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From marginal to conditional probability functions of parameters in a conceptual rainfall–runoff model: an event-based approach

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ABSTRACT
A parameter estimation strategy for a conceptual rainfall–runoff (CRR) model applied to a storm sewer system in an urban catchment (Chassieu, Lyon, France) is proposed on the basis of event-by-event Bayesian local calibrations. The marginal distribution formed by locally-estimated parameters is divided into conditional functions, clustering the event-based parameters based on their transferability to similar rainfall events. The conditional functions showed to be consistent with an observed bimodality in the marginal representation, reflecting two different hydrological conditions mainly related to the magnitude of the rainfall intensities (high or low). The improvements achieved by expressing the parameter probability functions into a conditional form are shown in terms of accuracy (Nash-Sutcliffe efficiency criterion), precision (average relative interval length) and reliability (percentage of coverage) for simulating flow rate in 255 and 110 calibration/verification events.

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Introduction

The urban drainage flow at the outlet of storm sewer systems can be seen as the result of multiple anthropogenic and non-anthropogenic complex processes developed at different temporal and spatial scales, of which the main driving force is the precipitation over the catchment (Leonhardt *et al.* 2014). Most model structures used nowadays in urban hydrology can be classified as conceptual rainfall–runoff (CRR) models (Wagener *et al.* 2003), offering a suitable balance between computational simplicity and physical meaning of their parameters (Zhang *et al.* 2015). Indeed, rainfall–runoff modelling in urban catchments by means of conceptual lumped models, i.e. accounting for the surface runoff and the sewer flow in a lumped description, can be considered as a suitable simplification for several purposes (e.g. Reed *et al.* 2004, Coutu *et al.* 2012). However, the performance of a given CRR model strongly depends on a comprehensive assessment of model parameters from calibration or experiments (Thyer *et al.* 2009, among many others). On the other hand, multiple studies have recognized the stochastic changes over model parameters at the inter-event scale as a fundamental uncertainty source in hydrological modelling (Brigode *et al.* 2013, Gharari *et al.* 2013, Sikorska *et al.* 2014, Thirel *et al.* 2015).

In this context, uncertainties in model parameters are principally estimated from calibration, based on a likelihood function that reflects the mismatch between model simulations and observations. For this purpose, two families of methodologies can be distinguished, whether this likelihood function is founded on a subjective selection (e.g. the generalized likelihood uncertainty estimation, GLUE; Beven and Binley 1992, Vrugt and Beven 2018), or as a formal error model using Bayesian statistics (e.g. the Bayesian Total Error Analysis, BATEA; Kavetski *et al.* 2006a, Del Giudice *et al.* 2016). Discussions and comparisons of informal and formal approaches are given by many researchers (e.g. Makowski *et al.* 2002, Montovan and Todini 2006, McMillan and Clark 2009, Jin *et al.* 2010, Dotto *et al.* 2012). However, Bayesian frames are preferred for this study, given that statistical assumptions about the modelling errors can be explicitly accounted for in the likelihood function (Vrugt *et al.* 2009, Vrugt 2016), besides reporting higher efficiencies in the exploration of the parametric space (Vrugt and Beven 2018). Among these Bayesian formal approaches, the BATEA (Kuczera *et al.* 2006, Kavetski *et al.* 2006a, 2006b) remains a very common framework to conceptualize the propagation of errors from data (input/output) and model structure, into the estimation of the posterior probability density function (hereinafter pdf) of model parameters (Yang *et al.* 2008). Drawbacks of BATEA in assessing the inter-event variability of CRR model parameters and rainfall measurement errors, especially when considering long calibration periods (e.g. 10 years), are mainly linked to the massive dimensionality of the inference, as further parameters or error characterization terms are defined as event-dependent rather than time-invariant (Thyer *et al.* 2009, Renard *et al.* 2011). On the other hand, Bayesian simplified inferences, i.e. without further characterizing each particular uncertainty source, have shown consistent results for problems with a lower dimensionality, despite the inherent imitations (Vrugt 2016).

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Therefore, simplified event-based Bayesian inferences (e.g. Singh and Bardossy 2012, Sun and Bertrand-Krajewski 2013a, Sun *et al.* 2017) may be sounder for exploring the inter-event variability of parameters by undertaking local event-by-event calibrations (e.g. Ajmal *et al.* 2015). From this implementation, local sets of parameters of satisfactory event-based calibrations can be marginalized for assessing a global pdf of the model parameters.

This study proposes a method to reduce the dispersion of this marginal pdf by clustering the estimated local sets of parameters, leading to the construction of alternative conditional representations of the marginal pdf. From this construction, the linkage between calibration rainfall events is represented by an adjacency matrix (e.g. Csardi and Nepusz 2006), based on the transferability (Bardossy and Singh 2008, Singh *et al.* 2016) of their locally-estimated parameters. The improvements achieved by expressing the parameter pdf into conditional functions, compared to the marginal representation, are shown in terms of accuracy, precision and reliability of the flow-rate simulations. The approach is tested by means of a lumped CRR model (single linear reservoir with Horton's infiltration equation), for an urban catchment with a separate sewer system in Lyon, France, considering 255 and 110 events for calibration and verification, respectively.

Methodology

Experimental set-up and data description

The proposed models are tested for 365 rainfall events across the Chassieu urban catchment (Lyon, France), measured between 2004 and 2011. Chassieu is one of the experimental sites of the OTHU (Observatoire de Terrain en Hyrdologie Urbaine/field observatory for urban hydrology) project[1] (Fig. 1).

The catchment is a 185-ha industrial area drained by a separate storm sewer system, with imperviousness ratio and runoff coefficients of about 0.72 and 0.43, respectively. The flow rate (L/s) at the outlet of the Chassieu catchment is measured in a 1.6-m circular concrete pipe with a 2-min time-step resolution. These flow measurements are carried out from periodically calibrated water depth and velocity sensors. Redundancy of sensors and field tests (e.g. tracing experiments, Lepot *et al.* 2014) allow errors to be minimized and a reduction in uncertainties in the flow-rate measurements, with relative measurement uncertainties ranging from 2% to 25% (Métadier 2011, Sun *et al.* 2017). Rainfall was measured with a time step of 1 min by a tipping-bucket raingauge installed in the catchment. Summarized statistics of different rainfall characteristics from the 365 rainfall events are presented in Table 1.

Hydrological model

The CRR model implemented in this study is lumped and consists of a single reservoir. The operation of the model is described by Equations (1)–(3). The effective rainfall $\boldsymbol{X}_{\mathrm{net}}(t)$ (L/s) is estimated from the observed rainfall $\boldsymbol{X}_{\mathrm{obs}}(t)$ (mm/h) by the Horton infiltration model (Equations (1) and (2)). The infiltration rate at time t, $\boldsymbol{f}(t)$ (mm/h) in Equation (1), involves three parameters that depend on soil characteristics: initial and final infiltration rates, f_0 (mm/h) and f_c (mm/h), respectively, and the decay constant k (min^{-1}). The impervious area of the catchment S is 80 ha (0.43 × 185 ha). The single reservoir lumped model is established in Equation (3), for estimating the simulated flow rate, $\boldsymbol{Y}_{\mathrm{sim}}(t)$ (L/s), as a function of $\boldsymbol{X}_{\mathrm{net}}(t)$. Three additional parameters are included in the linear reservoir model: the lag time of the reservoir K (min), an advective delay τ_d (min) and q (L/s) as an additive term of the output to represent baseflow (Equation (3)). The time step Δt of the simulations is equal to 2 min. The set of parameters $\boldsymbol{\theta}$ of the hydrological model (f_c, f_0, k, τ_d, K, q)

Figure 1. Aerial view of: the Chassieu catchment (Source: www.othu.org).

[1]www.othu.org.

Table 1. Summarized statistics of different rainfall characteristics. SD: standard deviation.

Rainfall characteristics	Mean	SD	Median	Minimum	Maximum
Rainfall depth (mm)	9.0	11.9	4.6	1.0	87.0
Mean intensity (mm/h)	1.7	2.3	1.0	0.1	23.1
Duration (h)	7.1	6.9	4.8	0.6	42.6
Maximum intensity (mm/h)	10.7	13.2	6.0	0.7	90.0
Antecedent dry period (h)	185.4	446.5	62.1	4.0	489.2

Table 2. Parameters for the model calibration, with min. and max. for uniform prior distributions.

Parameter	Units	Search range [min, max]
Final infiltration rate (f_c)	mm/h	[0, 5]
Initial infiltration rate (f_0)	mm/h	[0, 120]
Decay constant (k)	min^{-1}	[0, 5]
Advective delay (τ_d)	min	[0, 60]
Lag time of the reservoir (K)	min	[1, 120]
Baseflow (q)	L/s	[0, 20]

are listed in Table 2, including also their minimum and maximum values that are employed as calibration bounds (from Sun and Bertrand-Krajewski 2013a). The selection of this particular model structure is based on its performance capabilities in relation to its simplicity, as suggested by previous studies using the same dataset (Sun and Bertrand-Krajewski 2013b).

$$\boldsymbol{f}(t) = f_c + (f_c - f_0) \cdot \exp(-kt) \tag{1}$$

$$\boldsymbol{X}_{\text{net}}(t) = (\boldsymbol{X}_{\text{obs}}(t) - \boldsymbol{f}(t)) \cdot S \cdot 10000/3600 \tag{2}$$

$$\begin{aligned}\boldsymbol{f}_{\text{sim}}(t) = \exp\left(-\frac{\Delta t}{K}\right) \cdot \boldsymbol{Y}_{\text{sim}}(t - \Delta t) \\ + \left[1 - \exp\left(-\frac{\Delta t}{K}\right)\right] \boldsymbol{X}_{\text{net}}(t - T_{\mathbf{d}}) + q\end{aligned} \tag{3}$$

Event-based Bayesian calibrations

Simplified Bayesian inferences, widely used in hydrological modelling, allow one to calculate the posterior pdf $p(\boldsymbol{\theta}/\boldsymbol{Y})$, on the basis of a Gaussian likelihood function, a series of flow-rate observations $\boldsymbol{Y}_{\text{obs}}$ and prior knowledge of the distribution of parameters $p(\boldsymbol{\theta})$. A common implementation can lead to the calculation of $p(\boldsymbol{\theta}/\boldsymbol{Y})$ by means of Equation (4), numerically solved by the use of the DREAM algorithm (Vrugt 2016).

$$p(\boldsymbol{\theta}/\boldsymbol{Y}) = C\prod_{t=1}^{n}\frac{1}{\sqrt{2\pi\hat{\sigma}_t^2}} \cdot \exp\left[-\frac{1}{2}\left(\frac{\boldsymbol{Y}_{\text{sim}}(t,\boldsymbol{\theta}) - \boldsymbol{Y}_{\text{obs}}(t)}{\hat{\sigma}_t^2}\right)^2\right] \cdot p(\boldsymbol{\theta}) \tag{4}$$

where n is the number of flow-rate data $\boldsymbol{Y}_{\text{obs}}$; $\boldsymbol{Y}_{\text{sim}}(t, \boldsymbol{\theta})$ is the simulated flow rate by the model at a given time step t from the observed rainfall $\boldsymbol{X}_{\text{obs}}(t)$ and a set of parameters $\boldsymbol{\theta}$; $p(\boldsymbol{\theta})$ is the prior pdf for each parameter (uniform distribution); C is a normalization coefficient to guarantee that $\int p(\boldsymbol{\theta}/\boldsymbol{Y})\mathrm{d}\boldsymbol{\theta} = 1$ for the distribution $p(\boldsymbol{\theta}/\boldsymbol{Y})$ and $\hat{\sigma}_t^2$ is the residual variance, considered for this application to be equal to the flow-rate measurement error variance (from Métadier 2011).

When dealing with a significant number of rainfall events (e.g. more than 100), the application of Equation (4) by assigning a different set of parameters to each event under a multi-event simultaneous calibration approach (e.g. Kuczera 1990, Kuczera *et al.* 2006) might bring identifiability problems due to the massive dimension of the Bayesian inference (Thyer *et al.* 2009, Renard *et al.* 2011). In this sense, simplified event-based Bayesian calibrations are employed to explore the inter-event variability of the parameters, retaining the locally-estimated parameter pdfs estimated for events in which the statistical assumptions of Equation (4) are more likely to be held. Representing the modelling errors by means of Equation (4), i.e. by a normal joint distribution, uncorrelated, with zero mean and a variance dependent on the flow measurement error variance, can provide a reasonable approximation when applied to individual rainfall events for this CRR model and dataset (Sun *et al.* 2017). The logarithmic form of Equation (4) is implemented to ensure numerical stability of the DREAM algorithm in the event-based calibrations, including a maximum number of simulations of 10^4 with 30 parallel Markov chains to reach convergence (Gelman and Rubin convergence criteria > 1.2; see Gelman and Rubin 1992). For this implementation, event-based calibrations required a few minutes to be undertaken with an Intel Core CPU with 3.2GHz and 8GB RAM. For more complex problems that include a higher number of simulations, further alternatives such as parallel computing and surrogate modelling techniques can be implemented to reduce computational time (e.g. Razavi *et al.* 2012, Tsoukalas *et al.* 2016).

Rainfall measurement errors and initial conditions

For some events with large spatial heterogeneity and/or significant movement of rain cells over the catchment, a single raingauge cannot deliver representative rainfall intensities applicable to the entire catchment (Leonhardt *et al.* 2014). Indeed, the indetermination effect of multi-event simultaneous Bayesian inferences becomes even more intense when event-dependent terms are included for representing errors in rainfall data (e.g. rainfall multipliers) (Renard *et al.* 2011). Therefore, if one can establish that the selected CRR model constitutes a suitable event-based description of the rainfall–runoff processes, and the flow measurements at the outlet are accurate enough, one can suppose that poor quality in local event-based Bayesian calibration for a particular rainfall event are provoked by significant errors in rainfall measurements.

A first drawback for this hypothesis comes from the potential influence of previous storms over event-based calibrations. Conveniently, this influence might be negligible when the time elapsed from the last rainfall event, as measured with the raingauge, is higher than the time needed for the catchment to reach the dry weather initial conditions again (Métadier and Bertrand-Krajewski 2011). Indeed, for this separate sewer system, dry weather flows are practically equal to zero (Métadier 2011). On the other hand, a model is an effort to describe nature by means of mathematical abstractions and simplifications. Thus, the non-representativeness of complex processes throughout a given CRR model can also be a major cause of poor quality calibrations (adapted from Sandoval 2017). However, if unsatisfactory local calibrations are reported sporadically within a large enough set of storms (e.g. more than 200), causes might be linked to event-specific sources of uncertainty, such as errors in rainfall data. Accordingly, events with unsatisfactory local calibrations, suspected to be influenced by significant errors in rainfall data, are discarded in the construction of the marginal and conditional pdfs. Hypotheses about rainfall errors and initial conditions presented in this section are further discussed, once the proposed methodology has been implemented for the study case (see Discussion section).

Marginal and conditional pdfs of the model parameters

Local sets of parameters from satisfactory event-based calibrations by means of the proposed CRR model are marginalized for assessing a parametric marginal time-invariant pdf. This estimation is undertaken as follows:

Marginal pdf

The model is calibrated with the Bayesian method as implemented by the DREAM algorithm (Equation (4)), by using the observed data $\boldsymbol{X}_{\text{obs}}{}^{i}$ and $\boldsymbol{Y}_{\text{obs}}{}^{i}$ for the calibration rainfall event i. This procedure leads to the estimation of an optimal set of parameters $\boldsymbol{\theta}_{\text{opt}}{}^{i}$ (based on the maximum likelihood) and a posterior pdf $p(\boldsymbol{\theta}/\boldsymbol{Y})^{i}$. Rainfall events exhibiting a Nash-Sutcliffe efficiency (NSE) value lower than 0.75 in the local calibration are considered non-reproducible by the selected CRR model and the corresponding $\boldsymbol{\theta}_{\text{opt}}{}^{i}$ estimation is discarded as non-representative.[2] The global marginal pdf $p(\boldsymbol{\theta}/\boldsymbol{Y})$ is calculated from a marginalization of all the local pdfs $p(\boldsymbol{\theta}/\boldsymbol{Y})^{i}$, by exclusively considering the non-discarded events. The global set of optimal parameters $\boldsymbol{\theta}_{\text{opt}}$ is estimated as the multivariate mean of the marginal pdf $p(\boldsymbol{\theta}/\boldsymbol{Y})$.

However, the marginalization of various locally-estimated pdfs of parameters, obtained from Bayesian event-based calibrations, into a global pdf represents additional challenges. The dispersion of this global pdf in a marginal form can be massive, even if the events reporting unsatisfactory local calibrations are discarded. Indeed, local parameter pdfs might have been obtained from very dissimilar rainfall events and calibration periods (e.g. Gharari *et al.* 2013), leading to overestimated uncertainties in prediction (e.g. Dotto *et al.* 2011).

We propose to tackle this shortcoming by decomposing the global marginal into conditional pdfs based on the transferability concept, i.e. the capacity of a given local set of parameters to properly simulate other calibration rainfall events (Bardossy and Singh 2008, Singh *et al.* 2016). The transferability of each local set of parameters from one event to another (analogous to a leave-all-out cross-validation scheme) is represented by an adjacency matrix and, therefore, as an undirected graph (Csardi and Nepusz 2006). The graph is then analysed by a clustering technique to find groups of "connected" local sets of parameters and construct the conditional pdfs (see similar applications, e.g. by Singh *et al.* 2016). The methodology can be described as follows:

Conditional pdfs

The sets of optimal parameters $\boldsymbol{\theta}_{\text{opt}}{}^{i}$, calculated as for the marginal pdf, are used for constructing the conditional pdfs of the parameters. For this purpose, the main hypothesis is that two calibration rainfall events i and j are connected if the optimal set of parameters $\boldsymbol{\theta}_{\text{opt}}{}^{i}$ obtained for the event i is able to reproduce as well the flow generated by the rainfall event j and if $\boldsymbol{\theta}_{\text{opt}}{}^{j}$ is also able to reproduce the flow generated by the rainfall event i, in both cases with NSE > 0.75 (following a leave-all-out cross-validation scheme) (see Footnote 2). A symmetric adjacency matrix, AM, can be then constructed, with $\mathbf{AM}(i, j) = \mathbf{AM}(j, i) = 1$ if the calibration rainfall events i and j are connected and $\mathbf{AM}(i, j) = 0$ otherwise. The diagonal of $\mathbf{AM}(i = j)$ is filled with zeros, by convention. Indeed, the proposed AM represents an undirected graph (see Csardi and Nepusz 2006), in the sense that the rainfall events (or optimal local sets of parameters) are nodes and the connections between events i and j (or optimal local sets of parameters $\boldsymbol{\theta}_{\text{opt}}{}^{i}$ and $\boldsymbol{\theta}_{\text{opt}}{}^{j}$), when $\mathbf{AM}(i, j) = 1$, are the edges of the graph. A rainfall event i that is disconnected from the graph, i.e. $\mathbf{AM}(i,:) = 0$ and $\mathbf{AM}(:, i) = 0$ for all rows and columns, is labeled as unrepresentative and discarded from the analysis.

The number of clusters T for the AM needs to be established in order to define the number of conditional pdfs, classifying representative rainfall events into different groups, e.g. T_1 and T_2 for a number of clusters $T = 2$ (i.e. two conditional pdfs). For this clustering purpose, we propose to implement the graph-based "spinglass.community" cluster function, from the package "igraph" (Csardi and Nepusz 2006) in R (R Development Core Team 2018), by using the AM as the input, leading to a number of T clusters of representative events being delivered. This algorithm essentially seeks to maximize the connectivity density inside each of the T clusters and its compatibility with the case study comes from the symmetric, connected and binary properties of the proposed AM (adapted from Reichardt and Bornholdt 2006). Following the example of $T = 2$ and without losing generality, the global conditional pdfs, e.g. $p(\boldsymbol{\theta}/\boldsymbol{Y},T_1)$ and $p(\boldsymbol{\theta}/\boldsymbol{Y},T_2)$, are proposed to be calculated from a marginalization of the local estimations $p(\boldsymbol{\theta}/\boldsymbol{Y},T_1)^{i}$ contained in each of the T_1 and T_2 groups, separately. Consistently, the global sets of optimal parameters, e.g. $\boldsymbol{\theta}_{\text{opt}}T_1$ and $\boldsymbol{\theta}_{\text{opt}}T_2$, are calculated as the multivariate means of $p(\boldsymbol{\theta}/\boldsymbol{Y},T_1)$ and $p(\boldsymbol{\theta}/\boldsymbol{Y},T_2)$, respectively. Recommendations about the number of clusters T to be used for applying these conditional representations are dependent on the case study. However, we propose that the benefits of the conditional representations be evaluated by using the T value that reported the most satisfactory results for simulating flow rates in verification events.

[2]The selection of a threshold of NSE = 0.75 is based in values given from previous studies with the same dataset and similar models (Sun *et al.* 2017). In addition, further tests by varying the threshold value for the NSE from 0.7 to 0.8 showed not to significantly affect the estimations of either the marginal or the conditional pdfs.