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UNIVERSITY OF BOLOGNA
Alma Mater Studiorum

DATAERROR
Research Project

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Is deterministic physically-based hydrological modeling a feasible target? Incorporating physical knowledge in stochastic modeling of uncertain systems

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A premise on terminology

Physically-based, spatially-distributed and deterministic are often used as synonyms. This is not correct.

Sir Isaac Newton
(1689, by Godfrey Kneller)

- Physically-based model: based on the application of the laws of physics. In hydrology, the most used physical laws are the Newton's law of the gravitation and the laws of conservation of mass, energy and momentum.

- Spatially-distributed model: model's equations are applied at local instead of catchment scale. Spatial discretization is obtained by subdividing the catchment in subunits (subcatchments, regular grids, etc).

- Deterministic model: model in which outcomes are precisely determined through known relationships among states and events, without any room for random variation. In such model, a given input will always produce the same output

A premise on terminology

Fluid mechanics obeys the laws of physics. However:

- Most flows are turbulent and thus can be described only probabilistically (note that the stress tensor in turbulent flows involves covariances of velocities).
- Even viscous flows are au fond described in statistical thermodynamical terms macroscopically lumping interactions at the molecular level.

It follows that:

- A physically-based model is not necessarily deterministic.

A hydrological model should, in addition to be physically-based, also consider chemistry, ecology, etc.

In view of the extreme complexity, diversity and heterogeneity of meteorological and hydrological processes (rainfall, soil properties…) physically-based equations are typically applied at local (small spatial) scale. It follows that:

- A physically-based model often requires a spatially-distributed representation.

A premise on terminology

In fact, some uncertainty is always present in hydrological modeling. Such uncertainty is not related to limited knowledge (epistemic uncertainty) but is rather unavoidable.

It follows that a deterministic representation is not possible in catchment hydrology.

The most comprehensive way of dealing with uncertainty is statistics, through the theory of probability.

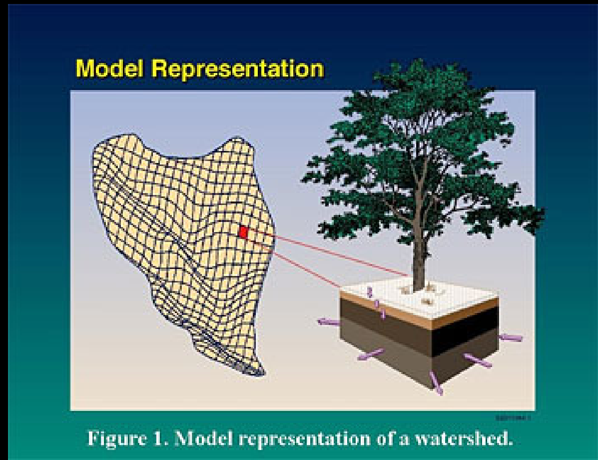

Figure taken from http://hydrology.pnl.gov/

Therefore a stochastic representation is unavoidable in catchment hydrology (sorry for that...).

The way forward is the stochastic physically-based model, a classical concept that needs to be brought in new light.

Formulating a physically-based model within a stochastic framework

Hydrological model:

in a deterministic framework, the hydrological model is usually defined as a single-valued transformation expressed by the general relationship:

$$Q_p = S\,(\varepsilon, \mathbf{I})$$

where Q_p is the model prediction, S expresses the model structure, $\mathbf{I}$ is the input data vector and ε the parameter vector.

In the stochastic framework, the hydrological model is expressed in stochastic terms, namely (Koutsoyiannis, 2010):

$$f_{Qp}\,(Q_p) = K f_{\varepsilon, I}(\varepsilon, \mathbf{I})$$

where f indicates the probability density function, and K is a transfer operator that depends on model S.

Formulating a physically-based model within a stochastic framework

Assuming a single-valued (i.e. deterministic) transformation $S(\boldsymbol{\varepsilon}, \mathbf{I})$ as in previous slide, the operator K will be the Frobenius-Perron operator (e.g. Koutsoyiannis, 2010).

However, K can be generalized to represent a so-called stochastic operator, which corresponds to one-to-many transformations S.

A stochastic operator can be defined using a stochastic kernel $k(e, \boldsymbol{\varepsilon}, \mathbf{I})$ (with e intuitively reflecting a deviation from a single-valued transformation; in our case it indicates the model error) having the properties

$$k(e, \boldsymbol{\varepsilon}, \mathrm{I}) \geq 0 \quad \text{and} \quad \int_e k(e, \boldsymbol{\varepsilon}, \mathrm{I})\, de = 1$$

Formulating a physically-based model within a stochastic framework

Specifically, the operator K applying on $f_{\boldsymbol{\varepsilon},\mathbf{I}}(\boldsymbol{\varepsilon},\mathbf{I})$ is then defined as (Lasota and Mackey, 1985, p. 101):

$$K f_{\boldsymbol{\varepsilon},\mathbf{I}}(\boldsymbol{\varepsilon},\mathbf{I}) = \int_{\boldsymbol{\varepsilon}} \int_{\mathbf{I}} k(e,\boldsymbol{\varepsilon},\mathbf{I})\, f_{\boldsymbol{\varepsilon},\mathbf{I}}(\boldsymbol{\varepsilon},\mathbf{I})\, d\boldsymbol{\varepsilon}\, d\mathbf{I}$$

If the random variables $\boldsymbol{\varepsilon}$ and $\mathbf{I}$ are independent, the model can be written in the form:

$$f_{Qp}(Q_{\mathrm{p}}) = K\,[f_{\boldsymbol{\varepsilon}}(e)\, f_{\mathbf{I}}(\mathbf{I})]$$

$$f_{Qp}(Q_{\mathrm{p}}) = \int_{\boldsymbol{\varepsilon}} \int_{\mathbf{I}} k(\mathrm{e},\boldsymbol{\varepsilon},\mathbf{I})\, f_{\boldsymbol{\varepsilon}}(\varepsilon)\, f_{\mathbf{I}}(\mathbf{I})\, d\boldsymbol{\varepsilon}\, d\mathbf{I}$$

Formulating a physically-based model within a stochastic framework

Estimation of prediction uncertainty:

Further assumptions:

1) model error is assumed to be independent of input data error and model parameters.

2) Prediction is decomposed in two additive terms, i.e. :

$$Q_p = S(\boldsymbol{\varepsilon}, \mathbf{I}) + e$$

where S represents the deterministic part and the structural error e has density $f_e(e)$.

4) Kernel independent of $\boldsymbol{\varepsilon}$, $\mathbf{I}$ (depending on e only), i.e.:

$$k(e, \boldsymbol{\varepsilon}, \mathbf{I}) = f_e(e)$$

By substituting in the equation derived in the previous slide we obtain:

$$f_{Q_p}(Q_p) = \int_{\boldsymbol{\varepsilon}} \int_{\mathbf{I}} f_e(Q_p - S(\boldsymbol{\varepsilon}, \mathbf{I}))\, f_{\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon})\, f_{\mathrm{I}}(\mathbf{I})\, d\boldsymbol{\varepsilon}\, d\mathbf{I}$$

Formulating a physically-based model within a stochastic framework

Symbols:

- Q_p — true (unknown) value of the hydrological variable to be predicted
- $S(\varepsilon,\mathbf{I})$ — Deterministic hydrological model
- e — Model structural error
- ε — Model parameter vector
- $\mathbf{I}$ — Input data vector

From the deterministic formulation:

$$Q_p = S(\boldsymbol{\varepsilon}, \mathrm{I})$$

to the stochastic simulation:

$$f_{Q_p}(Q_p) = \int_{\boldsymbol{\varepsilon}} \int_{\mathbf{I}} f_e(Q_p - S(\boldsymbol{\varepsilon}, \mathrm{I}))\, f_{\varepsilon}(\boldsymbol{\varepsilon})\, f_{\mathrm{I}}(\mathbf{I})\, d\boldsymbol{\varepsilon}\, d\mathbf{I}$$

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Formulating a physically-based model within a stochastic framework

An example of application: model is generic and possibly physically-based. Let us assume that input data uncertainty can be neglected, and that probability distributions of model error and parameters are known.

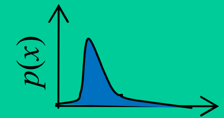
Repeat *j* times

Pick up a parameter vector ε from the model parameter space accordingly to probability $f_{\varepsilon}(\varepsilon)$

Input data vector (certain)

Compute model output and add *n* realisation of model error from probability distribution $f_e(e)$

Obtain n • *j* points lying on $f_{Qp}(Q_p)$ and infer the probability distribution



Problems:
1)computational demands;
2)estimate $f_{\varepsilon}(\varepsilon)$ and $f_e(e)$

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Example: linear reservoir rainfall-runoff model at monthly time scale

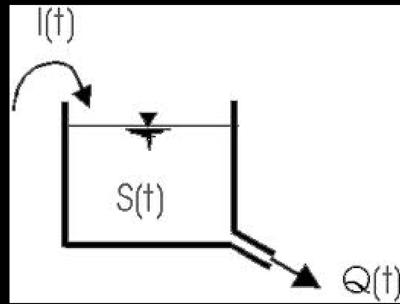
Synthetic data: monthly rainfall is Gaussian and independent. Monthly river flow $Q'(t)$ is generated with a linear reservoir model with parameter g = 800.000 s. Finally, river flow data are corrupted to account for model structural uncertainty:

$$Q(t) = Q'(t) + c(t)\, Q'(t)$$

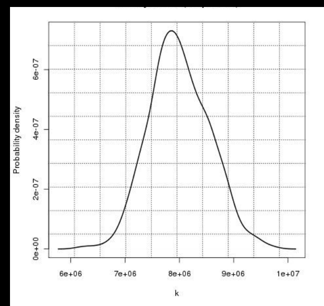
where $c(t)$ is a realisation from a Gaussian white noise.

Calibration of g was performed over a sample of 1500 observations by using DREAM (Vrugt and Robinson, 2007).

Probability density distribution of g turned out to be Gaussian with mean value equal to 800.000.



Linear reservoir



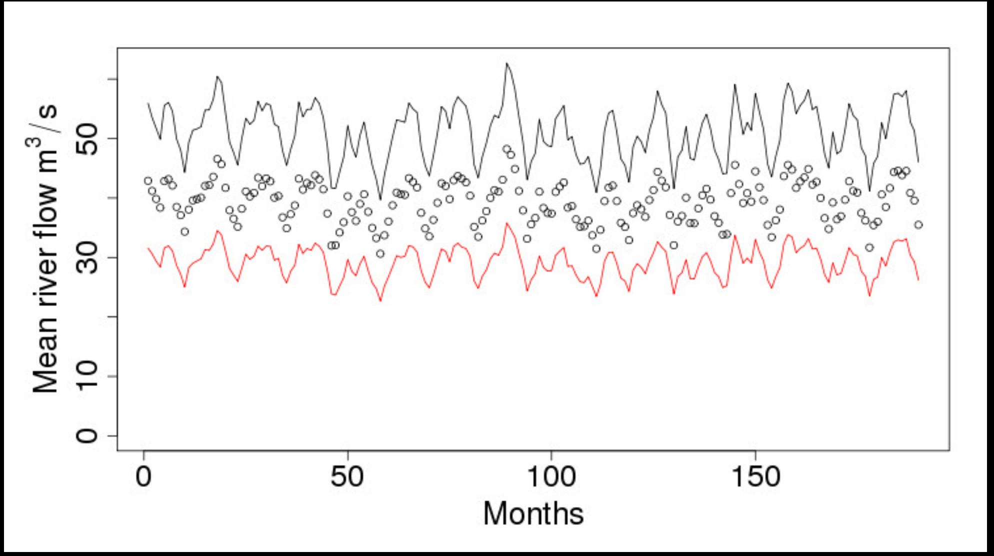
Probability density of g

Estimation of the predictive distribution

We estimated model predictive distribution by using 1500 “new” rainfall data in input to the linear reservoir model. We sampled 200 values from the parameter distribution and generated 200 “deterministic predictions”.

Then, to each prediction and for each time *t* we added 100 outcomes from the probability distribution of the model error e.

95% confidence bands and true values



Research challenges

To include a physically-based model within a stochastic framework is in principle easy. Nevertheless, relevant research challenges need to be addressed:

- numerical integration (e.g. by Monte Carlo method) is computationally intensive and may result prohibitive for spatially-distributed models. There is the need to develop efficient simulation schemes;
- a relevant issue is the estimation of model structural uncertainty, namely, the estimation of the probability distribution $f(e)$ of the model error. The literature has proposed a variety of different approaches, like the GLUE method (Beven and Binley, 1992), the meta-Gaussian model (Montanari and Brath, 2004; Montanari and Grossi, 2008), Bayesian Model Averaging. For focasting, Krzysztofowicz (2002) proposed the BFS method;
- estimation of parameter uncertainty is a relevant challenge as well. A possibility is the DREAM algorithm (Vrugt and Robinson, 2007).

Concluding remarks

- A deterministic representation is not possible in hydrological modeling, because uncertainty will never be eliminated. Therefore, physically-based models need to be included within a stochastic framework.
- The complexity of the modeling scheme increases, but multiple integration can be easily approximated with numerical integration.
- The computational requirements may become very intensive for spatially-distributed models.
- How to efficiently assess model structural uncertainty is still a relevant research challenge, especially for ungauged basins.

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