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Equifinality, data assimilation, and uncertainty estimation in mechanistic modelling of complex environmental systems using the GLUE methodology

Keith Beven*, Jim Freer

Institute of Environmental and Natural Sciences, Lancaster University, Lancaster LA1 4YQ, UK

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Abstract

It may be endemic to mechanistic modelling of complex environmental systems that there are many different model structures and many different parameter sets within a chosen model structure that may be behavioural or acceptable in reproducing the observed behaviour of that system. This has been called the equifinality concept. The generalised likelihood uncertainty estimation (GLUE) methodology for model identification allowing for equifinality is described. Prediction within this methodology is a process of ensemble forecasting using a sample of parameter sets from the behavioural model space, with each sample weighted according to its likelihood measure to estimate prediction quantiles. This allows that different models may contribute to the ensemble prediction interval at different time steps and that the distributional form of the predictions may change over time. Any effects of model nonlinearity, covariation of parameter values and errors in model structure, input data or observed variables, with which the simulations are compared, are handled implicitly within this procedure. GLUE involves a number of choices that must be made explicit and can be therefore subjected to scrutiny and discussion. These include ways of combining information from different types of model evaluation or from different periods in a data assimilation context. An example application to rainfall-runoff modelling is used to illustrate the methodology, including the updating of likelihood measures. © 2001 Elsevier Science B.V. All rights reserved.

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1. Equifinality in modelling complex environmental systems

It will be argued in this paper that, given current levels of understanding and measurement technologies, it may be endemic to mechanistic modelling of complex environmental systems that there are many different model structures and many different parameter sets within a chosen model structure that may be behavioural or acceptable in reproducing the observed behaviour of that system. Hornberger and Spear (1981), whose work originally inspired what follows here, noted that this is not simply a problem of identifying a correct or optimal model given limited data. Indeed, to focus attention on a rejection of the concept of the optimal model in favour of multiple possibilities for producing simulations that are acceptable simulators in some sense, this idea has been called elsewhere equifinality (Beven, 1993, 1996a,b). Equifinality should not be a surprising concept. It can often be argued on grounds of physical

* Corresponding author. Fax: +44-1524-593-985.
E-mail address: k.beven@lancaster.ac.uk (K. Beven).

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theory that there should be sufficient interactions among the components of a system that, unless the detailed characteristics of these components can be specified independently, many representations may be equally acceptable.

The idea of searching for a single optimal representation of reality is, however, very strong in environmental science. It is part of the normal working paradigm that research should lead to a realistic description of the real processes and characteristics. It is rarely considered that such a description may not be possible or uniquely identifiable despite the fact that for many systems the working descriptions are wrong and are known to be wrong (see the analysis of Morton, 1993), and that many system components may not be accessible to adequate observation given current measurement technologies (particularly, as in hydrology, where much of the active components of the system are below the ground surface). Thus, modelling of complex environmental systems generally involves the indirect identification of model components or parameters by posing an inverse problem. Often, such inverse problems involve multiple parameters and observations that are only indirectly related to the parameters of interest, or which may be at different scales to the variables and parameters used in the model calculations. A particular problem occurs in distributed predictions where the use of global parameters will result in error in predicting local responses at points with unique characteristics (Beven, 2000). In such cases, the inverse problem will not be well posed and identification of an optimal solution will be neither easy nor robust to a change of data set. This has been the subject of considerable study in the groundwater literature (e.g. McLaughlin and Townley, 1996), but has not been much studied in the more difficult case of distributed rainfall-runoff modelling.

This, in itself, should not be sufficient to reject the idea of an optimal model but a search of the feasible model structure and parameter space will commonly reveal many behavioural models with similar levels of performance in reproducing observational data. The concept of the optimal model must then be seriously questioned. Such searches have, until recently, not been computationally possible and remain computationally demanding or impossible for many complex models, such as long runs of global coupled ocean–atmosphere circulation models. Thus, it has only recently been possible to recognise the ubiquitous nature of the equifinality problem. Simulations of a variety of different systems, however, have now demonstrated that even moderate levels of model complexity start to reveal equifinality. This has been shown for rainfall-runoff models (Beven and Binley, 1992; Duan et al., 1992; Beven, 1993; Romanowicz et al., 1994; Freer et al., 1996; Fisher et al., 1997; Piñol et al., 1997; Franks et al., 1998; Lamb et al., 1998; Dunn et al., 1999; Beven, 2001; Beven and Freer, 2001); flood frequency and inundation models (Romanowicz et al., 1996; Romanowicz and Beven, 1998; Aronica et al., 1998; Cameron et al., 1999); river dispersion models (Hankin et al., 1998); soil–vegetation–atmosphere models (Franks and Beven, 1997a,b, 1999; Franks et al., 1999); groundwater flow and transport models (Buckley et al., 1995); and soil geochemical models (Zak et al., 1997; Zak and Beven, 1999; Schulz et al., 1999).

2. Equifinality as a working paradigm

One implication of rejecting the concept of an optimal parameter set and accepting the concept of equifinality is that the uncertainty associated with the use of models in prediction might be wider than has hitherto be considered, since if there are several (many?) different acceptable model structures or many acceptable parameter sets scattered throughout the parameter space, all of which are consistent in some sense with the calibration data, the range of any predicted variables is likely to be greater than might be suggested by a linearised analysis of the area of parameter space around the ‘optimum’. This suggests that the predictions of all the acceptable models (from here on model will be used to mean a particular model structure/parameter set combination) should be included in the assessment of prediction uncertainty, weighted by their relative likelihood or level of acceptability. Such an approach allows the nonlinearity of the response of acceptable model using different parameter sets to be taken into account in prediction.

This appears to lead quite naturally to a form of Bayesian averaging of models and predictions, in which prior distributions of models are assessed in terms of some likelihood measure relative to the observations and a posterior distribution calculated that can then be used in prediction. This is the basis of the generalised likelihood uncertainty estimation (GLUE) methodology proposed by Beven and Binley (1992), which has now been used in a variety of modelling contexts with a variety of likelihood measures in the applications noted above. Updating of the model likelihood distributions as new calibration data become available is handled easily within the Bayesian framework.

In the GLUE methodology, some prior information about feasible ranges of parameter values is used to control the generation of independent random parameter sets for use in each model. An input sequence is used to drive each model and the results are compared with the available calibration data. The model simulations may have either a deterministic or a stochastic dependence on the parameters and input data, but the methodology has to date been primarily used with deterministic models. A quantitative measure of performance or likelihood measure is used to assess the acceptability of each model based on the modelling residuals.

Effectively, each model run represents a sample on the response surface of the likelihood measure within the model space. The comparison of models in Fig. 1a–c represents a projection of the sampled response surface onto a single parameter axis. Each dot on these plots represents the results of a single realisation of a multiple parameter model, expressed in terms of a single summary likelihood measure, here based on a sum of squared errors criterion. The large number of models giving high values of the likelihood measure is an expression of the equifinality in modelling this data set. In this case, the large number of good or behavioural models are from different parameter sets within a single model structure. Extension to multiple competing model structures is simple, provided that a directly comparable likelihood measure may be used, which only requires that the different model structures included in the analysis must predict a variable that can be compared with a common set of available observations or other consistent information.

As projections, Fig. 1a–c do not reveal any obvious structure in the response surface arising from interaction between different parameter values. In general, of course, such interactions may be of great interest in guiding the modeller as to the sensitivity of the predictions to different combinations of parameter values and to where model reformulation and simplification might be appropriate. However, in the present context it is sufficient to note that it is the set of parameter values that is important in giving either good or poor performance, and that it is the set of models giving good performance that is of greatest interest and that is spread across the ranges of the individual parameters.

Other performance criteria have also been suggested and proposed (Beven and Binley, 1992) including fuzzy possibility measures (Aronica et al., 1998; Franks and Beven, 1998; Franks et al., 1998) and likelihood functions based on specific error models (Romanowicz et al., 1994, 1996; Romanowicz and Beven, 1998). The choice of likelihood measure is an important issue in this methodology.

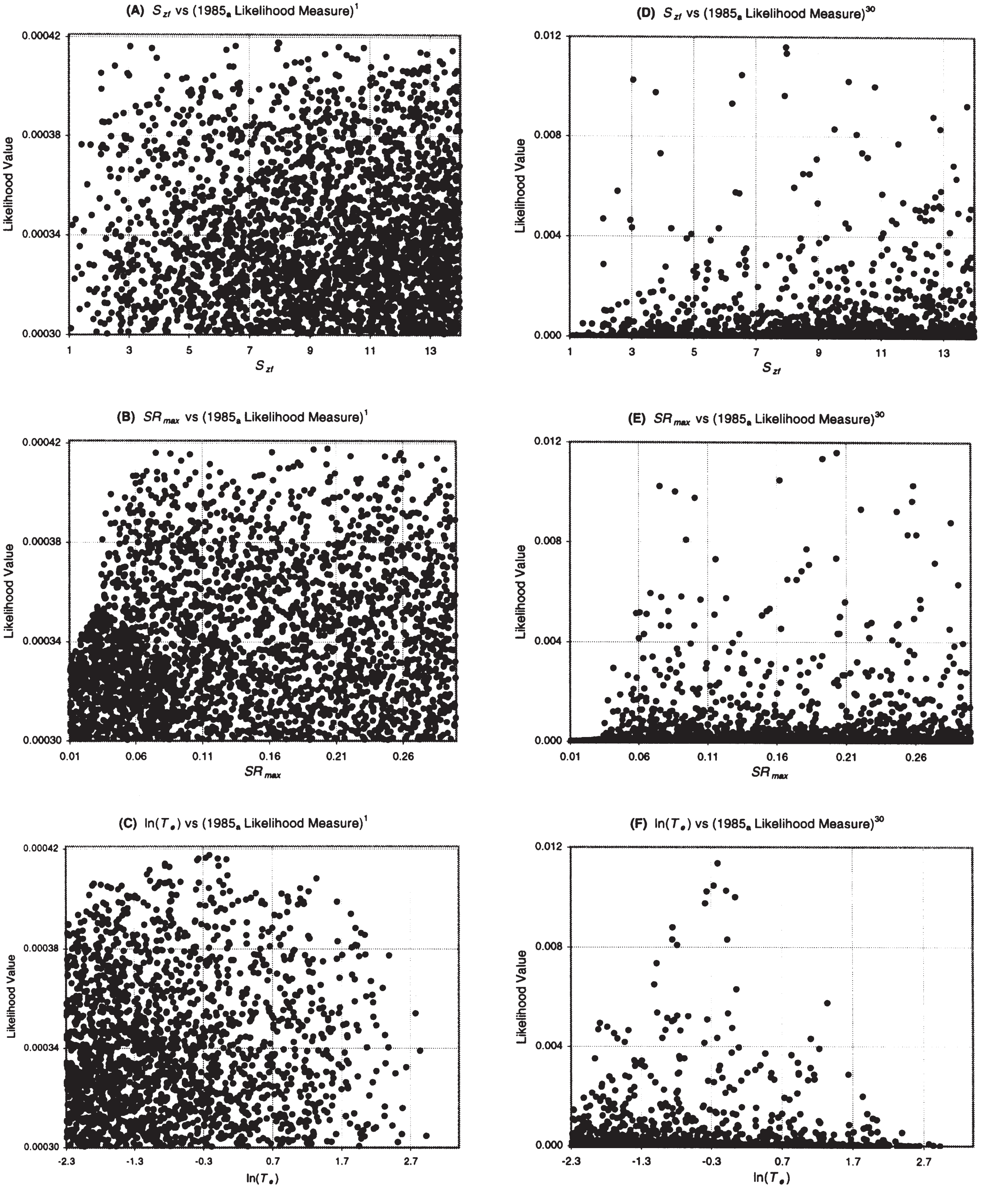
3. The choice of an appropriate likelihood measure

Many environmental modelling problems involve the modelling of time series or spatial patterns of observations, sometimes a single observed output or state variable, sometimes multiple observations at each time step. The model may involve multiple parameters and multiple model state variables not all of which will be measured or, indeed, observable. The model residuals, or errors, when compared with the observations will often have a complex structure. Experience suggests that they may show non-stationary bias, non-stationary variance, non-stationary skewness, and autocorrelation over one or more time steps.

However, for an initial analysis, consider the following traditional approach to likelihood estimation. We assume, perhaps after a suitable transformation, an error model of additive type, with Gaussian autocorrelated errors. Let Z_t be the observed time series, $M_t(\mathbf{\Theta},Y)$ the model output at time t, given the times series of inputs Y and the set of parameter values $\mathbf{\Theta}$, so that

$$Z_t = M_t(\mathbf{\Theta}, Y) + \epsilon_t(\Phi) \quad (1)$$

where $\epsilon_t(\Phi)$ represents the error model with parameters Φ. For a nth order Gaussian autoregressive


(A) S_{zf} vs (1985$_a$ Likelihood Measure)^1
Likelihood Value
0.00042
0.00038
0.00034
0.00030
1
3
5
7
9
11
13
S_{zf}
(D) S_{zf} vs (1985$_a$ Likelihood Measure)^{30}
Likelihood Value
0.012
0.008
0.004
0.000
1
3
5
7
9
11
13
S_{zf}
(B) SR_{max} vs (1985$_a$ Likelihood Measure)^1
Likelihood Value
0.00042
0.00038
0.00034
0.00030
0.01
0.06
0.11
0.16
0.21
0.26
SR_{max}
(E) SR_{max} vs (1985$_a$ Likelihood Measure)^{30}
Likelihood Value
0.012
0.008
0.004
0.000
0.01
0.06
0.11
0.16
0.21
0.26
SR_{max}
(C) ln(T_e) vs (1985$_a$ Likelihood Measure)^1
Likelihood Value
0.00042
0.00038
0.00034
0.00030
-2.3
-1.3
-0.3
0.7
1.7
2.7
ln(T_e)
(F) ln(T_e) vs (1985$_a$ Likelihood Measure)^{30}
Likelihood Value
0.012
0.008
0.004
0.000
-2.3
-1.3
-0.3
0.7
1.7
2.7
ln(T_e)

model AR(n)

$$\epsilon_t = \mu + \sum_{i=1}^{n} \alpha_i(\epsilon_{t-1} - \mu) + \sigma^2 \delta_t \qquad (2)$$

where δ_t should be $N[0,1]$. For the simplest first order correlation case, $\Phi = (\mu, \sigma, \alpha)$ the likelihood function is then given by

$$L(Z|\Theta, \Phi, Y) = (2\pi\sigma^2)^{-\tau/2}(1 - \alpha^2)^{1/2} \times \exp\left[-\frac{1}{2\sigma^2}\left\{(1 - \alpha^2)(\epsilon_1 - \mu)^2 + \sum_{t=2}^{\tau}(\epsilon_t - \mu - \alpha(\epsilon_{t-1} - \mu))^2\right\}\right] \qquad (3)$$

where τ is the number of time steps in the simulation. Note that if the quantities Z_t and $M_t(\Theta,Y)$ are taken to be log transformed observations and model outputs, respectively, then this same model can be used for multiplicative errors, which allows for the effects of an error variance that changes with the magnitude of the observation (one possible heteroscedastic case). Transformations, such as Box–Cox transforms, of the observed and predicted variables may also be used to stabilise the error variances (Box and Cox, 1964).

It is, of course, possible to use more complex likelihood functions but this will serve for illustrative purposes. Mechanistic environmental model simulations may involve a large number of time steps. The magnitude of the likelihood function then tends to be dominated by the first bracketed term on the RHS, $(2\pi\sigma^2)^{-\tau/2}$, essentially the error variance raised to a large negative power. The remaining terms correct for any model bias effects and the reduction in information content of the errors at successive time steps resulting from the correlation of the residuals. The result of $\tau/2$ being very large is to greatly accentuate the peak values of likelihood in the parameter space. This is, of course, an advantage if an optimum is being sought, since essentially only the simulations having the minimum variance will survive an operation that may involve powers of hundreds or even thousands. Thus, the concept of an optimum parameter set necessarily survives in this framework, and in finding the maximum likelihood solution the calculations can be carried out in log space so that $\tau/2$ becomes a multiplier and the numerical problems of using such large powers are avoided. To some extent this obscures the fact that, because of using such large powers, there is only information in the likelihood surface in the immediate vicinity of the 'optimum'. An example of such a transformation, in this case with the shaping factor $N = 30$ (see Table 1 (1b)), is shown in Fig. 1d–f.

This would suggest, therefore, that the parameters are extremely well identified. However, it is clear from Fig. 1a–c that this might be a misleading impression. There are many simulations from different parts of the parameter space that, on the basis of the error variance alone, are virtually indistinguishable from one another. These are clearly two extreme cases, one of which may overestimate parameter identifiability, the other may underestimate parameter identifiability. However, one implication of the difference between them is that, because of the extreme transformation inherent in Eq. (3) the maximum likelihood parameter set may not survive the use of a different calibration data set or sub-set.

In addition, once the maximum likelihood model has been found, the calculation of uncertainty in the predictions, and estimates of the variance and covariance of the parameters, generally involves an assumption of local linearity of the log-likelihood in the neighbourhood of the optimum. However, one of the features of environmental models is that they are often highly nonlinear. In this case it may be necessary to evaluate the complete likelihood surface (including the error parameters Φ) to assess the uncertainty in the predictions properly, by means of evaluating likelihood ratios, parametric bootstrapping or Monte Carlo Markov Chain methods (e.g. Tarantola, 1987; Kuczera and Parent, 1998). In different parts of this parameter space, it may be that the calculated residuals will not have the same assumed structure, even if that is the case at the maximum likelihood point. Also, remember that in this analysis we have actually added (at least) three additional parameters of the error model, that could result in the error model compensating for deficiencies in the

Fig. 1. Dotty plot of likelihood values for selected TOPMODEL parameters from Monte Carlo simulations of the Maimai catchment conditioned on the 1985a discharge period (a–c) using (1b) of Table 1 with $N = 1$; d–f using (1b) of Table 1 with $N = 30$).

Table 1
Example likelihood measures used in GLUE applications, where $\Phi = (\mu, \sigma, \alpha)$ and τ are defined in the text; σ_ϵ^2 is the error variance; σ_0^2 is the variance of the observations. $M(\mathbf{\Theta}_i|\mathbf{Y}_T, \mathbf{Z}_T)$ indicates the ith model, conditioned on input data $\mathbf{Y}_T$ and observations $\mathbf{Z}_T$

Based on autocorrelated Gaussian error model (Romanowicz et al., 1994, 1996)	$L[\mathbf{Z}_T|\mathbf{\Theta}, \Phi, \mathbf{Y}_T] = (2\pi\sigma^2)^{-\tau/2}(1-\alpha^2)^{1/2} \exp[-(1/2\sigma^2)\{(1-\alpha^2)(\epsilon_1-\mu)^2 + \sum_{t=2}^{\tau}(\epsilon_t - \mu - \alpha(\epsilon_{t-1}-\mu))^2\}]$	(1)
Based on inverse error variance with shaping factor N (Beven and Binley, 1992)	$L[M(\mathbf{\Theta}|\mathbf{Y}_T, \mathbf{Z}_T)] = (\sigma_\epsilon^2)^{-N}$	(1a)
Based on Nash and Sutcliffe efficiency criterion with shaping factor N (Freer et al., 1996)	$L[M(\mathbf{\Theta}|\mathbf{Y}_T, \mathbf{Z}_T)] = (1 - \sigma_\epsilon^2/\sigma_0^2)^N$ for $\sigma_\epsilon^2 < \sigma_0^2$	(1b)
Based on exponential transformation of error variance with shaping factor N (Freer et al., 1996)	$L[M(\mathbf{\Theta}|\mathbf{Y}_T, \mathbf{Z}_T)] = \exp(-N\sigma_\epsilon^2)$	(1c)

mechanistic model such that a simulation with a consistent bias might have a better profile likelihood value than an unbiased simulation, since Eq. (3) does not penalise against such a bias when applied locally in the response surface.

This situation arises because the likelihood function implicitly assumes that there is a true model of the observations so that the appropriate error model for the residuals is easily evaluated. This is not often the case in environmental modelling. Errors arise due to model structure, errors in boundary and forcing conditions and error in the observations, with which the model is compared. It may be very difficult indeed to separate these sources of error. The likelihood function is defined as the likelihood of the observations, given the model and error model. In environmental modelling we are generally more interested in the likelihood of the mechanistic model as a simulator of the system given, and conditional on, the (non-error-free) input data and (non-error-free) observations.

We are still, however, interested in the combination of states of information that underlies the likelihood principle. This suggests a more generalised approach to likelihood based parameter estimation, in which it is the likelihood of different models (parameter sets and/or structures) that is being investigated.

4. Generalised likelihood uncertainty estimation

Beven and Binley (1992) pointed out that, viewed in this light, many different likelihood measures might be appropriate in a given application setting. The aim is to assess the performance of different models in a way that allows different measures (calculated for different variables or different periods) to be combined in a suitable way. They outlined a number of ways of formulating both likelihood measures and ways of combining likelihood measures, including the following form of Bayes equation:

$$L[M(\mathbf{\Theta})] = L_0[M(\mathbf{\Theta})]L_T[M(\mathbf{\Theta}|\mathbf{Y}_T, \mathbf{Z}_T)]/C \tag{4}$$

where $L_0[M(\mathbf{\Theta})]$ is a specified prior likelihood for the model $M(\mathbf{\Theta})$ with parameter vector, $\mathbf{\Theta}$, $L_T[M(\mathbf{\Theta}|\mathbf{Y}_T, \mathbf{Z}_T)]$ is a likelihood measure calculated for the model over period T with input vector $\mathbf{Y}_T$ and observed variable vector $\mathbf{Z}_T$, and C is a scaling constant. Note that it is now the likelihood of the model (parameter set and/or structure), $M(\mathbf{\Theta})$, that is being assessed, rather than the value of an observation or of the individual parameters. Application of Eq. (4) implies that the values of the likelihood measures calculated for different models can be considered independent. Hence the attempt in traditional likelihood measures to achieve a residual series δ_t that is white, and that can be tested for its whiteness as a test of the error model used.

In general such orthogonality cannot be assured for mechanistic environmental models. However, by using model parameter sets that are chosen independently from some specified distributions, independence in sampling the likelihood surface can be assured, at least within a chosen parameter metric. This is easily done in a Monte Carlo sampling framework using either an importance sampling technique (so that the shape of the response surface is represented by the density of sampling and each model simulation is given equal weight in forming a distribution of predictions) or a uniform sampling technique (so that each model simulation is associated with a likelihood value reflecting the shape of the response surface). Both are ways of characterising the response surface in the model parameter space. Applications of GLUE have used the latter, trading off the inefficiency of uniform sampling against ease of implementation and minimal assumptions about the shape of the response surface. The results of each model can then be compared with the data and a likelihood measure calculated, so that Eq. (4) can then be applied in the form

$$L[M(\boldsymbol{\Theta}_i)] = L_0[M(\boldsymbol{\Theta}_i)]L_T[M(\boldsymbol{\Theta}_i|\mathbf{Y}_T, \mathbf{Z}_T)]/C \qquad (5)$$

where $M(\boldsymbol{\Theta}_i)$ indicates the ith model. If appropriate, the likelihood $L_T[M(\boldsymbol{\Theta}_i|\mathbf{Y}_T, \mathbf{Z}_T)]$ might be of the form of a measure defined by the likelihood function of Eq. (3), but a more application oriented, rather than error oriented, measure might be more appropriate, particularly if the model is not a particularly good representation of the data (as is often the case). Examples of likelihood measures used in different applications are given in Table 1. The likelihood measure will reflect the performance of a particular model, given the model nonlinearity and errors in model structure, inputs and observations. Since the likelihood measure value is associated with a parameter set, it will reflect all these sources of error and any effects of the covariation of parameter values on model performance implicitly. The only constraint is that it should increase monotonically with increase in model performance (however, that is defined) and that model simulations that are considered as non-behavioural should have a likelihood of zero. Equifinality in model performance will be reflected directly by different models having similar values of the chosen likelihood measure.

Given a large enough sample of Monte Carlo simulations, the range of likelihood weighted predictions may then be evaluated to obtain prediction quantiles at any time step. This is most easily done if the likelihood values are renormalised such that $\sum_{i=1}^{B} L[M(\boldsymbol{\Theta}_i)] = 1$, where $M(\boldsymbol{\Theta}_i)$ now indicates the ith behavioural Monte Carlo sample, so that at any time step t

$$P(\hat{Z}_t < z) = \sum_{i=1}^{B} L[M(\boldsymbol{\Theta}_i)|\hat{Z}_{t,i} < z] \qquad (6)$$

where $\hat{Z}_{t,i}$ is the value of variable Z at time t simulated by model $M(\boldsymbol{\Theta}_i)$. The prediction quantiles, $P(\hat{Z}_t < z)$ obtained in this way are conditional quantiles: conditioned on the inputs to the model; the model responses for the particular sample of parameter sets used; the choice of likelihood measure; and the observations used in the calculation of the likelihood measure. In such a procedure the simulations contributing to a particular quantile interval may vary from time step to time step, reflecting the nonlinearities and varying time delays in model responses. It also allows for the fact that the distributional characteristics of the likelihood weighted model predictions may vary from time step to time step (sometimes dramatically, see Freer et al., 1996). Note that Eq. (6) implicitly reflects the fact that the independence in sampling the parameter sets does not imply independence of the predicted variables of interest resulting from the similar (if not identical) input data and boundary conditions used to force the model (Bernardo and Smith, 1994). Model outputs will tend to be correlated, even for models judged to be non-behavioural.

If more than one period of data is available, Bayes' equation (5); (Box and Tiao, 1973) can be reapplied to update the likelihood weights on a parameter set by parameter set basis, reflecting the independence of the parameter sampling. The posterior from one application of Eq. (5) becomes the prior for the next application. The likelihood measures for a given parameter set for the periods may be correlated, indeed it should be hoped (if not necessarily expected) that if a model performs well in one calibration period, it will continue to perform well in other periods. If this is not the case then its combined likelihood measure will be reduced.

It is possible that, in combining two measures from different observed variables during the same calibration period, there will be a correlation in model performance against different variables, i.e. a model that produces good simulations of one output variable might equally produce good simulations of an observable internal state variable (although it has to be said that this does not necessarily follow in many applications). A simple application of Eq. (5) to the weights associated with each model separately will be effectively ignoring this correlation. It will have the desired effect that if a model produces good simulations on both variables its likelihood will be raised, if it does not, it will be lowered but a fully rigorous application of Eq. (5) would

Table 2
Examples of likelihood measure combination equations (before renormalisation), where ω_0 and ω_1 are weighting coefficients for different periods or different variables. $M(\boldsymbol{\Theta}_i|\mathbf{Y}_T, \mathbf{Z}_T)$ indicates the ith model, conditioned on input data $\mathbf{Y}_T$ and observations $\mathbf{Z}_T$

Bayes' multiplication (e.g. Beven and Binley, 1992; Romanowicz et al., 1994, 1996)	$L[M(\boldsymbol{\Theta}_i)] \propto L_0[M(\boldsymbol{\Theta}_i)]L_1[M(\boldsymbol{\Theta}_{1i}\vert Y_1, Z_1)]$	(5)
Weighted addition (Zak et al., 1997)	$L[M(\boldsymbol{\Theta}_i)] \propto \varpi_0 L_0[M(\boldsymbol{\Theta}_i)] + \varpi_1 L_1[M(\boldsymbol{\Theta}_i\vert Y_1, Z_1)]$	(5a)
Fuzzy union	$L[M(\boldsymbol{\Theta}_i)] \propto \mathrm{Min}[L_0[M(\boldsymbol{\Theta}_i)], L_1[M(\boldsymbol{\Theta}_i\vert Y_1, Z_1)]]$	(5b)
Fuzzy intersection	$L[M(\boldsymbol{\Theta}_i)] \propto \mathrm{Max}[L_0[M(\boldsymbol{\Theta}_i)], L_1[M(\boldsymbol{\Theta}_i\vert Y_1, Z_1)]]$	(5c)
Weighted fuzzy combination (Aronica et al., 1998)	$L[M(\boldsymbol{\Theta}_i)] \propto \varpi_0 \mathrm{Min}[L_0[M(\boldsymbol{\Theta}_i)], L_1[M(\boldsymbol{\Theta}_i\vert Y_1, Z_1)]] + \varpi_1 \mathrm{Max}[L_0[M(\boldsymbol{\Theta}_i)], L_1[M(\boldsymbol{\Theta}_i\vert Y_1, Z_1)]]$	(5d)

require a proper assessment of the information content of each measure.

The choice of method of combining likelihood measures may have implications for the choice of the measure itself, in particular if it is required that multiple combinations, for example of measures from different periods of data, have the same result as treating the data as a single continuous period (where this is possible). Repeated application of Eq. (5) would not lead to this end if, for example, the likelihood measure was a linear function of the inverse error variance for each separate period of data. The successive multiplications would result in the most recent period of data having the greatest weight in the determination of the likelihoods after resampling (which may, of course, give the desired effect if the system is thought to be changing over time). The use of a likelihood measure that is a constant linear function of the inverse exponential of the error variance, would result in an equivalence of final posterior likelihood (Table 1, Eq. (1c)).

There are also other ways of combining likelihood measures. As one example, the likelihood measures may be re-interpreted directly as fuzzy possibility measures so that the techniques of fuzzy union (Table 2, Eq. (5b)) and fuzzy intersection (Table 2, Eq. (5c)) could also be used. The value of additional data in refining the likelihood measure distribution associated with the parameter sets can be evaluated using different uncertainty measures (see Beven and Binley, 1992).

In essence, a generalised likelihood framework is being proposed, in which a variety of likelihood measures (including traditional likelihood functions) could be used. The choice of likelihood measure, and the way of combining likelihood measures, are subjective but, clearly, reasonable choices should be made for any particular application. An important point to be made, however, is that the choices must be made explicit so that the analysis can be reproduced at any time to check calculations, to compare different model structures or the effects of using different calibration variables etc. Being explicit, they can also be the subject of discussion and justification.

5. Generating parameter sets

The proposed methodology separates parameter sampling, to ensure independence of chosen parameter sets, with likelihood evaluation. As such it varies from much of the recent work in Monte Carlo Markov Chain and similar techniques that attempt to sample the parameter space according to likelihood power, with the hope of making considerable savings in computer time in defining the likelihood surface. Such methods may work well when there is a well defined surface, but for surfaces with lots of local maxima or plateaux, the advantages may not be great.

The shape of the response surface will, of course, reflect the likelihood function used. The choice of a likelihood measure, for example $(2\pi\sigma^2)^{-\tau/2}$ that is the dominant term of Eq. (3) with τ large, that emphasises the peak will then be advantageous but only if the resulting distributions of likelihood weighted predictions are reasonable in comparison with the observations. Raising the peak likelihood, relative to other values in the response surface, will generally have

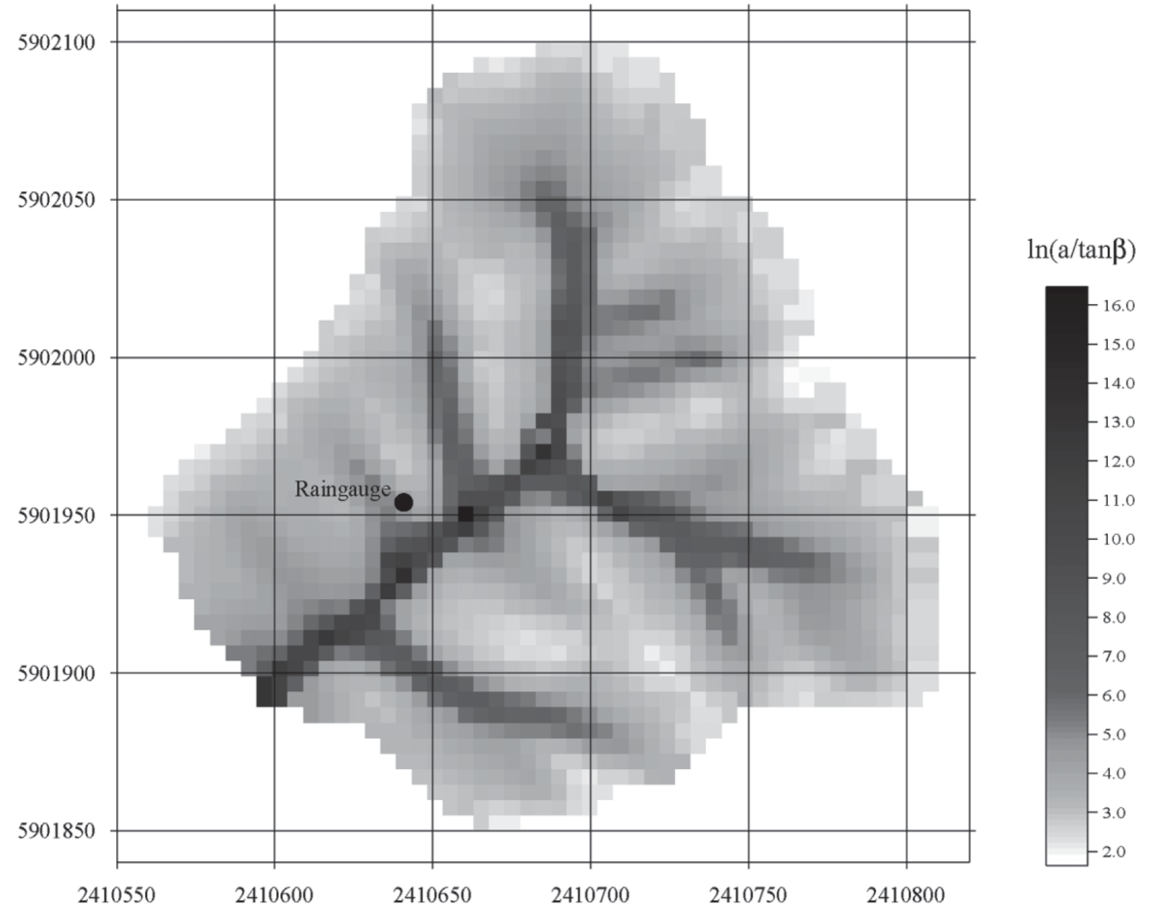


Fig. 2. Spatial distribution of the ln(*a*/tan *β*) topographic index for the Maimai M8 catchment, New Zealand.

the effect of narrowing the tails of the distributions of predictions, perhaps in some cases too much to allow the prediction limits to encompass many of the observations (e.g. Freer et al., 1996).

Thus the whole of the response surface may be of interest. Getting an adequate definition of that surface will be computationally expensive in high dimensional parameter surfaces. Both uniform Monte Carlo and Latin Hypercube sampling could be used to obtain parameter sets that are distributed throughout the parameter space and independent within that metric. Only the feasible parameter range and the scaling of the parameter axis must be specified for uniform sampling. Latin Hypercube sampling can be used to generate minimally correlated parameter sets in the case where there is some prior information about parameter covariation. With anything more than a small number of parameters, a large number of samples will be required for a proper characterisation of the response surface.

Prior information about parameters may take a number of forms. The first would be some sense of expected distribution and covariance of the parameter values. Some parameter sets, within the specified ranges, may be known a priori as not being feasible on the basis of past performance or mechanistic arguments. Then each parameter set might be given a prior likelihood (perhaps of zero): this need not change the sampling strategy but does mean that if the prior likelihood is zero it will not be necessary to run the model thereby saving computer time. It must be remembered that any parameter values outside the specified range are being given an a priori likelihood of zero, even while it will be commonly found that behavioural models may be found right up to the edge of this range (see Fig. 1a, b and many of the studies quoted above).

Table 3

Parameter ranges used in Monte Carlo simulations for Maimai catchment. *Estimates are shown for comparison, the details of this analysis has been given in Freer and Beven, 1994, ** ranges for T_0 and K_0 shown also in log to relate to the graph scales

Parameter	Minimum value	Maximum value	Sampling strategy	Mean field estimates*
S_{zf} (m)	1.00	14.00	Uniform	9.425
$SR_{\max}$ (m)	0.01	0.30	Uniform	0.086
$\Delta\theta_1$ (fraction)	0.01	0.25	Uniform	0.070
K_0 (m h^{-1})	0.10	60.00	Uniform log values	5.026
	** (−2.33)	(4.1)		
T_e (m^2 h^{-1})	0.10	30.00	Uniform log values	0.833
	** (−2.33)	(3.4)		
P_{mac} (fraction)	0.00	0.60	Uniform	0.195

There may also be some idea of the form of the expected response surface. This might be used to specify a different noninformative prior than the uniform prior suggested above, for example to use a prior that is conjugate with the expected posterior (see Bernardo and Smith, 1994). Again, however, this need not change the uniform sampling strategy, but each parameter set would not be given a uniform prior likelihood in this case. Alternatively, much more efficient sampling of the response surface might be achieved in such cases using a Monte Carlo Markov Chain (MCMC) algorithm or the structured tree algorithm of Spear et al. (1994).

An interesting question arises when there are measured values available of one, some or all parameter values in the model. In some (rare) cases it may even be possible to specify distributions and covariances for the parameter values on the basis of measurements. These could then be used to specify prior likelihood weights in the (still uniformly) sampled parameter space. Although it is often the case that such measurements are the best information that we have about parameter values, there is, however, no guarantee that the values measured at one scale will reflect the effective values required in the model to achieve satisfactory functional prediction of observed variables (Beven, 1989; Beven, 1996b). It might then be possible to feed disinformation into the prior parameter distributions but the repeated application of Eq. (5) or some other way of combining likelihood measures should result in the performance of the model increasingly dominating the shape of the response surface, unless prior likelihood weights assigned as zero have wrongly excluded some of the parameter space from consideration. In some cases this will be obvious, such as where initial results indicate that resampling of parameter sets beyond the prior specified sampling ranges should be carried out.

6. An example application: rainfall-runoff modelling of the Maimai M8 catchment, New Zealand, with the assimilation of successive periods of data

The small Maimai M8 (3.8 ha) catchment is located in the Tawhai State Forest, North Westland, South Island, New Zealand. It has been the focus for a variety of studies of hydrological processes (see Rowe et al., 1994, and Brammer and McDonnell, 1996). The catchment has a mean annual gross precipitation of 2600 mm, producing some 1550 mm of runoff from 1950 mm net precipitation with little seasonal variation. The catchment is underlain by a compact early Pleistocene conglomerate, called the Old Man Gravels, that is thought to be essentially impermeable. Slopes in the catchment are short and steep with a relief of 100–150 m. The soils are spatially variable in depth (0.2–1.8 m) and hydraulic conductivity, but are generally highly permeable. The vegetation is a mixed evergreen forest with an understory of tree ferns and shrubs.

This wet environment and sloping terrain is a suitable test environment for the rainfall-runoff model TOPMODEL (Beven and Kirkby, 1979; Beven et al., 1995; Freer et al., 1996; Beven, 1997; Beven, 2001; Beven and Freer, 2001), which assumes that dynamic changes in the saturated zone on the hillslopes can be represented as a succession of steady

Table 4
Summary of the Maimai catchment hydrometric data records used in the discharge simulations. ** Due to data limitations the same monthly PET data from 1987 has been used for all years

	Flow data (1 h timesteps)					
Data	1985-a	1985-b	1985-c	1985-d	1986	1987
Time period (days)	144	32	67	115	365	365
No. significant events >1 mm h^{-1}	3	2	4	4	19	25
P (mm)	622.8	223.5	584.1	721.0	2245.9	2667.7
Q (mm)	284.0	176.8	440.1	379.9	1311.1	1757.4
PET (mm)	374.7	28.9	85.3	321.7	**837.6	**837.6
Q/P (%)	45.6	79.0	75.3	52.7	58.41	65.8
Q_{peak} (mm h^{-1})	2.9	7.8	4.8	8.5	6.1	6.6
W. balance (mm)	− 35.9	17.8	58.7	19.4	97.56	72.74

states, in which downslope flow is everywhere equal to the product of an upslope contributing area and a mean recharge rate. This allows the catchment to be represented in terms of the soil-topographic index ($a/T_0 \tan \beta$) where a is the local upslope contributing area per unit contour length, T_0 is the transmissivity of the soil at saturation, and $\tan \beta$ is the local slope angle, which is derived from an analysis of the catchment topography and estimates of the soil transmissivity (see Beven et al., 1995; Quinn et al., 1995). The topographic index then acts as an index of hydrological similarity. Every point in the catchment with the same value of the index is predicted as responding in a hydrologically similar way (Fig. 2). The use of a constant upslope contributing area in the topographic index may not be a good assumption in drier environments (Barling et al., 1994; Western et al., 1999) but should be reasonable here. Assessing spatial variation in soil transmissivity is a problem in any catchment and Woods and Rowe (1996) and Freer et al. (1997) have shown that better predictions of subsurface flow can be achieved by taking account of variations in soil depth in calculating index values. However, in most catchments this type of information is not readily available and it is usually necessary to assume an effective transmissivity profile all over the catchment.

In the version applied here, TOPMODEL has six parameters that must be specified (Table 3). We have investigated the calibration of these parameters, within the GLUE methodology, by starting with a short period of rainfall-runoff data and gradually including more and longer periods of observations to be available. At each stage the new data are assimilated into the analysis by a Bayesian combination of likelihood measures using Eq. (5).

The periods of data used are listed in Table 4. The first year included in this study (1985) was, in fact, a year with a significantly different distribution of storm events (larger and less frequent), with longer drier periods than average. At each stage in the analysis, the predictions of a sample of models are compared with observations using a likelihood measure based on the efficiency measure of Nash and Sutcliffe (1970), expressed in the form of equation 1b of Table 1 with the shaping parameter, N. After each model evaluation, these likelihoods are used in Eq. (5) to derive a posteriori likelihood weights that can be used to derive prediction quantiles using Eq. (6), as discussed above. In this application, the likelihood associated with each model and the prediction quantiles are updated as each new period of data is assimilated into the analysis. The results are compared by successive prediction of the 1987 hydrographs, the last period of the records considered here. Thus, until the data from 1987 are included in the analysis, the 1987 period is therefore acting as a 'validation' period for predictions made with the posterior likelihood weights after updating at earlier periods.

Dotty plots of this likelihood measure for each parameter are shown in Fig. 1a–c. Each point on this plot represents a randomly sampled point on the response surface in the parameter space projected onto a single parameter axis. It is clearly not possible to show all the complex interactions between

Table 5
Summary results from the GLUE simulations of TOPMODEL for all discharge periods showing the effect of updating the likelihood weights

Results	Discharge data periods					
	1: 1985-a	2: 1985-b	3: 1985-c	4: 1985-d	5: 1986	6: 1987
Total no. simulations > 0.6 R^2	2946	3906	19108	17687	7164	7086
No. behavioural (retained)	2946	1319	1171	1168	1165	1026
Posterior entropy	11.52	10.35	10.18	10.16	10.14	9.96
Peak R^2 value	0.835	0.899	0.92	0.915	0.89	0.87

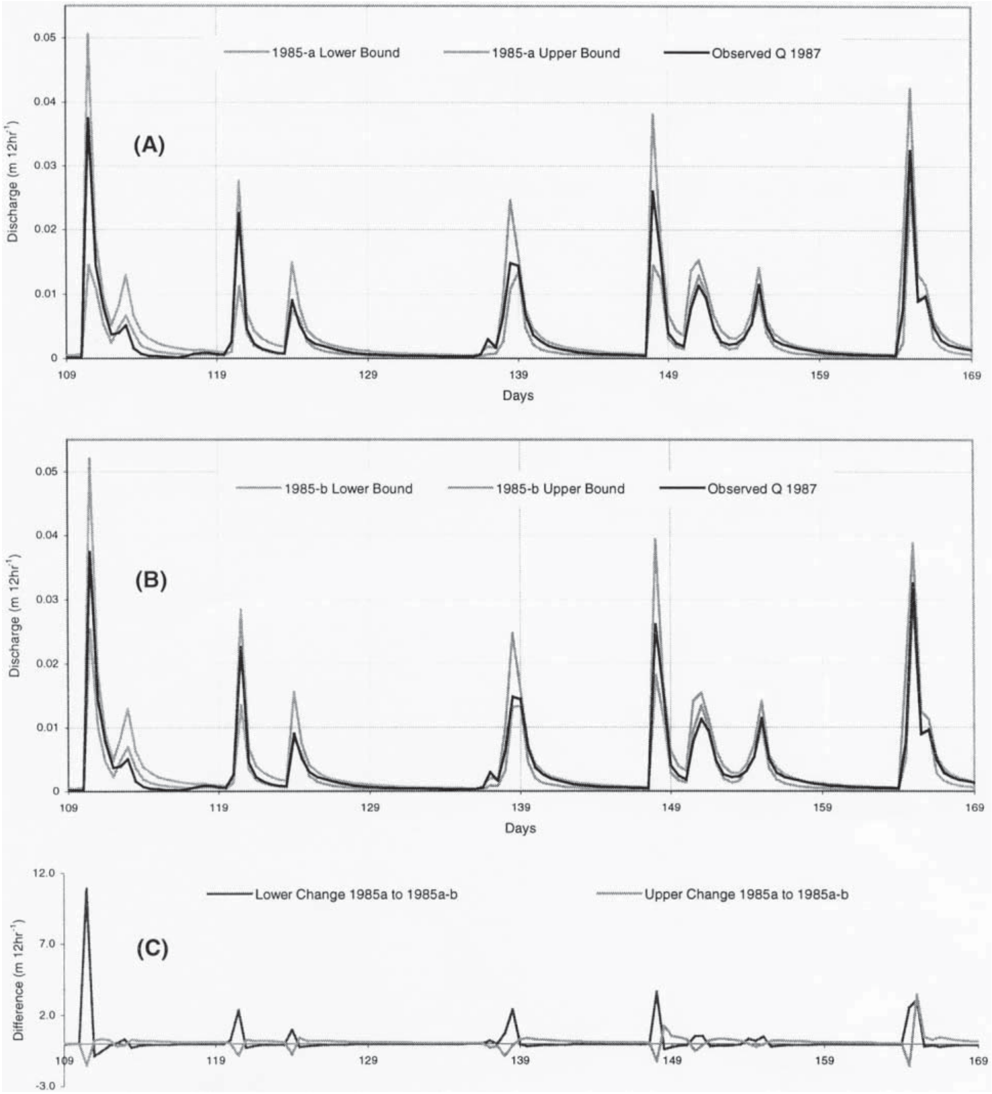


Fig. 3. Comparison of prediction limits shown for a selected period of the 1987 data set (19th April–18th June) having updated the likelihood weights using periods (A) 1985a; (B) 1985a–b; (D) 1985a–c and (F) all six periods. Changes to the prediction limits are shown for likelihood weights updated from (C) 1985a to 1985a–b (E) 1985a–b to 1985a–c.

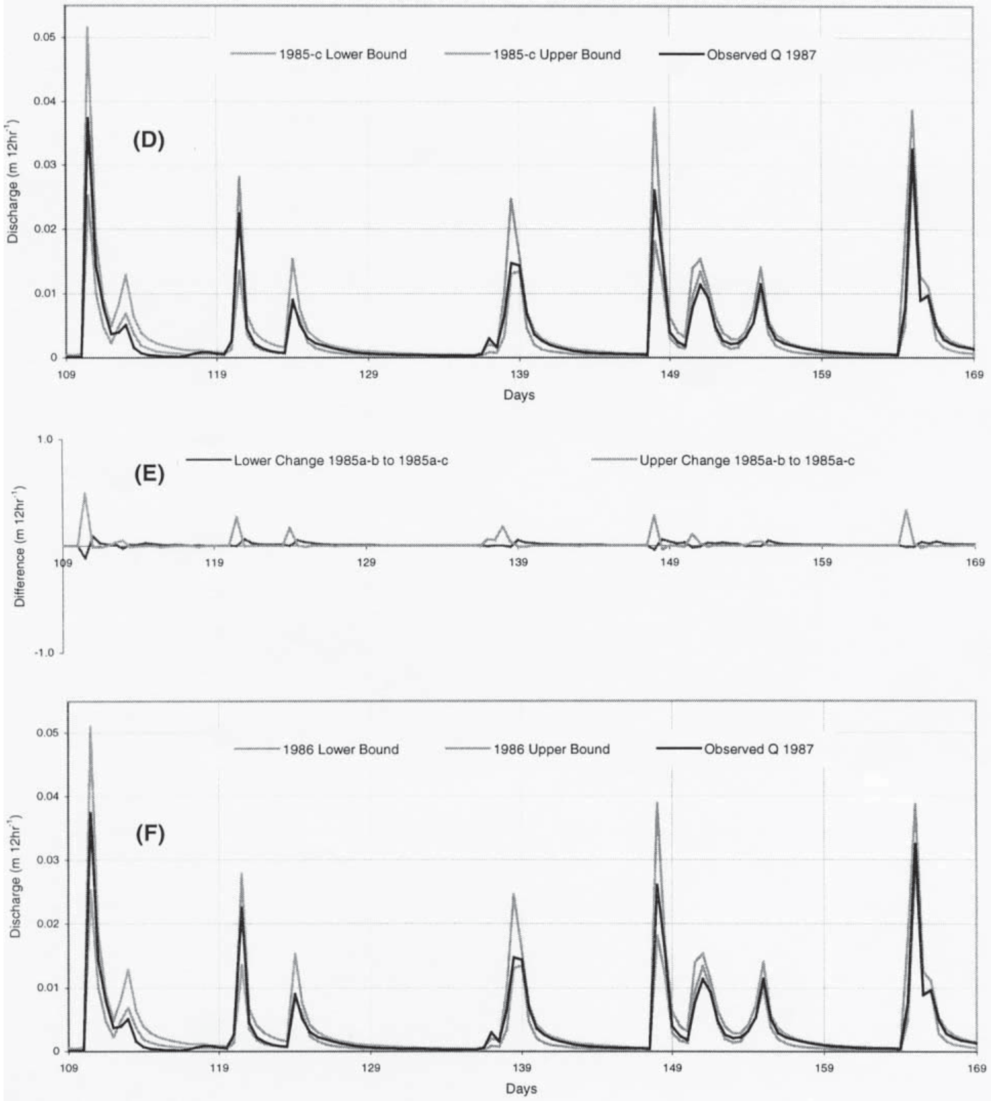


Fig. 3. (*continued*)

parameters in forming the response surface in such a one-dimensional plot. This is not, however, the point of such plots. The point is that there very often seems to be an upper limit of model performance that is reached, or almost reached, by different combinations of parameter values scattered through the model space. This is a reflection of equifinality in modelling such systems (and may also be extended to multiple model structures).

A decision must be made at this point. What level of goodness of fit to the observations will be considered acceptable, so that only the models that achieve that level will be retained for making predictions? From the dotty plots of Fig. 1a–c there is clearly no obvious cut-off between behavioural and non-behavioural models but rather a range of performance from good to bad for most parameter values. The decision is therefore generally subjective. It can be achieved in different ways. One way is to increase the power N so that it reduces the relative weight associated with poor models until the prediction limits reflect the power of the model in predicting the data. The value of N is then an index of the information content of the data in conditioning the set of feasible models. Application of Eq. (3) is effectively assuming a very high power of N, which will result in a very peaked likelihood surface. Experience suggests that this will tend to underestimate the uncertainty in the simulations.

Eq. (3) is essentially based on an assumption that a true model of the process exists, such that a likelihood of predicting the observations given this true model can be found. This is the traditional statistical approach towards defining a likelihood function, but it does not take adequate account of the possibility of model structural error. GLUE provides an estimate of the likelihood of a model given the observations and thereby includes the effects of model structural error implicitly. The resulting prediction limits are, however, quantiles of the model predictions, not direct estimates of the probability of simulating a particular observation (which is not easily estimated given model structural error). It could be argued that likelihood functions, such as Eq. (3), are a special case within the GLUE framework. The value of N will be necessarily a subjective choice but can be used to control the shape of the distribution of simulated variables and resulting prediction quantiles.

Another strategy for defining the set of behavioural models is to define some threshold of acceptability, ensuring that a sufficient sample of models remains to form a meaningful cumulative weighted distribution of predictions. This has been used satisfactorily in previous studies. Here we have chose a threshold efficiency measure of 0.6 ($N = 1$), before rescaling, as a boundary, below which models are rejected as being non-behavioural and given a likelihood of zero. All the points plotted in Fig. 1a–c are, in fact, behavioural in this sense. The likelihood values shown in Fig. 1 are rescaled values over the set of all behavioural models retained in the analysis.

Table 5 records the total number of model simulations out of 60 000 Monte Carlo parameter sets that achieved this efficiency threshold of 0.6 for each simulated period. It is notable that the two periods at the beginning of the record in the dry year of 1985 had smaller numbers of behavioural simulations than later wetter periods. This is partly, of course, because the use of a smaller observed mean discharge in drier periods means that a smaller residual variance is required to achieve the 0.6 behavioural threshold. Table 5 also shows how many simulations remain behavioural after updating the posterior likelihood weights as each successive period is added. In this case, starting with the relatively small number of behavioural simulations in periods 1985a and b, the posterior weights converge quite quickly to a common set of models. The later wetter periods do not add much information in terms of rejecting more of the models considered behavioural at the end of periods 1985b and 1985c. Note that only 1.7% of the original sample of models has been retained as behavioural after these successive updatings. Raising the behavioural threshold would reduce this percentage further.

A comparison of the predictions of the 1987 evaluation period after successive updatings of the prediction limits is shown in Fig. 3a,b,d,f. For the most part, the predictions bracket the observations but there are periods when it appears that the behavioural models (according to the definition used here) cannot reproduce the observations. This may be the result of inherent structural errors in the model, errors in the input data, or error in the discharge observations themselves (see also Freer et al., 1996, who discuss the specific problem of modelling snowmelt in this respect). This reinforces the point that these prediction limits are conditional on a particular model, sequence of input data, series of observations and likelihood measure used in conditioning. It remains difficult to separate out these potential sources of error, and it may not really be necessary provided that the conditional nature of the prediction limits is recognised. Just as it is difficult to justify a unique optimal model of the system, so it is difficult to justify a unique set of prediction limits in this type of environmental modelling (remembering that we do not generally expect to be able to demonstrate that a simple stationary error model is valid). Fig. 3c,e further emphasises the comments noted for Table 5 regarding the amount of information later periods add to rejecting behavioural models by showing the changes to the prediction limits before and after updating the likelihood weights. Significant changes to the prediction limits, primarily during the larger storm events, only occur for the first 1 or 2 updating sequences (a positive change indicates that the individual prediction limits have moved towards the mean prediction for that timestep).

For every time step the distribution of behavioural

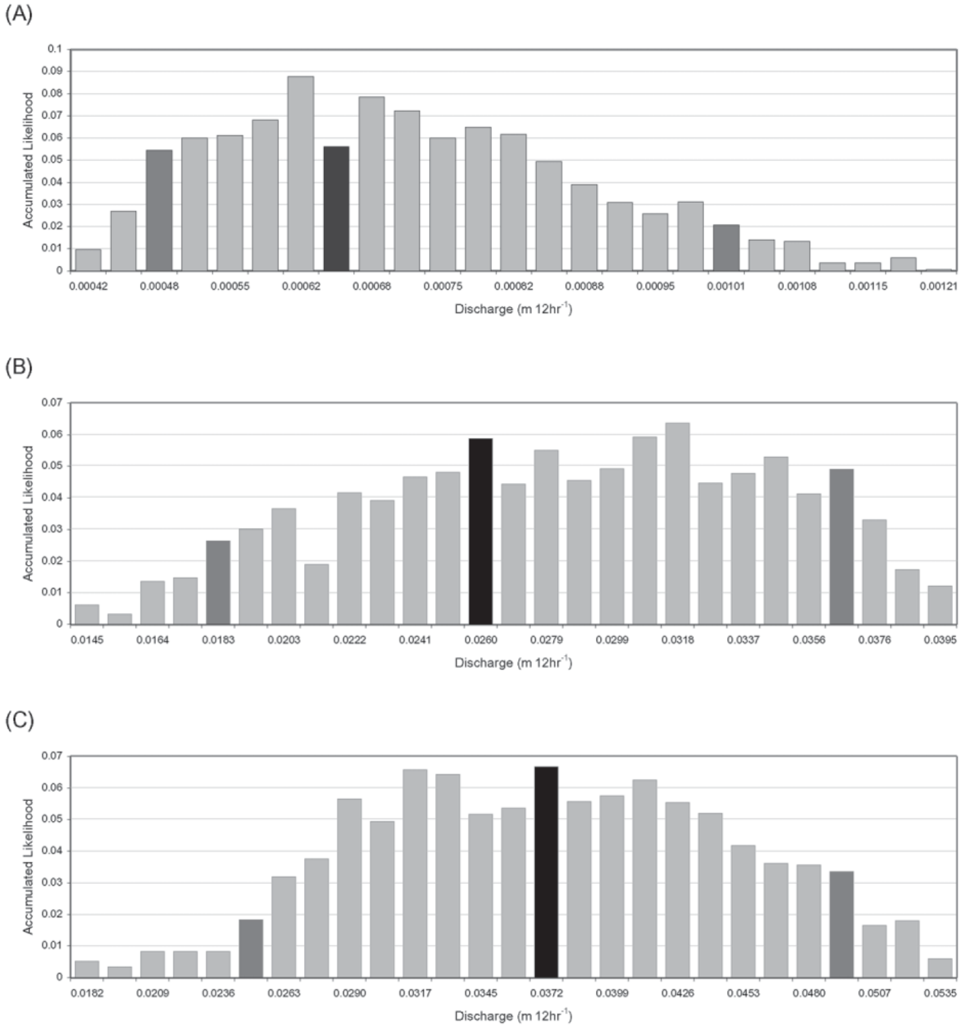


Fig. 4. Distribution of simulated discharges at selected timesteps predicted from behavioural parameter sets conditioned using all the flow periods for three different observed discharges (Q) –(A) 20th April, $Q = 0.037$ m 12h^{-1}; (B) 28th May, $Q = 0.026$ m 12h^{-1}; (C) 9th May, $Q = 0.00064$ m 12h^{-1} (black denotes observed discharge and dark grey denotes prediction limits for the timestep).

model discharge predictions can also be analysed to show the variability in the distribution characteristics. Fig. 4 shows the results of such an analysis for three different flow magnitudes. The plots show that these distributions are clearly non-Gaussian, having characteristics, which are changing shape and variance over time. These results are consistent with the formulation of the prediction limits as outlined in the GLUE methodology in Section 5.

It is also important to recognise that the performance of each sample model (whether behavioural or non-behavioural) is dependent on the set of parameter values. The likelihood weight associated with each parameter set will implicitly reflect the complex interactions between parameter values in any simulation. In some cases, however, information about individual parameters is of interest. Fig. 5 shows the cumulative marginal distributions for each parameter (compared with the initial uniform distribution in each case) for the final behavioural simulations after all updatings of the likelihood weights. Those parameters showing a strong deviation from the original uniform distribution may be considered the most sensitive in that they have been most strongly conditioned by the model evaluation process. Those that are still uniformly distributed across the same parameter

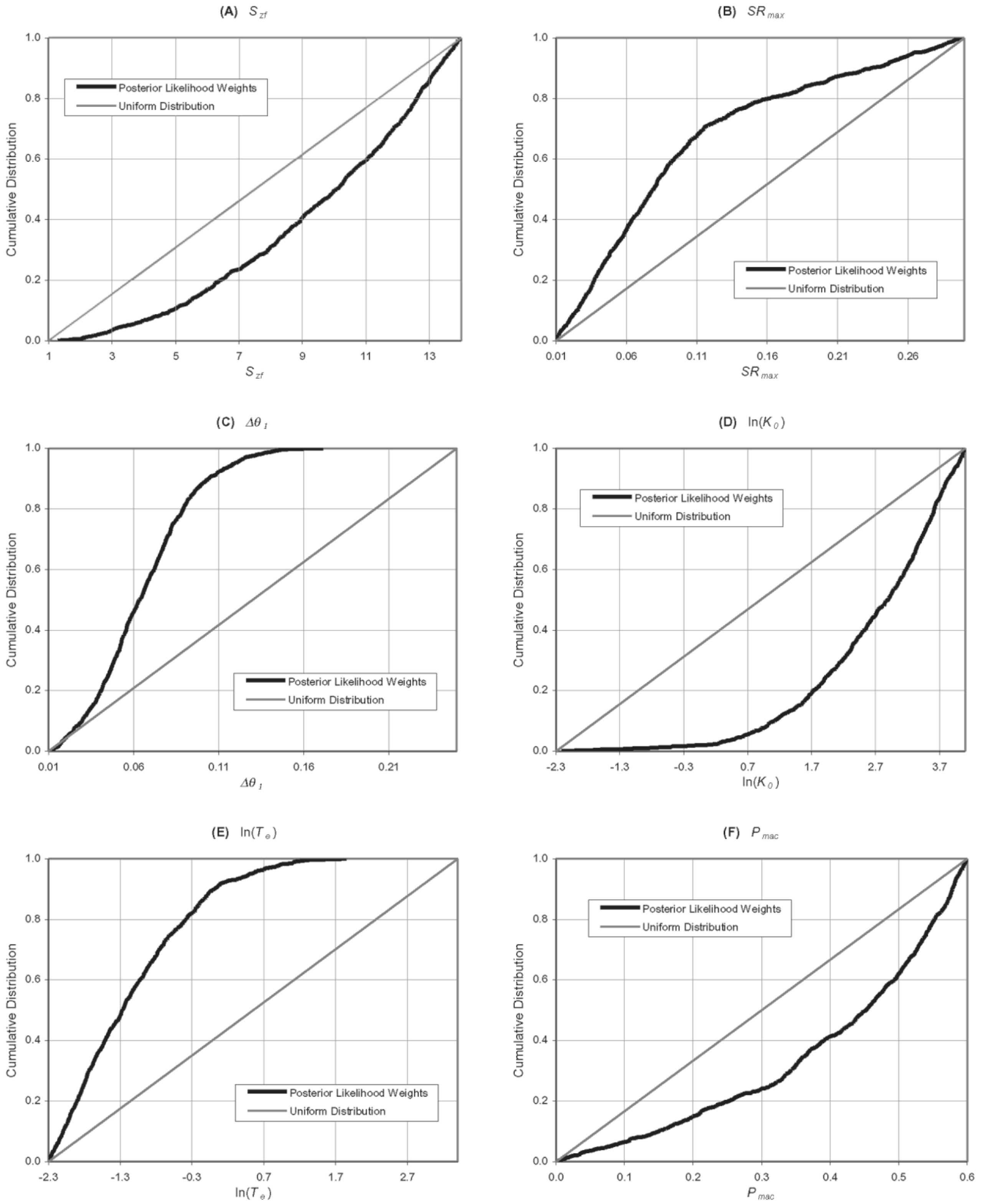


Fig. 5. Cumulative marginal likelihood distributions for all six model parameters from behavioural parameter sets with likelihood weights after updating using all the available discharge data. Uniform distributions across the prior ranges of feasible parameter values for each parameter (see Table 3) are shown to highlight the effects of the conditioning on the individual parameters.

ranges show less sensitivity. Such plots must be interpreted with care, however. The visual impression will depend on the original range of parameters considered, while the value of a parameter that continues to show a uniform marginal distribution may still have significance in the context of a set of values of the other parameters. Experience suggests that fixing the value of such parameters may constrain the performance of the model too much.

7. Conclusions

A generalised likelihood framework has been proposed for the analysis of environmental models and the uncertainty in their predictions. The methodology is extremely simple conceptually and easily implemented for any model that can be feasibly subjected to Monte Carlo simulation. There are a number of subjective elements to the methodology, including the definition of an appropriate likelihood measure (including the specification of non-behavioural models with likelihood zero), and the choice of a way of combining likelihood measures, but these choices must be made explicit and can be therefore subjected to scrutiny and discussion. The problem of equifinality of different model structures and parameter sets is handled naturally within this framework.

Any effects of model nonlinearity, covariation of parameter values and errors in model structure, input data or observed variables, with which the simulations are compared, are handled implicitly within this procedure. In effect, each parameter set within a model structure is handled as a unit. It is possible to calculate likelihood weighted marginal distributions for individual parameters (e.g. Fig. 4) but it is always the performance of the parameter set that is evaluated. The likelihood weighted model simulations can be used to estimate prediction quantiles in a way that allows that different models may contribute to the ensemble prediction interval at different time steps and that the distributional form of the predictions may change (in some cases dramatically) from time step to time step.

A demonstration Windows software package aimed at introducing the GLUE principles, including options for the transformation and combination of likelihood measures, and the types of plots presented in this paper can be downloaded over the Internet from the site http://www.es.lancs.ac.uk/hfdg/hfdg.html

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