Evaluating the effect of Tikhonov regularization schemes on predictions in a variable-density groundwater model

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ABSTRACT

Calibration of highly-parameterized numerical models typically requires explicit Tikhonov-type regularization to stabilize the inversion process. This regularization can take the form of a preferred parameter values scheme or preferred relations between parameters, such as the preferred equality scheme. The resulting parameter distributions calibrate the model to a user-defined acceptable level of model-to-measurement misfit, and also minimize regularization penalties on the total objective function.

To evaluate the potential impact of these two regularization schemes on model predictive ability, a dataset generated from a synthetic model was used to calibrate a highly-parameterized variable-density SEAWAT model. The key prediction is the length of time a synthetic pumping well will produce potable water. A bi-objective Pareto analysis was used to explicitly characterize the relation between two competing objective function components: measurement error and regularization error. Results of the Pareto analysis indicate that both types of regularization schemes affect the predictive ability of the calibrated model.

INTRODUCTION

The purpose of ground-water model calibration is to reduce model error to an acceptable level in the hope that this will translate to acceptable predictive error. In coastal settings, this prediction typically involves determining the position of the freshwater-saltwater interface relative to groundwater extraction and monitoring points. The calibration process typically involves adjusting model parameters until the difference between observed data and the corresponding model-simulated values are minimized to an acceptable level, while maintaining parameter plausibility.

In a highly-parameterized variable-density model, Tikhonov regularization is typically used to control parameter plausibility. Including regularization information into a single-objective calibration requires aggregation of the regularization information and the observation data into a single measure of calibration. This aggregation requires specification of group-specific weights to balance the contribution of each objective function component (Madsen 2000).

An alternative to aggregation is a multi-objective approach, where the goal is to find non-dominated or Pareto-optimal solutions (Gupta *et al* 1998). Each member of the Pareto-optimal set is defined as a solution that cannot be minimized further with respect to one objective without further sacrificing the minimization of other objectives (Srinivas and Deb 1994). By casting the highly-parameterized calibration process as an explicit multi-objective inversion, the resulting solution set explores the trade-off between observation residual minimization and regularization enforcement.

METHODS

A SEAWAT (Langevin *et al* 2008) model was constructed consisting of 25 100-meter rows, 50 100-meter columns, 15 layers and two 5-year stress periods. Sequential Gaussian simulation was used to generate a synthetic, lognormally-distributed hydraulic conductivity field, which was assigned to each of the 15 model layers, resulting in vertically homogeneous hydraulic conductivity. Monthly concentration and head data from stress period 1 (calibration period) were extracted from 20 randomly-selected observation points to serve as the calibration dataset. Two pumping wells were used to simulate the encroachment of seawater. Well #1 extended from model layers 5 through 15, and was made active only during the calibration period. Withdrawals from this well induced approximately 1.5 kilometers of landward migration of the freshwater-saltwater interface over the 5-year calibration period. Well #2, located 800 meters cross gradient, extended from model layers 5 through 12, and was made active only during stress period 2 (prediction period). The length of time this well produced potable water was treated as the key prediction of the model. The subsequent calibration attempted to reproduce the observed data, using 50 hydraulic conductivity pilot points, distributed throughout the model domain on a 500-meter spacing.

Two types of regularization were evaluated. Preferred-value regularization was applied with preferred values assigned the mean value of the synthetic hydraulic conductivity field. Preferred-equality regularization was distance-weighted using the same variogram used to generate the synthetic hydraulic conductivity field (Doherty 2003).

Two separate calibrations were completed resulting in four separate Pareto evaluations. One calibration used the same recharge value as used by the synthetic model. The other calibration was assigned a recharge value of 20 percent less than the synthetic recharge to induce explicit structural noise into the inverse problem.

RESULTS AND DISCUSSION

The results of the Pareto analyses are shown in Figures 1 and 2. Parameter standard deviation is shown as a measure of heterogeneity and parameter plausibility (the standard deviation of the synthetic hydraulic conductivity distribution is 98.2 meters/day). The minimum measurement objective function for the synthetic and reduced-recharge calibrations was 0.01 and 1.68, respectively.

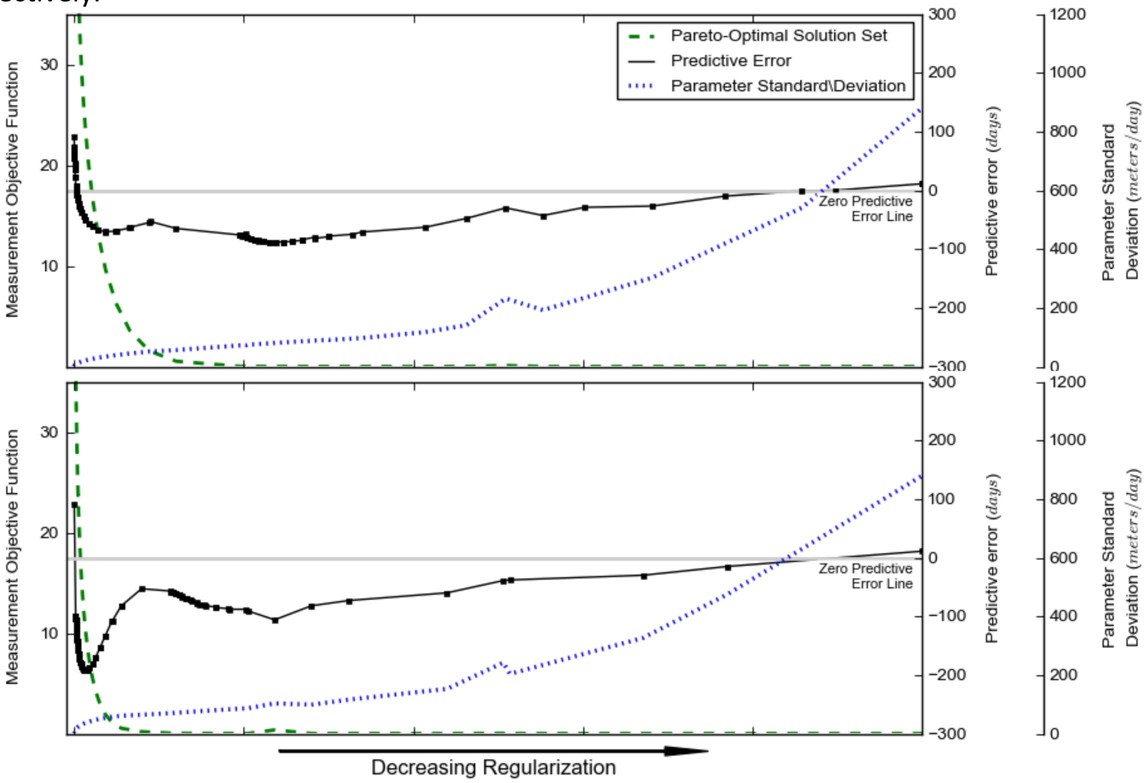

Figure 1. Comparison of the normalized preferred value (top) and the normalized preferred-equality (bottom) Pareto analyses with the synthetic recharge value.

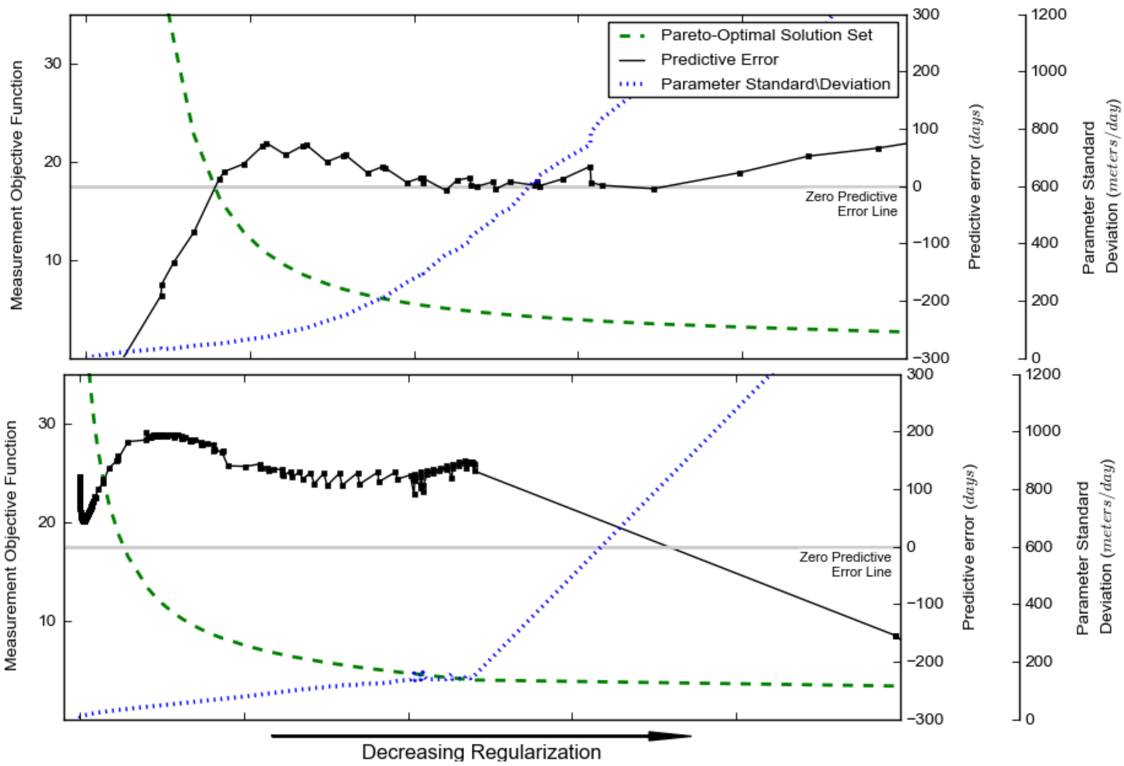

Figure 2. Comparison of the normalized preferred value (top) and normalized preferred-equality (bottom) Pareto analyses with the reduced recharge. Solutions with less than 20 times the synthetic variability shown.

In the absence of structural noise, less regularization appears to be positively correlated with better predictive ability. This finding suggests that Tikhonov regularization inhibits the ability of the calibration process to resolve the small-scale hydraulic conductivity variability, to which the prediction is sensitive. It appears the high level of the heterogeneity is compensating for the inability of the pilot points to fully resolve all of the small-scale variability of the synthetic field.

Unlike the synthetic recharge case, the addition of structural noise results in a non-linear relation between high levels of parameterization and improved predictive ability, suggesting these high levels of parameterization are attempting to resolve variability, which is masked by structural noise (over fitting). Regularization is needed to reign in the parameterization to a more realistic level of variability, while still including as much of the prediction-sensitive fine detail as possible.

When explicit structural noise is included in the Pareto analysis, the amount of heterogeneity must increase to compensate for the noise. Preferred-equality and preferred-value regularization exceed the variability of the synthetic case for measurement error values less than 6.4 and 8.5, respectively. At this level of parameterization, preferred-equality regularization over-predicts the useable life of Well #2 by 130 days, while the preferred-value over-predicts by 70 days (Figure 3). Even though preferred-equality regularization is better calibrated, it is a worse predictor of the useable life of Well #2.

The preferred-value regularization displays a broad region of less than 100 days of predictive error for a measurement objective function less than 10, while the preferred-equality regularization over-predicts the potable production period of Well #2 over the same range of solutions. Also, when normalized by maximum regularization penalty, the prediction sensitivity to the preferred-equality regularization is higher compared to the preferred-value regularization. Raising the measurement objective function from 3.0 to 4.0 resulted in a change of 300 days of predictive error, indicating highly non-linear behavior (Figure 3).

CONCLUSION

For the cases evaluated, Tikhonov regularization is shown to have a negative impact on the ability to accurately predict the time it would take for simulated production wells to be influenced by saltwater. Even for cases, where parameterization is the sole source of error (i.e., no explicit structural noise), even slight regularization decreases the predictive ability of the model and causes under prediction of the time until the production wells are impacted by saltwater. With explicit structural noise, high levels of parameterization adversely affect the predictive ability of the model by introducing artificial heterogeneity.

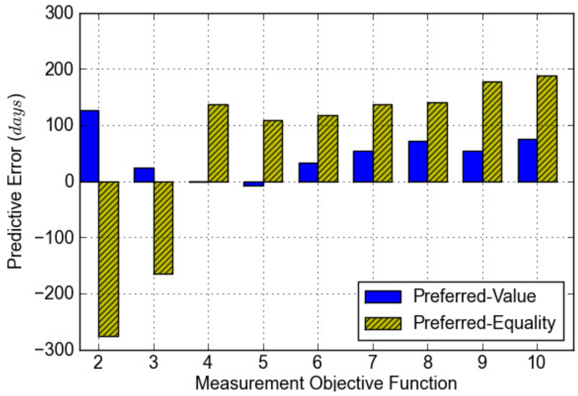

Figure 3. Comparison of predictive error and measurement objective function

For problems including structural noise, preferred-value regularization displayed a broad region of decreased predictive error for parameterizations with 2 to 10 times the variability of the synthetic distribution, while preferred-equality regularization over-predicts the useable life of the production wells over the same range. Also, finding solutions in this range of variability is difficult due to the extreme sensitivity of the preferred-equality regularization, when compared to the preferred-value regularization. Given these difficulties and the propensity for the preferred-equality regularization to over-predict the useable life of the extraction well in the range of potential solutions, the preferred-value regularization appears to provide better regularization for this synthetic case.

It is critical to understand how regularization in the presence of structural noise can affect the predictive ability of a model because highly-parameterized variable-density groundwater flow and transport models are actively being applied in saltwater intrusion studies. These results suggest that consideration of model variability, relative to known or expected ranges, can be used to guide the level of regularization used to calibrate a model to known stresses and give some confidence that it can be used to predict how chloride concentrations and heads might respond to future stresses.

REFERENCES

Doherty, J.2003.Ground Water Model Calibration Using Pilot Points and Regularization. *Ground Water* 2003:47:170-177

Gupta, H.V., S. Sorooshian and P.O. Yapo. 1998. Toward Improved Calibration of Hydrologic Models: Multiple and Noncommensurable Measures of Information. *Water Res Research* vol 34, no. 4:751-763

Langevin, C.D., D.T. Thorne Jr., A.M. Dausman, and M.C. Sukop. 2008. SEAWAT Version 4: A Computer Program for Simulation of Multi-Species Solute and Heat Transport. US Geological Survey Techniques and Methods Book 6, Chapter A22.

Madsen, H. 2001. Automatic Calibration of Conceptual Rainfall-Runoff Model Using Multiple Objectives. *Journal of Hydrology* no. 235:276-288

Srinivas, N. and K. Deb. 1994. Multiobjective Optimization Using Nondominated Sorting in Genetic Algorithms. *Journal of Evolutionary Computation* vol. 2 no. 3:221-248

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