UCODE - Eileen P. Poeter and Mary C. Hill

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a) Introduction:

The computer program UCODE performs inverse modeling, posed as a parameter-estimation problem, using nonlinear regression. Any application model or set of models can be used; the only requirement is that they have numerical (ASCII or text only) input and output files and that the numbers in these files have sufficient significant digits. Application models can include pre-processors and post-processors as well as models related to the processes of interest (physical, chemical, and so on), making UCODE extremely powerful. An estimated parameter can be a quantity that appears in the input files of the application model(s), or that can be used in conjunction with user-defined functions to calculate a quantity that appears in the input files. Observations to be matched in the regression can be any quantity for which a simulated equivalent value can be produced, and simulated equivalent values are calculated using values that appear in the application model output files and a set of additive and multiplicative functions. Prior, or direct, information on estimated parameters also can be included in the regression. The nonlinear regression problem is solved by minimizing a weighted least-squares objective function with respect to the parameter values using a modified Gauss-Newton method. Sensitivities needed for the method are calculated approximately by forward or central differences, and problems and solutions related to this approximation are discussed. Statistics are calculated and printed for use in (1) diagnosing inadequate data and identifying parameters that probably cannot be estimated; (2) evaluating estimated parameter values; (3) evaluating the model representation of the actual processes; and (4) quantifying the likely uncertainty of model simulated values. UCODE is intended for use on any computer operating system: it consists of algorithms programmed in perl, a freeware language designed for text manipulation, and Fortran90, which efficiently performs numerical calculations.

b) Advantages

- The modified Gauss-Newton method is very fast for well-posed problems -- that is, problems for which the observations provide substantial information about the parameters being estimated. It is typically 10 to 100 times faster than global search methods.
- Uncertainty of all defined parameters is propagated to predictions, and any aspect of a system can be defined using parameters, including boundary conditions.
- The defined parameters can include estimated and un-estimated parameters This means that the uncertainty related to undefined parameters can be propagated to measures of prediction uncertainty. For the un-estimated parameters, prior information can be used to represent independent information on the parameter so that the prediction uncertainty is not exaggerated.
- Though based on linear theory, the methods have proven to perform well in many problems with substantial nonlinearity.
- UCODE is freeware and is open source. We invite others to take advantage of any part of the program that appears to be useful to them.

c) Disadvantages

- Can not find global minimum if multiple minima occur.
- The optimization and statistical methods would perform poorly in extremely nonlinear parts of a solution. For example, in biological systems where everything dies if the pH gets to a certain level, it would perform poorly at near that pH value.

d) Assumptions

The model is not too nonlinear with respect to the parameters. In practice, models with significant nonlinearity have been evaluated very effectively with the methods in UCODE.

e) Most appropriate application areas

Models characterized with few estimated parameters relative to the number of observations. Here, observations are related to dependent variables such as simulated concentrations. The meaning of 'relatively few' depends on how much information the observations provide on the parameters. In all cases, the number of observations need to exceed the number of defined parameters. A warning is printed if the number of parameters is more than one-third the number of observations to encourage users to consider this aspect of their problem.

Any type of system can be considered as long as the model input and output can be ASCII of text only.

f) Reading list

Poeter, E.P. and Hill, M.C., 1998, Documentation of UCODE, a computer code for universal inverse modeling: U.S Geological Survey Water-Resources Investigations Report 98-4080, 122p. http://pubs.water.usgs.gov/wri984080/

Hill, M.C., 1998, Methods and guidelines for effective model calibration: U.S Geological Survey Water- Resources Investigations Report 98-4005, 90p. http://pubs.water.usgs.gov/wri984005/

g) Software availability

Open-source freeware

h) Web links or other information

http://water.usgs.gov/software/ucode.html

http://www.mines.edu/igwmc/freeware/ucode/

i) Figures

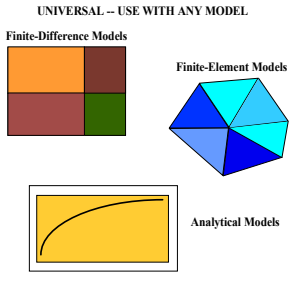

Figure 1: 'Covering Figure' for U-code

j) Delegates Comments (please add !!)