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Bayesian Analysis Diagnostics: Diagnosing Predictive and Parameter Uncertainty for Hydrological Models

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All scientific and statistical analysis, particularly in natural sciences, is based on approximations and assumptions. For example, the calibration of hydrological models using approaches such as Nash-Sutcliffe efficiency and/or simple least squares (SLS) objective functions may appear to be "assumption-free". However, this is a naïve point of view, as SLS assumes that the model residuals (residuals=observed-predictions) are independent, homoscedastic and Gaussian. If these assumptions are poor, parameter inference and model predictions will be correspondingly poor. An essential step in model development is therefore to verify the assumptions and approximations made in the modeling process. Diagnostics play a key role in verifying modeling assumptions. An important advantage of the formal Bayesian approach is that the modeler is required to make the assumptions explicit. Specialized diagnostics can then be developed and applied to test and verify their assumptions. This paper presents a suite of statistical and modeling diagnostics that can be used by environmental modelers to test their modeling calibration assumptions and diagnose model deficiencies. Three major types of diagnostics are presented:

Residual Diagnostics

Residual diagnostics are used to test whether the assumptions of the residual error model within the likelihood function are compatible with the data. This includes testing for statistical independence, homoscedasticity, unbiasedness, Gaussianity and any distributional assumptions.

Parameter Uncertainty and MCMC Diagnostics

An important part of Bayesian analysis is assess parameter uncertainty. Markov Chain Monte Carlo (MCMC) methods are a powerful numerical tool for estimating these uncertainties. Diagnostics based on posterior parameter distributions can be used to assess parameter identifiability, interactions and correlations. This provides a very useful tool for detecting and remedying model deficiencies. In addition, numerical diagnostics are provided to test the convergence of the MCMC sampling chains.

Diagnostics for Probabilistic Predictions

Quantifying predictive uncertainty is becoming a standard part of the modeling process. However, simply providing probability limits on the predictions provides little information on the reliability of these estimates. A series of methods are presented to verify and quantify predictive reliability, resolution and accuracy. A series of hydrological modeling case studies are used to demonstrate the use of these diagnostics for testing statistical and modeling assumptions and diagnosing model deficiencies. Guidance is given on the interpretation of these diagnostics. The practical implications of poor modeling assumptions is highlighted. Recommendations are provided on the general methodologies for improving the modeling assumptions and reducing modeling deficiencies. The suite of diagnostics is available as an R package, enabling modelers to apply them to their own model development and application endeavours.