem of characterizing the uncertainty in the output with respect to changes in the distribution of the input. In other words, the sensitivity indices are found by computing the distance between the two different cumulative distributions. This method is different from other methods where the output uncertainty is studied by sampling a particular input parameter with a fixed distribution.

In this method, the Euclidean distance between two output cumulative distributions is computed. The output CDF when all the inputs have their nominal distribution is noted \( F_Y \). The output CDF when the distribution of
input $i$ is changed is noted $F_i$. In this method, this distance is normalized by the mean of $Y$ as

$$SI_i = \frac{\left(\int [F_i(y) - F_Y(y)]^2 dy\right)^{1/2}}{E(Y)}.$$  \hspace{1cm} (2.20)

This method can measure the effect of an input distribution on the output distribution (both mean and variance of output). In addition, the concept of this method is simple and the indices can be calculated easily. However, the precise distribution of output is required.

### 2.4.6 Moment independence measures

Borgonovo [Bor07] explains that the variance based SA methods cannot provide complete information about the influence of input parameters on output, because variance is just one of the distribution moments (mean is another moment of distribution) and also the variance-based methods assume that inputs are independent.

In addition, monotonic transformation $T$ is used in some engineering applications to obtain convergence and stable estimations. However, using variance-based SA with transformation can be misleading because the variance-based SA are not invariant to monotonic transformation which means given any monotonic function $T$, the variance-based sensitivity of $T(Y)$ to any input is dependent on $T$ [BB13, BTPM14]. Consequently, sensitivity indices that are independent of any given monotonic transformation $T$ are required.

Some sensitivity indices, which are invariant under monotonic transformation (the sensitivity of $T(Y)$ to any input is independent of the monotonic function $T$), are proposed in [BB13, BTPM14]. These sensitivity indices are based on the distance between distributions [BB13, Bor07, BTPM14] and are defined as

$$SI_i = E_i \left[ \text{distance} \left( P_Y, P_{Y|X_i} \right) \right], \hspace{1cm} (2.21)$$

where, $P$ is probability. The measure used in [Bor07] is based on the $L^1$-distance between densities as

$$SI_{i}^{\text{Bor}} = \frac{1}{2} \int f_{X_i}(x_i) \left[ \int \left| f_Y(y) - f_{Y|X_i}(y) \right| dy \right] dx_i. \hspace{1cm} (2.22)$$

If $Y$ is independent of $X_i$, then $SI_i$ equals zero. The sensitivity index of a subset including all inputs $SI_{1,2,\ldots,d}$ is 1. If inputs are independent then
2.5 Surrogate-based methods for expensive function models

$SI_{1,2,...,d} = SI_i + ... + SI_d = 1$ [Bor07]. This sensitivity index is efficiently estimated in [PBS13]. It should be noted that it is possible that Borgonovo’s method and the variance-based methods provide different importance ranking of inputs because they are based on different mechanisms [Bor07].

The sensitivity measures in [BB13, BTPM14] are based on the cumulative distribution functions ($SI_i = E_i[\text{distance}(F_Y, F_Y|X_i)]$) and use the Kolmogorov-Smirnov metric ($KS$) and Kuiper metric ($Ku$) as

$$
SI_i^{KS} = E\left[\sup_y \{|F_Y(y) - F_Y|X_i(y)\}|\right],
$$

$$
SI_i^{Ku} = E\left[\sup_y \{|F_Y(y) - F_Y|X_i(y)\}| + \sup_y \{F_Y|X_i(y) - F_Y\}\right].
$$

(2.23)

The $SI_i^{KS}$ and $SI_i^{Ku}$ are better than $SI_i^{Bor}$, because they are based on the cumulative distribution functions and the cumulative distribution functions are defined for all distributions even if the distribution of output does not admit a probability density function (if the distribution of $X$ admits a probability density function, then $E[X] = \int_{-\infty}^{\infty} x f_X(x)dx$) [BB13]. Therefore, $SI_i^{Bor}$ cannot be used in such cases that the output distribution does not admit a probability density function (for example, the Cantor distribution).

In addition, $SI_i^{KS}$ and $SI_i^{Ku}$ always converge but $SI_i^{Bor}$ may not converge [BTPM14]. Baucells et al. also suggest using $SI_i^{KS}$ and $SI_i^{Ku}$ with focus on $SI_i^{Ku}$ [BB13].

2.5 Surrogate-based methods for expensive function models

In some SA methods, computing the sensitivity indices requires a lot of function evaluations, which is impractical for expensive model functions. Therefore, constructing approximation models becomes necessary. The approximating model is known as a surrogate model, metamodel, emulator or response-surface model. We now describe the Gaussian Process (GP) that not only builds a surrogate model, but also accounts for the uncertainty in evaluating the parameters.

Let $(x_s, y_s), s = 1, 2, ..., N$ be a sample set of $d$-dimensional input and output. Then the GP surrogate is defined as

$$
\hat{G}(x) = g(x)\beta + Z(x),
$$

(2.24)
where \( g(.) \) is a \( 1 \times h \) vector of arbitrary regression functions of \( x \) (the choice of \( g(x) \) is arbitrary, but it should fit the samples), \( \beta \) is a \( h \times 1 \) vector of parameters that should be estimated, and the function \( Z(x) \) is a Gaussian process that has mean 0 and variance \( \sigma^2 \) [OO04]. The covariance between \( Z(x') \) and \( Z(x'') \) (\( x' \) and \( x'' \) are two input vectors) is

\[
\text{Cov}[Z(x'), Z(x'')] = \sigma^2 C(x', x''),
\]

where \( C(\cdot, \cdot) \) is a correlation function that decreases as \( |x' - x''| \) increases and \( C(x, x) = 1 \) [OO04]. A popular choice for \( C(\cdot, \cdot) \) is

\[
C(x', x'') = \prod_{j=1}^{d} \exp(-\theta_j |x'_j - x''_j|^{v_j}),
\]

where \( \theta_j \) and \( 0 < v_j < 2 \) are estimated from the sample set [SW06]. Schonlau and Welch [SW06] used the maximum likelihood to estimate \( \beta \) in Equation (2.24), \( \sigma^2 \) in Equation (2.25), \( \theta_j \) and \( v_j \) in Equation (2.26). Alternatively, Oakley and O’Hagan. [OO04] adopt a Bayesian approach for finding the unknown parameters.

**GP — variance**

Schonlau et al. [SW06] compute the ANOVA decomposition of the GP surrogate, which can then be used to compute the Sobol indices. Alternatively, Oakley and O’Hagan [OO04] and Farah and Kottas [FK14] apply a Bayesian approach to the GP surrogate and account for the uncertainty in estimating the parameters when computing the Sobol indices.

**GP advantages and disadvantages**

The GP interpolates the observed data and is highly efficient for sensitivity analysis [OO04]. Unlike other metamodelling methods, applying a Bayesian approach to the GP accounts for uncertainty in using the surrogate in place of the original function when estimating the Sobol indices.

The disadvantages of the GP is that it requires various parameters to be estimated and the correlation function \( C \) is difficult to be chosen properly. Inappropriate values for these parameters or a bad choice for the correlation function may lead to a poor surrogate [BO09].

### 2.6 Sensitivity indices for multivariate outputs

This section is devoted to the sensitivity analysis of models with multivariate output. The multivariate output can be static, e.g., a vector of
2.6. Sensitivity indices for multivariate outputs

different measurements, or dynamic (same measurement is observed over multiple time points; sometimes referred to as functional output). A static model is time-invariant while a dynamic model is time-dependent. In other words, the output of a dynamic model at time $t^*$ is dependent on inputs at time $t < t^*$. The dynamic output is multivariate although it is a scalar at each specific time.

Most of the multivariate SA methods are devoted to dynamic models, while Gamboa et al. [GJKL13] generalize Sobol’s method to static models with high dimensional outputs.

2.6.1 Multivariate Sobol sensitivity analysis

Gamboa et al. [GJKL13] study the Sobol sensitivity indices for a static model that has a vector output. By a Monte Carlo estimator, the sensitivity index for a set of input $(X_R)$ is computed as

$$SI_R = \frac{\sum_{j=1}^{l} \left( \sum_{s=1}^{N} y_{j,s} y_{j,s}^* - \frac{1}{2N} \left( \sum_{s=1}^{N} y_{j,s} + y_{j,s}^* \right)^2 \right)}{\sum_{j=1}^{l} \left( \frac{1}{2} \sum_{s=1}^{N} y_{j,s}^2 + \left( y_{j,s}^* \right)^2 - \frac{1}{2N} \left( \sum_{s=1}^{N} y_{j,s} + y_{j,s}^* \right)^2 \right)},$$

where $y = (Y_1, ..., Y_l) = G(x)$, $y^* = (Y_1^*, ..., Y_l^*) = G(x_R, x'_R)$ and $x'_R$ is another independent sample for $x_R$. We note $y_{j,s}$ the $s$th sample for $Y_j$ and $y_{j,s}^*$ the $s$th sample for $Y_j^*$. The advantage of this method is that the influence of each input on the outputs of a multivariate model is shown by just one index. This method may be expensive when the model output is high dimensional.

2.6.2 Sequential sensitivity analysis

The sequential sensitivity analysis method is introduced as a multivariate global SA for a dynamic model [PCS+96]. The output is stored in a $N \times T$ matrix. Each column of this matrix shows the value of the output at a given time and each row presents the output for a given input.

By ANOVA (described in Subsection 2.4.1), the sensitivity of the output at each time (each column) is computed and the sensitivity indices are plotted.

The benefit of this method is that it shows when the influence of the input parameters decreases or increases. The interactions between input parameters can be computed and shown for any dynamic model with one or more outputs.
2.6. Sensitivity indices for multivariate outputs

This method is practical when the outputs at different times are not correlated.

2.6.3 PCA-based multivariate sensitivity analysis

Campbell et al. [CMW06, LML+09, LMM11] suggest to implement PCA on the output to find the non-correlated principal components. The sensitivity index for each principal component is computed by ANOVA (described in Subsection 2.4.1).

The benefit of this method is that it can be used not only for the time-dependent outputs but also for any functions of any continuous inputs such as the distance. The first order and the total sensitivity indices can be studied. The weakness of this method is that the different principal components lead to different importance rankings of inputs. Therefore, the sensitivity indices obtained from all the principal components should be presented graphically.

2.6.4 Variance-based multivariate sensitivity analysis

The output of a dynamic model at time \( t \) is affected by the inputs at time \( t \) \( (x(t)) \) and also the inputs before time \( t \) \( (x(t'), t' < t) \). Therefore, factor sensitivity indices and time sensitivity indices based on variance are proposed by Cao et al. [CDD13].

The factor sensitivity index measures the whole influence of an input on the current output while the time sensitivity indices find the contribution of an input variance at a specific time to the current output variance (both indices are based on ANOVA).

The time sensitivity index that studies the sensitivity of the current output \( y(t_y) \) to the input \( x_i \) at the time \( t^* \) is computed as

\[
\text{time } SI_i(t^*) = \frac{V\left[E\left[Y(t_y)|X_i(t^*)\right]\right]}{V[Y(t_y)]},
\]

and the factor sensitivity index is obtained by

\[
\text{factor } SI_i = \frac{V\left[E\left[Y(t_y)|X_i\right]\right]}{V[Y(t_y)]},
\]

where factor \( SI_i \) studies the sensitivity of the current output to the input \( x_i \) at all times prior to time \( t_y \).
2.7 Numerical examples and discussion

In this section, three studies are done. In the first study 2.7.1, the Pearson, Spearman and Sobol (which is a popular nonlinear SA method) methods are implemented on four functions to determine the differences between linear, monotonic and nonlinear sensitivities indices. In the second study, some SA methods are compared with each other and in the third study the sensitivity of an engineer model is analyzed.

2.7.1 Study 1

The Pearson, Spearman and Sobol methods (that are respectively linear, monotonic and nonlinear SA methods) are implemented on the four following function

\[
F_1(x) = 0.70x_1 + 0.05x_2 + 0.25x_3, \\
F_2(x) = 0.70x_1 + 0.05x_2 + 0.25x_3 + x_1x_2 + x_1x_3 + x_2x_3 + x_1x_2x_3, \\
F_3(x) = 0.3x_1 + 0.3x_2 + 0.3x_3, \\
F_4(x) = x_1^2 + x_2 + x_3.
\]  

Among these functions, the first and third functions are linear \((F_1 \text{ and } F_3)\). The Pearson, Spearman and the main Sobol sensitivity indices of these functions \((2.27)\) are shown in Table 2.1.

As Table 2.1 shows all the SA methods find the important input regardless of linear or nonlinear function. However, the linear SA method studies if the function can be approximated by a linear function while ignoring unimportant inputs. For example, The Pearson and Spearman methods indicate that functions \(F_1\) and \(F_4\) can be approximated by a linear function while considering the important input \(x_1\) and ignoring the unimportant inputs \(x_2\) and \(x_3\). It should be noted that function \(F_1\) is linear while function \(F_4\) is nonlinear.

In addition, the linear SA method shows that the input effects of \(F_2\) functions (on the functions outputs) are not linear. Therefore, these functions cannot be approximated by a linear function regardless to that \(F_2\) is nonlinear and \(F_3\) is linear.

Consequently, these methods do not give information about the models but give information about the effect of inputs on the model output.
2.7. Numerical examples and discussion

Table 2.1: The Pearson, Spearman and the main Sobol sensitivity indices of four functions (2.27).

<table>
<thead>
<tr>
<th>Function</th>
<th>SI</th>
<th>Pearson</th>
<th>Spearman</th>
<th>Sobol</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$S_I^1$</td>
<td>0.94</td>
<td>0.94</td>
<td>0.88</td>
</tr>
<tr>
<td>$F_1$</td>
<td>$S_I^2$</td>
<td>0.07</td>
<td>0.06</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>$S_I^3$</td>
<td>0.34</td>
<td>0.32</td>
<td>0.11</td>
</tr>
<tr>
<td></td>
<td>$S_I^1$</td>
<td>0.68</td>
<td>0.71</td>
<td>0.46</td>
</tr>
<tr>
<td>$F_2$</td>
<td>$S_I^2$</td>
<td>0.45</td>
<td>0.44</td>
<td>0.20</td>
</tr>
<tr>
<td></td>
<td>$S_I^3$</td>
<td>0.52</td>
<td>0.52</td>
<td>0.27</td>
</tr>
<tr>
<td></td>
<td>$S_I^1$</td>
<td>0.58</td>
<td>0.57</td>
<td>0.33</td>
</tr>
<tr>
<td>$F_3$</td>
<td>$S_I^2$</td>
<td>0.58</td>
<td>0.57</td>
<td>0.33</td>
</tr>
<tr>
<td></td>
<td>$S_I^3$</td>
<td>0.58</td>
<td>0.57</td>
<td>0.33</td>
</tr>
<tr>
<td></td>
<td>$S_I^1$</td>
<td>0.91</td>
<td>0.94</td>
<td>0.98</td>
</tr>
<tr>
<td>$F_4$</td>
<td>$S_I^2$</td>
<td>0.10</td>
<td>0.17</td>
<td>0.01</td>
</tr>
<tr>
<td></td>
<td>$S_I^3$</td>
<td>0.10</td>
<td>0.17</td>
<td>0.01</td>
</tr>
</tbody>
</table>

2.7.2 Study 2

In this section, the Pearson, Spearman, Borgonovo, Mckay, Sobol, EFAST, Morris and Wei methods are implemented on the Ishigami Function. The Ishigami function \([IH90]\) is

\[
I(x) = \sin(x_1) + ax_2^2 + bx_3^4 \sin(x_1),
\]

where \(x_i \in [-\pi, \pi], i = 1, 2, 3, a = 7\) and \(b = 1/8\), see Figure 2.3.

In the second study 2.7.2, the complexity and the assumptions of the Pearson, Spearman, Borgonovo, Mckay, Sobol, EFAST, Morris and Wei methods are compared. Finally, In the third study 2.7.3, the sensitivity of an engineering model is analyzed.

The Morris (2.16), Sobol (2.3) and FAST (2.9) codes can be found in SALib [Her15], SIMLAB [SH08], the R package [GBA\(^+\)15], SAinterface [Jac06] and the GSAT [Can14] libraries. The SIMLAB [SH08] library also includes code for the Tarantola (2.13), (2.14), Mckay (2.11) and Pearson (2.1) formulas.

The Pearson and Spearman indices are computed using the MATLAB function corr. The codes of the Borgonovo’s, Mckay’s and Morris’ methods are obtained from [Jac06], but the FAST code is obtained from GSAT [Can14] because the maximum number of inputs in GSAT is greater than the number
2.7. Numerical examples and discussion

of inputs in SAinterface [Jac06]. The code for EFAST (Equation (2.10)) is obtained from SAinterface [Jac06]. For estimating the Sobol indices Equation (2.6) is used. The Wei indices for the Ishigami function (2.28) are obtained from [WLS13].

The number of model runs in Pearson’s, Spearman’s and Borgonovo’s methods is $dN$ ($d$ is the dimension and $N$ in the number of samples). The number of model runs in Sobol’s and Morris’ methods is $(d+1)N$. Let $w_{\text{max}}$ be the maximum frequency in the FAST method. The number of model runs in the FAST method is $20w_{\text{max}} + 1$ and the number of model runs for finding the total sensitivity indices of the EFAST method is $(20w_{\text{max}} + 1)d$. The maximum number of samples considered in Mckay’s method code is $N_{\text{max}} = 100$ and the number of model runs is $(2d + 1)(N^2/2)$.

The level ($p$) in Morris’ method is set to 4 (which can be between 4 to 10). The number of samples ($N$) is not the same for all the methods but the maximum number of model runs considered for all the methods is about 1000$(d + 1)$. The results are shown as the average (ave) and the standard deviation (std) of the sensitivity indices obtained from 100 runs of the SA methods. The estimated sensitivity indices of the linear SA methods for the Ishigami function (2.28) are shown in Table 2.2. The variable $x_1$ has a small linear effect on the output and the methods in Table 2.2 do not provide any information about the influence of the inputs $x_2$ and $x_3$ on the output.

The sensitivity indices of the nonlinear methods for the Ishigami func-
Table 2.2: The sensitivity indices of the linear and monotonic methods for the Ishigami function.

<table>
<thead>
<tr>
<th>inputs/SI</th>
<th>$x_1$</th>
<th>$x_2$</th>
<th>$x_3$</th>
<th>Model runs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spearman (ave)</td>
<td>0.46</td>
<td>0</td>
<td>0</td>
<td>3,000</td>
</tr>
<tr>
<td>Spearman (std)</td>
<td>0.02</td>
<td>0.03</td>
<td>0.03</td>
<td></td>
</tr>
<tr>
<td>Pearson (ave)</td>
<td>0.45</td>
<td>0</td>
<td>0</td>
<td>3,000</td>
</tr>
<tr>
<td>Pearson (std)</td>
<td>0.02</td>
<td>0.03</td>
<td>0.3</td>
<td></td>
</tr>
</tbody>
</table>

Table 2.3: The numerical values of the Mckay and Sobol indices obtained from symbolic integration in Maple for the Ishigami function.

<table>
<thead>
<tr>
<th>inputs/SI</th>
<th>$x_1$</th>
<th>$x_2$</th>
<th>$x_3$</th>
<th>sum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mckay ($\eta_i$)</td>
<td>0.341</td>
<td>0.354</td>
<td>0</td>
<td>0.695</td>
</tr>
<tr>
<td>Sobol ($SI_i$)</td>
<td>0.342</td>
<td>0.354</td>
<td>0</td>
<td>0.695</td>
</tr>
<tr>
<td>Sobol ($SI_i^{tot}$)</td>
<td>0.645</td>
<td>0.354</td>
<td>0.304</td>
<td>-</td>
</tr>
</tbody>
</table>

Numerical examples and discussion

The Sobol, EFAST and Wei total sensitivity indices show that $x_1$ has the highest interaction with other inputs. In the following, the information provided by each method is explained.

The Borgonovo indices indicate the influence of the input distribution on the output distribution. The Mckay, Sobol and EFAST indices show the contribution of inputs to the output variance. Table 2.4 shows that the EFAST is more efficient than Sobol’s and Mckay’s methods because it uses the smallest number of model runs. Morris’ method indices show the average and the standard deviation of the output when one input is changed. Morris indices rank the inputs as $x_1 > x_2 > x_3$.

The Wei indices show $x_1$ is the most important input because by reducing its distributions, the output variability is highly affected. The Wei
Table 2.4: The average of sensitivity indices of different nonlinear methods for the Ishigami function.

<table>
<thead>
<tr>
<th>inputs/SI</th>
<th>$x_1$</th>
<th>$x_2$</th>
<th>$x_3$</th>
<th>sum</th>
<th>Model runs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Borgonovo$^{ave}$</td>
<td>0.28</td>
<td>0.30</td>
<td>0</td>
<td>0.58</td>
<td>3,000</td>
</tr>
<tr>
<td>Borgonovo$^{std}$</td>
<td>0.02</td>
<td>0.02</td>
<td>0</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Mckay $\eta_i^{ave}$</td>
<td>0.34</td>
<td>0.36</td>
<td>0</td>
<td>0.70</td>
<td>4,046</td>
</tr>
<tr>
<td>Mckay $\eta_i^{std}$</td>
<td>0.04</td>
<td>0.04</td>
<td>0.02</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Sobol $SI_i^{ave}$</td>
<td>0.34</td>
<td>0.35</td>
<td>0</td>
<td>0.69</td>
<td>4,000</td>
</tr>
<tr>
<td>Sobol $SI_i^{std}$</td>
<td>0.03</td>
<td>0.03</td>
<td>0.05</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Sobol $SI_i^{tot,ave}$</td>
<td>0.64</td>
<td>0.36</td>
<td>0.30</td>
<td>-</td>
<td>4,000</td>
</tr>
<tr>
<td>Sobol $SI_i^{tot,std}$</td>
<td>0.05</td>
<td>0.02</td>
<td>0.02</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>EFAST $SI_i^{ave}$</td>
<td>0.34</td>
<td>0.39</td>
<td>0</td>
<td>0.73</td>
<td>301</td>
</tr>
<tr>
<td>EFAST $SI_i^{tot,ave}$</td>
<td>0.64</td>
<td>0.37</td>
<td>0.30</td>
<td>-</td>
<td>903</td>
</tr>
<tr>
<td>Morris $\mu_i^{ave}$</td>
<td>9.24</td>
<td>7.87</td>
<td>7.82</td>
<td>-</td>
<td>4,000</td>
</tr>
<tr>
<td>Morris $\mu_i^{std}$</td>
<td>0.22</td>
<td>0</td>
<td>0.23</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Morris $\sigma_i^{ave}$</td>
<td>0.24</td>
<td>0.24</td>
<td>0.34</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Morris $\sigma_i^{std}$</td>
<td>0</td>
<td>0</td>
<td>0.23</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Wei $SI_i^{ave}$</td>
<td>0.25</td>
<td>0.19</td>
<td>0.06</td>
<td>-</td>
<td>2,048</td>
</tr>
<tr>
<td>Wei $SI_i^{std}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Wei $SI_i^{tot,ave}$</td>
<td>0.72</td>
<td>0.53</td>
<td>0.56</td>
<td>-</td>
<td>2,048</td>
</tr>
<tr>
<td>Wei $SI_i^{tot,std}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

total sensitivity indices confirm that if the input distributions reduce, the input $x_1$ has the most interactions with others. It should be noted that the small number of model runs (2,048) in Wei’s method is due to the use of a surrogate.

As each method gives a specific information, it can be concluded the inputs $x_1$ and $x_2$ have the most influences on the output sensitivity and $x_1$ has the most interactions with other inputs (the total sensitivity of $x_1$ is higher than the other inputs). The results match Formula (2.28): first order sensitivity indices for $x_1$ (resp. $x_2$) is responsible for around 34% (resp. 35%) of the variation due to the term $\sin(x_1)$ (resp. $a\sin^2(x_2)$). There is a nonlinear interaction since first-order interactions sum to 69%; it is the $bx_3^3\sin(x_1)$ term that appears as a 64% total variation index for $x_1$ so 30% is due to higher order interactions while $x_3$ only exhibits a 30% higher order
2.7. Numerical examples and discussion

2.7.3 Study 3

We consider a simple road design model [KL10, Mor96] which minimizes the construction cost. Figure 2.4 shows the ground, and the road. The vertical dashed lines indicate the sections. The road is divided into 3 segments (pieces on which the road is a quadratic function) as indicated as darker dashed vertical lines. The first, second and third segments are divided into 2, 2 and 4 sections, respectively.

The general parameters in this model are $n$ the number of sections, $n_g$ the number of sections in each segment, $A_i$ the area of section $i$, $h_i$ average ground height of section $i$, $x_i$ the start point of section $i$, and $t_g$ the $x$-coordinate at the end of segment $g$.

The cost parameters are $q_d$ the cost of embanking to a landfill (dump) pit, $p_b$ the cost of excavating from a borrow pit, $p$ the cost of excavating from each section, $q$ the cost of embanking to each section, $C_{ij}$ (or $C_{id}$) the cost of transporting one cubic unit from section $i$ to $j$ (or to the dump pit), and $C_{bi}$ the cost of transporting one cubic unit from the borrow pit to section $i$.

The decision variables are $u_i$ the height of earth removed from section $i$, $v_i$ the height of earth added to section $i$, $T_{ij}$ the number of units transported from section $i$ to $j$ ($A_i T_{ij}$ is the transferred volume), and $a_{gk}$ the coefficient of $x^k$ in the quadratic model of the road on segment $g$. 

Figure 2.4: The road and ground profiles.
2.7. Numerical examples and discussion

The quadratic model for each segment is

\[ P_g(x) = a_{g0} + a_{g1}x + a_{g2}x^2, \quad x \in [t_{g-1}, t_g], \quad i = 1, \ldots, n_g, \quad g = 1, 2, 3. \]

The objective function in this linear programming model is to minimize the total cost of embankment, hauling and excavation, i.e.

\[
\min \text{Cost} = \sum_{i=1}^{n} (pA_i u_i + qA_i v_i) + \sum_{i=1}^{n} \sum_{j=1, i \neq j}^{n} C_{ij} A_i T_{ij} + \sum_{i=1}^{n} ((C_{id} + q_d) A_i T_{id} + (C_{bi} + p_b) A_i T_{bi})
\]

The following constraint ensures that the transported volume to or from a section is equal to the work done at that section

\[
\sum_{j=1, i \neq j}^{n} A_i (T_{ij} - T_{ji}) = A_i (u_i - v_i), \quad i = 1, 2, \ldots, n.
\]

which can be simplified into

\[
\sum_{j=1, i \neq j}^{n} T_{ij} - T_{ji} = u_i - v_i, \quad i = 1, 2, \ldots, n.
\]

The smoothness and continuity constraints of splines are

\[
P_g(t_g) = P_{g+1}(t_g), \quad g = 1, 2,
\]
\[
P'_g(t_g) = P'_{g+1}(t_g), \quad g = 1, 2.
\]

The gap constraint is

\[
h_i(x_{g,i+1} - x_{g,i}) - \int_{x_{g,i}}^{x_{g,i+1}} P_g(x) = (u_i - v_i)(x_{g,i+1} - x_{g,i}); \quad i = 1, \ldots, n_g, \quad g = 1, 2.
\]

The slope constraints are

\[
\max_{x \in [t_{g-1}, t_g]} P'_g(x) \leq U \quad g = 1, 2, 3,
\]
\[
\min_{x \in [t_{g-1}, t_g]} P'_g(x) \geq L \quad g = 1, 2, 3,
\]

where \( t_0 = x_1 = 0 \). The road height at the initial point and final point should be 32m and 31m, respectively. The sensitivity analysis is implemented on
2.7. Numerical examples and discussion

This model to find the importance of ground height and cost parameters. The sensitivity of the ground heights at the start and end points are not studied because changing them may make the problem infeasible, and these values are usually known with much greater accuracy. The range of cost parameters is \((0, 5)\) and the height parameters range is \((20, 40)\) (these ranges are suggested by experts).

All the SA methods can be implemented on this problem but we chose the FAST method as a nonlinear variance based SA method. This problem is not high dimensional (7 height parameters and 5 cost parameters) and the number of inputs is smaller than the maximum number of inputs for the FAST method. In addition, when a model is not high dimensional, FAST is the cheapest method among the other variance based SA methods.

Since the FAST and Sobol’s methods provide the same information, we also implemented Sobol’s method to increase confidence in the results. Another verification method is to run Sobol’s method several times and verify that the standard deviation is small enough.

Table 2.5: The Sobol and FAST indices for Moreb’s problem.

<table>
<thead>
<tr>
<th>inputs/SI</th>
<th>SIave</th>
<th>SI_sd</th>
<th>SIave</th>
<th>SI_sd</th>
<th>SI</th>
<th>SIave</th>
<th>SI_sd</th>
<th>SIave</th>
<th>SI_sd</th>
</tr>
</thead>
<tbody>
<tr>
<td>(p)</td>
<td>0.07</td>
<td>0.03</td>
<td>0.07</td>
<td>0.00</td>
<td>0.06</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(q)</td>
<td>0.06</td>
<td>0.03</td>
<td>0.07</td>
<td>0.00</td>
<td>0.06</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(p_b)</td>
<td>0.00</td>
<td>0.03</td>
<td>0.00</td>
<td>0.03</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(q_d)</td>
<td>0.00</td>
<td>0.03</td>
<td>0.00</td>
<td>0.02</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(C)</td>
<td>0.26</td>
<td>0.02</td>
<td>0.33</td>
<td>0.01</td>
<td>0.25</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(h_2)</td>
<td>0.11</td>
<td>0.03</td>
<td>0.20</td>
<td>0.01</td>
<td>0.11</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(h_3)</td>
<td>0.03</td>
<td>0.03</td>
<td>0.13</td>
<td>0.01</td>
<td>0.03</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(h_4)</td>
<td>0.00</td>
<td>0.03</td>
<td>0.05</td>
<td>0.01</td>
<td>0.01</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(h_5)</td>
<td>0.01</td>
<td>0.03</td>
<td>0.09</td>
<td>0.01</td>
<td>0.01</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(h_6)</td>
<td>0.02</td>
<td>0.03</td>
<td>0.10</td>
<td>0.01</td>
<td>0.02</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(h_7)</td>
<td>0.02</td>
<td>0.03</td>
<td>0.11</td>
<td>0.01</td>
<td>0.03</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(h_8)</td>
<td>0.12</td>
<td>0.03</td>
<td>0.23</td>
<td>0.01</td>
<td>0.13</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\text{sum})</td>
<td>0.70</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.71</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

In our tests, Equation (2.3) resulted in large negative indices so we used Equation (2.6). To verify the result, we compared Sobol’s with FAST indices (Sobol’s method uses 13,000 model runs and the FAST method uses 5,861 model runs). In addition, Sobol’s method was run 20 times. The av-
average and standard deviation of the Sobol indices with the FAST indices are shown in Table 2.5. For expensive models, we suggest to run Sobol’s method (Formula (2.6)) once and compare the result with the FAST method.

The FAST method is deterministic, so we ran it once. We could not use the EFAST method in the SAinterface [Jac06] library since it is limited to 10 inputs for finding the total sensitivity indices.

As Table 2.5 shows the C parameter, which is the transportation cost, is the most important parameter while the \( p_b \) and \( q_d \) are unimportant and have no interaction with other inputs. However, we cannot simplify the model by removing the dump and borrow pits since they are used at the optimal solution.

2.8 Discussion

Figure 2.5 summarizes the SA methods for non-expensive models with a decision tree.

The SA methods have different assumptions and mechanisms and a proper method for a specific goal should be used. For the factor prioritization, factor fixing and model structure goals, the screening or the variance based methods can be applied. The monotonic SA method and plotting the ANOVA decomposition (plotting \( G(x) \) versus \( G_i(x_i) \) (Equation 2.2)) can be used for the model structure goal. The Wei method can be used for the stability goal.

While stability goal applies to linear programming (LP) problems [BP16], a parametric LP analysis (which is not studied in this paper) can also be used [BBM03, Fil11]. A Matlab-based toolbox for parametric LP analysis can be found in [MPT].

In addition to sensitivity analysis objectives, the complexity of each SA method should be taken into account for choosing a proper method. The maximum numbers of inputs for FAST (in GSAT library [Can14]) and EFAST (in SAInterface library [Jac06]) are 50 and 10, respectively (in their implementation). However, using EFAST with 50 inputs is still expensive and Saltelli et al [SRTC05, SRTC12] suggest to use the variance based methods when the model inputs are smaller than 20 or the model requires a small amount of CPU time (up to 1 min per run). When the model is low dimensional, the number of function evaluations of EFAST is smaller than the number of function evaluations used in the Sobol method. In this case, we suggest to use the EFASTT method instead of the Sobol method.

Saltelli et al [SRTC05, SRTC12] suggest to use the screening method
2.8. Discussion

Figure 2.5: Summary of SA methods for inexpensive models.

Based on radial sampling (Subsection 2.4.3) when the CPU time for each run of the model takes up to 10 min per run or the number of inputs is up to 100.

Increasing the number of samples, increases the accuracy of sensitivity indices. In this paper, the number of samples for Sobol’s method is set to 1,000. If 1,000 samples is expensive for a model (because each run of model takes more than 10 min or the number of inputs is more than 100), using the surrogate methods described in Section 2.5 is suggested for this expensive model. Among all the surrogate methods, we suggest the Gaussian process because it accounts for uncertainty.

In case of multivariate output models which are specific problems, different methods are discussed in Section 2.6. If the model is static, the Gamboa et al. [GJKL13] method is suggested. The sequential SA or the PCA based SA is recommended to graphically present the sensitivity indices of a dy-
Cao et al. \cite{CDD13} introduce two different indices (time and factor sensitivity indices) for dynamic models. The time index finds the sensitivity of output at time $t_y$ ($y(t_y)$) to an input at specific time ($t^*$) and the factor index finds the sensitivity of ($y(t_y)$) to an input at all time prior to time $t_y$.

Sobol’s and FAST methods are implemented on a road design model. The importance of cost and height parameters are studied for specific input ranges. The most important parameter was found to be the transportation cost. In the future, a more thorough study of the importance of all parameters of this model is needed to compute a range for each input on which the optimal solution is meaningful.
Chapter 3

Section positioning in the road design vertical alignment problem

The road design problem is usually split into horizontal alignment, vertical alignment, and earthwork. After the horizontal alignment is fixed, the vertical alignment problem considers a discretization of the ground into sections. The number of sections is directly linked to the computation time. A large number of sections increases the calculation time to find the optimal vertical alignment. We study different methods to approximate the ground with non-uniformly spaced sections. The presented methods are compared with a commercial road design software.

3.1 The road design problem

A country’s economic development is highly correlated with the quality of its road network. A reliable road network connects people, markets, services and knowledge together. In other words, the road network has a huge impact on the economic growth. However, the road construction and its maintenance are expensive activities. Therefore, the road design model should be optimized by minimizing the construction cost and considering safety constraint, environmental and socioeconomic impacts [HHLR14, HAMM13].

In the road design problem, the ground profile is discretized into segments and sections as shown in Figure 3.1. In this figure, the $i$th section is shown by $S_i$ and Segment $j$ is presented by $Seg_j$. Considering numerous sections in optimizing the road design model is too time consuming to be practical. Therefore, we present different methods to select a reasonable number of sections and position them in a way that still provide enough accuracy on the resulting road alignment.

The inputs to these methods consist of the number of sections ($N$), their
3.2. The road design model

For a good accuracy, the ground profile and the construction cost should be estimated well. The cost is dependent on the material volume and the ground profile. A linear programming road design model which has multi-material and side slope features is presented in this section. This model consists of several parameters, variables and constraints, which are introduced as they appear.

In this model, the ground profile is discretized into \( N \) sections and each section is presented by its height \( h_i \) and the start point \( (x_i) \). Sections are grouped into segments and the number of sections in each segment is shown by \( n_g \) [HHLR14, KL10, Mor96]. For example, the number of sections \( n_g \) in segments 1, 2 and 3 of Figure 3.1 are 4, 8 and 3, respectively. The \( x \)-coordinate at the end of segment \( g \) is shown by \( t_g \) and the quadratic road model for each segment is defined as

\[
\begin{align*}
\frac{1}{2} a_g x^2 + \frac{1}{2} x^2 + b_g x + c_g &= \text{(Road profile)} \\
&\quad \text{for } x_1 \leq x \leq x_2
\end{align*}
\]

This paper is organized as follows. Section 3.2 presents the model. Section 3.3 is devoted to explaining the methods used for section positioning and reducing the number of sections. These methods are implemented on different grounds and compared with each other in Section 3.4. Finally, conclusions are provided in Section 3.5.

3.2 The road design model

Figure 3.1: The vertical alignment of the ground profile.
3.2. The road design model

\[ P_g(x) = a_{g0} + a_{g1}x_i + a_{g2}x_i^2, \quad x_i \in [t_{g-1}, t_g], \quad i = 1, ..., n_g, \quad g \in G. \]

where \( G \) is the index of segments. A quadratic function is used to avoid sharp connections and have linear programming problem. If cubic or higher order spline is used, then the constraints cannot be enforced with linear programming.

The road should be smooth and continuous which means the height and the slope of the ending section of a segment should be equal to the height and slope of the beginning section of the next segment. The smoothness and continuity constraints of splines are

\[
\begin{align*}
P_g(t_g) &= P_{g+1}(t_g), \quad g \in G - 1, \\
P'_g(t_g) &= P'_{g+1}(t_g), \quad g \in G - 1.
\end{align*}
\]

(3.1)

The slope constraints, which are considered for safety, are

\[
\begin{align*}
\max_{x \in [t_{g-1}, t_g]} P'_g(x) &\leq U \quad g \in G, \\
\min_{x \in [t_{g-1}, t_g]} P'_g(x) &\geq L \quad g \in G.
\end{align*}
\]

(3.2)

During the road construction, not only may some material need to be moved between sections, but also some materials may be brought from Borrow pits to sections or dumped from sections to Waste pits. Thus, the Borrow and Waste pits are considered as the external sections in the road design problem.

Let the variables \( V^+_i \) and \( V^-_i \) represent the total cut and fill material volumes of section \( i \), respectively. The cost parameters are

- \( q_d \): the cost of embanking to a Dump pit,
- \( p_b \): the cost of excavating from a Borrow pit,
- \( p \): the cost of excavating from each section,
- \( q \): the cost of embanking to each section,
- \( C_{ij} \): the cost of transporting one cubic unit from section \( i \) to \( j \),
- \( C_{iw} \): the cost of transporting one cubic unit from section \( i \) to the Waste pit, and
- \( C_{bi} \): the cost of transporting one cubic unit from the Borrow pit to section \( i \).

The objective function in this linear programming model is to minimize
the total cost of embankment, hauling and excavation,

\[
\begin{align*}
\text{min } \text{Cost} &= \sum_{i=1}^{n} (pV_i^+ + qV_i^-) + \\
&\quad \sum_{i=1}^{n} \sum_{j=1, i \neq j}^{n} C_{ij}T_{ij} + \sum_{i=1}^{n} ((C_{iw} + q_w)T_{iw} + (C_{bi} + p_b)T_{bi}),
\end{align*}
\tag{3.3}
\]

where the variables \(T_{ij}, T_{bi}\) and \(T_{iw}\) represent the transferred volume from section \(i\) to \(j\), the transferred volume from Borrow pit to section \(i\) and the transferred volume from section \(i\) to Waste pit, respectively.

The material volume moved from section \(i\) to other sections or Waste pit should be equal to the volume cut from section \(i\). Similarly, The material volume brought from other sections or Borrow pit to section \(i\) should be equal to the volume filled to section \(i\). These constraints, which are called balance constraint, are defined as

\[
\begin{align*}
\sum_{j=1, i \neq j}^{N} T_{ij} + T_{iw} &= V_i^+, \quad i, j \in N, \\
\sum_{j=1, i \neq j}^{n} T_{ji} + T_{bi} &= V_i^-, \quad i, j \in N.
\end{align*}
\tag{3.4}
\]

In order to make the road durable, side-slopes are used. Side-slope refers to gradual increase (decrease) in height from a fill (cut) section of the ground profile to the height of the road profile [HHLR14]. In Figure 3.2, the cross-section of a road with and without side-slopes for a cut and a fill are shown respectively.

To model the side-slopes, trapezoid shaped cross-sections are approximated with several rectangles. Each rectangle is presented by an index (level), the altitude of the \(l^{th}\) rectangle at section \(i\) is shown by the Offset \(L_{i,l}\) and the variable \(u_i\) is the difference between the ground and road heights at section \(i\) as

\[
P(x_i) - h_i = u_i, \quad i \in N.
\tag{3.5}
\]

An example of a side-slope for a cut area is shown in Table 3.1 and Figure 3.3. Assume \(u_i = 7\)m, then \(l\) should be 5 and the cut volume can be computed easily by \(R_{i,4}^+ + \frac{R_{i,5}^+ - R_{i,4}^+}{L_{i,5} - L_{i,4}} (L_{i,5} - u_i) = 215.25\).
3.2. The road design model

Figure 3.2: The cross-section of a road with and without side-slopes.

Figure 3.3: Approximation of side-slopes for a cut area.

In other words, the gap constraint are

\[
V^+ = R^+_{i,l} + \frac{R^+_{i,l+1} - R^+_{i,l}}{L_{i,l+1} - L_{i,l}} (L_{i,l+1} - u_i), \quad i \in N, l \in \{l' | L_{i,l'} \leq u_i < L_{i,l'} + 1\},
\]

\[
V^- = R^-_{i,l} + \frac{R^-_{i,l+1} - R^-_{i,l}}{L_{i,l+1} - L_{i,l}} (L_{i,l+1} - u_i), \quad i \in N, l \in \{l' | L_{i,l'} \leq u_i < L_{i,l'} + 1\},
\]

(3.6)

where \( R^+_{i,l} \) and \( R^-_{i,l} \) are the cut and fill volumes at section \( i \) and level \( l \), respectively.

While the shrink and swell factors and compaction are material dependent, the model uses banked units to compute the transportation costs and thus avoids the complexity of tracking material dependent factors without any loss in approximation [Koc10, Remark 1.6].

44
3.3. Section positioning methods

Table 3.1: Approximation of Cut volumes using side-slopes for a cut area.

<table>
<thead>
<tr>
<th>Level $l$</th>
<th>Offset $L_{i,l}$</th>
<th>Cut Volume $R^+_{i,l}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>0.08</td>
</tr>
<tr>
<td>3</td>
<td>4</td>
<td>70.06</td>
</tr>
<tr>
<td>4</td>
<td>6</td>
<td>168.44</td>
</tr>
<tr>
<td>5</td>
<td>8</td>
<td>262.06</td>
</tr>
</tbody>
</table>

The optimization time for this model is dependent on the number of sections (the cost model is an aggregate model that does not go into the details of construction duration). Considering a lot of sections approximates the ground profile well but increases the optimization time. Keeping the approximation accuracy while reducing the optimization time can be done by the section positioning methods presented in the following section.

3.3 Section positioning methods

The methods used for section positioning are the heuristic method used in the RoadEng software, the regression tree [JWH14], and the piecewise constant approximation method [KK88]. These methods are explained in the following Subsections.

3.3.1 Method 1: The heuristic method

In this method, $N_1$ uniform sections are picked from $N$ uniform sections and the optimal cost is computed. If $\frac{|\text{Cost}_{N_1} - \text{Cost}_{2N_1}|}{\text{Cost}_{N_1}} < \epsilon$ is not satisfied, then $N_1$ is doubled until $\frac{|\text{Cost}_{N_1} - \text{Cost}_{2N_1}|}{\text{Cost}_{N_1}} < \epsilon$ is passed and $2N_1$ is returned as the number of sections. Three iterations of this method are presented in Figure 3.4.

3.3.2 Method 2: The regression tree

In this method, $x$ is the feature of sections and $h$ is the response. First, all sections are considered as a single section (all sections are considered in a single leaf). Afterward, $\hat{h}_{\text{leaf}}$ and $S$ presented in equation (3.7) are calculated and two leaves are added by examining all the binary splits of all variables value to find a value which leads to the largest decrease in $S$. This
3.3. Section positioning methods

Figure 3.4: Three iterations of the heuristic method.

procedure continues until a stopping criterion is reached ($S_{\text{new}} < \delta S_{\text{old}}$, $\delta$ is small and defined by user) [JWH14]. The pseudo-code of this method is presented in Algorithm 1.

\[
\bar{h}_{\text{leaf}} = \frac{1}{m_{\text{leaf}}} \sum_{i \in \text{leaf}} h_i,
\]

\[
S = \sum_{\text{leaf} \in \text{leaves(Tree)}} \sum_{i \in \text{leaf}} (h_i - \bar{h}_{\text{leaf}})^2. 
\] (3.7)

Algorithm 1: The regression tree

1: Consider all sections in a single leaf.
2: Calculate $S$ (3.7).
3: Search over all binary splits. Take a split which can reduce $S$ as much as possible and add two new leaves.
4: If the largest decrease in $S$ is less than $\delta S$, go to Step 5. Otherwise, go to Step 2.
5: Return the number of Sections $N'$ ($N' \leq N$).

Three iterations of the regression tree are presented in Figure 3.5. As this figure shows, two sections (leaves) are added by binary split.

3.3.3 Method 3: Piecewise constant approximation

Suppose $f(x)$, the ground profile is a piecewise constant function on an interval $x$. The piecewise constant approximation approximates $f(x)$ by $g^*(x)$ which has the minimum number of constant pieces ($(n(g^*))$) or the number of sections). In other words, the piecewise constant approximation solves
3.3. Section positioning methods

Figure 3.5: Three iterations of the regression tree.

\[
\min n(g) \\
\text{s.t. } \|g - f\|_\infty \leq \epsilon',
\]  
(3.8)

where \(\|g\|_\infty\) is the infinity norm of \(g\) [KK88]. For each section, the following variables are computed

\[
u_i = f_i + \epsilon', \\
l_i = f_i - \epsilon',
\]  
(3.9)

and the algorithm connects section \(j\) to \(i\) if

\[
(i) \min\{u_t | i < t \leq j\} \geq \max\{l_t | i < t \leq j\}, \\
(ii) u_i \geq \max\{l_t | i < t \leq j\}, \\
(iii) l_i \leq \min\{u_t | i < t \leq j\}.
\]  
(3.10)

This method has linear complexity and is optimal for finding the number of constant pieces with the constraint in Equation (3.8) [KK88]. Three iterations of this method are shown in Figure 3.6.

In this method, the best value of input \(\epsilon'\) is unknown and can also be obtained by

\[
\min \|g - f\|_2, \\
\text{s.t. } n(g) \leq k,
\]  
(3.11)

where \(k\) is the minimum value of \(n(g)\) obtained from Equation (3.8). The complexity of problem (3.11) is \(O(kn^2)\) [KK88] but Fulop et al. improved this complexity to \(O(n^2 + kn \log n)\) [FP92].

In the road design model, the number of sections which provides a trade-off between optimization time and approximation accuracy is unknown. Therefore, Equation 3.11 cannot be used to obtain \(\epsilon'\) since \(k\) in this Equation,
3.4 Results and Discussion

The three methods presented in this thesis are implemented on four different grounds. The number of sections \( N \), the number of levels \( n_l \), the optimal cost and the time for building a road from these grounds are shown in Table 3.2 and Figure 3.1. In Table 3.2, \( N \) presents the number of sections, \( n_l \) indicates the number of levels for approximation the cut and fill volumes and \( T_{\text{Solve}} \) is the optimization time (sec). It should be noted that these grounds are small part of real grounds and used as case studies in the present thesis.

Optimizing road construction from these grounds were solved using a C++ code in Visual Studio 2012 that called CPLEX 12.5.1.0 on a Windows 7, 64 bit computer with 4 cores hyper threading and 3.2 GHz.

In order to reduce the number of sections, similar and close sections are merged and represented as one section. The height of the new section is the height of the first section in the merged sections. The average and median of the merged sections heights can also be considered for the height of the

which is the appropriate number of sections, is unknown. Consequently, the value of \( \epsilon' \) for section positioning problem need to be defined by numerical tests.

The values of \( \delta S \) and \( \epsilon' \) are not related in this research as there are different metrics to relate these values and we do not know which one is the best. More details about these values are provided in Subsection 3.4.1.
3.4. Results and Discussion

Table 3.2: Four different grounds.

<table>
<thead>
<tr>
<th>Ground</th>
<th>N</th>
<th>n_l</th>
<th>Cost ($)</th>
<th>T_Solve</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>2,368</td>
<td>22</td>
<td>493,306</td>
<td>27</td>
</tr>
<tr>
<td>B</td>
<td>941</td>
<td>42</td>
<td>163,953</td>
<td>12</td>
</tr>
<tr>
<td>C</td>
<td>2,309</td>
<td>62</td>
<td>3,780,000</td>
<td>26</td>
</tr>
<tr>
<td>D</td>
<td>948</td>
<td>42</td>
<td>232,582</td>
<td>64</td>
</tr>
</tbody>
</table>

new section. As the sectioning methods merge the consecutive sections that have similar heights, all the metrics for presenting the new section height may lead to similar results.

In order to approximate the side-slopes for this new section, Algorithm 2 is used and an example for merging three sections with four levels is shown in Figure 3.8. According to this Figure, the properties of the new section from merging three sections are as described in the following paragraphs.

Algorithm 2: The algorithm for approximating the side-slopes of merged sections

1: Find the minimum \( h_{j,\text{min}}' \) and the maximum \( h_{j,\text{max}}' \) \((j \in N')\) of \( h_i + L_{i,l}, i \in \text{the merged sections} \).
2: Divide \( h_{j,\text{max}}' - h_{j,\text{min}}' \) to equal \( n_l \) Offsets and obtain all \( L_{j,l}' \).
3: The material volume related to the Offset \( L_{j,l}' \) is the sum of volume of rectangles (slabs) which satisfies the constraints \( h_j' + L_{j,l}' - 1 < h_i + L_{i,l} \) and \( h_j' + L_{j,l}' \geq h_i + L_{i,l} \) \((j \in N', i \in \text{the merged sections and } l,l' \geq 1)\).

The height of the new section is equal to the height of the first section \( (h' = h_1) \) and the number of levels in the new section and the merged sections are equal. In addition, the maximum height of the new section slab \( (h_{\text{max}}') \) is equal to the maximum height of the merged sections slabs \( (h_1 + L_{1,4}) \). Similarly, the minimum height of the new section slabs \( (h_{\text{min}}' = h' + L_{0,1}) \) is equal to the minimum height of the merged sections slabs \( (h_3 + L_{3,0}) \).

In Figure 3.8, the volumes in the slabs of the merged sections are appeared in the slabs of the new section based on the third step of Algorithm 2. According to this Algorithm, the volume of each slab of the new section is the sum of the volumes of the slabs of the merged sections that \( h_j' + L_{j,l'-1} \leq h_j' + L_{j,l'} \) \((l,l' \geq 1)\). For example, the bottom slab of the new section contains \( V_{3,1} \) but not \( V_{2,1} \) and \( V_{1,1} \) because
3.4. Results and Discussion

Figure 3.7: Four ground profiles.

\( h' + L'_0 < h_3 + L_{3,1} \leq h' + L'_1 \) but \( h' + L'_0 < h_2 + L_{2,1} \not\leq h' + L'_1 \) and \( h' + L'_0 < h_1 + L_{1,1} \not\leq h' + L'_1 \). Consequently, \( V_{2,1} \) and \( V_{1,1} \) are in the second slab of the new section because \( h' + L'_1 < h_1 + L_{1,1} \leq h' + L'_2 \) and \( h' + L'_1 < h_2 + L_{2,1} \leq h' + L'_2 \).

3.4.1 Comparing the three methods

As \( \delta \) in the regression tree and \( \epsilon' \) in the piecewise constant approximation method are unknown, 20 values for them are considered (\( 10^{-9} \leq \delta \leq 10^{-1} \) and \( 10^{-2} \leq \epsilon' \leq 10^{0.5} \)). For the heuristic method, six iterations are considered and in each iteration, \( N_1 \) sections (\( N_1 \approx N/(2^7-\text{iteration}) \)) are picked (7 is the number of iterations +1). We considered smaller number of iterations for the heuristic method than the other methods because if 20 iterations are considered for this method, then the number of iterations +1 = 21 and \( N_1 \approx N/(2^{21-\text{iteration}}) \) returns very small number of sections in the first
3.4. Results and Discussion

As each $\delta$ in the regression tree, each $\epsilon'$ in the approximation method and each iteration of the heuristic method returns a specific number of sections, comparison of these methods with a lot of numbers of sections is hard. Therefore, two stopping criteria are considered to return a specific number of sections for each method (stopping criterion 1 is obtained from the heuristic method explained in Subsection 3.3.1).

Stopping criterion 1: Relative cost error between two iterations of a method $\leq 0.05$ (the results which can satisfy this criterion are shown by the cyan color).

Stopping criterion 2: Relative cost error between original ground and each iteration of a method $\leq 0.05$. In addition, The root of mean squared errors ($RMSE$) between the height of approximated ground and the original ground $\leq 0.25m$ (the results which can satisfy this criterion are shown by the green color).

The following tables present the methods performances on the grounds shown in Table 3.2 and in these tables, the number of sections is shown.
by Section. $MaxE$ and $RMSE$ present the maximum absolute error and root mean squared error between the heights of the original and approximated grounds. The relative cost error between two consecutive iterations is indicated by $RelCost_{i,i+1}$. The relative and absolute errors between the cost of an iteration and the original ground cost are shown by $RelCostE$ and $AbsCostE$, respectively. Implementation time of the methods (in Matlab R2013b) is shown by $T_{method}$ and $T_{Solve}$ shows the solving time (optimizing the model by C++ code).

The cost and the height of the original ground are respectively shown by $Cost$ and $h$. The height and the cost of the approximated ground at iteration $i$ are respectively presented by $h'$ and $Cost'_{i}$. The number of sections of the approximated ground is smaller than the number of sections of the original ground. Therefore, the number of elements in $h'$ is smaller than $h$.

In order to compute $MaxE$ and $RMSE$ (3.12), we need to have the same number of elements for $h$ and $h'$. For this case, assume $x_{j'}$ ($j' \in N'$ and $N'$ is the number of sections of the approximated ground) is the number of merged sections from the original ground to make the $j^{th}$ section of the approximated ground. Therefore, any section of the approximated ground is replicated for $x_{j'}$ times to have the same length for $h$ and $h'$. Consequently, $MaxE$, $RMSE$, $RelCost_{i,i+1}$, $RelCostE$ and $AbsCostE$ are defined as

$$MaxE = \max |h - h'|,$$
$$RMSE = \sqrt{\frac{1}{N}(h_j - h'_j)}, j \in N,$$
$$RelCost_{i,i+1} = \frac{|Cost'_{i+1} - Cost'_{i}|}{Cost'_{i}},$$
$$RelCostE = \frac{|Cost - Cost'_{i}|}{Cost},$$
$$AbsCostE = |Cost - Cost'_{i}|.$$  

(3.12)

For stopping criterion 1, $Total\_Time$ is sum of $T_{method}$ and $T_{Solve}$ from the first iteration till the iteration that satisfies this criterion. According to stopping criterion 1, the method that returns the smallest Section, $Total\_Time$ and $RelCost_{i,i+1,i+2}$ is the winner. We also consider $RelCost_{i,i+1,i+2}$ since the approximation is good enough if both $RelCost_{i,i+1}$ and $RelCost_{i+1,i+2}$ are small.

For stopping criterion 2, $Total\_Time$ is sum of $T_{method}$ and $T_{Solve}$ from the iteration that has $RMSE \leq 0.25$ until the iteration that satisfies this criterion. Based on stopping criterion 2, the method that returns the smallest Section and $Total\_Time$ is the winner.
3.4. Results and Discussion

For comparing the performances of the regression tree and the piecewise constant approximation method, two studies are done. In the first study, the methods are implemented as they are explained in Subsections 3.3.2 and 3.3.3. In other words, the ground elevation is used as a criterion to merge sections. In the second study, the material volume is used instead of the ground elevation as the criterion for merging sections.

It should be noted that the heuristic method requires neither ground elevation nor material volumes and this method just picks uniform sections. Therefore, the heuristic results in both studies are the same.

Study 1: Comparison based on ground elevation

Ground elevation is used as a criterion for merging sections and the performances of the heuristic method, the regression tree and the piecewise constant approximation method on Ground A (2,368 sections and the road construction cost is $493,306) are presented in Tables 3.3, 3.4 and 3.5, respectively. These tables are summarized based on the two stopping criteria in Table 3.6.

Table 3.3: The performance of the heuristic method on Ground A.

<table>
<thead>
<tr>
<th>Iteration</th>
<th>Section</th>
<th>MaxE</th>
<th>RMSE</th>
<th>RelCost_{i+1}</th>
<th>RelCostE</th>
<th>AbsCostE</th>
<th>T_Method</th>
<th>T_Solve</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>37</td>
<td>3.46</td>
<td>1.11</td>
<td>0.20</td>
<td>0.30</td>
<td>149830</td>
<td>0.0</td>
<td>0.5</td>
</tr>
<tr>
<td>2</td>
<td>74</td>
<td>1.92</td>
<td>0.57</td>
<td>0.02</td>
<td>0.05</td>
<td>24238</td>
<td>0.5</td>
<td>1.0</td>
</tr>
<tr>
<td>3</td>
<td>148</td>
<td>1.16</td>
<td>0.28</td>
<td>0.01</td>
<td>0.02</td>
<td>11315</td>
<td>1.6</td>
<td>0.8</td>
</tr>
<tr>
<td>4</td>
<td>296</td>
<td>0.94</td>
<td>0.14</td>
<td>0.01</td>
<td>0.01</td>
<td>7249</td>
<td>2.4</td>
<td>1.2</td>
</tr>
<tr>
<td>5</td>
<td>592</td>
<td>0.82</td>
<td>0.06</td>
<td>0.01</td>
<td>0.01</td>
<td>3762</td>
<td>3.5</td>
<td>2.8</td>
</tr>
<tr>
<td>6</td>
<td>1184</td>
<td>0.68</td>
<td>0.03</td>
<td>0.00</td>
<td>0.00</td>
<td>1000</td>
<td>6.3</td>
<td>9.2</td>
</tr>
</tbody>
</table>

In Table 3.4, the relative cost error between \(\delta\) equals to 0.0008 and 0.0003 is small (\(RelCost_{i,i+1} = 0.05\)) but \(RelCost_{i,i+1}\) between \(\delta\) equals to 0.0003 and 0.0004 is not small (\(RelCost_{i,i+1} = 0.12\)). Therefore, considering stopping criterion 1 is not necessarily satisfactory to obtain a good approximation since \(RelCost_{i,i+1}\) may become bigger than 0.05 in the next iterations. In addition, the absolute cost error for this delta (0.0003) is huge.
3.4. Results and Discussion

Table 3.4: The performance of the Regression tree on Ground A.

<table>
<thead>
<tr>
<th>Delta</th>
<th>Section</th>
<th>MaxE</th>
<th>RMSE</th>
<th>RelCostE</th>
<th>AbsCostE</th>
<th>T_method</th>
<th>T_Solve</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>3</td>
<td>29.65</td>
<td>12.87</td>
<td>0.39</td>
<td>2.76</td>
<td>1362194</td>
<td>0.0</td>
</tr>
<tr>
<td>4E-02</td>
<td>4</td>
<td>18.34</td>
<td>9.34</td>
<td>0.16</td>
<td>4.23</td>
<td>2086554</td>
<td>0.1</td>
</tr>
<tr>
<td>1E-02</td>
<td>6</td>
<td>16.03</td>
<td>6.67</td>
<td>0.51</td>
<td>5.08</td>
<td>2507834</td>
<td>0.3</td>
</tr>
<tr>
<td>5E-03</td>
<td>8</td>
<td>9.77</td>
<td>4.68</td>
<td>0.08</td>
<td>2.00</td>
<td>987854</td>
<td>0.4</td>
</tr>
<tr>
<td>2E-03</td>
<td>10</td>
<td>9.11</td>
<td>4.02</td>
<td>0.34</td>
<td>1.76</td>
<td>867594</td>
<td>0.4</td>
</tr>
<tr>
<td>8E-04</td>
<td>16</td>
<td>5.03</td>
<td>2.36</td>
<td>0.05</td>
<td>0.82</td>
<td>405703</td>
<td>0.6</td>
</tr>
<tr>
<td>3E-04</td>
<td>18</td>
<td>4.80</td>
<td>2.13</td>
<td>0.12</td>
<td>0.74</td>
<td>363373</td>
<td>0.5</td>
</tr>
<tr>
<td>1E-04</td>
<td>30</td>
<td>3.70</td>
<td>1.28</td>
<td>0.15</td>
<td>0.53</td>
<td>260887</td>
<td>0.6</td>
</tr>
<tr>
<td>4E-05</td>
<td>35</td>
<td>2.54</td>
<td>1.08</td>
<td>0.09</td>
<td>0.30</td>
<td>149966</td>
<td>0.6</td>
</tr>
<tr>
<td>2E-05</td>
<td>57</td>
<td>2.09</td>
<td>0.68</td>
<td>0.06</td>
<td>0.19</td>
<td>94012</td>
<td>0.7</td>
</tr>
<tr>
<td>6E-06</td>
<td>71</td>
<td>1.33</td>
<td>0.54</td>
<td>0.01</td>
<td>0.12</td>
<td>59974</td>
<td>0.5</td>
</tr>
<tr>
<td>2E-06</td>
<td>110</td>
<td>1.03</td>
<td>0.35</td>
<td>0.05</td>
<td>0.11</td>
<td>52876</td>
<td>0.6</td>
</tr>
<tr>
<td>9E-07</td>
<td>138</td>
<td>0.66</td>
<td>0.27</td>
<td>0.00</td>
<td>0.05</td>
<td>26039</td>
<td>1.2</td>
</tr>
<tr>
<td>3E-07</td>
<td>208</td>
<td>0.62</td>
<td>0.18</td>
<td>0.03</td>
<td>0.06</td>
<td>28095</td>
<td>1.0</td>
</tr>
<tr>
<td>1E-07</td>
<td>270</td>
<td>0.33</td>
<td>0.13</td>
<td>0.00</td>
<td>0.03</td>
<td>13114</td>
<td>1.6</td>
</tr>
<tr>
<td>5E-08</td>
<td>397</td>
<td>0.25</td>
<td>0.09</td>
<td>0.02</td>
<td>0.03</td>
<td>15291</td>
<td>1.82</td>
</tr>
<tr>
<td>2E-08</td>
<td>535</td>
<td>0.17</td>
<td>0.06</td>
<td>0.00</td>
<td>0.01</td>
<td>7309</td>
<td>3.3</td>
</tr>
<tr>
<td>7E-09</td>
<td>718</td>
<td>0.11</td>
<td>0.04</td>
<td>0.01</td>
<td>0.02</td>
<td>8102</td>
<td>3.8</td>
</tr>
<tr>
<td>3E-09</td>
<td>979</td>
<td>0.07</td>
<td>0.03</td>
<td>0.01</td>
<td>0.03</td>
<td>12706</td>
<td>5.2</td>
</tr>
<tr>
<td>1E-09</td>
<td>1288</td>
<td>0.04</td>
<td>0.02</td>
<td>0.02</td>
<td>0.02</td>
<td>7729</td>
<td>9.4</td>
</tr>
</tbody>
</table>

Based on stopping criterion 1 in Table 3.6, the regression tree returns the smallest number of section. However, the $RelCost_{i+1,i+2}$, $RelCostE$ and $RMSE$ of the regression tree is the worst. Consequently, there is no winner according to stopping criterion 1 for Ground A. Based on stopping criterion 2 in Table 3.6, the number of sections of all methods are close to each other but the Total Time of the piecewise approximation method is the biggest time. Therefore, the heuristic method and the regression tree are the winners for Ground A.

The results for Ground B, C and D are presented in Tables 3.7, 3.8 and 3.9, respectively.

Based on stopping criterion 1, the heuristic method has the smallest $RelCost_{i+1,i+2}$ and Total Time for Ground B but returns the biggest number of sections. For Ground C and D, the regression tree returns the smallest number of sections and Total Time but largest $RelCost_{i+1,i+2}$. Therefore, stopping criterion 1 is not good enough to find the best method for section positioning problem.
3.4. Results and Discussion

Table 3.5: The performance of the piecewise constant approximation method on Ground A.

<table>
<thead>
<tr>
<th>Epsilon</th>
<th>Section</th>
<th>MaxE</th>
<th>RMSE</th>
<th>RelCostE</th>
<th>AbsCostE</th>
<th>T_method</th>
<th>T_Solve</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1623</td>
<td>21</td>
<td>2.08</td>
<td>0.90</td>
<td>0.12</td>
<td>0.64</td>
<td>313255</td>
<td>1.7</td>
</tr>
<tr>
<td>2.3357</td>
<td>29</td>
<td>1.55</td>
<td>0.65</td>
<td>0.04</td>
<td>0.43</td>
<td>214204</td>
<td>1.7</td>
</tr>
<tr>
<td>1.7252</td>
<td>39</td>
<td>1.23</td>
<td>0.49</td>
<td>0.10</td>
<td>0.37</td>
<td>183334</td>
<td>1.5</td>
</tr>
<tr>
<td>1.2743</td>
<td>52</td>
<td>0.86</td>
<td>0.36</td>
<td>0.08</td>
<td>0.23</td>
<td>113097</td>
<td>1.4</td>
</tr>
<tr>
<td>0.9412</td>
<td>72</td>
<td>0.82</td>
<td>0.27</td>
<td>0.04</td>
<td>0.13</td>
<td>66533</td>
<td>1.2</td>
</tr>
<tr>
<td>0.6952</td>
<td>95</td>
<td>0.43</td>
<td>0.20</td>
<td>0.01</td>
<td>0.09</td>
<td>46664</td>
<td>1.2</td>
</tr>
<tr>
<td>0.5135</td>
<td>128</td>
<td>0.34</td>
<td>0.15</td>
<td>0.04</td>
<td>0.10</td>
<td>50860</td>
<td>1.2</td>
</tr>
<tr>
<td>0.3793</td>
<td>172</td>
<td>0.24</td>
<td>0.11</td>
<td>0.01</td>
<td>0.06</td>
<td>29256</td>
<td>1.1</td>
</tr>
</tbody>
</table>

The Piecewise Constant Approximation Method

<table>
<thead>
<tr>
<th>Stopping Criterion</th>
<th>Methods</th>
<th>Section</th>
<th>RMSE</th>
<th>RelCostE</th>
<th>Total_Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Heuristic</td>
<td>148</td>
<td>0.28</td>
<td>0.01</td>
<td>0.02</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>18</td>
<td>2.13</td>
<td>0.12</td>
<td>0.74</td>
</tr>
<tr>
<td></td>
<td>Piecewise approx.</td>
<td>39</td>
<td>0.49</td>
<td>0.10</td>
<td>0.37</td>
</tr>
<tr>
<td>2</td>
<td>Heuristic</td>
<td>296</td>
<td>0.14</td>
<td>0.01</td>
<td>0.01</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>270</td>
<td>0.13</td>
<td>0.02</td>
<td>0.03</td>
</tr>
<tr>
<td></td>
<td>Piecewise approx.</td>
<td>230</td>
<td>0.08</td>
<td>0.00</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Table 3.6: Comparing methods on Ground A according to two stopping criteria.
3.4. Results and Discussion

Table 3.7: Comparing methods on Ground B according to two stopping criteria.

<table>
<thead>
<tr>
<th>Stopping Criterion</th>
<th>Methods</th>
<th>Section</th>
<th>RMSE</th>
<th>RelCostE</th>
<th>RelCost$t_{i+1,i+2}$</th>
<th>Total_Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Heuristic</td>
<td>118</td>
<td>0.54</td>
<td>0.01</td>
<td>0.01</td>
<td>3.0</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>9</td>
<td>2.89</td>
<td>0.01</td>
<td>0.25</td>
<td>1.1</td>
</tr>
<tr>
<td></td>
<td>Piecewise</td>
<td>33</td>
<td>0.62</td>
<td>0.04</td>
<td>0.10</td>
<td>3.5</td>
</tr>
<tr>
<td></td>
<td>approximation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Heuristic</td>
<td>471</td>
<td>0.11</td>
<td>0.00</td>
<td>0.00</td>
<td>7.9</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>185</td>
<td>0.23</td>
<td>0.00</td>
<td>0.01</td>
<td>1.8</td>
</tr>
<tr>
<td></td>
<td>Piecewise</td>
<td>125</td>
<td>0.20</td>
<td>0.00</td>
<td>0.00</td>
<td>1.9</td>
</tr>
<tr>
<td></td>
<td>approximation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3.8: Comparing methods on Ground C according to two stopping criteria.

<table>
<thead>
<tr>
<th>Stopping Criterion</th>
<th>Methods</th>
<th>Section</th>
<th>RMSE</th>
<th>RelCostE</th>
<th>RelCost$t_{i+1,i+2}$</th>
<th>Total_Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Heuristic</td>
<td>145</td>
<td>1.13</td>
<td>0.04</td>
<td>1.29</td>
<td>10</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>70</td>
<td>1.52</td>
<td>0.18</td>
<td>1.30</td>
<td>15</td>
</tr>
<tr>
<td></td>
<td>Piecewise</td>
<td>83</td>
<td>0.65</td>
<td>0.02</td>
<td>2.25</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td>approximation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Heuristic</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Piecewise</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>approximation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3.9: Comparing methods on Ground D according to two stopping criteria.

<table>
<thead>
<tr>
<th>Stopping Criterion</th>
<th>Methods</th>
<th>Section</th>
<th>RMSE</th>
<th>RelCostE</th>
<th>RelCost$t_{i+1,i+2}$</th>
<th>Total_Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Heuristic</td>
<td>119</td>
<td>0.43</td>
<td>0.02</td>
<td>0.70</td>
<td>15</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>4</td>
<td>4.44</td>
<td>0.40</td>
<td>0.62</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>Piecewise</td>
<td>32</td>
<td>0.45</td>
<td>0.16</td>
<td>0.72</td>
<td>76</td>
</tr>
<tr>
<td></td>
<td>approximation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Heuristic</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Piecewise</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>approximation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
3.4. Results and Discussion

Table 3.7 confirms that stopping criterion 1 is not good enough to evaluate the methods because the regression tree and the piecewise approximation methods return small number of sections but their ground approximations are bad (large \( \text{RMSE} \) and \( \text{RelCostE} \)). As Table 3.7 shows, based on the Stopping criterion 2, the regression tree and piecewise approximation methods are winners for Ground B.

Tables 3.8 and 3.9 highlight that stopping criterion 1 is not good enough to evaluate the methods. In addition, no methods can satisfy stopping criterion 2, thus the rows are blank. Therefore, there is no winner based on stopping criterion 2 in these tables.

As the cost approximation error should be small and cost is dependent on the material volume, the volumes of materials are used instead of ground elevation in the following study.

Study 2: Material volumes instead of ground elevation

In this study, the effect of using material volumes instead of ground elevation for the regression tree and the piecewise constant approximation method is studied. The methods are compared and the summarized results based on two criteria are presented in the following Tables.

Table 3.10: Comparing methods on Ground A based on the material volumes and according to two stopping criteria.

<table>
<thead>
<tr>
<th>Stopping Criterion</th>
<th>Methods</th>
<th>Section</th>
<th>( \text{RMSE} )</th>
<th>( \text{RelCostE} ) (_{1,1+2} )</th>
<th>( \text{RelCostE} )</th>
<th>( \text{Total Time} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Heuristic</td>
<td>148</td>
<td>0.28</td>
<td>0.01</td>
<td>0.02</td>
<td>2.4</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>213</td>
<td>0.22</td>
<td>0.00</td>
<td>0.00</td>
<td>3.3</td>
</tr>
<tr>
<td></td>
<td>Piecewise approx.</td>
<td>577</td>
<td>0.25</td>
<td>0.00</td>
<td>0.00</td>
<td>28.3</td>
</tr>
<tr>
<td>2</td>
<td>Heuristic</td>
<td>296</td>
<td>0.14</td>
<td>0.01</td>
<td>0.01</td>
<td>3.5</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>213</td>
<td>0.22</td>
<td>0.01</td>
<td>0.00</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td>Piecewise approx.</td>
<td>577</td>
<td>0.25</td>
<td>0.01</td>
<td>0.00</td>
<td>2.2</td>
</tr>
</tbody>
</table>
### 3.4. Results and Discussion

Table 3.11: Comparing methods on Ground B based on the material volumes and according to two stopping criteria.

<table>
<thead>
<tr>
<th>Stopping Criterion</th>
<th>Methods</th>
<th>Section</th>
<th>RMSE</th>
<th>RelCostE</th>
<th>Total_Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Heuristic</td>
<td>118</td>
<td>0.54</td>
<td>0.01</td>
<td>0.01</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>90</td>
<td>1.02</td>
<td>0.02</td>
<td>0.07</td>
</tr>
<tr>
<td></td>
<td>Piecewise approx</td>
<td>624</td>
<td>1.05</td>
<td>0.00</td>
<td>0.16</td>
</tr>
<tr>
<td>2</td>
<td>Heuristic</td>
<td>471</td>
<td>0.11</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Piecewise approx</td>
<td>733</td>
<td>0.18</td>
<td>0.00</td>
<td>0.01</td>
</tr>
</tbody>
</table>

Table 3.12: Comparing methods on Ground C based on the material volumes and according to two stopping criteria.

<table>
<thead>
<tr>
<th>Stopping Criterion</th>
<th>Methods</th>
<th>Section</th>
<th>RMSE</th>
<th>RelCostE</th>
<th>Total_Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Heuristic</td>
<td>145</td>
<td>1.13</td>
<td>0.04</td>
<td>1.29</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>389</td>
<td>0.38</td>
<td>0.23</td>
<td>1.67</td>
</tr>
<tr>
<td></td>
<td>Piecewise approx</td>
<td>2090</td>
<td>0.04</td>
<td>0.21</td>
<td>1.90</td>
</tr>
<tr>
<td>2</td>
<td>Heuristic</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Piecewise approx</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 3.13: Comparing methods on Ground D based on the material volumes and according to two stopping criteria.

<table>
<thead>
<tr>
<th>Stopping Criterion</th>
<th>Methods</th>
<th>Section</th>
<th>RMSE</th>
<th>RelCostE</th>
<th>Total_Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Heuristic</td>
<td>119</td>
<td>0.43</td>
<td>0.02</td>
<td>0.70</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>96</td>
<td>1.17</td>
<td>0.39</td>
<td>0.67</td>
</tr>
<tr>
<td></td>
<td>Piecewise approx</td>
<td>382</td>
<td>0.14</td>
<td>0.02</td>
<td>0.72</td>
</tr>
<tr>
<td>2</td>
<td>Heuristic</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Regression Tree</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Piecewise approx</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

In this study, stopping criterion 2 is not successful to evaluate methods and the heuristic method is mostly the winner based on the stopping criterion 1.
3.5 Summary of the section positioning methods

This Chapter presents heuristic method, regression tree and piecewise constant approximation for section positioning in road design model. Two stopping criteria are considered for these methods and the methods performances are compared in two studies.

In the first study, the ground elevation is used in the regression tree and piecewise constant approximation method and the material volumes are used in the second study for these methods. The heuristic method results are the same in both studies, as this method just picks uniform sections regardless of considering ground elevation or volumes.

The results show there is no specific method that is the best for all grounds. Therefore, all methods should be implemented on a small part of a real ground and the method which has the best performance should be implemented on the whole of real ground.
Chapter 4

Conclusion

This thesis is based on two research projects. In the first project (Chapter 2), an extensive survey on the sensitivity analysis methods is done which helps the practitioners decide the most appropriate SA method. In addition, the most appropriate methods are implemented on a road design model. In the second project (Chapter 3), three methods are compared to obtain a trade-off between reducing number of sections and accuracy.

The contributions of this thesis are

1. Sensitivity analysis (Chapter 2): Categorizing the most efficient sensitivity analysis methods, comparing sensitivity analysis methods in each category, helping practitioners decide the most appropriate sensitivity analysis method and analyzing the sensitivity of a road design model.

2. Section positioning (Chapter 3): proof of concept that has great potential for reducing the number of variables considered and subsequently reducing the computation time. In this thesis, up to 90% reduction in number of section was observed while maintaining acceptable accuracy that translate to 88% savings in computation time. This is a proof of concept supported by 4 use cases that show tremendous potential.

The limitations of this thesis are:

1. Only construction cost was considered in the road design model while in practice, environmental, users, and other costs should be taken into account.

2. Only vertical alignment was considered but SA should also be applied to horizontal alignment; similarly, section reduction was applied to vertical alignment but may also give huge savings on the horizontal alignment.

3. Even with only building costs considered, several approximation assumption were made e.g. no details on what machine was used, wages, construction duration etc. were used to keep the model tractable.
Future work based on Chapter 2 could consider obtaining safe ranges of road design model inputs such as cost parameters. The true cost parameters cannot be known until after construction, and even then it may be difficult to estimate the true cost parameters. Therefore, ranges for the unit costs should be found such that the construction cost is not sensitive to these unit costs ranges.

Suppose $UC$ is the actual unit cost and $UC_1$ is the uncertain unit cost. For a given set of standards and constraints (assume constant), function $F_a$ returns an alignment for a given set of unit costs. For a given alignment, the total earthwork construction cost ($C$) can be estimated by the cost function $F_c$.

\begin{equation}
A = F_a(UC), \quad C = F_c(A, UC),
\end{equation}

where $A$ and $C$ are the actual alignment and construction cost, respectively. As the designers do not have the actual unit costs, they use the uncertain unit costs ($UC_1$) and find an alignment ($A_1 = F_a(UC_1)$). The cost of constructing this alignment is $C_{1T}$ that can be calculated by estimating the actual unit costs and plugging them in the cost function $C_{1T} = F_c(A_1, UC)$.

The designers expect $C_{1T}$ and $C$ to be close to each other. In other words, they expect $\frac{C_{1T} - C}{C}$ to have a small value. Therefore, designing a cost model that helps to find an insensitive construction cost is required.

Future work based on Chapter 3 is comparing the section positioning methods on a large number of grounds. In addition, the grounds should be categorized into flat, hilly, and etc. For each category of grounds, specific values for the methods parameters ($\delta$ and $\epsilon'$) could be defined.
Bibliography


Bibliography


Bibliography


Bibliography


Bibliography


Bibliography


70


