a more precise characterization of system behavior in heterogeneity.

Structural Parameter Optimization A good general guideline for all modeling is to start simple and add complexity as appropriate. In bgaPEST, this goal is achieved by starting with small values of variogram parameters (slope for the linear, variance for the nugget or exponential) such that the solution will be very smooth. By optimizing for structural parameters, roughness will be introduced by the algorithm until convergence at the optimal level of roughness. At the early, exploratory stages of a project, it might be desirable to set `sig_opt=1` to see what level of fit may be achievable, but the user should be prepared to override this in later stages as allowing too much roughness to be introduced. For the prior distribution variogram parameters, however, optimization should always be employed in keeping with the Empirical Bayes perspective the algorithm was designed with.

## Limitations to Version 1.0

bgaPEST marks the first widely available implementation of BGA for use by practitioners. Limitations, of course, accompany this first implementation. Version 1.0 does not have an explicit parallelization facility. This can be overcome by using external programs for derivatives and calling a parallel Jacobian calculation package such a BeoPEST (Schreüder, 2009) or GENIE (Muffels and others, 2012) whenever a Jacobian matrix is required. The impact of this is on the run times required to obtain a solution.

A practical upper limit on the number of parameters estimated is on the order of 100,000. To estimate a larger number of parameters, machines with a large amount of random access memory (RAM) must be used. At some greater limit, methods such as periodic embedding or other decompositions must be incorporated to mitigate the expense of storing and calculating the prior covariance matrix.

The source code is written in Fortran-90 and should be compilable on any platform with a Fortran compiler. Special care was taken to avoid obscure and nonstandard language features. Nonetheless, it is possible that some platform- or compiler-specific problems may be encountered.

It is possible to use bgaPEST with a small number of parameters, but the assumption from the start is that parameters in at least part of the spatio-temporal domain represent a field of correlated instances (e.g. model nodes, discrete times) that often outnumber the number of data observations. A combination of homogeneous parameters in zones with a refined area of interest that is distributed is a common application and, as implemented through beta associations, this mix of distributed and zoned parameters is supported and encouraged. Typically, sufficient data to support a distributed parameter set is limited to part of a model domain in space or time.

In considering uncertainty, version 1.0 presents posterior covariance values. For some applications, conditional realizations may be desired to capture candidate roughness of solutions within the ensemble distribution of solutions. Details for conditional realizations are provided by Kitanidis (1995).

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