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Asserting predictive uncertainty of regulated river system model

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Abstract: Sound water resource planning is assisted by hydrologic model simulation of alternative resource management scenarios. Asserting the predictive uncertainty of the simulation is important in the comparison of planning options. The valley wide regulated river system model is a cluster of independently calibrated component models such as irrigation model, a number of rainfall-runoff models, a number of hydrologic river routing models etc. Assigning confidence bands to simulation outputs is onerous as the multivariate residual errors are spatially related with strong serial correlation and unstable variance. For example, during spill periods the residual error of the reservoir level variable resets at every time step whilst during recession residuals exhibits long memory. Non linear error propagation towards both the upstream and downstream direction in the system is notable. Different calibration periods and the sample size of different component models mean that a multivariate set of residuals with sufficient sample size is often nonexistent.

This paper uses a meta Gaussian approach to infer the simulation error. It does so by first transposing all the variable of interests using a Normal Quantile Function. The calibration error is then measured in the transformed space. A linear model is then fitted to the calibration error where the predictors are chosen from other simulated variable that exhibits physical dependence to this error. The linear model allows the separation of the bias and white noise portion of the calibration error. The confidence interval is then inferred from the fitted cumulative distribution of the white noise.

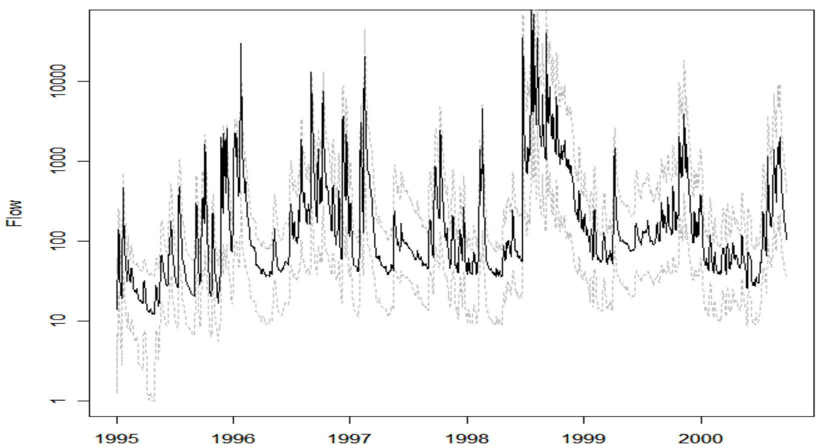

Figure 1. Simulated flow at Carroll Gap with 95% confidence band.

The case study examined the simulations of the river system model known as the Integrated Quantity Quality Model (IQQM). The study selects the Peel River system of which the variables of interest are flow at three key locations, irrigation and urban water usage and storage volume. The calibration version of the full ensemble runs for 1982 to 2000 and long term planning model simulates from 1892 to 2005. The paper presents the predictive uncertainty of the flow at Carroll Gap by computing confidence band of the simulation. It does so by developing a linear model in meta Gaussian space where the predictors of flow residuals are storage volume, total diversion and the flow persistence. It filters the biased naïve residuals into white noise and thus infers confidence interval to long term flow simulation as shown in Figure 1. The paper also discusses various relevant unresolved issues for example calibration uncertainty versus predictive uncertainty and unstable transformation that offer foresight into future research opportunities.

Keywords: *Uncertainty, River System Model, IQQM, Peel River.*

1. INTRODUCTION

River system simulation of resource management scenarios is important for optimising the management of a regulated river. The hydrologic model simulates inflows to the system, river flows, storage levels and spills, regulated release to meet various water use demands (irrigation, domestic etc) and environmental watering all subject to the jurisdictional management plans. It is important to assert the predictive uncertainty of the simulations as any conclusive impact of alternative scenarios is required to exceed the simulation noise (Bormann, 2005). However, assigning predictive uncertainty to simulated variables is onerous for reasons that are discussed in the next section. The aim of this paper is to aid the development of a practice manual on uncertainty band determination for river system simulations. Note that no unique definition of uncertainty exists in scientific literature (Montanari, 2007). This paper refers to uncertainty as the quantum of departure of simulation from the respective true value; the departure can be quantified by objective measures such as variance, squared error or confidence interval. So measurement of uncertainty requires simulation of observed variables. The next paragraph provides the background of the development of the hydrologic models used for water resources planning, the appreciation of this development steps is relevant to this paper.

Various components of a river system model are first independently calibrated and later assembled together. This is called '*the calibration version*' of the model. For water resources planning reference, the various components of the calibrated models are frozen at a certain reference development level. The components may be maximum irrigable land, population of a town, size of a reservoir etc on a particular year. Then the proposed planning rules and a level of development are imposed on the model components, such as minimum flow requirement at a location, storage reserve, accounting methods of irrigation diversions, environmental watering regime and so on. This is called '*the planning version*' of the model. The simulation of the planning version is carried out for a set of input time series (rainfall, evaporation, temperature etc) for a period representative of climatic variability of the catchment. Conventionally representativeness is achieved using long period observed time series (e.g. 1895 to 2009), however a synthetically generated set of time series with sufficient length can also be used. The simulation provides probabilistic outcome for the proposed planning rules such as percentage of time the storage falls below critical level or reliability of irrigation allocation. A planning model assumes a given physical development level and planning rules, it can neither hindcasts past events nor forecasts future possibilities where the level of development or planning rules are different, which is normally the case. Hence the conventional method of error inference based on difference in simulation and observation (of past or notional future event) is not possible.

The literature on uncertainty for a full river system model is limited to using efficiency measures of monthly flow simulation (van Dijk, A. *et al*., 2008). However river flow is only one of the many variables of interest; storage levels, various diversions or resource allocation are also important for planning. Assigning uncertainty bands in isolation and ignoring spatial dependences to other variables is not robust. The monthly statistics inadequately reflects the flow simulation in daily time step which is essential to analyse various environmental flow regimes. Besides the analysis by van Dijk *et al*. (2008) assumes 'the planning version' of a reference development (baseline model) as 'the calibration version'. Various complexities of estimating the simulation error of the planning version are discussed in the following section.

2. UNCERTAINTY IN RIVER SYSTEM SIMULATIONS

In numerical modelling terms, regulated river system model is a hierarchical cluster of independently calibrated component modules such as irrigation demand module, a number of rainfall-runoff modules, a number of hydrologic river routing modules. The multivariate response includes daily time series of river flow at various locations, extraction volumes and reservoir levels. The conventional practice of assigning predictive uncertainty (of mainly univariate response) often assume that the residuals are random numbers that are unbiased, with stable variance, and free of serial correlation. In contrast, the multivariate residual errors of a river system model are spatially related with strong serial correlation and unstable variance along with challenges as discussed below.

Significant spatial and temporal dependence of the columns of multivariate error matrix is expected due to feedback loops of various component models. Unlike a simple one dimensional flow path, residual error may travel upstream. For example, any overestimation of irrigation demand at a location nonlinearly overestimates regulated release from the head water reservoir. Non contiguity causes additional challenge to extract the multivariate error matrix since the component models are often calibrated at different time period and at different time steps (daily, monthly and annual). Finally the distribution of the residuals often does not conform any design distribution limiting any parametric inference.

2.1. Prior Assumptions

There are a number of prior assumptions that leads to the proposed computation. The assumptions can be explained based on various sources of total uncertainty. The total uncertainty in hydrological models can be traced into three broad sources which are 1) inaccuracy of input variables, 2) imprecise calibration variable and 3) structural uncertainty.

Input error: The uncertainty in hydrological model inputs, if ignored, introduces systematic bias in the parameters estimated. The methods of eliminating parameter biases (Chowdhury and Sharma 2007; Huard and Mailhot 2006; Kavetski et al., 2002) are computationally expensive for such a highly parameterized river system models. Instead, this paper assumes stationary input error with stable variance and hence input error is implicitly reflected in the total error of the simulation.

Imprecise calibration variable: In practice, hydrologist often uses expert judgment during calibration to minimize calibration biases caused by imprecise observations. Besides any local optima in parameter space may corrupt calibration as well. For simplicity, this paper ignores any imprecision in calibration variable as narrow band of white noise. The proposed computation here does not add any external noise to the simulation to account for observation errors.

Structural uncertainty: This is the error that would prevail even if the true input time series were known and unbiased calibration is achieved due to availability of the true response variable. The uncertainty estimate in this paper in fact aims to reflect this imperfection due to simplification of the natural process.

The above details on error characteristics and underlying assumption set the background of the methodology as described next.

3. METHODOLOGY

Consider a river system model where observed time series of interest are $\mathbf{Y}^*$.

$$\mathbf{Y}^* = \{\mathrm{Q}_t, \mathrm{S}_t, \mathrm{D}_t, \ldots; t=1, 2, 3, \ldots\}^* \quad [1]$$

where,

$\mathrm{Q}_t{}^* = \{q_{1,t}\,; q_{2,t}\,; q_{3,t} \ldots\}^*$: flow time series at location 1, 2, 3…and so on.

$\mathrm{S}_t{}^* = \{s_{1,t}\,; s_{2,t}\,; s_{3,t} \ldots\}^*$: storage volume time series of reservoir 1, 2, 3…and so on.

$\mathrm{D}_t{}^* = \{d_{1,t}\,; d_{2,t}\,; d_{3,t} \ldots\}^*$: irrigation diversion time series of irrigator 1, 2, 3…and so on.

The proposed error model largely follows the methodology introduced by Montanari and Brath (2004). It begins with a normal quantile transformation *NQT*(.) prior to any analysis. This empirical transformation forces any vector into a perfect normal distribution.

$$\mathbf{Y} = NQT_i(\mathbf{Y}^*) \quad [2]$$

where index i denotes the flexibility of using separate functions for each variable of interest such as flow, storage and diversion.

The variables without a star indicate computations post transformation. The complementary set of variables from simulation of the full ensemble of the river system model is shown as $\hat{\mathbf{Y}}$.

Now the multivariate time series of error $\mathbf{E}$ is (assuming $\mathbf{Y}$ is available):

$$\mathbf{E} = \mathbf{Y} - \hat{\mathbf{Y}} \quad [3]$$

The dimension of $\mathbf{E}$ is the number of variable of interest multiplied by the time steps of calibration; note that the bold notation indicates matrices (multiple time series). The problem is now confined to separating the predictable portion of error (say $\hat{\mathbf{E}}$) and the associated left over white noise (say $\boldsymbol{\varepsilon}$). Let us name the error at time t of a variable (eg. flow at 2nd location, $q_{2,t}$) is E_t, then a multiple linear model is fitted as follows:

$$E_t. = \alpha + \sum \mathrm{X}_t\,\beta + \varepsilon_t \quad [4]$$

Where, X_t : appropriate predictor variables, for example$\{q_{2,t}\,; q_{2,t-1}\,; d_{1,t}\,; d_{2,t}$ and so on$\}$;

β : regression parameter $\beta_1, \beta_2, \beta_3 \ldots$ up to size of X_t ;

α : regression intercept;

ε_t : white noise or unexplained leftover residual.

In theory, a properly fitted generalised linear model assigns an exponential distribution to ε = {ε_t; t=1,2,3.. max calibration length} from which inference of confidence interval can be drawn. For example, in case of Gaussian distribution the 95% confidence band is given by adding ±1.96 times of standard deviation to the predictable portion of E_t. (first two terms of Equation [4]). However, this study advocates a generic approach where the confidence interval is estimated after a fitting smooth curve to the cumulative frequency plot F(ε). Hence the 95% confidence band (±2.5%) of flow at 2nd location ($q_{2,t}$*) can be given by the following formula:

$$\text{Upper limit} = q_{2,t}^* + NQT_q^{-1}(\hat{E}_t + F(\varepsilon)|F=97.5\%) \qquad [5]$$

$$\text{Lower limit} = q_{2,t}^* + NQT_q^{-1}(\hat{E}_t + F(\varepsilon)|F=2.5\%)$$

4. THE REGULAED PEEL RIVER SYSTEM

4.1. Integrated Quantity Quality Model

The case study looks at the simulations of a conceptual river system model known as Integrated Quantity Quality Model (IQQM). The hydrologic model IQQM was progressively developed in the 1990s by the NSW Department of Water and Energy and its predecessors (Simons et al., 1996). This is a conceptual deterministic model that mainly simulates (using a node link structure) daily rainfall runoff, river routing, reservoir operation, irrigation demand and associated extractions subject to legal compliance (Hameed and Podger, 2001). The model has been extensively used for water resource planning of NSW and partly in Queensland (CSIRO, 2007).

4.2. Peel River

The study selects the Peel River system which is situated about 400 km North West of Sydney. The rural catchment is located within the Murray Darling Basin. The river flows generally in a north westerly direction; it drains a catchment area of 4700 sq km. The surface water resource of the Peel River is mainly regulated by the Chaffey Dam with a maximum capacity of $61.8\text{x}10^6$ m^3. There is a smaller Dungowan Dam ($6.3\text{x}10^6$ m^3) which supplies urban population of Tamworth City, any shortfall is supplemented from the Chaffey Dam. Tamworth is a major regional centre which uses about $9\text{x}10^6$ m^3 of water on an average year. Another significant water usage is irrigation of annual and perennial crops, which is about $5\text{x}10^6$ m^3 on average at present

Peel IQQM is an ensemble of hierarchical component time series models where each component is independently calibrated. The major modules of this rural catchment include 2 reservoirs, 4 clusters of irrigators, 1 town water use, 3 flow routing reaches, 5 rainfall runoff modules and various conceptualisations of lateral inflow and loss. The calibration periods vary from modules to modules based on available boundary time series. Indicative calibration period of various modules are as follows:

Rainfall runoff (daily): 1936 to 2000, 1965 to 2000, 1974 to 1993.

Flow routing and loss (daily): mainly 1959 to 1996

Irrigation diversion (monthly): 1983 to 2000

Urban water usage (monthly): 1997 to 1999

Chaffey Dam (daily): 1982 to 2000

Dungowan Dam (monthly): 1984 to 1990

The version of Peel IQQM used in this paper was calibrated during early 2000s. Peel IQQM is continuously evolving as driven by the changing need and new information. Hence the results shown here may not represent the current state of the Peel IQQM. The variables of interest are flow at three key locations, irrigation and town water usage and storage volume. The calibrated Peel IQQM has been applied in various water management studies (CSIRO, 2007). The full ensemble of the calibration version of Peel IQQM runs from 1982 to 2000. The planning version of Peel IQQM runs for 1892 to 2005.

4.3. Flow at Carroll Gap

This study attempts to assign confidence band to flow simulation at Carroll Gap, which is situated at the downstream end of the Peel River. The author first analyses the error structure using partial auto correlation function (ACF). Partial ACF computes lagged correlation of a time series after earlier lags being removed, for example the partial correlation of lag 3 is the correlation of current time step to 3 time step earlier after removing lag 1 and 2 dependencies. The partial ACF of the Carroll Gap flow simulation error shown in Figure 2 indicates daily (up to 2 days), weekly and monthly dependence of the error structure. The daily dependence can be attributed to routing error of a hydrograph tail. Weekly and monthly dependence may be reflective of calibration time interval of diversion such as irrigation and town water supply.

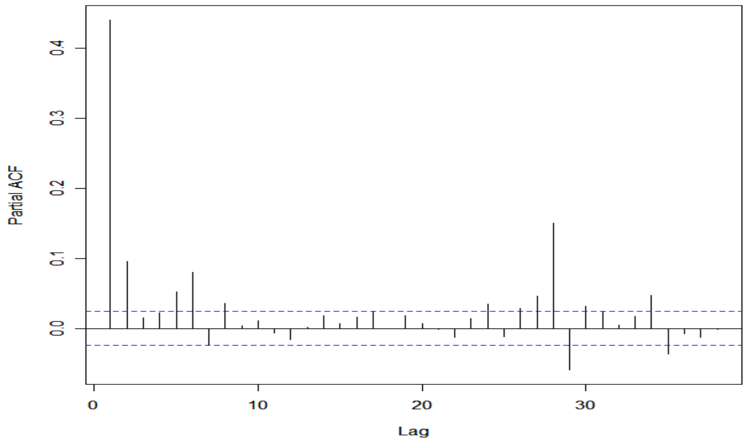

Figure 2. Partial auto correlation of the flow simulation error. Note the traces of daily, weekly and monthly trend.

The next phase of the analysis involves quantile transformation *NQT*(.) of the observed and simulated flow, simulated total diversion and simulated storage volume time series. Figure 3 shows such transformation of Carroll Gap flow. Note that storage and total diversion (all irrigation plus town water usage) applied their own *NQT*(.) function. The error time series of flow simulation, E_t, is determined after the transformation.

The prospective error time series predictor include diversion, flow at other locations, storage volume, last seven days flow, sine wave with seasonal cycle. Note that all the predictors are in transformed space, except the sine wave. The following predictor time series (1982 to 2000) are retained in the final model.

X = total diversion, storage volume, last 3 days flow in Carroll Gap.

The fitting of linear model (Equation [4]) to flow error separates the white noise ε_t for inferring confidence band. Figure 4 next shows the scatter plot of the error ε and naïve error against the flow at Carroll Gap. Naïve error refers to raw error of the calibration results prior to any transformation. Note the clear funnel pattern of the naïve error with increasing flow, while **ε** is exhibiting a more uniform scatter across all flow ranges. The uniform scatter signifies that **ε** may be taken as white noise for inferring error bound.

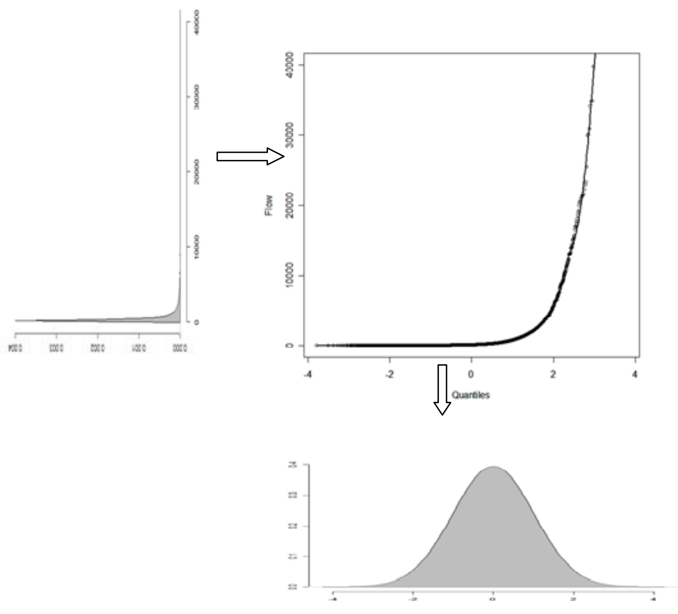

Figure 3. Transforming flow into normal distribution using NQT.

The author fits a smooth curve on the cumulative frequency of the error **ε** and the ordinate against 97.5% and 2.5% give the necessary information to compute Equation [5]. Now the information is used to provide 95% confidence band of the simulation (planning version) extending from 1895 to 2005. Figure 1 has shown a 15 year window out of 110 year of simulation of the planning version.

5. CALIBRATION VERSUS PREDICTIVE UNCERTAINTY

One of the major unaddressed issues in the conceptualisation of the proposed method is the assumption that the calibration error equals predictive uncertainty of the full simulation. Note that the calibration version of a model returns minimal error. One can progressively increase the number of parameters in order to reduce the error during calibration period without necessarily having any foresight of those parameters being valid beyond that period. The optimal number of parameter depends on the length of calibration time series. While any increase in model complexity beyond that optimal number further decreases calibration error, it increases error of the full simulation (predictive error). This understanding of numerical model behaviour is well established in environmetrics, biometrics and data mining (Hastie et al., 2000). The optimal parameter issue is visited in the field of rainfall runoff model as well (Perrin et al., 2001, 2003).

The complexities of the river system and small numbers of measured time series indicate the possibility of over parameterisation of such models. So an understanding of the inflation of the calibration error to simulation error is important. Hydrological studies usually analyse the ‘validation runs’ in a way to seek the predictive error of the simulations. Unfortunately, systems like the Peel River come with a small multivariate concurrent observed data set. Hence the production of multiple validation versions of sufficient length (without degrading calibration accuracy) is not possible. The way forward in this area may be first to conceptualise the likely increase of calibration uncertainty to predictive uncertainty based on relevant known factors, such as: a) variation between climates of calibration period and full simulation period, b) divergence of calibration model error to null model error, c) increase in errors of individual module to full ensemble model. Later a fuzzy logic based schematics can be drawn to elements (a) to (c) to derive an inflation factor (or a set of factors). The confidence band (as estimated in this paper) will be widened by multiplying the inflation factor to derive ultimate predictive uncertainty of the planning simulations. This will be addressed in future studies.

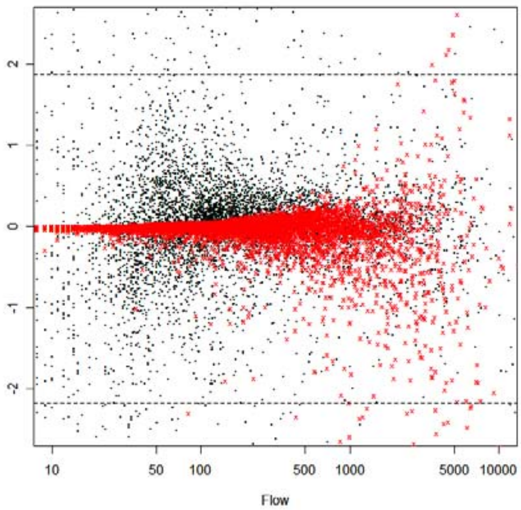

Figure 4. The naïve residual error (red x) and final residual error (black dot) are drawn against observed flow. For clarity the flow is in log scale, the residual errors are standardised for comparison. The 95% confidence band of the final residual error is within the two broken horizontal line.

6. DISCUSSION

The case study presented here is limited to flow output from the full river system simulation. The application to flow simulation is a relatively simpler problem when compared to other variable of interest like diversion or storage volume. In NSW, the diversion (irrigation, town water usage) records are usually available in monthly format or sometime in irregular interval (monthly to seasonal or whenever the meter is read). The additional uncertainties arising from the disaggregation methods adopted needs to be included in the proposed method. In case of storage volume, the memory of residual error needs to be pre processed using methods like differencing. These challenges should be addressed in continuation of this study.

This study used meta Gaussian method by using normal quantile transformation (NQT). The empirical NQT relies heavily on observed time series and may not be stationary (large change correspond to small change in time window). The different NQT of different variables (flow, diversion, storage) masks any meaningful interpretation of the regression relationship. The author asserts that the proposed transformation does not need to be limited to NQT. Other transformations that dampen skews and stabilise variances can also be used such as modified Box-Cox transformation (Wang et al., 2009: Yeo and Johnson, 2000). Further comparative studies on suitable transformation will be advantageous to this research.

One aspect of simplification is to model multivariate **E** (Equation [3]) using univariate linear regression of E_t.(Equation [4]). It is expected that the loss of multivariate characteristics of **E** may be compensated by the use of some common set of predictor variables $\{X_t\}$ for every E_t. Nevertheless, this simplification clearly weakens the spatial dependence of the confidence band among various variables. The solution lies in the multivariate extension (or alternative) of Equation [4].

The case study is based on the software IQQM. The methodology is not software dependant and intended to inform future version of such modelling practises. The findings of this research will inform the next generation of river system models in development such as *RiverManager*.

7. CONCLUSION

This paper presents the methodology of a comprehensive attempt of defining uncertainty band of simulations of regulated river system model. It sets the background by first introducing the characteristics of the river system models used for planning purpose. The example is drawn from an application of Integrated Quantity Quality Model (IQQM) to the rural catchment of the Peel River in Eastern Australia. Peel IQQM is an ensemble of hierarchical component time series modules of independently calibrated 2 reservoirs, 4 clusters of irrigators, 1 town water use, 3 flow routing reaches, 5 rainfall runoff models and various conceptualisations of lateral inflow and loss. The flow at Carroll Gap is chosen as variable of interest. Calibration error of Carroll Gap (1982 to 2000) shows daily, weekly and monthly serial correlation reflective of error propagation of various modules in the system. The analyses are carried out after applying normal quantile transformation. Linear association of the flow calibration error to storage volume and total diversion is identified. Accordingly the fitted linear model filtered out the white noise of flow error. The 95% confidence band is inferred from this white noise. This analysis enables assigning confidence band to the planning version of the Carroll Gap flow simulation (1892 to 2005). The paper discusses a number of further research needs relevant to this work. They include estimating likely amplification of calibration error into predictive uncertainty, some unique features of other variables of interest and stronger representation of spatial statistics.

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