## Review and improvements to methods of parameter space exploration of ecological models using R

Authors Andre Chalom

Paulo Inacio Prado

Date 03/16/2012

Affiliation Department of Ecology,

University of Sao Paulo

#### Abstract

In recent years, both the scientific community and policy makers are gaining confidence in the formulation and use of mathematical models in ecological studies. We are thus seeing a flourishing of more elaborate and complex models, and the questions related to the efficient, systematic and error-proof exploration of parameter spaces are of great importance to better understand, estimate confidences and make use of the output from these models. In this work, we investigate some of the relevant questions related to parameter space exploration, in particular using the technique known as Latin Hypercube Sampling and focusing in qualitative and quantitative output analysis. We present improvements to the methods discussed, and assess how are these questions being currently addressed in the literature. Full working examples are given in the R language, included at the appendix.

NOTA: Vão ser incluidas muito mais refs posteriormente!

#### 1 Introduction

There is a growing trend in the use of mathematical modelling tools in the study of many areas of the biological sciences. The use of models is essencial as they present an opportunity to address questions that are impossible or impractical to answer in either in purely theoretical analyses or in field or laboratory experiments, and to identify the most important processes which should then be investigated by experiments. Of particular interest are the Individual Based Models (IBM), which represent individuals that move and interact in space, according to some decision-making rules. These models permit a great level of detail and realism to be included, as well as linking multiple levels of complexity in a system.

On the other hand, more realistic models employ a vast selection of input parameters, from temperature and rainfall to metabolic and encounter rates, which may be difficult to accurately measure. While variations in some of those parameters will have negligible impact on the model output, other parameters may profoundly impact the validity of a model's predictions, and it may be impossible to determine *a priori* which are the most important parameters. In theory, this could be done by evaluating the model at all possible combinations of parameters, however this would require a prohibitive number of model runs, specially considering that a single run of those models may take days to complete. Our challenge then consists in providing the best estimates for the importance of the several parameters, requiring the least number of model runs.

The disciplines of uncertainty and sensivity analysis have been developed in the context of the physical sciences and engineering, and have been greatly developed in the 1980 and 1990 decades by researches such as Saltelli, Helton, Iman, Conovoer, Sobol' and McKay. More recently, these analyses have been successfully applied to biological models, in order to explore the possible outcomes from the model output, estimate their probability distribution and the dependency of the output on different combinations of parameters, and to assess which parameters require more experimental effort in order to be more confidently estimated. This kind of parameter space exploration is considered a fundamental step prior to using the model in management decisions [?].

One approach to the parameter space exploration, which will be described here, is to generate samples from the parameter space, run the model with these samples, and analyse the qualitative or quantitative differences in the model output. Section 2 will present the sampling techniques, with empashis on the Latin Hypercube method, while sections 3 and 4 will deal with qualitative and quantitative analyses, respectively. Then, we briefly review some relevant research papers which have used such techniques in the exploration of ecological models in section 5, and present a full working example of the sampling and analysis in the Appendixes.

#### 1.1 Parameter spaces

In order to better pose our questions, we need first to have a precise definition of what is the parameter space (or PS for short) of our models, and to distinguish the general use of this expression by the statistical and the modeling community [?].

#### TOD0

Also, it should be mentioned that the parameter space may be constrained or unconstrained. This will have an impact on some of the available sampling and analysis techniques.

For example, let us consider the space of all triangles with one fixed side. We will use as parameters the angles of the triangle (fig. 1),  $a_1$ ,  $a_2$  and  $a_3$ . As the sum of the angles is  $180^o$ , we can fix  $a_3 = 180^o - a_1 - a_2$ . In addition, the sum of  $a_1 + a_2$  must not exceed  $180^o$ . The condition

$$a_1 + a_2 \le 180^o \tag{1}$$

is called a constraint, and limits the values that the parameter vector may assume. We will return to questions related to constrained parameter spaces in section 2.2.

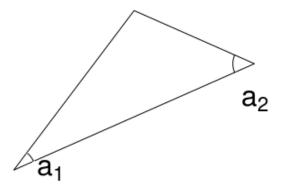


Figure 1: A sample triangle with the angles  $a_1$  and  $a_2$  highlighted.

#### 1.2 Problems in parameter space exploration

Next, we turn our attention to the kind of problems we might want to address with the exploration of the parameter space. First, the simplest case is asking "is there a region of my parameter space where condition X holds?" This condition might be, for example, the extinction or coexistance of species, some pattern of distribution or abundance of species. We also might be interested in mapping where are these regions. In complex models, where several different regions might exist where the qualitative results of the models are very different, we may ask how many of these regions are there, as well as map the frontiers between them. We will explore some tools that deal with these qualitative problems in section 3.

Another class of problems arises when the model produces some quantitative response, and we are interessed in determining the dependency of this response to the input parameters. For example, when modeling the dynamics of a population, we might want to know how the final population varies with each of the input parameters. In this context of quantitative analysis,

the questions are divided in two classes: first, how much the variation of the input parameters is translated into the total variation of the results, which is the topic of uncertainty analysis, and second, how much of the variation in the results can be ascribed to the variation of each individual parameter, which is the topic of sensitivity analysis [7, 8]. We will present the techniques and results from both uncertainty and sensitivity analysis in section 4.

All these problems may be formulated in a general way, defining some response from the model  $\mathbf{Y}$  as a function of the input parameter vector  $\mathbf{x}$ :

$$\mathbf{Y} = \mathbf{f}(\mathbf{x}) \tag{2}$$

In the equation 2, all the quantities are vectors, indicated by the boldface. Here,  $\mathbf{x} = [x_1, x_2, \dots, x_m]$  represent the parameters to the model  $\mathbf{f}$ , and  $\mathbf{Y} = [y_1, y_2, \dots, y_n]$  represent the some quantitative responses from the model. In some sections, we will discuss the response as a single value y, without loss of generality.

Each of the input parameters  $x_i$  is associated with a probability distribution  $D_i(x)$ , which represent our degree of knowledge about the values that  $x_i$  may assume (see figure 2 for examples).

Conseguir dados reais para gerar Dis

## 2 Sampling Techniques

There are several strategies that can be used to choose the samples from the parameter space that will be used as input to our model of interest. Here, we will present some of them, along with their limitations, to justify our choice for the Latin Hypercube Sampling, which we will describe in section 2.1.

One way of exploring the parameter space is to choose a number of possible values for each parameter, and run the model for every combination of those values. This is called full parameter space exploration, as done in [5], and altough it possesses many advantages, it may become very costly in terms of computer time. In addition, the number of possible combinations increases exponentially with the number of parameter dimensions considered.

To circumvent the exponential increase in the number of samples, it is usual to explore the parameter space in the following fashion: holding all but one parameter constant, we analyse how the output of a model is affected by one parameter dimension at a time (as done in [11]). This kind of analysis, called individual parameter perturbance, is, however, limited by the fact

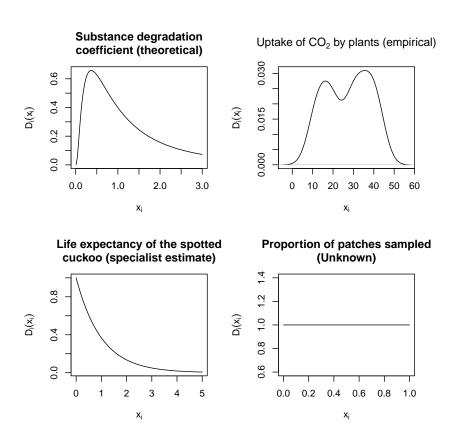


Figure 2: Four different possible origins from  $D_i$  \*TODO\* melhorar explicacao

that the combinations of changed parameters may give rise to complex and unexpected behaviours.

Another viable option would be to chose N random samples from the entire space, in order to analyse both the effect of each parameter and the combined effect of changing any combined number of parameters. This sampling scheme is called random sampling, or Monte Carlo sampling, and has been applied to many biological models [9].

Stratified sampling strategies, which are a special case of Monte Carlo sampling, consist in strategies for chosing these random samples while, at the same, making sure that every subdivision (or *strata*) of the distribution is well represented. As shown on [12], the estimatives of the statistical properties (such as the mean or the variance) of the model output are better represented by stratified random sampling than by simple random sampling (see figure 3 for examples). As we shall see in the next session, the Latin Hypercube sampling is a practical and easy to understand stratified sampling strategy.

#### 2.1 Latin Hypercube: Definition and use

In this section, we describe the Latin Hypercube Sampling, and show how it can be used to efficiently solve the questions posed in section 1. We also discuss what are the available methods for obtaining the LHS.

Firstly, let us define, in the context of statistical sampling, what is a Latin Square:

**Definition** If we divide each side in a square in N intervals, and then take samples from the square, the resulting square will be called Latin if and only if there is exactly one sample in each row and each column.

A Latin Hypercube is simply the generalization of the Latin Square to an arbitrary number of dimensions m. From these definitions, it is clear that the number of samples is fixed as N We will show how to estimate the optimal N in section 4.7, but for now it is relevant to note that N does not depend on the number of parameters considered.

We will now construct the Latin Hypercube. Let's fix our attention in one parameter dimension i of the parameter space. The first step we should take is to divide the range of  $x_i$  in N equally probable intervals. In order to do so, we will turn our attention to the probability distribution of  $x_i$ , defined on section 1.1 as  $D_i$ . Recall that this probability distribution must be chosen in a way that represents our current understanding of the biology of the given system. This function might be estimated by an expert in the field, it might represent a data set from field or laboratory work, or in some cases it may

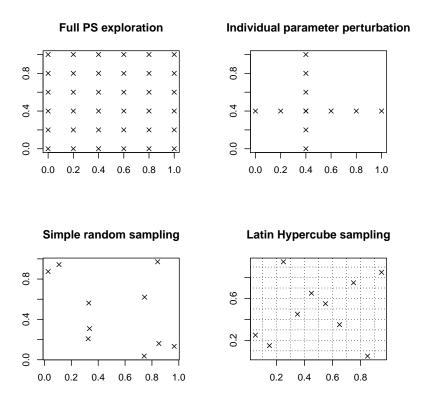


Figure 3: Illustration of four sampling methods. While the full parameter space exploration is clearly representative of the whole space, it requires a very large number of samples. The individual parameter perturbation chooses samples by holding one parameter constant and varying the other, and clearly cannot take into account interactions between parameters. The random sampling uses information about the whole parameter space with a small number of samples, but can oversample some regions while undersampling others. The Latin Hypercube (section 2.1) samples all the intervals with equal intensity.

be simply the broadest possible set of parameters, in some cases where the actual values are unknown or experiments are unfeasible (see fig. ??).

In possession of the distribution function  $D_i$ , we must sample one point from each equally probable interval. There are two approaches used here: it is possible to choose a random value from within the interval (as proposed by [12]), or instead, we can use the midpoint from each interval [2]. We will use the second approach here.

The integral of the distribution function is called the cumulative distribution function  $F_i(x)$ . This function relates the values x that the parameter may assume with the probability p that the parameter is less than or equal to x. We will refer to the inverse of the cumulative distribution function,  $F_i^{-1}$ , as the quantile function of the parameter  $x_i$ , as it associates every probability value p in the range (0,1) to the value x such that  $P(x_i \leq x) = p$ . We divide the range (0,1) in N intervals of size 1/N, and use this quantile function to determine the x values as the midpoints of each interval. Summarizing, we take the N points, represented as  $x_{i,k}$ ,  $k \in [1, N]$ , from the inverse cumulative distribution  $F_i^{-1}(x)$  as:

$$x_{i,k} = F_i^{-1} \left( \frac{k - 0.5}{N} \right) \tag{3}$$

The samples from each dimension are subsequently shuffled, to randomize the order in which each value will be used (see example on figure 4). As the samples come from the distributions  $D_i$ , and are only reordered, their (marginal) distribution will remain that of  $D_i$ . However, the joint distribution of the parameters is still not well defined. In particular, this simple shuffling may result in some of the parameters to be positively or negatively correlated with each others, which might be undesirable. Some techniques have been developed to eliminate these correlation terms or to impose different correlations between the variables, and will be presented on section 2.2.

It should be noted that, in the mathematical literature, it is usual to refer to a somewhat different object as a Latin Square: this would be a square whose sides are divided in N intervals, and is filled with N different symbols, such that for each row and column there is exactly one occurrence of each symbol. The figure 5 shows an example of one "full" Latin Square.

#### 2.2 Algorithms and extensions

As described above, the LH sampling generates an uniform distribution of samples in each parametric dimension. However, there is no guarantee that

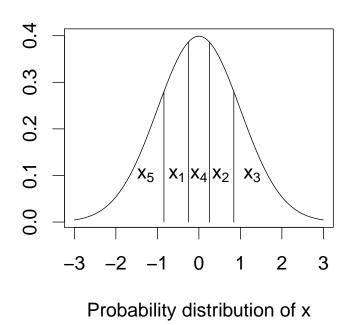


Figure 4: Sample normal probability distribution, with 5 samples collected and shuffled. Note that the first sample correspond to the second interval, the second sample correspond to the fourth interval, and so on.



Figure 5: A stained glass window at the Caius College, Cambridge, showing a full Latin Square. Notice how there is only one occurence of each color in each row and in each column.

the correlation between two or more parameters will be zero, and the classical algorithm from McKay [12] usually produces correlations as high as 0.3 between pairs of factors, which can difficult or even compromise further analyses. In this section, we will present one algorithm designed to take into account the correlation between the parameter variables [2], using a single-switch-optimized sample reordering scheme. We will present the general case of prescribing a correlation matrix, and will also present results for the trivial case of zero correlation terms. Other methods have been proposed to address this problem [10, 4, 1], including methods that deal with higher-order correlation terms [?] using orthogonal designs. These methods, however, impose severe restrictions on the number of samples that must be chosen.

In order to obtain the samples with prescribed correlation terms, we define the desired  $m \times m$  correlation matrix between the variables, in which  $C_{i,j}^*$  stands for the correlation between  $x_i$  and  $x_j$ .

The next step is done iteratively for each parameter dimension, starting with the second one. Suppose that the method has already been applied to i = 1, 2, ..., l - 1, and we will apply it to i = l. The square sum of the errors in the correlations between  $x_l$  and the anterior parameters is given by

$$E = \sum_{k=1}^{l-1} \left( C_{l,k} - C_{l,k}^* \right)^2 \tag{4}$$

Afterwards, we calculate, for each pair of values sampled from the parameter dimension l, what would be the error in the correlation if they were switched. The pair that corresponds to the greater error reduction is then switched, and the procedure is repeated iteratevely until the error is acceptably small.

Here, we also consider how to treat a constrained parameter space, as described in section 1.1 (the case in which  $a_1 + a_2 < 180^{\circ}$ ). Clearly, this parameter space is not square, in the sense that, if we define the ranges of the variables  $a_1$  and  $a_2$  independently as (0,180), not all combinations of parameters will be meaningful. What can be done in this case is to create a new parameter  $\hat{a_1}$ , defined as

$$\hat{a_1} = \frac{a_1}{180 - a_2} \tag{5}$$

This new parameter varies between 0 and 1, and all combinations of  $\hat{a_1}$ ,  $a_2$  are points from our parameter space. Now, care must be exercised after applying such transformations in order to preserve the marginal distributions from the original variables, as exemplified on figure 6.

a1 + b\*a2 < X

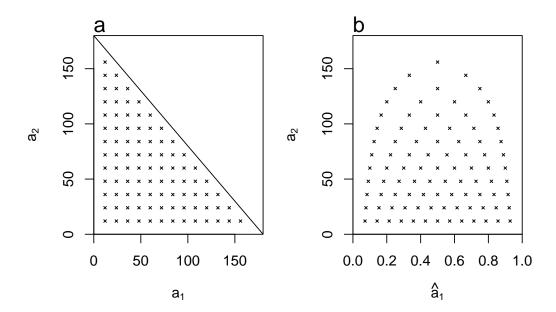


Figure 6: a. The constrained parameter space considered, with the line representing  $a_1 + a_2 = 180$ . The symbols represent a uniform sample taken from the space. b. The transformed parameter space  $\hat{a_1}, a_2$  (see eq. 5), showing the same sampled points.

```
a1 - b*a2 < X
a1 * a2 < X -> escala exp
a1 / a2 < X -> escala log
cacar envelopes, EcoSim macroecologia
J Biogeogr
For a given transformation T, how are the D_i affected?
```

#### 2.3 Stochastic models

When dealing with stochastic models, like several relevant individual based models (IBM), the questions presented become complicated by the fact that running the same model with exactly the same parameters might wield largely different results, both quantitative and qualitatively. In this scenario, we must be able to differentiate the variation in responses due to the variation of the parameters with the variation in response due to stochastic effects.

We will proceed first by defining the variation due to the input parameters as the epistemic uncertainty. This uncertainty arises from the fact that we do now know what are the correct values for a given parameter in a given natural system, and is related to the probability distributions  $D_i$ , presented in section 1.2. The variation in the behaviour of the model which is caused by stochastic effects is called stochastic uncertainty, and is inherent to the model.

It is important to note that the two uncertainty components are impossible to disentangle in general stochastic models. This has prevented the general analysis of such models until recently. In recent years, studies have shown that the important parameters and their effects can be correctly identified by running such models repeatedly for the same input variables and then averaging the output [?], given that the following conditions are respected:

- Sample sizes should be large, relative to the aleatory uncertainty.
- The output values should be unimodal, that is, the output values for a given parameter choice should be clustered around a central value.
- The correct analysis tools should be used (as PRCC, which will be discussed on session 4).

Here, we also give an overview of Markov Chain Monte Carlo methods, and their relation with LHS.

#### 2.4 Adaptative refinement

After generating the N Latin Hypercube samples and running the model with the determined parameters, it may become necessary to increase the number of samples. In simple Monte Carlo simulations, increasing the number of samples can be done easily by generating new random points and running the model with them. However, to maintain the desirable properties of the Latin Hypercube, care must be taken to (1) keep the marginal distribution of the points equal to the parameter original distribution and (2) keep the correlation terms equal to zero, or equal to the ascribed values.

We refer to this increase in the number of sample points as a sampling refinement, and as it is done on demand after examining the already generated outputs, we refer to it as an adaptative sampling refinement. This technique can be applied while estimating Iman and Conover's TDCC, which will be used to determine the optimum N size (section 4.7).

To our knowledge, no adaptative sampling refinement technique has been formally proposed on the literature for Latin Hypercube sampling. Our construction will start by defining a new sequence of values  $\gamma_i$  for every parameter dimension, with

$$\gamma_{i,k} = F_i^{-1} \left( \frac{k - 1/6}{N} \right) \tag{6}$$

$$\gamma_{i,2k} = F_i^{-1} \left( \frac{k - 5/6}{N} \right) \tag{7}$$

For every  $k \in [1, N]$ , and so  $\gamma_i$  has 2N elements. Following this, Huntington & Lyrintzis' algorithm [2] is applied on the set of  $\gamma_i$  in order to minimize the correlation between them. The extended Latin Hypercube is formed by concatenating the original  $x_i$  values to the  $\gamma_i$  values, and obtaining a cube with 3N samples defined as  $z_i$ , of which just 2N must be calculated.

**Theorem 2.1** The extended Latin Hypercube presents the following desirable properties:

- The expected sample mean is equal to the distribution mean for each parameter:  $\langle \bar{z}_i \rangle = \langle D_i \rangle$
- The expected sample variance is equal to the distribution variance for each parameter:  $\langle \bar{\sigma}(z_i) \rangle = \langle \sigma(D_i) \rangle$
- The correlation between any two variables is bounded by the following expression:  $\rho_{z_i z_j}^2 \leq \rho_{x_i x_j}^2 + \rho_{\gamma_i \gamma_j}^2$

The proof of these affirmations, along with code examples for the implementation of this algorithm, are showed on the Appendixes.

## 3 Qualitative output analysis

Most of the times, after applying the Latin Hypercube Sampling to an ecological model, it is possible to identify qualitatively different behaviours of the model, possibly clustered into separate regions. In this section, we will focus on tools to identify the different regions.

Descrever o problema e tecnicas para resolve-lo. ConvexHull?

## 4 Quantitative output analysis

#### 4.1 Uncertainty analysis and visualization

The first question we would like to answer, in the context of quantitative analysis, is what is the probability distribution of the response variable y given that we know the join probabilities of the input parameters  $\mathbf{x}$  (see definitions in section 1.2), which is the subject of uncertainty analysis [7].

This can be done by fitting a density curve to the output y or an empiric cumulative distribution function (ecdf). If there is any theoretical reason to believe that the distribution of y should follow one given distribution, it is possible to fit this function to the actual output data and estimate the distribution parameters. If the input parameter distibution functions  $D_i$  correspond to the actual probability of some natural system to exhibit some given parameter value (as opposed to the case where we have no biologically relevant estimates for some parameters), the estimate represented by the density and ecdf functions approaches the actual distribution that the variable y should present in nature.

The next reasonable step is to construct and interpret scatterplots relating the result to each input parameter. These scatterplots may aid in the visual identification of patterns, and altough they cannot be used to "prove" any relationship between the model response and input, they may direct the research effort to the correct analyses. There are extensive reviews of the use of scatterplots to identify the important factors and emerging patterns in sensitivity analyses [6].

We will present here some quantitative analyses tools, aimed at identifying increasingly complex patterns in the model responses. It should be stressed that no single tool will capture all the relations between the input and output. Instead, several tools should be applied to any particular model.

#### 4.2 Linear relation

The most straightforward relationship between y and  $x_i$  is the linear, represented by  $y \sim x_i$ . This is case if, every time  $x_i$  is increased, y increases by approximately the same ammount. The Pearson correlation coefficient is the commonly used measure to test for a linear correlation:

$$\rho_{yx_i} = \frac{\sigma_{yx_i}}{\sigma_y \sigma_{x_i}} \tag{8}$$

Where  $\sigma_a$  is the variance of a and  $\sigma_{ab}$  is the covariance between a and b. The correlation coefficient is a measure of the predicted change in y when  $x_i$  is changed one unit, relative to its standard deviations, and, as such, approaches  $\pm 1$  when there is a strong linear relation between the variables. The square of  $\rho$ , usually written as  $R^2$ , measures the fraction of the variance in the output that can be accounted for by a linear effect of  $x_i$ . Is is usual to test the significance of this linear relation by a t-test [?].

Other than examining the individual relationships between the parameters and the output, we can investigate the joint effect of several  $x_i$ , as  $y \sim x_1 + x_2 + \cdots + x_m$ . In this case, the multiple  $R^2$  represent the fraction of the variance on the output due to linear effects of all the  $x_i$  considered.

However, a measure of  $\rho$  close to zero does not mean that no relationship exists between y and  $x_i$  - for instance,  $x^2 + y = 1$ ,  $x \in [-1, 1]$  presents  $\rho = 0$ , so clearly other methods might be needed.

The Partial Correlation Coefficient (PCC) between  $x_i$  and y is the measure of the linear effect of  $x_i$  on y after the linear effects of the remaining parameters have been discounted. In order to calculate the PCC, first we fit a linear model of  $x_i$  as a function of the remaining parameters:

$$\hat{x}_i \sim x_1 + x_2 + \dots + x_{i-1} + x_{i+1} + \dots + x_m \tag{9}$$

A corresponding model is done with y:

$$\hat{y} \sim x_1 + x_2 + \dots + x_{i-1} + x_{i+1} + \dots + x_m \tag{10}$$

The PCC is calculated as the correlation between the residuals of these two models:

$$PCC(y, x_i) = \rho((y - \hat{y}), (x_i - \hat{x}_i))$$
 (11)

#### 4.3 Monotonic relation

Let us refer to each value of y as  $y_k$  and each value of  $x_i$  as  $x_{ik}$ . The rank transformation of y, represented by  $r(y_k)$  can be found by sorting the values

 $y_k$ , and assigning rank 1 to the smallest, 2 to the second smallest, etc, and N to the largest. The rank of  $x_{ik}$ ,  $r(x_{ik})$ , can be found in a similar way.

If there exists a strictly monotonic relation between y and  $x_i$ , that is, if every time  $x_i$  increases, y either always increase or always decreases by any positive ammount, it should be clear that the ranks of y and  $x_i$  present a linear relationship:  $r(y) \sim r(x_i)$ .

The correlation between r(y) and  $r(x_i)$  is called the Spearman correlation coefficient  $\eta_{yx_i}$ . The same analyses presented on section 4.2 can also be applied for the rank transformed data, including significance testing and multiple regression.

If the procedure described to calculate the PCC is followed on rank transformed data, that is, if y and  $x_i$  are rank transformed and fitted as linear models of the remaining parameters, the correlation between the residuals is called PRCC, or Partial Rank Correlation Coefficient. This measure is a robust indicator of monotonic interactions between y and  $x_i$ , and is subject to significance testing as described in [3]. As shown on figure 7, this measure will perform better with increasing N.

#### 4.4 Trends in central location

Even if the relation between y and  $x_i$  is non monotonic, it may be important and well-defined. The case in which  $y \sim x_i^2$ ,  $x_i \in (-1,1)$  is a common example. This relation may be difficult to visualize, and sometimes may not be expressed analytically. In these cases, the Kruskal-Wallis rank sum test may be used to indicate the presence of such relations [6].

In order to perform the test, the distribution of  $x_i$  must be divided into a number  $N_{test}$  of disjoint intervals. The model response y is then grouped with respect to these intervals, and the Kruskal-Wallis test is used to investigate if the y values have approximately the same distribution in each of those intervals. A low p-value for this test indicates that the mean and median of y is likely to be different for each interval considered, and thus that the parameter  $x_i$  have a (possibly non monotonic) relationship with y.

The number of intervals  $N_{test}$  is not fixed as any "magical number", and may have a large impact on the test results. It is then recommended that this test should be repeated with different values to obtain a more comprehensive picture of the interactions between  $x_i$  and y (fig. 8).

## 4.5 Trends in variability

Other than the central tendency of the results, their dispersal may be dependent on the input parameters.

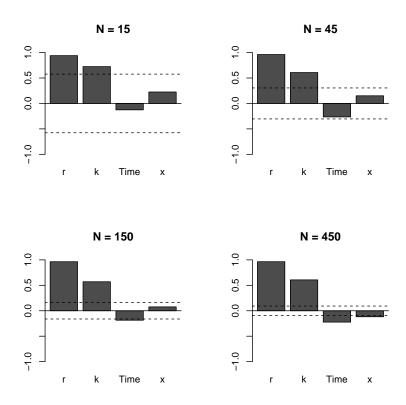


Figure 7: PRCC coefficients for 4 input variables on a model. Values between the dashed lines are not statistically significant. The four panels present results from different sample sizes.

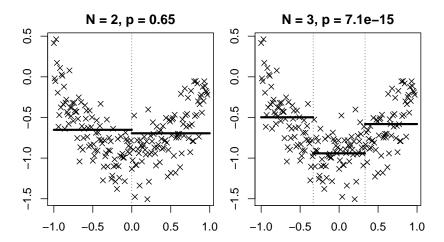


Figure 8: Example of application of the Kruskal-Wallis test on the same data set, which present a strong quadratic component, by dividing the range in 2 intervals (right) or 3 intervals (left). The dashed lines are the divisions between the intervals, and the strong horizontal lines are the sample means for each interval.

Descrever eFAST ANOVA-like SOBOL Kleijnen p17

Pauleira demais? Serah que fazemos essa parte??

## 4.6 Statistical independence

Fazer ou nao? Chi-square testing Kleijnen p18

#### 4.7 Top-down correlation coefficient

Metodo de TDCC do Conover. Pesquisar fonte e descrever

## 4.8 Time dependency

In models where time is an explicit variable, it may be useful to consider how are the correlation and variance-decomposition indexes varying with time.

Descrever o problema com mais detalhe, mostrar mais indices

Figure 9 shows as an example the evolution of the PRCC of a three-dimensional hypercube with parameters r, K and  $X_0$ .

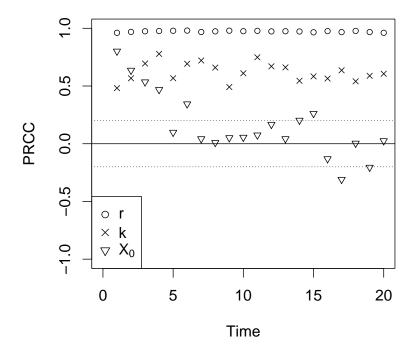


Figure 9: Time dependency of the PRCC values from the model. Values between the dashed lines are not significant.

#### 4.9 Averaging stochastic model runs

Here, we must discuss the averaging of model runs in Segovia04

## 5 Use of Latin Hypercube in ecological studies

Here we present some relevant papers in the ecological literature that made use of LH sampling or similar parameter space exploration techniques. We also try to summarize what are the prerequisites that a model must fulfill in order to use it, what are the cautions that must be taken in running the sampling, what are the potential pitfalls interpreting the results.

Discutir Fisher10, e Thebault10, Johnson12.
Fazer uma sistematica? revisao da literatura
efeito fundador
trabalhos que usaram lhs pra resvoler A, B ou C (din pop? sad? etc)
alguma medida de sucesso de uso?
% dos artigos publicados em Amer Nat, Ecolog, J Ecol, Oikos e Oecol
deiferentes tecnicas de analise, mplementacoes??
selecionar as revistas de (engenharia vs. eco vs. biogeral)

# 6 Appendix: An R implementation of the sampling and analysis methods

In this section, we perform a code analysis of some possible implementations for the sampling and analysis methods described in the R language. These implementations are not necessarily the most efficient, but are designed to be clearly understandable and to illustrate the points made in this work.

Usar Sweave para inserir os exemplos de codigo aqui

## 7 Appendix: Proof of Theorem 1

TODO

## Acknowledgements

We would like to thank Camila Castanho (IB/USP) for the several insightful comments. This work was supported by a CAPES scholarship.

## References

- [1] Florian A. An efficient sampling scheme: Updated latin hypercube sampling. *Probabilistic Engineering Mechanics*, 7:123–130, 1992.
- [2] Huntington D.E. & Lyrintzis C.S. Improvements to and limitations of latin hypercube sampling. *Prob. Engng. Mech.*, 13:245–253, 1998.

- [3] Marino S.; Hogue I.B.; Ray C.J. & Kirschner D.E. A methodology for performing global uncertainty and sensivity analysis in systems biology. *Journal of Theoretical Biology*, 254:178–196, 2008.
- [4] Steinberg D.M. & Lin D.K. A construction method for orthogonal latin hypercube designs. *Biometrika*, 93:279–288, 2006.
- [5] Turchin P. & Hanski I. An empirically based model for latitudinal gradient in vole population dynamics. *The American Naturalist*, 149:842–874, 1997.
- [6] Kleijnen J.P.C. & Helton J.C. Statistical analyses of scatterplots to identify important factors i large-scale simulations, 1: Review and comparison of techniques. *Reliability Engineering and System Safety*, 65:147–185, 1999.
- [7] Helton J.C. & Davis J.D. Latin hypercube sampling and the propagation of uncertainty in analyses of complex systems. *Reliability Engineering and System Safety*, 81:23–69, 2003.
- [8] Helton J.C.; Davis F.J. & Johnson J.D. A comparison of uncertainty and sensivity analysis results obtained with random and latin hypercube sampling. *Reliability Engineering and System Safety*, 89:304–330, 2005.
- [9] Letcher B.H.; Rice J.A.; Crowder L.B. & Rose K.A. Variability in survival of larval fish: disentangling components with a generalized individual-based model. *Can. J. Fish. Aquat. Sci.*, 53:787–801, 1996.
- [10] Ye K.Q. Orthogonal column latin hypercubes and their application in computer experiments. *Journal of the American Statistical Association*, 93:1430–1439, 1998.
- [11] Yang Y. & Atkinson P.M. Parameter exploration of the raster space activity bundle simulation. *J. Geograph. Syst.*, 10:263–289, 2008.
- [12] McKay M.D. & Beckman R.J. A comparison of three methods for selecting values of input variables in the analysis of output from a computer code. *Technometrics*, 21:239–244, 1979.