Uncertainty estimation for environmental predictions: the BLUECAT approach and software

Session HS4.3

Alberto Montanari[1] and Demetris Koutsoyiannis[2]

[1]Department of Civil, Chemical, Environmental and Material Engineering, University of Bologna
[2]School of Civil Engineering, National Technical University, Athens

May 1st, 2025

The quest for certainty blocks the search for meaning. Uncertainty is the very condition to impel man to unfold his powers.
Erich Fromm (1900-1980)

This study was partially supported by (1) the European Union Next-GenerationEU (National Recovery and Resilience Plan – NRRP, Mission 4, Component 2, Investment 1.3 – D.D. 1243 2/8/2022, PE0000005) and (2) the Italian Science Fund, grant number J53C23003860001

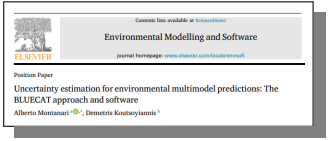
What is BLUECAT

www.albertomontanari.it/bluecat

- BLUECAT is a method for estimating uncertainty of predictions provided by a deterministic **calibrated** model;

  Koutsoyiannis and Montanari (2022) & Montanari and Koutsoyiannis (2024).

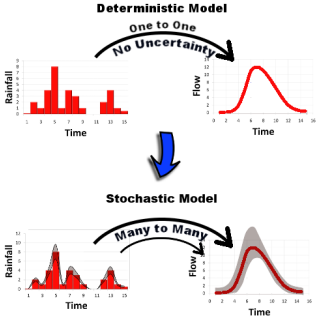
- BLUECAT is ready to use, with a software in Python and R that comes with help facilities and examples of application (https://github.com/albertomontanari)
- BLUECAT is accompanied by procedures for rigorously testing the reliability of the estimated uncertainty bands.



BLUECAT: looking for simplicity and operational efficiency

BLUECAT transforms a deterministic prediction model into a stochastic prediction model.

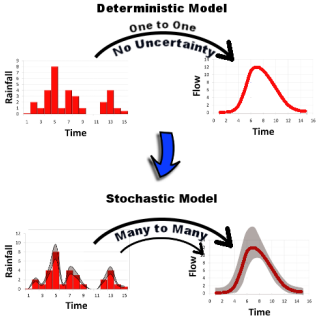
- From a point prediction we obtain the probability distribution of the predictand. From the above probability distribution we estimate the average (or median) prediction along with its confidence band for an assigned confidence level.
- BLUECAT is more than an uncertainty assessment method: it is rather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



BLUECAT: looking for simplicity and operational efficiency

BLUECAT transforms a deterministic prediction model into a stochastic prediction model.

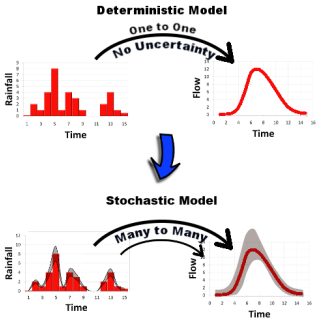
- From a point prediction we obtain the probability distribution of the predictand. From the above probability distribution we estimate the average (or median) prediction along with its confidence band for an assigned confidence level.
- BLUECAT is more than an uncertainty assessment method: it is rather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



BLUECAT: looking for simplicity and operational efficiency

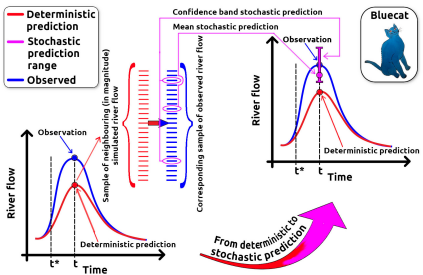
BLUECAT transforms a deterministic prediction model into a stochastic prediction model.

- 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.



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: 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:

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

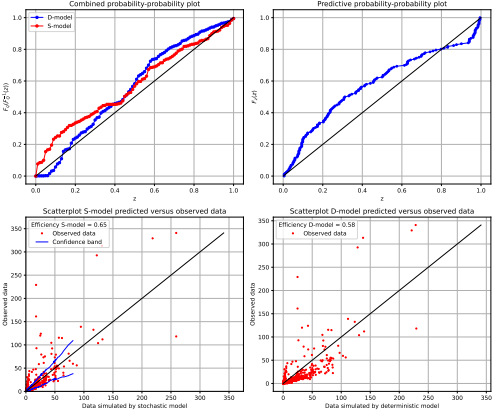
where q and Q are concurrent observed and simulated flow, respectively, and stochastic variables are underlined.
If Q and q are concurrent time series, each of size n, and if $Q_{(i:n)}$ is the *ith* smallest value in Q and $q_{(j:n)}$ is the *jth* smallest value in q, then the approximations $F_Q(Q_i) \approx i/n$ 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

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

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

Hypothesis testing

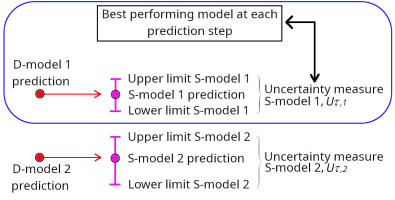
- Testing stochastic physically-based assumptions through validation of the confidence band of the prediction.
- Verification of the reliability of uncertainty assessment.
- The only solution to quantitative testing of uncertainty assessment is comparison with observed data.
- Combined probability-probability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



Ensemble simulation with BLUECAT

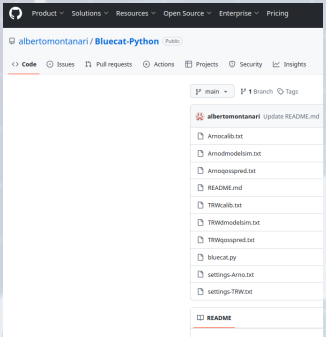
- Multimodel simulation is attractive (for example, a rainfall-runoff model with different parameters for different regimes).
- Two challenges: (a) how to combine different predictions (Bayesian averaging is an option) (b) how to estimate uncertainty for the obtained combination (remember: the pure ensemble 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).

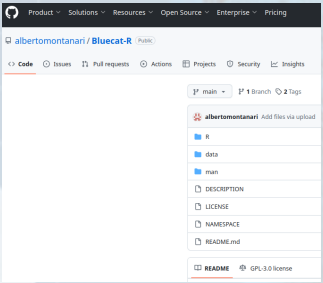
A single model prediction corresponding to the least uncertain ensemble member, that is identified through a proper measure, is picked up at each prediction step.

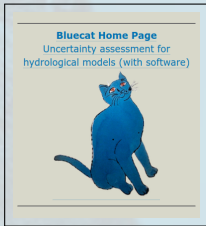


BLUECAT software (www.albertomontanari.it/bluecat)

- 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.

Take home message: try it and please let me know!

References

- Koutsoyiannis, D., Stochastics of Hydroclimatic Extremes - A Cool Look at Risk, Edition 3 (2023). ISBN: 978-618-85370-0-2, 391 pages, doi:10.57713/kallipos-1, Kallipos Open Academic Editions, Athens, 2023. Open access.
- Koutsoyiannis, D., & Montanari, A. (2022). Bluecat: A local uncertainty estimator for deterministic simulations and predictions. Water Resources Research, 58(1), e2021WR031215.
- Laio, F., & Tamea, S. (2007). Verification tools for probabilistic forecasts of continuous hydrological variables. Hydrology and Earth System Sciences, 11(4), 1267-1277.
- Montanari, A., & Koutsoyiannis, D. (2012). A blueprint for process-based modeling of uncertain hydrological systems. Water Resources Research, 48(9).
- Montanari, A., & Koutsoyiannis, D. (2025). Uncertainty Estimation for Environmental Multimodel Predictions: The Bluecat Approach and Software. Environmental Modelling and Software, 188, 106419.
- Montanari, A., Merz, B., & Blöschl, G. (2024). HESS Opinions: The sword of Damocles of the impossible flood. Hydrology and Earth System Sciences, 28(12), 2603-2615.
- Sikorska, A. E., Montanari, A., & Koutsoyiannis, D. (2015). Estimating the uncertainty of hydrological predictions through data-driven resampling techniques. Journal of Hydrologic Engineering, 20(1), A4014009.