Sensitivity Analysis with DiffEqSensitivity.jl

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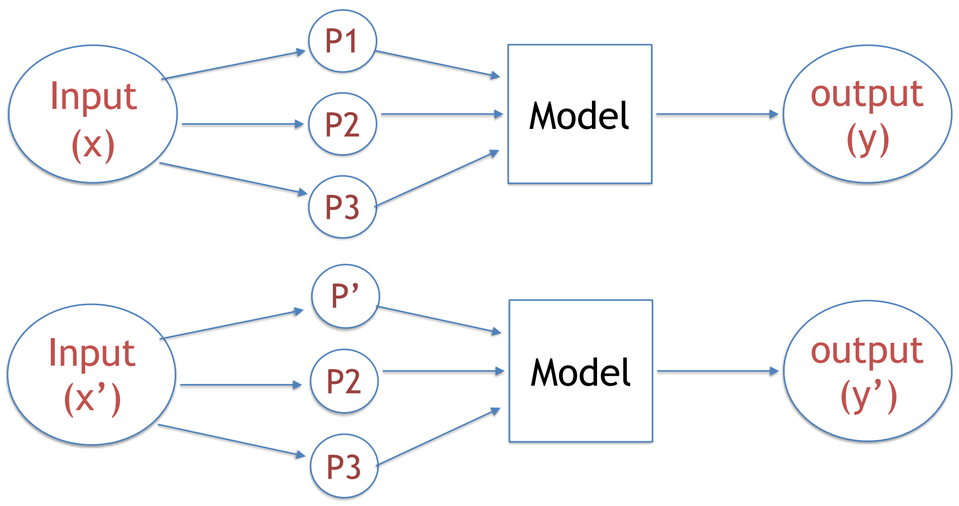
Abstract

Sensitivity analysis is the study of how the uncertainty in the output of a mathematical model or system (numerical or otherwise) can be apportioned to different sources of uncertainty in its inputs.

DiffEqSensitivity.jl aims to expand the JuliaDiffEq suite's Sensitivity Analysis tools by providing various methods of Global Sensitivity Analysis and also Local Sensitivity Analysis

For an ODE $\dot{\mathbf{x}}(\mathrm{t}) = f(\mathrm{x}(\mathrm{t}), \mathrm{u}, \mathrm{t} \mid \theta)$
the sensitivity problem is the variation in x(t), the solution of the ODE w.r.t. variation in θ, the parameters of the ODE.

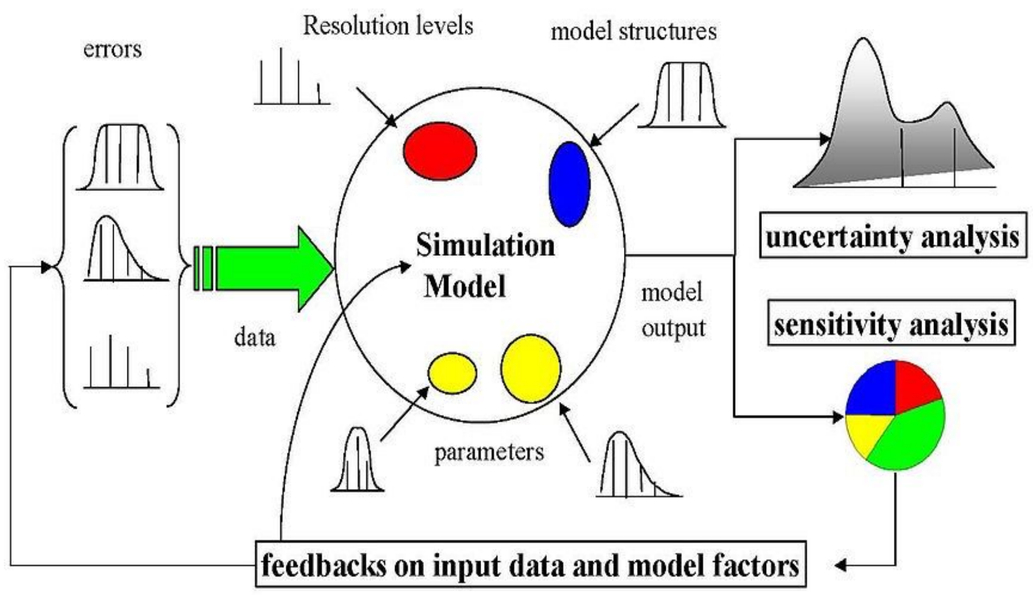
Motivation



One at a time type (OAT) methods

Dynamical systems modelled by differential equations contain parameters whose values are not precisely known. Uncertainty in those parameter values produces uncertainty in the output of the model. Understanding and quantifying this uncertainty using sensitivity analysis is an important part of the development and use of models

Sensitivity analysis methods are applicable to a variety of fields, like systems pharmacology, and because of this wide area of applications, there exists several different broad techniques and specific methods. DiffEqSensitivity.jl is aimed at improving the analysis tooling in the JuliaDiffEq suite.



Uncertainty arising from different sources – errors in the data, parameter estimation procedure, alternative model structures – are propagated through the model for uncertainty analysis and their relative importance is quantified via sensitivity analysis.

Background

Sensitivity analysis methods involve quantification of uncertainty and the relationship between the changes the input parameters and the obtained values.
Sensitivity Analysis methods are divided into

1. One at a time methods
2. Local methods, based on $\frac{\partial Y}{\partial X_i}$
3. Scatter Plots
4. Regression Analysis
5. Variance-based Methods
6. Screening Methods
7. Emulators/ Surrogate models
8. FAST

$$Y = f_0 + \sum_{i=1}^{d} f_i(X_i) + \sum_{i<j}^{d} f_{ij}(X_i, X_j) \ldots + f_{1,2\ldots d}(X_1, X_2, \ldots X_d)$$

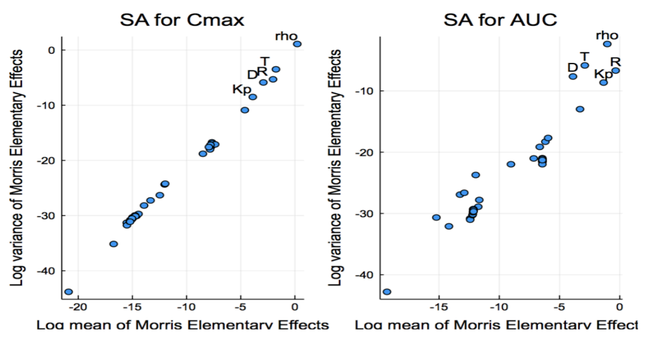
$$Var(Y) = \sum_{i=1}^{d} V_i + \sum_{i<j}^{d} V_{ij} + \ldots + V_{1,2\ldots,d}$$

Variance decomposition used in Sobol Method and other variance-based methods

Results and Discussion

DiffEqSensitivity.jl provides both local and global sensitivity analysis methods. For local sensitivity analysis, **ODELocalSensitivityProblem** type is used and for global methods a uniform interface is provided for the methods implemented, a **DEProblem** is passed with the method specific arguments.

Sensitivity Analysis is a computationally expensive task. The performance of these methods is hindered because of the need for large model number of evaluations.



Morris sensitivity analysis for the ACAT model parameters on Theophylline Cmax (maximum concentration) and AUC (total drug exposure).

Conclusion and Future Work

There are still a lot of methods that need to be implemented and some of the methods require optimisations. Currently the package supports Morris Method, Sobol Method, Regression Analysis, Local and Adjoint sensitivity Analysis. The adjoint sensitivity calculation techniques requires checkpointing and other memory reduction techniques for use on partial differential equation systems.

References/Acknowledgements

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