Supplement of Hydrol. Earth Syst. Sci., 27, 2935–2950, 2023
https://doi.org/10.5194/hess-27-2935-2023-supplement

Hydrology and Earth System Sciences
Open Access

Supplement of

Bayesian parameter inference in hydrological modelling using a Hamiltonian Monte Carlo approach with a stochastic rain model

Simone Ulzega and Carlo Albert

Correspondence to: Simone Ulzega (simone.ulzega@zhaw.ch)

Supplementary Materials

S1

We shall first describe the general procedure to derive the prior probability density $f(\xi)$ for a generic nonlinear SDE model, hence examine the specific case of the model used in this study (Eq. 2).

Let us consider a SDE model in the form,

$$\dot{\xi} = F(\xi,t) + G(\xi,t)\eta(t)\,, \tag{S1.1}$$

interpreted according to the Itô convention, where η indicates white noise, with $\langle \eta(t)\eta(t')\rangle = \delta(t-t')$, and F and G are generic, possibly nonlinear, functions. The probability density for a full model realization can be written as the probability density for the corresponding noise realization η, that is,

$$f(\eta) \propto \exp\left[-\frac{1}{2}\int_0^T \eta^2(t)dt\right]\,, \tag{S1.2}$$

where $[0,T]$ is the observation time interval. Then, the probability density $f(\xi)$ is easily obtained by changing coordinates from the noise η to the state variable of interest ξ, using the model of Eq. S1.1, that is,

$$\eta(t) = \frac{\dot{\xi}(t) - F(\xi,t)}{G(\xi,t)}\,. \tag{S1.3}$$

Depending on the SDE convention, this transformation might generate additional terms stemming from the Jacobian $d\xi/d\eta$ (Lau and Lubensky, 2007). Finally, it is convenient to write the probability density $f(\xi)$ in terms of an action $\mathcal{S}(\xi,\dot{\xi})$ as,

$$f(\xi) \propto \exp\left[-\mathcal{S}(\xi,\dot{\xi})\right]\,. \tag{S1.4}$$

Let us consider now the specific case of the stochastic process of Eq. 2. Using the procedure described above, the action $\mathcal{S}$ can be written in its continuous form (Lau and Lubensky, 2007) as,

$$\mathcal{S}(\xi,\dot{\xi}) = \int_0^T \frac{\tau}{4}\left(\dot{\xi}(t) + \frac{\xi(t)}{\tau}\right)^2 dt\,, \tag{S1.5}$$

where T is the total measurement time. Following Albert et al. (2016), we rewrite Eq. S1.5 in the form,

$$\mathcal{S}(\xi,\dot{\xi}) = \int_0^T \left(\frac{\tau}{4}\dot{\xi}^2 + \frac{\xi^2}{4\tau} + \dot{\xi}\frac{\partial U(\xi,t)}{\partial \xi}\right) dt\,, \tag{S1.6}$$

with $U(\xi,t) = \xi^2(t)/4$. Using $\dot{\xi}\frac{\partial U}{\partial \xi} = \frac{dU}{dt} - \frac{\partial U}{\partial t}$ and $\frac{\partial U}{\partial t} = 0$, it is straightforward to obtain,

$$\mathcal{S}(\xi,\dot{\xi}) = \frac{\xi^2(T)}{4} - \frac{\xi^2(0)}{4} + \int_0^T \left(\frac{\tau}{4}\dot{\xi}^2 + \frac{\xi^2}{4\tau}\right) dt\,, \tag{S1.7}$$

which yields the discretized expression of Eq. 16.

S2

The first harmonic term of the discretized action (Eq. 16) can be written in the form,

$$\sum_{i=2}^{N} \frac{\tau}{4dt}\left(\xi_i - \xi_{i-1}\right)^2 = \frac{\tau}{4}\sum_{s=1}^{n_P}\left[\frac{(\xi_{(s-1)j_P+1} - \xi_{sj_P+1})^2}{j_P dt} + \sum_{k=2}^{j_P}\frac{k}{(k-1)dt}(\xi_{(s-1)j_P+k} - \xi^*_{(s-1)j_P+k})^2\right], \tag{S2.1}$$

with $\xi^*_{(s-1)j_P+k}$ defined by Eq. 19. Using the coordinate transformations of Eqs. 17 and 18, it is straightforward to rewrite S2.1 as,

$$\sum_{i=2}^{N} \frac{\tau}{4dt}\left(\xi_i - \xi_{i-1}\right)^2 = \frac{\tau}{4j_P dt}\sum_{s=1}^{n_P}(u_{(s-1)j_P+1} - u_{sj_P+1})^2 + \frac{k\tau}{4(k-1)dt}\sum_{s=1}^{n_P}\sum_{k=2}^{j_P} u^2_{(s-1)j_P+k}\,. \tag{S2.2}$$

Moreover, using Eqs. 17 and 20 one obtains,

$$\sum_{i=2}^{N}\xi_i^2 = \sum_{s=1}^{n_P}\left[u^2_{sj_P+1} + \sum_{k=2}^{j_P}\left(\sum_{l=k}^{j_P+1}\frac{k-1}{l-1}u_{(s-1)j_P+l} + \frac{j_P-k+1}{j_P}u_{(s-1)j_P+1}\right)^2\right]. \tag{S2.3}$$

Finally, using S2.2 and S2.3, the action $\mathcal{S}(\boldsymbol{\xi})$ (Eq. 16) can be formulated in the space of u-coordinates as in Eq.21.

S3

The runoff observation model $f\left(\boldsymbol{Q}_{\text{obs}} \mid \boldsymbol{\xi}, \boldsymbol{\theta}, \sigma_z\right)$ of Eq. 8 needs to be formulated in the u- rather than ξ-space. The only term affected by this coordinate transformation is obviously the ξ-dependent term $Q^{(\xi)}_{M,(s-1)j_Q+1}$ in the model predicted discharge $Q_{M,(s-1)j_Q+1}(\boldsymbol{\xi},\boldsymbol{\theta})$, with $s = 1,...,n_Q+1$ (see Eqs. 6 and 7). Using the definition of Eq. 7, straightforward calculations yield the recursive form,

$$Q^{(\xi)}_{M,(s-1)j_Q+1} = \left(1-\frac{dt}{K}\right)^{j_Q} Q^{(\xi)}_{M,(s-2)j_Q+1} + \left(1-\frac{dt}{K}\right)^{j_Q-1} r\left(\xi_{(s-2)j_Q+1}\right) + \sum_{k=2}^{j_Q}\left(1-\frac{dt}{K}\right)^{j_Q-k} r\left(\xi_{(s-2)j_Q+k}\right), \tag{S3.1}$$

and then with the transformations of Eqs. 17 and 20, after replacing the number of discretization bins for the precipitation data j_P with that for the discharge data j_Q,

$$\begin{aligned} Q^{(u)}_{M,(s-1)j_Q+1} &= \left(1-\frac{dt}{K}\right)^{j_Q} Q^{(u)}_{M,(s-2)j_Q+1} + \left(1-\frac{dt}{K}\right)^{j_Q-1} r\left(u_{(s-2)j_Q+1}\right) \\ &\quad + \sum_{k=2}^{j_Q}\left(1-\frac{dt}{K}\right)^{j_Q-k} r\left(\sum_{l=k}^{j_Q+1}\frac{k-1}{l-1}u_{(s-2)j_Q+l} + \frac{j_P-k+1}{j_P}u_{(s-2)j_Q+1}\right), \end{aligned} \tag{S3.2}$$

with $s = 2,...,n_Q+1$ and $Q^{(u)}_{M,1} = 0$. Finally, one has,

$$Q_{M,(s-1)j_Q+1}(\boldsymbol{u},\boldsymbol{\theta}) = \frac{S_1}{K}\left(1-\frac{dt}{K}\right)^{(s-1)j_Q} + A\frac{dt}{K}Q^{(u)}_{M,(s-1)j_Q+1} + \left[1-\left(1-\frac{dt}{K}\right)^{(s-1)j_Q}\right]Q_{\text{gw}}\,. \tag{S3.3}$$