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Supplement of

Large-scale assessment of Prophet for multi-step ahead forecasting of monthly streamflow

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S.1 Definitions and background information

Let us consider a time series of N observations. Let us also consider a prediction made for the next n observations.

If the total information utilized for this prediction is past available information (with respect to the prediction period), the prediction is also considered as a **forecast**.

For $n = 1$, the forecast is considered as an **one-step ahead forecast**.

For $n > 1$, the forecast is considered as a **multi-step ahead forecast**.

The forecasted variable(s) are called **predictand (or dependent) variables** and result via regression on the **predictor (or independent) variables**.

The latter can be **endogenous** or **exogenous**. According to Hyndman and Kostenko (2006) the former are variables, the values of which are determined within the system, and the latter are variables, the values of which are determined outside of the system.

Box S.1. Basic forecasting terminology.

Let $\{\underline{x}_t\}$, $t = 1, 2, \dots$ be a **Hurst-Kolmogorov process**. The latter is a three-parameter normal stationary stochastic process in discrete time. Its parameters μ , σ and H are defined by Equations S.1-S.3 (Tyrallis and Koutsoyiannis 2011).

$$\mu := E[\underline{x}_t] \quad (\text{S.1})$$

$$\sigma := (\text{Var}[\underline{x}_t])^{1/2} \quad (\text{S.2})$$

$$\rho_k := \text{Corr}[\underline{x}_t, \underline{x}_{t+k}] = |k+1|^{2H} / 2 + |k-1|^{2H} / 2 - |k|^{2H}, k = 0, 1, \dots, H \in (0, 1) \quad (\text{S.3})$$

The parameter μ is the mean of the stochastic process and the parameter σ is its standard deviation. The parameter H represents the magnitude of long-range dependence, i.e. the tendency of wet or dry years to be clustered in long time periods (persistence), while the autocorrelation function ρ_k increases with H . High values of H denote strong long-term persistence, while when $H < 0.5$, the resulting stochastic process is antipersistent, but still stationary. $H = 0.5$ is equivalent to a stochastic process of independent variables.

Box S.2. Definition of the Hurst-Kolmogorov process. This box is an adapted reproduction from Tyrallis et al. (2018).

The **AutoRegressive Fractionally Integrated Moving Average (ARFIMA)** models are widely used in hydrology. The reader is referred to Wei (2006, pp. 6-65, 489-494) for their detailed definitions. Let $d \in (-0.5, 0.5)$. The stochastic process $\{\underline{x}_t\}$ is an ARFIMA(p, d, q), if Equation S.4 holds.

$$\varphi_p(B)(1-B)^d \underline{x}_t = \theta_q(B) \underline{a}_t \quad (\text{S.4})$$

where

$$\varphi_p(B) := 1 - \varphi_1 B - \dots - \varphi_p B^p \quad (S.5)$$

$$\theta_q(B) := 1 + \theta_1 B + \dots + \theta_q B^q \quad (S.6)$$

$$B^j \underline{x}_t = \underline{x}_{t-j} \quad (S.7)$$

B is an operator, $\varphi_1, \dots, \varphi_p, d$ and $\theta_1, \dots, \theta_q$ are parameters of the model, and $\{a_t\}$ is a white noise process. The parameter d is a measure of the estimated long-range dependence of the time series (see also Box S.2). The parameters p and q are the orders of the AutoRegressive and Moving Average components of the ARFIMA model. The ARFIMA forecasting method fits an ARFIMA(p, d, q) model to the fitting set. The fitting procedure is explained in Hyndman et al. (2017). The parameters p and q are estimated using the Hyndman and Khandakar (2008) algorithm and the parameter d is estimated using the Haslett and Raftery (1989) algorithm. The method combines functions from the fracdiff (Fraleay et al. 2012) and forecast (Hyndman et al. 2018) R packages. The fitted model is used for forecasting future values.

The **Simple Exponential Smoothing (SES)** model, introduced by Brown (1959) and described in Hyndman et al. (2008, p. 13), computes the forecast of the next period based on the forecast of the previous period, the latter adjusted using its error according to Equation S.8.

$$f_{t+1} = f_t + a(x_t - f_t), a \in (0, 1) \quad (S.8)$$

The estimation of the parameters of the SES model is performed using procedures of the forecast R package (Hyndman et al. 2018).

The **Prophet** model, introduced by Taylor and Letham (2018) and implemented through the prophet R package (Taylor and Letham 2017), considers time series forecasting as a curve-fitting exercise, while it does not explicitly consider the temporal dependence of the time series. It simultaneously uses a decomposable time series model. The Prophet model is inspired by the nature of the time series forecasted at Facebook, which are characterized by trend, multiple seasonality and holidays.

Box S.3. Brief description of the ARFIMA, SES and Prophet models. This box is an adapted reproduction from Papacharalampous et al. (2018c).

For the definitions we consider a time series of N observations. Let us also consider a forecast of the last n observations. Let x_1, x_2, \dots, x_n represent the last n observations and f_1, f_2, \dots, f_n represent the forecasted values.

The **Root Mean Square Error (RMSE)** metric is defined by Equation S.9.

$$\text{RMSE} := \sqrt{(1/n) \sum_{i=1}^n (f_i - x_i)^2} \quad (S.9)$$

Let \bar{x} be the mean of the observations, which is defined by Equation S.10.

$$\bar{x} := (1/n) \sum_{i=1}^n x_i \quad (\text{S.10})$$

The **Nash-Sutcliffe Efficiency (NSE)** metric is defined by Equation S.11 (Nash and Sutcliffe 1970).

$$\text{NSE} := 1 - (\sum_{i=1}^n (f_i - x_i)^2 / \sum_{i=1}^n (x_i - \bar{x})^2) \quad (\text{S.11})$$

The **index of agreement (d)** metric is defined by Equation S.12 (Krause et al. 2005).

$$d := 1 - (\sum_{i=1}^n (f_i - x_i)^2 / \sum_{i=1}^n (|f_i - \bar{x}| + |x_i - \bar{x}|)^2) \quad (\text{S.12})$$

Let s_x be the standard deviation of the observations, which is defined by Equation S.13.

$$s_x := \sqrt{(1/(n-1)) \sum_{i=1}^n (x_i - \bar{x})^2} \quad (\text{S.13})$$

Let \bar{f} be the mean of the forecasts and s_f be the standard deviation of the forecasts, which are defined by Equations S.14 and S.15 respectively.

$$\bar{f} := (1/n) \sum_{i=1}^n f_i \quad (\text{S.14})$$

$$s_f := \sqrt{(1/(n-1)) \sum_{i=1}^n (f_i - \bar{f})^2} \quad (\text{S.15})$$

The Pearson's correlation coefficient (Pr) metric is defined by Equation S.16 (Krause et al. 2005).

$$\text{Pr} := (\sum_{i=1}^n (x_i - \bar{x})(f_i - \bar{f})) / (\sum_{i=1}^n (x_i - \bar{x})^2 \sum_{i=1}^n (f_i - \bar{f})^2)^{0.5} \quad (\text{S.16})$$

The **Kling-Gupta Efficiency (KGE)** metric is defined by Equation S.17 (Gupta et al. 2009).

$$\text{KGE} := 1 - \sqrt{(\text{Pr} - 1)^2 + ((s_f/s_x) - 1)^2 + ((\bar{f}/\bar{x}) - 1)^2} \quad (\text{S.17})$$

Box S.4. Definition of the RMSE, NSE, d and KGE metrics. This box is an adapted reproduction from Papacharalampous et al. (2018a, supplementary material).

S.2 Additional figures

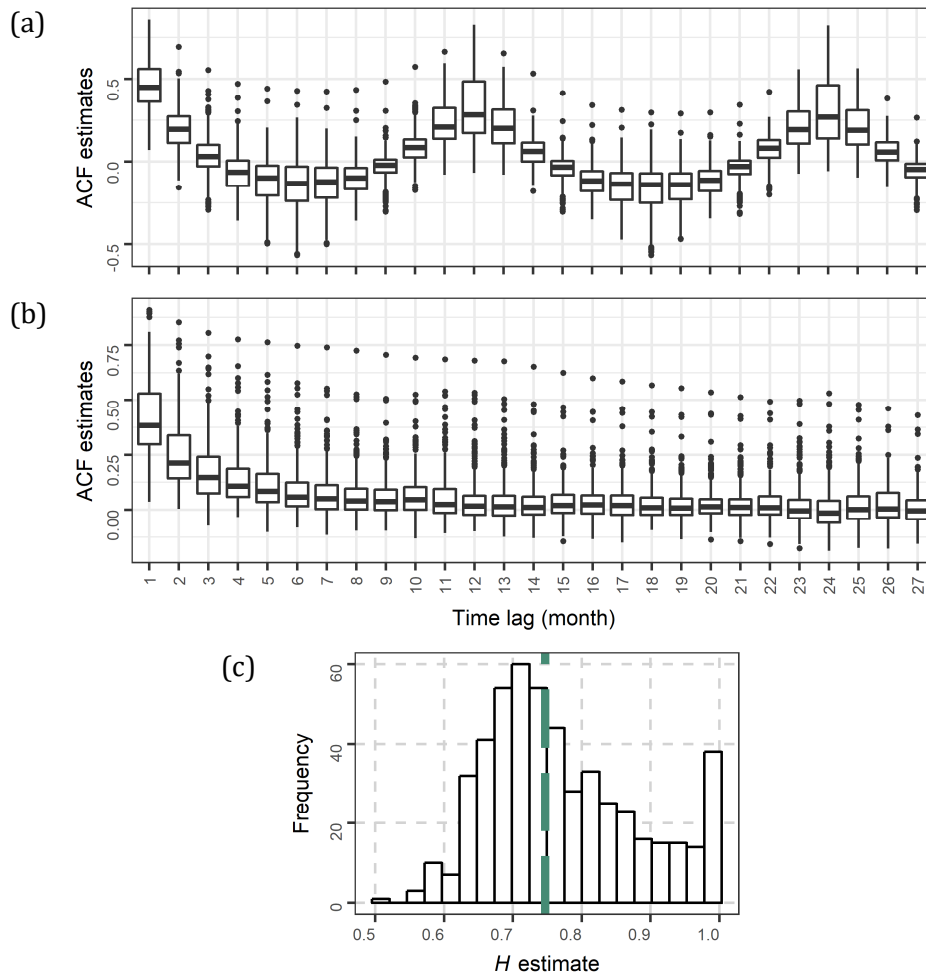


Figure S.1. Exploration of the monthly streamflow data examined in the forecasting experiment: (a) AutoCorrelation (ACF) estimates of the original time series, (b) ACF estimates of the deseasonalized time series and (c) Hurst parameter (H) estimates of the deseasonalized time series; their median is denoted with a green dashed line. The ACF and H estimates for the 513 catchments are presented in an aggregated form.

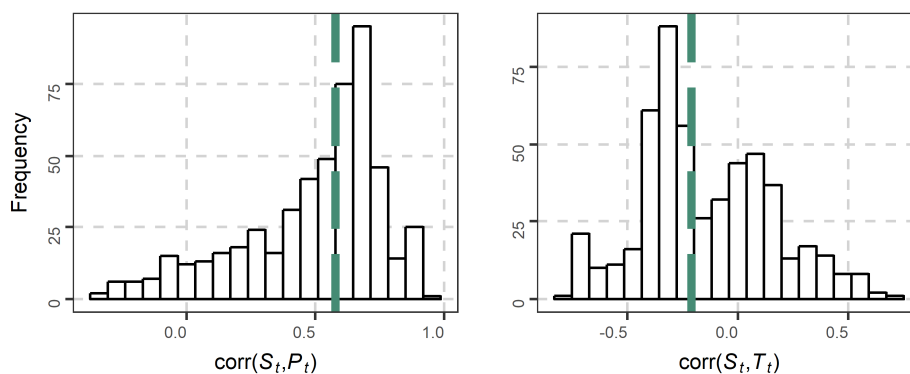


Figure S.2. Pearson's correlations between the monthly streamflow and precipitation variables ($\text{corr}(S_t, P_t)$), and the monthly streamflow and temperature variables ($\text{corr}(S_t, T_t)$) computed for the 513 catchments examined in the forecasting experiment. The correlations are presented in an aggregated form. Their medians are denoted with green dashed lines.

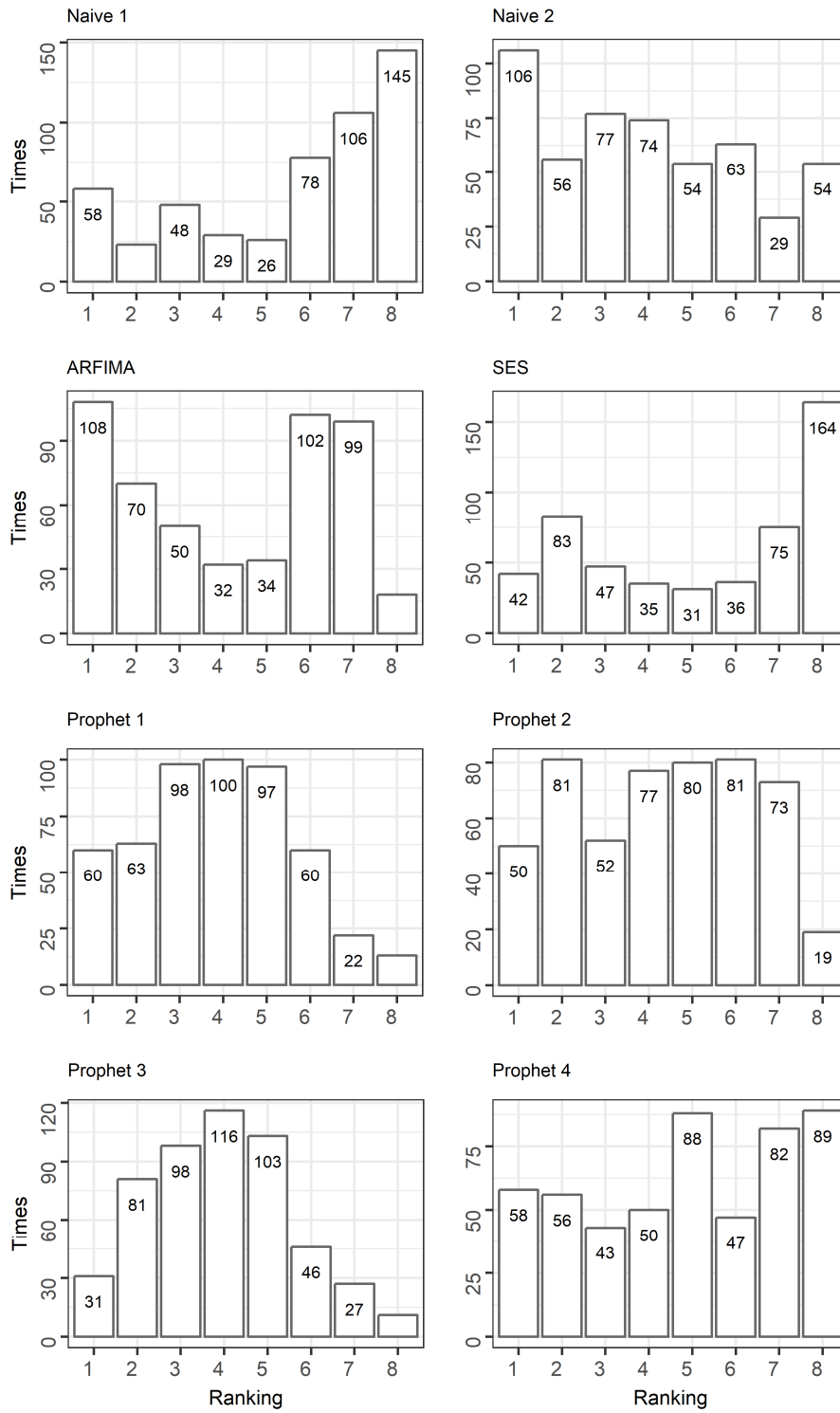


Figure S.3. Number of times that each algorithm is ranked from best (1st) to worst (8th) according to the RMSE metric.

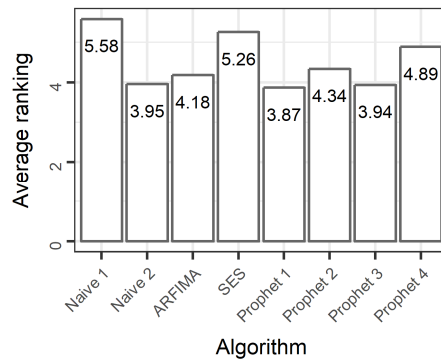


Figure S.4. Average rankings of the algorithms according to the RMSE metric. The algorithms are ranked from best (1st) to worst (8th).

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