Uncertainty and sensitivity analysis

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Nomenclature

D	Random distribution of x
S_i	First order sensitivity index
S_{Ti}	Total order sensitivity index
x	Stochastic model input
y	Stochastic model output
α	Percentage outside credible region

1 Introduction

This section begins with a discussion of how it is possible to perform an uncertainty analysis to analyse stochastic model results. Then different methods of performing sensitivity analysis methods will be surveyed, with an identification of the most suitable technique to apply for computationally inexpensive models with relatively low numbers of variables. Finally the uncertainty and sensitivity analysis techniques will be summarised with a description of a modelling process which uses both in order to produce useful analysis from a scientific model.

Uncertainty analysis and sensitivity analysis serve similar yet separate tasks. This difference is described in the following manner; for a given deterministic model, the results $\mathbf{y}(\mathbf{x}) = [y_1(\mathbf{x_1}), y_2(\mathbf{x_2}), ..., y_n(\mathbf{x_n})]$ are functions of the uncertain inputs $\mathbf{x} = [x_1, x_2, ..., x_{nX}]$. Uncertainty in $\mathbf{x}$ results in an uncertainty in y. Uncertainty analysis is answering the question of identifying the uncertainty in $\mathbf{y}(\mathbf{x})$ given the uncertainty in $\mathbf{x}$. Sensitivity analysis is the identification of how individual elements of $\mathbf{x}$ contribute towards the uncertainty in $\mathbf{y}$ (Helton et al., 2006; Saltelli et al., 2006, 2008)). Global sensitivity analysis studies the effects of input variations on the input parameters in the entire allowable range, with the result they account for the effects of interactions between different parameters (Baroni and Tarantola, 2014)).

2 Uncertainty analysis

There are two main categories of uncertainty regarding scientific models; type A and type B. Type A uncertainty, also known as aleatory uncertainty, refers

to the inherent randomness in the behaviour of a system under study. Type B uncertainty, also known as epistemic uncertainty, is that derived from a lack of knowledge about the value to use for a parameter assumed to have a fixed value for a specific analysis (ISO, 2008)). There are two types of statistical error that can occur in the analysis of data; type 1 and type 2 (Neyman and Pearson, 1928)). Type 1 error is the incorrect rejection of a true null hypothesis, whereas type 2 error is the failure to reject a false null hypothesis. It is important to understand the difference when attempting to model the behaviour of an engineering artefact of uncertain dimensions. At the exploratory stage it may be more important to model the behaviour of an artefact across a wider range of dimensions to see where the global optimums might be. However, if smaller regions of parameters were studied then it may be possible that Type 2 error occurs and incomplete analysis might be returned.

There are multiple uncertainty analysis methods which may be applied towards understanding complex models. For models with large computational costs surrogate models can be used to simulate the performance of the model (Forrester and Keane, 2009)). They use an experimental design procedure to minimise the number of model points to be tested (Lucia Faravelli, 1990; Simpson et al., 2001; Helton and Davis, 2003b)). Other methods which may be applied include differential analysis (Jackson, 1995)), variance decomposition (Saltelli et al., 2000b)) and sampling based techniques (Helton et al., 2006)).

Note that the methods discussed so far are all probabilistic characterisations of uncertainty. It is possible to use other methods such as fuzzy logic (Ross, 2004)) to explore possibilistic characterisations of uncertainty. The use of possibilistic techniques rely on successfully identifying how to derive the correct possibilities using linguistic variables. In fuzzy logic, for example, this involves identifing the correct membership function to describe the relationship between a physical parameter and the likelihood of it occuring given a possibility. However if this membership function is judged incorrectly due to a paucity of information then it may be possible that Type 2 error is encountered. It may be possible in future analysis to use possibilistic methods to identify 'more-likely' parameter ranges which can then be analysed using probabilistic methods. For now the use of a deterministic physics based model which is analysed using probabilistic methods will be discussed. This provides a methodology which can then be adapted to recieve parameter regions selected using fuzzy logic.

Sampling-based techniques, also known as Monte-Carlo techniques are suitable for use with models that are computationally inexpensive that have relatively low numbers of parameters (Helton et al., 2006)). The process for implementing a sampling based methodology for uncertainty analysis is described;

1. Define the distributions $D_1, D_2, ..., D_{nX}$ that characterise the epistemic uncertainty in the elements $x_1, x_2, ..., x_{nX}$ of $\mathbf{x}$.
2. Generation of a sample $x_1, x_2, ..., x_{nX}$ in consistency with the distributions $D_1, D_2, ..., D_{nX}$.
3. Propagation of the sample through the model to produce a mapping $[\mathbf{x_i}, \mathbf{y}(\mathbf{x_i})], i = 1, 2, ..., nS$ from model inputs to model results.
4. Perform uncertainty analysis

Identifying the sample distributions D that describe the epistemic uncertainty of input parameters to the modelling process is key to the success of the

analysis process. This stage is usually completed using expert insight or experimental results (Helton et al., 2006)). However, at the exploratory analysis stage or for situations such as archaeological investigations with scarce information it's possible to use simple definitions for $D_1, D_2, ..., D_{nX}$. This allows exploration in the variation in the model output (avoiding type 1 error) rather than for a specific application of the model.

There are multiple methods for generating a sample for each input parameter distribution. Selecting a methodology at this stage involves identifying the computational cost of running the model, the number of input parameters of the model and the requirement for accuracy of analysis. Furthermore, the consideration of the purpose of the uncertainty analysis or sensitivity analysis to be performed also influences the accuracy and the number of model runs required (Saltelli et al., 2008)).

Three main groups of sampling methods have been identified; importance sampling, Latin hyper-cubes, and random sampling (Helton et al., 2006)). Importance sampling involves sampling x_i independently from a density $p(x)$ given a probability density $q(x)$. The improvement over random methods is that through sampling from a density $p(x)$ which is over the region where the supposedly more important results exist, it is possible to get more representative model results (Owen and Zhou, 2000)). However, the disadvantage of this method is that the individual sample elements do not have equal weight of occurrence (Helton et al., 2006)), therefore leading to results which are dependent on the model and the researcher performing the analysis and leading to Type 2 error.

Latin hypercubes are an example of a space filling technique, where the sample space is sampled in such a manner to achieve coverage of the main variations (McKay et al., 1979; Morris, 1991)). Latin hyper-cube sampling is performed in the following manner in order to generate a sample of size nS from the distributions $D_1, D_2, ..., D_{nX}$ associated with the elements $x_1, x_2, ..., x_{nX}$ of $\mathbf{x}$. The range of each x_j is exhaustively divided into nS disjoint intervals of equal probability and one value x_{ij} is randomly selected from each interval. The nS values for x_1 are randomly paired without replacement with the nS value for x_2 to produce nS pairs. These pairs are then randomly combined without replacement with the nS values for x_3 to produce nS triples. The procedure is followed until a set of nS nX-tuples $\mathbf{x_i} = [x_{i1}, x_{i2}, ..., x_{i,nX}], i = 1, 2, ..., nS$ is obtained (Helton and Davis, 2003a)). This method is known to be more efficient than random sampling techniques for analysing models when low order terms are present (Kucherenko et al., 2015)), and is often chosen for computationally expensive models. However, random sampling methods allow more accurate results for computationally inexpensive models.

Random sampling techniques draw samples from the probability distributions D. These samples can be drawn independently of each other, i.e. in a crude manner, or, these samples can be drawn in a manner so that they are dependent on each other. The latter method can be done using Markov Chain Monte Carlo techniques which use Markov chains to simulate a prior distribution for a given variable (Brooks, 1998)). At the exploratory stage it's more important to study the model and higher-order effects rather than to represent the distributions of the input parameters exactly. Furthermore, existing techniques for generating random numbers often have large periods, such as the mersenne twister with a period of $2^{19937} - 1$ which is implemented in the Numpy Python package (Stéfan van der Walt and Varoquaux, 2011)). Therefore it is

possible to get fairly accurate results using crude random sampling methods.

In order to identify how to conduct an uncertainty analysis the statistical framework used to analyse the results must be identified. Philosophically there are two approaches to statistical analysis, the Bayesian approach and the Frequentist approach. The subject of what framework to use has been the subject of much debate throughout the 20th century, (Jaynes, 1976)) for example. Frequentists understand probabilities as being fundamentally related to frequencies of events, whereas Bayesians understand probabilities as being fundamentally related to their own knowledge about an event. The consensus is that it is possible to frame pertinent questions about a given data set using the language of Bayesian statistics in a simpler and more accurate manner than frequentist statistics (VanderPlas, 2014)).

The question of interest is the identification of the probable performance of a given sailing craft. In the language of Bayesian statistics this is the identification of a credible region CR_y which the measurement result y lies within. If this credible region contains the result y_0 at least $100(1-\alpha)\%$ of the time given any value of y_0 in repeated samples, then CR_y is the $100(1-\alpha)\%$ credible region for the parameter y (Gelman et al., 2014)).

There are two methods of estimating the bounds of a credible region, either identifying a quantile based interval (Hitchcock, 2012a)) or calculating the bounds of the highest posterior density interval (Hitchcock, 2012b)). If y_L^* is the $\alpha/2$ posterior quantile for y, and y_U^* is the $1-\alpha/2$ posterior quantile for y, then (y_L^*, y_U^*) is the $100(1-\alpha)\%$ credible interval for y. However, if the posterior distribution is skewed then quantile based intervals give incorrect intervals and it is more appropriate to use the bounds given by the highest posterior density region. This region is a subset $\mathcal{C} \in y$ defined by $\mathcal{C} = y : \pi(y|\mathbf{x}) \geq k$ where k is the largest number such that $\int_{y:\pi(y|\mathbf{x})\geq k} \pi(y|\mathbf{x})dy = 1-\alpha$. As the posterior distribution of sailing craft performance is unknown, it is appropriate to use the highest posterior density region to provide credible performance estimates.

3 Sensitivity analysis

Sensitivity analysis techniques either focus on local or global approaches. Local approaches vary each model parameter in turn in order to study the influence around a single point in the model parameter region. These approaches are often computationally cheap to run, however do not study the result of interaction between parameters or the influence of the whole parameter region. However, global sensitivity analyses allow the influence of parameter variation over the whole input parameter space on model output space (Saltelli et al., 2000b)). Local sensitivity analyses are found often in ship science research for two reasons; often the parameter region is well defined, such as in kayak performance (Jackson, 1995)) and a global analysis might not be required, or the model or experiment is simply too expensive to run for the whole region. Global sensitivity analyses may be defined using the two properties below (Saltelli et al., 2000a)), and are particularly suitable for applications where relatively little is known about the behaviour of the model.

1. The sensitivity analysis incorporates the effect of the range and the shape of their probability density functions.

2. The sensitivity estimates of individual factors are evaluated varying all other factors as well.

The model considered for this research, a sailing craft velocity prediction program, is comparatively lightweight to other engineering simulation techniques and there is a large associated parameter range for the input designs to be considered, therefore global sensitivity analysis techniques provide the only way of examining the impact of the archaeological uncertainty of the Polynesian voyaging canoe design. GSA require a large number of model runs in order to attempt to explore the impact of parameter influence on the model inputs. Identifying the purpose of a sensitivity analysis is crucial for interpreting its results. Four main purposes, or settings have been identified for sensitivity analysis methods (Saltelli et al., 2000b, 2002, 2008)):

1. **Factor prioritisation** allows the identification of the factor, which, if known, would lead to the greatest reduction in the variance of the target output Y.
2. **Factor fixing** simplifies the model through identifying and fixing non-influential factors.
3. **Variance cutting** is used to reduce the output variance below a specified tolerance. This is where the analyst seeks to reduce the output uncertainty through acting on the smallest number of factors.
4. **Factor mapping** is used to study which values of input parameters lead to model realisations in a given range of the output space.

For the application to an archaeological performance prediction problem the factor prioritisation and factor fixing settings are the aims of the sensitivity analysis process. This because the primary aim is to identify what the most influential parameters are, and thus identify the key archaeological implications from the modelling process. The factor fixing process is also useful as it would reduce the number of parameters that would need to be considered in a given voyaging craft design. When the modelling process requires an identification of the most significant parameters that influence performance in a specific area, the factor mapping setting can then be used.

A useful sensitivity analysis technique must possess the properties described below (Saltelli et al., 2008)). There are a range of sensitivity analysis techniques which meet these criteria and are also suitable for application to the settings described above. Table 1 gives a brief overview of the categories of technique available.

1. Sensitivity measure is independent of the model
2. Capacity to capture the influence of the full range of variation of each input factor
3. Appreciation of interaction effects among input factors
4. Capacity to tackle groups of input factors

The practice of performing local sensitivity analysis is limited in application through not investigating the whole model space, which is crucial for this investigation. The method of Morris (Morris, 1991; Campolongo et al., 2007)) is effective for the ranking of different parameters, however doesn't provide a measure of how each parameter contributes towards the total model uncertainty.

Type	**Morris**	**Variance**	**Factorial**	**Monte Carlo**	**Local SA**
Model independent?	Yes	Yes	Yes	Yes	Yes
Sample source	Levels	Distributions	Levels	Distributions	Levels
No. factors	20 - 100	<20	>100	<20	<100
Factor range	Global	Global	Global	Global	Local
Multi-factor variation	Yes	Yes	Yes	Yes	No
Correlated factors?	No	No	Yes	Yes	No
Cost (for k factors)?	10 (k+1)	500(k+2)	k ->2k	500 + 1	2(k + 1)
Estimated CPU	1 day	11 days	3 hours	$\approx$ 2 days	1 hour

Table 1: Overview of sensitivity analysis techniques available, (Usher, 2016)) adapted from Saltelli et al. (2008)). Time calculations computed assuming 5 minutes run time per simulation and 30 factors.

Fractional factorial methods (Saltelli et al., 2008, p. 71)) are able to cope with non-linear models, however don't process input factors as belonging to distributions and lack accuracy compared to variance based techniques. Variance based techniques are able to quantify the contribution each parameter makes to the uncertainty in a model output and they are able to calculate the impact each factor has in co-ordination with other factors. This makes them suitable for application to understand how different design parameters contribute towards the uncertainty in a performance estimate.

Variance based techniques propose that model uncertainty can be measured using its variance. They use this measurement to proportion how uncertainty in input parameters have impacted it. The variance based technique identified for use is named the "Sobol Sensitivity Analysis" (Sobol, 2001; Saltelli, 2002; Saltelli et al., 2010)) and is chosen for its wide application to many different problems (Saltelli et al., 2008)).

The first variance based technique was the Fourier amplitude sensitivity test (FAST) described in (Cukier et al., 1973)) which introduced conditional variances for a sensitivity analysis based on first-order effects. A methodology for decomposing the output of a function into contributions of different dimensions was introduced by (Sobol, 1993)), using Mont Carlo simulations to generate samples. This method allowed the computation of first order and higher order indices. Progress in this methodology was described further in (Sobol, 2001)). In order to reduce the computational cost of performing the sensitivity analysis to widen application, (Saltelli, 2002)) introduces methods which reduce the cost of computing the first order and total order sensitivity indices. This work demonstrated that Sobols method outperforms FAST, with the ability to calculate an extra parameter which can identify non influential parameters for no extra computational cost. Sobols method was also showed to be successful for application to non-linear and non-additive physical models. Sobols method was developed further in Saltelli et al. (2010)) with the identification of more efficient methods of generating samples which cover the model region and methods of calculating the sensitivity indices. The use of Sobol quasi-random sequences, which generate samples of $X_1, X_2, ..., X_R$ as uniformly as possible over the unit hyper cube ω, using radial sampling was identified as being the most effective. Quasi-random sequences generate samples based on knowledge of existing samples which allows more efficient sets of samples to be generated.

There are two key measures of the influence a generic factor X_i has on the

results of a model, S_i and S_{Ti} (Homma and Saltelli, 1996)). Equations (1) (2) describe the calculation of the first order sensitivity measure and the total order sensitivity measure. It's noted that sensitivity analysis includes examining the influence a parameter has interacting with other parameters as well as on its own.

$\mathbf{X}_{\sim_\mathbf{i}}$ is the matrix of all factors but X_i, thus the inner expectation operator in Equation 1 is that the mean of Y is taken over all possible values of $\mathbf{X}_i$ while keeping X_i fixed. $\mathbf{X}_{\sim\mathbf{i}}$ denotes the matrix of all factors but X_i. S_i is a normalised index as $V_{X_i}(X_{\mathbf{X}_{\sim\mathbf{i}}}(Y|X_i))$ varies between 0 and $V(Y)$. S_{Ti} measures the total effect, i.e. first and higher order interactions of the factor X_i. It can be calculated through subtracting the first order effect of $\mathbf{X}_{\sim\mathbf{i}}$, $V_{\mathbf{X}_{\sim i}}(E_{X_i}(Y|\mathbf{X}_{\sim i}))$ from the variance $V(Y)$ which gives all the contribution of the terms in the variance decomposition which do include X_i.

$$S_i = \frac{V_{X_i}(X_{\mathbf{X}_{\sim\mathbf{i}}}(Y|X_i))}{V(Y)} \tag{1}$$

$$S_{Ti} = \frac{X(\mathbf{X}_{\sim\mathbf{i}}(V_{X_i}(Y|\mathbf{X}_{\sim\mathbf{i}}))}{V(Y)} = 1 - \frac{V_{\mathbf{X}_{\sim i}}(E_{X_i}(Y|\mathbf{X}_{\sim i}))}{V(Y)} \tag{2}$$

One methodology which is able to combine uncertainty and sensitivity anaylsis techniques within a single framework is described in Baroni and Tarantola (2014)) as the "General Probabilistic Framework for uncertainty and global sensitivity of deterministic models". This framework, shown in Figure 1, is able to cope with non-scalar sources of uncertainty without any constraint and can be applied to models of unknown linearity, monotonicity and additivity. It has been successfully applied to understanding environmental models. It's possible to use this diagram to show how the uncertainty and sensitivity analysis being performed in this report fit into the process of evaluating Polynesian canoe performance.

Glossary

sampling based Sampling based techniques, also known as Monte Carlo techniques (Metropolis and Ulam, 1949)), involve the exploration of a mapping between input and output parameters through the generation of random samples for input into the model.. 2

surrogate Surrogate models aim to simulate the results from computationally expensive engineering methods through creating models from sampled points of the response of the method given a series of sample points. 2

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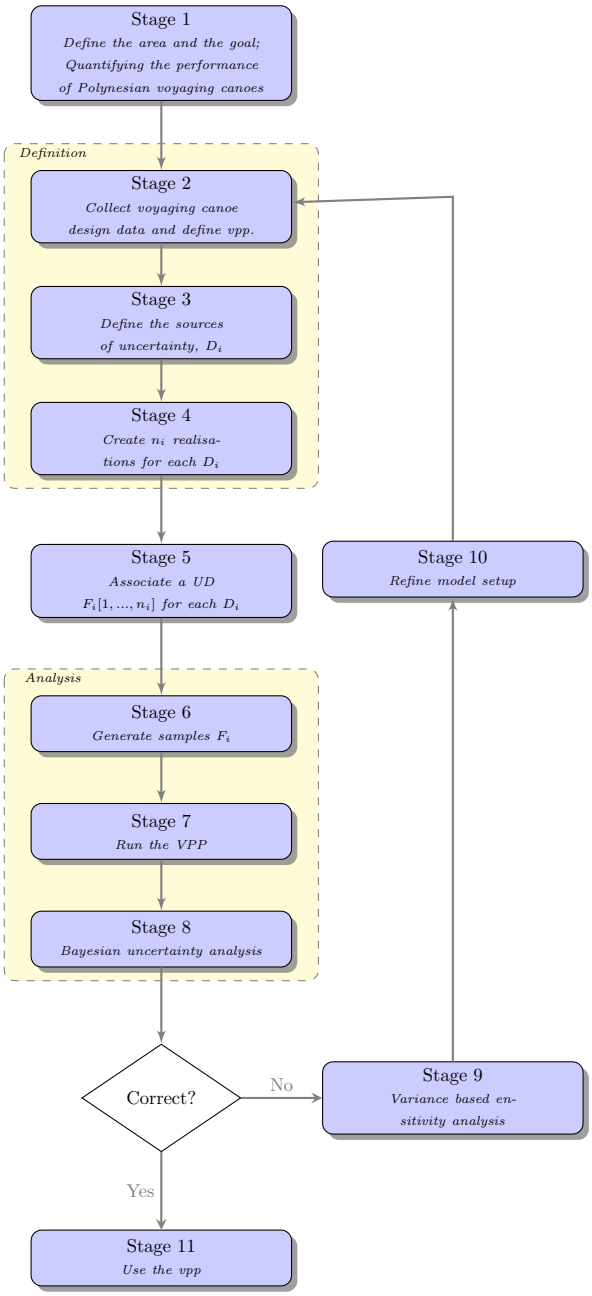

Figure 1: Diagram showing how it is possible to apply the general probabilistic model to perform analysis of a physical model. Modified from Baroni and Tarantola (2014)).

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