Robust Solution of Normal (Kriging) Equations

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The underlying estimator for most geostatistical modeling algorithms is Kriging. There are many variants of Kriging. Each type leads to a system of linear equations built from positive definite covariance models, correlations, constraints and/or polynomial coefficients for an external drift. Resulting systems are solved using various techniques such as Gaussian elimination; however, solutions are not always acceptable. Research in Geostatistics is yielding more complex techniques such as Direct Sequential Simulation and Kriging in the presence of locally varying anisotropy; such techniques may generate systems of equations that are close to being non positive definite. Solutions to these systems can produce extreme solution weights or negative Kriging variances. This paper introduces a robust solver that detects problematic systems and makes adjustments so that extreme weights are mitigated and negative variances do not occur.

Introduction

Two trends in geostatistical research are resulting in problematic Kriging systems of equations: (1) striving to include as much information as possible into the modeling process, and (2) development of more complex modeling techniques. An example of (1) is Bayesian updating (Deutsch and Zanon, 2007). This technique can incorporate many secondary attributes and correlates them to any primary variables of interest. Indefinite correlation matrices have been encountered in this method due to missing data in sample sets and contradictory information. An example of (2) is accounting for locally varying anisotropy (Boisvert, Manchuk and Deutsch, 2007). This method relies on optimization to find the minimum anisotropic distance between geospatial data and often yields systems that are geometrically infeasible in the dimensionality of the given problem. In both examples, problematic systems result in extreme solution weights and/or negative Kriging variances.

Many types of Kriging exist for geological modeling: simple, ordinary, universal, collocated, generalized cokriging and others. Application of any one of these Kriging types to modeling of a geological resource can involve setting up and solving thousands to millions of systems of equations. Depending on the type and complexity of the modeling technique many unacceptable, i.e. indefinite or ill-conditioned systems, may be encountered. These systems can be referred to as unstable to the cause of Kriging. It is unreasonable to identify all of these problematic systems and analyse them to recover the cause of instability. Causes include contradictory correlations among multiple variables, overly redundant information and spatial screening effects. These are not straightforward problems to identify or correct, especially when systems can involve tens to hundreds of equations.

Solutions to indefinite and/or nearly singular systems of equations may cause one or both of the following: extreme solution (Kriging) weights and negative Kriging variance. Extreme Kriging weights can result in excessive estimates of the variable of interest, potentially far beyond the acceptable range of that variable. For example, extreme weights in a petroleum context may produce a negative porosity estimate or one that is higher that 100%. The same situation could occur in a mining context for gold grade. The later result, negative Kriging variance, is illogical in terms of assessing uncertainty. In the context of stochastic simulation, Kriging provides a parametric distribution from which a value is randomly drawn. The distribution cannot have negative variance.

This paper introduces a robust solver specifically for systems of equations built within a Kriging framework. For the remainder of the paper, this solver will be referred to as RSOL. Input systems are constructed in the manner that the type of Kriging demands and with the appropriate covariance model, correlation coefficients, constraints and/or polynomial coefficients. Upon receiving the system for processing, RSOL automatically detects the following problematic cases: (1) extreme Kriging weights, (2) negative Kriging variance, and (3) indefinite systems. Adjustments are made to the system by minimizing an objective function that will be discussed. Minimization was designed to lessen identified problems before calculating a final solution.

Existence of Unstable Systems

This section of the paper motivates the need for RSOL. It identifies three situations in geological modeling via Kriging that result in unacceptable solution weights and estimates. The simplest of scenarios shows spatial screening with only two conditioning data. An example of a correlation matrix from inconsistent data used in Bayesian updating will be shown next followed by an example of the geometrically infeasible systems that can result from locally varying anisotropy.

Consider two conditioning data used to estimate porosity at an unknown location in 2-dimensional space. Conditioning data follow a Gaussian distribution derived from applying a normal score transform to the original variable which is from a true data set. Assume that the underlying covariance structure has already been modeled and was found to be isotropic spherical with zero nugget effect and a range, r, of 50 units (Equation 1). The configuration and values of conditioning data relative to the estimate location are summarized in Table 1. The system of equations setup to solve this estimation problem is shown by Equation 2 along with the solution weights.

$$\gamma(h) = \sigma^2\left[1 - \tfrac{h}{r}\left(1.5 - 0.5\left(\tfrac{h}{r}\right)^2\right)\right] \quad (1)$$

Table 1: Two data Kriging scenario

	Porosity Value	Easting	Northing	Normal Score
Conditioning 1	3.02	34.8	9.4	-1.747
Conditioning 2	3.52	35.0	9.1	-1.585
Estimate	N/A	5.0	5.0	N/A

$$\begin{bmatrix} 1.000 & 0.989 \\ 0.989 & 1.000 \end{bmatrix}\begin{bmatrix} 0.240 \\ -0.035 \end{bmatrix} = \begin{bmatrix} 0.206 \\ 0.203 \end{bmatrix} \quad (2)$$

In this example screening has resulted in a redundant system of equations where the solution weights are problematic. One would expect both samples to receive approximately equal weighting since they are nearly equidistance from the estimate location. This issue of screening can be projected into much more complex scenarios where the outcome would cause problems with the estimate and the Kriging variance; however, this simple example is useful for explaining the robust solution.

Another problematic scenario occurs in Bayesian updating, an approach to geological modeling that is gaining in popularity due to its ability to incorporate an abundance of secondary information with a simple methodology. Deutsch and Zanon (2007) provide a discussion of the method for interested readers. One component of Bayesian Updating is a correlation matrix that relates all variables. It is used in calculating a likelihood distribution. Equation 3 shows the system of equation for calculating the likelihood. It is composed of secondary to secondary correlations, ρ_{ij}, and primary to secondary correlations, ρ_{ik}, $i,j=1,\ldots,n$ and $k=1,\ldots,m$ where n is the number of secondary and m the number of primary variables. Solution weights, λ_{ik}, are solved column-wise, each column being associated with a particular primary variable.

$$\begin{bmatrix} \rho_{11} & \cdots & \rho_{1n} \\ \vdots & \ddots & \vdots \\ \rho_{n1} & \cdots & \rho_{nn} \end{bmatrix}\begin{bmatrix} \lambda_{11} & \cdots & \lambda_{1m} \\ \vdots & \cdots & \vdots \\ \lambda_{n1} & \cdots & \lambda_{nm} \end{bmatrix} = \begin{bmatrix} \rho_{11} & \cdots & \rho_{1m} \\ \vdots & \ddots & \vdots \\ \rho_{n1} & \cdots & \rho_{nm} \end{bmatrix} \quad (3)$$

This example uses an actual correlation matrix from the application of Bayesian updating to a reservoir. Five secondary variables are used to generate the likelihood distribution for one of the primaries. The system of equations for this scenario (Equation 4) results in a likelihood variance of -0.388. This is an impractical result occurring from poor conditioning of the secondary to secondary correlation matrix. In this case, an ill-conditioned system is caused by two common problems with sample data: (1) missing samples and (2) an inadequate number of samples to maintain a contiguous set for correlation calculations. In other cases, indefinite systems may occur.

$$\begin{bmatrix} 1.000 & 0.502 & 0.226 & 0.120 & -0.329 \\ 0.502 & 1.000 & 0.496 & 0.569 & -0.273 \\ 0.226 & 0.496 & 1.000 & 0.832 & -0.707 \\ 0.120 & 0.569 & 0.832 & 1.000 & -0.358 \\ -0.329 & -0.273 & -0.707 & -0.358 & 1.000 \end{bmatrix} \begin{bmatrix} -1.365 \\ 0.869 \\ -0.289 \\ 0.065 \\ -0.098 \end{bmatrix} = \begin{bmatrix} -0.954 \\ 0.105 \\ -0.043 \\ 0.191 \\ 0.295 \end{bmatrix} \tag{4}$$

A final example will be taken from a recent development in geostatistical modeling, that being Kriging in the presence of locally varying anisotropy (LVA). LVA has been used in the past (Xu, 1996), but not in the fashion that it is used in its most recent implementation (Boisvert, 2007). In this example, the resulting system is indefinite and results in problematic weights, an extreme estimate and negative variance. The scenario involves 10 conditioning data positioned through-out a 2-dimensional LVA field (Figure 1). Table 2 summarizes the locations of conditioning data and estimate, sample values (synthetic), and the resulting solution weights for the initial system.

Table 2: LVA example data and results.

Data	X	Y	Value	Weight	Covariance
Conditioning	10	1	6	-0.445	0.869
	10	5	10	0.921	0.893
	18	1	-8	0.958	0.649
	18	5	-5	-0.300	0.623
	2	1	-5	-0.281	0.635
	10	10	-3	-1.325	0.194
	2	5	-10	1.281	0.599
	18	10	-4	-0.025	0.559
	2	10	-12	0.702	0.475
	10	15	12	-0.665	0.006
Estimate	11	1	-23.36		
Variance			-0.519		

The resulting estimate and variance are unacceptable, especially given the data configuration: the estimate is quite close to the top 5 data based on covariances in Table 2 indicating that it should be within the range of those data to some extent.

These three examples have shown that problematic systems are possible from the simplest of Kriging algorithms to those that are more complex. It is imperative that these systems be identified and dealt with in applications otherwise unacceptable solutions may be carried through a geostatistical study. For example, some transfer functions such as flow simulation can be very sensitive to extreme values that can inject a bias into results. After describing RSOL in the next sections of this paper, these problematic systems will be revisited and the robust solutions analysed.

RSOL

There are three components that contribute to the idea of robustly solving a system of equations built within a Kriging algorithm: (1) detection of unstable systems, (2) forcing indefinite systems to be positive definite, and (3) stabilizing the systems to mitigate undesirable outcomes. Undesirable outcomes include extreme Kriging weights and negative Kriging variances, which will have an impact in other areas of a geostatistical modeling application. These outcomes are used to detect an unstable system. The following components of RSOL will be discussed in more detail:

- Identifying unstable systems.
- Indefinite and ill-conditioned systems.
- Stabilization of the systems.

Identifying Unstable Systems

Detection methods for identifying unstable systems involve first solving the system. In the event that there is no solution, the system of equations is said to be singular. Singular systems can result in a spatial setting if two samples of a particular variable share the same location. They can also result in Bayesian updating if two variables are perfectly correlated. Occurrences of singular systems are a product of how the systems were built or from inadequate cleaning and analysis of input data to a Kriging application. These systems will not be dealt with by RSOL.

Solution weights and Kriging variance are checked once a system is solved. Negative Kriging variance is straightforward to detect and will not be discussed further. However, what is the definition of a problematic Kriging weight? It has been noted that negative weights or those greater that 1 may cause deranged estimates (Chiles and Delfiner, 1999).

The definition of a problematic (extreme) weight in this paper does agree that a weight greater than 1 is problematic when dealing with standardized covariance; however, this is not the only case. Consider a system of equations in a geospatial Kriging context: covariance values between conditioning data and a location to estimate are a measure of the information those conditioning data can provide. If solution weights are considered to be a ratio of that information that is used in making an estimate, then one should not exceed a ratio of 1:1 or 100%. Extreme weights, λ_i, i=1,…,n, are therefore defined as those which exceed the right hand side values, C_{0i}, i=1,…,n, to which they are associated in absolute value (Equation 5). C's may represent covariance values, correlations or polynomial coefficients. If a system is not identified at this point as being problematic its solution is deemed acceptable. No further operations are done by RSOL.

$$\begin{bmatrix} C_{11} & \cdots & C_{1n} \\ \vdots & \ddots & \vdots \\ C_{n1} & \cdots & C_{nn} \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \vdots \\ \lambda_n \end{bmatrix} = \begin{bmatrix} C_{01} \\ \vdots \\ C_{0n} \end{bmatrix} \rightarrow \begin{bmatrix} C_{11} & \cdots & C_{1n} & C_{01} \\ \vdots & \ddots & \vdots & \vdots \\ C_{n1} & \cdots & C_{nn} & C_{0n} \\ C_{01} & \cdots & C_{0n} & 1 \end{bmatrix} \tag{5}$$

$$\text{Extreme Weights: } |\lambda_i| > |C_{0i}|, i = 1,...,n$$

Systems deemed unstable are combined into a single matrix (Equation 5) prior to being made positive definite and/or stabilized. A matrix that contains all information accounts for instabilities present in the entire system of equations. It also simplifies the stabilization process where entries of both left and right hand side component of the system are changed.

Indefinite and Ill-conditioned Systems

Identified problematic systems will undergo a stabilization process to be described in the next section; however, one prerequisite is calculating the Eigen Decomposition of the system. If negative eigenvalues are detected, the system is indefinite and must first be made positive definite. A process used in several other areas of numerical computing is to increase the diagonals of the system until it is positive definite.

Diagonals are increased until all eigenvalues are positive. One eigenvalue will however be close to zero and the system will be nearly singular or ill-conditioned. This is due to the process of increasing diagonals: the magnitude of increments is slightly larger than the magnitude of the most negative eigenvalue, which has the effect of making that eigenvalue a very small positive. Even though the system has been made positive definite, it can still result in negative Kriging variance. Using the eigenvalues of the system, bounds on the variance can be defined. Consider a linear system of equations $Ax=b$ where A and b are populated with standardized covariance values. Once solved, the Kriging variance is defined by Equation 6. Substituting Ax for b the second term is recognized as the quadratic form (Equation 7). Positive definiteness of A ensures that the quadratic form is convex: the solution, x, is indeed minimizing variance and is guaranteed to be positive. However, this does not ensure that Equation 6 is positive. Using the minimum, $\lambda_{\min}$, and maximum, $\lambda_{\max}$, eigenvalues of A, bounds on the quadratic form can be calculated (Equation 8). The quadratic form must also meet the criteria in Equation 9 so that the variance is always positive and less than the global variance, σ^2.

$$\sigma_{SK}^2 = \sigma^2 - x'b \tag{6}$$

$$\sigma_{SK}^2 = \sigma^2 - x'Ax \tag{7}$$

$$\lambda_{min} x'x \le x'Ax \le \lambda_{max} x'x \tag{8}$$

$$0 \le x'Ax \le \sigma^2 \tag{9}$$

As the diagonals of A are increased, which is the technique used to enforce positive definiteness, the bounds in Equation 8 also become tighter. The magnitude of $x'x$ decreases. Should a positive definite system cause a negative Kriging variance, diagonal elements can be increased until a positive variance is achieved. Diagonal entries in A are equivalent to the variance, σ^2, of a variable. Changing diagonal entries does not imply a change in the variance of that variable. The calculation of Kriging variance (Equation 10), with A^* being the stabilized version of A, is not altered to accommodate changes made to these entries.

$$\sigma_{SK}^2 = \sigma^2 - x'A^*x \tag{10}$$

Stabilization

The scheme to stabilize a problematic system of equations was derived from the condition number of a matrix, which is a measure of precision loss for numerical analysis in using that matrix (Golub and Van Loan, 1989). Condition number is calculated as the ratio of the maximum to the minimum absolute eigenvalue of a matrix so large condition numbers are an indication of an unstable system. Stabilization accomplished in RSOL then amounts to lowering the condition number of the input system of linear equations. This can be done by altering entries in the system so that its eigenvalues are driven towards a single value: the average of all eigenvalues of the system.

Eigenvalues of a matrix can be related to its entries by a gradient, which is calculated using the similarity transform of the matrix to its Eigen Decomposition. Letting the matrix A represent the combined system of equations, the Eigen Decomposition can be written as Equation 11 where P is an orthogonal matrix of eigenvectors and D a diagonal matrix of eigenvalues. This equation can be rearranged and differentiated to give Equation 13, the gradient of each element of A with respect to each eigenvalue of D. The gradient is calculated strictly in magnitude as directional information is derived from the eigenvalues themselves in Equation 14 where *sgn* is the sign operator, *tr* is the trace operator and n is the dimension of A.

$$A = PDP' \tag{11}$$

$$D = P'AP \tag{12}$$

$$\frac{\partial D_{kk}}{\partial A_{ij}} = P_{ki} \left| A_{ij} \right| P_{jk} \tag{13}$$

$$\delta D = \operatorname{sgn}\left(\frac{tr(D)}{n} - D \right) \tag{14}$$

Equation 13 and 14 can be combined into Equation 15 and used to simultaneously update all elements of A so that the eigenvalues converge towards $tr(D)/n$. This will reduce the condition number and improve the stability of the system of equations that is contained within A. The equation for updating A is shown in Equation 16. An optimization method is required to calculate the step size, α, that makes the original system of equations stable, but does not alter it so much that all information is destroyed.

$$G_{ij} = \sum_{k=1}^{n} \delta D_{kk} \frac{\partial D_{kk}}{\partial A_{ij}} \tag{15}$$

$$A^* = A + \alpha G \tag{16}$$

A secondary objective function must be derived in order to calculate the step size. Unconstrained minimization of the condition number of *A* via Equation 16 would result in all eigenvalues being nearly equal; all dependencies in the system would be lost. The objective function to be developed is based on the Kriging weights and variance. Extreme Kriging weights are combined into a single measure of instability (Equation 17). Kriging variance will not be negative for the stabilization process as any indefinite systems would have been adjusted; however, it is used as a penalty. Because eigenvalues are driven towards a constant, the variance of the system increases. Equation 18 is used as a measure of information lost and penalizes optimization of α. One additional penalty is included in the objective function to provide the user with some control over how much a system is altered. Equation 19 describes a log barrier function used in some constrained optimization algorithms (Boyd and Vandenberghe, 2004). The measure of instability to be minimized is thus the sum of Equation 17, 18 and 19 (Equation 20).

$$W_\alpha = \sum_{k=1}^{n'} \delta\left(\lambda_k - C_k\right), \qquad \delta = \begin{cases} 0 \text{ if } \left|\lambda_k\right| \le \left|C_k\right| \\ 1 \text{ otherwise} \end{cases} \tag{17}$$

$$\Sigma_\alpha = \frac{\sigma_\alpha - \sigma_0}{1 - \sigma_0} \tag{18}$$

$$L_\alpha = -\frac{1}{t}\log\left(\frac{\alpha_{max} - \alpha}{\alpha_{max}}\right) \tag{19}$$

$$S_\alpha = W_\alpha + \Sigma_\alpha + L_\alpha \tag{20}$$

In Equations 17 to 20, *n'* is the dimension of the original system of equations, λ_k and C_k are solution weights and right hand side values, σ_0 and σ_α are the initial Kriging variance and that at α, α_{max} is the maximum permitted change that is to be made to elements of *A*, and W_α is the extreme weight measure for the solution at step α. Note that Equation 18 assumes a standardized variance. Also note that δ in Equation 17 is calculated once for the initial system. In this way, initial problematic weights detract from the measure of instability after they are corrected, acting like a momentum term in optimization.

Minimization of Equation 20 will result in mitigation of extreme weights at the expense of an increase in Kriging variance. Moreover, increasing the variance is implying that less information than was indicated by the initial system is actually known.

Unstable Systems Revisited

RSOL will be applied to the three problematic systems that were discussed above. Several aspects of the algorithm will be reviewed: shape of the objective function; change in solution weights and Kriging variance with α; solutions before and after stabilization; and runtimes. To look at the objective function a range of α values were evaluated along the gradient. Points along the function that were actually evaluated during optimization will be highlighted. Runtime will be evaluated by solving the same system a fixed number of times using a basic solver and using RSOL. Runtime will be longer for RSOL because of the added stabilization procedures.

The solution to the simple 2-data case (Equation 21) is more intuitive given the spatial orientation of the conditioning data and estimate. The maximum change made to any of the system entries was 0.033, which had the effect of changing solution weights by 0.103. In a spatial context, these changes are equivalent to dispersing the data that comprise the system, moving the two conditioning data further apart and further from the estimate. This has the effect of reducing redundancy in the system while incurring a slight 0.001 increase in Kriging variance for this example (Figure 2). Note that variance is plotted on the right y-axis for clarity. Minimization of the objective function only required 9 iterations; however, each iteration involves solving the system.

$$\begin{bmatrix} 1.000 & 0.956 \\ 0.956 & 1.000 \end{bmatrix} \begin{bmatrix} 0.137 \\ 0.070 \end{bmatrix} = \begin{bmatrix} 0.203 \\ 0.200 \end{bmatrix} \tag{21}$$

Example two provides a more problematic case as the Kriging variance is negative. RSOL detects this problem and increases the diagonal entries until the variance is positive. In this case, the initial system is not indefinite, but it may be ill-conditioned. Diagonals were increased from one to a value of 1.350. If the system is solved with this change, the resulting Kriging variance is 0.123. Once the variance was made positive practically no change was required to further improve the system (Equation 22). 4 out of 5 weights are not extreme by the definition given above, although the third weight is borderline. Using a standard solver, only 2 out of 5 weights were not extreme. Because nearly no change was observed for this example, aside from increasing diagonal entries, a graph will not be shown. Comparison can be made between Equation 4 and 22.

$$\begin{bmatrix} 1.3502 & 0.5016 & 0.2256 & 0.1198 & -0.3301 \\ 0.5016 & 1.3502 & 0.4954 & 0.5687 & -0.2741 \\ 0.2256 & 0.4954 & 1.3502 & 0.8323 & -0.7077 \\ 0.1198 & 0.5687 & 0.8323 & 1.3502 & -0.3589 \\ -0.3301 & -0.2741 & -0.7077 & -0.3589 & 1.3502 \end{bmatrix} \begin{bmatrix} -0.8244 \\ 0.3743 \\ -0.0511 \\ 0.1134 \\ 0.0956 \end{bmatrix} = \begin{bmatrix} -0.9548 \\ 0.1049 \\ -0.0428 \\ 0.1905 \\ 0.2940 \end{bmatrix} \quad (22)$$

Results for the LVA example are very similar to the Bayesian updating example: diagonal entries were increased until a positive variance was achieved and then stabilization was applied. Again, very little change after increasing the diagonals was made. Table 3 can be used to compare the results of solving the system in its initial state and after stabilization. Very little change can be seen in the right hand side covariances. Diagonal entries were increased from 1 to 1.494. A positive Kriging variance is realized along with an estimate that is more acceptable than that initially calculated. Only two of ten weights are extreme as compared to six of ten prior to stabilization. Those still extreme have been substantially reduced relative to the right hand side covariance.

Table 3: LVA example solved with RSOL.

				Initial			RSOL	
Data	X	Y	Value	Weight	Covariance		Weight	Covariance
Conditioning	10	1	6	-0.445	0.869		0.223	0.868
	10	5	10	0.921	0.893		0.233	0.891
	18	1	-8	0.958	0.649		0.221	0.649
	18	5	-5	-0.300	0.623		0.144	0.622
	2	1	-5	-0.281	0.635		0.133	0.635
	10	10	-3	-1.325	0.194		-0.311	0.194
	2	5	-10	1.281	0.599		0.185	0.599
	18	10	-4	-0.025	0.559		0.089	0.559
	2	10	-12	0.702	0.475		0.193	0.475
	10	15	12	-0.665	0.006		-0.305	0.006
Estimate	11	1	-23.36			-6.73		
Variance			-0.519			0.091		

A runtime study was carried out with these three systems to give an idea of how solving and stabilizing problematic systems compares to just solving those systems. Runs were done on a machine with an Intel Core 2 Duo T5500 processor rated at 1.67 GHz. When solving stable systems, RSOL compares to any basic solver in runtime; however, when dealing with unstable systems, it takes 50 to 60 times longer (Figure 3).

Conclusion

A method of automatically detecting and adjusting problematic systems of equations that are encountered in geostatistical modeling practices has been presented. RSOL detects extreme weights, negative estimation variance and indefinite systems and adjustments are made to mitigate the problems without user intervention. A measure of instability was created and used as an objective function to minimize indicators of unstable systems. Three examples showed that extreme weights are mitigated. Negative variance and indefinite systems are fixed by increasing diagonal entries, which did not show a negative impact on resulting estimates. One disadvantage is a substantially longer run-time when dealing with unstable systems; however, identification and finding root causes to problematic systems by hand will not be required.

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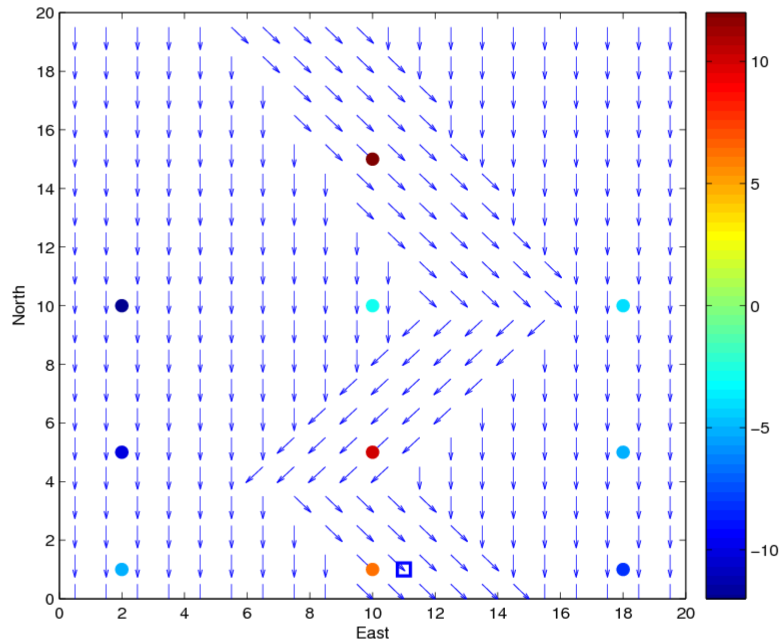

Figure 1: LVA field and data configuration. Bullets are conditioning data, the square is the estimate location, and arrows indicate major direction of anisotropy.

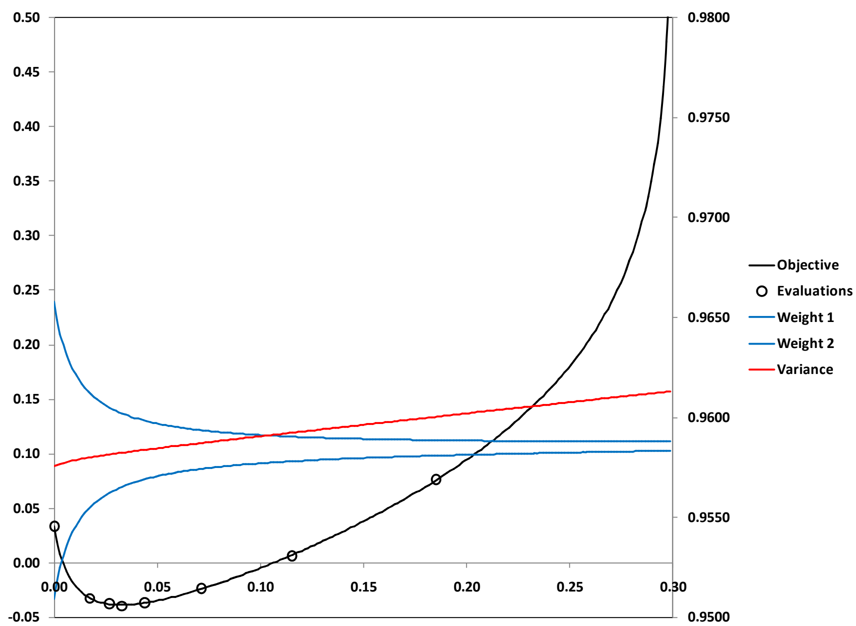

Figure 2: Stabilization of 2-data example.

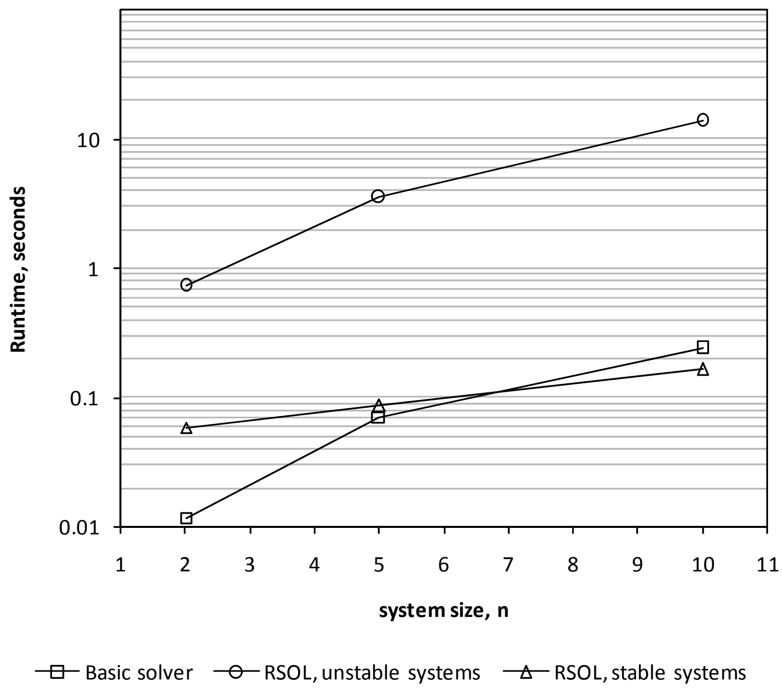

Figure 3: Runtime results based on solving systems 10,000 times.