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ORIGINAL PAPER

Application of the generalized likelihood uncertainty estimation (GLUE) approach for assessing uncertainty in hydrological models: a review

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Abstract The generalized likelihood uncertainty estimation (GLUE) technique is an innovative uncertainty method that is often employed with environmental simulation models. Over the past years, hydrological literature has seen a large increase in the number of papers dealing with uncertainty. There are now a lot of citations to their original paper which illustrates GLUE tremendous impact. GLUE's popularity can be attributed to its simplicity and its applicability to nonlinear systems, including those for which a unique calibration is not apparent. The GLUE was introduced for use in uncertainty analysis of watershed models has now been extended well beyond rainfall-runoff watershed models. Given the widespread adoption of GLUE analyses for a broad range or problems, it is appropriate that the validity of the approach be examined with care. In this article, we present an overview of the application of GLUE for assessing uncertainty distribution in hydrological models particularly surface and subsurface hydrology and briefly describe algorithms for sampling of the prior parameter in hydrologic simulation models.

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1 Introduction

Hydrology is a science that is highly uncertain. The main reason for this uncertainty is that the inherent dynamics of many surface and subsurface hydrological processes are not known. Many of hydrological control volumes such as subsurface preferential flow paths and river beds cannot be represented mathematically and consequently cannot be observed in details. The boundary and initial conditions of hydrological processes are still unknown to hydrologists. Finally, hydrologists are usually working under data insufficiency situation, which limits the efficiency of an inductive approach for tackling the above problems, so, according to the numerous contributions in recent scientific literature, uncertainty estimation in hydrological surface and subsurface modeling is receiving increasing attention from researchers and practitioners.

In hydrological modeling, the three fundamental sources contributing to modeling uncertainty are uncertainty in model parameters, uncertainties associated with input data and data for calibration, and imperfection in the model structure. (e.g., Refsgaard and Storm 1995). Engeland et al. (2005) showed that the effect of the model structural uncertainty on the total simulation uncertainty of a conceptual water balance model was larger than parameter uncertainty. Marshall et al. (2007) stated that the uncertainty in model structure requires developing alternatives where outputs from multiple models are pooled together in order to generate an ensemble of hydrographs that are able to represent uncertainty. Kavetski et al. (2002), and Chowdhury and

Sharma (2007) investigated input data uncertainty by artificially adding noise to input data and then formulating an empirical relationship between this noise and parameter error. Many other examples of the methods dealing with model and data uncertainty are available in the hydrological literature (e.g., Georgakakos et al. 2004; Cheng et al. 2007; Carpenter and Georgakakos 2004; Kavetski et al. 2006a, b).

To account for uncertainties, in the last two decades, many uncertainty-analysis techniques have been developed and applied to various catchments. The motivation for developing new or modified approaches may stem from the fact that the typical use of frequentist and Bayesian approaches which only consider parameter uncertainty and (independent) measurement error while neglecting input and model structure uncertainty leads to unrealistic prediction uncertainty bounds. The development follows three main categories: (i) Development of new approaches without rigorous statistical assumptions or ad-hoc modifications to existing statistical approaches. These approaches try to represent all uncertainties by an enhanced parameter uncertainty. Examples of such approaches are Generalized Likelihood Uncertainty Estimation (GLUE) (Beven and Binley 1992) and Sequential Uncertainty Fitting (SUFI-2) (Abbaspour et al. 2004, 2007). (ii) Approaches that account for the effect of input and model structural errors on the output by an additive error model which introduces temporal correlation of the residuals. e.g., Yang et al. (2007), and Schaefli et al. (2007). (iii) Development of improved likelihood functions that explicitly represent input errors and/or model structural error of the underlying hydrological model. These approaches include consideration of input uncertainty through integrated Bayesian uncertainty estimation (Ajami et al. 2007).

Despite the large number of suggested techniques, only rarely more than one technique was applied for comparing techniques in the same case study in the literature. Yang et al. (2008) compared five uncertainty analysis procedures: Generalized Likelihood Uncertainty Estimation (GLUE), Parameter Solution (ParaSol), Sequential Uncertainty FItting algorithm (SUFI-2), and a Bayesian framework implemented using Markov chain Monte Carlo (MCMC) and importance Sampling (IS) techniques. The results of this study showed that Application of GLUE based on the Nash–Sutcliffe coefficient. This application led to the widest marginal parameter uncertainty intervals of the model parameters and to a good prediction uncertainty in the sense of coverage of measurements by the uncertainty bands. On the other hand, the inefficiency of the global sampling procedure leads to problems in locating the maximum or maxima of the objective function. GLUE and SUFI-2 are very flexible by allowing for arbitrary likelihood measures/objective functions. On the other hand, GLUE and SUFI-2 lose their statistical basis when using this additional freedom. The real capability of exploring the parameter space is also seriously affected by the choice of the objective function. In ParaSol, though the objective function and the way to split the parameter set are statistically based, the underlying statistical assumptions are seriously violated.

The GLUE method is inspired by the Hornberger and Spear (1981) method of sensitivity analysis and operates within the context of Monte Carlo analysis coupled with Bayesian estimation and propagation of uncertainty. Since its introduction in 1992, GLUE has found widespread application in uncertainty assessment in many fields of study, including modeling of the rainfall-runoff transformation (Beven and Binley 1992; Freer et al. 1996; Lamb et al. 1998; Chen and Chau 2006), soil erosion (Brazier et al. 2001), tracer dispersion in a river reach (Hankin et al. 2001), groundwater and well capture zone delineation (Feyen et al. 2001; Jensen 2003), unsaturated zone (Mertens et al. 2004a, b), flood inundation (Romanowicz et al. 1996; Aronica et al. 2002a, b; Chau et al. 2005; Goodarzi et al. 2012), land–surface– atmosphere interactions (Franks et al. 1997), soil freezing and thawing (Hansson and Lundin 2006), crop yields and soil organic carbon (Wang et al. 2005), and ground radar-rainfall estimation (Tadesse and Anagnostou 2005). Recent applications of GLUE are also found in distributed hydrologic modeling (McMichael et al. 2006; Muleta and Nicklow 2005; Mirzaei et al. 2013a). The popularity of GLUE is probably best explained by its conceptual simplicity and relative ease of implementation, requiring no modifications to existing source codes of simulation models.

Recent contributions to the hydrologic literature have criticized GLUE for not being formally Bayesian, resulting in parameter and predictive distributions that are statistically incoherent, unreliable, and concluded that it therefore should not be used (Christensen 2004; Montanari 2005; Mantovan and Todini 2006; Vogel et al. 2008; Mirzaei et al. 2013b). The GLUE method is most often used with a statistically informal likelihood function, does not attempt to find the maximum likelihood estimate of the parameters to benchmark the performance of the best model, and does not explicitly consider model errors in the derivation and communication of predictive distributions. In recent years, a strong debate has emerged in the hydrologic community between those that adhere strongly to the underlying philosophy of GLUE and believe that the method is a useful working methodology for assessing uncertainty in non-ideal cases (see Beven 2006), and researchers and practitioners that strongly oppose incorrect usage of statistics and prefer to use coherent probabilistic approaches.

The aim of this study is to review the existing literature regarding the application of the GLUE Approach for assessing uncertainty in hydrological models.

We introduce the GLUE methodology, Parameter Sampling Strategies and GLUE likelihood measures. Next, GLUE application in water quality, Rainfall-Runoff modeling and groundwater is discussed. Lastly, recommendations and suggestions for future research and conclusions are elaborated.

2 The generalized likelihood uncertainty estimation methodology (GLUE)

In this section we briefly discuss the GLUE methodology, and describe algorithms for sampling of the prior parameter distribution.

2.1 The GLUE methodology

The GLUE methodology rejects the idea of one single optimal solution and adopts the concept of equifinality of models, parameters and variables (Beven and Binley 1992). Equifinality originates from the imperfect knowledge of the system under consideration, and many sets of models, parameters and variables may therefore be considered equal or almost equal simulators of the system. Using the GLUE analysis, the prior set of models, parameters and variables is divided into a set of non-acceptable solutions and a set of acceptable solutions. The GLUE methodology deals with the variable degree of membership of the sets. The degree of membership is determined by assessing the extent to which solutions fit the model, which in turn is determined by subjective likelihood functions. By abandoning the statistical framework the traditional definition of uncertainty is also abandoned and in general it will have to accept that to some extent uncertainty is a matter of subjective and individual interpretation by the hydrologist.

Considering the sources of mismatch between observed and simulated state variables, it can be argued that the mismatch is to a great extent due to vague and ambiguous interpretations. The GLUE methodology implementation is done through the 3 steps described in Fig. 1.

Step 1 is to determine the statistics for the models, parameters and variables that, prior to the investigation, are considered likely to be decisive for the simulation of the system

(a) Typically quite wide discrete or continuous uniform distribution is chosen—reflecting the fact that there is little prior knowledge of the uncertainties arising from the models, parameters and variables. In principle all available knowledge can be put into the prior distributions.

Step 2 is a stochastic simulation (b) based on the models' parameters and variables defined in step 1. The Monte Carlo or Latin Hypercube method may be used to do a random sample of the parameter sets. Step 2 gives us an unconditional estimate of the statistics of any system state variable (c).

In step 3 an evaluation procedure (d) is carried out for every single simulation performed in step 2. Simulations and thus parameter sets are rated according to the degree to which they fit observed data. If the simulated state variables are "close" to the observed values the simulation is accepted as having a given likelihood (l), whereas if the considered simulated state variables are unrealistic the simulation is rejected as having a zero likelihood.

In this fashion, a likelihood value is assigned to all accepted parameters set (zero for rejecting sets and positive for accepting sets). Thus, the direct result is a discrete joint likelihood function (DJPDF) for all the models' parameters and variables involved. The DJPDF can only be illustrated in two (maximum three) dimensions, and likelihood scatter plots are often used to illustrate the estimated parameters. In Fig. 1 the models' parameters and variables,, are considered independent, the likelihood is projected onto the parameter axis, and discrete density functions (e) are presented, Discrete likelihood functions for all types of system state variables can likewise be constructed (f).

2.2 Parameter sampling strategies in GLUE

Due to the lack of a prior distribution of a parameter, uniform distribution is chosen due to its simplicity (Muleta and Nicklow 2005; Lenhart et al. 2007; Migliaccio and Chaubey 2008). The range of each parameter is divided into n overlapping intervals based on equal probability and parameters are identically chosen from spanning the feasible parameter range. The drawback of a typical GLUE approach is its prohibitive computational burden imposed by its random sampling strategy. To sample the prior parameter distribution, practitioners of the GLUE methodology generally implement a latin hypercube sampling (LHS) strategy. Compared to random sampling, LHS can reduce sampling times and provide a 10-fold greater computing efficiency (Vachaud and Chen 2002). Therefore, LHS is used for random parameter sampling to enhance the simulation efficiency of the GLUE simulation. Values then are randomly selected from each interval.

This stratified random sampling method, though relatively simple to implement, is unlikely to densely sample the parameter space close to the global optimum with a dense distribution of points.

An adaptive sampling method that uses information from past draws to update the search direction is used in GLUE methodology. Such a method would probably result in parameter and prediction uncertainty estimates that are more reliable from a statistical point of view. Instead of randomly sampling the prior parameter space, the shuffled

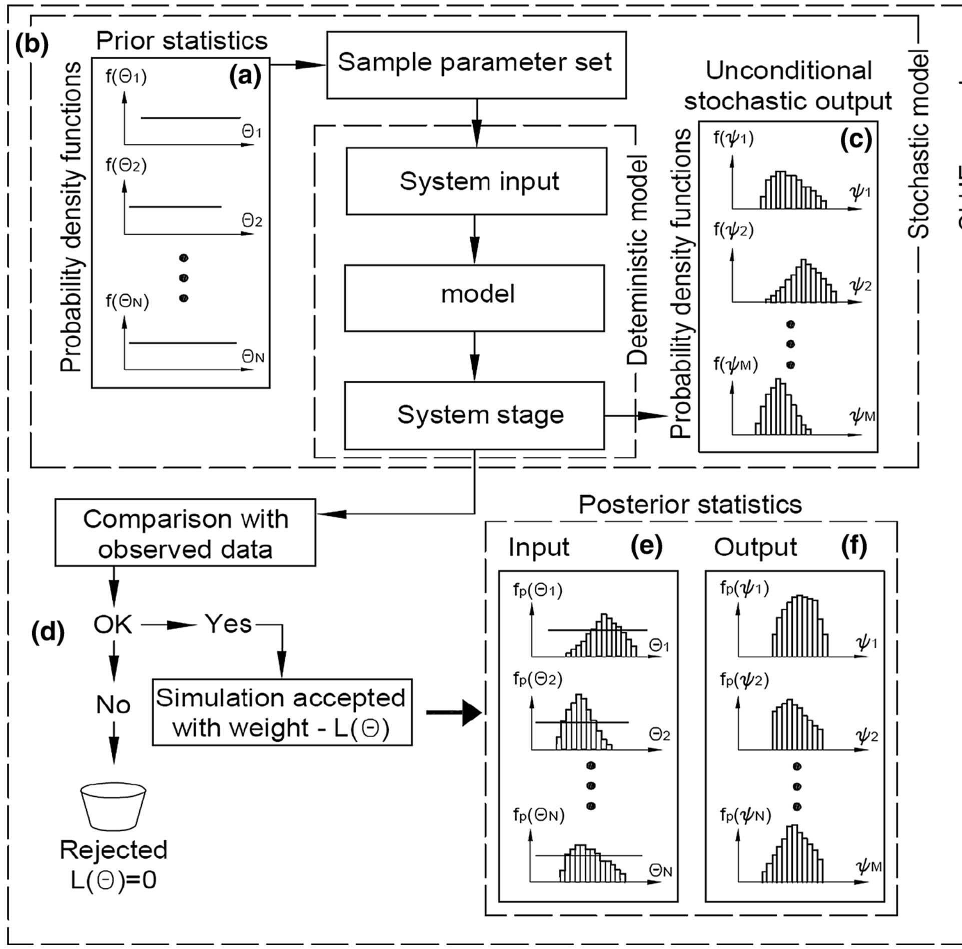

Fig. 1 The GLUE procedure, **a** prior statistics, **b** stochastic modelling, **c** unconditional statistics of system state variables, **d** evaluation procedure **e** posterior parameter likelihood functions and **f** likelihood functions for system state variables

complex evolution metropolis for uncertainty assessment (SCEM-UA algorithm generates a random walk through the parameter space such that any individual state is visited with a frequency proportional to its weight in the posterior PDF. In contrast to LHS, the SCEM-UA algorithm is an adaptive sampler that periodically updates the covariance (size and direction) of the sampling or proposal distribution during the evolution of the sampler toward the HPD region of the parameter space, using information from the sampling history induced in the transitions of the Markov Chain. Experiments using synthetic mathematical test functions have demonstrated that the SCEM-UA algorithm has the appropriate ergodic properties, and provides a more efficient sampling of the HPD region of the parameter space than traditional Metropolis–Hastings samplers (Vrugt et al. 2003). In the SCEM-UA algorithm, a predefined number of different Markov Chains are initialized from the highest likelihood values of the initial population. These chains independently explore the search space, but communicate with each other through an external population of points, which are used to continuously update the size and shape of the proposal distribution in each chain. The MC evolution is repeated until the Rstatistic of Gelman and Rubin (1992) indicates convergence to a stationary posterior distribution. An extensive description and explanation of the method appears in Vrugt et al. (2003) and so will not be repeated here.

2.3 GLUE likelihood measures

Various likelihood functions have been proposed in the literature (e.g. Beven and Binley 1992; Romanowicz 1994; Christensen 2004; Montanari 2005) as measures that quantify the closeness between model simulations and observations. Most of these functions are considered pseudo-likelihood functions because they do not adhere to formal Bayesian statistics, but instead are designed to implicitly account for errors in model structure and input data, and to avoid over conditioning to a single parameter set.

2.3.1 Model efficiency function

The model efficiency function is given as (Beven and Binley 1992)

$$L(\theta|\psi^*) = (1 - \sigma_\varepsilon^2/\sigma_0^2); \quad \sigma_\varepsilon^2 \geq \sigma_0^2 \rightarrow L(\theta|\psi^*) = 0$$

where

$$\sigma_\varepsilon^2 = (\psi^* - \psi(\theta))' V (\psi^* - \psi(\theta))/N_{obs}$$

is the weighted variance of the residuals and σ_0^2 is the weighted variance of the observations. Here V is a weight matrix. The likelihood equals one if all residuals are zero, and zero if the weighted variance of the residuals is larger then the weighted variance of the observations.

2.3.2 *Inverse error variance function*

Beven and Binley (1992) have suggested a function based on the inverse error variance with shaping factor N:

$$L(\theta|\psi^*) = (\sigma_\varepsilon^2)^{-N}$$

This function concentrates the weights of the best simulations as N increases. For N → ∞ all weight will be on the single best simulation and for small values of N all simulations will tend to have equal weight.

3 Application for investigating uncertainty in water resource modeling

3.1 Water quality modeling

Uncertainty in a water quality simulation model is inevitable due to the difficulty of identifying a single model (including grid-scale, process formulations and parameter values) that can accurately represent the water quality under all required model tasks (see the discussions of Beck 1987; Van Straten 1998; Adams and Reckhow 2001). Although we have extensive knowledge about water quality processes from laboratory experiments extrapolation of this knowledge to models of the real environment has consistently proven to be difficult. This is partly because the modelling scale is different to the laboratory scale, and the diversity of species and heterogeneity found in natural environments must (to some degree) be modelled approximately using lumped state variables.

In the last decades, uncertainty analysis has been used in water quality management. Lindblom et al. (2007) employed GLUE to assess the uncertainty embedded in model predictions of copper loads from storm water systems. Freni et al. (2008a, b) utilized GLUE to evaluate the uncertainty of the results from an integrated urban drainage model including a sewer network, a wastewater treatment plant (WWTP), and a receiving water body. They found high uncertainties in the water-quality model results, significantly higher than the uncertainties in the results of the water quantity or flow modules. Vezzaro et al. (2010) estimated the uncertainty of an integrated model in the assessment of the copper and total suspended solids. The uncertainty assessment enabled a wider application of the developed model and provided a tool for pollution-reduction strategies. GLUE, compared with other methods, is easy to implement and allows a flexible definition of the so-called likelihood function used to separate behavioral and nonbehavioral solutions. The likelihood function can include several variables, a feature that is particularly valuable for assessment of integrated and/or distributed models that operate with multivariable, multisite, and multi response criteria.

The main drawbacks of the GLUE technique are the subjectivity involved in the definition of the likelihood function, the threshold for defining the behavioral solutions, and the huge number of necessary model simulations (Freni et al. 2008a, b, 2009a, b, c). Mats Larsbo M. and Jarvis N. 2004, investigated uncertainty in simulating solute transport in a structured field soil, the GLUE analysis showed that observations of soil water contents, drain flow, and both flux and resident concentrations for both tracer and pesticide gave the highest degree of parameter conditioning. Mannina and Viviani (2009) presented the results of applying the GLUE methodology to a quality model aimed to assess the ecological status of small rivers. These results revealed that the model was unable to reproduce the pollutant discharges consistently and that the resulting predicted pollutant loads must be associated with significant uncertainty.

3.2 Rainfall-runoff modeling

In a rainfall-runoff model, parameter uncertainty estimation using GLUE accounts for all sources of uncertainty, i.e., input uncertainty, structural uncertainty, parameter uncertainty and response uncertainty; because "the likelihood measure value is associated with a parameter set and reflects all these sources of error and any effects of the covariation of parameter values on Rainfall-Runoff model performance implicitly" (Beven and Freer 2001). Also, from a practical point of view, "disaggregation of the error into its source components is difficult, particularly in cases common to hydrology where the model is non-linear and different sources of error may interact to produce the measured deviation" (Gupta et al. 2005). In GLUE, parameter uncertainty is described as a set of discrete "behavioral" parameter sets with corresponding "likelihood weights".

The GLUE method has become one of the most widely used and studied uncertainty assessment methods in Rainfall-Runoff modeling (Freer et al. 1996; Cameron et al. 1999; Aronica et al. 2002a, b; Blazkova & Beven 2002; Montanari 2005; Heidari et al. 2006; Mantovan &

Todini 2006; McMichael et al. 2006; Beven et al. 2008; Blasone et al. 2008a, b; Xiong & O'Connor 2008; Stedinger et al. 2008). Despite its popularity, there are still some critical problems facing GLUE application, such as: the efficiency of its prediction bounds in enveloping the observations, the subjectivity in choosing the threshold value for defining behavioural parameter sets, and the definition of likelihood measures. These problems have led to some in depth appraisal of the GLUE methodology (Montanari 2005; Mantovan & Todini 2006; Xiong & O'Connor 2008; Stedinger et al. 2008).

Xiong et al. (2009) applied GLUE for calculating indices for assessing the prediction bounds of rainfall-runoff models and application. They recommend that a broad set of such indices be always employed in carrying out such uncertainty assessment exercises. McMichael et al. (2006) used GLUE methodology for model calibration, testing, and prediction uncertainty estimation in the application of MIKE SHE (System Hydrologique European) hydrologic model for estimating monthly streamflow in a semi-arid Shrubland (chaparral) catchment in central California.

Blasone et al. (2008a, b, c, d) demonstrated the potential of improving GLUE method for sampling the prior distribution of a rainfall-runoff model parameters by employing the shuffled complex evolution metropolis (SCEM-UA) global optimization algorithm and GLUE. The combined SCEM-UA—GLUE method provided better predictions of the model output than a classical GLUE procedure based on random sampling.

Vrugt et al. (2008) compared a formal Bayesian approach that attempts to explicitly quantify the individual sources of uncertainty in the rainfall-runoff modeling process with the traditional GLUE method that maps all sources of uncertainty onto the parameter space. They showed that while the estimates of total uncertainty were similar in both methods, the GLUE method produced large estimates of parameter uncertainty which can lead to erroneous conclusions on the identification of model parameters.

3.3 Groundwater modelling

Groundwater modeling and decision making are beset with uncertainty caused by incomplete knowledge of the underlying system and/or uncertainty due to natural variability in system processes and field conditions. There are four main topics in groundwater model uncertainty that should be addressed in all groundwater reports, namely, conceptual model uncertainty, parameter uncertainty, calibration uncertainty, and predictive uncertainty. It is important to note that a well calibrated model and a unique solution do not necessarily mean that uncertainty in a groundwater model has been eliminated completely. If the conceptual model is poorly defined without investigation of the unknowns through a rigorous method, such as Monte Carlo analysis, there will be inherent uncertainties within the model unaccounted for. In addition, if the data was poorly collected and the errors in the data are not properly explored, the uncertainty will not be accounted for.

In groundwater modelling, parameter and output uncertainties have often been estimated by use of inverse methods like the nonlinear regression approach (e.g. Doherty 2005; Hill and Tiedeman 2007) and Monte Carlo based techniques such as Bayesian uncertainty estimation and generalized likelihood uncertainty estimation (GLUE) (Beven and Binley 1992).

4 Recommendations and suggestions for future research

Overall, this paper provided a detailed discussion on the application of generalized likelihood uncertainty estimation (GLUE) Approach for assessing uncertainty in hydrological models. Based on the reviewed literature, the potentials for future research on GLUE-based uncertainty analysis of watershed and hydrological modeling can be highlighted as follows;

(1) Defining likelihood functions in a more rigorous way instead of using goodness-of-fit measures,
(2) Directly factoring management concern(s) into the likelihood measure,
(3) Hydrological numerical simulation is influenced by more factors. Therefore, an integrated evaluation method is required to account for all uncertainty sources simultaneously for obtaining accurate and reliable assessment result,
(4) Developing more specific strategies for behavioral separation, and
(5) Treating the error terms in a more explicit way.

5 Conclusions

GLUE has the advantage of simple structure, easy operation, and wide applicability, so that it can be applied to the uncertainty analysis of various water resources and environmental models. GLUE is constructed based on Monte Carlo technique, which the efficiency and reliability of sampling algorithm are the key of the method. Traditionally, in water resources planning studies, GLUE takes advantage of a uniform sampling algorithm to obtain parameters' posterior distributions.

However, because of the ineffective sampling technique, this method requires a huge number of simulations to obtain the convergence of Monte Carlo simulation (Blasone R S, et al. 2008). Furthermore, for complex and high-dimensional uncertainty issues, it is likely to generate unreliable and inconsistent results. The combined SCEM-UA—GLUE method provides better predictions of the model output than a classical GLUE procedure based on random sampling. This improvement is obtained for the median GLUE estimates and best parameter estimates from the initial sample. At the same time, the Markov Chain sampler yields a reduction in the uncertainty of the output estimate, providing narrower confidence intervals than those obtained from the LHS dataset. The differences in the results from the two sampling methods increase with the model complexity and with N, the exponent of the likelihood function.

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