Investigation of the effect of the hyperparameter optimization and the time lag selection in time series forecasting using machine learning algorithms

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Abstract

The hyperparameter optimization and the time lag selection are considered to be of great importance in time series forecasting using machine learning (ML) algorithms. In this study, we investigate the effect of the hyperparameter optimization and the time lag selection in time series forecasting. The investigation is conducted using the following two large-scale simulation experiments: Within each of them we compare 12 methods on 2,000 simulated time series from the family of Autoregressive Fractionally Integrated Moving Average (ARFIMA) models. The methods are defined by the set (ML algorithms, hyperparameter selection procedure, time lag selection). We compare ML algorithms, i.e., Neural Networks (NN), Support Vector Machines (SVM), two procedures for hyperparameter selection, i.e., predefined hyperparameters or defining optimization and two regression strategies (using time lag 1 and/or 2, 21). After splitting each simulated time series into a fitting and a testing set, we optimize the models to the former set and compare their performance on the latter one. We quantify the methods’ performance using several metrics proposed in the literature and benchmark methods. Furthermore, we conduct a sensitivity analysis on the length of the fitting set to examine how it affects the robustness of our results.

The findings indicate that the hyperparameter optimization mostly has a small effect on the forecasting performance. This is particularly important, because the hyperparameter optimization is computationally intensive. On the other hand, the time lag selection seems to significantly affect the results. Another finding is that the use of all time lags can be beneficial in the fitting procedure. In general, the performed study indicates that the hyperparameter optimization mostly has a small effect on the forecasting performance. This is particularly important, because the hyperparameter optimization is computationally intensive. On the other hand, the time lag selection seems to significantly affect the results. Another finding is that the use of all time lags can be beneficial in the fitting procedure.

1. Introduction

Machine learning (ML) algorithms are widely used in geosciences and beyond as an alternative to stochastic methods. We present an overview of the state of the art in the field of ML algorithms and their applications in geosciences. The ML algorithms investigated were NN and SVM in the former study and NN, RF and SVM in the latter study. To describe the long-term persistence of the simulated time series, we estimate their index of agreement (d).

2. Methodological framework

We conduct 6 large-scale simulation experiments (SE_1, SE_2, SE_3, SE_4, SE_5, SE_6), which are determined by the simulated time series.

3. Metrics

To evaluate and compare the ML methods, we present the following metrics:

- The root mean square error (RMSE) is defined by
- The mean absolute error (MAE) is defined by
- The index of agreement (d) is defined by
- The Nash-Sutcliffe efficiency (NSE) is defined by
- The coefficient of determination (R²)
- The coefficient of efficiency (CE)
- The time series

4. Simulated time series

We simulate time series according to the ARFIMA(1,0.30,0) model. For the ARFIMA model, we consider the following parameter values: $n = 2000$, $s = 1000$, $i = 2$, $p = 21$, $q = 2$, $H = 0.3$, $d = 0.3$, $n_{test} = 500$, and $n_{fit} = 500$.

5. Forecasting methods

We compare 12 ML methods. We also use 2 benchmark methods.

- We apply the ML methods using the R package runner (2010, 2016), as also several built-in algorithms (R Core Team 2017) and the benchmark methods using the R package forecast (Hyndman and Khandakar 2008, Hyndman et al. 2017).

6. Results

The findings indicate that the hyperparameter optimization mostly has a small effect on the forecasting performance. This is particularly important, because the hyperparameter optimization is computationally intensive. On the other hand, the time lag selection seems to significantly affect the results. Another finding is that the use of all time lags can be beneficial in the fitting procedure. In general, the performed study indicates that the hyperparameter optimization mostly has a small effect on the forecasting performance. This is particularly important, because the hyperparameter optimization is computationally intensive. On the other hand, the time lag selection seems to significantly affect the results. Another finding is that the use of all time lags can be beneficial in the fitting procedure.

7. Comparison of the methods in terms of RMSE

The methods are compared in terms of RMSE.

8. Comparison of the methods in terms of d

The methods are compared in terms of d.

9. Comparison of the methods in terms of Pr

The methods are compared in terms of Pr.

10. Comparison of the methods in terms of NSE

The methods are compared in terms of NSE.

11. Contribution of the present study

The findings indicate that the hyperparameter optimization mostly has a small effect on the forecasting performance. This is particularly important, because the hyperparameter optimization is computationally intensive. On the other hand, the time lag selection seems to significantly affect the results. Another finding is that the use of all time lags can be beneficial in the fitting procedure. In general, the performed study indicates that the hyperparameter optimization mostly has a small effect on the forecasting performance. This is particularly important, because the hyperparameter optimization is computationally intensive. On the other hand, the time lag selection seems to significantly affect the results. Another finding is that the use of all time lags can be beneficial in the fitting procedure.

References