

NE 290 C

INTRODUCTION TO SENSITIVITY AND UNCERTAINTY ANALYSIS

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Summer 2002, Schedule: MWF 8:30 – 10:30

SUMMARY: The role of computer-assisted modeling and analysis of physical processes has increased tremendously in the last decade. This increase is driven by (and, in turn, has been driving) increases in computing speed, capacity, and versatility in both hardware and software. Since computers operate on mathematical models of physical reality, the computed results must be compared, whenever possible, to experimental measurements. As is well known, though, computational results seldom agree exactly with actual measurements. The disagreements between measurements and calculations arise because of uncertainties stemming not only from experimental measurements but also from the respective mathematical models and their numerical solutions.

A mathematical model comprises independent variables, dependent variables, and a system of relationships (e.g., equations, look-up tables, etc.) that relate the dependent to the independent variables. Even if a physical process is faithfully modeled mathematically, the numerical methods employed to solve the equations underlying the mathematical model introduce themselves numerical errors. Furthermore, mathematical models also include parameters (such as material properties, constitutive relations) stemming from experiments; as such, their actual values are not known precisely, but may vary within some ranges of uncertainty. The sensitivity/uncertainty analysis of a mathematical model becomes even more complicated if the numerical calculations are affected by chaotic attractors. Nevertheless, the effects of parameter uncertainties and variations on the uncertainty in the calculated result must be assessed. Broadly speaking, these are the tasks of *sensitivity* and *uncertainty analysis*. Once the sensitivities to all parameters are available, they can be used for various purposes, such as for ranking the respective parameters in order of their relative importance to the response, for assessing changes in the response due to parameter variations, for performing uncertainty analysis (using either the Bayesian approach or the response surface approach), or for data adjustment.

The simplest and also the most common procedure for assessing the effects of parameter variations on a model's result is to vary selected input parameters, rerun the code, and record the corresponding changes in the results (i.e., responses) calculated by the code. The model parameters responsible for the largest relative changes in the responses are then classified to be the most important. For complex models, though, the large amount of computing time needed by such recalculations severely restricts the scope of this sensitivity analysis procedure. In practice, this means, in particular, that the modeler can investigate only a few parameters that he judges *a priori* to be important.

Only relatively recently have methods been developed for sensitivity/uncertainty analysis of models that involve a large number of parameters and comparatively few responses. The most efficient method for sensitivity analysis of such large-scale, complex physical models is based on the use of **adjoint operators**.

The course will cover the following topics: 1) conceptual mathematical modelling of physical, engineering, biological, econometric, etc., systems; 2) review of selected concepts underlying the analysis of random processes: probability, measurement errors, uncertainties in experiments; 3) fundamental concepts of perturbation theory; 4) fundamental concepts of system sensitivity and uncertainty analysis: system response sensitivities to parameter perturbations, propagation of parameter uncertainties, system response uncertainties; 5) sensitivity analysis of systems of algebraic equations; 6) sensitivity analysis of ordinary and differential equations; 7) sensitivity analysis of integral and integro-differential equations. For each of the aforementioned mathematical models, the theoretical derivations will be underscored by performing sensitivity analysis of several practical problems, including: a paradigm neutron diffusion equation, Markov chains in system reliability modelling, a radiative-convective model of the atmosphere, transport (random walks in phase-space) processes in system reliability, conservation laws in fluid thermal-hydraulic systems, neutron and radiation transport, and selected numerical methods that are routinely used for solving differential and integral equations. The course will also provide a brief review of selected topics from linear algebra, operators in vector spaces, differential calculus in vector spaces, Gateaux- and Frechet-differentials and derivatives, Hilbert spaces and adjoint operators. In addition to standard homework problem assignments, the participants will also be assigned a Final Project.

Required background: Note that the course will provide a review of the basic mathematical tools needed for sensitivity and uncertainty analysis. These tools are assembled from linear algebra, differential and integral equations, numerical methods, operators in vector spaces, differential calculus in vector spaces, Hilbert spaces and adjoint operators. Therefore, prior knowledge about these mathematical topics would be useful, allowing the participant to concentrate fully on the concepts underlying sensitivity/uncertainty analysis.

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Course Outline

WEEK 1: Conceptual mathematical modelling of physical, engineering, biological, econometric, etc., systems: dependent & independent variables, parameters. Review of selected concepts underlying the analysis of random processes: probability, measurement errors, uncertainties in experiments. Basic concepts of perturbation theory. Basic concepts of system sensitivity and uncertainty analysis: system response sensitivities to parameter perturbations, propagation of parameter uncertainties, system response uncertainties. An introductory paradigm for sensitivity and uncertainty analysis: the second order algebraic equation.

WEEK 2: Mathematical background: selected results from linear algebra, operators in vector spaces, differential calculus in vector spaces, Gateaux- and Frechet-differentials and derivatives, Hilbert spaces and adjoint operators. Sensitivity analysis of systems of algebraic equations. (Homework #1).

WEEK 3: Sensitivity analysis of scalar linear and nonlinear ordinary differential equations. Sensitivity analysis of systems of ordinary differential equations. Practical illustrative examples: sensitivity analysis of a paradigm neutron diffusion equation, sensitivity analysis of Markov chains in system reliability modelling; sensitivity analysis of a radiative-convective model of the atmosphere. (Homework #2).

WEEK 4: Sensitivity analysis of integral equations. Practical illustrative example: transport (random walks in phase-space) processes in system reliability. (Homework #3).

WEEK 5: Sensitivity analysis of systems of partial differential equations. Practical illustrative example: conservation laws in fluid thermal-hydraulic systems. Sensitivity analysis of numerical methods routinely used for solving differential and integral equations. (Final Project)

WEEK 6: Sensitivity analysis of integro-differential equations. Practical illustrative example: neutron and radiation transport.

SELECTED REFERENCES

A. General References on Sensitivity Analysis

1. Frank, P. M., *Introduction to System Sensitivity Theory*, Academic Press, 1978.
2. Cacuci, D. G., Sensitivity Theory for Nonlinear Systems. I. Nonlinear Functional Analysis Approach, *J. Math. Phys.*, 22, 2794; 1981; and :Cacuci, D. G., Sensitivity Theory for Nonlinear Systems. II . Extensions to Additional Classes of Responses, *J. Math. Phys.*, 22, 2803; 1981.

3. Fiacco, A. V., *Introduction to Sensitivity and Stability Analysis in Nonlinear Programming*, Mathematics in science and engineering, volume 165, Academic Press, 1983.
4. Cacuci, D. G., *The Forward and the Adjoint Methods of Sensitivity Analysis*, in *Uncertainty Analysis*, Y. Ronen, Ed., CRC Press, Inc., Boca Raton, Florida, Chap. 3, 1988.
5. Cacuci, D. G., Global Optimization and Sensitivity Analysis, *Nucl. Sci. Eng.*, 104, 78, 1990.
6. Rosenwasser, E., Yusupov, R., *Sensitivity of automatic control systems*, CRC Press, 2000.
7. Eslami, M., *Theory of Sensitivity in Dynamic Systems: An Introduction*, Springer-Verlag, 1994.

B. Illustrative Applications of Perturbation Theory to Sensitivity Analysis of Nuclear Engineering Problems

1. Wigner, E. P., Effects of Small Perturbations on Pile Period, *Chicago Report P-G*, 3048, 1945.
2. Stacey, Jr., W. M., *Variational Methods in Nuclear Reactor Physics*, Academic Press, New York, 1974.
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4. Cacuci, D. G., Weber, C. F., Oblow, E. M., and Marable, J. H., Sensitivity Theory for General Systems of Nonlinear Equations, *Nucl. Sci. Eng.* 75, 88; 1980.
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8. Gandini, A., Generalized Perturbation Theory (GPT) Methods: A Heuristic Approach, *Advances in Nuclear Science and Technology*, Plenum Press, New York, Vol. 19, 1987.

C. Uncertainty Analysis

1. Smith, D. L., *Probability, Statistics, and Data Uncertainties in Nuclear Science and Technology*, American Nuclear Society, 1991.
2. Cowan, G., *Statistical data analysis*, Clarendon Press, 1998.
3. Rabinovich, S. G., *Measurement Errors and Uncertainties: Theory and Practice*, AIP Press, 1995, Second Edition, Springer-Verlag New York, 2000.
4. Myers, R. H., *Response Surface Methodology*, Allyn and Bacon, Boston, 1971.
5. Gandini, A., Uncertainty Analysis and Experimental Data Transposition Methods Based on Perturbation Theory, in *Uncertainty Analysis*, Ronen, Y., Ed., CRC Press, Inc., Boca Raton, Florida, 1988, Chap. 6; see also: Ronen, Y., Uncertainty Analysis Based on Sensitivity Analysis, in *Uncertainty Analysis*, Ronen, Y., Ed., op. cit.