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Weak-formed based objective functions in hydrology. Application to a 1D transport/degradation model

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The process of model calibration consists in bringing the simulated variable as close as possible to the measured one. The intuitive term "as close as possible" can be translated into a mathematical formulation of the error between simulation and observation: the objective function provides a measure of how close to zero the modeling error is.

The most widely used objective function in any scientific application is probably the Root Mean Squared Difference (RMSD), which is the euclidian distance between the observed and simulated variable. In hydrology, the well-known Nash-Sutcliffe efficiency, may also be considered as a measure of the distance between observations and simulation. Using distance-based objective functions, turns the model calibration process in an optimization problem: minimization if a cost function is used or maximization for an efficiency function. A general formulation of a distance-based cost function can be written as:

$$J_p = \alpha \sum_i |F(U_i, \phi) - V_i|^p$$

where α depends on the function definition, $F(U_i, \phi)$ is the model output (for different locations or times), with ϕ the parameter to be calibrated and V_i are the measurements. In case of an efficiency function, the form $1 - J_p$ can be used. In this formulation, the model is considered perfect if $J_p = 0$, i.e. if it reproduces exactly the measurements, but uncertainty on the latter can also be taken into account in the definition of the objective function.
Another category of objective functions is based on a weak formulation of the evaluation problem. This can be for example, the bias-indicator or cumulative error. The weak formulation can be written in the general form:

$$J_p = \alpha \sum_i \left(F(U_i, \phi) - V_i\right) |F(U_i, \phi) - V_i|^{p-1}$$

In contrast with the distance-based formulation, the weak-form based objective functions are monotone (and thus, can be negative). This has several practical consequences. The first one, is that the model calibration process is transformed into a root-finding problem, that can be solved using a simple, efficient gradient-based method (such as Newton's algorithm) rather than generally more complex global optimization algorithms. Moreover, the function monotony implies the unicity of the solution, thus avoiding multiple local optima. A model with N parameters can be calibrated by defining N weak form-based objective functions and finding their intersection in the parameter space. These functions can be defined by using different observation variables (or functions of these variables) or different values of p. Parameter redundancy can be evidenced when no intersection can be found between objective functions defined with the same observe variable but different values of p.

The weak-form based objective function is applied on the multi-criteria calibration of a hydrodynamic transport-degradation model. The parameter with respect to which the model is calibrated, is the degradation coefficient k. However, since it is time dependent, a piecewise linear function is defined with n values of k, leading to a n-criteria calibration. It appeared in this study that the classical distance RMSD failed to converge to a global optimum of the k_n vector. The use of n weak-form based objective functions, defined with n different values of p enables the model calibration with the classical Newton's algorithm.