

Data-based mechanistic modelling and forecasting of hydrological systems

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ABSTRACT

The paper presents a data-driven approach to the modelling and forecasting of hydrological systems based on nonlinear time-series analysis. Time varying parameters are estimated using a combined Kalman filter and fixed-interval-smoother, and state-dependent parameter relations are identified leading to nonlinear extensions to common time-series models such as the autoregressive exogenous (ARX) and general transfer function (TF). This nonlinear time-series technique is used as part of a data-based mechanistic modelling methodology where models are objectively identified from the data, but are only accepted as a reasonable representation of the system if they have a valid mechanistic interpretation. To this end it is shown that the TF model can represent a general linear storage model that subsumes many common hydrological flow forecasting models, and that the rainfall-runoff process can be represented using a nonlinear input transformation in combination with a TF model. One advantage of the forecasting models produced is that the Kalman filter can be used for real-time state updating leading to improved forecasts and an estimate of associated forecast uncertainty. Rainfall-runoff and flood routing case studies are included to demonstrate the power of the modelling and forecasting methods. One important conclusion is that optimal system identification techniques are required to objectively identify parallel flow pathways.

Key words | data-based mechanistic, flood forecasting, Kalman filter, system identification, nonlinear transfer function, state-dependent parameters

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INTRODUCTION

Many data-driven modelling techniques, such as neural networks, are black-box in nature. Although they provide an important predictive tool in many hydrological applications, they provide little physical insight into the dominant behavioural modes of the system, and are likely to be less robust than models that have a sound physical basis. Time-series analysis has often been used in the modelling and forecasting of hydrological systems since it has some important advantages such as optimal parameter estimation, and an inherently stochastic formulation that allows probabilistic predictions to be easily generated. Time-series modelling techniques are often thought of as black-box techniques and indeed they do provide powerful black-box signal processing methods of interpolation and forecasting (see Young (1999a) for an excellent review

of time-series analysis and forecasting). However, these tools can also be used within a data-based mechanistic (DBM) modelling framework (Young & Lees 1993; Young *et al.* 1996; Young 1998a,b) to produce physically acceptable models, or as a precursor to mechanistic modelling where the data-based mechanistic model indicates the required parsimony of the subsequent mechanistic model.

This paper demonstrates that one time-series model, the general transfer function (TF), can be directly related to well-known hydrological models such as linear reservoir based models, and if an extra step of checking the physical interpretability of the TF model is added to the identification procedure, then the resultant models can be considered to be data-based mechanistic: that is they are objectively identified from the data but are only accepted

as a reasonable representation of the system if they have a valid mechanistic interpretation. Note that this modelling approach is similar to the grey-box modelling methods of Jacobsen & Madsen (1996) and DeMoor & Berckmans (1996). These DBM models retain the forecasting advantages of time-series models but, since they are now constrained during identification to transfer function representations of linear stores in a general cascade/parallel structure, they are likely to be more robust when used in out-of-sample forecasting applications.

A commonly used time-series model in hydrology is the autoregressive exogenous model (ARX: Box & Jenkins 1976); because it is linear in the parameters, the estimation problem can be formulated as a linear regression. However, unless the noise inputs conform to a very restrictive, and in practice rather unlikely, form this method produces biased parameters that are not minimum variance estimates. It is for this reason that although parallel processes in hydrology are intuitively sensible due to different experimentally observed flow pathways, and indeed have been built into numerous conceptual models, it was not until optimal system identification methods such as the refined instrumental variable techniques of Young (1984) were used in conjunction with transfer function models that parallel structures were objectively identified from the data (Young 1992). These linear data-driven modelling techniques have subsequently been used in many other environmental modelling studies to produce models whose physical interpretation has sometimes questioned existing modelling paradigms. A good example of the application of this DBM modelling methodology in the area of water quality modelling is the development of the aggregated dead-zone (ADZ) model of solute transport (Beer & Young 1983; Lees *et al.* 1998a) that helped to objectively reveal the importance of dead-zone processes in the advection-dispersion process of natural channels.

Until recent nonlinear extensions to time-series modelling techniques (Priestly 1988; Young 1993), one disadvantage of linear time-series models in comparison with other data-driven modelling techniques was that they are poor descriptors of the nonlinear processes that are particularly important in the case of rainfall-runoff modelling, owing to the highly nonlinear effect of dynamic contributing areas. Time-series analysis has traditionally been

dominated by the *en-bloc* procedures of Box & Jenkins (1976) that do not provide information on the nature of the model parameter non-stationarity. Several researchers (Priestly 1988; Young 1993) realised that recursive state estimation based on the Kalman filter (Kalman 1960) provides a method of analysing the time-series directly in their non-stationary form so that time varying parameter models can be produced. This then enables state-dependent relations to be examined and finite forms of these parametric relations used to define nonlinear models.

Here, this new state-dependent parameter modelling technique is used to extend the data-based transfer function model to a nonlinear transfer function with the time variable parameters modelled as a generalised random walk class of the stochastic Gauss Markov model. Time variation in parameters could be the result of either changes in the system (e.g. land-use or climatic changes) or nonlinearity. It is well-known that many nonlinear hydrological models can be represented by small perturbation linearised models and that the linearised model parameters can be related to state variables: see for example Perumal (1994) and Camacho & Lees (1999). Therefore the time varying parameters can be considered as state-dependent parameters of a nonlinear model. Estimation of these state-dependent parameters is challenging since they vary rapidly. Two important developments in the identification of state-dependent parameter relations that are described in this paper are fixed-interval-smoothing (FIS) and dependent-state data sorting. FIS, which is a backward pass procedure that is carried out after the forward pass of the Kalman filter, helps to remove the inevitable filtering lag so improving the relation between the estimated variable parameters and states. Dependent-state sorting (Young 1998a) involves sorting the input and output data according to the ranked order of the dependent state so that parameter variations from one sample to the next are reduced, resulting in better defined relations as is demonstrated in one of the case studies described in this paper.

The aim of this paper is to describe these state-of-the-art time-series modelling techniques in the context of hydrological modelling and forecasting, and to illustrate the power of these techniques through rainfall-runoff and

flood routing case studies. The first part of the paper outlines the state-dependent parameter method of non-linear time series analysis, as applied to the dynamic autoregressive exogenous model that is most suitable for flow modelling applications; before describing the general linear transfer function and the associated simplified refined instrumental variable (SRIV) method of optimal parameter estimation. Next, the relation between DBM models and more conventional hydrological models is discussed and methods of real-time forecast updating are described. Finally, two illustrative case studies are presented that utilise the DBM models and associated identification, estimation and forecasting techniques.

NON-STATIONARY TIME-SERIES MODELS

The unobserved components model of Young (1999a) is a very general non-stationary time-series model that can be used in the DBM modelling of a wide range of environmental, biological, mechanical and economic data (Young 1998b). The model can be developed for multivariate systems, but since only univariate systems are considered here, for simplicity the following version is considered,

$$y_t = T_t + C_t + S_t + f(\mathbf{u}_t) + N_t + e_t, \quad (1)$$

where y_t is the observed time-series at the t th sampling instant; T_t is a trend component; C_t is a damped cyclical component; S_t is a seasonal component; $f(\mathbf{u}_t)$ captures the influence of an exogenous variable vector \mathbf{u}_t ; N_t is a stochastic perturbation model, for instance an autoregressive moving average (ARMA) model; and e_t is discrete time white noise with zero mean and variance σ^2 that accounts for any purely random component of the observed data.

For the particular case of hydrological flow systems where there is a clear input-output relation, the best predictive performance is usually obtained by a model that includes the exogenous variable, although good short lead-time forecasts can be derived solely from past flow values. As pointed out by Babovic & Keijzer (1999) in the context of rainfall-runoff modelling this has the advantage

that it does not require input measurements that are seriously affected by spatial measurement errors. However, to produce forecasts at the lead times specified for most operational uses, it is necessary to utilise the delay caused by the time of concentration of a catchment in the generation of forecasts. A useful model in this regard is the multi-input single-output (MISO) dynamic autoregressive exogenous (DARX) model,

$$y_t = \sum_{i=1}^r \frac{B_i(z^{-1})}{A(z^{-1})} u_{i,t-\delta_i} + \frac{1}{A(z^{-1})} e_t, \quad (2)$$

where

$$B_i(z^{-1}) = b_{0,i,t} + b_{1,i,t}z^{-1} + \dots + b_{m_i,t}z^{-m_i} \quad (3)$$

$$A(z^{-1}) = 1 + a_{1,t}z^{-1} + a_{2,t}z^{-2} + \dots + a_{n,t}z^{-n}$$

or in vector-matrix form,

$$y_t = \mathbf{z}_t \boldsymbol{\theta}_t^T + e_t, \quad (4)$$

where

$$\mathbf{z}_t = [-y_{t-1} \dots -y_{t-n} \ u_{1,t-\delta_1} \dots u_{1,t-m_1-\delta_1}] \quad (5)$$

$$\boldsymbol{\theta}_t = [a_{1,t} \dots a_{n,t} \ b_{0,1,t} \dots b_{m_1,t}].$$

Here $u_{i,t}$, $i = 1, 2, \dots, r$ are input variables; the triad $[n, m_i + 1, \delta_i]$ defines the model structure; z^{-p} is the backward shift operator, i.e. $z^{-p}x_t = x_{t-p}$; and $a_{1,t} \dots a_{n,t}$, $b_{0,1,t} \dots b_{m_1,t}$ and are time varying parameters (TVP) that are each defined by a two-dimensional stochastic state vector $\mathbf{x}_{i,t}$ which takes the form

$$\mathbf{x}_{i,t} = \begin{bmatrix} l_t \\ d_t \end{bmatrix}, \quad (6)$$

where l_t is the changing level and d_t is the changing slope of the TVP. The stochastic evolution of the state vector is described by the following generalised random walk process (GRW: Jakeman & Young 1984)

$$\mathbf{x}_{i,t} = \mathbf{F}_i \mathbf{x}_{i,t-1} + \mathbf{g}_i \eta_{i,t}, \quad (7)$$

where

$$\mathbf{F}_i = \begin{bmatrix} \alpha & \beta \\ 0 & \gamma \end{bmatrix}, \mathbf{g}_i = \begin{bmatrix} \chi \\ \varepsilon \end{bmatrix} \quad (8)$$

and $\eta_{i,t}$ is zero mean white noise with variance q_i . This general model comprises as special cases the random walk (RW: $\alpha = \gamma = 1$; $\beta = \varepsilon = 0$), integrated random walk (IRW: $\alpha = \beta = \gamma = \varepsilon = 1$; $\chi = 0$) and smoothed random walk (SRW: $0 < \alpha < 1$; $\beta = \gamma = \varepsilon = 1$; $\chi = 0$), which is an intermediate of the RW and IRW. In practice, the SRW is not often used since it introduces an additional meta-parameter that must be optimised. The use of a stochastic GRW process to describe the evolution of the parameters over time may seem complex, but it is just a statistical mechanism to allow for the estimation of parametric change.

Combining (4) with (7) leads to the following Gauss–Markov (GM) state-space equations,

$$\mathbf{x}_t = \mathbf{F}\mathbf{x}_{t-1} + \mathbf{g}\eta_t \quad (9)$$

$$y_t = \mathbf{H}_t\mathbf{x}_t + e_t$$

where \mathbf{x}_t is the state vector that is formed by concatenation of the $\mathbf{x}_{i,t}$ state vectors; \mathbf{H}_t is an appropriately defined observation vector formed from \mathbf{z}_t ; \mathbf{F} is the state transition matrix that is a block diagonal aggregation of the \mathbf{F}_i matrices; \mathbf{g} is a concatenation of the \mathbf{g}_i vectors; and η_t is an appropriately dimensioned vector of zero mean white noise sequences with covariance \mathbf{Q} that is independent of e_t (see Ng & Young (1990) for a more expansive description of this formulation).

STATE ESTIMATION

Since the DARX model has been formulated as a Gauss–Markov state-space model, a modified Kalman filter (KF) can be used to estimate the states that are actually unknown model parameters. The KF is termed modified because in the standard formulation of the KF the model parameters are known *a priori* and the filter is

then used to calculate state estimates from noise-corrupted measurement data. This is the algorithm used for so-called state updating in hydrological forecasting, as will be demonstrated later. Several researchers (Lee 1964; Young 1970) realised that by reversing the formulation of the Gauss–Markov model with the model parameters now treated as states, modified the KF into a powerful recursive parameter estimator. Where the context of parameter estimation is clear, the states will be referred to as parameter estimates.

The KF (Kalman 1960) can be written as follows:

repeat for $t = 1, 2, \dots, N$

Prediction

$$\hat{\mathbf{x}}_{t|t-1} = \mathbf{F}\hat{\mathbf{x}}_{t-1}$$

$$\mathbf{P}_{t|t-1} = \mathbf{F}\mathbf{P}_{t-1}\mathbf{F}^T + \mathbf{g}\mathbf{Q}\mathbf{g}^T \quad (10)$$

$$\hat{y}_{t|t-1} = \mathbf{H}_t\hat{\mathbf{x}}_{t|t-1}$$

Correction

$$v_t = 1 + \mathbf{H}_t\mathbf{P}_{t|t-1}\mathbf{H}_t^T$$

$$\hat{\mathbf{x}}_t = \hat{\mathbf{x}}_{t|t-1} + \mathbf{P}_{t|t-1}\mathbf{H}_t^T v_t^{-1} [y_t - \hat{y}_{t|t-1}]$$

$$\mathbf{P}_t = \mathbf{P}_{t|t-1} - \mathbf{P}_{t|t-1}\mathbf{H}_t^T v_t^{-1} \mathbf{H}_t\mathbf{P}_{t|t-1} \quad (11)$$

$$\hat{y}_t = \mathbf{H}_t\hat{\mathbf{x}}_t$$

where \mathbf{P}_t is the normalised parameter covariance matrix that is related to the parameter covariance matrix \mathbf{P}_t^* by $\mathbf{P}_t^* = \sigma^2\mathbf{P}_t$; v_t is the normalised output variance that is related to the output variance v_t^* by $v_t^* = \sigma^2v_t$; and \mathbf{Q}_r is defined as the noise variance ratio (NVR),

$$\mathbf{Q}_r = \frac{\mathbf{Q}}{\sigma^2} \quad (12)$$

which reduces the number of metaparameters that have to be optimised without losing any of the flexibility of the original KF algorithm. \mathbf{Q}_r is usually diagonal with a single

NVR specified for each parameter. Increasing the NVR for a particular state has the same effect as increasing the variance of the system noise in relation to the measurement noise, resulting in the error between the estimated output and the actual output having a larger effect on the parameter estimate. The NVR can also be shown to control the weighting effect of the data in the locality of the parameter estimate at sample t on the parameter estimate, with higher NVR values reducing the number of non zero weights (Young 1999a). Note also that the shape of the local weighting effect is controlled by the nature of the GRW with a RW having a Gaussian shape which applies maximum weight to the current data with declining weight each side.

For off-line application the forward pass KF can be combined with a backward pass fixed-interval-smoother (FIS) that produces optimal parameter estimates given all of the data rather than just the data up to sample t . Several FIS algorithms are available, and one that has been found to work well in practice is the following modified Bryson-Frazier fixed-interval smoothing algorithm (Bierman 1973),

repeat for $t = N - 1, N - 2, \dots, 1$

$$\begin{aligned}
 \mathbf{C} &= \mathbf{F}(\mathbf{I} - \mathbf{P}_{t|t-1}\mathbf{H}_t^T\mathbf{v}_t^{-1}\mathbf{H}_t) \\
 \mathbf{a} &= \mathbf{C}^T\mathbf{a} + \mathbf{H}_t^T[y_t - \hat{y}_{t|t-1}]\mathbf{v}_t^{-1} \\
 \mathbf{B} &= \mathbf{C}^T\mathbf{B}\mathbf{C} + \mathbf{H}_t^T\mathbf{H}_t\mathbf{v}_t^{-1} \\
 \hat{\mathbf{x}}_{t|n} &= \hat{\mathbf{x}}_{t|t-1} + \mathbf{P}_{t|t+1}\mathbf{a} \\
 \mathbf{P}_{t|n} &= \mathbf{P}_{t|t-1} - \mathbf{P}_{t|t-1}\mathbf{B}\mathbf{P}_{t|t-1} \\
 \hat{y}_{t|n} &= \mathbf{H}_t\hat{\mathbf{x}}_{t|n}
 \end{aligned} \tag{13}$$

The use of the fixed-interval-smoothing is very important for state-dependent modelling because, as with all filtering techniques, the time variable parameter estimates generated from the forward pass filtering are lagged. This means that any relations between the time varying parameters and states become very ill defined. Another important technique in the identification of state-dependent par-

ameter relations, which is possible if a single state dependent variable is used, is to sort the input and output data into the order of the ranked state-dependant variable (Young 1998a, 1999a). This sorting means that variations in the state-dependent parameter from one data step to the next are considerably smoother, which in turn means that lower NVRs can be specified while still adequately tracking the parameter variations resulting in less noise propagation.

FORECASTS

For on-line forecasting applications the prediction equations on the KF can be employed to calculate f -step-ahead forecasts: $f = 1, 2, \dots$,

$$\begin{aligned}
 \hat{\mathbf{x}}_{t+f} &= \mathbf{F}\hat{\mathbf{x}}_{t+f-1} \\
 \mathbf{P}_{t+f} &= \mathbf{F}\mathbf{P}_{t+f-1}\mathbf{F}^T + \mathbf{g}\mathbf{Q}\mathbf{g}^T \\
 \hat{y}_{t+f} &= \mathbf{H}_{t+f}\hat{\mathbf{x}}_{t+f} \\
 v_{t+f} &= 1 + \mathbf{H}_{t+f}\mathbf{P}_{t+f}\mathbf{H}_{t+f}^T
 \end{aligned} \tag{14}$$

where the forecast variance is given by $v_{t+f}^* = \sigma^2 v_{t+f}$. In on-line forecasting applications σ^2 must also be recursively estimated since it is not known *a priori*. It can be shown (Brown *et al.* 1975) that the variance of the normalised innovations d_n where,

$$d_{n,t} = \frac{y_t - \hat{y}_{t|t-1}}{\sqrt{v_t}} \tag{15}$$

is distributed as a normal Gaussian sequence with zero mean and variance σ^2 . Therefore an estimate $\hat{\sigma}_t^2$ of σ^2 can be obtained from the following recursion (Young 1984)

$$\hat{\sigma}_t^2 = \hat{\sigma}_{t-1}^2 + \frac{1}{t} [d_{n,t}^2 - \hat{\sigma}_{t-1}^2]. \tag{16}$$

METAPARAMETER ESTIMATION

To apply the KF and FIS, values of metaparameters or 'hyper-parameters' such as the elements of the NVR

matrix \mathbf{Q} , and parameters of the GRW need to be specified. As these are not known *a priori* they must be estimated either using modifications to the KF that are termed adaptive filtering (Mehra 1970; Wood & Szöllösi-Nagy 1980) or by using numerical optimisation of an appropriate performance criterion. While adaptive filtering is less computationally demanding, convergence is not guaranteed, and with improvements in computing power and optimisation algorithms, numerical optimisation is now the preferred method. Theoretically a maximum likelihood (ML) approach is most appealing and although it is not possible to form an analytical likelihood function due to the non-stationary nature of the model, prediction error decomposition (Schweppe 1965) leads to the following function based on the KF innovations and output variance which should be *minimised* so as to maximise the likelihood (see also Young 1999a),

$$J = (N-k) \log \left(\frac{1}{N-k} \sum_{t=k+1}^N \frac{d_t^2}{v_t} \right) + \sum_{t=k+1}^N \log v_t, \quad (17)$$

where k is the number of metaparameters.

Numerical optimisation can be performed using well-known local optimisation methods such as the simplex (Nelder & Mead 1965) or global optimisation methods such as the shuffled complex evolution (SCE) method (Duan *et al.* 1993). Since Equation (17) is based on one-step-ahead distribution properties, forecasting performance may be improved by metaparameter optimisation that is based on the root mean squared (f -step-ahead) prediction error, ($RMSE(f)$)

$$RMSE(f) = \left(\frac{1}{N-f} \sum_{t=1}^{N-f} \tilde{y}_{t+f}^2 \right)^{0.5}, \quad (18)$$

where $\tilde{y}_{t+f} = y_{t+f} - \hat{y}_{t+f}$ are the forecast residuals.

GENERAL TRANSFER FUNCTION

Up to this point, discussion has been predominantly related to non-stationary models and methods of par-

ameter estimation for the purpose of state-dependent parameter estimation. If the system is linear, or the non-linearity can be characterised as an input nonlinearity, then it is more efficient to estimate the linear parameters using a recursive least squares algorithm or *en-bloc* variant (see, for example, Young *et al.* 1996). The constant parameter version of the DARX model (the ARX model) could be used, although the autoregressive nature of the noise model is often inappropriate, and unless the actual noise process conforms to this structure the parameters will be biased. A more appropriate model structure is the general transfer function,

$$y_t = \sum_{i=1}^r \frac{B_i(z^{-1})}{A(z^{-1})} u_{i,t-\delta_i} + e_t, \quad (19)$$

where the model components are defined as a constant parameter version of the DARX model (Equation 2). This model is nonlinear in the parameters and must be transformed to the following vector matrix estimation form,

$$y_t = \mathbf{z}_t^T \boldsymbol{\theta}_t + \xi_t, \quad (20)$$

where $\xi_t = A(z^{-1})e_t$. This model is now linear in the parameters, although because the noise entering the system is coloured, the parameters will become biased as the signal:noise ratio reduces. However, one method to ensure unbiased (consistent) parameter estimates is to use an instrumental variable (IV; Young 1970) method of system identification, and in conjunction with data pre-filtering this method produces optimal parameter estimates for this model. Note that work is continuing (Young 1999b) on the development of an IV version of the KF/FIS parameter estimator that will enable optimal estimation of a dynamic transfer function model.

SIMPLIFIED REFINED INSTRUMENTAL VARIABLE PARAMETER ESTIMATION

The simplified refined instrumental variable (SRIV) method of identification and estimation for constant parameter transfer function models (Young 1985, 1991)

uses the following recursive least squares algorithm (Young 1984),

$$\hat{\theta}_t = \hat{\theta}_{t|t-1} + \mathbf{P}_{t|t-1} \mathbf{w}_t^T (1 + \mathbf{z}_t \mathbf{P}_{t|t-1} \mathbf{w}_t^T)^{-1} \times [y_t - \mathbf{z}_t \hat{\mathbf{x}}_{t|t-1}] \quad (21)$$

$$\mathbf{P}_t = \mathbf{P}_{t|t-1} - \mathbf{P}_{t|t-1} \mathbf{w}_t^T (1 + \mathbf{z}_t \mathbf{P}_{t|t-1} \mathbf{w}_t^T)^{-1} \mathbf{z}_t \mathbf{P}_{t|t-1}$$

where the data vectors are defined as follows,

$$\mathbf{z}_t = [-y_{t-1}^* \dots -y_{t-n}^* u_{i,t-\delta_i}^* \dots u_{i,t-m_i-\delta_i}^*] \quad (22)$$

$$\mathbf{w}_t = [-w_{t-1}^* \dots -w_{t-n}^* u_{i,t-\delta_i}^* \dots u_{i,t-m_i-\delta_i}^*]$$

in which w_t is the *instrumental variable*, defined as an estimate of the noise free system output and obtained from the following adaptive auxiliary model,

$$w_t = \sum_{i=1}^r \frac{\hat{B}_i(z^{-1})}{\hat{A}(z^{-1})} u_{i,t-\delta_i} \quad (23)$$

Here, the polynomials $\hat{A}(z^{-1})$ and $\hat{B}_i(z^{-1})$ are adaptive estimates of the TF model polynomials; and the star superscripts indicate that the associated variables are adaptively pre-filtered in the following manner,

$$y_t^* = \frac{1}{\hat{A}(z^{-1})} y_t; \quad u_{i,t}^* = \frac{1}{\hat{A}(z^{-1})} u_{i,t}; \quad w_t^* = \frac{1}{\hat{A}(z^{-1})} w_t \quad (24)$$

The adaption of both the auxiliary model and prefilters is performed within a three-step iterative procedure (Young 1984, 1991; Jakeman & Young 1984) and, at the end of the final iteration, the estimated parameter vector $\hat{\theta}_N$ is returned along with standard errors that can be calculated from the covariance matrix $\mathbf{P}_N^* = \sigma^2 \mathbf{P}_N$ (Young *et al.* 1996).

The SRIV algorithm is asymptotically optimal in a maximum likelihood sense if the noise e_t is serially uncorrelated white noise with a Gaussian amplitude distribution. If the noise is not white but can be assumed to follow an ARMA process, then the related but more complex refined instrumental variable (RIV) algorithm (Jakeman & Young 1984) is optimal and can be used instead. However, the IV aspect of the analysis ensures that the SRIV estimate $\hat{\theta}_N$ is always consistent, provided

the IV assumptions are applicable (e.g. Young 1984). Moreover, experience over many years suggest that the SRIV algorithm is very robust in practice and often yields good results when the more sophisticated RIV algorithm (and other related optimal algorithms, such as the ML approach of Box & Jenkins 1976) fail to yield acceptable models because of their need to *simultaneously* estimate the noise process.

MODEL ORDER IDENTIFICATION

Model order identification is based around the coefficient of determination, R_T^2 and the heuristic *YIC* criterion, which are defined as follows,

$$R_T^2 = 1 - \frac{\sigma^2}{\sigma_y^2}, \quad (25)$$

where σ_y^2 is the variance of the output time-series, and

$$YIC = \ln \left(\frac{\sigma^2}{\sigma_y^2} \right) + \ln \left(\sum_{i=1}^{np} \frac{\sigma^2 p_{ii}}{\hat{\theta}_i^2} \right), \quad (26)$$

where $np = n + m$ is the number of estimated parameters in the θ vector; $\sigma^2 p_{ii}$ is an estimate of the variance of the estimated uncertainty on the i th parameter estimate; and $\hat{\theta}_i^2$ is the square of the i th parameter in the θ vector.

The coefficient of determination R_T^2 is a statistical measure of how well the model explains the data: if the variance of the model residuals σ^2 is low compared with the variance of the data σ_y^2 , then R_T^2 tends towards unity; while if σ^2 is of similar magnitude to σ_y^2 then it tends towards zero. Note, however, that R_T^2 is based on the variance of the model residuals and it is *not* the more conventional coefficient of determination R^2 based on the variance of the one step ahead prediction errors: this is because R_T^2 is a more discerning measure than R^2 for TF model identification: while it is often quite easy for a model to produce small one step ahead prediction errors, since the model prediction is based on past measured values of the output variable y_t , it is far more difficult for it to yield small model response errors, where the model output is based only on the measured input variable u_t and does not refer to y_t .

The *YIC* is a more complex criterion that provides a measure of the balance between model fit and over-parameterisation. From the definition of R_T^2 it can be seen that the first term is simply a relative measure of how well the model explains the data: the smaller the model residuals the more negative the term becomes. The second term, on the other hand, provides a measure of model parsimony since as a model becomes over-parametrised the parameter covariance increases in value, often by several orders of magnitude, resulting in less negative values. Although heuristic, the *YIC* has proven very useful in practical identification terms over the past 10 years (see, for example, Young 1992; Young & Lees 1993).

ON-LINE UPDATING

If the forecasting model is either linear or nonlinear where the nonlinearity takes the form of an input nonlinearity, then state updating can be performed using the KF in its original form where the states are now model states rather than parameters, and the constant parameters are contained in the state equation transformation matrices. The general transfer function model can be formulated as the following GM state space equations,

$$\mathbf{x}_t = \mathbf{F}\mathbf{x}_{t-1} + \mathbf{G}\mathbf{u}_t + \boldsymbol{\eta}_t \quad (27)$$

$$y_t = \mathbf{H}\mathbf{x}_t + e_t$$

where \mathbf{x}_t is the state vector; \mathbf{u}_t is the input data matrix; \mathbf{H} is the observation vector; \mathbf{F} is an appropriately defined matrix containing the TF denominator parameters; \mathbf{G} contains the TF numerator model parameters, and $\boldsymbol{\eta}_t$ and e_t are as defined previously. Note that the KF prediction Equations (10) and the forecasting Equations (14) must be slightly modified to incorporate the $\mathbf{G}\mathbf{u}_t$ term. Until recently, a major practical problem in the application of the KF for real-time state updating has been determination of the NVRs which have an important effect on the updating performance since the values of the NVRs control the behaviour of the filter: if the NVRs are specified as too high, then the state estimate will be overly

influenced by the noise corrupted output, resulting in poor forecasts. However, numerical optimisation based on the $RMSE(f)$ criterion (Equation 18) provides an objective method of calibrating the NVR on historical data. This procedure is computationally intensive but since it is an off-line operation it has no impact on the use of the optimised KF on-line.

Parameter updating can also be performed using an on-line version of the KF to estimate real-time variable model parameter estimates (Equations 10 & 11). However, in practical applications (Lees *et al.* 1994), due to the limited information content of the data, it has been found to be more robust to estimate a single adaptive gain parameter g_t where the adaptive model can be defined as,

$$y_t = g_t \frac{B(z^{-1})}{A(z^{-1})} u_{t-\delta} + e_t \quad (28)$$

and the Gauss–Markov state equations required for input to the KF are a single parameter variant of (Equation 9) where the state equation is defined as a GRW and the observation vector contains outputs of the stationary forecast model.

State and parameter updating can be combined where parameter updating is used to correct long-term changes in the system caused by physical changes such as land-use changes in the case of rainfall-runoff modelling, or channel properties in the case of flood routing, and state-updating is used to incorporate past observations into forecasts in an optimal manner. This combined approach has been successfully used in practice in the Dumfries flood forecasting system (Lees *et al.* 1994).

DATA-BASED MECHANISTIC MODELLING AND FORECASTING METHODOLOGY

It is suggested that the DBM modelling methodology for input–output systems should be done in the following steps:

1. Identification and estimation of a linear TF model using the SRIV algorithm and associated identification criteria.

2. Visual examination of the model fit and residuals along with standard residuals tests such as calculation of the autocorrelation function. If the model fit is satisfactory and the properties of the residuals conform to white noise proceed to step 7.
3. Identify several different DARX models (as suggested by the identified linear TF structures) with all parameters modelled as GRW stochastic processes and the metaparameters estimated using numerical optimisation. If some parameters do not vary significantly, repeat the procedure with those parameters modelled as constant parameters, *i.e.* set their respective NVRs to zero.
4. Investigate state-dependent parameter relations using scatter plots.
5. If a single relationship emerges, repeat the TVP estimation with the data processed in order of the ranked dependent state to improve the state-dependent parameter relation.
6. In the case of gain nonlinearities, reformulate the model as an input-nonlinearity combined with a linear TF model and identify the TF model structure and estimate the parameters using the optimal SRIV method of system identification.
7. Investigate the physical interpretation of the different resultant models and favour any model that has a sensible mechanistic interpretation over models of equal in-sample predictive performance.
8. Calibrate the KF state updating algorithm on the calibration data if real-time forecasts are required. Investigate the additional use of on-line parameter adaptation to track slowly varying system changes.
9. Verify the models on a data period that is independent of the calibration period, and evaluate the real-time forecasting performance.

In cases where measured data are not available, the DBM techniques can still be used to investigate the dominant mode behaviour of systems. This is performed by experimentation on mechanistic models where the model is perturbed and output data collected. The techniques described in this paper are then used to investigate the dominant system processes and this information can then be used to guide the development of parsimonious mechanistic models. As a caveat here it should be noted that

care should be taken not to remove processes from the model that may be important during situations outside those captured in the calibration data. For instance, the snow-melt component of a rainfall-runoff forecasting model will obviously be unidentifiable if no snow fall is recorded during the calibration data period.

DATA-BASED MECHANISTIC HYDROLOGICAL MODELS

One of the major advantages of the TF over other conceptual hydrological models is that the structure is objectively identified as part of the modelling procedure so resulting in parsimonious models. At first sight to many hydrologists, this feature places the TF in the group of 'black-box' models along with neural network models since the estimated model parameters do not appear to have a physical interpretation. Indeed, identified TF models can have characteristics such as oscillatory responses that are clearly unacceptable given our current knowledge of hydrological processes. However, as suggested in the DBM modelling methodology, an investigation of any identified models for physical interpretation should also be performed prior to acceptance of the TF as a predictive model of the system. At this stage it is useful to examine the relation between certain single-input single-output (SISO) TF model structures, as defined by the triad $[n, m + 1, \delta]$, with more traditional rainfall-runoff models. It is easy to show that discretisation of the well-known linear storage model,

$$\frac{dQ}{dt} = \frac{1}{T} [u(t) - Q(t)], \quad (29)$$

where $Q(t)$ is the outflow at time t ; $u(t)$ is the inflow at time t ; and T is the residence time, results in the following first-order discrete TF $[1, 1, 0]$,

$$Q_t = \frac{b_0}{1 - a_1 z^{-1}} u_t; \quad b_0 = \frac{\Delta t}{T}, \quad a_1 = 1 - \frac{\Delta t}{T}, \quad (30)$$

where Δt is the discretisation step size. Introducing a lag element δ results in a TF with $[1, 1, \delta]$ structure that can

be rearranging into the following difference equation form,

$$Q_{t+\delta} = b_0 u_t + a_1 Q_{t+\delta-1}, \quad (31)$$

revealing that the model is identical to commonly applied flood forecasting models such as the linear input-storage-output (ISO; Lambert 1972). Using block diagram analysis it is easy to show that the SISO version of the transfer function model (Equation 19) can represent any combination of linear storage models as defined by (Equation 31) as is shown in Figure 1. To decompose an identified TF into its constituent linear storage structures requires partial fraction expansion (see Young 1992). Note that the transfer function is not constrained to the linear storage parameter relation $a_1 = 1 - b_0$, *i.e.* mass can be generated or lost: this is a very useful feature in cases where additional inflow such as flow from ungauged tributaries or lateral inflow occurs, as is demonstrated in the flood routing case study described below.

Having ascertained that the SISO TF can be considered to be a representation of common conceptual hydrological models questions the usefulness of the TF approach. However, as demonstrated in earlier sections, there are several advantages in posing the modelling problem in TF form including the availability of powerful system identification techniques for optimal parameter estimation; the ability to use state estimation methods to improve on-line forecasts; and increased structural flexibility. In particular, most simple conceptual and unit hydrograph based models do not attempt to include base-flow as an integral model component although it is well known that second-order flow dynamics can represent an important component of flood flows. TF modelling objectively reveals the most appropriate model structure for the

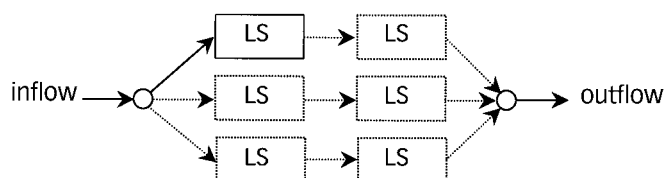


Figure 1 | General linear storage model.

study catchment as part of the modelling procedure, and the majority of cases studied so far suggest that the most appropriate structure is second order which can be decomposed into two linear stores representing ‘quick’ and ‘slow’ flow processes. This parallel storage structure is a common feature of several accepted rainfall-runoff models including PDM (Moore 1985) and IHACRES (Jakeman & Hornberger 1993).

The rainfall runoff process is inherently nonlinear owing to antecedent catchment wetness and the effect of dynamic contributing areas on runoff production. Some operational flood forecasting models ignore this non-linearity, instead relying upon real-time model correction, while many incorporate very simple rainfall loss methods of calculating an effective rainfall for input to the routing component of the model (e.g. RORB, Mein *et al.* 1974). The first nonlinear extension of a TF based rainfall runoff model, which is presented in Whitehead *et al.* (1979), consists of a rainfall pre-processor that calculates effective rainfall (er) as the product of rainfall (r) with a catchment wetness index (CWI) that is simply filtered rainfall,

$$er_t = r_t \times CWI_t; \quad CWI_t = \frac{1}{1+a_1 z^{-1}} r_t. \quad (32)$$

Here a_1 is related to the time constant (memory) of the filter through,

$$T_c = \Delta t / \ln(-a_1). \quad (33)$$

This rainfall loss function is closely related to the antecedent precipitation method of effective rainfall calculation since it can be shown that the output of a first-order filter is the summation of exponentially weighted past inputs. Extensions to this loss function have since been made to incorporate the effects of long-term changes in evaporation resulting in the IHACRES model (Jakeman & Hornberger 1993), which is one example of a new class of hybrid conceptual-metric (HYCOM) continuous simulation models that combine various conceptual loss functions with a metric TF routing model (Wheater *et al.* 1993; Lees *et al.* 1998b).

While a conceptual loss function is required for simulation purposes, in real-time flow forecasting applications measurements of antecedent flow are likely to provide

a better indicator of catchment wetness than the output from a model. Young & Beven (1994) propose the following simple loss function,

$$er_t = r_t \times Q_{t-\tau}^\alpha, \quad (34)$$

where τ is a shift parameter that is usually zero, and α is optimised using a nonlinear numerical optimisation method such as the simplex method. Excellent results have been reported for this loss function in a number of applications when it is combined with a parallel structure TF model (e.g. Young *et al.* 1997).

Obviously the power law form of this loss function is *subjective* and many other forms could be appropriate according to the specific catchment characteristics. The form of this nonlinearity can be objectively identified using the state-dependent modelling technique outlined in this paper using the DARX model (Equation 2). Relations between parameter variations and states provide a non-parametric representation of the nonlinearity. For example, it has been found that for the rainfall-runoff case the numerator parameter of a first-order model varies with flow in a manner that can often be approximated as a power law relation, and since this parameter acts solely on the input variable, the nonlinearity can be simplified to an input form. Although state-dependent parameter modelling provides an objective method of identifying the nature of the rainfall-runoff nonlinearity, at this point in time, due to the complexity of the methodology, it is more useful as a research tool to investigate the nature of other suitable nonlinear functions that would then be optimised using simpler numerical optimisation techniques. Note that there are clear parallels here between the nature of this nonlinearity and the dynamic contributing area concept of models such as PDM (Moore 1985) and TOPMODEL (Beven & Kirkby 1979).

REAL-TIME FLOOD FORECAST UPDATING

It has long been recognised by researchers that on-line forecast correction using the latest available flow data should be an important component of a real-time flood

forecasting system. However, with a couple of notable exceptions, many areas of the UK currently rely on forecasting systems that do not have any mechanism for the automatic real-time correction of flood forecasts. Although experienced operators can take account of systematic errors in hindcasts there is a concern that errors can be made under the pressurised conditions that occur during flooding events.

A number of different correction techniques exist that attempt to improve forecasts by examination of past forecast performance, and as such they can be thought of as an automation of the intuitive correction applied by a human operative. Most techniques can be classified as either state updating, parameter updating or error prediction methods. Error prediction methods can be applied to any type of forecasting model since they are based on the time-series modelling of the forecast error series (Bell & Moore 1998). State updating and parameter updating can be performed using a Kalman filter if the model is linear, or by an extended Kalman filter (EKF) if the model is nonlinear (Wood & Szöllösi-Nagy 1980). Bell & Moore (1998) also present an empirical state updating method for nonlinear forecasting models.

The TF model has the advantage that it can be easily converted to the Gauss-Markov (GM) state space Equations (27) and therefore the KF can be used to estimate an optimal state estimate, which in this case is flow. One major advantage of formulating the TF model as a stochastic GM model is that probabilistic forecasts are also produced by the KF. This capability could be of great potential use as an automated measure of forecast confidence since the KF generated uncertainty mimics an experienced operative's intuition as it is driven by past forecast performance. A common simplification of the KF state-updating technique is state replacement where the latest available flow measurements replace model output in forecast calculations. For example, the state updated forecasts for a first-order model with a 2 sample lead time can be calculated at each step by,

$$\hat{Q}_{t+1} = a_1 Q_t + b_0 u_{t-1} \quad (35)$$

$$\hat{Q}_{t+2} = a_1 \hat{Q}_{t+1} + b_0 u_t$$

where \hat{Q}_t is the flow forecast and Q_t is the measured flow. This method is of course equivalent to KF state updating with the NVR set to a large value such that the KF estimate closely tracks the output. Although this technique is very simple, it has the disadvantage that probabilistic forecasts are no longer produced.

Parameter updating refers to the on-line estimation of model parameters using a recursive estimator such as the KF with the state vector now containing the parameters. Owing to the limited information content contained within individual flood events, it is not possible to robustly estimate very many model parameters on-line. In many situations it is sufficient to estimate a scalar gain parameter that does not change the 'shape' of the hydrograph but simply shifts the output up or down (see Equation 28). Lees *et al.* (1994) report a successful application of adaptive gain updating to an operational TF based flood forecasting system for Dumfries in south-west Scotland.

CASE STUDY I: RAINFALL-RUNOFF MODELLING

To demonstrate the performance of the nonlinear rainfall-runoff model and different system identification techniques, a limited modelling exercise has been performed using data from the River Hafren, Plynlimon, Wales (Figure 2). This catchment, which is one of the UK Institute of Hydrology's experimental catchments, has been selected since the rainfall-runoff response is similar to many fast-responding UK catchments where production of flood forecasts typically relies on a rainfall-runoff model. Details of the catchment's climatic régime, geology and instrumentation can be found in Foster *et al.* (1997). Calibration was carried out on a 4 month period of hourly data between January and March 1994, and verification on a 4 month period between November 1994 and February 1995: see Figure 3. Winter periods, where the effects of evaporation do not influence the runoff significantly, have been selected since the purpose of the modelling here is for flood forecasting.

Initial linear TF identification using the SRIV method indicated that a first-order model with a 1 hour lag is the

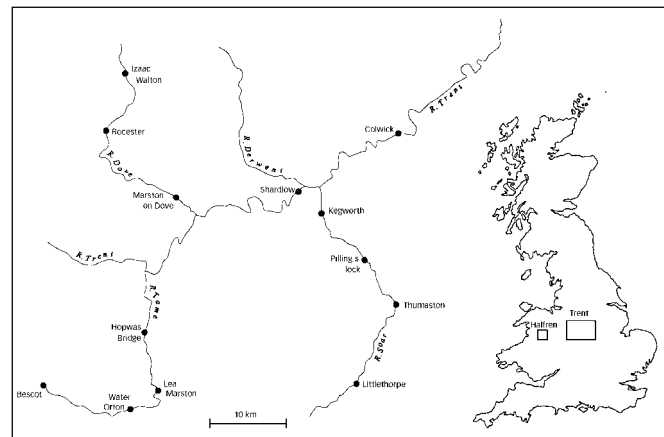


Figure 2 | River Trent catchment gauging stations and (inset) the Trent and Hafren locations.

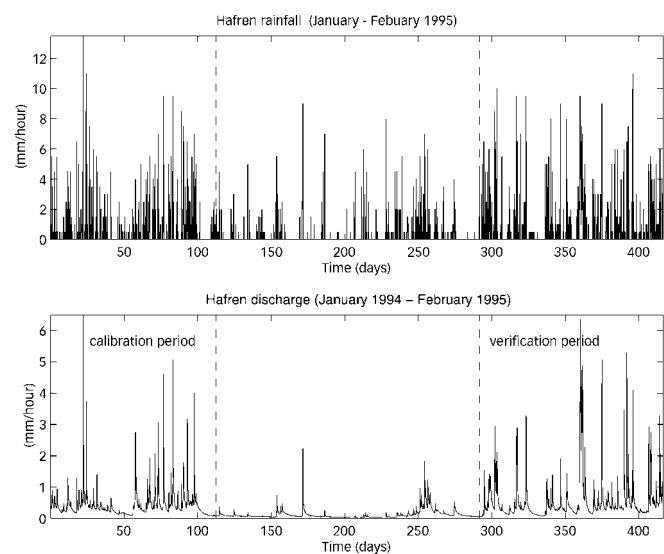


Figure 3 | Hafren rainfall and discharge.

most appropriate TF structure. This model explains approximately 75% of the runoff variance, although examination of the model fit shown in Figure 4 reveals that peak flows are significantly under-estimated, and the base-flow discharge component is very poorly modelled with the model flow tending to zero during dry periods. This lack of performance is caused by a combination of the inappropriateness of a linear model and the failure to identify a second-order (parallel) TF. Next, as suggested by previous DBM rainfall-runoff modelling studies (Young

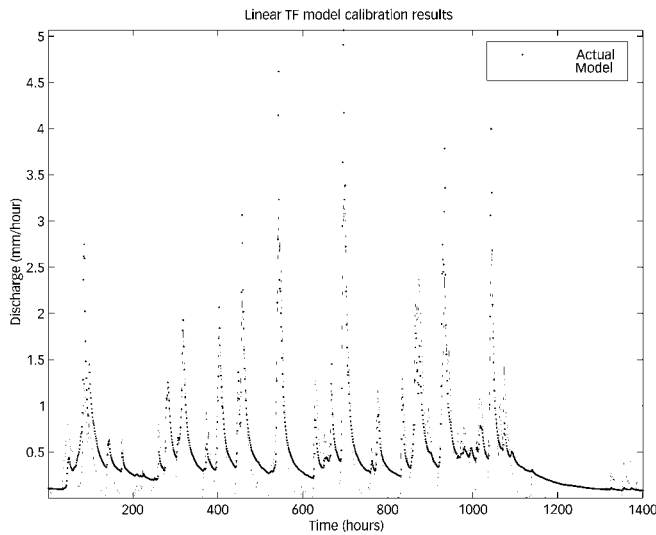


Figure 4 | Model fit for the best identified linear TF model.

1993; Young & Beven 1994), a time variable parameter DARX model is estimated with the b_0 parameter modelled as a RW process while the a_1 parameter is estimated as a constant parameter. Figure 5 shows the results of different variants of the state-dependent modelling procedure to show the importance of state-dependent sorting and fixed-interval-smoothing: Figure 5a shows the state-dependent relation produce by the Kalman filter with the data processed in time sequence; Figure 5b shows the same relation but with the data sorted according to the dependent state which is flow in this case; and Figure 5c shows the state-dependent relation using the Kalman filter with FIS and sorted data. It can be clearly seen that sorting the data according to the dependent-state results in a dramatically improved state-dependent parameter relation and that FIS also reduces the scatter considerably. Figure 5d, which shows the NVR optimisation results for the state parameter sorted and time ordered variants, reveals that the optimum NVR for the sorted data method is significantly lower. Since the data are sorted, changes in the variable parameter estimate from one step to the next are relatively small, and therefore the memory of the state estimator can be increased resulting in reduced noise propagation into the parameter estimates, and therefore improved state-dependent parameter relations. Figure 5e,

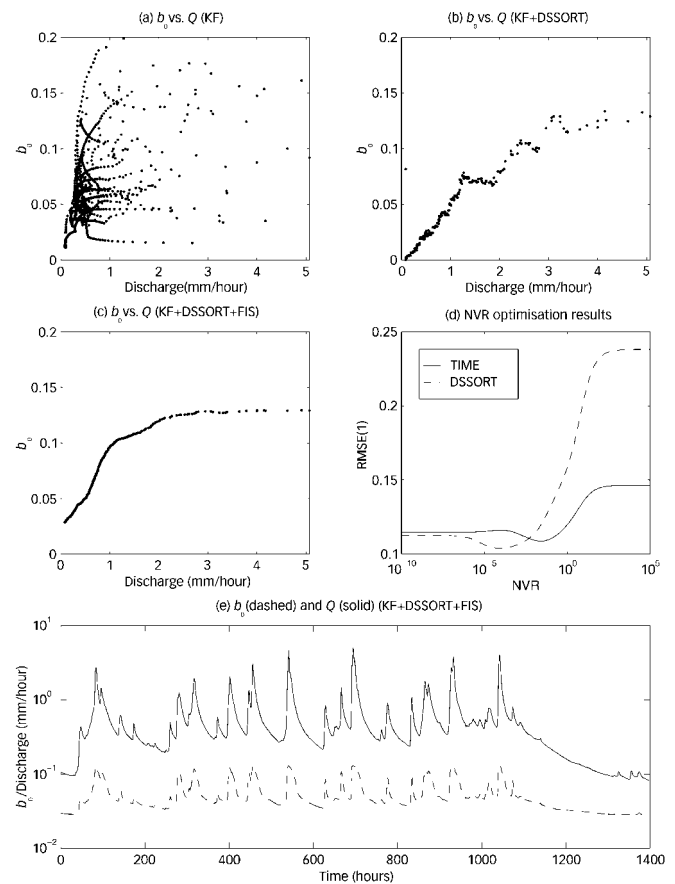


Figure 5 | State-dependent parameter estimation results: KF, Kalman filter; DSSORT, dependent-state sorting; FIS, fixed-interval-smoothing.

which shows the variable parameter estimate and the state re-ordered into time sequence after state ordering, reveals the clear relation between discharge and the b_0 parameter that controls the model gain, and that this relation is nonlinear with a cut-off point that can be interpreted as the point of catchment saturation, *i.e.* all rainfall is effective. Note that it was found that the $RMSE(1)$ based metaparameter optimisation method produced better predictive models in this application than the ML method that produced a higher estimated NVR.

Since the identified state dependent in this case is a gain nonlinearity, the overall nonlinear model can be represented as a TF model with an input nonlinearity. This reformulation allows the use of SRIV system identification to objectively identify the routing model structure and

Table 1 | ARX identification results.

Model [<i>n</i> , <i>m</i> +1, <i>d</i>]	<i>YIC</i>	R_T^2
1,1,1	- 6.6822	0.8182
1,2,1	- 4.9639	0.8398
2,2,1	- 4.0607	0.8344
3,1,1	- 3.7846	0.8191

Table 2 | SRIV TF identification results.

Model [<i>n</i> , <i>m</i> +1, <i>d</i>]	<i>YIC</i>	R_T^2
1,1,1	- 9.2241	0.8060
1,2,1	- 8.6000	0.8563
2,2,1	- 8.4761	0.8912
2,3,1	- 4.6898	0.8921

estimate the parameters. In order to investigate the difference in performance of an ARX model estimated using a constant parameter version of the KF and a TF model estimated using the SRIV algorithm, both modelling techniques were applied to the data where the rainfall data are transformed to effective rainfall as follows,

$$er_t = f(Q_t) \times r_t, \quad (36)$$

where $f(Q_t)$ is a finite form of the state-dependent relation shown in Figure 5c calculated using piece-wise linearisation. This method of fitting a relation has been found to be more flexible than previously used polynomial and power relations. Many model structures ranging from [1, 1, 0] to [3, 3, 3] were searched and identification results for the best four models are shown in Tables 1 and 2. The SRIV identification results reveal that the best model according to the *YIC* criterion is a first-order model [1, 1, 1]. However, the second-order model [2, 2, 1], has a significantly improved fit with a slightly higher *YIC*. The fact that this

model has two extra parameters and yet has only a slightly smaller *YIC* indicates that the parameters are estimated with certainty. Examination of the model fit shown in Figure 6 reveals that the second-order model is far superior with the recession component of the hydrographs well reproduced. The estimated second-order model takes the form,

$$\hat{Q}_t = \frac{1.7593(0.0018) - 1.6769(0.0014)z^{-1}}{1 - 1.5602(0.0003)z^{-1} + 0.5685(0.0002)z^{-2}} er_{t-1}, \quad (37)$$

where the parameter standard errors are given in parentheses. Verification of this model over the 4 month period from November 1994 to February 1995 results in an excellent model fit of $R_T^2 = 0.8681$ indicating that the model is robust. Partial fraction expansion of the second-order transfer function (Young 1992) results in the following parallel structure,

$$\hat{Q}_t = \frac{1.6404}{1 - 0.5800z^{-1}} 0.39er_{t-1} + \frac{0.1189}{1 - 0.9802z^{-1}} 0.61er_{t-1}, \quad (38)$$

where each first-order transfer function can be considered to be a linear store with 'quick' flow passing through one store and 'slow' flow through the other store. The time constants are calculated using Equation (33) as 1.83 hours for the quick store and 50 hours for the slow store with 61% of flow passing through the slow store.

In contrast to the SRIV identification results, the ARX results given in Table 1 reveal that none of the identified models are as well identified as the TF model as indicated by the higher *YIC* values. Also, there is no clear difference in terms of performance of the second-order model over the first-order model. Examination of the second-order model fit shown in Figure 7 reveals that the model is failing to capture the parallel flow dynamics in this case. The estimated second-order model is,

$$\hat{Q}_t = \frac{1.0725(0.0200) - 0.7952(0.0216)z^{-1}}{1 - 1.3637(0.0110)z^{-1} + 0.4148(0.0080)z^{-2}} er_{t-1}. \quad (39)$$

Note that the parameter standard errors are one order of magnitude larger than the SRIV identified model parameters.

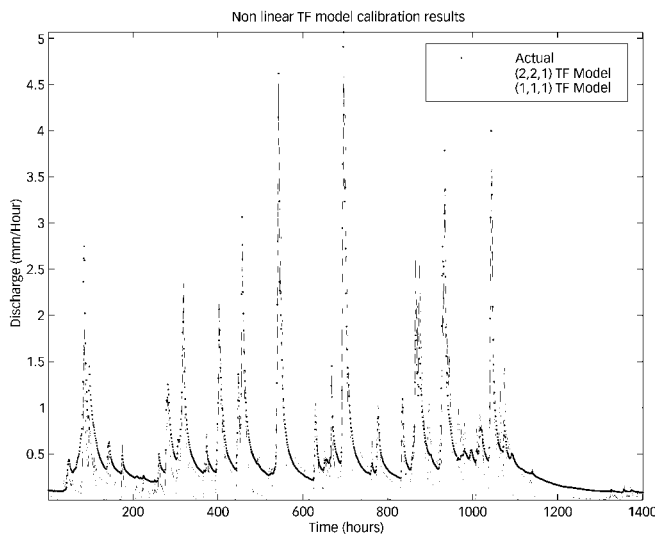


Figure 6 | Model fit comparison of first- and second-order nonlinear TF models.

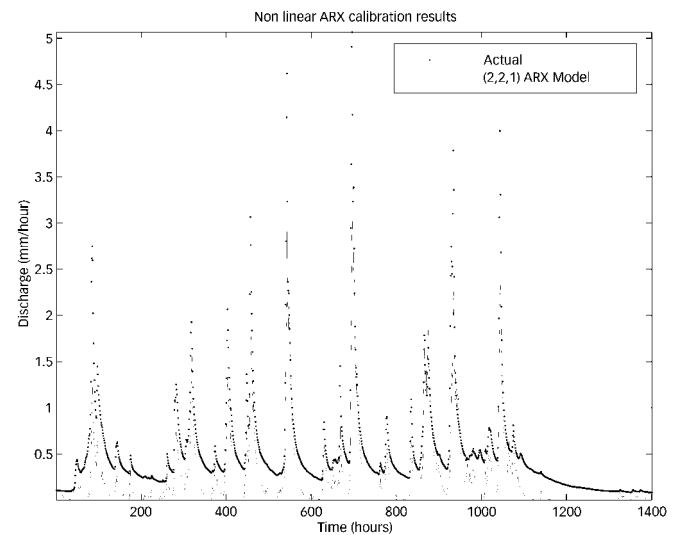


Figure 7 | Second-order ARX model fit.

CASE STUDY II: FLOOD ROUTING

Linear stores are a central component of several popular flood-routing techniques such as the Kalinin–Milyukov (Kalinin 1971) and Muskingum–Cunge (Cunge 1969) methods. It is an accepted fact that the propagation of a flood wave is a nonlinear process and therefore application of the linear models previously described may result in crude approximations of actual waves, particularly under conditions dominated by high resistance effects. Recently, these models have been extended into a nonlinear form where the parameters vary with flow producing a better representation of the flood routing dynamics: see for example Perumal's (1994) multilinear discrete lag-cascade model. Typically flood-routing model parameters are derived from hydrogeometric characteristics such as channel dimensions, slope and roughness (Dooge 1986). While this approach is attractive for situations where upstream and downstream discharge data are not available, if these data are available, data-driven modelling techniques such as those described in this paper are likely to provide improved forecasts, especially if real-time updating is employed. To illustrate the application of the data-based mechanistic modelling methodology to flood forecasting, this section outlines a typical flood routing case study.

Data for one year of hourly discharges from the Shardlow (*S*) gauging station on the River Trent in England are available along with data from two gauging stations approximately 50 km upstream: Izaak Walton on the River Dove (*IW*) and Hopwas Bridge on the River Tame (*HB*). The river network and location are shown in Figure 2. Examination of the data shown in Figure 8 reveals that the volume of the combined input discharges is significantly below the output discharge, indicating the important contribution of flow from the ungauged River Trent and possibly lateral inflow in this case. It can also be clearly seen that there is a significant anthropogenic effect on discharge in the River Tame in the form of a diurnal cycle that is probably the result of effluent discharges. The first half of the data are used for calibration and the second half for model verification.

Model identification proceeds with the estimation of a large number of model structures of the 2 input 1 output variant of the MISO TF model (Equation 19) using the SRIV algorithm. The best identified model with a *YIC* of -9.4636 and a R_T^2 of 0.9605 is,

$$\hat{S}_t = \frac{0.1439(0.00002)}{1-0.8652(0.00002)} HB_{t-8} + \frac{1.3543(0.00204)}{1-0.8652(0.00002)} IW_{t-8}. \quad (40)$$

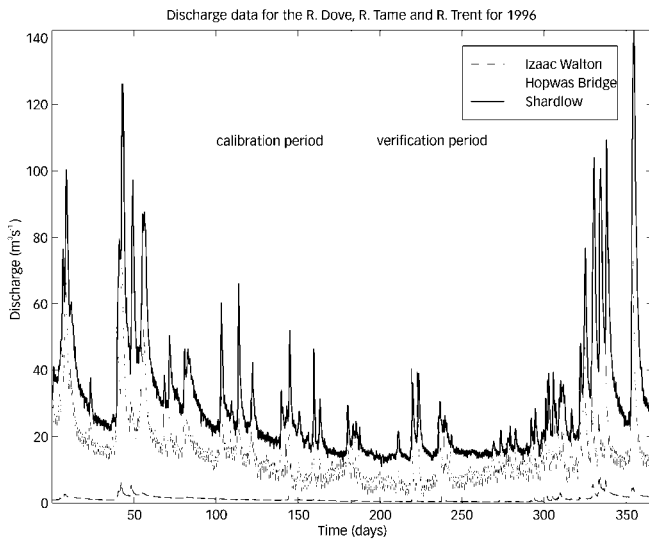


Figure 8 | Trent catchment discharge data.

Although the model fit is excellent in terms of explanation of output variance, examination of the model fit and residuals indicates a systematic under-estimation of peak flows. Figure 9, which shows the model fit over the period of highest flow, confirms that on the whole the model fit is excellent but that there is an underestimation of peaks. This discrepancy could result from the use of a rating curve which, as with most rating curves, is more uncertain at high flows, but analysis will proceed under the assumption that there is no systematic measurement error present.

The next stage in the modelling procedure is to fit a time variable parameter model to the data in order to investigate any state-dependent parameter relations. First, to simplify this procedure, the MISO transfer function is converted to an equivalent SISO form through combination of the input discharges according to their relative steady state gains (SSG, which is calculated by setting $z^{-P} = 1$ in the TF model). State-dependent parameter modelling where the b_0 parameter is allowed to vary produces a well-defined linear state-dependent relation between the b_0 parameter and lagged downstream discharge, with an increasing gain with flow. This can be approximated in finite form as the following linear equation,

Table 3 | Comparative modelling and forecasting results.

Model	Calibration		Verification: 8-hour forecasts	
	R_T^2	Peak Error [m^3/s]	R_T^2	Peak Error [m^3/s]
Linear TF	0.9605	8.2928	0.9254	24.303
Input NL TF	0.9670	1.4270	0.9432	11.450
Full NL TF	0.9674	2.0545	0.9513	14.320

$$b_0 = 0.0002 \times S_{t-8} + 0.1327. \quad (41)$$

Treating the state-dependent nonlinearity as an input nonlinearity and estimating the linear transfer function using the SRIV algorithm results in the following nonlinear transfer function model,

$$\hat{S}_t = \frac{1.1166(0.00073)}{1-0.8493(0.00001)} [(0.0002 \times S_{t-8} + 0.1327) \times \{HB_{t-8} + 9.4903IW_{t-8}\}]. \quad (42)$$

Figure 9 shows the significant performance improvement at peak flows of the nonlinear TF model, especially for the largest flow peak. State-dependent parameter modelling was also carried out with both the a_1 and b_0 parameters allowed to vary. Again good relations with flow resulted, with the b_0 parameter increasing with flow and the a_1 parameter reducing with flow. However, as indicated by the model fit given in Table 3, the model performance is little improved over the input-nonlinear model. Also, examination of the variation in time constant and SSG with flow reveals that the SSG increases with flow in a linear fashion and that the changes in the time constant are minimal. The most likely physical interpretation here is that there is an increasing contribution to outflow from lateral inflow as discharge increases.

Verification results, also given in Table 3, and shown in Figure 9 for the highest verification flow period, reveal a similar trend to the calibration results with all the models recording similar R_T^2 values but with the nonlinear models

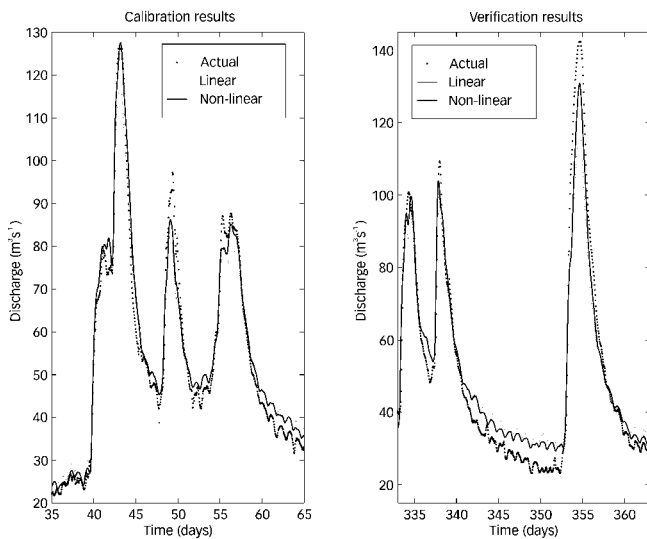


Figure 9 | Comparison of linear and nonlinear flow model performance for Shardlow.

producing significantly better performances at high flows as indicated here by the model error at the highest flow. However, as in calibration, the full nonlinear model does not provide improved performance in comparison to the input-nonlinear model.

Next, optimisation of a state updating procedure using the KF with the Gauss–Markov model specified as in (Equation 27) was performed for the linear (Equation 40) and nonlinear (Equation 42) TF models on the calibration period. Optimisation was performed using the $RMSE(8)$ criterion because 8-hour-ahead forecasts are the most important forecast output. Figure 10, which shows a comparison of the forecasting performance of the input-nonlinear model with and without state updating, reveals that state updating improves the 8 hour forecast performance but not dramatically so. However, Figure 11, which shows the state updated versus non-state updated performance over the range of lead times that are produced by the KF shows that as the lead time is reduced performance improves dramatically with an almost perfect fit to the observed discharge for the one-step-ahead forecasts. Figure 10 also shows the probabilistic 8 hour forecasts generated from the KF. As stated earlier these probabilistic forecasts are very useful in an operational context since a measure of the forecast accuracy is provided, and

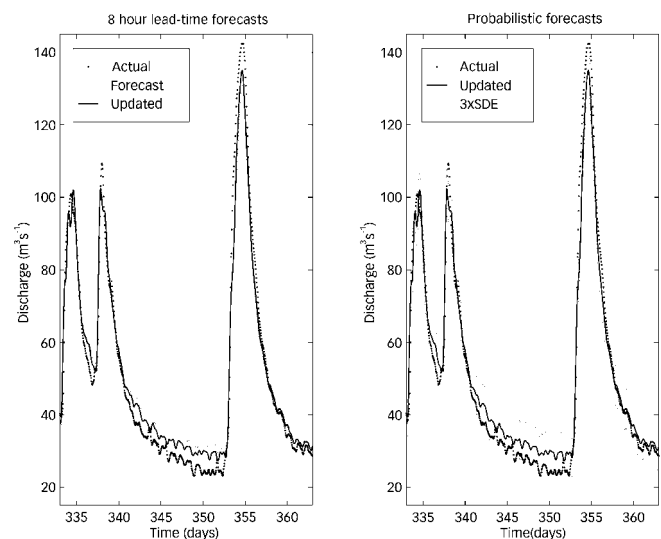


Figure 10 | Comparison of nonlinear TF model forecasting performance with and without state updating and probabilistic forecasts for the state updated model.

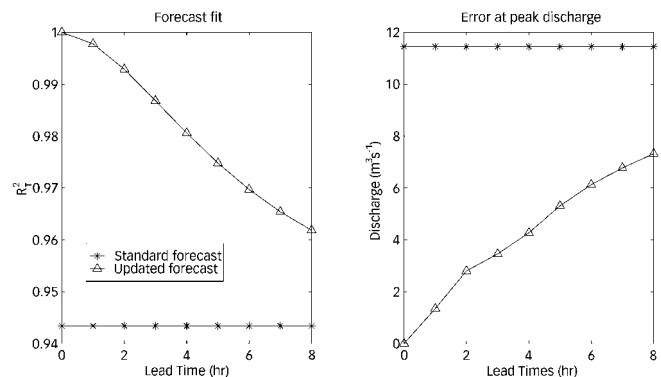


Figure 11 | Model forecasting performance.

naturally this accuracy improves with reduced lead times as the state updating procedure has more effect.

CONCLUSIONS

The paper has demonstrated that non-stationary models, in particular the DARX model estimated using a combined KF/FIS algorithm, can be used to estimate time variable parameters that can be related to state variables, such as discharge, resulting in nonlinear state-dependent

parameter models. In the special (although common) case that the identified nonlinearity is a gain nonlinearity then the nonlinear model can be represented by the combination of an input nonlinearity with a linear model. This particular nonlinear model formulation allows a linear TF model to be identified between the transformed input and the outflow. This is important for two reasons: first, optimal system identification techniques, in this case the SRIV algorithm, can be used to identify the model structure and estimate the model parameters; and secondly, because models in this form can be updated in real-time using a KF state updating procedure that enables improved forecasts to be produced along with an estimate of forecast uncertainty. Forecast uncertainty can provide very useful additional information on flooding likelihood, although there is much current debate in the UK as to what form probabilistic forecasts issued to the public should take. It should be noted here that the use of a sophisticated corrector is no substitute for a well identified forecast model, and also that in the case of rainfall-runoff modelling, forecasting performance is heavily influenced by the accuracy of the spatial rainfall input.

The idea of introducing a data-based mechanistic step into the modelling procedure is suggested as a way of ensuring the identified model is a hydrologically acceptable physical representation of the dominant dynamic processes. To this end, it is shown that the TF model can represent a general linear storage model that obeys the fundamental law of continuity where linear stores are combined both in series and in parallel, and that an identified TF model should not be accepted as a reasonable descriptor of the system unless it can be decomposed into a physically reasonable form. It is argued that this mechanistic interpretation helps to ensure that the model is robust for out-of-sample forecasting application.

Two case studies are included that demonstrate the utility of the DBM modelling methodology for the two most common hydrological forecasting applications: rainfall-runoff modelling and flood routing. The importance of FIS and dependent-state sorting in the identification of state-dependent parameter relations is demonstrated. Excellent results using nonlinear TF models are produced, and it is shown that SRIV system identification is required if appropriate second-order

parallel models are to be objectively identified from the data. This data-driven modelling approach allows the model structure to be objectively identified rather than subjectively conceptualised.

In conclusion, the DBM modelling and forecasting technique is a powerful objective data-driven technique that extends a class of widely-used linear storage based hydrological models into the hydroinformatic age where data availability and increasing computing power are becoming readily available. Many of the modelling techniques used in this paper are contained in the CAPTAIN MATLAB (Mathworks 1996) toolbox developed by the Systems and Control Group at Lancaster University, see <http://es-parto.lancs.ac.uk/captain/> and others are available from the author as MATLAB functions, see <http://ewre-www.cv.ic.ac.uk>.

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REFERENCES

- Babovic, V. & Keijzer, M. 1999 Forecasting of river discharges in the presence of chaos and noise. In *Coping With Floods: Lessons Learned From Recent Experience* (ed. J. Marsalek). NATO ASI Series. Kluwer, Dordrecht.
- Beer, T. & Young, P. C. 1983 Longitudinal dispersion in natural streams. *J. environ. Engng (ASCE)* **109**, 1049–1067.
- Bell, V. A. & Moore, R. J. 1998 A grid-based distributed flood forecasting model for use with weather radar data: Part 2. Case studies. *Hydrol. Earth Sys. Sci.* **2**, 283–298.
- Even, K. J. & Kirkby, M. J. 1979 A physically based, variable contributing area model of basin hydrology. *Hydrol. Sci. Bull.* **24**, 43–69.

- Bierman, G. J. 1973 Fixed interval smoothing with discrete measurements. *Int. J. Cont.* **18**, 65–75.
- Box, G. E. P. & Jenkins, G. M. 1976 *Time Series Analysis, Forecasting And Control*, revised edn. Holden-Day, Oakland, California.
- Brown, R. L., Durbin, J. & Evans, J. M. 1975 Techniques for testing the constancy of regression relationships over time. *Jl R. statist. Soc. B* **37**, 149–192.
- Camacho, L. A. & Lees, M. J. 1999 Multilinear discrete lag-cascade model for channel routing. *J. Hydrol.* (In the press.)
- Cunge, J. A. 1969 On the subject of a flood propagation computation method (Muskingum method). *J. hydraul. Res.* **7**, 205–230.
- DeMoor, M. & Berckmans, D. 1996 Building a grey box model to model the energy and mass transfer in an imperfectly mixed fluid by using experimental data. *Math. Comp. Simulat.* **42**, 233–244.
- Dooge, J. C. I. 1986 Theory of flood routing. In *River Flow Modelling and Forecasting* (ed. D. A. Kraijenhoff & J. R. Moll). John Wiley, Chichester.
- Duan, Q., Gupta, V. K. & Sorooshian, S. 1993 A shuffled complex evolution approach for effective and efficient global minimization. *J. Optimiz. Theory Applic.* **76**, 501–521.
- Foster, H. J., Alexander, S., Locks, T., Wheater, H. S., Lees, M. J. & Reynolds, B. 1997 Scale dependence of the episodic hydrochemical response of nested catchments at Plynlimon. *Hydrol. Earth Sys. Sci.* **1**, 639–651.
- Jacobsen, J. L. & Madsen, H. 1996 Grey box modelling of oxygen levels in a small stream. *Environmetrics* **7**, 109–121.
- Jakeman, A. J. & Young, P. C. 1984 Recursive filtering and the inversion of ill-posed causal problems. *Utilitas Mathematica* **35**, 351–376.
- Jakeman, A. J. & Hornberger, G. M. 1993 How much complexity is warranted in a rainfall-runoff model? *Wat. Resour. Res.* **29**, 2637–2649.
- Kalinin, G. P. 1971 *Global Hydrology Transactions*. (In Russian.) Israel Programme for Scientific Translations, Jerusalem, Israel.
- Kalman, R. E. 1960 A new approach to linear filtering and prediction problems. *J. bas. Engng, Trans. ASME D* **82**, 35–45.
- Lambert, A. O. 1972 Catchment models based on ISO-functions. *J. Inst. Wat. Eng.* **26**, 413–422.
- Lee, R. C. K. 1964 *Optimal Identification, Estimation and Control*. MIT Press, Cambridge, Mass.
- Lees, M. J., Young, P. C., Ferguson, S., Beven, K. J. & Burns, J. 1994 An adaptive flood warning scheme for the River Nith at Dumfries. In *2nd International Conference on River Flood Hydraulics* (ed. W. R. White & J. Watts), pp. 65–75. John Wiley & Sons, Chichester.
- Lees, M. J., Camacho, L. A. & Whitehead, P. 1998a Extension of the QUASAR river quality model to incorporate dead-zone mixing. *Hydrol. Earth Sys. Sci.* **2**, 353–365.
- Lees, M. J., Price, N., Wheater, H. S. & Peach, D. 1998b A flood simulation model for the South Galway region of Ireland. In *Proceedings of BHS International Symposium on Hydrology in a Changing Environment*, vol. III, pp. 93–104. John Wiley & Sons, Chichester.
- Mathworks 1996 *MATLAB Reference Guide*. Natick, Mass.
- Mehra, R. K. 1970 Approaches to adaptive filtering. *IEEE Trans. aut. Cont.* **AC-17**, 693–698.
- Mein, R. G., Laurenson, E. M. & McMahon, R. A. 1974 Simple nonlinear model for flood estimation. *Proc. ASCE* **11**, 1507–1518.
- Moore, R. J. 1985 The probability-distributed principle and runoff production at point and basin scales. *J. hydrol. Sci.* **30**, 273–297.
- Nelder, J. A. & Mead, R. 1965 A simplex method for function minimization. *Computer J.* **7**, 308–313.
- Ng, C. N. & Young, P. C. 1990 Recursive estimation and forecasting of nonstationary time series. *J. Forecasting* **9**, 173–204.
- Perumal, M. 1994 Multilinear discrete cascade model for channel routing. *J. Hydrol.* **158**, 135–150.
- Priestly, M. 1988 *Nonlinear and Nonstationary Time Series Analysis*. Academic Press, London.
- Schweppe, F. 1965 Evaluation of likelihood function for Gaussian signals. *IEEE Trans. Inform. Theory* **11**, 61–70.
- Wheater, H. S., Jakeman, A. J. & Beven, K. J. 1993 Progress and directions in rainfall-runoff modelling. In *Modelling Change in Environmental Systems* (ed. A. J. Jakeman *et al.*). John Wiley, Chichester.
- Whitehead, P., Young, P. C. & Hornberger, G. 1979 A systems model of stream flow and water quality in the Bedford-Ouse river–1. Stream flow modelling. *Wat. Res.* **13**, 1155–1169.
- Wood, F. & Szöllösi-Nagy, A. 1980 Real-time forecasting/control of water resource systems. Pergamon Press, Oxford.
- Young, P. C. 1970 An instrumental variable method for real-time identification of a noisy process. *Automatica* **6**, 271–287.
- Young, P. C. 1984 *Recursive Estimation and Time-Series Analysis*. Springer-Verlag, Berlin.
- Young, P. C. 1985 The instrumental variable method: a practical approach to identification and system parameter estimation, *Proc 7th IFAC/IFORS Symposium on Identification and System Parameter Estimation*, York, International Federation of Automatic Control, Vol 1, 1–15.
- Young, P. C. 1991 Simplified refined instrumental variable (SRIV) estimation and true digital control (TDC): a tutorial introduction. In *Proceedings of the First European Control Conference*, Grenoble, pp. 1295–1306.
- Young, P. C. 1992 Parallel processes in hydrology and water quality: a unified time-series approach. *J. Inst. Wat. Env. Manage.* **6**, 598–612.
- Young, P. C. 1993 Time variable and state-dependent modelling of non-stationary and nonlinear time series. In *Developments in Time Series Analysis* (ed. T. Subba Rao), pp. 374–413. Chapman & Hall, London.
- Young, P. C. 1998a Data-based mechanistic modelling of engineering systems. *J. Vibrat. Cont.* **4**, 5–28.
- Young, P. C. 1998b Data-based mechanistic modelling of environmental, ecological, economic and engineering systems. *Environ. Model. Soft.* **13**, 105–122.
- Young, P. C. 1999a Nonstationary time series analysis and forecasting. *Prog. env. Sci.* **1**, 3–48.

- Young, P. C. 1999b Development of an IV DTF parameter estimator. Personal communication.
- Young, P. C. & Lees, M. J. 1993 The active mixing volume, a new concept in modelling environmental systems. In *Statistics for the Environment* (ed. V. Barnett & K. Turkman), pp. 3–43. John Wiley, Chichester.
- Young, P. C. & Beven, K. J. 1994 Data-based mechanistic modelling and the rainfall-flow nonlinearity. *Environmetrics* **5**, 335–363.
- Young, P. C., Parkinson, S. & Lees, M. J. 1996 Simplicity out of complexity in environmental modelling: Occam's razor revisited. *J. appl. Stat.* **23**, 165–210.
- Young, P. C., Jakeman, A. J. & Post, D. A. 1997 Recent advances in data-based modelling and analysis of hydrological systems. *Wat. Sci. Technol.* **36** (5), 99–116.