Applied Numerical Computing for Scientists and Engineers

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This lecture discusses sensitivity analysis tools from Reading Assignment 8.

1. Outline

• Purpose:

Modelers may conduct sensitivity analyses for a number of reasons including the need to determine: (1) which parameters require additional research for strengthening the knowledge base, thereby reducing output uncertainty; (2) which parameters are insignificant and can be eliminated from the final model; (3) which inputs contribute most to output variability; (4) which parameters are most highly correlated with the output; and (5) once the model is in production use, what consequence results from changing a given input parameter. [1]

• Terminology:

- Uncertainty analysis (parameter importance)
- Sensitivity analysis (parameter sensitivity)

• Outline of procedures

Sensitivity analyses are conducted by: (a) defining the model and its independent and dependent variables (b) assigning probability density functions to each input parameter, (c) generating an input matrix through an appropriate random sampling method, calculating an output vector, and (e) assessing the influences and relative importance of each input/output relationship. [1]

• Local sensitivity analysis example

The following is the methods that are used in [2] to quantify the sensitivity of the model output variables C_{AII} relative to changes in the input parameters. First, the local sensitivity is determined by varying one parameter at a time while holding the other parameters fixed. We evaluate the local sensitivity at a single time of 2 h after dosing because that is when most of the experimental data is approaching the peak effects of the dose. The local sensitivity indices are the first-order partial derivatives of the model outputs with respect to the changing model parameter P_k , which can be approximated by a difference equation given small perturbations ΔP_k to the input parameter:

$$\frac{\partial f_i}{\partial P_k} = \lim_{\Delta P_k \to 0} \frac{f_i(P_k + \Delta P_k, P_{n \neq k}) - f_i(P_k, P_{n \neq k})}{\Delta P_k} \tag{1}$$

where $f_i(P)$ is the model prediction of the output variable i at time t=2 h evaluated at parameter set P. We select $\Delta P_k = 0.001 P_k$. Therefore, we decrease each parameter in turn by 0.1% fold from the fitted value obtained by parameter estimation. The local sensitivity is normalized to remove the effects of units:

$$S_{L_{i,k}} = \frac{\partial f_i}{\partial P_k} \frac{P_K}{f_i(P_k, P_{n \neq k})} \tag{2}$$

where $S_{L_{i,k}}$ is the normalized local sensitivity index for the *i*th output variable and the *k*th parameter in parameter set P.

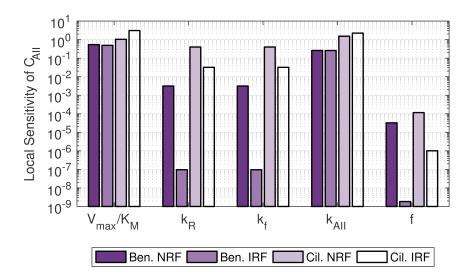


Figure 1: Ang II concentration sensitivity with respect to the model prediction at 2 h after dosing: local sensitivity analysis [2]

• Local sensitivity analysis in-class problem Start from ICPL14starting.m or ICPL14.mlx

For the model

$$f(x,p) = a\exp(bx) + c\exp(dx), \tag{3}$$

where $p = \{a, b, c, d\}$, use local sensitivity analysis to determine how sensitive the model output f(x, p) is to values of p given uniformly distributed values of each parameter in the range of [-10,10] and with the nominal values of 1 for each parameter.

References

- [1] D. M. Hamby. Review of techniques for parameter sensitivity analysis of environmental models. *Environmental Monitoring and Assessment*, 32:135–154, 1994.
- [2] A. N. Ford Versypt, G. K. Harrell, and A. N. McPeak. A pharmacokinetic/pharmacodynamic model of ACE inhibition of the renin-angiotensin system for normal and impaired renal function. *Comput Chem Eng*, 104:311–322, 2017.