Maximum Likelihood Bayesian Model Averaging (MLBMA) - Shlomo P. Neuman

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Uncertainty Analysis in Environmental Modelling
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a) Introduction:

Bayesian Model Averaging (BMA) (Draper, 1995; Kass and Raftery, 1995; see Hoeting et al., 1999, for an excellent tutorial and Newman, 1997, and van Gelder et al., 1999, for applications) provides an optimal way of combining the predictions of several competing models and assessing their joint predictive uncertainty. To render BMA computationally feasible in a hydrologic context, Neuman (2002, 2003) proposed adopting a Maximum Likelihood (ML) version (MLBMA) of BMA in which model posterior probability is approximated in terms of an information criterion (KIC) due to Kashyap (1982). The latter is closely related to an ML version of the Laplace approximation (e.g., Draper, 1995; Kass and Raftery, 1995) used successfully in the BMA context by statisticians (Hoeting et al., 1999) but conforms more directly to ML-based hydrologic model discrimination and parameter estimation frameworks proposed for deterministic models by Carrera and Neuman (1986a-c), for geostatistical models by Samper and Neuman (1989a-c), and for stochastic moment models by Hernandez et al. (2002, 2003). MLBMA allows but does not require using prior information about the parameters to estimate them on the basis of hydrologic observations. It being Bayesian, MLBMA allows updating both model probabilities (and choices) and parameter estimates (and parameterization schemes) whenever new information (knowledge- and/or data-based) about the system becomes available.

b) Advantages

- Provides a theoretical and working framework for prediction under uncertainty related to model - Structure (conceptual-mathematical model), Parameters and Forcing terms - in a manner consistent with available – Knowledge and Data
- Allows, but does not require, specifying prior information about model parameters.
- By relying on ML model calibration against hydrologic observations, with or without the use of prior information, MLBMA avoids the need for time-consuming Monte Carlo simulations to render hydrologic predictions and, in the case of geostatistical or stochastic moment models, to assess predictive uncertainty.
- MLBMA applies to both deterministic and stochastic models.
- Models considered in MLBMA may have different types and numbers of parameters.
- By relying on KIC, MLBMA favors models which, among a given set of alternatives, are least likely to be incorrect. It honors the principle of parsimony by favoring the least complex among models which, otherwise, fit observational data equally well. Among models of equal complexity, MLBMA favors those exhibiting the best fit. It additionally contains an information term which allows one to consider models of growing complexity as the dataset improves in quantity and quality. Stated otherwise, MLBMA recognizes that when the dataset is limited and/or of poor quality, one should assign relatively low weights to elaborate models with numerous parameters. One should weigh more heavily simpler models with fewer parameters that nevertheless reflect adequately the underlying hydrologic structure and phenomena.
- MLBMA allows updating both model probabilities (and choices) and parameter estimates (and parameterization schemes) whenever new information (knowledge- and/or data-based) about the system becomes available.
- MLBMA obviates the need for subjective model acceptance thresholds or criteria used in some other methodologies.

c) Disadvantages

- Results are conditional on choice of models and data.
- Models considered in MLBMA must be based on a single dataset. As an example, to analyze jointly two- and three-dimensional models via MLBMA, a given set of three-dimensional data must be used and either projected onto a two-dimensional plane or averaged in the third dimension for inclusion in the two-dimensional model(s).
- The question how to assign prior probabilities to models is not fully resolved

d) Assumptions

If Δ is a quantity one wants to predict, then its posterior distribution given a discrete set of data **D** is $p(\Delta|\mathbf{D}) = \sum_{k=1}^{K} p(\Delta|M_k,\mathbf{D})\, p(M_k|\mathbf{D})$ where **M** = $(M_1,\ldots,M_K)$ is the set of all models (or hypotheses) considered.
In other words, $p(\Delta|\mathbf{D})$ is the average of the posterior distributions $p(\Delta|M_k,\mathbf{D})$ under each model, weighted by their posterior model probabilities $p(M_k|\mathbf{D})$. The posterior probability for model M_k is given by Bayes' rule, $p(M_k|\mathbf{D}) = \frac{p(\mathbf{D}|M_k)\,p(M_k)}{\sum_{l=1}^{K} p(\mathbf{D}|M_l)\,p(M_l)}$ where $p(\mathbf{D}|M_k) = \int p(\mathbf{D}|\theta_k,M_k)\,p(\theta_k|M_k)\,d\theta_k$ is the integrated likelihood of model M_k, θ_k is the vector of parameters associated with model M_k, $p(\theta_k|M_k)$ is the prior density of θ_k under model M_k, $p(\mathbf{D}|\theta_k,M_k)$ is the joint likelihood of model M_k and its parameters θ_k, and $p(M_k)$ is the prior probability that M_k is the correct model.
All probabilities are implicitly conditional on **M.**

Given a set of alternative models **M**, one formally assumes that their prior probabilities sum up to one $\sum_{k=1}^{K} p(M_k) = 1$
The number of potential models is exceedingly large. Based on the idea of Occam's window one considers only a relatively small set of the most parsimonious models among those which, *a priori*, appear to be hydrologically most plausible in light of all knowledge and data relevant to the purpose of the model and, *a posteriori*, explain the data in an acceptable manner.
Working with a few plausible models is better than the usual hydrologic practice of adopting a single model, whereas working with many models would render the approach impractical.

MLBMA consists of replacing θ_k by its maximum likelihood estimate $\hat{\theta}_k$ based on the likelihood $p(\mathbf{D}|\theta_k,M_k)$.
$p(M_k|\mathbf{D})$ is approximated in terms of an information criterion (*KIC*) due to *Kashyap* (1982).

e) Most appropriate application areas

Any set of competing hydrologic/environmental models that can be compared on the basis of a common data base.

f) Reading list

Neuman, S.P., Maximum likelihood Bayesian averaging of alternative conceptual-mathematical models, Stochastic Environmental Research and Risk Assessment, 17(5), 291-305, DOI: 10.1007/s00477-003-0151-7, 2003.

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

g) Software availability - none

h) Web links or other information - none

i) Figures

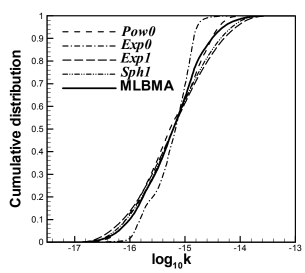

Figure 1. Cumulative distribution of kriged log10k estimates obtained using various models and MLBMA.

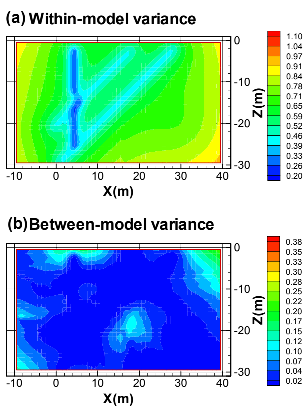

Figure 2. (a) Within- and (b) between-model variance of MLBMA log10*k* estimates at *y* = 6.5 m.

j) Delegates Comments (please add !!)