

Forecasting of geophysical processes using stochastic and machine learning algorithms

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Abstract: We perform an extensive comparison between four stochastic and two machine learning (ML) forecasting algorithms by conducting a multiple-case study. The latter is composed by 50 single-case studies, which use time series of total monthly precipitation and mean monthly temperature observed in Greece. We apply a fixed methodology to each individual case and, subsequently, we perform a cross-case synthesis to facilitate the detection of systematic patterns. The stochastic algorithms include the Autoregressive order one model, an algorithm from the family of Autoregressive Fractionally Integrated Moving Average models, an Exponential Smoothing State Space algorithm and the Theta algorithm, while the ML algorithms are Neural Networks and Support Vector Machines. We also use the last observation as a Naïve benchmark in the comparisons. We apply the forecasting methods to the deseasonalized time series. We compare the one-step ahead as also the multi-step ahead forecasting properties of the algorithms. Regarding the one-step ahead forecasting properties, the assessment is based on the absolute error of the forecast of the last observation. For the comparison of the multi-step ahead forecasting properties we use five metrics applied to the test set (last twelve observations), i.e. the root mean square error, the Nash-Sutcliffe efficiency, the ratio of standard deviations, the index of agreement and the coefficient of correlation. Concerning the ML algorithms, we also perform a sensitivity analysis for time lag selection. Additionally, we compare more sophisticated ML methods as regards to the hyperparameter optimization to simple ones.

Key words: Stochastic algorithms, machine learning algorithms, multiple-case study, cross-case synthesis, multi-step ahead forecasting, one-step ahead forecasting, time lag selection, hyperparameter optimization

1. INTRODUCTION

Machine learning (ML) algorithms are widely used for the forecasting of geophysical processes as an alternative to stochastic algorithms. Popular ML algorithms are the rather well established Neural Networks (NN) and the new-entrant in most scientific fields Support Vector Machines (SVM). The latter was presented in its current form by Cortes and Vapnik (1995; see also Vapnik, 1995, 1999). The large number of the relevant applications is imprinted in Maier and Dandy (2000) and Raghavendra and Deka (2014).

As a result, the research in geophysical sciences often focuses on comparing stochastic to ML forecasting algorithms. The comparisons performed are usually based on single-case studies (e.g. Koutsoyiannis et al., 2008; Valipour et al., 2013), which offer the benefit of studying the phenomena in detail as also in their context and thus can provide interesting insights. On the other hand, single-case studies do not allow generalizations to any extent (Achen and Snidal, 1989). Generalizations could be derived by examining a sufficient number of different cases, as implemented in Papacharalampous et al. (2017). Within the latter study large-scale computational experiments based on simulations are conducted to compare several stochastic and ML methods regarding their multi-step ahead forecasting properties. A statistical analysis is performed and the results are presented accordingly.

Here we conduct a multiple-case study composed by 50 individual cases, each of them based on geophysical time series data from Greece. We apply a fixed methodology to each individual case for the comparison between several stochastic and ML methods regarding their one-step ahead and

multi-step ahead forecasting properties. Concerning the ML methods, we also perform a sensitivity analysis for time lag selection. Additionally, we compare more sophisticated ML methods as regards to the hyperparameter optimization to simple ones. Finally, we perform a cross-case synthesis to facilitate the detection of systematic patterns. We believe that the multiple-case study method can be useful for the comparative assessment of forecasting methods, as it can provide a form of generalization named “contingent empirical generalization”, while retaining the immediacy of the single-case study method (Achen and Snidal, 1989).

2. DATA AND METHODS

2.1 Time series

We use 50 time series of total monthly precipitation and mean monthly temperature observed in Greece. We select only those with few missing values (blocks with length equal or less than one). Subsequently, we use the Kalman filter algorithm from the zoo R package (Zeileis and Grothendieck, 2005) for filling in the missing values. We use the deseasonalized time series for the application of the forecasting methods for the improvement of the forecasting quality, as suggested in Taieb et al. (2012). The deseasonalization is performed using a multiplicative model of time series decomposition.

The basic information about the time series is provided in Table 1. To describe the long-term persistence of the deseasonalized time series, we estimate the Hurst parameter H for each of them using the maximum likelihood method (Tyrallis and Koutsoyiannis, 2011) implemented with the HKprocess R package (Tyrallis, 2016).

2.2 Forecasting methods

We use four stochastic and two ML forecasting algorithms. The stochastic algorithms include the Autoregressive order one model (AR(1)), an algorithm from the family of Autoregressive Fractionally Integrated Moving Average models (auto_ARFIMA), an Exponential Smoothing State Space algorithm (BATS) and the Theta algorithm. The ML algorithms are Neural Networks (NN) and Support Vector Machines (SVM). We also use the last observation as a Naïve benchmark in the comparisons. We apply the stochastic algorithms using the forecast R package (Hyndman and Khandakar, 2008; Hyndman et al., 2016) and the ML using the rminer R package (Cortez, 2010, 2015). The Naïve, AR(1), auto_ARFIMA and BATS algorithms apply Box-Cox transformation to the input data before fitting a model to them.

While the stochastic forecasting methods are simply defined by the stochastic algorithm, the ML methods are defined by the set {ML algorithm, hyperparameter selection procedure, time lags}. We compare two procedures for hyperparameter selection, i.e. predefined hyperparameters or defined after optimization, and 21 regression matrices, each using the first n time lags, $n = 1, 2, \dots, 21$. The hyperparameter optimization is performed with the hold-out method.

Hereafter, we consider that the ML models are used with predefined hyperparameters and that the regression matrix is built only by the first time lag, unless mentioned differently. We use two ML forecasting methods (one for each algorithm) in the comparisons conducted between stochastic and machine learning. We also use 42 forecasting methods (21 for each algorithm) to perform a sensitivity analysis for time lag selection and four ML forecasting methods (two for each algorithm) for the investigation of the effect of the hyperparameter optimization.

2.3 Metrics

Regarding the one-step ahead forecasting properties, the assessment is based on the absolute

error (AE) of the forecast of the last observation. For the comparison of the multi-step ahead forecasting properties we use the root mean square error (RMSE), the Nash-Sutcliffe efficiency (NSE), the ratio of standard deviations (rSD), the index of agreement (d) and the coefficient of correlation (Pr) applied to the test set. These metrics quantify the forecasting methods' performance according to several criteria related to the accuracy, the capture of the variance and the correlation between the forecasted and their respective observed values. For the definitions of the metrics NSE, d and Pr the reader is referred to Krause et al. (2005), while for the definition of the rSD to Zambrano-Bigiarini (2014).

Table 1. Time series examined. The Hurst parameter H is estimated for the deseasonalized time series.

| s/n | Process | Code | Location | Station id | Reference | Start | End | Length (months) | H |
|-----|---------------|--------------|----------------|------------|--------------------------------|----------|----------|--------------------|------|
| 1 | Precipitation | prec_1 | Agrinion | 16672000 | Peterson and Vose (1997) | Jan 1956 | Dec 1987 | 384 | 0.48 |
| 2 | | prec_2 | Alexandroupoli | 16627000 | | Jan 1951 | Dec 1990 | 480 | 0.59 |
| 3 | | prec_3 | Aliartos | 16674000 | | Jan 1907 | Dec 1990 | 1008 | 0.53 |
| 4 | | prec_4 | Anogeia | 16754001 | | Jan 1919 | Dec 1939 | 252 | 0.52 |
| 5 | | prec_5 | Anogeia | 16754001 | | Jan 1950 | Dec 1979 | 360 | 0.53 |
| 6 | | prec_6 | Araxos | 16687000 | | Jan 1949 | Dec 2000 | 624 | 0.51 |
| 7 | | prec_7 | Athens | 16714000 | | Jan 1860 | Dec 1881 | 264 | 0.48 |
| 8 | | prec_8 | Athens | 16714000 | | Jan 1887 | Dec 2005 | 1428 | 0.53 |
| 9 | | prec_9 | Athens | 16716000 | | Jan 1929 | Dec 1945 | 204 | 0.52 |
| 10 | | prec_10 | Fragma | 16715001 | | Jan 1926 | Dec 1990 | 780 | 0.54 |
| 11 | | prec_11 | Heraklion | 16754000 | | Jan 1946 | Dec 1990 | 540 | 0.50 |
| 12 | | prec_12 | Igoumenitsa | 16641001 | | Jan 1951 | Dec 1990 | 480 | 0.49 |
| 13 | | prec_13 | Ioannina | 16642000 | | Jan 1951 | Dec 1990 | 480 | 0.58 |
| 14 | | prec_14 | Kalamata | 16726000 | | Jan 1956 | Dec 1970 | 180 | 0.51 |
| 15 | | prec_15 | Kalo Chorio | 16756001 | | Jan 1950 | Dec 1984 | 420 | 0.50 |
| 16 | | prec_16 | Kastelli | 16760001 | | Jan 1949 | Dec 1976 | 336 | 0.55 |
| 17 | | prec_17 | Kerkyra | 16641000 | | Jan 1952 | Dec 1996 | 540 | 0.51 |
| 18 | | prec_18 | Kythira | 16743000 | | Jan 1951 | Dec 1973 | 276 | 0.48 |
| 19 | | prec_19 | Kos | 16742000 | | Jan 1958 | Dec 1990 | 396 | 0.49 |
| 20 | | prec_20 | Kozani | 16632000 | | Jan 1955 | Dec 1987 | 396 | 0.57 |
| 21 | | prec_21 | Larissa | 16648000 | | Jan 1951 | Dec 1997 | 564 | 0.55 |
| 22 | | prec_22 | Lemnos | 16650001 | | Jan 1951 | Dec 2000 | 600 | 0.52 |
| 23 | | prec_23 | Methoni | 16734000 | | Jan 1951 | Dec 1991 | 492 | 0.49 |
| 24 | | prec_24 | Milos | 16738000 | | Jan 1951 | Dec 1990 | 480 | 0.57 |
| 25 | | prec_25 | Mytilene | 16667000 | | Jan 1952 | Dec 1990 | 468 | 0.55 |
| 26 | | prec_26 | Naxos | 16732000 | | Jan 1955 | Dec 1971 | 204 | 0.46 |
| 27 | | prec_27 | Patra | 16689000 | | Jan 1901 | Dec 1984 | 1008 | 0.52 |
| 28 | | prec_28 | Sitia | 16757000 | | Jan 1960 | Dec 1983 | 288 | 0.56 |
| 29 | | prec_29 | Skyros | 16684000 | | Jan 1955 | Dec 1987 | 396 | 0.50 |
| 30 | | prec_30 | Thessaloniki | 16622000 | | Jan 1931 | Dec 1997 | 804 | 0.58 |
| 31 | prec_31 | Thessaloniki | 16622002 | Jan 1961 | Dec 1970 | 120 | 0.56 | | |
| 32 | prec_32 | Trikala | 16645001 | Jan 1951 | Dec 1990 | 480 | 0.56 | | |
| 33 | prec_33 | Tripoli | 16710000 | Jan 1951 | Dec 1985 | 420 | 0.53 | | |
| 34 | Temperature | temp_1 | Araxos | 16687001 | Lawrimore et al. (2011) | Jan 1951 | Dec 1980 | 360 | 0.66 |
| 35 | | temp_2 | Athens | 16714000 | | Jan 1858 | Dec 1975 | 1416 | 0.67 |
| 36 | | temp_3 | Athens | 16714000 | | Jan 1989 | Dec 2001 | 156 | 0.68 |
| 37 | | temp_4 | Athens | 16716000 | | Jan 1951 | Dec 2012 | 744 | 0.65 |
| 38 | | temp_5 | Heraklion | 16754000 | | Jan 1950 | Dec 2015 | 792 | 0.69 |
| 39 | | temp_6 | Kalamata | 16726000 | | Jan 1956 | Dec 2015 | 720 | 0.74 |
| 40 | | temp_7 | Kerkyra | 16641000 | | Jan 1951 | Dec 2016 | 792 | 0.67 |
| 41 | | temp_8 | Larissa | 16648000 | | Jan 1899 | Dec 2016 | 1416 | 0.64 |
| 42 | | temp_9 | Lemnos | 16650000 | | Jan 1951 | Dec 1998 | 576 | 0.75 |
| 43 | | temp_10 | Methoni | 16734000 | | Jan 1951 | Dec 1972 | 264 | 0.59 |
| 44 | | temp_11 | Methoni | 16734000 | | Jan 1975 | Dec 2000 | 312 | 0.61 |
| 45 | | temp_12 | Patra | 16689000 | | Jan 1951 | Dec 1989 | 468 | 0.69 |
| 46 | | temp_13 | Samos | 16723000 | | Jan 1955 | Dec 1969 | 180 | 0.64 |
| 47 | | temp_14 | Samos | 16723000 | | Jan 1974 | Dec 2003 | 360 | 0.64 |
| 48 | | temp_15 | Souda | 16746000 | | Jan 1961 | Dec 2015 | 660 | 0.71 |
| 49 | | temp_16 | Thessaloniki | 16622000 | | Jan 1892 | Dec 2016 | 1500 | 0.67 |
| 50 | | temp_17 | Thessaloniki | 16622001 | | Jan 1961 | Dec 1970 | 120 | 0.48 |

2.4 Methodology outline

We conduct 50 single-case studies by applying a fixed methodology to each time series (see Section 2.1), as explained subsequently. First, we split the time series into a fitting and a test set. The latter is the last observation for the one-step ahead forecasting experiments and the last 12 observations for the multi-step ahead forecasting experiments. Second, we fit the models to the deseasonalized fitting set, within the context determined by each forecasting method (see Section 2.2), and make predictions corresponding to the test set. Third, we add the seasonality to the predicted values and compare them to their corresponding observed using the metrics (see Section 2.3). Finally, we conduct the cross-case synthesis presented in Section 3 to demonstrate similarities and differences between the single-case studies conducted.

3. RESULTS AND DISCUSSION

We visualize the results within and across the individual cases using heatmaps. For the quantitative form of the latter graphs, as well as for Figures S1 and S2, the reader is referred to the Supplementary material, which is available at: <https://doi.org/10.17632/p8sw8pzkcd.3>.

As regards the heatmaps of the present study, they are formed under the following conditions: a) the darker the colour the better the forecasts and b) the scaling is performed in the row direction. White color rows indicate that no scaling is taking place. The latter happens when the forecasting methods under comparison perform equally well regarding the criterion tested.

In Figures S1 and 1 we present the heatmaps formed for the comparison between the stochastic and two of the ML forecasting methods on precipitation and temperature time series data respectively. As we observe, the results of the single-case studies vary significantly. We also observe that in every individual case examined the following applies. There is no best or worst forecasting method regarding all the criteria set simultaneously. In other words, none of the forecasting methods is uniformly better or worse than the rest. The former observations apply equally to the stochastic and the ML forecasting methods, while it is noteworthy that the Naïve benchmark is as competent as the forecasting methods regarding all the criteria set.

The observations outlined above are particularly important, because they reveal that the forecasting quality is subject to limitations. Each forecasting method has some specific theoretical properties and, due to the latter, it performs better or worse than other forecasting methods regarding specific criteria and in specific cases. Thus, the conduct of a single-case study using fewer criteria would have led to a very different overall picture. We note that the metrics RMSE and NSE give almost the same information about the forecast quality regarding the multi-step ahead forecasting experiments, a fact that does not apply to any other pair of metrics.

It is also interesting that the forecasting methods AR(1) and auto_ARFIMA are the least proper to use on precipitation data, while they are competent on the temperature time series data. This is actually a systematic pattern, which can be explained, when tracing back to the single-case studies using precipitation time series data. In more detail, those two forecasting methods predict zero precipitation in contrast to the rest, as a result to the zero precipitation observations in the summer months.

Finally, by studying the numerical results we note that the forecasts for temperature are remarkably better than the forecasts for precipitation. This may be explained by the fact that the variability in temperature is more regular than that in precipitation.

In Figures 2 and S2 we present the heatmaps formed for the sensitivity analysis on the time lags in time series forecasting using the NN and the SVM algorithms respectively. In both figures we observe significant variations in the results across the individual cases, in an extent that it is impossible to decide on a best or worst ML forecasting method among the single-case studies. Regarding the SVM algorithm (Figure S2), we observe no systematic patterns and the variations seem to be rather random, while for the case of the NN algorithm (Figure 2) we observe that the left parts of the heatmaps are smoother with no white cells.

- (1) one-step ahead forecasting - AE (2) multi-step ahead forecasting - RMSE (3) multi-step ahead forecasting - NSE
 (4) multi-step ahead forecasting - rSD (5) multi-step ahead forecasting - d (6) multi-step ahead forecasting - Pr

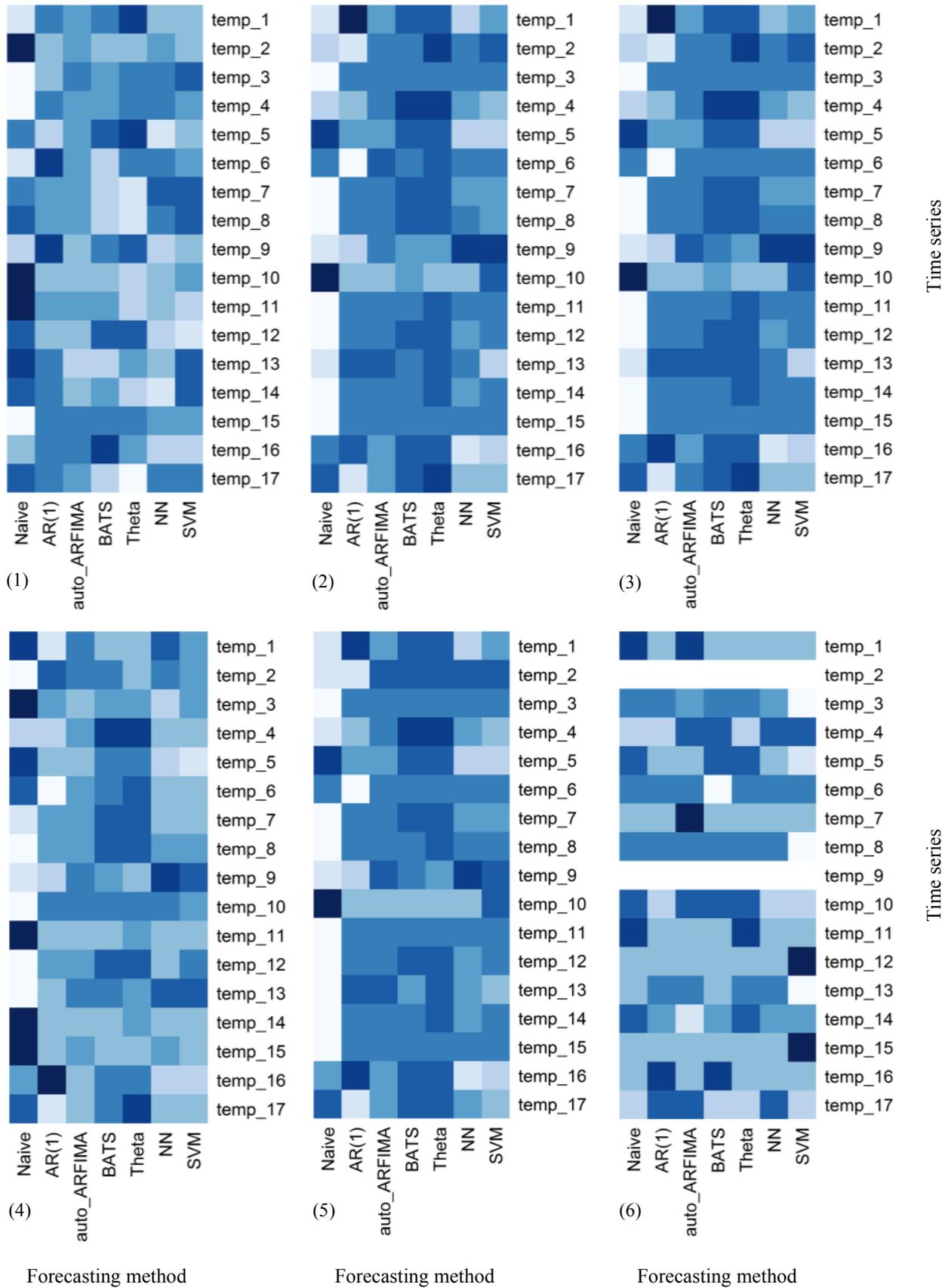


Figure 1. Heatmaps for the comparison between stochastic and ML methods on temperature time series.

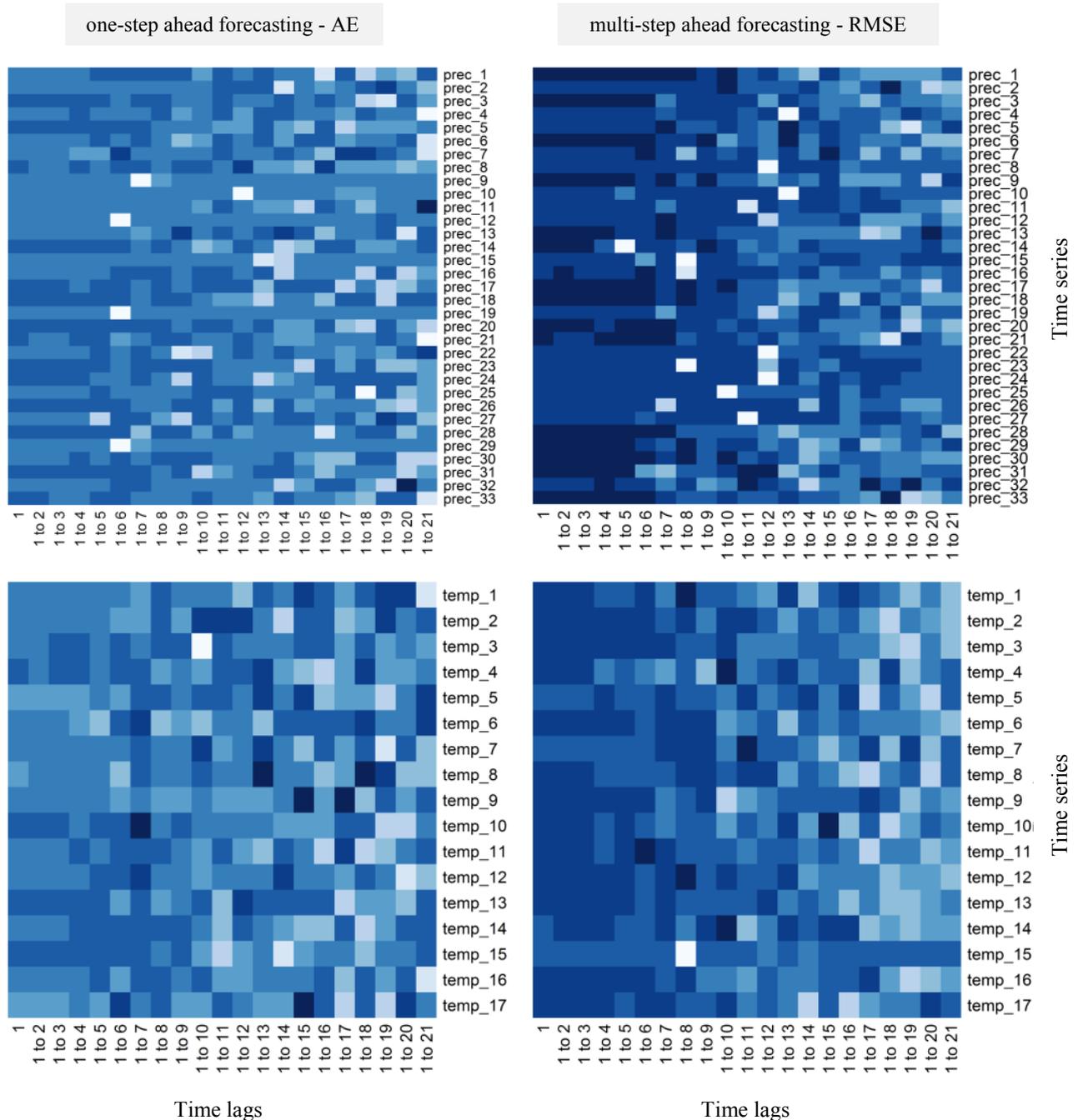


Figure 2. Heatmaps for the sensitivity analysis on the time lags in time series forecasting using the NN algorithm.

In Figure 3 we present the heatmaps formed for the investigation of the effect of the hyperparameter optimization. The results vary across the single-case studies in a rather random manner, which indicates that the hyperparameter optimization does not necessary lead to better forecasts for the NN and SVM algorithms.

4. CONCLUSIONS

The multiple-case study conducted must be encountered as a contingent empirical evidence on several issues that have drawn the attention in the field of time series forecasting. The findings suggest that the stochastic and ML methods can perform equally well, but always under limitations. The best forecasting method depends on the case examined and the criterion of interest, while it can be either stochastic or ML. However, the ML methods are computationally intensive. Regarding the time lag selection, the best choice seems to depend mainly on the case, while the ML algorithm

might has also some effect. Finally, for the algorithms used in the present study hyperparameter optimization does not necessarily lead to better forecasts.

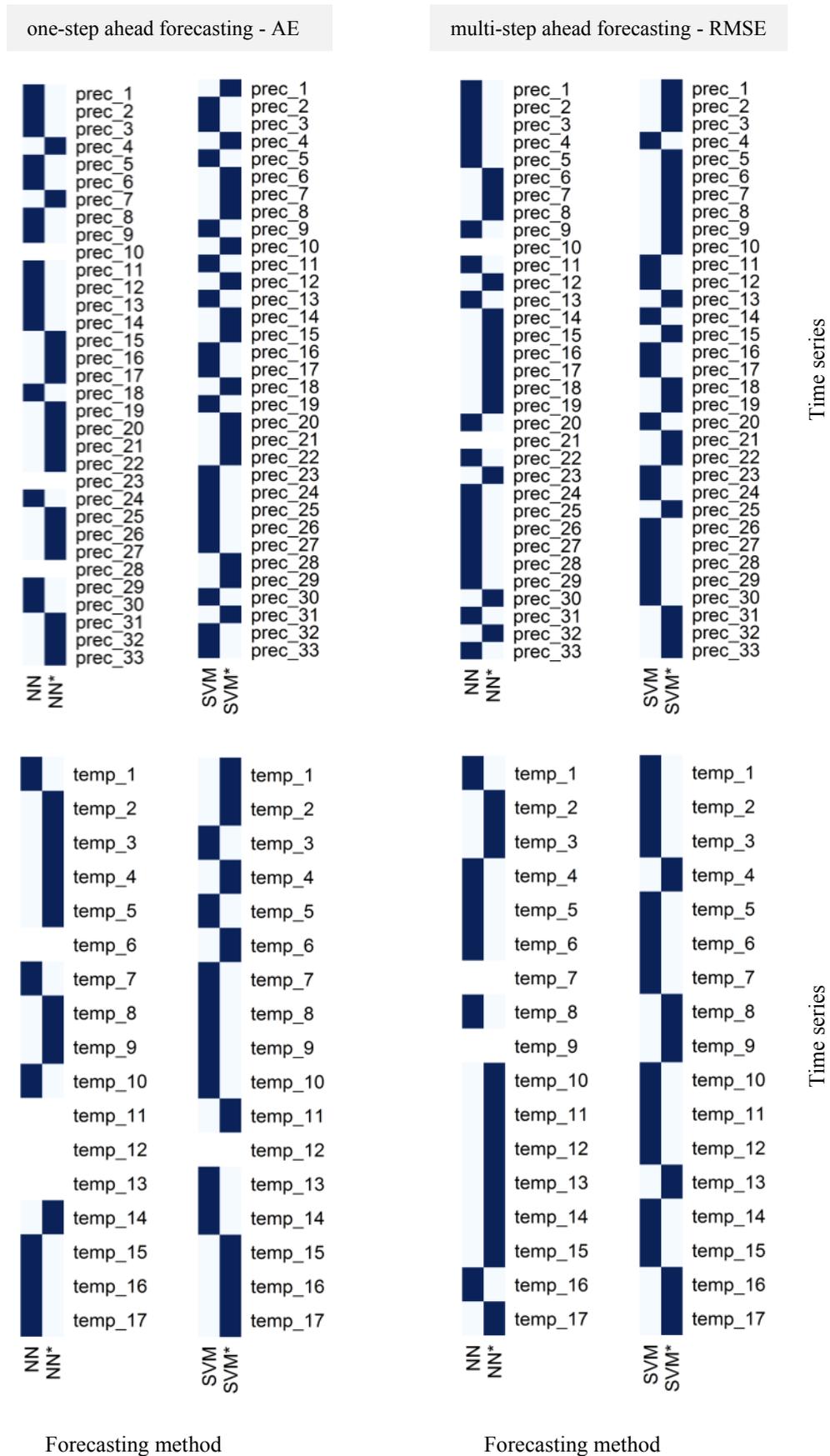


Figure 3. Heatmaps for the investigation of the effect of hyperparameter optimization on the forecast quality. The symbol * in the name of a forecasting method denotes that the model's hyperparameters have been optimized.

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