Approaches in Highly Parameterized Inversion–bgaPEST: A Bayesian Geostatistical Approach Implementation with PEST–Documentation and Instructions

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Introduction

Environmental modeling can facilitate informed management of natural resources. In most cases, models represent physical processes such as groundwater flow, contaminant

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transport, surface water flood routing, etc. Simulating the physics and chemistry with governing equations and concepts such as conservation of mass and momentum is only part of the challenge. Once a model adequately represents the processes of the problem, it is still a general tool until estimates of the physical characteristics are tuned to observations from the specific area to be managed.

Input values that control the behavior of a model at a given site are called "parameters" and they represent specific characteristics (for example, hydraulic conductivity, recharge rate, chemical decay rate) of the natural system encountered at a specific area. The values appropriate for parameters in natural systems are often difficult or impossible to measure directly. However, observations of system state (for example, water levels, streamflow magnitudes, chemical concentrations) are often easier to measure and they correspond to output values from the model. The output values corresponding to observation data from the model are dependent on the values of parameters: indeed, if parameter values are changed in a model, the system state also typically changes. "Parameter estimation" and "calibration" are both terms describing the process of incorporating site-specific information into a model as a means to improve its representativeness, thus making it more suitable for use supporting management decisions. In essence, this process uses observation data to infer appropriate values for parameters.

This concept is so important that one may interpret a model as a data-processing tool that tests conceptualizations of a system as much as a simulator of physical processes; the data processing being a pipeline from field observation to model parameters and ultimately to predictions. Put in terms of a Bayesian description, this process is one in which the model is a vehicle for updating soft- or expert-knowledge (*a priori* understanding) of the system to an understanding that is filtered by a measure of the ability to simulate the natural world informed, or updated, by site-specific information (*a posteriori* understanding). In such an approach, the ability to simulate features of the natural world "condition" or narrow the wide range of possible outcomes that result from general soft-knowledge alone. This Bayesian approach is adopted here and will be discussed in more detail. First, however, the concept of conditionality must be emphasized.

Bayes' theorem is at the heart of the techniques in this report:

$$p\left(\mathbf{s}|\mathbf{y}\right) \propto L\left(\mathbf{y}|\mathbf{s}\right) p\left(\mathbf{s}\right) \tag{1}$$

where: $\mathbf{s}$ is a vector of parameter values, $\mathbf{y}$ is a vector of observations, $p(\cdot)$ indicates a probability density function (pdf), $L(\cdot)$ indicates a likelihood function, and $|$ indicates conditionality. In words, Bayes' theorem states that the posterior probability of parameters conditional on the observations $p(\mathbf{s}|\mathbf{y})$, is proportional to the prior probability of the parameters $p(\mathbf{s})$ updated with the likelihood function $L(\mathbf{y}|\mathbf{s})$ that expresses how well $\mathbf{y}$ is estimated using the model and a candidate parameter set $\mathbf{s}$. The pdfs in all cases are assumed to follow Gaussian distributions. This assumption is important and somewhat restrictive, but is made for computational simplicity. Active research is ongoing on alternatives to this approach, but the traditional Gaussian assumption is adopted in this report.

In the Bayesian context, expressing the parameters and the likelihood function as probability distributions formally incorporates an estimate of the uncertainty rather than treating the parameters as perfectly known values. All *a posteriori* (also called posterior) distributions are conditional upon the specific data used in the calibration process. ~~Perhaps less obviously,~~ posterior distributions are also conditional on all other modeling and data assumptions and decisions that go into formulating the problem: which model and what model options are chosen, numerical considerations such as discretization and solver convergence criteria, boundary conditions that may or may not be considered static and known, variance values and weights given to individual observations and parameters, and others. As a result, if any of these underlying assumptions and decisions change, it is expected, in the Bayesian context, that the parameters estimated will also change.

The conditionality includes *all* decisions made in the process of constructing a model and incorporating data, however, not all of this information is explicitly addressed by the modeler. In fact, the only *explicit* conditionality is on the observation data. The information contained in the prior pdf ($p(\mathbf{s})$) in eq. 1 is critical because it represents the state of knowledge about the parameters in the system prior to updating through the calibration process. In this report, assumptions made prior to calibration are intentionally limited and are restricted to the assignment of a mean value (unknown) of each distinct parameter type and region within the model domain (beta association–described below), and a characteristic about continuity or smoothness of the parameter field. The degree to which this continuity characteristic is enforced is dictated by the observations included and the subsequent performance of the model. This construction is similar (and in some cases, mathematically equivalent) to Tikhonov regularization

(*Tikhonov*, 1963a,b; *Aster et al.*, 2005). Sufficient limitation of the information assumed *a priori* is similar to assuming a low or diffuse level of *a priori* soft-knowledge (called an ignorance prior in *Jaynes and Bretthorst* 2003, chapter 12). In this case, the resulting model is driven more by information obtained from site-specific observations than from prior assumptions based on soft-knowledge. A goal of this approach is to limit the subjective information used in favor of an objective and repeatable result based on observation data. Additionally, so-called structural parameters that enforce the characteristic are estimated. As algorithm that encompasses all of these aspects is considered an Empirical Bayes approach.

The concept of a beta association is an important one that is revisited throughout this report. The term "beta" refers to the mathematical symbol used to represent the mean value for a specific parameter type (for example, hydraulic conductivity in a groundwater model) in a specific region of a model. In the methodology described in this report, parameter values are estimated by estimating a mean value (termed β in the mathematics) and fluctuations about that mean. Each parameter, therefore, must be associated with a mean value.

It would be tempting to use another term such as "zone" or "facies" to describe this concept, but the term "beta association" was selected specifically to highlight the flexibility of the concept. The important idea is that the method described in bgaPEST depends on being able to associate each parameter with a mean value. In the case of distributed parameters (for example, hydraulic conductivity or recharge being distributed throughout a region in a model in which each model cell or node is assigned a unique value), the subdivision of the entire model domain into beta associations accounts for hydrogeologic contacts or facies to be delineated. This delineation prevents correlation across these natural divisions. Similarly, parameters of one type are typically not correlated with parameters of a different type. Beta associations allow the inclusion of multiple parameter types and the delineation of important geologic features in distributed parameter sets.

The likelihood function in eq. 1, $L(\mathbf{y}|\mathbf{s})$, expresses the correspondence of model outcomes with field observations collocated in space and time. This correspondence is expressed as the sum of the squared differences between outcomes and observations, weighted by a covariance matrix, which expresses the relative certainty of each observation. This is effectively equivalent to the weighted measurement objective function in PEST (*Doherty*, 2010a). These elements of Bayes' equation form the fundamental

basis for the bgaPEST software described here.

Purpose and Scope

This Report is intended to serve two main purposes. First, a Bayesian approach to parameter estimation–expressed in the context of the Bayesian Geostatistical Approach (BGA)–is introduced to provide an accessible and general tool for moving a model from a general simulator of a physical process to a more optimal tool, tuned to a set of calibration information, which, in turn, can be used for management of a particular site and issue. Second, a computer code–bgaPEST–is introduced and documented in which BGA is deployed using the protocols and input/output concepts developed in the free and open-source PEST suite of software *Doherty* (2010a). The bgaPEST input framework is consistent with the input block and keyword concepts described by the JUPITER project *Banta et al.* (2006). To our knowledge, this marks the first implementation of BGA available for general use.

The input/output concepts in PEST enable the use of PEST with nearly any computer model. The only restriction is that input can be provided to the model using a text (ascii) file and that output can be generated from the model also using a text file. This restriction can be relaxed, provided that a translation utility can be deployed that converts data of another format–for example, binary–to or from ascii, as appropriate. The only kind of model that PEST cannot easily control is one in which any changes to model input or the reading of model output must take place in a graphical user interface. This generality of model compatibility is a powerful capability that bgaPEST is able to take advantage of by virtue of efficient open-source modules that make this external control of a model possible using the same protocols as PEST.

As discussed elsewhere in this report, bgaPEST must control the model for two purposes: to evaluate the likelihood function (assessing the correspondence between model output and collocated observation data, given a candidate set of parameter values) and to calculate the "Jacobian" or "sensitivity" matrix that is required for solving the calibration equations. To enable PEST (and bgaPEST) to write input for a model, template files are created that provide a mapping of named parameters into their proper place in input files for the model. More than one template file can be used corresponding to multiple model input files. To enable reading of output files, instruction files are created

that contain a set of instructions (including locating specific line numbers or searching for specific text) that enable extraction of output values to be compared with observation data. Leveraging the modules that implement the PEST input/output protocols takes advantage of the flexibility and generality of PEST. It also makes it possible to take advantage of some of the utility programs already created to be compatible with the PEST suite of software. Programs created using the JUPITER program employ a very similar set of protocols by virtue of the PEST modules being provided to the JUPITER project. As a result, template and instruction files created to work with a model are largely interchangeable among projects implemented in PEST, bgaPEST, and programs created using JUPITER.

A full description of the format of template and instruction files is not part of the scope of this work: detailed descriptions are provided in the PEST documentation (*Doherty*, 2010a, chapter 3). All options implemented in template and instruction files in PEST are available in bgaPEST.

This initial implementation is written in FORTRAN-90. The calculation of the Jacobian (sensitivity or derivatives) matrix can either be implemented using a script written by the user, or employing a Python script provided with bgaPEST. The Python script depends on several utilities that are standard with PEST and available for download at http://www.pesthomepage.org. The necessary executable files are also provided with bgaPEST. For users on the Windows operating system, installation of Python is optional as the Python codes are compiled into executables using py2exe that can be called by the main program. For users on Macintosh or Linux systems, all the code must be compiled for the native platform and Python should already be installed so the Python scripts may be called directly without need to compile them separately. The use of external derivatives (sensitivity) calculation with PEST and Python will be replaced by integration of a general parallel run management suite (GENIE, Muffels and others, in review) as part of future work. Parallelization is possible using beoPEST (REF), but the entire process, including starting and stopping all parallel computer (slave) programs must be encapsulated in a script that is called by bgaPEST.

An important concept discussed in this report is based on a distributed parameterization scheme that is meant to be flexible in that certain regions of primary interest and with sufficient data in the model (called beta associations) have unique parameter values estimated for each model node or cell. This leads to a large number of parameters which is accompanied by computational challenges. Alleviating these computational

challenges is an active area of ongoing research.

The remainder of this report provides some details on the mathematical theory behind BGA, followed by detailed instructions for using the computer program. Conventions and assumptions for using the program are included in the discussion.

Bayesian Geostatistical Approach Overview

The Bayesian geostatistical approach is described in detail in *Kitanidis and Vomvoris* (1983); *Hoeksema and Kitanidis* (1984); *Kitanidis* (1995); *Nowak and Cirpka* (2004) among others. In this Section, we provide a conceptual overview of the method. A more detailed description, including more mathematical details, is included in Appendix C.

The core of the Bayesian geostatistical inverse method is Bayes' theorem, which states

$$p(\mathbf{s}|\mathbf{y}) \propto L(\mathbf{y}|\mathbf{s})p(\mathbf{s}) \tag{2}$$

where $\mathbf{y}$ are the measured data, $\mathbf{s}$ are the unknown parameters, $p(\mathbf{s}|\mathbf{y})$ is the posterior probability density function (pdf) of $\mathbf{s}$ given $\mathbf{y}$, $L(\mathbf{y}|\mathbf{s})$ is the likelihood function, and $p(\mathbf{s})$ is the prior pdf of $\mathbf{s}$. Details of these pdfs are explained below.

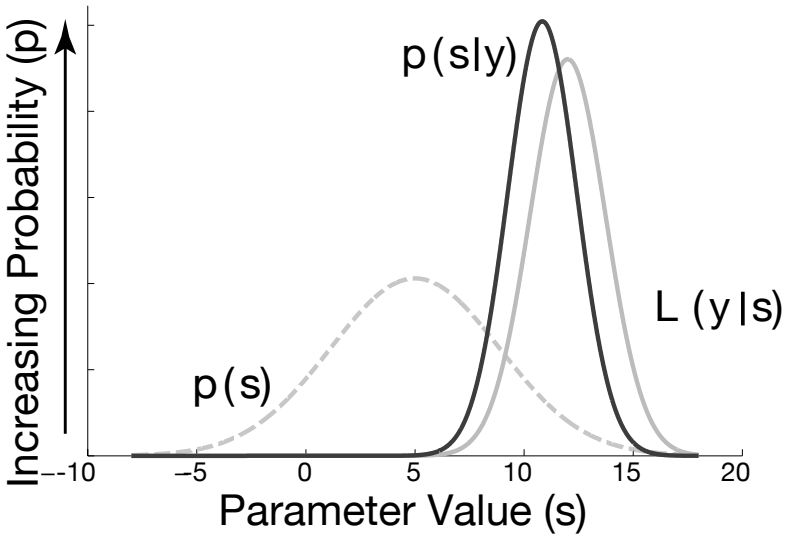


Figure 1: Graphical illustration of Bayes' theorem.

Figure 1 depicts one-dimensional distributions graphically illustrating Equation 2. In

this example, the prior distribution $p(\mathbf{s})$ is diffuse, meaning the variance is relatively high and, correspondingly, commitment to a particular value is low. The likelihood function $L(\mathbf{y}|\mathbf{s})$, on the other hand, has lower variance, suggesting a process that brings a higher level of certainty to the estimation of the parameters ($\mathbf{s}$) than is indicated by the prior distribution only. The resulting posterior distribution $p(\mathbf{s}|\mathbf{y})$ is a convolution of the prior and likelihood functions. The peak is shifted significantly from the prior toward the likelihood and is higher. The posterior distribution also has lower variance than the prior as illustrated by the spread in the figure. Since the likelihood function is more focused (less spread) and higher than the prior, the attributes of the likelihood contribute more to the posterior than the prior does.

In bgaPEST, an empirical Bayes (*Robbins*; *Casella*, 1985) perspective is adopted. Empirical Bayes means that the general characteristics of the prior and (optionally) epistemic covariances introduced above are provided in the model setup, but the values of "structural" parameters that control the structure of the system–the balance between smoothness and misfit–are estimated from the observation data. In other words, the level of roughness in the solution is dictated by the information content of the observation data rather than specified by the user ahead of time.

The prior distribution is the main mechanism by which soft-knowledge about the parameter field is imparted on the parameter estimation process. In the Empirical Bayes perspective, this soft-knowledge is intentionally limited such that significant flexibility is available to the algorithm and a specific practitioner's preconceived notions, which are more subjective, are replaced by the objective power of the site-specific observations. This idea is inspired, also, by the concept of multiple working hypotheses (*Chamberlin*, 1890). Chamberlin warned of scientists falling victim to a "paternalistic affection" for his or her initial explanation of a phenomenon such that they are blind to other explanations that may be more appropriate. This is not to discount the value of soft-knowledge–indeed, the general characteristics imparted through specification of the prior information and the interpretation of the results of using BGA rely deeply on expertise–but it highlights a goal of leaving as much flexibility as possible in the process.

In bgaPEST, then, the practitioner specifies a type of variogram (nugget, linear, or exponential) that is used to control the variability–smoothness or roughness–of parameters within a beta association, but the *degree* to which this characteristic is enforced is determined by restricted maximum likelihood (RML). In RML, the value of structural

parameters that control the variogram behavior is treated as a probability distribution and the most likely values resulting in either the best possible fit (if the epistemic error term is estimated) or a user-specific level of fit (if the epistemic error term is fixed) are estimated. "Fit," in this context, refers to the correspondence between observation data and model outputs collocated in space and time with the measured observations. Fit and epistemic error are discussed in more detail in the next section. A danger, when providing a model with substantial flexibility, is an "overly complex" model that is "overfit" (e.g. *Draper and Smith*, 1966; *Hill*, 2006). To mitigate this issue, the RML approach is consistent with the principle of maximum entropy such that the smoothest solution is chosen, based on the structural parameters estimated from the data. For a discussion of subtle formal differences from minimum relative entropy, see *Rubin* (2003, p. 333-342).

An extension to this approach is the inclusion of information about the prior mean (*Nowak and Cirpka*, 2004). Although the mean is estimated in the solution, a prior value and covariance can be supplied to constrain the estimate. Typically, a relatively high covariance magnitude is used so the constraint on the estimated mean is weak or "diffuse." Thus the prior mean principally serves the role of providing numerical stability rather than compelling the solution to adhere closely to prior values. Similarly, prior information and covariance can be supplied on the structural parameters to constrain the estimated values to more closely follow an initial conception of the parameter field variability.

The forward model is constructed to provide outputs of values collocated in space and time with measured observations. The likelihood function quantifies the difference (misfit) between the model simulated outputs and associated observations. In all modeling, perfect correspondence between forecasts and observations is neither attainable nor desirable. The observations themselves are corrupted by measurement errors and there is usually a lack of perfect correspondence between the exact nature of the measurements and the simulated counterparts. This corruption is due to uncertainty from sources including the paucity of observations, imperfections in the conceptual model, and approximations made to codify the physics of the phenomena into a numerical model framework. All of these sources of uncertainty are described by the overarching term "epistemic uncertainty" (*Rubin*, 2003, p. 4). This epistemic uncertainty characterizes the expected misfit between simulated and observed equivalents , and is expressed through a covariance function. As a result, the likelihood function can be characterized

by a Gaussian distribution with zero mean and covariance defined by the epistemic uncertainty.

With both the prior pdf and likelihood function expressed as Gaussian distributions, the resulting posterior pdf is also Gaussian. The values of the parameters $\mathbf{s}$ that result in the maximum value of the posterior pdf are therefore the most likely solution on a point-by-point basis. The solution as a whole is always a somewhat smoothed version of reality, but the influence of small-scale variability can be approximated through conditional realizations. The balance between the strength of smoothing and the level of fit between simulated and observed equivalents is found through calculation of optimal values for the structural parameters. Optionally, this can include a value to quantify the epistemic uncertainty. The result will favor smoothness, but may achieve a level of fit corresponding to an unrealistically low level of epistemic uncertainty. As a result, it is generally most appropriate to fix the level of epistemic uncertainty but allow the other structural parameters to be estimated.

Structural Parameters

The term "structural parameters" may be unfamiliar to users. Like the more general term "parameters," structural parameters are variable values that are estimated in the bgaPEST algorithm. Unlike general parameters, however, structural parameters do not *directly* control physical aspects of the system in the way that, for example, hydraulic conductivity or stream roughness do in hydrologic models. Instead, structural parameters control the structure of the general parameters. For example, the variogram values (e.g. variance, slope, and correlation length) that control to roughness of distributed parameter fields are structural parameters, as is the value of variance controlling epistemic uncertainty. Because these parameters must be estimated but are not directly connected to the physics of the problem, they are also in other work referred to as "nuisance" parameters or "hyperparameters." We adopt the term "structural" to highlight the fact that the impact these parameters has on the solution is control of the shape or structure of the distributed parameter fields.

Beta Associations

In an idealized problem, a single covariance model (for example, a single variogram) is flexible enough to encompass the entire variability of the hydraulic parameters. However, in many hydrogeologic applications, lithologic contacts and unconformities can

create discontinuities in parameter values that a single covariance model cannot characterize. Partitioning the field based on either the data (e. g. *Fienen et al.*, 2004) or through interrogation of preliminary solutions (e. g. *Fienen et al.*, 2008) can greatly improve the parameter estimation results. This partitioning is implemented by imposing discontinuities in the stochastic field that censor correlation among all cells that do not occur in the same partition. In this context, "stochastic" refers to the entity being partitioned (namely the correlation structure of the parameter field) but we emphasize here that the locations of the imposed discontinuities are themselves considered deterministic and certain. This concept of partitioning is consistent with zonal boundaries in models made up of homogeneous zones but allows more flexibility by allowing properties within the zone to vary. Furthermore, multiple types of parameters (for example, in a flow and transport model, hydraulic conductivity and porosity) are commonly estimated. While at the physical level, these parameters may be related, they must correspond to different mean values, so similar censoring of correlation among different types of parameters is also necessary in most applications through partitioning.

For hydrogeologic applications, the term "facies association," from the facies architecture field, is a good description for these partitions (*Fienen et al.*, 2009). The term "facies association" typically refers to descriptive properties of a subset of a medium in the field or at least for a specific project. "Architectural elements" is used in the broader case where the characteristics are more formally defined, (see *Collinson* (1969); *Walker* (1984, 1992); *Swift et al.* (2003)). It would be appropriate to use the less restrictive and less transferable term "facies association" in hydrogeologic applications because when we subdivide the correlation structure of the medium, we often base the stochastic discontinuities (bounding surfaces, or contacts) on perceived hydraulic properties. These properties will often coincide with differences in age, provenance, or depositional environment, but such coincidence is not required for or by their use. In all cases, partitioning into facies associations are most effective when based on readily observable hydrologic or lithologic attributes.

For bgaPEST to be a more general tool (not limited to hydrogeologic modeling), we have broadened this concept by adopting the term "beta association." As shown in Equation 8, the Greek letter β stands for the mean of a region of distributed parameters. Beta associations can, therefore, delineate regions of a distributed parameter field that have similar statistical properties and correspond to the same mean value. However, importantly, beta associations can also refer to completely different parameter types

(for example, hydraulic conductivity and recharge).

To clarify our terminology in this work, partitions delineated by stochastic discontinuity within a distributed parameter field are referred to as "beta associations," whereas zones of piecewise continuity are referred to as "homogeneous zones." The beta associations delineate sub-regions of the model domain that share correlation characteristics and are uncorrelated from neighboring beta associations; they are usually delineated by features that are easily identified in measured data or geologic conceptualizations of a given site area. In beta associations, variability of parameter values within each cell is allowed and constrained by the *a priori* covariance structure, whereas in homogeneous zones, a single parameter value represents the property for the entire zone. Beta associations also delineate regions in the model (whether defined by one or more parameter values) that correspond to different mean values (β).

Beta Associations and Zones: ***Why aren't "beta associations" just called "zones"?*** Beta associations are a term specific to bgaPEST. As discussed in the main text, this term evolved from the term "facies association," which describes partitioning of parameter fields based on hydrogeologic characteristics. This term was used in place of "zones" because of a long history of zones referring to regions of piecewise constant homogeneity (one parameter value applied to every node within a region). Beta associations are *not* homogeneous, so a distinct term was sought that describes the characteristic of regions partitioned due to their characteristics and how these characteristics correlation to regions around them. To generalize beyond hydrogeologic applications, and to account for the fact the distinct parameter types require distinct partitions, "beta associations" was the term chosen. Each of these parameter partitions has a distinct mean value (β) to be estimated within the region, so the partitioning of the problem results in different β values; because the parameter type and/or region must be associated with a mean value (β), we use the term "beta associations."

Running bgaPEST

The bgaPEST program uses a single input control file, template and instruction files to control the underlying model, and generates several output files. These files are discussed in the context of progression of the bgaPEST program in the remainder of this section. Figure 2 shows the general progression of a bgaPEST parameter estimation run. The entire process is controlled by variables in the input `.bgp` file discussed below.

To obtain an optimal solution to the parameter estimation problem, it is necessary to perform multiple iterations. An iteration is defined as a single run of the entire estimation process with a particular set of values. Multiple iterations are required due to the nonlinearity of the problem and due to the necessity of estimating structural parameters separately from model parameters. Appendix C provides more detail about the methodology used to obtain a solution for a set of optimal parameters and structural parameters in bgaPEST.

Outer iterations (also called bga iterations) are wrapped around the traditional parameter estimation process with values of the structural parameters held constant. Inner parameter estimation iterations are performed to account for the (restricted maximum likelihood) estimation of structural parameters. If structural parameters are not chosen to be estimated, then a single outer iteration is performed using the initial values of structural parameters and inner iterations are performed until convergence or until the number of iterations reaches `it_max_phi`. If a linesearch is requested, this is performed within the inner iterations. If structural parameter optimization is requested, it is performed after convergence or maximum inner iterations are reached. Then, restricted maximum likelihood is performed to estimate a new set of structural parameters. The interdependence between structural parameters and model parameters requires reiteration of the inner iterations and structural parameter estimation until both have converged or the maximum number of outer iterations has been reached. At the end of both inner and outer iteration convergence, or exceedance of maximum iterations, posterior covariance is calculated, if requested.

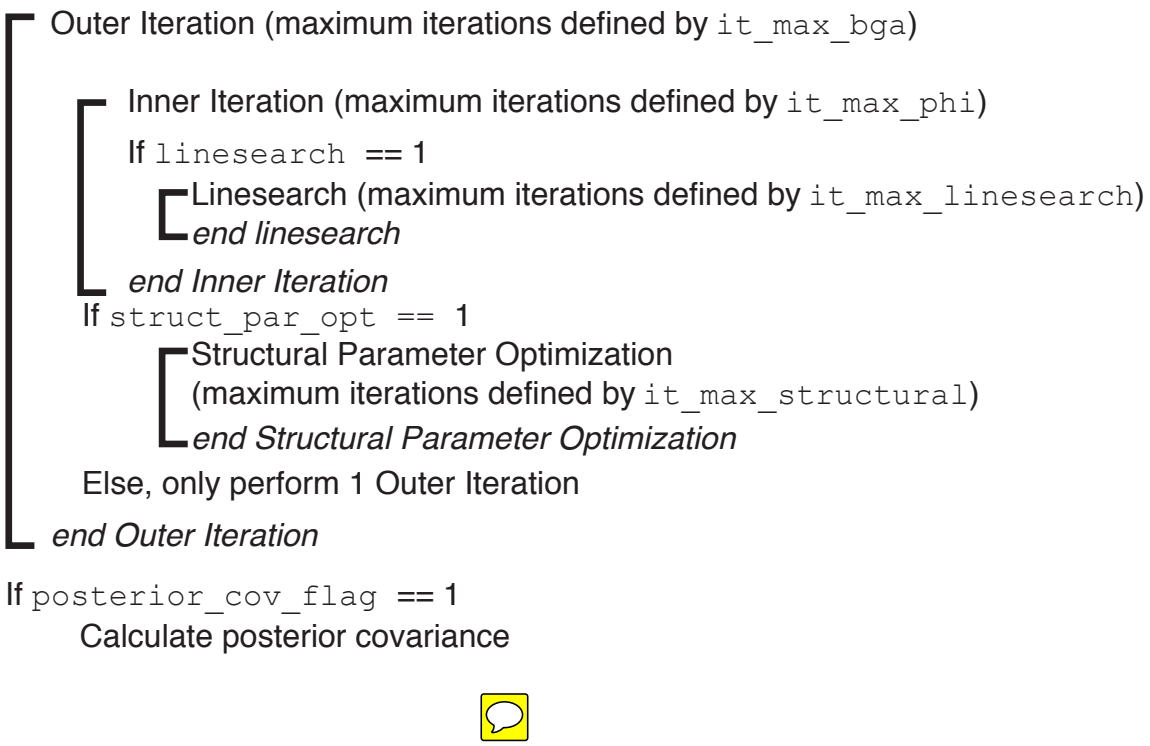


Figure 2: Abbreviated flowchart showing the progression of the major bgaPEST procedures.

bgaPEST Control Variables

Two types of variables are used in bgaPEST: data variables and control variables. Data variables are values such as model parameters, observations, file names, and other data that are needed by the bgaPEST program. Control variables, on the other hand, drive the actions that are performed on these data elements. As such, control variables are abstracted on level from data variables and control either the reading/writing of data or the progression of the algorithm. Many control variables are straightforward (for example, `it_max_phi`, an integer, is the total number of iterations allowed in each quasi-linear inner estimation optimization. *default=10).* Such variables are defined in the context of the input instructions in Appendix A. However, other control variables are accompanied by important conventions regarding their impact on the performance of the algorithm. For these cases, in this section, more detail is provided about certain control variables.

`structural_conv` *float* Convergence criterion for structural parameter convergence.

Positive or negative values can be used to trigger two different measures of convergence, as noted below. In either case, however, convergence is compared to the absolute value of `structural_conv`.
If positive, convergence is based on the absolute difference in structural parameter objective function over consecutive iterations.

$$\text{conv} = \text{abs}\left(\mathbf{\Phi}_{S,i} - \mathbf{\Phi}_{S,i-1}\right) \tag{3}$$

where i is the current structural parameter optimization iteration, $i-1$ is the previous structural parameter optimization iteration, and $\mathbf{\Phi}_S$ is the structural parameter objective function.
If negative, convergence is based on the norm of the difference between consecutive structural parameter values.

$$\text{conv} = \sqrt{\left(\theta_i - \theta_{i-1}\right)^T \left(\theta_i - \theta_{i-1}\right)} \tag{4}$$

where i and $i-1$ are as defined above, and θ is a vector containing all structural parameters currently being estimated (may include epistemic uncertainty, if requested). *default=0.001*

`phi_conv` *float* Convergence criterion for objective function convergence. The convergence at each inner iteration is evaluated as the absolute difference from one inner iteration to the next. This is evaluated as

$$\text{conv} = \text{abs}\left(\mathbf{\Phi}_{T,i_{in}} - \mathbf{\Phi}_{T,i_{in}-1}\right) \tag{5}$$

where i_{in} is the current inner iteration, and $\mathbf{\Phi}_T$ is the total objective function (Equation 36). *default=0.001*

`bga_conv` *float* Convergence criterion for objective function outer iterations. The convergence at each outer iteration is evaluated as the absolute difference from one outer iteration to the next. This accounts for both convergence of $\mathbf{\Phi}_T$ and $\mathbf{\Phi}_S$. The convergence is evaluated as

$$\text{conv} = \text{abs}\left(\mathbf{\Phi}_{T,i_{out}} - \mathbf{\Phi}_{T,i_{out}-1}\right) \tag{6}$$

where i_{out} is the outer iteration, and $\mathbf{\Phi}_T$ is the total objective function (Equation

36). *default*=10×`phi_conv`

`Q_compression_flag` *integer* Flag to determine how to calculate Q_0 [0] = no compression– calculate full Q_0 matrix, [1] = Calculate separate Q_0 matrix for each beta association. In addition to controlling the behavior of prior covariance compression, this flag also determines whether a full posterior covariance matrix or only the diagonal are calculated. *default=0*

`posterior_cov_flag` *integer* Flag to determine whether posterior covariance matrix should be calculated. [0] = do not calculate posterior covariance matrix, [1] = calculate posterior covariance. If `Q_compression_flag=1`, only the diagonal of the posterior covariance matrix is calculated. If `posterior_cov_flag=0` then 95% confidence intervals are not calculated and the output file `<casename>.bpp.fin` discussed below does not include confidence intervals.

Input Files

The bgaPEST program is run from the command line by typing `bgaPEST.exe <casename>.bgp` where `<casename>` is a filename containing input instructions. Detailed input instruction are in Appendix A.

Output Files

Several output files are generated throughout the progression of a single bgaPEST run. These files are summarized in this section.

bgaPEST Record File `<casename>.bpr`

The main output file for bgaPEST is called `<casename>.bpr`. Initial values of bgaPEST input are repeated to form a record for the bgaPEST run. After each inner iteration, as defined above, the objective function is reported and external files are written that include current parameter values and observation values. After each outer iteration, structural parameter values are also reported for each beta association in which structural parameter estimation was requested and for the epistemic uncertainty term, if requested. After the final outer iteration, all structural parameter values–including those which were not estimated–are reported to make a complete record.

bgaPEST Parameter Value Files <casename>.bpp.<#Oi>_<#Ii>

The parameter values are written to files called <casename>.bpp.<#Oi>_<#Ii> where <#Oi> is the outer iteration number and <#Ii> is the inner iteration number. These ascii files are printed in columns with the following headers: ParamName; ParamGroup; BetaAssoc; ParamVal. At the beginning of a bgaPEST run, a file <casename>.bpp.0 is written in the same format to record the initial parameter values used. This is done to avoid cluttering the <casename>.bpr file with what is often a very long list of parameters and their values. Parameter values that were subjected to logarithmic transformation are reported in their linear space, *not* log-transformed space.

Another special case of parameter value files is written at the end of a bgaPEST run and called <casename>.bpp.fin. This file contains the final parameter values estimated as optimal by bgaPEST. Furthermore, if posterior covariance calculation was requested, two additional columns are added: 95pctLCL and 95pctUCL which are the 95% lower and upper confidence limits, respectively. These confidence limits are obtained by applying the subtraction and addition, respectively, of $2 \times \sqrt{\mathbf{V}_{ii}}$ to $\mathbf{s}_i$–the i^{th} optimal parameter value. In this case, $\mathbf{V}$ is the posterior covariance, so $\sqrt{\mathbf{V}_{ii}}$ is the standard deviation of the i^{th} parameter. The 95% confidence limits are reported in linear space, *not* log-transformed space, so for log-transformed parameters, the upper and lower 95% percent confidence limits are not symmetrical about the parameter value.

bgaPEST Observation Value Files <casename>.bre.<#Oi>_<#Ii>

The observation values obtained by running the forward model with the currently estimated parameters are written to files called <casename>.bre.<#Oi>_<#Ii> following a similar convention as with the <casename>.bpp files above. The ascii files are printed with the following headers: ObsName; ObsGroup; Modeled; Measured. These files may be easily copied into a spreadsheet or read with a plotting program to calculate and plot residuals.

Posterior Covariance File <casename>.post.cov

If the input variable posterior_cov_flag=1, then posterior covariance of the parameters $\mathbf{s}$ is calculated. In addition to this information being used to report 95% confidence limits as described above, the posterior covariance matrix is also written to the

file `<casename>.post.cov`. If the variable `Q_compression_flag=1`, then compression is used for saving the prior covariance matrix. This is done when a large number of parameters is used and, thus, the full covariance matrices are unwieldy. Based on this choice, the posterior covariance is either reported as the diagonal of the posterior covariance matrix ($diag\,(\mathbf{V})$) if `Q_compression_flag=1` or the full covariance matrix $\mathbf{V}$ if `Q_compression_flag=0`. The output formats are discussed at the end of Appendix A.

Posterior Covariance and Parameter log-Transformations In this section, it was indicated that in the `<casename>.bpp.fin` file, parameter values and 95% confidence intervals are reported in linear (untransformed) space while in the `<casename>.post.cov` file, posterior covariance values are reported in estimation (log-transformed) space. Why the difference? The two files are serving slightly different purposes. The parameter output file presents values in the units they are entered in (and, presumably, the units "seen" by the forward model). As a result, 95% confidence intervals are reported in the same way. Furthermore, the addition and subtraction of $2 \times \sqrt{\mathbf{V}_{ii}}$ must be applied to the parameters before back-transformation, which explains the asymmetry of the confidence limits. On the other hand, the full posterior covariance matrix is intended for other analysis (propagation of variance through to predictions, conditional realizations, and others) in which the information should be retained in estimation (log-transformed) space. In the end, the decision of how to report these values is one of convention, and this side box is intended to make clear which was chosen in each case.

Suggestions and Guidelines for Initial Use

The Bayesian Geostatistical Approach is a highly parameterized method that is appropriate for some, but not all applications. In this section, we outline a few considerations to aid in the decision about whether to use bgaPEST on a given problem based on the history and characteristics of the method. We also provide a few guidelines to help avoid potential pitfalls in the application of bgaPEST.

This report documents the first release of bgaPEST and, to our knowledge, the first implementation of BGA available in a generalized package. As a result, users of this version will be among the first to apply this software outside of academia where custom programs have been the rule. Nonetheless, the method has a 20 year history. The ma-

jority of applications have been to groundwater modeling projects including (but not limited to): pumping test analysis (*Snodgrass and Kitanidis*, 1998); hydraulic tomography (*Li et al.*, 2007; *Fienen et al.*, 2008; *Li et al.*, 2008; *Cardiff and Kitanidis*, 2009); borehole logging (*Fienen et al.*, 2004); contaminant source identification (*Snodgrass and Kitanidis*, 1997; *Michalak and Kitanidis*, 2002, 2003); and nonparametric tracer test analysis (*Fienen et al.*, 2006). The main application to date that does not involve groundwater is in atmospheric modeling (ANNA'S PAPERS).

Characteristics for Suggested Use

The characteristics that unite these applications form a solid guide when deciding if bgaPEST is appropriate for a given application. First, and foremost, there must be a parameter set that varies either in space or time. For example, a time series of chemical concentrations (a breakthrough curve), a hydraulic conductivity field, a recharge field, ATMOSPHERIC EXAMPLE? These parameters should vary continuously over reasonably substantial areas for a variogram to be an adequate descriptor of the shape of the parameter field. Sub-areas delineated by geologic contacts, or in the case of time series, punctuated by known events, can be partitioned into beta associations, as discussed throughout this report. Another consideration is a more practical one–model run time.

The nature of bgaPEST is that many parameters are to be estimated. Throughout the parameter estimation process, a Jacobian sensitivity matrix must be calculated, requiring one model run per parameter. This computational burden must be considered and, potentially mitigated. In academic settings, many researchers have taken advantage of adjoint state to make the calculation of the Jacobian matrix more efficient in the case where parameters greatly outnumber observations. Adjoint state versions of commercial and government codes are not typically available, however, but bgaPEST is equipped to handle Jacobian matrices calculated outside of bgaPEST so users who are able to write such codes can make use of them. Similarly, parallelization of the Jacobian calculations is a feature that will be added in the future. For now, through clever scripting, it is possible to use beoPEST outside of bgaPEST to parallelize the calculations of the Jacobian matrix. In this initial release of bgaPEST, however, it may be more practical to stick with models with short run times, run Jacobian calculations in series and just recognize that the computational burden may be high.

A common occurrence in groundwater modeling applications is that parameters far ex-

ceed observations in number. This, of course, can change in transient simulations where, if each measurement in time at a single measurement location is considered an observation, the numbers of observations and parameters may equalize. bgaPEST is most appropriate for the latter case–where parameters outnumber observations, typically by a large margin. Several programming and mathematical accommodations are made to enable the number of parameters to grow very large (testing has been performed with 90,000 parameters). However, if the number of observation grows significantly, computer memory will become a limitation in many cases. For transient problems, one should consider the information content of each measurement point in time. Often, the number of observation points can be effectively reduced by considering moments rather than discrete points (*Li et al.*, 2005) or by other time series processing such as methods available in R (REF) or TSPROC (REF).

Guidelines

The number of applications of bgaPEST this far is limited. As new software and a relatively novel technique, it will take time for users to "get a feel" for the behavior and characteristics of the tool. In this section, we provide a few guidelines that we hope will help users avoid pitfalls. In future releases, building on the experience of a larger user base, more guidelines will become available.

Run Times For a typical groundwater model, somewhere between 5 and 15 outer iterations will often be required. For each outer iteration, it is likely that about 5 inner iterations are necessary. This means up to 75 calculations of the Jacobian matrix may be required. Without parallelization or adjoint state, users should carefully consider how many parameters can be accommodated as run times grow in length. For planning, assume that the time required for each Jacobian calculation is NPAR $\times$ Run Time.

Beta Associations Beta associations provide the ability to include knowledge about contacts and other partitions in the parameter fields. Some beta associations can have a separate parameter value in each node, while others can be treated as homogeneous zones. This is accomplished through the design of the template file. In addition to allowing for the inclusion of well-known structures such as lithologic contacts, beta associations also allow for some regions–either because of greater importance to the

ultimate management decisions, due to greater density of data, or both–to have a large number of parameters whereas other regions have homogeneous values. By only allowing a large number of parameters in focused areas of interest, the overall number of parameters can be reduced, thus mitigating some of the concerns about run times.

Line Search The purpose of the line search is similar to the purpose of the Levenberg-Marquardt adjustment used in PEST; it is to make a correction to the search direction when the optimization algorithm might otherwise stray from the optimal direction. The linesearch, therefore, serves its greatest purpose in its first iteration or two. After that, the value of the linesearch is limited for mathematical reasons having to do with linearization of the problem (see Appendix C for more details). As a result, a value of between 2 and 5 for `it_max_linesearch` in the control variables is generally adequate. If the linesearch algorithm does not converge, a warning will be issued and, while it is good to know that this took place, the linesearch has served its purpose and little gain will be achieved by increasing `it_max_linesearch.`

Level of Fit "With great power comes great responsibility." In applications where parameters outnumber observations, a real danger lurks of overfitting. In other words, parameters can be adjusted to achieve a level of correspondence between simulated and observed equivalents that exceeds a reasonable level. The danger of this is that some of the *lack* of correspondence is often due to random epistemic error and is not representative of actual system behavior. However, if the parameters are adjusted to match observations within this margin of error, they are "fitting the noise." The ramifications of this are mainly a diminishment of predictive power of the model and unrealistic roughness of the parameter fields estimated. There are two means of avoiding this problem. One is the maximum entropy property of BGA. The algorithm is designed to find the *smoothest* solution consistent with the level of fit. If all structural parameters–including σ_R–are estimated, the algorithm will try to achieve perfect fit with the smoothest solution that can do so. This may still lead to overfitting, however, so in most cases, it is more appropriate to set the level of fit using `sig_0` in the Epistemic Error Term input block described below to a level of fit chosen by the user to be appropriate given known and suspected uncertainties about both the observation quality and the model. Weights on observations can account for different levels of quality in different observations. In most cases, the user should also set `sig_opt=0` to force the algorithm to use

a consistent value for epistemic uncertainty and thus to manually control the level of fit. If set this way, the algorithm will adjust the other structural parameters to achieve the smoothest possible solution corresponding to the specified level of fit.

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.

A Input Instructions

In this appendix, the general strategy for input instructions is described. The input is arranged in a file called `<casename>.bgp`, which is made up of input blocks, as discussed below. Following a discussion of more detail of the general input protocols, subsections in which specific input blocks are discussed including variables and data that can be input in them are presented.

General Structure of Input

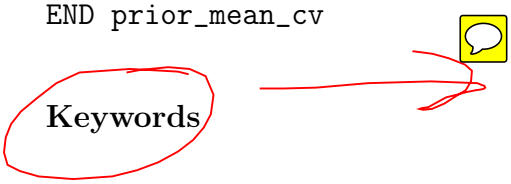
The general input structure is designed on a subset of the JUPITER protocol (*Banta et al.*, 2006). The advantage of this protocol over XML or the previous input format for PEST is that annotations that are easily read by humans are part of the input protocol. The full JUPITER protocol, however, has memory and computational overhead that can become a problem for large and complicated data sets. The protocol used here, therefore, is simplified but should be easily recognizable to users of other JUPITER-compatible programs.

The strategy for input is designed to use BLOCKS that are made up of either KEYWORDS for individual variables or TABLES for a series of data. The specification of whether a given block uses KEYWORDS or TABLES is preordained and the input blocks defined below indicate which is required.

Blocks

Input Blocks are allowed to take one of two forms: either KEYWORDS or TABLES. All input blocks are delineated by the words BEGIN and END. The header line also includes the name and type of the block and the final line contains the name of the block. For example:

```
BEGIN prior_mean_cv KEYWORDS
prior_betas=1
beta_cov_form = 0
END prior_mean_cv
```



Keywords

Keyword variables correspond to single values identifies with an "=" sign. Multiple KEYWORDS can be entered on each line in an input file but no spaces are allowed in KEYWORDS names or variable values. An example is: `prior_betas=1.`

Tables

Table variables are used for tabular data series that have multiple values in categories. Tables are identified by listing the number of rows (nrow), number of columns (ncol), and providing the keyword columnlabels. This is followed by nrow rows of data, with values arranged in ncol columns, corresponding to the same order as the columnlabels, and delimited by one or more spaces. For example:

```
BEGIN Q_compression_cv TABLE
nrow=2 ncol=5 columnlabels
BetaAssoc Toep_flag Nrow Ncol Nlay
1 0 21 21 1
2 1 21 21 1
END Q_compression_cv
```

Files

A user may want to shorten the length of the main input file by ~~redirecting certain input to~~ retrieving input from external text files. This can be done by signaling an input block with the word `FILES`, to read a file containing the entire set of information for the block. Regardless of whether the external text file contains a `KEYWORDS` or `TABLE` block, a block definition must be in place directing the program to the external file. For example:

```
BEGIN Q_compression_cv FILE
compression.txt
END Q_compression_cv
```

In this example, the contents of the file compression.txt would be:

```
BEGIN Q_compression_cv TABLE
nrow=2 ncol=5 columnlabels
BetaAssoc Toep_flag Nrow Ncol Nlay
1 0 21 21 1
2 1 21 21 1
END Q_compression_cv
```

bgaPEST Input Blocks

is the ordering of the blocks hard wired? required?

The specific input blocks used in bgaPEST are discussed, in order of appearance in the `<casename>.bgp` file. For each block, data types are identified either as *float*, *integer*, or *string*. Values entered as *float* can include scientific/engineering notation, but in all cases should contain a "." even if no fractional detail is included. Conversely, *integers* must not contain ".". Variables identified as *string* may not include spaces because whitespace is used as the delimiter for rows in tables and separating keywords.

Each block is also defined with a suffix of "cv" for "control variables," or "data" for data. Control variables are those that govern the behavior of the algorithm as a whole as opposed to data points (such as parameter values, structural parameter values, etc.).

A note on default variable values In the input instructions below, some variables list a default value. Part of the design strategy of this software was to not burden users with determining appropriate values for each and every variable that controls the algorithm. As a result, default values are provided for some variables. In those cases, input by the user in the `.bgp` file is optional. If no value is provided by the user, the default value will be used by bgaPEST. If a variable not listed with a default value in these input instructions is omitted by a user, bgaPEST will return with an error indicating that the variable is not present.

Algorithmic Control Variables `algorithmic_cv` KEYWORDS

The following `KEYWORDS` variables are in the `algorithmic_cv` block.

`structural_conv` *float* Convergence criterion for structural parameter convergence. If positive, convergence is based on the absolute difference in structural parameter objective function over consecutive iterations. If negative, convergence is based on the norm of the difference between consecutive structural parameter values. Used only if at least one structural parameter is to be estimated. *default=0.001*

`phi_conv` *float* Convergence criterion for objective function inner iterations. *default=0.001*

`bga_conv` *float* Convergence criterion for objective function outer iterations. *default*=10×`phi_conv`

`it_max_structural` *integer* Total number of iterations allowed in structural parameter optimization. *default=10*

`it_max_phi` *integer* Total number of iterations allowed in each quasi-linear estimation optimization. *default=10*

`it_max_bga` *integer* Total number of outer iterations allowed for the entire algorithm. *default=10*

`linesearch` *integer* Flag to determine whether a line search should be conducted. [0] = do not use linesearch, [1] = use linesearch. *default=0*

`it_max_linesearch` *integer* Total number of outer iterations allowed for the line search. Used only if `linesearch` = 1. *default=4*

`theta_cov_form` *integer* Form of the theta covariance matrix. [0] = none, [1] = diagonal, [2] = full matrix. [0] means no prior covariance on theta provided and it is assumed totally unknown. Used only if at least one structural parameter is to be estimated. *default=0*

`Q_compression_flag` *integer* Flag to determine how to calculate Q_0 [0] = no compression– calculate full Q_0 matrix, [1] = Calculate separate Q_0 matrix for each beta association. *default=0*

`par_anisotropy` *integer* Flag to determine whether parameter anisotropy should be considered when making the **Q** matrix: [0] = do not consider anisotropy, [1]=consider anisotropy. If anisotropy is considered, a `parameter_anisotropy` block should be included, as defined below. *default=0.*

`deriv_mode` *integer* Flag to determine whether sensitivities are calculated using an external call to PEST or using a user-supplied program (such as adjoint state). [0] = use PEST, [1] = use external program identified below in the `model_command_lines` block. *default=0*

`posterior_cov_flag` *integer* Flag to determine whether posterior covariance matrix should be calculated. [0] = do not calculate posterior covariance matrix, [1] = calculate posterior covariance matrix. If `Q_compression_flag = 1`, only the diagonal of the posterior covariance matrix is calculated. *default=0*

`jacobian_file` *string* Name of the file generated by an external program if `deriv_mode = 1`. If `deriv_mode = 0`, this value is ignored and left at its default value. *default="scratch.jco"*

`jacobian_format` *string* Format of the file indicated in jacobian_file. [binary] indicates a binary file formatted as a JCO file from PEST, [ascii] indicates a file of a standard PEST matrix format, discussed below in this documentation. If `deriv_mode = 0`, this value is ignored and left at its default value. *default="binary"*

Prior Mean Control Variables `prior_mean_cv` KEYWORDS

The following `KEYWORDS` variables are in the `algorithmic_cv` block.

REQUIRED

`prior_betas` *integer* Flag indicating whether information about prior mean (β) will be supplied. [0] = no, [1] = yes.

`beta_cov_form` *integer* Form of the prior mean (β) covariance matrix ($\mathbf{Q}_{\beta\beta}$). [0] = none, [1] = diagonal, [2] = full matrix. This value is used only if `prior_betas = 1`. *default=0*

Beta Association Data `prior_mean_data` TABLE

This table must contain the same number of rows as there are beta associations to be defined. The rows must be in ascending order of beta association numbers. This is also the block where beta associations are defined, even if prior means are not defined.

`BetaAssoc` *integer* Identifier of each beta association (one per row). These should be sequential integers.

`Partrans` *string* Transformation indicator determining whether β values will be in physical or estimation space. Acceptable values are `log` and `none`.

`beta_0` *float* Value of prior mean value (β_0) for the row's beta association. This value is used only if `prior_betas = 1`.

`beta_cov_#` *float* The number of values provided is based on the value of `beta_cov_form` specified above:

If `beta_cov_form = 1`, one value is provided.

If `beta_cov_form = 2`, `nrow` values are provided, corresponding to the current row of the beta covariance matrix ($\mathbf{Q}_{\beta\beta}$).
This value is used only if `prior_betas = 1`.

Structural Parameter Control Variables `structural_parameter_cv` TABLE

This table must contain the same number of rows as there are beta associations to be defined. The rows must be in ascending order of beta association numbers.

`BetaAssoc` *integer* Identified ~~of~~ for ? each beta association (one per row). These should be sequential integers.

`prior_cov_mode` *integer* Flag to indicate whether prior covariance of parameters ($\mathbf{Q_{ss}}$) is supplied or calculated. This is reserved for future use - currently $\mathbf{Q_{ss}}$ is always calculated, so this value is ignored if present.

`var_type` *integer* This is a flag to indicate which variogram type is used to express the prior covariance ($\mathbf{Q_{ss}}$). Acceptable choices are [0] = pure nugget, [1] = linear, [2] = exponential. *default=1*

`struct_par_opt` *integer* Flag for whether structural parameters are meant to be optimized or not. This can be chosen for each structural parameter individually. [0] = do not optimize (hold at initial value), [1] = optimize using a marginal distribution. *default=1*

`trans_theta` *integer* Flag for whether a power transformation should be applied to the structural parameters in the current row. [0] = do not transform, [1] = transform. This value is only used of `struct_par_opt = 1`. *default=0*

`alpha_trans` *float* Exponent of the power transformation used only if `trans_theta = 1`. *default = 50*

Structural Parameter Data `structural_parameter_data` TABLE

This table must contain the same number of rows as there are beta associations to be defined. The rows must be in ascending order of beta association numbers.

`BetaAssoc` *integer* Identifier of each beta association (one per row). These should be sequential integers.

`theta_0_1` *float* Initial value of $\theta_{1,0}$ which is the starting value of the first structural parameter for prior covariance.

`theta_0_2` *float* Initial value of $\theta_{2,0}$ which is the starting value of the second structural parameter for prior covariance. If using a linear or nugget variogram, an arbitrary negative value should be entered here indicating that the value will be ignored. For an exponential variogram, this parameter is the correlation length.

Structural Parameter Covariance Data `structural_parameter_cov` TABLE

The only covariance model currently supported is diagonal, so there must be one covariance value for each θ parameter. This block is only read if `theta_cov_form` is not zero.

`theta_cov_1` *float* Variance of the current row's θ parameter. If using an exponential variogram, then a single beta association will have two structural parameters. To handle this possibility, the variance values should be listed, one per line, in the order of beta associations, then in order θ_1 then θ_2. Even structural parameters that will not be estimated (e.g. that are held at their initial values, as indicated by `struct_par_opt` above, must have a placeholder value entered here to maintain the order–the placeholder value is arbitrary and will be ignored.

Epistemic Error Term `epistemic_error_term` KEYWORDS

`sig_0` *float* Initial value of the epistemic error (σ_o).

`sig_opt` *integer* Flag indicating whether epistemic error should be optimized for or not. [0] = do not optimize, [1] = optimize. If `sig_opt = 0`, then the value of `sig_0` is used throughout the inversion.

`sig_p_var` *float* Prior variance on σ. `sig_p_var = 0` means no prior variance on epistemic error is provided and it is assumed totally unknown. This value is used only if `sig_opt = 1`. *default=0.*

`trans_sig` *integer* Flag for whether a power transformation should be applied to the epistemic error. [0] = do not transform, [1] = transform. This value is used only if `sig_opt = 1`. *default=0*

`alpha_trans` *float* Exponent of the power transformation, used only if `trans_sig = 1`. *default = 50*

Parameter Control Values `parameter_cv` KEYWORDS

`ndim` *integer* Number of dimensions over which parameters span.

Prior Covariance Compression Control Variables `Q_compression_cv` TABLE

This table must contain the same number of rows as there are beta associations to be defined. The rows must be in ascending order of beta association numbers. This block is only read if `Q_compression_flag` = 1.

`BetaAssoc` *integer* Identified of each beta association (one per row). These typically are sequential integers.

`Toep_flag` *integer* This is a flag to determine whether a Toeplitz transformation should be applied to the prior covariance matrix ($\mathbf{Q_{ss}}$) . [0] = do not use Toeplitz transformation, [1] = do use Toeplitz transformation.

`Nrow` *integer* Number of rows in the current beta association (only read if `Toep_flag` = 1).

`Ncol` *integer* Number of columns in the current beta association (only read if `Toep_flag` = 1).

`Nlay` *integer* Number of layers in the current beta association (only read if `Toep_flag` = 1).

Parameter Groups `parameter_groups` TABLE

Each row of this table corresponds to one of the parameter groups. These groups are used to group together parameters by type and are not the same as beta associations.

`groupname` *string* Name of the group in the current row. Note that these cannot contain spaces.

Parameter Data `parameter_data` TABLE

Each row of this table provides information for one parameter.

`ParamName` *string* Name for the parameter.

`StartValue` *float* Staring parameter value.

`GroupName` *string* Name of the group to which the parameter belongs. This name must be defined in the `parameter_groups` block.

`BetaAssoc` *integer* Beta association to which this parameter belongs.

`SenMethod` *integer* Sensitivity method used for this parameter type. This parameter may now be arbitrary–it is reserved for future use and currently is ignored.

`x1` *float* Location in the first dimension.

`x2` *float* Location in the second dimension. Only read if `ndim >= 2`.

`x3` *float* Location in the third dimension. Only read if `ndim = 3`.

Observation Groups `observation_groups` TABLE

Each row of this table corresponds to one of the observation groups. These groups are used to group together observations by type and are used to report portions of the objective function.

`groupname` *string* Name of the group in the current row. Note that these cannot contain spaces.

Observation Data `observation_data` TABLE

One observation is presented on each line.

`ObsName` *string* Name of an observation.

`ObsValue` *float* Value of the observation.

`GroupName` *string* Name of the group to which the observation belongs. This name must be defined in the `observation_groups` block.

`Weight` *float* A relative weight that gets applied to the epistemic error.

Model Command Lines `model_command_lines` KEYWORDS

Currently a single forward model command and an option derivative model command can be supplied here. These string keywords can include path information if the command line batch files or shell scripts are not located in the current working directory, but spaces are not allowed.

`Command` *string* This is the batch file or shell script that runs the forward model.

`DerivCommand` *string* This is the optional batch file or shell script that is used to calculate derivatives. This is only used if `deriv_method = 1` in the `algorithmic_cv` block.

Model Input Files `model_input_files` TABLE

Each row of this table includes a matched template file and model input file. This allows the program to create the correct input files for the model.

`TemplateFile` *string* Name of a template file for making model input. Must end in `.tpl`.

`ModInFile` *string* Name of the model input file corresponding to the TemplateFile identified on the same row.

Model Output Files `model_output_files` TABLE

Each row of this table includes a matched instruction file and model output file. This allows the program to read the results of model runs correctly.

`InstructionFile` *string* Name of an instruction file for reading model output. Must end in `.ins`.

`ModOutFile` *string* Name of the model output file corresponding to the InstructionFile identified on the same row.

Parameter Anisotropy `parameter_anisotropy` TABLE

Each row of this table contains information for parameter anisotropy for a beta association. This block is read only if the variable `par_anisotropy` =1 in the `algorithmic_cv` block.

`BetaAssoc` *integer* Identifier of a beta association.

`horiz_angle` *float* Angle, in degrees of the principal direction of anisotropy in a horizontal plane. See Figure 4 for details.

`horiz_ratio` *float* Ratio of maximum to minimum principal property values in the horizontal plane. See Figure 4 for details.

`vertical_ratio` *float* Ratio of maximum to minimum principal property values in the vertical direction. See Figure 4 for details. This value is only read if `ndim=3`.

PEST Matrix Formats for Jacobian and Posterior Covariance

On two occasions in `bgaPEST` a matrix text file format from `PEST` is used to store matrices: when posterior covariance output from `bgaPEST` is specified as a full matrix; and when Jacobian sensitivity matrix information is exchanged from an external code with `bgaPEST`. (e g Python script?)

The posterior covariance matrix may take two forms: a full matrix; or a diagonal matrix. These options are discussed below. Two options are available for Jacobian sensitivity matrices (**H**) to be read by `bgaPEST`. If `deriv_mode=0`, `PEST` is used, external to `bgaPEST`, to calculate the Jacobian matrix resulting in a binary file with the extension `.jco`. If `deriv_mode=1` then an external program is used to calculate **H** and a file written by the external program must be communicated to `bgaPEST`. This file can either be a `.jco` file or a `.jac` file which is an ASCII file following the format of a standard matrix file used by `PEST`, as described in *Doherty* (2010b), Section 4.4.3. An example and description of the format of a standard `PEST` matrix follow, quoting from *Doherty* (2010b).

Figure A depicts an example matrix file holding a matrix with three rows and four columns.

```
   3   4   2
3.4423    23.323    2.3232   1.3232
5.4231    3.3124    4.4331   3.4442
7.4233    5.4432    7.5362   8.4232
* row names
apar1
apar2
apar3
* column names
aobs1
aobs2
aobs3
aobs4
```

Figure 3: Example of a standard PEST matrix file, adapted from *Doherty* (2010b).

The first line of a matrix file contains 3 integers. The first two indicate the number of rows (NROW) and number of columns (NCOL) in the following matrix. The next integer (named ICODE) is a code, the role of which will be discussed shortly. Following the header line is the matrix itself, in which entries are space-separated and wrapped to the next line if appropriate. The maximum line length is 500 characters, so wrapping to the next line must occur within 500 characters. It is recommended to wrap lines after 8 values and to maintain maximum possible precision.

In use for Jacobian matrices by bgaPEST, ICODE is set to 2, so the string "`* row names`" is printed next, followed by NROW names (of 20 characters or less in length), containing the names associated with rows of the matrix. NCOL column names follow in a similar format, following the string "`* column names`".

Other options for ICODE are described in *Doherty* (2010b) and are used in bgaPEST for output of the posterior covariance matrix. The two options for posterior covariance output both refer to square matrixes that have the same names of columns and rows. As a result, only one list of names follows the data following the string "`* row and column names`".

If compression is used in the prior covariance matrix, bgaPEST only outputs the diagonal elements of the posterior covariance. In this case, ICODE=-1 and only the diagonal entries are listed, one per line, after the header line. If compression is not used, the entire posterior covariance matrix is printed using ICODE=1 with 8 values per line.

B Quick Start Instructions

One advantage of using block input and keywords, as discussed in Appendix A, is that default values are provided within bgaPEST so they can be skipped by a user. The values provided as defaults have general applicability and will all be reported in the `<casename>.bpr` file. In this section, then, the bare minimum level of input is described to get a project running.

Forward Model The forward model must exist and have the ability–either inherently or through pre- and post-processing–to receive input and provide output using text (ascii) files. For bgaPEST to be able to run the model, template files (`.TPL`) and instruction files (`.INS`) must be provided corresponding with model input and output, respectively. Details of the contruction of these files are in (*Doherty*, 2010a, chapter 3). The template and instruction files are detailed in the `model_input_files` and `model_output_files` blocks, respectively. The `model_command_lines` block must also be included with an entry for either a batch file or shell script in the `command` keyword that runs the model.

Observations The `observation_groups` block must be completed. All observations can belong to the same group if desired. Groups are reported in output to assist in interpretation of results. The `observation_data` block must also be completed.

Beta Associations Beta associations are first defined in the `prior_mean_data` block. If no prior information about mean values and their covariance is to be supplied, the only information necessary is a row for each beta association in the `prior_mean_data` block and a decision about whether to transform the value with a logarithmic transform or not. Note that beta associations indicate regions and groups that will have the same mean value estimated regardless of whether prior information about the mean is provided or not.

Structural Parameters Each beta association must have a variogram specified for it, defined by structural parameters. Therefore, the `structural_parameters_cv` and `structural_parameter_data` blocks must be completed. Whether or not to optimize

for structural parameter values, and whether or not to provide prior information about the values is optional.

Parameters The `parameter_groups` block must be completed and, like with observations, it is acceptable for all parameters to be in a single group, and groups do not need to correspond with beta associations. The `parameter_cv` keyword `ndim` must be provided, and the `parameter_data` block must be completed.

Algorithmic Control Variables The `algorithmic_cv` block contains variables that all have default values. However, bgaPEST must find the `algorithmic_cv` block - even if it is empty. If the `algorithmic_cv` block is empty, all default values will be used.

C Details of the Method

The Bayesian geostatistical approach is described in detail in *Kitanidis and Vomvoris* (1983); *Hoeksema and Kitanidis* (1984); *Kitanidis* (1995); *Nowak and Cirpka* (2004) among others. The mathematics are reviewed here.

The Bayesian Geostatistical Approach

In the Bayesian geostatistical approach, the posterior pdf is calculated as

$$p(\mathbf{s}|\mathbf{y}) \propto \underbrace{\exp\left(-\frac{1}{2}\left(\mathbf{y}-\mathbf{h}(\mathbf{s})\right)^T \mathbf{R^{-1}} \left(\mathbf{y}-\mathbf{h}(\mathbf{s})\right)\right)}_{\mathrm{L}(\mathbf{y}|\mathbf{s})} \underbrace{\exp\left(-\frac{1}{2}(\mathbf{s}-\mathbf{X}\beta^*)^T \mathbf{G_{ss}^{-1}} (\mathbf{s}-\mathbf{X}\beta^*)\right)}_{\mathrm{p}(\mathbf{s})} \tag{7}$$

where $\mathbf{s}$ is the vector of parameter values at distributed spatial locations in the model, $\mathbf{X}\beta^*$ is the prior mean, $\mathbf{G_{ss}}$ is the prior covariance of $(\mathbf{s}-\mathbf{X}\beta^*)$, $\mathbf{h}(\mathbf{s})$ is the modeled forecasts collocated with observations $(\mathbf{y})$, and $\mathbf{R}$ is the epistemic uncertainty covariance, modeled as $\sigma_R^2\mathbf{I}$ where σ_R^2 represents epistemic uncertainty, and $\mathbf{I}$ is an identity matrix. In general terms, the likelihood function $(L(\mathbf{y}|\mathbf{s}))$ characterizes the misfit between model forecasts and observations while the prior pdf $(p(\mathbf{s}))$ defines a characteristic (such as smoothness or continuity) that is assumed to apply to the parameter field. The prior pdf also serves the role of regularization.

The best estimate of $\mathbf{s}$ maximizes the posterior pdf. A computationally efficient method to find the best estimates of $\mathbf{s}$ and β $\left(\hat{\mathbf{s}} \text{ and } \hat{\beta}, \text{ respectively}\right)$ is through

$$\hat{\mathbf{s}} = \mathbf{X}\hat{\beta} + \mathbf{Q_{ss}}\mathbf{H^T}\xi \tag{8}$$

which is the superposition of the prior mean (first term) and an innovation term which considers deviations of the predictions from the observations (second term). In this context, β in the first term is not the prior mean, but is the best estimate of the mean (mapped onto the parameter field through the $\mathbf{X}$ matrix) while the second term is fluctuations about the estimated mean. $\mathbf{H}$ in the second term (often referred to as the Jacobian, sensitivity, or susceptibility matrix) is the sensitivity of observation values to parameter values where $H_{ij} = \frac{\partial \mathbf{h}(\mathbf{s})_i}{\partial \mathbf{s}_j}$, which can be calculated using either finite difference or adjoint-state methods. In bgaPEST, finite-difference calculations for $\mathbf{H}$ are calculated using PEST whereas adjoint-state calculations depend on the specific model being used and must be calculated using an external program.

The values for $\hat{\beta}$ and ξ are found by solving the $(n+p) \times (n+p)$ linear system of cokriging equations

$$\begin{bmatrix} \mathbf{Q_{yy}} & \mathbf{HX} \\ \mathbf{X}^T\mathbf{H}^T & -\mathbf{Q}_{\beta\beta}^{-\mathbf{1}} \end{bmatrix} \begin{bmatrix} \xi \\ \hat{\beta} \end{bmatrix} = \begin{bmatrix} \mathbf{y} \\ -\mathbf{Q}_{\beta\beta}^{-\mathbf{1}}\beta^* \end{bmatrix} \tag{9}$$

where $\mathbf{Q_{yy}}$ is the auto-covariance matrix of the observations, defined as $\mathbf{HQ_{ss}H^T} + \mathbf{R}$, n is the number of observations, and p is the number of beta associations.

In hydrogeologic applications, the numerical forward model is typically nonlinear. Further nonlinearity can be induced by using a logarithmic transformation, which is a convenient way to enforce non-negativity on parameters and is often an appropriate transformation for hydraulic conductivity parameters in groundwater models.

Provided that the nonlinearities introduced are not too extreme, a solution can be obtained through successive linearizations following the quasi-linear extension (*Kitanidis*, 1995). The forward model, $\mathbf{h}(\mathbf{s})$ is expanded about the current best estimate of the parameters $\tilde{\mathbf{s}}$

$$\mathbf{h}(\mathbf{s}) \approx \mathbf{h}(\tilde{\mathbf{s}}) + \tilde{\mathbf{H}}(\mathbf{s} - \tilde{\mathbf{s}}) \tag{10}$$

where $\tilde{\mathbf{H}}$, as a function of $\tilde{\mathbf{s}}$, is evaluated at each linearization. We assign the subscript $_k$ to indicate iteration number, and correct the measurements for the k^{th} linearization

as

$$\mathbf{y}_k^{'} = \mathbf{y} - \mathbf{h}(\tilde{\mathbf{s}}_k) + \tilde{\mathbf{H}}_k \tilde{\mathbf{s}}_k. \tag{11}$$

Then the cokriging equations (Equation 9) are updated

$$\begin{bmatrix} \tilde{\mathbf{Q}}_{\mathbf{yy},k} & \tilde{\mathbf{H}}_k \mathbf{X} \\ \mathbf{X}^T \tilde{\mathbf{H}}_k^T & -\mathbf{Q}_{\beta\beta}^{-\mathbf{1}} \end{bmatrix} \begin{bmatrix} \xi_k \\ \hat{\beta}_k \end{bmatrix} = \begin{bmatrix} \mathbf{y}_k^{'} \\ -\mathbf{Q}_{\beta\beta}^{-\mathbf{1}} \beta^* \end{bmatrix} \tag{12}$$

where $\tilde{\mathbf{Q}}_{\mathbf{yy},k} = \tilde{\mathbf{H}}_k \mathbf{Q}_{\mathbf{ss}} \tilde{\mathbf{H}}_k^T + \mathbf{R}$. From this set of equations, the next estimate of $\mathbf{s}$ is

$$\tilde{\mathbf{s}}_{k+1} = \mathbf{X}\hat{\beta}_k + \mathbf{Q}_{\mathbf{ss}} \tilde{\mathbf{H}}_k^T \xi_k. \tag{13}$$

This can be iterated until there is no difference in the parameter estimates, or when there is no further improvement in the objective function. The objective function, which we seek to minimize, is $-\ln p(\mathbf{s}|\mathbf{y})$ which is equivalent to maximizing Equation 7

$$\mathbf{\Phi} = -\ln p(\mathbf{s}|\mathbf{y}) = (\mathbf{s} - \mathbf{X}\beta^*)^T \mathbf{G}_{\mathbf{ss}}^{-\mathbf{1}} (\mathbf{s} - \mathbf{X}\beta^*) + (\mathbf{y} - \mathbf{h}(\mathbf{s}))^T \mathbf{R}^{-\mathbf{1}} (\mathbf{y} - \mathbf{h}(\mathbf{s})) \tag{14}$$

Line Search

In some cases, numerical instability makes convergence difficult. A line search is implemented in which a linear search is performed between the most recent best estimate of the parameters ($\hat{\mathbf{s}}$) and the current linearization of the parameters ($\widetilde{\mathbf{s}}$), seeking a parameter value that minimizes an objective function.

The linesearch optimizes a single parameter, ρ, along a linear dimension between $\hat{\mathbf{s}}$ and $\widetilde{\mathbf{s}}$ as

$$\mathbf{s}_{opt} = \hat{\mathbf{s}}\rho + \widetilde{\mathbf{s}}(1 - \rho) \tag{15}$$

where $\mathbf{s}_{opt}$ minimizes the objective function, Φ, using a Nelder-Mead simplex (see, e.g., *Press et al.*, 1992), which guarantees monotonic decrease in $\mathbf{\Phi}$ over successive iterations. It is recommended to limit the number of linesearch iterations to a relatively low number, as the goal of handling weak linearity is balanced against the computations required to perform the line search. The greatest advantage is likely achieved in the first few (less than five) iterations. The role of the line search is not to find a minimum value of $\mathbf{\Phi}$ because the nonlinearity of the overall problem prevents it. Rather, the line search is meant to be a correction of search direction for stability.

Parameter Field Anisotropy

In distributed parameter fields, such as hydraulic conductivity in groundwater models, it is common to encounter anisotropy along an axis that may or not be aligned with the coordinate (x, y, z) axes. bgaPEST allows the definition of anisotropy in a horizontal plane at any angle from the x-axis and also in the vertical direction. The general layout of horizontal anisotropy is illustrated in Figure 4. The angle from the x-axis (specified in degrees) is defined by `horiz_angle` and the amount of anisotropy is defined by `horiz_ratio`. `p_max` refers to the direction with maximum parameter values and `p_min` refers to the direction of minimum parameter values. The ratio is used to adjust the effective distance (and thereby the covariance values) along that principal direction. The user supplies values for `horiz_angle` and `horiz_ratio` for each beta association. If some beta associations are not meant to exhibit anisotropy, the user may simply set `horiz_ratio=1.0`. If none of the beta associations exhibit anisotropy, the entire `parameter_anisotropy` block can be eliminated by setting the algorithmic control variable `par_anisotropy=0` which means the block, if present, is ignored.

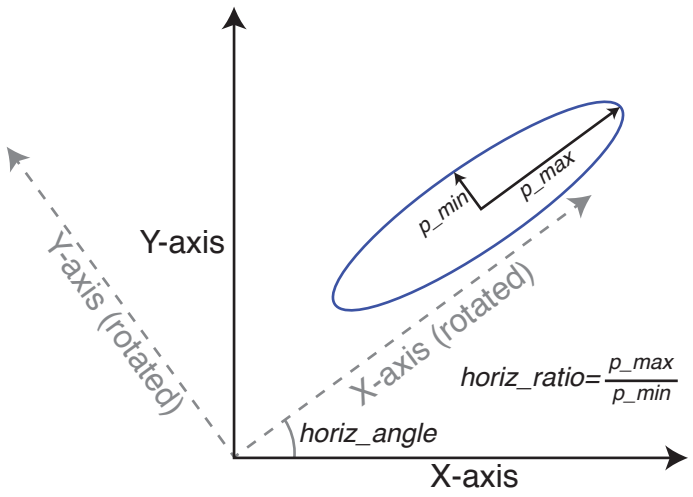


Figure 4: Schematic diagram of horizontal anisotropy defining conventions for bgaPEST.

Anisotropy is introduced in the calculation of distances that are, then, used in the calculation of the prior covariance matrix $\mathbf{Q}_{\mathbf{ss}}$ discussed below. For every pair of points, they must first be rotated into the principal direction orientation. This is accomplished

using a rotation matrix:

$$\begin{bmatrix} x_{rot,i} \\ y_{rot,i} \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} x_i \\ y_i \end{bmatrix} \tag{16}$$

where i indicates the i^{th} point of the pair ($i = 1, 2$), θ is the angle (in degrees) specified by `horiz_angle`, x and y are the point coordinates in the original coordinate system, and x_{rot} and y_{rot} are the location projected into the coordinate system corresponding to the orientation of horizontal anisotropy.

Once this projection is made, the horizontal distance is calculated as

$$distance = \sqrt{(x_{rot,1} - x_{rot,2})^2 + \texttt{horiz\_ratio} \times (y_{rot,1} - y_{rot,2})^2} \tag{17}$$

For three-dimensional parameter fields, a second anisotropy ratio may be specified as `vertical_ratio`. In the vertical direction, no angle is specified, so the rotation step is not required and distance is calculated as

$$distance = \sqrt{\begin{array}{c} (x_{rot,1} - x_{rot,2})^2 \\ +\texttt{horiz\_ratio} \times (y_{rot,1} - y_{rot,2})^2 \\ +\texttt{vertical\_ratio} \times (z_{rot,1} - z_{rot,2})^2 \end{array}} \tag{18}$$

Prior Probability Density Function

The prior pdf of $\mathbf{s}$ can be characterized as multi-Gaussian through its mean and covariance. The $(m \times 1)$ unknown parameter vector, $\mathbf{s}$, is modeled as a random process with mean

$$E[\mathbf{s}] = \mathbf{X}\beta \tag{19}$$

where $E[\cdot]$ indicates expected value, m is the number of parameters, β is a $(p \times 1)$ vector of drift coefficients, and $\mathbf{X}$ is an $(m \times p)$ matrix of base functions. In the absence of prior drift, the β are the beta association mean values and $\mathbf{X}$ is a selection matrix mapping each value in $\mathbf{s}$ and β into their appropriate beta association. $\mathbf{X}$ contains all zeros except for $\mathbf{X}_{ij}^{th}$ element, which maps the i^{th} parameter to the j^{th} beta association, that contains the value of one. Subdivision into beta associations within distributed parameter domains have been critical to success in hydrogeologic settings which include

strong contrasts in parameter values indicative of geologic contacts [see e.g. *Fienen et al.*, 2004 and *Fienen et al.*, 2008]. Prior drift is accounted for in $\mathbf{X}$ through trends expressed in the nonzero terms, although this is not currently implemented in bgaPEST.

The prior covariance ($\mathbf{Q_{ss}}$) of $\mathbf{s}$ for a known β is

$$\mathbf{Q_{ss}}(\theta) = E[(\mathbf{s}-\mathbf{X}\beta)(\mathbf{s}-\mathbf{X}\beta)^T] \tag{20}$$

where $\mathbf{Q_{ss}}$ is a covariance function with structural parameters θ. In bgaPEST, allowable covariance functions include:

1. the nugget
$$\mathbf{R}(\mathbf{d}) = \sigma^2 \tag{21}$$

2. and the exponential covariance function
$$\mathbf{R}(\mathbf{d}) = \sigma^2 \exp(-\frac{|\mathbf{d}|}{\ell}) \tag{22}$$

where $|\mathbf{d}|$ is separation distance, σ^2 is variance, and ℓ is integral scale. If the integral scale is set such that $\ell > \max(|\mathbf{h}|)$ we can substitute $\sigma^2 = \theta\ell$ and restate Equation 22 as

$$\mathbf{Q_{ss}}(\mathbf{h}, \theta) = \theta\ell \exp(-\frac{|\mathbf{d}|}{\ell}) \tag{23}$$

We can also set $\ell = 10 \times \max(|\mathbf{d}|)$ so the behavior of the covariance function will be as a linear variogram (*Fienen et al.*, 2008) which enforces continuity at a scale determined by the single free structural parameter θ. The motivation for this covariance function choice is to impart minimal assumptions about parameter structure onto the solution. The appropriate value of θ is calculated through restricted maximum likelihood. For the remainder of this derivation, θ is assumed known. In bgaPEST, as discussed below in the input instructions, either the exponential or linear variogram models may be used.

Assembling the mean and covariance, the prior pdf is

$$p(\mathbf{s}|\beta) \propto \exp\left[-\frac{1}{2}(\mathbf{s} - \mathbf{X}\beta)^{\mathrm{T}}\mathbf{Q_{ss}^{-1}}(\mathbf{s} - \mathbf{X}\beta)\right] \tag{24}$$

In the case of no knowledge about the prior mean, the prior pdf of β can be modeled

as uniform over all space as $p(\beta) \propto \mathbf{1}$ and both $\mathbf{s}$ and β are estimated together, so that the conditional distribution in Equation 24 is replaced by a joint distribution

$$p(\mathbf{s}, \beta) \propto \exp\left[-\frac{1}{2}(\mathbf{s} - \mathbf{X}\beta)^{\mathrm{T}}\mathbf{Q}_{\mathbf{ss}}^{-\mathbf{1}}(\mathbf{s} - \mathbf{X}\beta)\right]. \tag{25}$$

Frequently, at least diffuse knowledge about the prior mean is available and can be modeled as multi-Gaussian with mean β^* and covariance $\mathbf{Q}_{\beta\beta}$. Typically, $\mathbf{Q}_{\beta\beta}$ is modeled as a diagonal matrix with variance values on the diagonal indicating independence among the β^*. Incorporating the prior information yields a prior pdf for $\mathbf{s}$

$$p(\mathbf{s}) \propto \exp\left[-\frac{1}{2}(\mathbf{s} - \mathbf{X}\beta^*)^{\mathrm{T}}\mathbf{G}_{\mathbf{ss}}^{-\mathbf{1}}(\mathbf{s} - \mathbf{X}\beta^*)\right] \tag{26}$$

where $\mathbf{X}\beta^*$ is the prior mean, and $\mathbf{G}_{\mathbf{ss}} = \mathbf{Q}_{\mathbf{ss}} + \mathbf{X}\mathbf{Q}_{\beta\beta}\mathbf{X}^{\mathbf{T}}$ is the prior covariance (*Nowak and Cirpka*, 2004).

The incorporation of prior mean information, even assuming very high variance values in $\mathbf{Q}_{\beta\beta}$, can provide numerical stability without overly biasing the results.

Prior Covariance Matrix Storage Issues

In underdetermined problems suitable for bgaPEST, the number of parameters can be very large. The prior covariance matrix discussed above can, therefore, grow to such large dimensions that it cannot be practically stored in computer memory. However, two techniques are provided to alleviate some of this storage stress: compression and Toeplitz transformation.

Compression takes advantage of the fact that values in the $\mathbf{G}_{\mathbf{ss}}$ matrix relating parameters in different beta associations, by definition, have the value of zero. As a result, a general $\mathbf{G}_{\mathbf{ss}}$ matrix can be viewed as a partitioned matrix of nonzero blocks ($\mathbf{G}_{\mathbf{ss},\beta i}$) and zero blocks

$$\mathbf{G}_{\mathbf{ss}} = \begin{bmatrix} \mathbf{G}_{\mathbf{ss},\beta 1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{G}_{\mathbf{ss},\beta 2} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{G}_{\mathbf{ss},\beta p} \end{bmatrix}. \tag{27}$$

There is no need to store the zero elements provided that accommodations are made to avoid multiplications that involve the zeros. These accommodations have been made

in bgaPEST and compression is, therefore, allowed.

In cases where spacial spacing is constant in respective directions, $\mathbf{G}_{\mathbf{ss},\beta i}$ is a Toeplitz matrix (*Gray*, 2005). A square, symmetric $j \times j$ matrix is Toeplitz in form if it has diagonals that all have the same value as in this example

$$\mathbf{T} = \begin{bmatrix} t_0 & t_1 & \dots & t_{j-2} & t_{j-1} \\ t_1 & t_0 & t_1 & \ddots & t_{j-2} \\ \vdots & t_1 & t_0 & \ddots & \vdots \\ t_{j-2} & \ddots & \ddots & \ddots & t_1 \\ t_{j-1} & t_{j-2} & \dots & t_1 & t_0 \end{bmatrix}. \tag{28}$$

This matrix has the properties that there are only j unique values, and these values occur in a regular order such that only a vector of length j needs to be stored from which individual rows can be constructed to perform matrix multiplication operations. The spacing, as indicated above, must be constant. For example, in a spatial model such as properties in a groundwater model, Δx, Δy, and Δz must be constant, but these values do not need to be equal to each other. While this is restrictive in the sense that it implies a regular grid that may not correspond to geometry in the field. However, the regular grid required to take advantage of Toeplitz storage and operations can be assigned to one beta association with a surrounding, irregular grid put in another beta association with fewer parameter values.

In order to use Toeplitz structure in three dimensions, there must be a three-level embedding of Toeplitz matrices (*D'Oria*, 2010). The first level corresponds to the model layers, the second level corresponds to model rows, and the third level corresponds to model columns. Inspection of the schematic example in Fig. 5 shows that every distinct value represented in the entire matrix is found in the first (leftmost) column. Cycling of rows or columns, relative to the single stored vector, can be used to reconstruct any row or column of the main matrix to be used in multiplication operations. In bgaPEST, a combination of Toeplitz and complete blocks can make up the $\mathbf{G}_{\mathbf{ss}}$ matrix in Compressed form, as discussed above.

Detailed input instructions for bgaPEST are presented in Appendix A. It is important to note, however, that if Toeplitz compression is invoked, parameters must be listed in the `.bgp` input file in order, sorted first by layer, then by column, and finally by row.

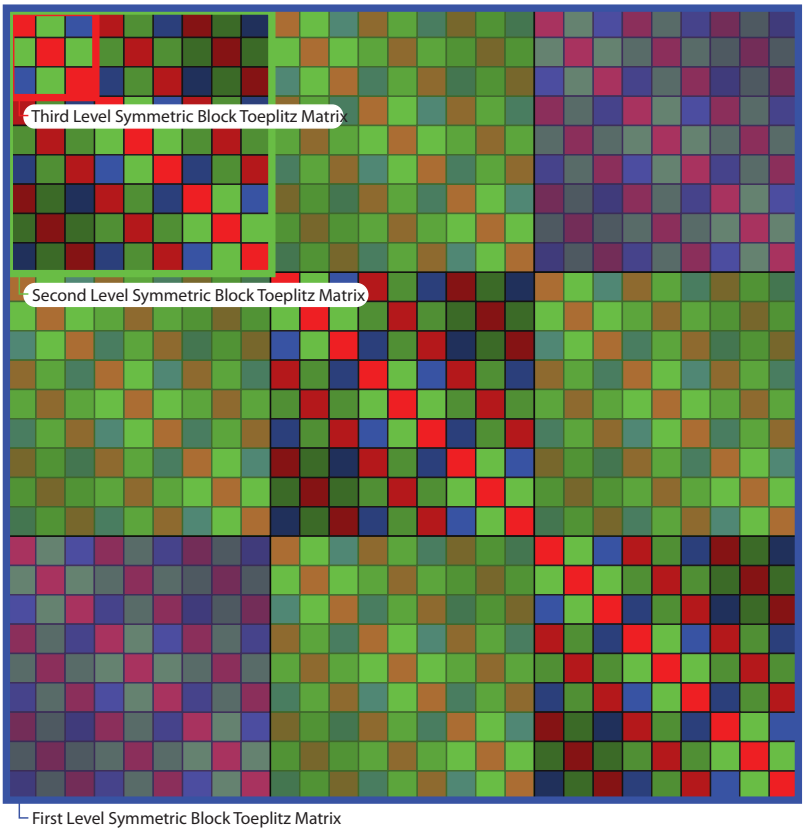


Figure 5: Schematic graphical visualization of a three-level embedded set of Toeplitz blocks in a covariance matrix (modified from *D'Oria* (2010)). The smallest squares represent individual matrix entries (values) and the colors correspond to distinct values. In this synthetic example, it is assumed that there are three rows, three columns, and three layers in the underlying model.

Likelihood Function

The parameters $\mathbf{s}$ are related to observations $\mathbf{y}$ through a measurement equation

$$\mathbf{y} = \mathbf{h}(\mathbf{s}) + \mathbf{v} \tag{29}$$

where $\mathbf{y}$ is an $(n \times 1)$ vector of observations, such as hydraulic heads or solute concentrations, $\mathbf{h}(\mathbf{s})$ is a transfer function or numerical model that calculates predictions which are collocated spatially and temporally with the observation values, and $\mathbf{v}$ is an $(n \times 1)$ vector of epistemic uncertainty terms, modeled as a random process with zero mean

and covariance matrix $\mathbf{R}$. Epistemic uncertainty is the result of imperfect or sparse measurements and an incomplete or inappropriate conceptual model (*Rubin*, 2003, p. 4). The epistemic uncertainty terms are assumed independent and uncorrelated so

$$\mathbf{R} = \sigma_{\mathbf{R}}^{\mathbf{2}}\mathbf{W} \tag{30}$$

where σ_R^2 is the epistemic uncertainty parameter and $\mathbf{W}$ is an $(n \times n)$ diagonal weight matrix in which each element is $\mathbf{W}_{ii} = \frac{1}{\omega_i^2}$ where ω_i is the i^{th} weight, specified by the user. The purpose of the values of ω is to allow for different confidence in different individual observations or groups of observations.

In reality, the component of epistemic uncertainty due to measurement error is likely uncorrelated, but the component due to modeling and conceptual uncertainty is likely systematic and correlated (*Gaganis and Smith*, 2001). A significant portion of this uncertainty may be reduced by not lumping parameters into homogeneous zones (*Gallagher and Doherty*, 2007), and the means to characterize the structure of $\mathbf{R}$ are rarely available. If information about $\mathbf{R}$ is available, however, it could be included and Equation 30 could be replaced by a more complicated matrix. This option is currently not available in bgaPEST, however. Proceeding with Equation 30 the likelihood function, assumed multi-Gaussian, is

$$L(\mathbf{y}|\mathbf{s}) \propto \exp\left[-\frac{1}{2}\left(\mathbf{y} - \mathbf{h}(\mathbf{s})\right)^{\mathrm{T}}\mathbf{R}^{-\mathbf{1}}\left(\mathbf{y} - \mathbf{h}(\mathbf{s})\right)\right]. \tag{31}$$

The structural parameter for the likelihood function is σ_R^2 and is calculated along with θ using restricted maximum likelihood.

Posterior Probability Density Function

Applying Bayes' theorem with the product of Equations 26 and 31 yields the posterior pdf

$$p(\mathbf{s}|\mathbf{y}) \propto \exp\left[-\frac{1}{2}(\mathbf{s} - \mathbf{X}\beta^*)^{\mathrm{T}}\mathbf{G}_{\mathbf{ss}}^{-\mathbf{1}}(\mathbf{s} - \mathbf{X}\beta^*) - \frac{1}{2}\left(\mathbf{y} - \mathbf{h}(\mathbf{s})\right)^{\mathrm{T}}\mathbf{R}^{-\mathbf{1}}\left(\mathbf{y} - \mathbf{h}(\mathbf{s})\right)\right] \tag{32}$$

The best estimate of $\mathbf{s}$ maximizes the posterior pdf. A computationally efficient method

to find the best estimates of $\mathbf{s}$ and β $\left(\hat{\mathbf{s}} \text{ and } \hat{\beta}, \text{ respectively}\right)$ is through

$$\hat{\mathbf{s}} = \mathbf{X}\hat{\beta} + \mathbf{Q_{ss}}\mathbf{H^T}\xi \tag{33}$$

which is the superposition of the prior mean (first term) and an innovation term which considers deviations of the model outputs from the observations (second term). $\mathbf{H}$ in the second term (often referred to as the Jacobian, sensitivity, or susceptibility matrix) is the sensitivity of observation values to parameter values where $H_{ij} = \frac{\partial \mathbf{h}(\mathbf{s})_i}{\partial \mathbf{s}_j}$ is calculated using either finite-difference or adjoint-state methods.

The values for $\hat{\beta}$ and ξ are found by solving the $(n+p) \times (n+p)$ linear system of cokriging equations

$$\begin{bmatrix} \mathbf{Q_{yy}} & \mathbf{HX} \\ \mathbf{X}^T\mathbf{H}^T & -\mathbf{Q_{\beta\beta}^{-1}} \end{bmatrix} \begin{bmatrix} \xi \\ \hat{\beta} \end{bmatrix} = \begin{bmatrix} \mathbf{y} \\ -\mathbf{Q_{\beta\beta}^{-1}}\beta^* \end{bmatrix} \tag{34}$$

where $\mathbf{Q_{yy}}$ is the auto-covariance matrix of the observations, defined as $\mathbf{HQ_{ss}H^T} + \mathbf{R}$.

Quasi-Linear Extension

As discussed by *Kitanidis* (1995), we must adjust calculations of the posterior pdf to account for nonlinearity. To do this, we expand the solution in a first-order Taylor expansion, resulting in an updated set of cokriging equations from Equation 34

$$\begin{bmatrix} \mathbf{Q_{yy}} & \mathbf{HX} \\ \mathbf{X}^T\mathbf{H}^T & -\mathbf{Q_{\beta\beta}^{-1}} \end{bmatrix} \begin{bmatrix} \xi \\ \hat{\beta} \end{bmatrix} = \begin{bmatrix} \mathbf{y} - \mathbf{h}\left(\tilde{\mathbf{s}}\right) + \mathbf{H}\tilde{\mathbf{s}} \\ -\mathbf{Q_{\beta\beta}^{-1}}\beta^* \end{bmatrix} \tag{35}$$

At each iteration (later referred to as inner iterations), the system in Equation 35 is solved, resulting in an updated estimate of $\hat{\mathbf{s}}$ calculated through Equation 33. At each iteration, the objective function, based on minimizing the negative logarithm of the posterior pdf (Equation 32) is evaluated using the current value of $\hat{\mathbf{s}}$: this is equivalent to finding the values of $\mathbf{s}$ that *maximize* the posterior probability. Switching to a minimization problem and taking the logarithm has computational advantages.

The objective function, then, is

$$\mathbf{\Phi}_T = \mathbf{\Phi}_M + \mathbf{\Phi}_R \tag{36}$$

where $\mathbf{\Phi}_T$ is the total objective function, $\mathbf{\Phi}_M$ is the misfit objective function (also corresponding to the likelihood function) and $\mathbf{\Phi}_R$ is the regularization objective function (also corresponding to the prior pdf). The components of Equation 36 are

$$\mathbf{\Phi}_M = \frac{1}{2}\left(\mathbf{y} - \mathbf{h}(\hat{\mathbf{s}})\right)^T \mathbf{R^{-1}} \left(\mathbf{y} - \mathbf{h}(\hat{\mathbf{s}})\right) \tag{37}$$

and

$$\mathbf{\Phi}_R = \frac{1}{2}(\hat{\mathbf{s}} - \mathbf{X}\beta^*)^T \mathbf{G_{ss}^{-1}} (\hat{\mathbf{s}} - \mathbf{X}\beta^*) \tag{38}$$

where both the negative signs and exponentiation are obviated by taking the negative logarithm of $p\left(\mathbf{s}|\mathbf{y}\right)$.

Implementation of Partitions into Beta Associations

The concept of beta associations is discussed above and details of their implementation are explained here. First, the prior covariance matrix $\mathbf{Q_{ss}}$ is censored by assigning a value of zero to each element which characterizes covariance between cells of different regions or parameter types, as defined by beta associations. It is not required that the covariance model be the same for each beta association. If different covariance models are used for different zones, this is reflected in the appropriate parts of $\mathbf{Q_{ss}}$. Furthermore, in some applications, a single structural parameter, θ, may be estimated and applied to all of $\mathbf{Q_{ss}}$. In other cases, and necessarily if the covariance model differs in various beta association, multiple elements of θ are estimated.

A distinct prior mean parameter β^* is assigned for each beta association, and the matrix $\mathbf{X}$ (Equation 19) is determined as explained in above. In cases where the mean of each zone is completely unknown, no values for β^* are provided, but the $\mathbf{X}$ matrix is constructed nonetheless and in both cases a value of $\hat{\beta}$ is calculated for each beta association.

Structural Parameters and Restricted Maximum Likelihood

A vital element to the method outlined above is proper selection of the structural parameters. Structural parameters–also called hyperparameters–or nuisance parameters, are the parameters that characterize the covariance structure of both the epistemic

uncertainty related to the observations, and the inherent variability of the parameters. In this work, structural parameters may include the epistemic uncertainty term in Equation 30 (σ_R^2) and the prior pdf variogram parameters in Equation 23 (θ) . These parameters are estimated using Restricted Maximum Likelihood consistent with the approaches of *Kitanidis and Vomvoris* (1983), *Kitanidis* (1995) and *Li et al.* (2007).

Applying Bayes' theorem to the structural parameters, given the measurements, we calculate

$$p\left(\theta|\mathbf{y_k^{'}}\right) \propto L\left(\mathbf{y}_k^{'}|\theta\right) p\left(\theta\right) \tag{39}$$

The likelihood function evaluates how closely the observations and predictions match, given the current linearization and the current set of structural parameters

$$L\left(\mathbf{y}_k^{'}|\theta\right) \propto \det\left(\mathbf{G_{yy}}\right)^{-\frac{1}{2}} \exp\left[-\frac{1}{2}\left(\mathbf{y}_k^{'} - \mathbf{H}\mathbf{X}\beta^*\right)^T \mathbf{G_{yy}^{-1}}\left(\mathbf{y}_k^{'} - \mathbf{H}\mathbf{X}\beta^*\right)\right] \tag{40}$$

where $\mathbf{G_{yy}}$ is the measurement autocovariance defined as

$$\mathbf{G_{yy}} = \mathbf{Q_{yy}} + \mathbf{H}\mathbf{X}\mathbf{Q}_{\beta\beta}\mathbf{X}^T\mathbf{H}^T. \tag{41}$$

Prior information about the structural parameters may also be included, with prior mean θ^* and covariance matrix $\mathbf{Q}_{\theta\theta}$.

$$p\left(\theta\right) \propto \det\left(\mathbf{Q}_{\theta\theta}\right)^{-\frac{1}{2}} \exp\left[-\frac{1}{2}\left(\theta - \theta^*\right)^T \mathbf{Q}_{\theta\theta}^{-1}\left(\theta - \theta^*\right)\right] \tag{42}$$

The posterior pdf is the product of Equations 42 and 40

$$p\left(\theta|\mathbf{y_k^{'}}\right) \propto \det\left(\mathbf{Q}_{\theta\theta}\right)^{-\frac{1}{2}} \det\left(\mathbf{G_{yy}}\right)^{-\frac{1}{2}} \exp\left[\begin{array}{c} -\frac{1}{2}\left(\theta - \theta^*\right)^T \mathbf{Q}_{\theta\theta}^{-1}\left(\theta - \theta^*\right) \\ -\frac{1}{2}\left(\mathbf{y}_k^{'} - \mathbf{H}\mathbf{X}\beta^*\right)^T \mathbf{G_{yy}^{-1}}\left(\mathbf{y}_k^{'} - \mathbf{H}\mathbf{X}\beta^*\right) \end{array}\right]. \tag{43}$$

To find the most likely values for θ we minimize $-\ln\left(p\left(\theta|\mathbf{y_k^{'}}\right)\right)$ resulting in the objective function

$$\mathbf{\Phi}_S = \frac{1}{2}\ln\left(\det\left(\mathbf{G_{yy}}\right)\right) + \frac{1}{2}\left[\left(\theta - \theta^*\right)^T \mathbf{Q}_{\theta\theta}^{-1}\left(\theta - \theta^*\right) + \left(\mathbf{y}_k^{'} - \mathbf{H}\mathbf{X}\beta^*\right)^T \mathbf{G_{yy}^{-1}}\left(\mathbf{y}_k^{'} - \mathbf{H}\mathbf{X}\beta^*\right)\right] \tag{44}$$

where unchanging quantities are absorbed into the constant of proportionality including $\det\left(\mathbf{Q}_{\theta\theta}\right)^{-\frac{1}{2}}$. The optimal values for θ are found using the Nelder-Mead simplex

algorithm (e.g. *Press et al.*, 1992, p. 408-410). Non-negativity in the θ parameters is enforced using a power transformation (*Box and Cox*, 1964). As indicated by *Kitanidis* (1995), nonlinearity requires that structural parameters are estimated iteratively with the estimation of hydraulic parameters. This is accomplished through a sequence of coupled inversion as follows.

1. Initialize hydraulic parameters as ($\mathbf{s_0}$) and structural parameters ($\theta_\mathbf{0}$).
2. Solve for a new estimate of hydraulic parameters ($\hat{\mathbf{s}}$) holding θ constant.
3. Solve for a new estimate of structural parameters $\left(\hat{\theta}\right)$ holding $\mathbf{s}$ constant.
4. Repeat steps 2 and 3 until the change in θ in two consecutive outer iterations of steps 2 and 3 decreases below a specified tolerance.

Posterior Covariance

The posterior covariance can be calculated based on the inverse of the Hessian of the objective function (for example, *Nowak and Cirpka*, 2004). In closed form, the equation for the full posterior covariance matrix is:

$$\mathbf{V} = \mathbf{G_{ss}} - \mathbf{G_{sy}}\mathbf{G_{yy}^{-1}}\mathbf{G_{sy}^{T}} \tag{45}$$

where $\mathbf{G_{sy}} = \mathbf{G_{ss}}\mathbf{H}^T$ and $\mathbf{G_{yy}} = \mathbf{H}\mathbf{G_{ss}}\mathbf{H}^T + \mathbf{R}$. In the case where compression of $\mathbf{Q}$ is not used, the full matrix $\mathbf{V}$ is calculated and reported. Where compression of $\mathbf{Q}$ is used, however, the diagonal of $\mathbf{V}$ is returned as a vector of variances on parameters. This information is reported in a separate file, but also used to calculated posterior 95% confidence intervals. The full matrix, when reported, can be used to calculate conditional realizations (*Kitanidis*, 1995, 1996).

D Single Layer Example Application

The first example application presented is a single-layer groundwater model. The forward model is a steady-state, MODFLOW-2005 model with 21 rows and 21 columns with constant row and column spacing of 1 m. The hydraulic conductivity field is heterogeneous, varying from 6.068×10^{-05} to 0.048 meters/day. The true hydraulic

conductivity field is depicted in Figure 6. Observations of head at the locations shown in Figure 9 were used for parameter estimation. To generate observations representing what would be field measurements in a non-synthetic case, the model was run forward using the true synthetic hydraulic conductivity values and the resulting head values were perturbed with normally distributed noise with mean of zero and standard deviation of 0.01 m.

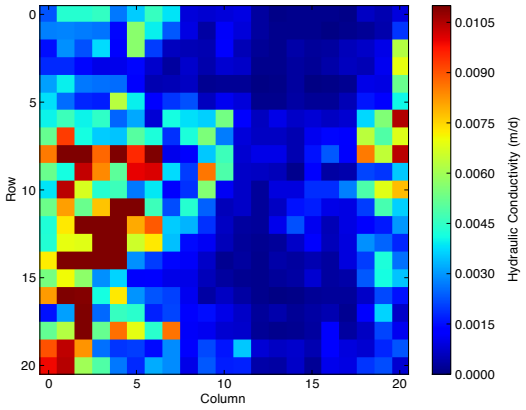


Figure 6: True hydraulic conductivity field for the single layer example application.

The boundary conditions are constant head, highest at the northwest corner and linearly decreasing to the southeast, as depicted in Figure 7. There is a well at row 13, column 6, extracting water at a constant rate of 0.231 liters/minute. No recharge is simulated in this case.

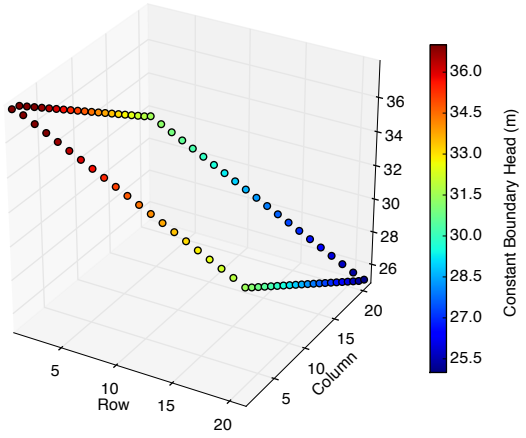


Figure 7: Boundary condition (constant head) for the single layer example application.

Two options exist to calculate sensitivity (Jacobian) matrices: an experimental adjoint-state version of MODFLOW, or finite difference calculations using the python linkage and PEST, as capable in the released version of bgaPEST. Two scenarios were tested as well: a case in which the epistemic error term (σ_R^2) is estimated, and one where σ_R^2 is fixed at a value approximately the same as the artificial noise used to corrupt the synthetic "true" values previously generated by the model–$1.0m$. This level of epistemic uncertainty is intended to be unrealistically high, but also encompasses both measurement and modeling error and was used to demonstrate a case where overfitting would be avoided at all costs.

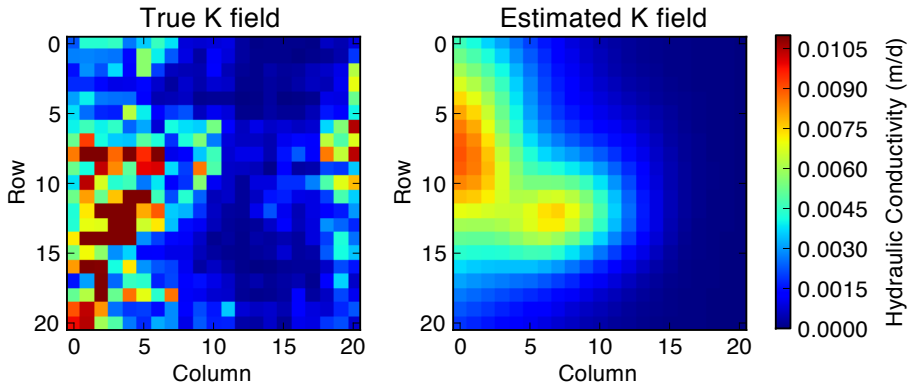


Figure 8: Parameters (hydraulic conductivity field) estimated for the 1 layer example application using bgaPEST with σ_R^2 fixed at $1.0m$.

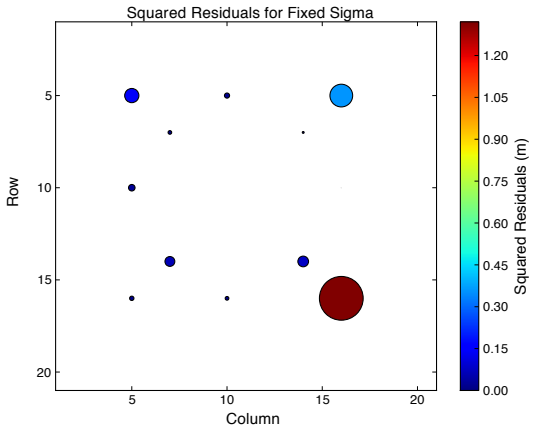


Figure 9: Squared residuals, plotted at their locations in the model, for the 1 layer example application using bgaPEST with σ_R^2 fixed at $1.0m$.

Figures 8 and 9 show the estimated parameter field and the corresponding squared residuals, respectively, for the case in which σ_R^2 is fixed at $1.0m$. In this case, the relatively high value ascribed to epistemic uncertainty certainly prevents overfitting. The solution, in fact, is quite smooth, and the linear variogram slope parameter θ was estimated to be 3.66×10^{-01}. Appropriately, the most structure expressed in the parameter field, and the correspondingly lowest residuals, are found in the vicinity of the pumping well where the greatest stress (and therefore the greatest amount of information) is found. This phenomenon is discussed in further detail by *Fienen et al.* (2008).

The smoothness of the parameter field is as expected by the bgaPEST algorithm and consistent with the maximum entropy property of the algorithm. In other words, the true hydraulic conductivity field is quite rough but the algorithm estimates parameters that smooth over these rough areas. The "smearing" of higher values across a larger area than in reality is also consistent with maximum entropy and also information content– an anomalous region of high hydraulic conductivity emanates from the area of the well due to the focus of stress (and therefore information) near the pumping well.

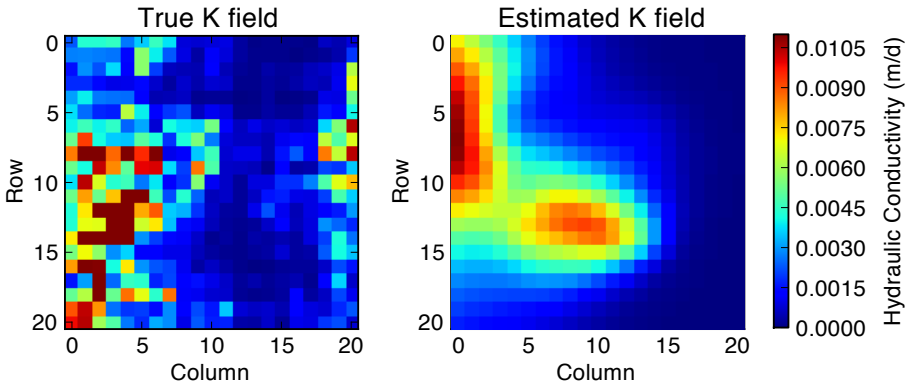


Figure 10: Parameters (hydraulic conductivity field) estimated for the 1 layer example application using bgaPEST with σ_R^2 estimated by the bgaPEST algorithm.

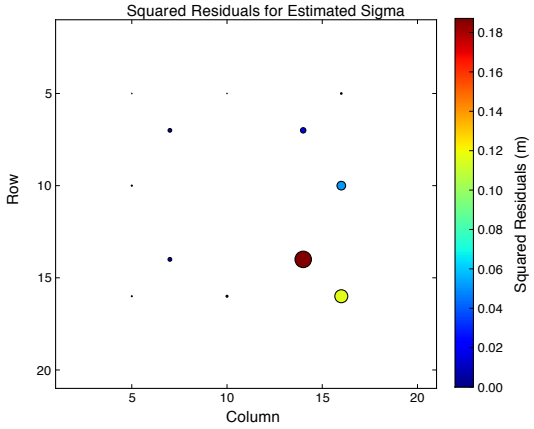


Figure 11: Squared residuals, plotted at their locations in the model, for the 1 layer example application using bgaPEST with σ_R^2 estimated.

Figures 10 and 11 show the estimated parameter field and the corresponding squared residuals, respectively, for the case in which σ_R^2 is estimated by the bgaPEST algorithm. The estimated value for epistemic uncertainty was 1.007×10^{-01} and the variogram slope (θ) was 2.836×10^{-01}. These results are similar to the case in which σ_R^2 was held constant. The parameter field shows a similar shape and smoothness level, although Figure 10 shows a bit more structure (roughness). Correspondingly, the residuals are generally lower. A key point here, however, is that the pattern of the residuals is similar and, again, reflects the general information content of the stress induced on the system.

E Three Layer Example Application

A three layer groundwater model is presented to explore the use of multiple beta associations, anisotropy, and a larger number of parameters. In this case, the model is 40 rows by 35 columns across three layers. The row spacing is 2.0 m while the column spacing is 1.5 m. The layers, from shallowest to deepest, are 1.8 m, 1.4 m, and 1.8 m in thickness, respectively. The disparate row, column, and layer spacing was used to test the Toeplitz compression option. The model has constant head boundaries on all sides (set at the same elevation–60 meters) and a single well at row 18, column 17, extracting at 0.01 liters/minute from each layer. This low flow rate is not meant to represent typical field conditions, but rather highlights what can be learned with even a very small stress on the system.

Similarly

The true parameter field, shown in Figure 12, varies from 0.01 to 0.075 meters/day.

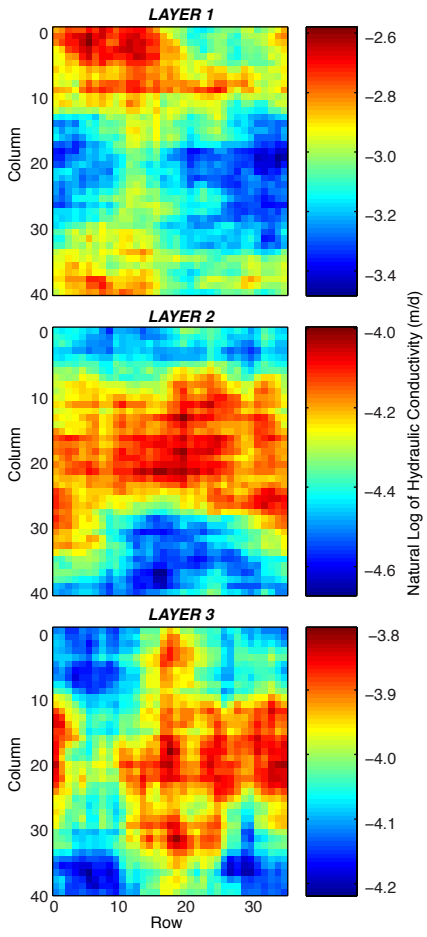


Figure 12: True synthetic hydraulic conductivity field for each layer in the three layer example application. Values are shown in natural logarithm space to make the differences more visible.

Five cases are illustrated here, as summarized in Table 1. In all cases, each layer is treated as a separate beta association. In each of these layers, the initial value for the prior structural parameter (the linear variogram slope, θ) is 1.0×10^{-5}. Cases 1 and 2 illustrate how the level of fit (and, therefore, the degree of roughness of the solution) can be influenced by adjusting the epistemic uncertainty term (σ_R^2), so in these cases, σ_R^2 is set at a fixed value. In Case 3, σ_R^2 is set low (1.0×10^{-5}) and the restricted maximum likelihood algorithm is given the freedom to estimate it. This is to illustrate the best achievable fit that one might achieve given the specific observation set provided without regard for overfitting. In Cases 5 and 6, estimates are made with specification of anisotropy in the prior covariance. Inspection of the true parameter field in Figure 12

suggests a possible correlation along the horizontal axis, indicative of a channel feature. In Cases 5 and 6, therefore, an arbitrarily chosen ratio of 100 is applied with a rotation angle of zero. In Case 5, like in Case 3, σ_R^2 is estimated to achieve the best possible fit, while in Case 6, σ_R^2 is held constant at 1.0×10^{-1}.

	Scenario	Case 1	Case 2	Case 3	Case 5	Case 6
	Initial σ_R^2	1.00E-01	1.00E-02	1.00E-05	1.00E-04	1.00E-01
	Estimated σ_R^2	-	-	7.79E-08	1.18E-05	-
Prior Parameters						
Beta Association 1	*Initial* θ	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-05
	Estimated θ	2.46E-03	1.55E-02	1.25E-02	5.54E-03	3.61E-03
Beta Association 2	*Initial* θ	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-05
	Estimated θ	6.16E-03	2.47E-02	1.34E-02	3.19E-03	7.97E-03
Beta Association 3	*Initial* θ	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-05
	Estimated θ	2.46E-03	1.55E-02	1.21E-02	2.51E-03	7.73E-05
Anisotropy Parameters						
Beta Association 1	*horiz_angle*	-	-	-	0.0	0.0
	horiz_ratio	-	-	-	100.0	100.0
	verical_ratio	-	-	-	1.0	1.0
Beta Association 2	*horiz_angle*	-	-	-	0.0	0.0
	horiz_ratio	-	-	-	100.0	100.0
	verical_ratio	-	-	-	1.0	1.0
Beta Association 3	*horiz_angle*	-	-	-	0.0	0.0
	horiz_ratio	-	-	-	100.0	100.0
	verical_ratio	-	-	-	1.0	1.0

Table 1: Summary of the five cases investigated. The table shows which structural parameters were estimated and fixed, and also indicates anisotropy when used.

Figures 13 and 14 show the estimated hydraulic conductivity field and squared differences between measured and observed head values, respectively, for Case 1. In this case, meant to be conservative with respect to overfitting, the squared differences are smaller in magnitude than the specified value of σ_R^2 (1.0×10^{-1}) and very little roughness in the solution is required to achieve the level of fit desired.

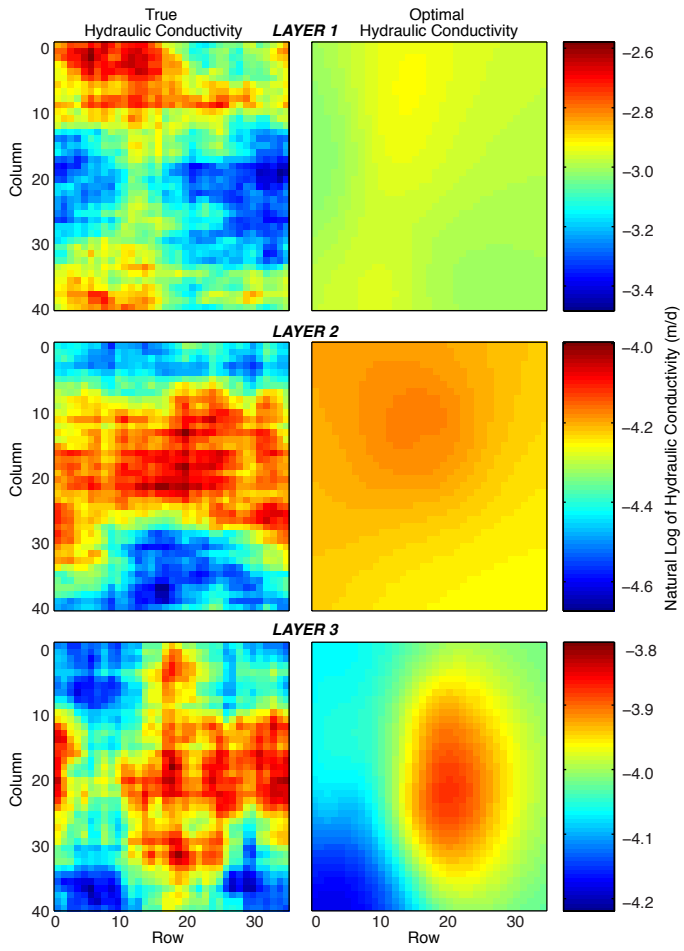


Figure 13: Case 1: Hydraulic conductivity fields estimated using bgaPEST compared to the true, synthetic hydraulic conductivity field.

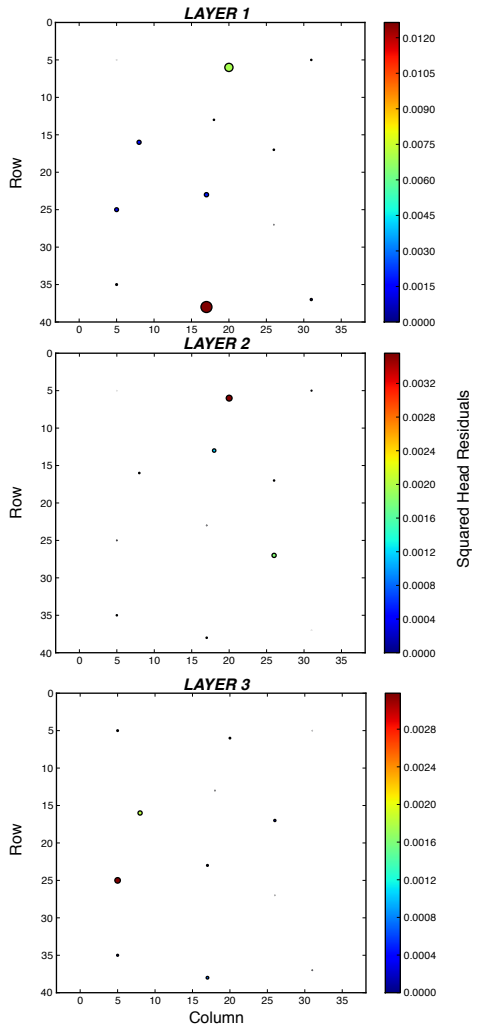


Figure 14: Case 1: Squared differences between modeled and "true" head values. Symbol size qualitatively indicates magnitude while color scale quantifies magnitude. Locations of the circles indicate observation location in the model domain in plan view.

Figures 15 and 16 show the estimated hydraulic conductivity field and squared differences between measured and observed head values, respectively, for Case 2. In this case, the specified value of σ_R^2 (1.0×10^{-2}) is lower and , accordingly, the squared head differences are lower, and more structure (roughness) is observed in the parameters, as expected. Note that, in this case, even with very low residuals, the parameter fields estimated are a smoothed representation of the "truth."

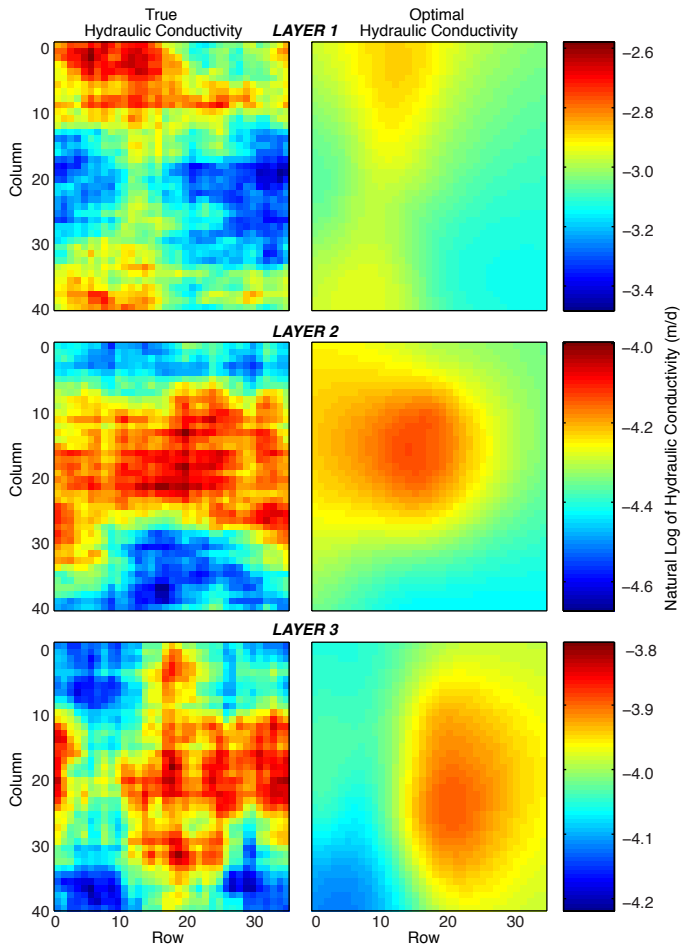


Figure 15: Case 2: Hydraulic conductivity fields estimated using bgaPEST compared to the true, synthetic hydraulic conductivity field.

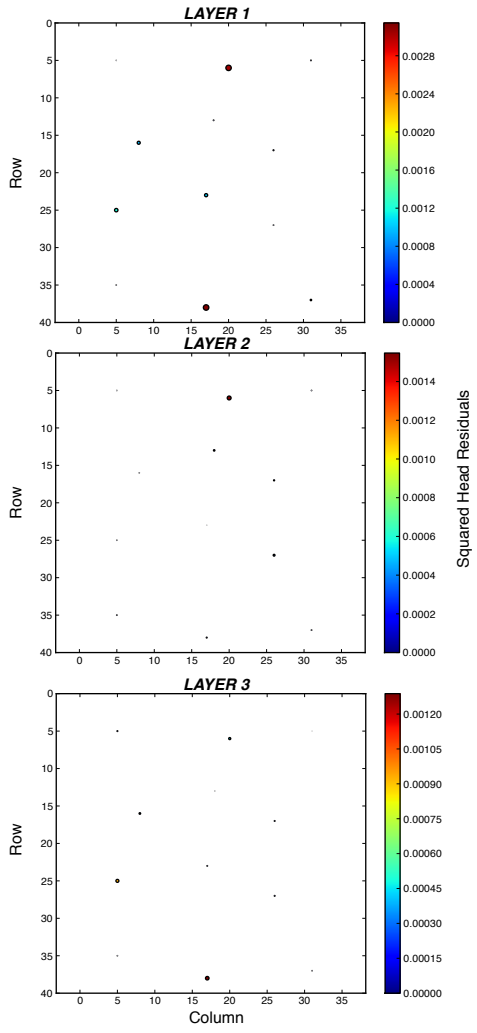


Figure 16: Case 2: Squared differences between modeled and "true" head values. Symbol size qualitatively indicates magnitude while color scale quantifies magnitude. Locations of the circles indicate observation location in the model domain in plan view.

Figures 17 and 18 show the estimated hydraulic conductivity field and squared differences between measured and observed head values, respectively, for Case 3. In this case, the value of σ_R^2 is estimated by the restricted maximum likelihood value algorithm. The head values match perfectly to machine precision, and the roughness of the field is the greatest of Cases 1 through 3, as expected. The major features of the "true" hydraulic conductivity field are reproduced by this solution although they are smoothed, somewhat, as expected. Importantly, while the highest hydraulic conductivity values in layer

2 are slightly offset to the west, no artifacts are introduced that would be considered spurious in this solution.

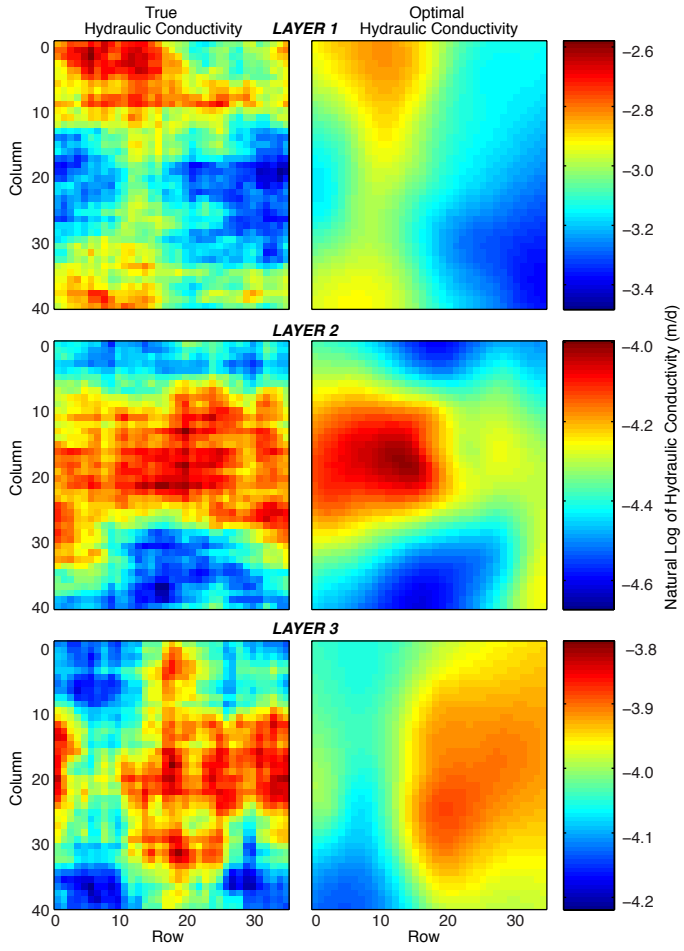


Figure 17: Case 3: Hydraulic conductivity fields estimated using bgaPEST compared to the true, synthetic hydraulic conductivity field.

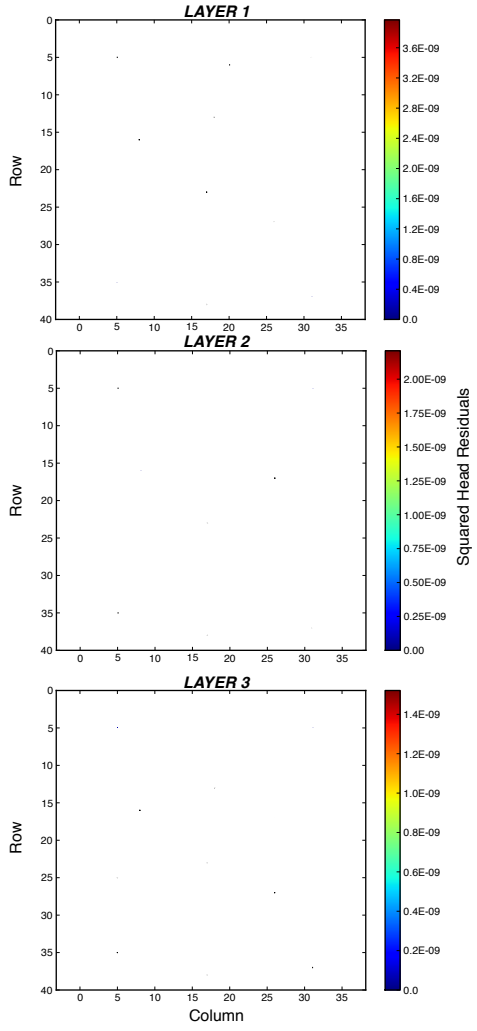


Figure 18: Case 3: Squared differences between modeled and "true" head values. Symbol size qualitatively indicates magnitude while color scale quantifies magnitude. Locations of the circles indicate observation location in the model domain in plan view.4

Figures 19 and 20 show the estimated hydraulic conductivity field and squared differences between measured and observed head values, respectively, for Case 5. In this case, the value of σ_R^2 is set at a very low value (1.0×10^{-4}) to attempt to achieve excellent fit while introducing anisotropy with the principal direction aligned with the horizontal axis. In layer 1, a somewhat spurious artifact is found in the form of a high hydraulic conductivity zone near the middle of the field. The head targets almost match within machine precision, however, and all other features are reasonable. This

highlights the fact that, within a single beta association, if anisotropy is used, *all* features estimated will roughly correspond to that framework so, in a Bayesian sense, the answer is *conditional* on the prior assumption that the anisotropy is an appropriate general characteristic shape of the parameter field. Such assumptions must be made cautiously.

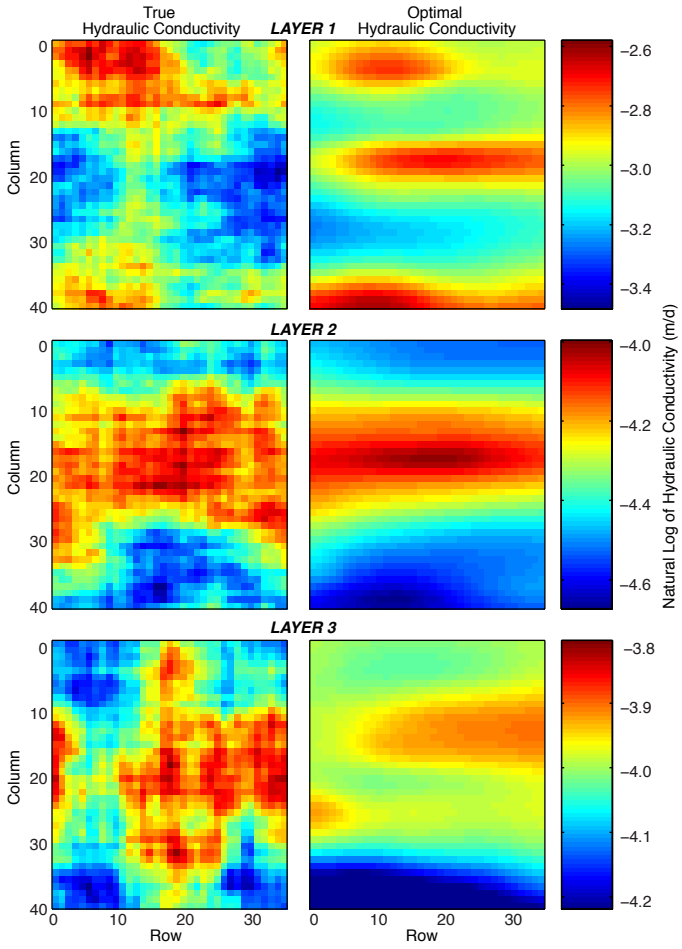


Figure 19: Case 5: Hydraulic conductivity fields estimated using bgaPEST compared to the true, synthetic hydraulic conductivity field.

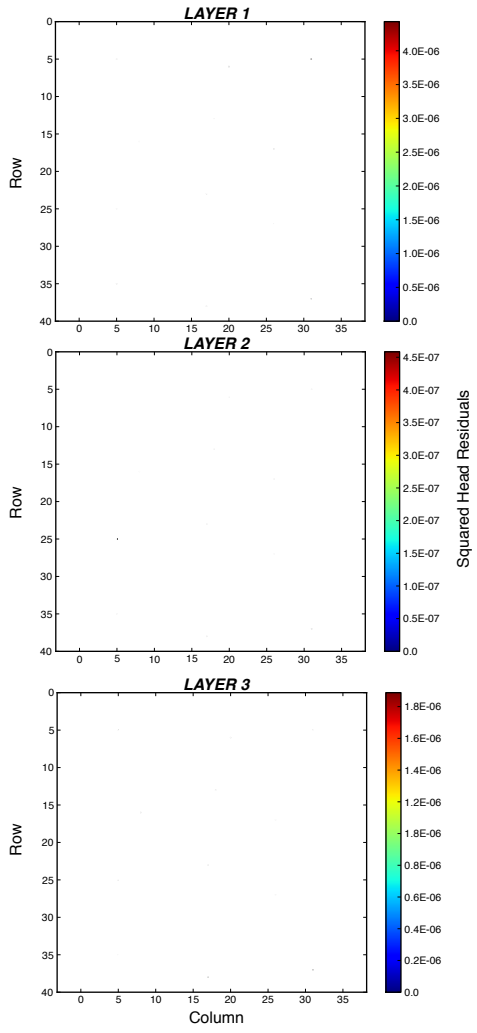


Figure 20: Case 5: Squared differences between modeled and "true" head values. Symbol size qualitatively indicates magnitude while color scale quantifies magnitude. Locations of the circles indicate observation location in the model domain in plan view.

Figures 21 and 22 show the estimated hydraulic conductivity field and squared differences between measured and observed head values, respectively, for Case 6. In this case, the value of σ_R^2 is set at a the same value as Case 1 (1.0×10^{-1}) to compare a solution with and without anisotropy assumed. Since anisotropy is a reasonable characteristic of the "true" field in this case, better fits are achieved (nearly an order of magnitude lower residuals) and the general pattern of the parameter field is better in Case 6 using anisotropy than in Case 1 without anisotropy. This highlights the power

that anisotropy can bring to a parameter estimation problem when it is appropriate even when σ_R^2 is set conservatively to avoid overfitting. As discussed above, however, this will, in a sense, force the solution to conform to such a shape, so it's use should be approached with caution.

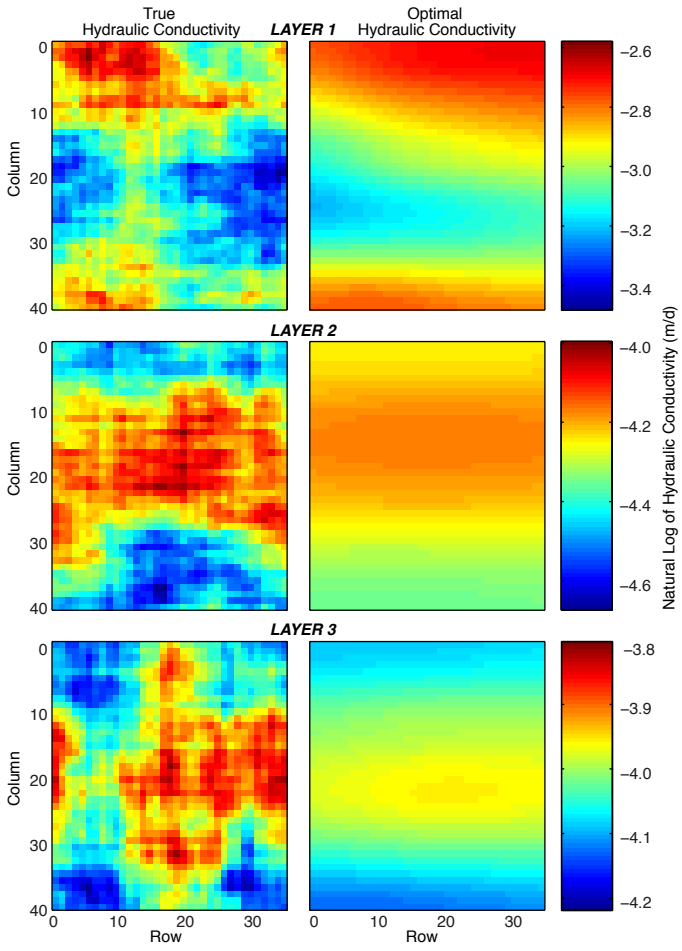


Figure 21: Case 6: Hydraulic conductivity fields estimated using bgaPEST compared to the true, synthetic hydraulic conductivity field.

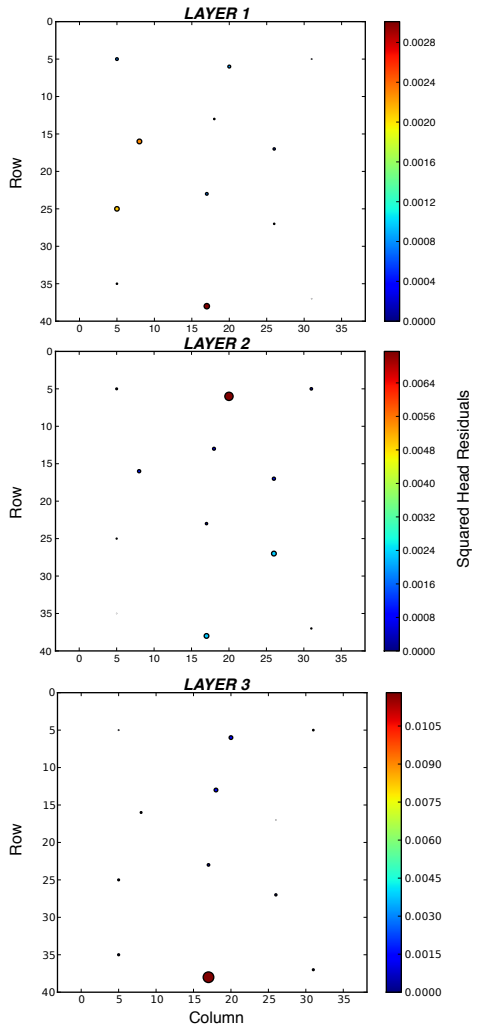


Figure 22: Case 6: Squared differences between modeled and "true" head values. Symbol size qualitatively indicates magnitude while color scale quantifies magnitude. Locations of the circles indicate observation location in the model domain in plan view.

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