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Quantification of model uncertainty in environmental modeling

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The last few decades have seen considerable progress in the quantification of environmental model uncertainty. Initially the emphasis has been on uncertainty in model parameters. A more recent trend has been to consider uncertainties in both model structure and parameters, most commonly by analyzing jointly predictions generated by several alternative models of the environment. This has been motivated by a growing recognition that the open and complex nature of environmental systems renders them suitable to multiple conceptualizations and mathematical descriptions. Predictions generated by a single model are prone to statistical bias (by reliance on an invalid model) and underestimation of uncertainty (by under-sampling the relevant model space) (Neuman 2003; Neuman and Wierenga 2003).

Some multimodel approaches blend or average statistical results generated by a set of alternative models. A common approach to model averaging is to (1) postulate several alternative models for a site, (a) associate each model with a weight or probability, and (c) generate weighted average predictions and statistics of all the models. Ways to accomplish this have varied; some are included in a public-domain code (Multimodel Analysis or MMA by Poeter and Hill 2007) recently reviewed by Ye (2010). This special issue of SERRA focuses on such and other emerging methods of model and parameter uncertainty quantification.

The special issue contains seven papers devoted to model averaging. Diks and Vrugt compare model averaging methods that weigh models in different ways, without always requiring that the weights sum up to unity. The methods are applied to two sites and compared in term of their predictive performance measured by out-of-sample root mean squared prediction error. Sain and Furrer estimate weights based on variation and correlation of alternative hierarchical models. They use a Bayesian hierarchical model to estimate correlation between models and the impact of parameter estimation uncertainty on the weights.

Ajami and Gu use the Bayesian Model Averaging (BMA) approach of Raftery et al. (2005) to assess uncertainty in a suite of biogeochemical models having various levels of complexity to simulate the fate and transport of nitrate at a field site in California. Their results demonstrate that whereas single models, regardless of their complexity levels, are incapable of representing all active processes at the site, the 95% uncertainty bounds of BMA bracket 90% to 100% of the observations.

Tsai use a variance-window (Tsai and Li 2008) version of Maximum Likelihood (ML) BMA (MLBMA; Neuman 2003; Ye et al. 2004) to quantify model uncertainty in managing groundwater within a thick sandy aquifer in Louisiana where saltwater intrusion is of concern. Alternative models are postulated to reflect uncertainty in conceptualizing hydraulic head boundaries and geostatistical parameterization through variogram models. The results

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show that using model-average predictions in the management problem requires relatively high injection and pumping rates to avoid violating constraints associated with multiple models. Morales-Casique et al. also use variance-window with MLBMA to quantify uncertainty associated with five variogram and gas flow models for unsaturated fractured tuff in Arizona. Cross-validation indicates that, whereas MLBMA is far superior to individual models in one validation test (as measured by predictive coverage and log score), it is second to last in another such test, the estimated weights depending on calibration data.

Singh et al. develop an Interactive Multi-Objective Genetic Algorithm (IMOGA) to assess model uncertainty at the Waste Isolation Pilot Plant (WIPP) site in New Mexico. IMOGA can use either MLBMA or the Generalized Likelihood Uncertainty Estimation method (GLUE; Beven and Binley 1992) to estimate model weights. Their approach incorporates subjective expert knowledge in the weight estimation process. The authors find GLUE to yield more uniform weights than MLBMA, which tends to favor one model which fits observed data best. Reeves et al. use GLUE to assess model uncertainty in simulating radionuclide flux at the Climax Mine area of the Nevada Test Site. Model uncertainty arises from 25 possible hydrostratigraphy-recharge combinations at the regional scale as described by Ye et al. (2010). The breakthrough of a conservative radionuclide is used to evaluate the influence of model and parameter uncertainty on radionuclide mass flux predictions.

In one of the three remaining papers, Winter compares the performance of alternate stochastic environmental system models based on a normalized Mahalanobis distance measure. This may be appropriate when data are too limited to allow computing likelihood ratios or Bayes factors for model averaging. Computational experiments are used to evaluate the measure's ability to identify a "true" model and to single out good models.

Bulygina and Gupta develop a Bayesian Estimation of Structure (BESt) approach to quantify model uncertainty without averaging. They consider situations in which an adequate conceptual model is available but the mathematical structure of this model is uncertain. BESt uses iterative data assimilation to update model structure using physically-based prior knowledge of the structure and observed system behavior. The authors use synthetic data to investigate the extent to which model structure can be identified with little, no or incorrect prior knowledge of its functional form.

Faybishenko combines probability and possibility theories to assess model uncertainty through a fuzzy-probabilistic approach. Fuzzy methods are useful when probabilities for some uncertain variables are not available. Model uncertainty in this hybrid approach is characterized by several possible combinations of probability densities and fuzzy numbers. A total of eight possible combinations are considered in simulating soil water balance and quantifying uncertainty at the Hanford Site in Washington.

In conclusion, we hope that this special issue of SERRA will help define the state of the art in model uncertainty assessment and help inspire additional advances in this important area of environmental modeling.

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References

Beven KJ, Binley A (1992) The future of distributed models: model calibration and uncertainty prediction. Hydrol Process 6:279–298

Neuman SP (2003) Maximum likelihood Bayesian averaging of alternative conceptual-mathematical models. Stoch Environ Res Risk Assess 17(5):291–305. doi:10.1007/s00477-003-0151-7

Neuman SP, Wierenga PJ (2003) A comprehensive strategy of hydrogeologic modeling and uncertainty analysis for nuclear facilities and sites, NUREG/CR-6805, USA. Nuclear Regulatory Commission, Washington, DC

Poeter EP, Hill MC (2007) MMA: a computer code for multi-model analysis. U.S. Geological Survey Techniques and Methods TM6-E3

Raftery AE, Gneiting T, Balabdaoui F, Polakowski M (2005) Using Bayesian model averaging to calibrate forecast ensembles. Mon Weather Rev 133:1155–1174

Tsai FT-C, X Li (2008) Inverse groundwater modeling for hydraulic conductivity estimation using Bayesian model averaging and variance window. Water Resour Res 44(9):W09434. doi:10.1029/2007WR006576

Ye M (2010) MMA: a computer code for multimodel analysis. Ground Water 48(1):9–12. doi:10.1111/j.1745-6584.2009.00647.x

Ye M, Neuman SP, Meyer PD (2004) Maximum likelihood Bayesian averaging of spatial variability models in unsaturated fractured tuff. Water Resour Res 40(5):W05113. doi:10.1029/2003WR002557

Ye M, Pohlmann KF, Chapman JB, Pohll GM, Reeves DM (2010) A model-averaging method for assessing groundwater conceptual model uncertainty. Ground Water doi:10.1111/j.1745-6584.2009.00633.x