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Mechanical model comparison using Sobol' indices

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Abstract. Models are mathematical representations capable of describing phenomena in different scenarios. Usually, two or more models are available for the same phenomenon, which leaves the choice of the most suitable model to the user. In practice, simplified models can be as precise as more refined ones and, simultaneously, less demanding in terms of computational power. In this work, we present a novel approach for measuring the discrepancy between models when considering the randomness of the variables. We first define a uniformly distributed random variable that chooses which model is employed to evaluate the response. A global sensitivity analysis (GSA) is then performed by determining Sobol' total index of the response with respect to this variable. The result reveals the importance of choosing between one model or another and indicates the level of discrepancy between them in the stochastic context. Two numerical examples are presented, indicating the kind of insight the proposed approach produces.

Keywords: Model comparison, Mechanical models, Global sensitivity analysis, Sobol' indices

1 Introduction

Two or more models are usually available to represent a particular phenomenon, which leaves analysts with the question of which model to choose to achieve efficient and precise analysis. Hence, the model choice is an important question when dealing with the mathematical representation of phenomena. Establishing comparison approaches that measure how discrepant two or more models are is essential. In this work, we address the problem of model comparison considering variables' uncertainty to support decision making, i.e. we aim to determine if the discrepancy between models is significant concerning input randomness.

Although employing different approaches, mathematical model comparison has been the subject of study in almost every field of science, as seen in Bauer and Tyacke [1], Heywood and Cheng [2], Vorel et al. [3] and Allen et al. [4]. Comparison of regression models to empirical data and stochastic model comparison are often contexts to which the term "model comparison" refers.

Here, the proposed approach is cast in the global sensitivity analysis (GSA) framework [5] by defining a random variable that chooses which mathematical model is employed to evaluate the response. Sobol' total index [6] is then determined, which indicates the importance of model choice to the response obtained and the level of discrepancy between the models.

The rest of this paper is organized as follows. The next section briefly presents a review of GSA and Sobol' indices concepts. The proposed approach for models comparison is then presented in section 3, while section 4 demonstrates two numerical examples of model comparison. Finally, conclusions are discussed in the last section.

2 Variance-based global sensitivity analysis

Sensitivity analysis (SA) refers to quantifying the importance of each input parameter to the output of a model. It allows to determine how uncertainty in the output can be attributed to different sources of uncertainty in the model input [7]. See Borgonovo and Plischke [8], Iooss and Lemaître [9] and Silva and Ghisi [10] for a comprehensive review of SA methods and their capabilities.

Here we employ variance-based GSA, which measures the importance of an input variable according to the expected reduction of the output variance by fixing this variable. Consider the response $Y = f(\mathbf{X})$, where $f : \mathbb{R}^m \to \mathbb{R}$ is the mathematical model and $\mathbf{X} \in \mathbb{R}^m$ is the vector of input variables. Sobol' first order sensitivity index (S_i) concerning random variable X_i is defined as [6]

$$S_i = \frac{\mathbb{V}_i(Y)}{\mathbb{V}(Y)} = \frac{\mathbb{V}\left[\mathbb{E}\left[Y|X_i\right]\right]}{\mathbb{V}(Y)} \tag{1}$$

where $\mathbb{E}\,[.]$ and $\mathbb{V}\,[.]$ represent the expected value and variance, respectively, while $\mathbb{E}\left[Y|X_i\right]$ is the expected value of Y conditioned to X_i.

Sobol' first order indices do not measure the effect of interaction between variables, which may be significant depending on the model and the analysis context. Saltelli et al. [5] mention the factor fixing context, in which one employs GSA to determine whether an input variable is unimportant. In these cases, Sobol' total index (S_{T_i}) is preferred since it includes interaction effects between variables. Sobol' total index is given by [5]

$$S_{T_i} = 1 - \frac{\mathbb{V}\left[\mathbb{E}\left[Y|\mathbf{X}_{\sim i}\right]\right]}{\mathbb{V}\left[Y\right]} \tag{2}$$

where $\mathbb{V}\left[\mathbb{E}\left[Y|\mathbf{X}_{\sim i}\right]\right]$ is the expected value Y conditioned to all variables but X_i.

3 Approach for model comparison

The following strategy is employed to compare the mathematical models $f_1, f_2, ..., f_m$ using GSA framework presented previously [11]. Consider the random variable W with discrete uniform distribution and mass function

$$p(w) = \begin{cases} 1/m, & \text{if } \; w = 1 \\ 1/m, & \text{if } \; w = 2 \\ \vdots & \\ 1/m, & \text{if } \; w = m \end{cases} \tag{3}$$

The response Y is defined as

$$Y = f(\mathbf{X}, W) = \begin{cases} f_1(\mathbf{X}), & \text{if } \; w = 1 \\ f_2(\mathbf{X}), & \text{if } \; w = 2 \\ \vdots & \\ f_m(\mathbf{X}), & \text{if } \; w = m \end{cases} \tag{4}$$

Therefore, the response Y equals the model $f_i(\mathbf{X})$ according to the realized value of W, which is determined randomly with a probability of $1/m$. Thus, the variable W is employed to select one of the m models to evaluate the response.

We can apply the global sensitivity analysis from this definition to determine how significant the model choice is to the response obtained. The Sobol' total sensitivity index of Y with respect to W is given by

$$S_{T_W} = 1 - \frac{\mathbb{V}\left[\mathbb{E}\left[Y|\mathbf{X}_{\sim W}\right]\right]}{\mathbb{V}\left[Y\right]} \tag{5}$$

The index S_{T_W} represents how much reduction of $\mathbb{V}\left[Y\right]$ would be achieved, on average, by fixing W. A small S_{T_W} means that W has little impact on $\mathbb{V}\left[Y\right]$, and thus $f_1, f_2, ..., f_m$ can be considered similar. On the other hand, if S_{T_W} is high, W is responsible for a relevant part of the variance of the response, and the choice between $f_1, f_2, ..., f_m$ becomes significant.

In this way, S_{T_W} can be viewed as a measure of discrepancy between models in the stochastic context. It means that the comparison depends on the degree of randomness of the variables and their influence on the response. Consequently, discrepant models in the deterministic context may end up being similar in the stochastic context if individual variables account for most part of $\mathbb{V}[Y]$.

Note that, as described, the proposed approach for model comparison is cast in the context of variance-based GSA, which provides the method with the sound mathematical basis of Sobol' indices [6] and the efficient computational techniques available [12].

4 Numerical examples

Two examples are presented in this section to illustrate the applicability of the proposed approach. The first example compares a quadratic function and its first order Taylor expansion. In the second example, we compare two models employed to determine the ultimate bending moment of reinforced concrete beams. Sobol' indices presented here have been evaluated through the MATLAB toolbox GSAT developed by Cannavó [13].

4.1 Mathematical models

Two mathematical models are described in eq. (6) and eq. (7). As illustrated in Fig. 1, the model f_2 is the first order Taylor expansion of f_1 at $(x_1, x_2) = (6, 6)$. Variables are taken as independent and normally distributed, and indices were determined with a sample size equal to 10^5.

$$f_1(X_1, X_2) = X_1^2 + X_2^2 + X_1X_2 \tag{6}$$

$$f_2(X_1, X_2) = 108 + 18(X_1 - 6) + 18(X_2 - 6) \tag{7}$$

Three comparison cases are considered according to the statistical parameters shown in Table 1. At first we take expected values $\mathbb{E}[X_1] = \mathbb{E}[X_2] = 6$ and standard deviations $\sqrt{\mathbb{V}[X_1]} = \sqrt{\mathbb{V}[X_2]} = 1$, i.e. random variables are centered at the point at which both models are equivalent. The Sobol' total indices obtained in this case are presented in the second line of Table 1. The index S_{T_W} resulted in close to 0.3%, which indicates that both models are very similar when randomness is taken into account.

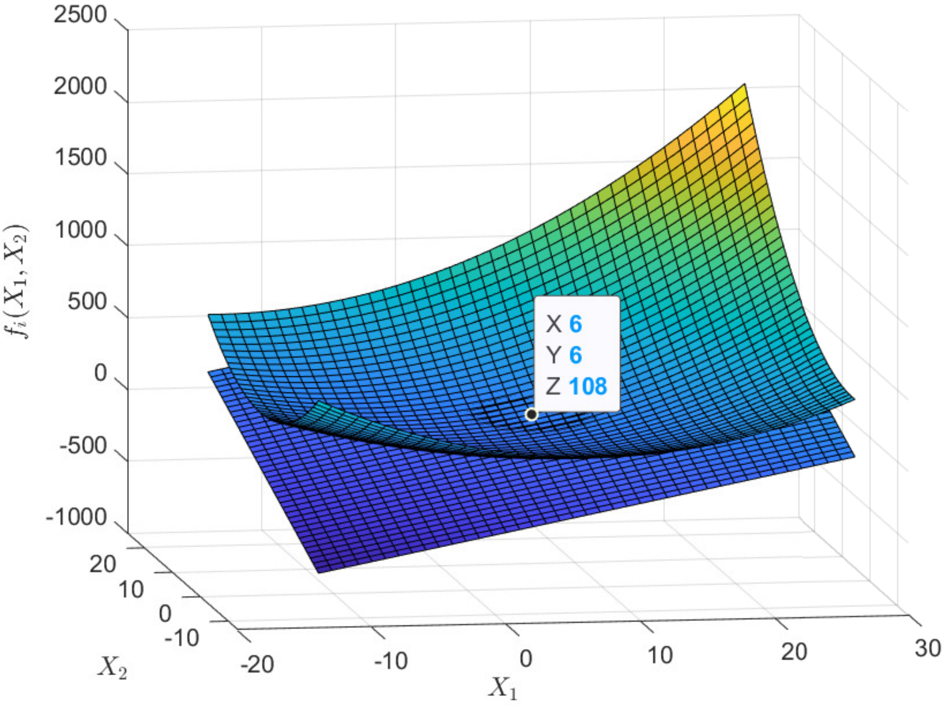
Table 1. Total sensitivity indices in each case.

Statistical parameters	S_{T_W}	S_{T_1}	S_{T_2}
$X_1 \sim \mathcal{N}(6, 1)$, $X_2 \sim \mathcal{N}(6, 1)$	**0,0027**	0,4976	0,5032
$X_1 \sim \mathcal{N}(9, 1)$, $X_2 \sim \mathcal{N}(10, 1)$	**0,2854**	0,3653	0,3872
$X_1 \sim \mathcal{N}(9, 2^2)$, $X_2 \sim \mathcal{N}(10, 3^2)$	**0,1311**	0,2729	0,6477

In the second case, we take $\mathbb{E}[X_1] = 9$, $\mathbb{E}[X_2] = 10$ and keep the standard deviations unchanged. Here the index S_{T_W} resulted close to 29%, meaning that now f_1 and f_2 are considerably discrepant, and model choice is relevant to the response. It happens because now the expected values are different from $(x_1, x_2) = (6, 6)$, the point at which f_2 approximates f_1.

Finally, in the third case, expected values are kept unchanged from the second case, but standard deviations are higher ($\sqrt{\mathbb{V}[X_1]} = 2$ and $\sqrt{\mathbb{V}[X_2]} = 3$). The sensitivity index with respect to W resulted in lower than previously ($S_{T_W} \approx 13\%$), which suggests that the discrepancy between f_1 and f_2 is lower (i.e. the models are more similar). This is explained because X_1 and X_2 have higher variability and thus are responsible for a more considerable portion of $\mathbb{V}[Y]$. Note, too, that differently from the previous cases in which X_1 and X_2 had similar or slight different indices, here $S_{T_1} \approx 27\%$ and $S_{T_2} \approx 65\%$, indicating that X_2 has a much higher impact than X_1.

Figure 1. Models f_1 and f_2.



4.2 Ultimate bending moment

The ultimate bending moment (M_u) is an important question in the structural design of reinforced concrete beams. It tells us the maximum bending moment a beam can resist before failure and depends on parameters such as the geometry of the beam, resistance of materials and stress distribution.

One simple model to determine the ultimate bending moment for a given reinforced concrete cross section under flexure is given by

$$M_u = zA_s f_y \tag{8}$$

where z is the lever arm between compression and tension forces, A_s is the steel area, and f_y is the steel yielding stress. For preliminary estimation purposes, M_u can be approximated by taking $z = 0.9d$, where d is the cross section's effective depth.

In the second model, we determine the moment-curvature relation and maximum bending moment through the integration of the stress field over the cross section. Although more computationally demanding, this method can handle any cross section shape and constitute law of materials. MATLAB routines proposed by Melo et al. [14] have been employed to generate moment-curvature relations. Bilinear constitutive law is considered for steel, with tensile stress given by

$$\sigma_s = \begin{cases} \varepsilon_s E_s, & 0 \leq |\varepsilon_s| \leq \varepsilon_{sy} \\ f_y \varepsilon_s / |\varepsilon_s|, & \varepsilon_{sy} \leq |\varepsilon_s| \leq \varepsilon_{su} \\ 0, & |\varepsilon_s| > \varepsilon_{su} \end{cases} \tag{9}$$

where ε_s is the strain in the steel, f_y is the yielding stress, $E_s = 210GPa$ is the modulus of elasticity of the steel, $\varepsilon_{sy} = f_y/E_s$ and $\varepsilon_{su} = 10‰$

In the case of concrete, Hognestad constitutive law [15] has been employed. No tension resistance has been considered. Compressive stress is given by

$$\sigma_c = \begin{cases} 0.9 f_c \left[\frac{2\varepsilon_c}{\varepsilon_0} - \left(\frac{\varepsilon_c}{\varepsilon_0} \right)^2 \right], & \varepsilon_c \leq \varepsilon_0 \\ 0.9 f_c - 0.135 f_c \frac{\varepsilon_c - \varepsilon_0}{\varepsilon_{cu} - \varepsilon_0}, & \varepsilon_0 < \varepsilon_c \leq \varepsilon_{cu} \end{cases} \tag{10}$$

where ε_c is the strain in the concrete, f_c is the compressive strength, $\varepsilon_0 = 1.62 f_c / E_c$ and $\varepsilon_{cu} = 3.8‰$. The modulus of elasticity is taken as $E_c = 4700\sqrt{f_c}$ for normal weight concrete [16].

Here we take a rectangular reinforced concrete cross section with width b, effective depth d and steel area A_s. Mean (μ) and coefficient of variation (COV) values according to Nowak et al. [17] are presented in Table 2 for basic random variables. Beam height (h) is taken as $d/0.9$ and steel area is equivalent to 0.15%, 0.5%, 1%, 1.5% and 2% reinforcement ratio (ρ). Steel nominal yield strength equals 500MPa, and concrete nominal compressive strength varies from 20MPa to 50MPa.

Table 2. Statistical parameters for variables.

Category	Variable	Unit	Distribution	Nominal	μ	COV
Geometry	Width b	mm	Normal	200	202	0.04
	Effective depth d	mm	Normal	400	396	0.04
Steel	Area A_s	mm^2	Normal	ρbh	ρbh	0.015
	Yield strength f_y	MPa	Normal	500	565	0.03
Concrete	Compressive strength f_c	MPa	Normal	20	26.40	0.17
			Normal	25	31.75	0.16
			Normal	30	36.60	0.14
			Normal	35	41.30	0.13
			Normal	40	46.40	0.12
			Normal	45	51.30	0.12
			Normal	50	56.00	0.12

Total sensitivity indices were evaluated with a sample size $N = 2000$. Table 3 presents the results using concrete nominal strengths and reinforcement ratios tested. The results show that, in general, the models tend to agree more (i.e. sensitivity indices are lower) for lower reinforcement ratios combined with lower concrete strengths and higher reinforcement ratios combined with higher concrete strengths.

The dark blue region in Fig. 2 reveals f_c and ρ values for which models present high similarity. Note that standard deviations for concrete strength are higher for higher values of f_c (although COV values are lower), which is partly responsible for the lower sensitivity indices observed at the top of Fig. 2.

Models are significantly discrepant when extreme reinforcement ratios (0.15% and 2.0%) are considered, independent of f_c. In these cases, lever arm $z = 0.9d$ does not provide a good approximation for the ultimate bending moment. Using the same approach, we can adjust the coefficient to obtain a better fit, which can be further investigated in future works.

5 Conclusions

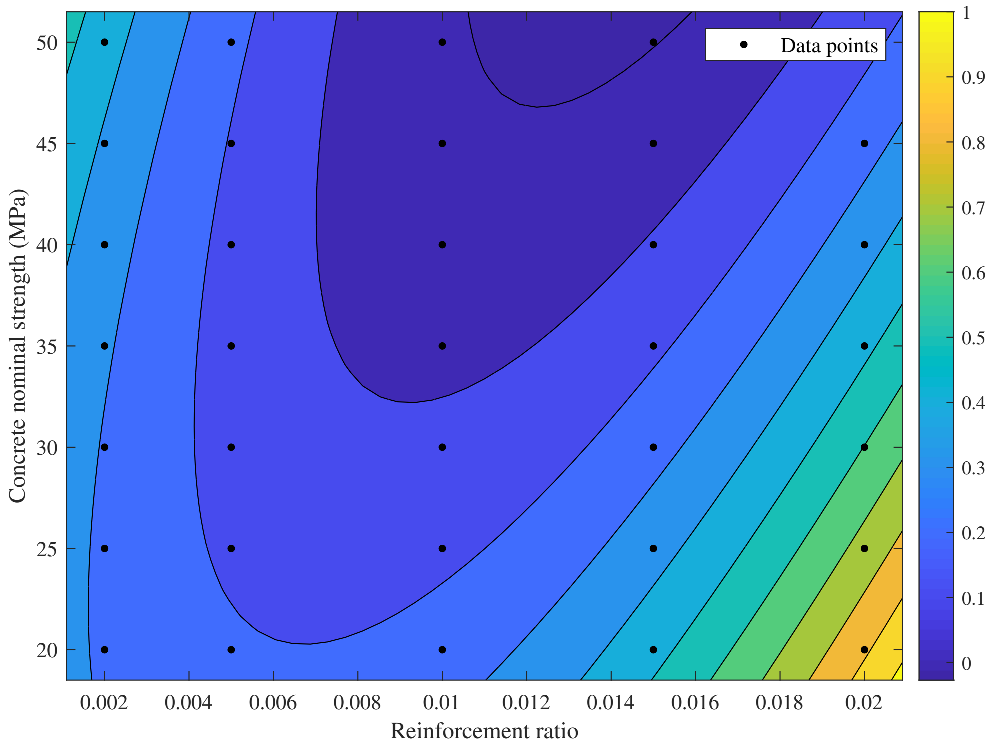
This work presented an approach to comparing mathematical models in the stochastic context. The method allows to measure the discrepancy between models considering the uncertainty in the input. Consequently, variables' randomness affects directly how discrepant two or more models are, which does not happen in a deterministic analysis. Besides, variance-based GSA provides the approach with a solid theoretical basis and efficient computational techniques.

The numerical examples presented practical applications by measuring the discrepancy between the models described. The second example demonstrated the cases in which a simple model is similar to a more complex one and thus can be adopted without loss of precision.

Table 3. Total sensitivity indices according to reinforcement ratio and concrete strength

Concrete nominal strength (MPa)	Reinforcement ratio 0.15%	0.5%	1.0%	1.5%	2.0%
20	0.3253	0.0855	0.2441	0.6185	0.8241
25	0.3433	0.1232	0.0955	0.4700	0.7093
30	0.3601	0.1618	0.0384	0.3062	0.6056
35	0.3549	0.1809	0.0228	0.1883	0.4805
40	0.3610	0.2015	0.0255	0.0889	0.3419
45	0.3657	0.2142	0.0552	0.0404	0.2488
50	0.3693	0.2236	0.0621	0.0269	0.1709

Figure 2. Total sensitivity index isolines representing the fitted surface with $R^2 = 0.928$.



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References

[1] J. Bauer and J. Tyacke. Comparison of low reynolds number turbulence and conjugate heat transfer modelling for pin-fin roughness elements. *Applied Mathematical Modelling*, vol. 103, pp. 696–713, 2022.

[2] N. Heywood and D.-H. Cheng. Comparison of methods for predicting head loss in turbulent pipe flow of non-newtonian fluids. *Transactions of the Institute of Measurement and Control*, vol. 6, n. 1, pp. 33–45, 1984.

[3] J. Vorel, M. Marcon, G. Cusatis, F. Caner, G. Di Luzio, and R. Wan-Wendner. A comparison of the state of the art models for constitutive modelling of concrete. *Computers Structures*, vol. 244, pp. 106426, 2021.

[4] C. B. Allen, N. V. Taylor, C. L. Fenwick, A. L. Gaitonde, and D. P. Jones. A comparison of full non-linear and reduced order aerodynamic models in control law design using a two-dimensional aerofoil model. *International Journal for Numerical Methods in Engineering*, vol. 64, n. 12, pp. 1628–1648, 2005.

[5] A. Saltelli, M. Ratto, T. Andres, F. Campolongo, J. Cariboni, D. Gatelli, M. Saisana, and S. Tarantola. *Global sensitivity analysis: the primer*. John Wiley & Sons, 2008.

[6] I. M. Sobol. Global sensitivity indices for nonlinear mathematical models and their monte carlo estimates. *Mathematics and computers in simulation*, vol. 55, n. 1-3, pp. 271–280, 2001.

[7] A. Saltelli, S. Tarantola, F. Campolongo, and M. Ratto. *Sensitivity analysis in practice - A guide to assessing scientific models*. John Wiley & Sons, 2004.

[8] E. Borgonovo and E. Plischke. Sensitivity analysis: A review of recent advances. *European Journal of Operational Research*, vol. 248, pp. 869–887, 2016.

[9] B. Iooss and P. Lemaître. A review on global sensitivity analysis methods. *Uncertainty management in simulation-optimization of complex systems*, pp. 101–122, 2015.

[10] A. S. Silva and E. Ghisi. Evaluation of capabilities of different global sensitivity analysis techniques for building energy simulation: experiment on design variables. *Ambiente Construído*, vol. 21, pp. 89–111, 2021.

[11] A. Torii, R. Begnini, O. M. I. Matar, and H. M. Kroetz. Global sensitivity analysis for mathematical models comparison. *Submitted for publication*, 2022.

[12] A. Saltelli. Making best use of model evaluations to compute sensitivity indices. *Computer Physics Communications*, vol. 145, n. 2, pp. 280–297, 2002.

[13] F. Cannavó. Sensitivity analysis for volcanic source modeling quality assessment and model selection. *Computers & Geosciences*, vol. 44, pp. 52–59, 2012.

[14] G. F. d. Melo, A. J. Torii, E. M. d. Medeiros, and A. K. L. Kzam. Matlab computational routines for moment-curvature relation of reinforced concrete cross sections. *Revista IBRACON de Estruturas e Materiais*, vol. 14, 2021.

[15] E. Hognestad, N. W. Hanson, and D. McHenry. Concrete stress distribution in ultimate strength design. In *Journal Proceedings*, volume 52, pp. 455–480, 1955.

[16] A. Pauw. *Static modulus of elasticity of concrete as affected by density*. University of Missouri, 1960.

[17] A. Nowak, A. Rakoczy, and E. K. Szeliga. Revised statistical resistance models for r/c structural components. *American Concrete Institute, ACI Special Publication*, vol. 284, pp. 61–76, 2011.