An impossible dream: The deterministic hydrologic prediction

IAHS Peter Loucks Lecture

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Emphasis is also on a basic element of uncertainty which seems to pervade nature and our knowledge of it. It is expressed by Gödel's incompleteness theorem, by fuzzy logic, by Heisenberg's uncertainty relation, by other random fluctuations and random measuring errors etc, which have fascinated the imagination of mathematicians, physicists, astronomers and geodesists since C.F. Gauss.
H. Moritz in Science, Mind and the Universe

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My web site: open education, teaching, research, software, data

Impossible dream

No deterministic models

Stochastic models of Nature

Examples

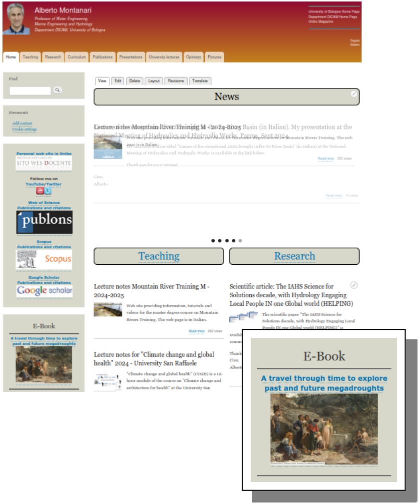
Stochastics: How to?

Fitting randomness with stochastics

Climate impact amplification

Take home messages

- This presentation is available in my website at www.albertomontanari.it.
- Everything is open, can be copied and reproduced (citation is appreciated).
- Everything I do is there. Lecture notes (in English), videos of lectures, scientific papers, presentations, software.
- Highlights: A travel through time to explore past and future megadroughts (interactive ebook); Floods, ten concepts to get protected; Climate change and water: lecture to students.
- Openness stands for dissemination and inclusivity.



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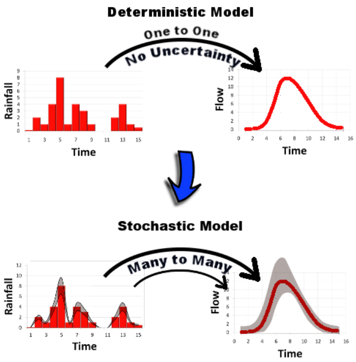
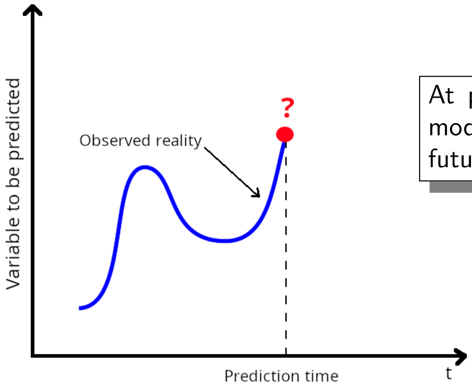
Deterministic and stochastic: definitions



- A deterministic model with a particular input and initial state, will always produce the same output.
- A stochastic model with a particular probability distribution of input and initial state will always produce the same probability distribution of output.

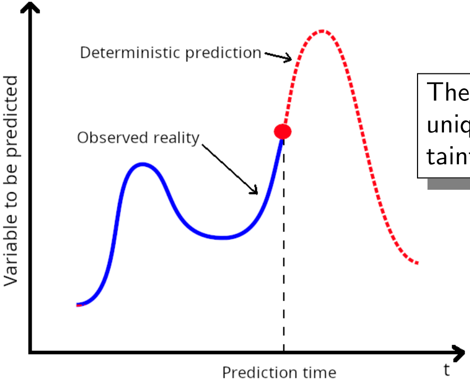
Note: The systems studied in chaos theory are deterministic. If the initial state were known exactly, then the future state of such a system could theoretically be predicted. However, knowledge about the future state is limited by the precision with which the initial state can be measured, and chaotic systems are characterized by a strong dependence on the initial conditions.

The impossible dream



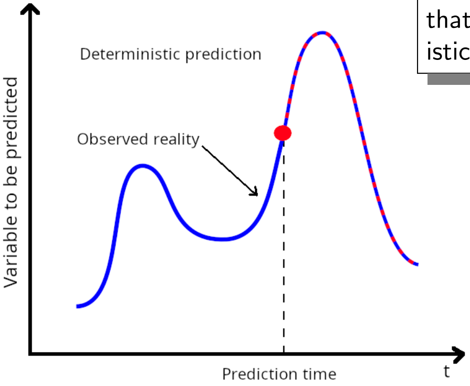
At prediction time, a deterministic model is usually applied to obtain a future prediction

The impossible dream



The deterministic model predicts a unique trajectory, with no uncertainty

The impossible dream

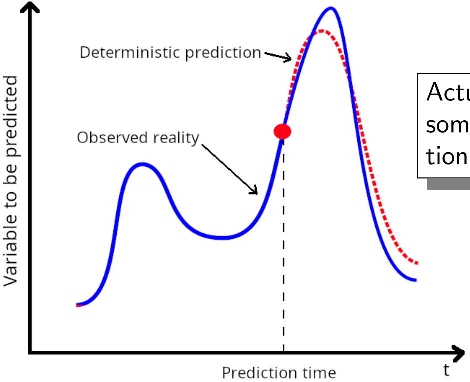


The dream is an evolution of reality that perfectly matches the deterministic prediction

The dream may not look impossible because:

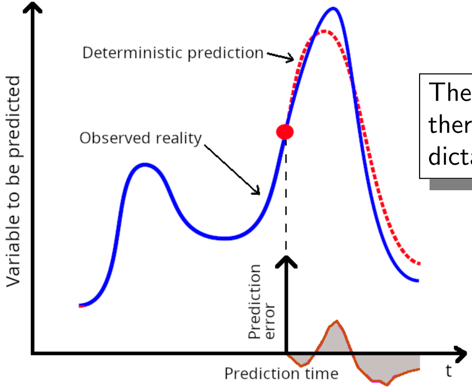
- Hydrology (conservation equations) is not subjected to chaotic expansion.
- In principle we may be able to obtain huge information with big data etc.

Dream does not come true



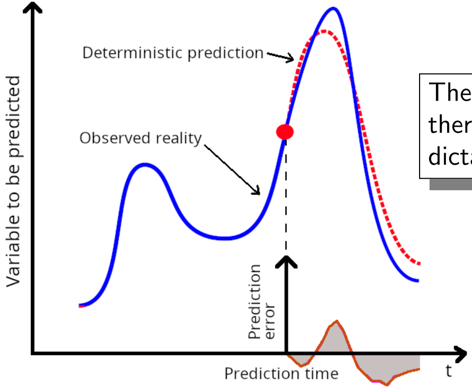
Actually, the outcome is for sure something different from the prediction: there is a prediction error

Dream does not come true



The presence of error means that there is a lack of deterministic predictability: uncertainty!

Dream does not come true



The presence of error means that there is a lack of deterministic predictability: uncertainty!

Error cannot be predicted by the deterministic model

Some considerations on the prediction error

Behaviours of the error of the deterministic prediction:

- Error cannot be predicted by the deterministic model, but actually often looks predictable to some extent. Thus, the deterministic model can be updated.
- Eventually a part of error remains that is unpredictable with a deterministic approach.
- The latter is then a random component, which means uncertainty (Koutsoyiannis, 2023).
- The presence of a random component means that the deterministic model is eventually not correct.

Uncertainty $\Longleftrightarrow$ Lack of deterministic predictability

Rational (usual) interpretation of uncertainty

Uncertainty means that:

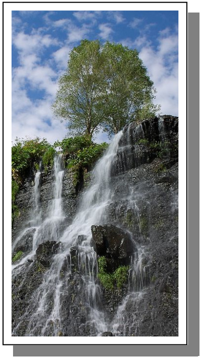
- Our interpretation (understanding) of patterns and dynamics is not correct or at least incomplete.
- Uncertainty $\Longrightarrow$ lack of understanding.
- Model needs to be improved basing on improved understanding.
- With a refined interpretation, model and monitoring, uncertainty can be eliminated.
- Once uncertainty disappears, deterministic models will allow prediction for arbitrarily extended lead time.

Arthur Hughes, **Uncertainty**, 1878, oil on canvas, Public domain, via Wikimedia Commons

An alternative vision (still knowledge-based, more creative?)

Uncertainty: an inherent behaviour of our understanding of nature

- "....He does not throw dice" (Einstein, on quantum mechanics). I fully agree and I would say: **The World of Nature is Unpredictable**.
- Models for reproducing nature are inherently uncertain (Bloeschl and Montanari, 2010; Farmer and Vogel, 2016).
- Measurements, control volume (catchment), initial conditions, numerical approximation $\Longrightarrow$ Uncertainty. Remember: computers do not play with real numbers.
- **Becomes essential when living species (people) are involved**. Would you be willing to discard uncertainty in your everyday life?



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An alternative vision: challenges

Embracing uncertainty requires that:

- We recognise the concept that uncertainty is an added value to modelling, an opportunity for improvement.
- We realise that uncertainty does not mean that physical laws do not apply. Quite the opposite: they fully apply in terms of probabilities. Testing is more rigorous and more useful.
- Validation of a physical law (hypothesis testing) that fails in a deterministic setting may succeed in terms of probability.
- We recognise that lack of deterministic predictability does not preclude that a process can be predicted in terms of probabilities. These are VERY useful in risk management.

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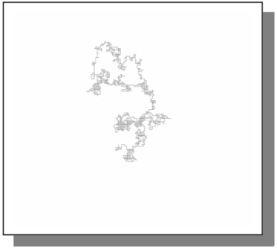
An alternative vision: challenges

Embracing uncertainty requires that:

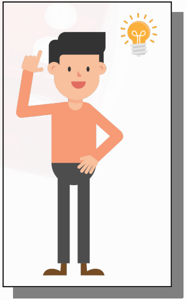
- We set up a knowledge base $\Longrightarrow$ theory $\Longrightarrow$ workflow.
- We elaborate an understanding of the physical - process based - nature of uncertainty and explain its deterministic part.
- **We identify a model for uncertainty**.
  This is not easy: prediction errors of hydrological models refuse an easy and reliable probabilistic description (Beven, 2006). This is why the topic became so popular in hydrology and why the related literature flourished (search for "uncertainty" and "hydrology" or "water" in Google Scholar).



Random Walk. László Németh, CC0, via Wikimedia Commons

Conceptions on uncertainty

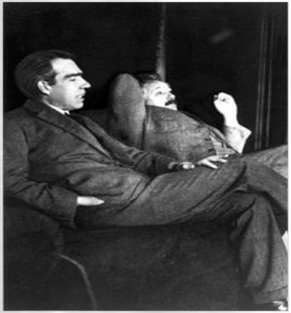
- Uncertainty can be **reduced**. Reducing uncertainty to its purely random component is our target.
- Uncertainty can be modelled by following alternative approaches.
- **Traditionally** it is modelled by using **probability and stochastics**.
- **Possible alternatives**: data-driven approaches, fuzzy logic, machine learning, ..., many others.
- Probabilistic description of prediction errors may entail a deterministic component. It **necessarily** includes a **random component**.



Historical remarks on uncertainty in physics

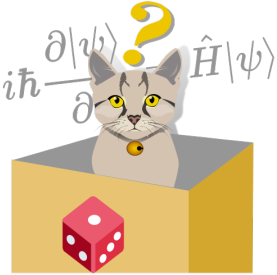
From Wikipedia: "The Bohr–Einstein debates were a series of public disputes about quantum mechanics between Albert Einstein and Niels Bohr. [...] and the outcome of Bohr's version of quantum mechanics becoming the prevalent view—form the root of the modern understanding of physics.

- In 1926 Max Born proposed that a particle's position in quantum mechanics was to be understood as a probability without any causal explanation.
- In a 1926 letter to Max Born, Einstein wrote: "I, at any rate, am convinced that He [God] does not throw dice." Einstein did not reject the idea that positions in space-time could never be completely known but did not want to allow the uncertainty principle to necessitate a seemingly random, non-deterministic mechanism by which the laws of physics operated.



Niels Bohr with Albert Einstein at Paul Ehrenfest's home in Leiden (1925; From Wikimedia Commons)

An historical analogy: Schrodinger's cat paradox



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Schrödinger's cat is a thought experiment concerning quantum statistical mechanics (QSM). A hypothetical cat is closed into a box for 1 hour and its fate is linked to the random release of a letal poison with probability of 50%. Then, according to probability theory the cat may be considered simultaneously both alive and dead. A paradox.

The thought experiment was conceived by physicist Erwin Schrödinger in 1935 in a letter to Einstein.

Schrodinger meant to express a criticism on the probabilistic description of quantum mechanics. However, its paradoxical experiment turned to be supportive of QSM as it demonstrate that a deterministic prediction is not possible.

Example: Galton board

The Galton board consists of a vertical board with interleaved rows of pegs. Beads are dropped from the top and bounce either left or right as they hit the pegs. Eventually they are collected into bins at the bottom.

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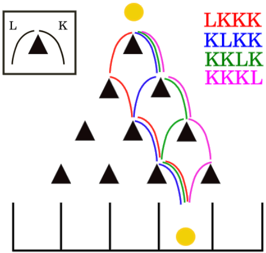

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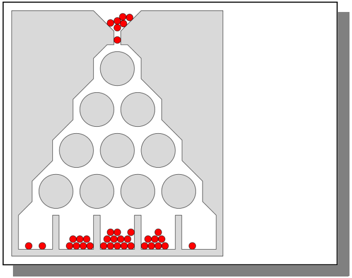
- Physics of the system is fully known.
- However, fitting a deterministic model trying to predict the position of each bead at a given time step would deliver a erroneous solution.

Example: Galton board

- A stochastic model assigning equal probability through a binomial distribution to left and right turn at each peg, would deliver a perfect probabilistic prediction, given by the **Gaussian distribution**.
- Knowledge of the physical basis and geometry of the system is essential to assign probabilities of left and right turn and parameters of the resulting probability distribution.



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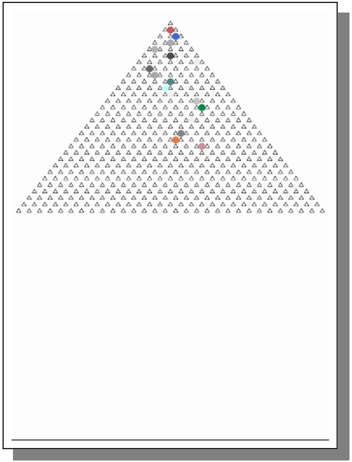
Example: Galton board

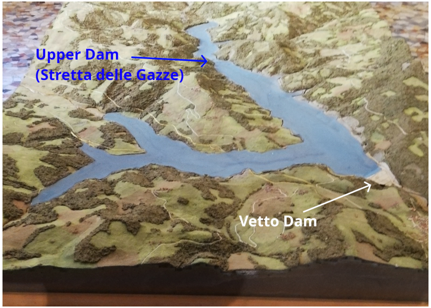
- A stochastic model assigning equal probability through a binomial distribution to left and right turn at each peg, would deliver a perfect probabilistic prediction, given by the **Gaussian distribution**.
- Knowledge of the physical basis and geometry of the system is essential to assign probabilities of left and right turn and parameters of the resulting probability distribution.
- **Note**: testing is essential to make sure that the interpretation is correct.



Example: Vetto Dam (socio-hydrology)

Water resources management in the Enza Valley (Italy) under climate change.

The Enza Valley provides irrigation water for the Parmesan Cheese production area, and civil and industrial water supply to the cities of Reggio Emilia and Parma. Enza valley historically suffers from water scarcity, that may be resolved by an artificial reservoir.



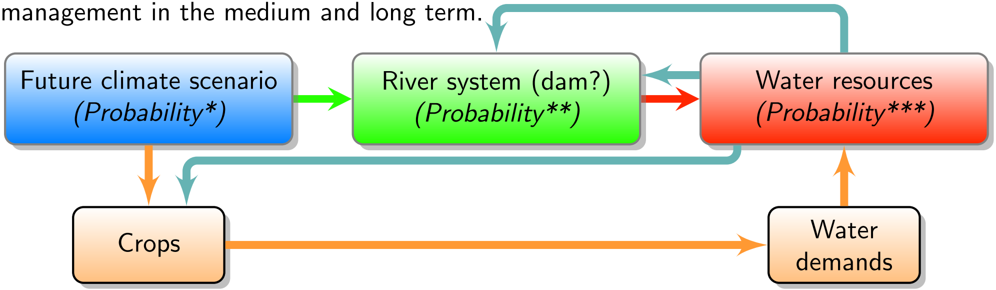
Three alternatives:

- No dam, improved water resources management.
- "Vetto Dam", storage $103 \cdot 10^6 m^3$;
- "Stretta delle Gazze Dam", storage $27 \cdot 10^6 m^3$.

Technical question: downstream water resources management under climate change.

Example: Vetto Dam (socio-hydrology)

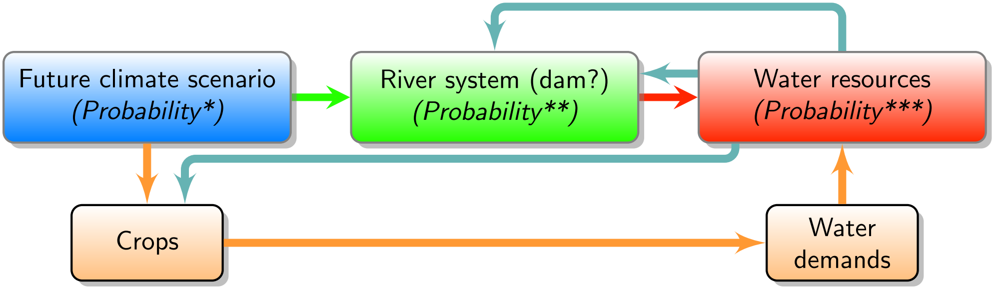
The Vetto Dam has a long history. The first project dates back to 1865. Construction of the dam started twice: in 1922 and 1980. Now the debate has restarted, another evaluation of possible solutions is ongoing. A prediction is needed of downstream water resources management in the medium and long term.



The Enza Valley system is impossible to model in deterministic terms at least because:

- Climate scenario is uncertain.
- Deterministic prediction of "dam" vs "no dam" is not possible.

Example: Vetto Dam (socio-hydrology)



We argue that the most rigorous approach is a stochastic model relying on meaningful probabilities of future climate and river system structure and dynamics.

In particular we need:

- Probability of future climate scenario (*), and
- Probabilities of alternatives for the river system (**),

to obtain probabilistic prediction of the future state of water resources (***).

Some considerations on probabilities

Key challenges of the proposed approach (reasons why stochastic models are not popular):

- Probability of future climate scenario (*): essential for making realistic (correct) predictions. Another impossible dream: How to estimate such probability?
  Note: ensemble simulation does not necessarily deliver probabilities of future climate.
- Probabilities for the river system (**): Not only the probability of "dam"/"no dam", which can be estimated with a socio-economic-political analysis. We also need uncertainty assessment for the river system model.
- Other uncertainties may be included, for instance by using stochastic equations for the feedbacks (blue arrows).

Note: climate models usually do not include a stochastic component. Ensemble simulation by different parameters/initial conditions may not encompass all uncertanties.
Possible solution: combination of stochastic and deterministic models.

Stochastic hydrological models with physical basis: how to

There are several options for framing a hydrological model in a stochastic setting:

- The "traditional approach" (ARIMA, FARIMA, etc).
- Data-driven approaches: neural networks, random forests, etc. These can be "physics informed".

These may not meet the target of providing a physically-based interpretation of the underlying dynamics.

- Deterministic models with stochastic input, parameters etc., including models based on stochastic differential equations
- Deterministic models coupled with stochastic error models.

Whatever the approach, the validity of the stochastic interpretation of physical processes should be tested.

Stochastic physically-based modelling: a generalised theory of pattern modelling with uncertainty

Montanari and Koutsoyiannis (M&K, 2012), proposed a blueprint to reframe in a stochastic setting a deterministic process-based model. From the deterministic model

Model prediction **Deterministic model**

$$Q = S(\Theta, \mathrm{X})$$

Parameters **Input data**

We move to its stochastic counterpart

Probability distribution of model prediction **Transfer operator from deterministic to stochastic**

$$f_Q(Q) = K_S f_{\Theta,\mathrm{X}}(\Theta, \mathrm{X})$$

Parameters **Input data**

After some math development we end up to:

Probability distribution of model prediction **Probability distribution of model error**

$$f_Q(Q) = \int_\Theta \int_\mathrm{X} f_e(Q - S(\Theta, \mathrm{X}) | \Theta, \mathrm{X}) f_\Theta(\Theta) f_\mathrm{X}(\mathrm{X}) \, d\Theta d\mathrm{X}$$

Input data **Parameters**

Definition of the probability distribution of model error is the key step

Stochastic physically-based modelling: a generalised theory of pattern modelling with uncertainty

Probability distribution of model prediction

Probability distribution of model error

$$f_Q(Q) = \int_{\Theta} \int_{X} f_e(Q - S(\Theta, X)\,|\Theta, X)\, f_{\Theta}(\Theta)\, f_X(X)\, d\Theta dX$$

Input data **Parameters**

This is a general theory. Includes, as a specific case, the traditional stochastic black box models

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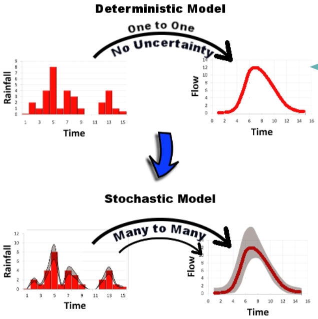
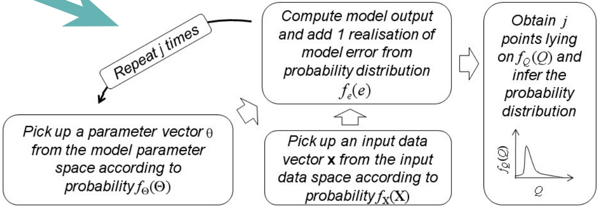




Definition of the probability distribution of the model error

Several alternatives:

- ARIMA modelling of model error through autocorrelation (Toth et al., 1999).
- Meta-Gaussian approach (Krzysztofowicz, 2002).
- Simulation and resampling methods (GLUE, Beven & Binley, 1992).
- Ensemble simulation.
- Modified Meta-Gaussian approach (M&K, 2012): Statistics of model error depend on the simulated river flow.
- Sikorska et al. (2015): resampling by nearest neighbour depending on predicted value.
- Data driven modelling depending on input data and system state (Tran et al., Auer et al., 2024).
- BLUECAT (K&M, 2022; M&K 2024, under review, available online).

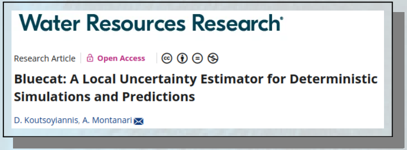
In blue the methods that explicitly estimate the distribution of model error.

BLUECAT: looking for simplicity and operational efficiency

www.albertomontanari.it/bluecat

Koutsoyiannis and Montanari (2022) & Montanari and Koutsoyiannis (2024). BLUECAT transforms a deterministic prediction model into a stochastic prediction model.

- From a point prediction we obtain the probability distribution of the predictand. From the above probability distribution we estimate the average (or median) prediction along with its confidence band for an assigned confidence level.
- BLUECAT is more than an uncertainty assessment method: it is rather a new prediction model with a stochastic structure. BLUECAT can be applied in conjunction with any deterministic prediction model.


Water Resources Research

Research Article | Open Access

Bluecat: A Local Uncertainty Estimator for Deterministic Simulations and Predictions

D. Koutsoyiannis, A. Montanari

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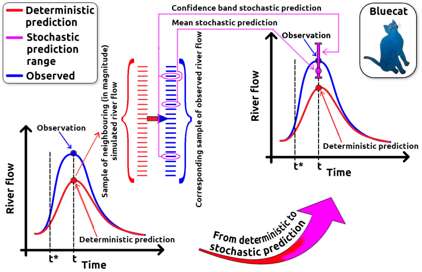
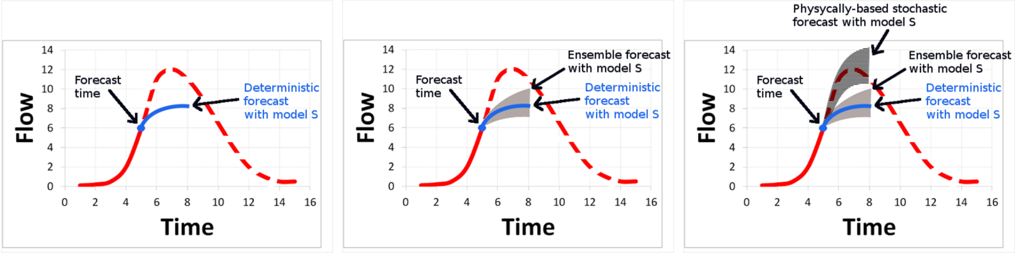
BLUECAT: workflow

- A point prediction is obtained with a deterministic model.
- A sample of neighbouring (in magnitude to the point prediction) simulated river flows is collected from the calibration period.
- A corresponding sample of observed river flows is collected. This is used to estimate (from data) the probability distribution of the predictand.
- Mean (or median) value is extracted along with the confidence bands.
- The stochastic prediction is obtained along with uncertainty assessment.



BLUECAT: features

Note: the previous point prediction is not necessarily included in the confidence band. The latter is displaced around the stochastic prediction (not around the point prediction).



- BLUECAT updates the model.
- Uncertainty is not necessarily displaced around the deterministic prediction. BLUECAT corrects the bias, which may vary with the river flow.

BLUECAT: assumptions

Note: in what follows, deterministic and stochastic model are D-model and S-model, respectively. BLUECAT assumptions:

- The stochastic processes describing the modelled variables are stationary during the calibration and application period. Non-stationarity can be accounted for by using non-stationary D-models.
- The calibration data set is extended enough to ensure that sufficient information is available to upgrade the D-model into the S-model.
- Uncertainty is not subdivided in different components as BLUECAT is assumed to automatically incorporate all types, including the uncertainty in input data and parameters, for which no particular provision is necessary.

Why BLUECAT

"Brisk Local Uncertainty Estimator for generiC simulations And predic-Tions"

BLUECAT refers to the pop-art by Andy Warhol (1928–1987), a success creation stimulated by a simple idea that gives a feeling of positive thinking and optimism.

BLUECAT: a bit of theory

To advance from the D-model to the S-model in we need to specify the conditional distribution:

$$\boxed{F_{q|Q}(q|Q) = P\left\{\underline{q} \leq q | \underline{Q} = Q\right\},}$$

where q and Q are concurrent observed and simulated flow, respectively, and stochastic variables are underlined.
If Q and q are concurrent time series, each of size n, and if $Q_{(i:n)}$ is the *ith* smallest value in Q and $q_{(j:n)}$ is the *jth* smallest value in q, then the approximations $F_Q(Q_i) \approx i/n$ and $F_q(q_j) \approx j/n$ can be used. After mathematical development we we prove that $F_{q|Q}$ can be obtained by minimizing the quantity

$$\boxed{A := \sum_{j=1}^{n} (B_j - j)^2 = \sum_{j=1}^{n} \left(\sum_{i=1}^{n} F_{q|Q}\left(q_{(j:n)}|Q_{(i:n)}\right) - j \right)^2 ,}$$

therefore getting the desired conditional distribution which leads to the formulation of the S-model corresponding to the D-model.

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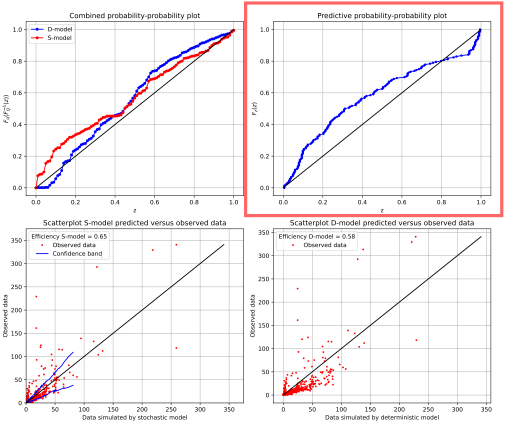
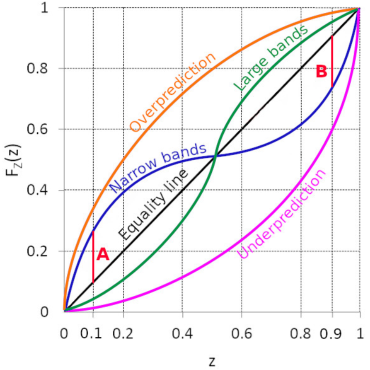
Hypothesis testing

- Testing stochastic physically-based assumptions through validation of the confidence band of the prediction.
- Verification of the reliability of uncertainty assessment.
- The only solution to quantitative testing of uncertainty assessment is comparison with observed data.
- Combined probability-probability plot (CPP), Predictive probability-probability plot (PPP).
- Embedded in the BLUECAT software.



Predictive probability-probability plot (PPP)

- Rigorous approach, surprisingly not much popular (perhaps because it is rigorous).
- First proposed by Laio and Tamea (2007). And then discussed by several authors, including Eslamian (2014), K&M (2022), M&K (2024).
- It tests whether probability of the observed data evaluated by BLUECAT are uniform. A straightforward and quick test.
- PPP plots the above probabilities against the sample frequency of the observed values. These are expected to fall within the BLUECAT confidence band with probability $1 - \alpha$ where α is the significance level.



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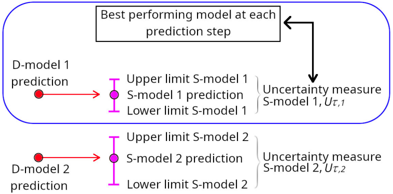
Ensemble simulation with BLUECAT

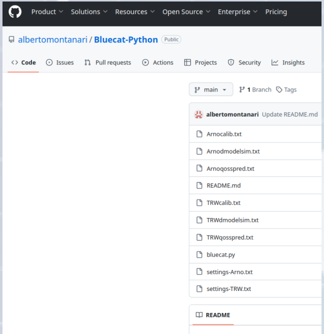
- Multimodel simulation is attractive (for example, a rainfall-runoff model with different parameters for different regimes).
- Two challenges: (a) how to combine different predictions (Bayesian averaging is an option) (b) how to estimate uncertainty for the obtained combination (remember: the pure ensemble spread does not suffice to provide a comprehensive estimate of uncertainty).
- BLUECAT: uncertainty of each model estimated at each prediction step as a criteria to select the optimal ensemble member (M&K, 2024).

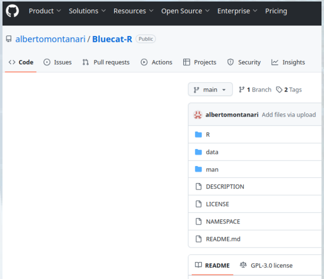
A single model prediction corresponding to the least uncertain ensemble member, that is identified through a proper measure, is picked up at each prediction step.

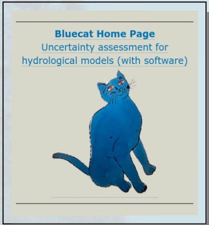


BLUECAT software (www.albertomontanari.it/bluecat)

- Python: https://github.com/albertomontanari/Bluecat-Python
- R: https://github.com/albertomontanari/Bluecat-R



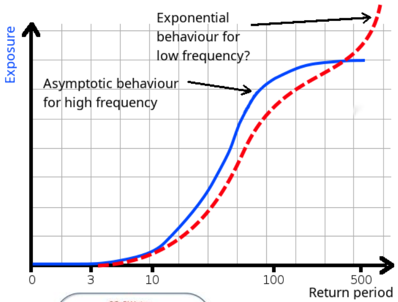




Software are accompanied by embedded help and examples of applications for full reproducibility.

Looking forward to a stochastic future
Climate impact amplification

Hydrology is not subjected to chaotic expansion, but hydrological risk is, through exposure that may evolve with a markedly non linear pattern dictated by hazard, vulnerability and socio-economic conditions. The presence of thresholds and marked step changes in risk pattern is one of the causes of "impossible flood" (Montanari, Merz and Bloeschl, 2024), namely, the "surprise" effect (Merz et al., 2015).

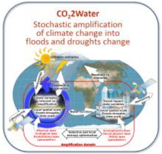


"Climate impact amplification" is defined as a step change in the impact of flood and droughts – impossible flood – triggered by a minor change in climatic drivers. It is determined by the concurrency of critical conditions in the climatic, hydrological and socio-economic systems.

FIS Advanced Grant project: $CO_2$2Water

Italian Science Fund

www.albertomontanari.it/co22water



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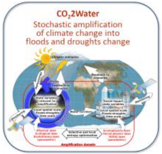
Climate impact amplification: searching for events

$CO_2$2Water is activating a search for events where climate impact got suddenly amplified and communities were taken by surprise.

- Flash and large scale floods.
- Droughts with unexpected impact.
- Debris flow events.



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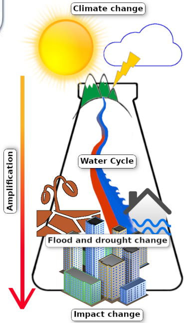

The purpose is to elaborate a large data set of surprise events at global scale to propose a checklist for identifying the climatic, hydrological and socio-economic conditions leading to amplification and surprise.
Such checklist may support the identification of areas exposed to risk.
We need data! **Interested in participating** and contribute to papers?
Stay tuned at www.albertomontanari.it/co22water!

Take home messages

"Uncertainty is an uncomfortable position. But certainty is an absurd one"
Voltaire, 1694 - 1778

- **"The World of Nature is unpredictable".** Trying to predict what is unpredictable is meaningless, misleading and a limit to our understanding.
- From Schrodinger's cat to **BLUECAT**: embracing uncertainty as an inherent feature of hydrological models within a creative vision of the water cycle.
- Relevant implications in **communication and policy making**. Explaining to stakeholders that a probabilistic prediction of water resources is useful.
- Physically-based (or physics informed) stochastics is the way to interpret randomness and **understanding predictability**.
- Understanding probabilities means **inspecting its physical basis** and **testing** with data (or other information).

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From Science to People:
Expecting the unexpected in flood and drought risk management

Thursday June 19, 2025 - Friday June 20, 2025

A focus on surprise in risk assessment and management

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- Surprise in floods and droughts
- Amplification of climate signal
- Hydrological change and non-stationarity

First flyer to come soon!