FORECASTING WITH SKTIME:
DESIGNING SKTIME’S NEW FORECASTING API AND APPLYING IT TO REPlicate AND EXTEND THE M4 STUDY

ABSTRACT

We present a new open-source framework for forecasting in Python. Our framework forms part of sktime, a machine learning toolbox with a unified interface for different time series learning tasks, like forecasting, but also time series classification and regression. We provide a dedicated forecasting interface, common statistical algorithms, and scikit-learn compatible tools for building composite machine learning models. We use sktime to both replicate key results from the M4 forecasting study and to extend it. sktime allows to easily build, tune and evaluate new models. We investigate the potential of common machine learning techniques for univariate forecasting, including reduction, boosting, ensembling, pipelining and tuning. We find that simple hybrid models can boost the performance of statistical models, and that pure machine learning models can achieve competitive forecasting performance on the hourly data sets, outperforming the statistical algorithms and coming close to the M4 winner model.

Keywords: Forecasting competitions, M competitions, Forecasting accuracy, Time series methods, Machine learning methods, Benchmarking methods, Practice of forecasting

Pre-release

The design and results presented in this paper depend on sktime version 0.4.0 which is currently being prepared for release and not yet available. In addition, we will add more tests to check if found performance differences are statistically significant.

1 Introduction

Time series forecasting is ubiquitous in real-world applications. Examples include forecasting demand to fill up inventories, predicting economic growth to inform policies, and forecasting stock prices to guide trading decisions. Forecasting is also a fruitful area for machine learning research, and pure and hybrid machine learning models have recently achieved state-of-the-art performance [1, 2].

In practice, forecasting involves a number of steps. We need to specify, fit and select an appropriate model, and evaluate and deploy it. There are various open-source toolboxes that help us implement these steps. However, most existing toolboxes are limited in important respects. Some support only specific model families (e.g. ARIMA or neural networks). Others provide more generic frameworks for forecasting, but no interfaces to existing machine learning toolboxes like scikit-learn [3]. Still others offer functionality for only some steps of a typical modelling workflow (e.g. feature extraction). In addition, existing toolboxes are often incompatible with each other. So, despite the success of machine learning in forecasting, to our knowledge, there is no open-source toolbox that allows to interface existing machine learning toolboxes and to build, tune and evaluate composite machine learning models for forecasting.

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To close this gap, we present a new open-source, scikit-learn compatible forecasting framework in Python. We provide a dedicated forecasting interface and all the necessary functionality to build, tune and evaluate forecasting models. Our framework is embedded in sktime [4], a machine learning toolbox for time series with a unified interface for multiple learning tasks that arise in a temporal data context, including forecasting, but also time series classification and regression among others.

In this paper, we first motivate and describe the design of our forecasting framework. We then use it to replicate key results from the M4 forecasting study. In addition, we extend the M4 study by evaluating univariate composite machine learning models using common techniques such as reduction, boosting, pipelining and tuning.

In our replication, we find no differences for the naïve models, small differences for statistical algorithms, and large improvements for machine learning models. In our extension, we find that hybrid machine learning models can boost the performance of statistical models, and that pure machine learning models can achieve competitive performance on the hourly data set, outperforming statistical models and coming close to the best M4 models.

Finally, with sktime, we hope to streamline open-source capabilities for machine learning with time series in Python, making algorithmic performance comparisons more transparent and reproducible.

Summary of contributions

sktime’s forecasting framework. To the best of our knowledge, we are the first to present an open-source machine learning toolbox for forecasting that allows to easily build, tune and evaluate composite machine learning models and is compatible with existing machine learning toolboxes, like scikit-learn.

Replication and extension of the M4 study. To our knowledge, we are the first to replicate the M4 study [5, 6] and check the validity of the published results. In addition, we extend the M4 study by evaluating new machine learning approaches, including reduction, boosting, pipelining and tuning.

The remainder of the paper is organised as follows:

- Section 2 states the problems we are trying to solve with sktime’s new forecasting framework.
- Section 3 motivates and describes the framework.
- Section 4 reviews related software and literature.
- Section 5 presents the results from reproducing and extending the M4 study.
- Section 6 concludes by suggesting future directions of research and development.

2 Problem statement

We consider two problems: the practitioner’s problem of making accurate forecasts, and the developer’s problem of designing a good application programming interface (API) for solving the practitioner’s problem.

2.1 Forecasting

For the practitioner’s problem, we consider the classical univariate forecasting problem with discrete time points. We task is to use the observations \( y = (y(t_1) \ldots y(t_T)) \) of a single time series observed up to time point \( t_F \) to find a forecaster \( \hat{f} \) which can make accurate temporal forward predictions \( \hat{y}(h_i) = \hat{f}(h_i) \) for the given time points \( h_1 \ldots h_H \) of the forecasting horizon. To evaluate the forecasting accuracy, we use performance metrics. Two common metrics, which are also used in the M4 study, are MASE (mean absolute scaled error) and sMAPE (symmetric mean absolute percentage error):

\[
\text{sMAPE} = \frac{1}{H} \sum_{i=1}^{H} \frac{|y(h_i) - \hat{y}(h_i)|}{|y(h_i)| + |\hat{y}(h_i)|}, \quad \text{MASE} = \frac{1}{H} \sum_{i=1}^{H} \frac{1}{1+H-m} \sum_{j=m+1}^{T} \frac{|y(t_j) - y(t_{j-m})|}{y(t_j) + \hat{y}(h_i)}
\]

where the denominator of MASE is the naïve seasonal in-sample forecasts and \( m \) the seasonal periodicity (or periods per year) of the data (e.g. 12 for monthly data). MASE and sMAPE are scale-independent metrics and hence appropriate for comparing forecasting algorithms across different data sets [11]. Note that we here assume equidistant time points, but our forecasting framework is flexible enough to support unequally-spaced series. It is also worth emphasising that we focus on univariate forecasting where only a single series is required for training. By contrast, many of the machine learning models submitted to the M4 study need multiple series for training.

For an overview of the classical forecasting setting, see e.g. [7, 8, 9, 10].
2.2 API design

The developer’s problem is to find a good API to help solve the practitioner’s forecasting problem, subject to a few extra requirements. Forecasting, like any other machine learning task, involves a number of mathematical concepts and operations. Designing an API is about mapping these concepts and operations onto classes and methods in Python.

Our extra requirements are that the API should be compatible with scikit-learn, so that we can re-use much of their functionality, including the regression algorithms. The API should also have a common interface for forecasting algorithms and other core functionality, ensuring that the API is modular and composable, and thereby allowing us to develop modular tools for building composite models that work with any forecaster or regressor.

Evaluating the goodness of an API is less straightforward than evaluating forecasting accuracy. Throughout the paper, we will make qualitative arguments to support our design choices drawing on the similarity to well established APIs, notably scikit-learn [3], and adherence to common design patterns and principles for object-oriented software development [12].

3 Forecasting API

3.1 Motivation

Before we describe sktime’s forecasting framework in detail, we want to briefly motivate why we develop sktime. There are a number of reasons why we believe extending toolbox capabilities for time series analysis is important:

- **Rapid prototyping.** Toolboxes allow for rapid implementation and exploration of new models, allowing users and researchers to quickly and systematically evaluate and compare models.

- **Reproducibility.** Reproducibility is essential to scientific progress, and in particular to machine learning and forecasting research [13, 14, 15, 16]. Toolboxes, like sktime, with a principled and modular interface, enable researchers to easily replicate results from available models and compare them against new models.

- **Transparency.** By providing a consistent interface for algorithms and composition functionality, toolboxes make algorithms and workflows more readable and transparent, helping users and researchers to better understand how forecasts are generated.

In addition, there are a number of reasons why we develop our forecasting framework as part of sktime’s unified API, as opposed to a self-standing forecasting toolbox:

- **Reduction.** Many time series algorithms are highly composite and often involve reduction from complex to simpler learning tasks. Reduction relations exist between many time series related learning tasks, including forecasting and tabular (or cross-sectional) regression, but also time series regression, multivariate (or panel) forecasting, and time series annotation (e.g. anomaly detection) [4]. Only a unified toolbox like sktime allows to fully exploit these relations. Reduction is discussed in more detail in section 3.3.1.

- **Reduce confusion/errors.** When learning with time series, there are various related but distinct learning tasks and models that can solve them. A single API, supported by a clear taxonomy of tasks and models, helps reduce confusion. It helps to clarify the task one wants to solve and the kind of model that can solve it, and it helps to avoid common issues when evaluating and comparing model performances. An often seen example is that performance estimates of the reduced regression setting are mistaken for performance estimates for the forecasting setting, which are in general not the same [17]. The crucial difference is that in the regression setting, it is usually assumed that we have independent samples, whereas in the forecasting setting we usually do not have independent samples, as observations are dependent on past observations. Another example is given by the M4 study, which includes univariate and multivariate models, without distinguishing them explicitly. By univariate models we mean those models that use a single series for training (e.g. all of the statistical models in table 10), by multivariate models those that use multiple series for training and hence can make use of consistent patterns across series (e.g. the winner [1], the runner-up [18], and the best pure ML submission by Trotta). Comparing both univariate and multivariate models is problematic for two reasons. First, by training models on multiple series, the performance estimates on individual series are not longer independent. However, the performance estimates are only reliable to the extend that they are based on independent samples. Second, it may seem unfair to compare multivariate models with univariate ones, especially when this is not made explicit. We believe a unified API will help distinguish these cases more clearly.

- **Re-usability.** Many time series learning tasks require common functionality (e.g. feature extraction, time series distances, or pre-processing routines). Providing them in a consistent and modular interface allows us to re-utilise them for different tasks.
3.2 Forecaster interface

We start discussing sktime’s new forecasting framework by describing our basic interface for forecasting algorithms (or forecasters). We encapsulate forecasters in classes with a common interface, as is standard in existing toolboxes. The advantages of a common interface are clear: we can interchange forecasters at run-time and we can compose them, allowing us to write tools that work with any forecaster and to easily build composite models (e.g. ensembles or tuning routines).

Example 1: Base forecaster interface

```python
forecaster = ExponentialSmoothing(trend="additive")
forecaster.fit(y_train)  # y_train is the training series
y_pred = forecaster.predict(fh=1)  # single-step ahead forecasting horizon (fh)
```

What is less obvious is what a common interface for forecasters should look like. We list the methods we consider essential in table 1 and discuss them in more detail below. Example 1 shows what our common interface looks like in practice.

| Functionality       | Description                                         | Method             |
|---------------------|-----------------------------------------------------|--------------------|
| Specification       | Building and initialising models, setting of hyper-parameters | __init__          |
| Training            | Fitting model parameters to training data           | fit                |
| Forecasting         | Generating in-sample or out-of-sample predictions based on fitted parameters | predict            |
| Updating            | Updating fitted parameters using new data           | update             |
| Dynamic forecasting | Making and updating forecasts dynamically using temporal cross-validation | update_predict    |
| Inspection          | Retrieving hyper-parameters and fitted parameters   | get_params, get_fitted_params |

- **Specification.** Like scikit-learn, but unlike statsmodels, we separate model specification from the training data, following the general design principles of modularisation and decoupling.

- **Training.** Once specified, the model can take in training data for parameter fitting, and optionally the forecasting horizon. Models that fit separate parameters for each step of the forecasting horizon will require the forecasting horizon during training.

- **Forecasting horizon.** The forecasting horizon specifies the time points we want to predict. It could be specified in a number of ways. In sktime, we specify it as the steps ahead relative to the end of the training series. A relative horizon, as opposed to an absolute one, as in statsmodels, has the advantage that it allows us to update our forecasts when time moves on without having to simultaneously update the forecasting horizon. Similarly, specifying the forecasting horizon as an interval of time points as in statsmodels, or simply the number of steps ahead as in pmdarima, is not enough. Forecasters may fit separate parameters for each step and hence need to know the exact steps to avoid needless computations. As a consequence, we specify in-sample forecasts as negative steps, going backwards from the end of the training series. Another consequence is that forecasters need to keep track of the last point of the training series, what we call the cutoff point.

- **Forecasting.** Once fitted, the forecaster can generate forecasts. We expose a single method for in-sample and out-of-sample forecasts, even though generating them may involve different operations. The key advantage of a single method is that a composition forecaster does not have to distinguish between different method calls of its component forecasters, and instead can delegate that decision to the component forecasters. We discuss detrending as an example of this case in section 3.3.2.

- **Updating.** In addition to fitting, we introduce a method for updating forecasters with new data. This allows to keep track of the cutoff point as time moves on, but also to update fitted parameters without having to re-fit the whole model.

- **Dynamic forecasting.** We also introduce a method for making and updating forecasts more dynamically. This is useful for temporal cross-validation, where we generate and evaluate multiple forecasts based on different windows of the data. The method takes in test data and an iterator that encodes the temporal cross-validation scheme.

- **Inspection.** In addition to the common hyper-parameter interface from scikit-learn, we also propose a new uniform interface for fitted parameters. This enables us to have composite models which make use of fitted parameters of component models. We discuss feature extraction as a typical example in section 3.3.5.
3.3 Composition

With the common forecaster interface in place, we propose a number of composition forecasters that enable us to build composite models based on one or more component forecasters. As is standard, composition forecasters (or meta-forecasters) share the common interface of the base forecasters, allowing us treat simple and composite forecasters uniformly. Our composition forecasters include adaptations of common tabular meta-estimators from scikit-learn to the forecasting setting, like pipelining, ensembling and tuning, but also novel meta-forecasters for reduction, detrending and feature extraction.

3.3.1 Reduction

As described in section 3.1, one of the main reasons for developing a unified API is reduction, i.e. the insight that algorithms that can solve one task, can also be used to solve another task. Many machine learning approaches to forecasting work through reduction.

For example, a common approach is to solve forecasting via regression. We typically do this as follows: We first split the training series into fixed-length windows and stack them on top of each other. This gives us a matrix of lagged values in a tabular format, and thus allows us to apply any tabular regression algorithm [19]. This approach is sometimes also called lagged variable regression, dynamic regression or auto-regression. To generate forecasts, there are multiple strategies. The most popular one is the recursive strategy, in which we use the last window as input to the fitted regressor to generate the first step ahead forecast. To make multi-step ahead forecasts, we can update the last window recursively with the previously forecasted values. Other strategies are the direct and hybrid strategies.

While reductions are not new, we are the first to propose encapsulating them as meta-estimators. Reductions have several key properties that make them well suited to be expressed as meta-estimators:

- **Modularity.** Reductions convert any algorithm for a particular task into an algorithm for a new task. Applying some reduction approach to \( n \) base algorithms gives \( n \) new algorithms for the new task. Any progress on the base algorithm immediately transfers to the new task, saving both research and software development effort [20, 21].

- **Tunability.** Most reductions require modelling choices that we may want to optimise. For example, we may want to tune the window length or select among different strategies for generating forecasts [22, 19]. By expressing reductions as meta-estimators, we expose these choices via the common interface as tunable hyper-parameters.

- **Composability.** Reductions are composable. They can be composed to solve more complicated problems [20, 21]. For example, we can first reduce forecasting to time series regression which in turn can be reduced to tabular regression via feature extraction.

- **Adaptor.** Reductions adapt the interface of the base algorithm to the interface required for solving the new task, allowing us to use the common tuning and model evaluation tools appropriate for the new task.

Due to the current lack of a unified toolbox, reductions are often hand-crafted, the M4 study being a case in point. The consequence is that they are neither adaptors, nor modular, tunable or composable. Example 2 shows what reduction to tabular regression looks like in sktime, and we make heavy use of it in section 5 to replicate and extend the M4 study. We also provide a meta-forecaster for reduction to time series regression, so that any of sktime’s time series regressor can be use to solve a forecasting task.

Example 2: Solving forecasting via reduction to tabular regression

```python
regressor = RandomForestRegressor () # from scikit-learn
forecaster = ReducedRegressionForecaster ( regressor , window_length = 10, strategy = "recursive ")
forecaster . fit ( y_train )
y_pred = forecaster . predict ( fh = 1 )
```

3.3.2 Detrending

sktime provides a number of transformers which allow to apply data transformations. Similar to scikit-learn, they share a common interface for fitting, transforming and, if available, the inverse transformation. In contrast to scikit-learn’s transformers, the transformers presented here operate on a single series. But sktime provides modular functionality to apply the single-series transformers on data frames with multiple series, so that they are re-usable for different learning tasks.

In particular, we introduce a new modular detrending transformer, a composite transformer which works with any forecaster. It works by first fitting the forecaster to the input data. To transform data, it uses the fitted forecaster to
generate forecasts for the time points of the passed data and returns the residuals of the forecasts. Depending on the passed data, this will require to generate in-sample or out-of-sample forecasts. Example 3 shows how we can use the detrending transformer to remove a linear trend from the time series.

Example 3: Detrending

```python
forecaster = PolynomialTrendForecaster(degree=1)
transformer = Detrender(forecaster)  # linear detrending
transformer.fit(y_train)
yt = transformer.transform(y_train)  # returns in-sample residuals
```

The detrender also works in a pipeline as a form of boosting, by first detrending a time series and then fitting another forecaster on the residuals. We investigate the potential of boosting a statistical method with machine learning algorithms in section 5.5.

3.3.3 Pipelining

Following scikit-learn, we provide a composition forecaster for chaining one or more transformers with a final forecaster. When fitting the pipeline, the data is first transformed before being passed to the forecaster. To make forecasts, the forecaster first generates forecasts which are then inverse-transformed before being returned. Since the transformers work on the target series to be forecasted, we follow scikit-learn in calling this meta-estimator TransformedTargetForecaster.

Example 4 shows how the Naïve2 strategy from the M4 study, described in table 10, can be expressed as a pipeline of a deseasonalisation step and a naïve forecaster. But note that our implementation allows to chain multiple transformations.

Example 4: Pipeline

```python
forecaster = TransformedTargetForecaster([  
    ("deseasonalise", Deseasonaliser(sp=12)),  # monthly seasonal periodicity  
    ("forecast", NaiveForecaster(strategy="last"))  
])
forecaster.fit(y_train)
y_pred = forecaster.predict(fh=1)
```

3.3.4 Ensembling

Following scikit-learn, we provide a simple meta-forecaster for ensembling multiple base forecasters. The ensemble forecaster fits each component forecaster separately and combines forecasts using a simple arithmetic mean. Given sktime’s modular structure, it is straightforward to add other approaches to combine forecasts like weighted averages or stacking.

3.3.5 Feature extraction

Forecasting algorithms can not only be used to solve forecasting tasks, but can also help solve other related learning tasks. A common approach is to use forecasting algorithms as a feature extraction method for solving learning tasks such as time series regression, classification or clustering. This works by first fitting a forecaster to the available time series, then retrieving their fitted parameters, and finally using them as features for tabular estimator. There are both bespoke models which make use of this approach (see e.g. the random interval spectral ensemble for time series classification, which makes use of auto-regressive coefficients) and toolkits like tsfresh which allow to extract numerous features from time series, including fitted parameters from certain forecasting algorithms. Note that in this case forecasters offer one way to reduce a time series task to its tabular counterpart.

To allow for more configurable feature extraction, we propose a feature extraction transformer, which is a meta-estimator that extracts the fitted parameters from a forecaster. To ensure full modularity of the transformer, we propose a new common inspection interface for retrieving fitted parameters in a uniform manner, as described in section 3.2.

Example 5 shows how this transformer could be used in a pipeline for time series classification.

Example 5: Feature extraction for classification

```python
forecaster = ARIMA()
classifier = Pipeline([[
```
To our knowledge, we are the first to propose a common interface for fitted parameters, but we strongly encourage, and hope, that other toolboxes like scikit-learn follow us. This would allow to extract features from composite models with scikit-learn components and open a number of other possibilities for model composition.

### 3.4 Model selection

Similar to scikit-learn, we have a tuning meta-forecaster. It performs grid-search cross-validation based on cross-validation iterator encoding the cross-validation scheme, the parameter grid to search over, and optionally the evaluation metric for comparing model performance. As in scikit-learn, tuning works through the common hyper-parameter interface which allows to repeatedly fit and evaluate the same forecaster with different hyper-parameters.

**Example 6: Model selection**

```python
forecaster = ReducedRegressionForecaster(RandomForestRegressor(), window_length=3)
param_grid = {"window_length": [3, 5, 7]}
cv = SlidingWindowSplitter()  # cross-validation object
gscv = ForecastingGridSearchCV(forecaster, param_grid, cv)
gscv.fit(y_train)  # performs temporal grid-search CV
y_pred = gscv.predict(fh=1)  # makes predictions based on best model found via CV
```

### 3.5 Technical details

sktime is available via PyPI and can be installed using Python’s package manager `pip`. We distribute compiled files for Windows, MacOS and Linux. The forecasting framework is available starting from version 0.4.0.

sktime requires Python 3.6 or later, and has a number of core dependencies, including NumPy\(^5\) [32, 33], SciPy\(^5\) [34, 35], pandas\(^5\) [36], scikit-learn\(^5\) [37, 38], statsmodels\(^5\) [39], numba\(^5\) [40] for just-in-time compilation, and joblib\(^5\) for parallelisation. For deep learning, sktime has a companion package, called sktime-dl\(^5\), which is based on TensorFlow\(^6\) [41] and Keras\(^6\).

We use continuous integration services for unit testing and code quality checks. Our functionality is documented online with interactive tutorial notebooks on Binder\(^5\), allowing users to try out sktime without installation. Development takes place on GitHub\(^5\). sktime is distributed under a permissive, open-source BSD-3-clause license.

### 4 Related work

#### 4.1 Related software

There are various well-developed toolboxes for the tabular (or cross-sectional) setting, which have established key design patterns for machine learning APIs: most notably, scikit-learn\(^3\) [37, 3, 38] in Python, Weka\(^4\) [44, 45] in Java, MLJ\(^4\) in Julia, and mlr\(^4\) [47] or caret\(^4\) [48, 49] in R, all of which implement common interfaces for fitting, predicting and hyper-parameters, and support composite model building and tuning.

Beyond the cross-sectional setting, toolbox capabilities remain limited\(^5\). There are a few toolboxes that extend tabular toolboxes and provide frameworks for time series learning tasks closely related to the cross-sectional setting, such as time series classification, regression and clustering. This includes pyts\(^7\) [50], seglearn\(^8\) [51] and tselearn\(^5\) in Python and tsml\(^8\) [29] in Java. However, none of them have a dedicated forecasting API. Other toolboxes extend tabular

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\(^5\)https://github.com/joblib/joblib
\(^6\)https://github.com/sktime/sktime-dl
\(^7\)https://github.com/alan-turing-institute/sktime/wiki/Related-software
\(^8\)https://github.com/uea-machine-learning/tsml/
toolboxes by providing functionality to solve specific steps of a time series modelling workflow, most prominently, feature extraction toolboxes such as tsfresh [31, 30], Featuretools [52] and hctsa [53, 54, 55]. In addition, there are a number of smaller toolkits for specific reduction approaches from tabular toolboxes to different time series learning tasks, such as time series regression and forecasting [56].

There are also a few toolboxes specifically for forecasting. However, most of them have important limitations. Arguably one of the most popular and comprehensive toolboxes for forecasting is the forecast library [57, 9] in R. Together with its companion libraries, forecast provides extensive functionality for statistical and encapsulated machine learning algorithms, as well as for pre-processing, model selection and evaluation. Similarly, gluonts [58] in Python provides deep-learning models for probabilistic forecasting and interfaces other packages like forecast. But both are limited in their support for composite model building and do not integrate with available machine learning libraries like scikit-learn. Other forecasting toolboxes in Python are further limited to specific model families. statsmodels [39] provides extensive tools for time series analysis, including forecasting, but is limited to statistical models (e.g. ARIMA, exponential smoothing and state space models), pmdarima [59] ports forecast’s Auto-ARIMA algorithm [57] into Python and provides additional tools for seasonality testing, pre-processing and pipelining, but is limited to the ARIMA family. Similarly, PyFlux [60] is limited to generalised auto-regressive models (e.g. GARCH, GAS), and fbprophet [61] to general additive models.

Finally, there are a number of repositories which collect and combine popular forecasting models via interfaces to existing libraries with tools to automate workflows, such as atsky [62] and the Microsoft forecasting repository, but none of them support composite model building.

4.2 Related literature

There is a long history of empirical comparison of forecasting algorithms. The M4 study [6, 5] is the latest in an influential series of forecasting competitions organised by Spyros Makridakis since 1982 [63], with the fifth edition currently running on Kaggle. Previous competitions include one on energy demand [64], one on tourism data [65], and the M3 competition [66, 67, 68]. In addition, several articles have reviewed the competition results, including a special issue of the International Journal of Forecasting [69, 70, 71, 72, 22]. While machine learning approaches have received special attention in all of the previous competitions, they have also been reviewed in [73, 74, 75] with a focus on deep learning.

5 Experiments: Reproducing & extending the M4 study

We use sktime’s new forecasting framework to replicate and extend the M4 study. This allows us to test our algorithm implementations and to showcase the usefulness of our framework. In addition, it enables us to cross-check published results from the M4 study and to further investigate the potential of machine learning models for forecasting.

5.1 Data

We use the 100k-series data set of the M4 study provided by [6, 76, 5]. The data set consists of data frequently encountered in business, financial and economic forecasting. The series are grouped by sampling frequency into yearly, quarterly, monthly, weekly, daily and hourly data sets. Tables 8 and 9 in the appendix present summary statistics, showing wide variability in time series characteristics and lengths of the available training series.

5.2 Model evaluation

We only evaluate point forecasts in this paper, but hope to extend support for interval and probabilistic forecasts to all forecasters in sktime in the future. To evaluate the accuracy of point forecasts on a single series, we use sMAPE and MASE as defined in section 2.1. In addition, we use OWA (overall weighted average), which is used in the M4 study to rank entries. OWA is an aggregate performance metric over multiple series:

\[
OWA = \frac{1}{2} \left[ \frac{\frac{1}{N} \sum_i sMAPE_i}{\frac{1}{N} \sum_i sMAPE_{i, \text{Naive2}}} + \frac{\frac{1}{N} \sum_i MASE_i}{\frac{1}{N} \sum_i MASE_{i, \text{Naive2}}} \right]
\]

where \( N \) is the number of time series we aggregate over, the subscript \( i \) denotes the index of an individual series, and \( sMAPE_{i, \text{Naive2}} \) and \( MASE_{i, \text{Naive2}} \) are the respective metrics for series \( i \) and the Naïve2 forecaster described in table 10.

9 https://github.com/microsoft/forecasting
10 https://www.kaggle.com/c/m5-forecasting-accuracy/overview
5.3 Technical implementation

The code for reproducing and extending the M4 study can be found on GitHub. We ran the experiments on machines with Linux CentOS 7.4, 32 CPUs and 189 GB RAM.

For all forecasters and composition tools, we use sktime. Forecasters are specified as composite models whenever possible, using the composition classes described in section [5]. For all regressors except XGB, we use scikit-learn [3]. For XGB, we use xgboost [77].

5.4 Reproducing the M4 study

5.4.1 Models

To replicate key results from the M4 study, we implement and re-evaluate all baseline forecasters of the M4 study in sktime, except the automatic exponential smoothing model (ETS). We also evaluate the improved Theta model by Legaki & Koutsouri, the best statistical model in the M4 study. We give an overview of the replicated forecasters in table 10 in the appendix.

For each model, we compare our findings against published results. We focus on average performance and computational run time.

5.4.2 Results

For each model, we compare our findings against published results. We focus on average performance and computational run time.

Our main results are presented in table 2, which shows the percentage differences between replicated and published sMAPE values for the data sets grouped by sampling frequency. Corresponding results for MASE and OWA are shown in the appendix in tables 11 and 12. We also test whether the found differences are statistically significant using a paired t-test. Detailed results of the significance tests for sMAPE and MASE values are shown in the appendix in tables 13 and 14 respectively. Aggregate results are summarised in table 3. Our main findings are as follows:

Table 2: sMAPE percentage difference between replicated and published results

| Model       | Yearly | Quarterly | Monthly | Weekly | Daily | Hourly |
|-------------|--------|-----------|---------|--------|-------|--------|
| Naïve       | 0.000  | 0.000     | 0.000   | 0.000  | 0.000 | 0.000  |
| Naïve2      | 0.000  | 0.000     | 0.000   | 0.000  | 0.000 | 0.000  |
| sNaïve      | 0.000  | 0.000     | 0.000   | 0.000  | 0.000 | 0.000  |
| SES         | −0.004 | 0.069     | 0.016   | −0.005 | 0.011 | 0.000  |
| Holt        | 4.063  | −1.528    | 3.916   | −3.365 | 0.286 | −4.347 |
| Damped      | 1.586  | −1.024    | 0.010   | −0.694 | 1.036 | −0.783 |
| Com         | 1.659  | −0.615    | 1.123   | −1.418 | 0.498 | −1.538 |
| ARIMA       | 1.617  | 4.572     | 2.418   | 0.851  | −2.142| −2.017 |
| Theta       | −1.514 | 0.046     | 0.078   | 0.174  | 0.057 | 0.008  |
| Theta-bc    | −0.948 | −0.096    | −0.092  | −0.043 | 0.050 | 3.378  |
| MLP         | −11.936| −24.109   | −27.567 | −52.596| −61.727| −4.558 |
| RNN         | −22.728| −29.329   | −30.815 | −25.979| −33.001| −9.332 |

Notes: Rows show forecasters described in table 10. Columns show M4 data sets grouped by sampling frequency. Values show the percentage difference between replicated and published mean sMAPE values relative to the published values. Negative values indicate that replicated results are lower/better than published ones.

- For all naïve forecasters, we can replicate the published results perfectly, barring negligible differences due to numerical approximations. This validates our experiment orchestration and evaluation workflow.
- For the statistical models, we find small but often statistically significant differences. The largest difference we find for sMAPE is 4% for the Holt forecaster on the yearly data set. There appears to be no clear trend in the differences: in some cases, published results are better, in others ours. A possible explanation of the differences is the randomness involved in the optimisation routines used during fitting. However, we do not run the same forecaster multiple times on the same series and hence cannot reliably quantify this source of variation. Differences may also be due to algorithmic differences in the packages we interface and bugs.[11]

[11] For example, statsmodels’ exponential smoothing model seems to return wrong forecasts in a few cases (see https://github.com/statsmodels/statsmodels/issues/5877). We also discovered that the M4 study used...
Table 3: Summary of replicated results

| Mean rank (sMAPE) | Replicated | Original | Change | Replicated metrics | Running time (min) | Replicated | Original | Factor |
|------------------|------------|----------|--------|-------------------|-------------------|------------|----------|--------|
| Theta-bc         | 5.454      | 5.242    | -0.212 | 11.952            | 1.583             | 0.876      | 8.100    | 25.00  | 0.3    |
| Theta            | 5.649      | 5.437    | -0.212 | 12.264            | 1.669             | 0.900      | 6.268    | 12.70  | 0.5    |
| Com              | 5.726      | 5.454    | -0.271 | 12.668            | 1.687             | 0.914      | 69.473   | 33.20  | 2.1    |
| Damped           | 5.925      | 5.635    | -0.291 | 12.992            | 1.718             | 0.920      | 53.448   | 15.30  | 3.5    |
| ARIMA            | 5.748      | 5.473    | -0.275 | 13.090            | 1.885             | 0.970      | 5.902    | 8.10   | 0.7    |
| Holt             | 6.001      | 5.780    | -0.222 | 14.160            | 1.830             | 0.997      | 11.720   | 13.30  | 0.9    |
| Naïve2           | 7.029      | 6.736    | -0.292 | 13.564            | 1.912             | 1.000      | 3.664    | 2.90   | 1.3    |
| RNN              | 6.784      | 8.314    | 1.529  | 15.122            | 1.902             | 1.067      | 38941.684| 64857.10| 0.6    |
| Naïve            | 7.337      | 7.050    | -0.287 | 14.208            | 2.044             | 1.072      | 1.035    | 0.20   | 5.2    |
| NaNaiive         | 8.046      | 7.729    | -0.316 | 14.657            | 2.057             | 1.105      | 1.028    | 0.30   | 3.4    |
| MLP              | 7.513      | 8.450    | 0.937  | 16.480            | 2.079             | 1.156      | 157.884  | 1484.37| 0.1    |

Notes: Rows show forecasters described in table 10. Replicated running times are scaled to the number of CPUs used in the original M4 study.

- For MLP and RNN, we find larger and statistically significant differences. Differences are entirely negative, ranging from $-11\%$ for MLP on the yearly data set to $-61\%$ on the daily data set. Negative differences indicate that our results are better than those of the M4 study. Again, fitting these models involves randomness, but given the exclusively negative differences, it is likely that the underlying algorithms in scikit-learn and TensorFlow have been improved since the M4 study. This is also suggested by the improved run times shown in table 3.

- In addition, we compare the computational run times between sktime and the M4 study, which for most parts relies on the forecast library in R. Note, however, that run times are not directly comparable, as we used machines to replicate the results (see section 5.3 for more details). To make run times more comparable, we scale our obtained run times to the number of CPUs used in the M4 study. The scaled values are shown in table 3. Most notably, ARIMA takes approximately 5x longer than in the M4 study. This is likely because R’s forecast library supports the conditional sum of square approximation technique for model estimation [78, p. 209ff.], which is considerably faster, especially for long series, but currently not supported by pmdarima and statsmodels. MLP and RNN, based on scikit-learn and TensorFlow, are now substantially faster than in the M4 study. The remaining run times compare favourably: SES, Holt and Theta are slightly faster when using sktime, the naïve forecasters and Damped slightly slower.

5.5 Extending the M4 study

5.5.1 Research questions

Having replicated key results from the M4 study, we extend it by evaluating new machine learning models. The main motivation for extending the M4 study is twofold: First, we want to showcase the usefulness of sktime for solving practical forecasting problems. sktime allows to easily build, tune and evaluate new models thanks to its modular API, including common machine techniques like pipelining, reduction, boosting, and tuning. Second, we want to further investigate the potential of machine learning models for forecasting. In contrast to most of the machine learning entries of the M4 study, we focus on univariate forecasting models that require only a single series during training and hence cannot make use of consistent patterns across multiple series. Our extension is guided by three research questions, which we discuss in turn below:

1. Can standard tabular regression algorithms via reduction outperform statistical models?
2. Can we improve upon Theta-bc, the best statistical model in the M4 study, by residual boosting with standard tabular regressors?
3. Does tuning the window length hyper-parameter of the reduction from forecasting to tabular regression help improve performance?

[ inconsistent seasonality tests for Python and R which we take into account for reproducing the results (see https://github.com/Mcompetitions/M4-methods/issues/25).]
5.5.2 Models

To explore these questions, we evaluate five different machine learning approaches. We describe them in detail in table 4.

The simplest approach uses reduction to tabular regression without applying any seasonal adjustments. Instead, we set the window length so that it covers at least a full seasonal period. As in the M4 study, we apply linear detrending in all approaches, as the window slicing of the reduction approach makes it difficult for the models to pick up long-term trends. We evaluate each of the approaches with four standard regression algorithms: Linear regression (LR), K-nearest-neighbours (KNN), random forest (RF), and gradient boosted trees (XGB). We evaluate a total of 20 new models. For more details on the regressors and their hyper-parameter settings, see table 15 in the appendix.

Table 4: Machine learning models

| # | Name | Category | Description |
|---|------|----------|-------------|
| 1 | {regressor} | ML | Regression via reduction, using the standard recursive strategy for generating predictions described in section 3.3.1. No seasonal adjustment, but linear detrending and standardisation (removing the mean and scaling to unit variance) is applied. The window length is set to \( \min(sp, 3) \), where \( sp \) is the seasonal periodicity of the data. |
| 2 | {regressor}-s | ML | Like #1, but with seasonal adjustment as in Naïve2. |
| 3 | {regressor}-t-s | ML | Like #2, but with tuning of the window length. We use a simple temporal cross-validation scheme, in which we make a single split of the training series, using the first window for training and the second window for validation. The validation window has the same length as the forecasting horizon (i.e. the test series). We search over the following window length values: 3, 4, 6, 8, 10, 12, 15, 18, 21, 24. |
| 4 | {regressor}-Theta-bc | Hybrid | Residual boosting of Theta-bc. Standardisation is applied as in #1 to the Theta-bc residuals. Window length is set as in #1. |
| 5 | {regressor}-Theta-bc-t | Hybrid | Like #4, but with tuning of the window length as in #3. |

Notes: {regressor} is a placeholder for the tried out tabular regression algorithms described in the appendix in table 15.

5.5.3 Results

**Question 1:** Can standard tabular regression algorithms via reduction to forecasting outperform statistical models?

We present OWA results in table 5. We also report selected M4 entries as a reference for comparison, including the M4 winner [79, 1], the runner-up [18], the best pure machine learning model (a convolutional neural network adapted to time series submitted by Trotta), and Theta-bc as the best statistical forecaster. Detailed results for all models are reported in the appendix in tables 16, 17, 18, and 19. Our key findings are as follows:

In line with previous findings [69, 80], we find that the tried out machine learning models, on average, cannot outperform statistical models over the whole of the M4 data set. However, on the hourly data set machine learning models perform better than statistical ones and the best pure machine learning entry of the M4 study. The best model, XGB-s with a OWA of 0.496 even comes close to the multivariate, hybrid models of the M4 winner (0.44) and runner-up (0.484). RF-s (0.493) and LR-s (0.501) achieve slightly worse, but still competitive performances.

As pointed out in [69], it appears that the characteristics of the series as well as their length may be a critical factor determining the performance of univariate machine learning methods. This suggests that certain forecasting problems can benefit from more systematic exploration of machine learning approaches.

**Question 2:** Can we improve upon Theta-bc, the best statistical model in the M4 study, by residual boosting with standard tabular regressors?

To explore the second question, we compare results for Theta-bc with their boosted variants based on the RF and XGB regression algorithms. We also include the tuned versions of the boosted models. Results are shown in table 6. Our key findings are as follows:

Boosting Theta-bc with RF and XGB models slightly improves performance on data sets of weekly, daily and hourly frequency. For example, on the daily data set boosting with RF improves the OWA of Theta-bc from 0.996 to 0.988, and from 1.009 to 0.985 on the hourly data set. For the weekly data set, tuning is required to improve accuracy beyond that of Theta-bc. For the other yearly, monthly and quarterly data sets, boosting leads to worse performance.

**Question 3:** Does tuning the window length hyper-parameter of the reduction from forecasting to tabular regression help improve performance?
To explore the last question, we compare the performance of each regressor, once with tuning of the window length and once without it. Results are shown in table 7. Our key findings are as follows:

Tuning the window length does generally not help improve performance. Exceptions are the weekly data set and the KNN regressor. On the weekly data set, all tried out regressors benefit from tuning, with the biggest OWA improvement being 0.082 for XGB. KNN additionally benefits from tuning on the yearly and hourly data set.

It is worth emphasising that other temporal cross-validation schemes are possible and may prove to be more beneficial to overall performance, for example using a sliding window validation. In addition, we only try to optimise the window length used in the reduction, but one may want to tune other hyper-parameters like the strategy to generate forecasts as discussed in section 3.3.1. Of course, we may also want to optimise the hyper-parameters of regressor using tabular cross-validation schemes. But note also that tuning comes at the cost of a considerable increase in computational running time, as reported in the appendix in table 19.

### Table 5: Performance of new machine learning models (OWA)

|                        | Yearly | Quarterly | Monthly | Weekly | Daily | Hourly | Total |
|------------------------|--------|-----------|---------|--------|-------|--------|-------|
| M4 winner              | 0.778  | 0.847     | 0.836   | 0.851  | 1.046 | 0.44   | 0.833 |
| M4 runner-up           | 0.799  | 0.847     | 0.858   | 0.796  | 1.019 | 0.484  | 0.847 |
| Theta-bc               | 0.776  | 0.893     | 0.904   | 0.964  | 0.996 | 1.009  | 0.876 |
| Com                    | 0.886  | 0.885     | 0.93    | 0.911  | 0.982 | 1.506  | 0.914 |
| M4 best pure ML        | 0.859  | 0.939     | 0.941   | 0.996  | 1.071 | 0.634  | 0.926 |
| RF-s                   | 0.967  | 1.014     | 0.994   | 1.015  | 1.078 | 0.493  | 0.994 |
| Naïve2                 | 1.0    | 1.0       | 1.0     | 1.0    | 1.0   | 1.0    | 1.0   |
| XGB-s                  | 1.022  | 1.091     | 1.118   | 1.113  | 1.149 | 0.496  | 1.088 |
| LR-s                   | -      | 1.037     | 2.16    | 0.964  | 1.07  | 0.501  | -     |

**Notes:** Rows show forecasters described in table 4. Columns show M4 data sets grouped by sampling frequency. We exclude results for LR model when generated forecasts were unstable/exploding due the little available data and linear extrapolation.

### Table 6: Performance of boosted Theta-bc models (OWA)

|                        | Yearly | Quarterly | Monthly | Weekly | Daily | Hourly | Total |
|------------------------|--------|-----------|---------|--------|-------|--------|-------|
| Theta-bc               | 0.776  | 0.893     | 0.904   | 0.964  | 0.996 | 1.009  | 0.876 |
| RF-Theta-bc-t          | 0.854  | 0.938     | 0.933   | 0.959  | 0.999 | 0.987  | 0.919 |
| RF-Theta-bc            | 0.864  | 0.957     | 0.932   | 1.052  | 0.988 | 0.985  | 0.925 |
| XGB-Theta-bc           | 0.898  | 1.017     | 0.971   | 1.153  | 1.023 | 0.993  | 0.968 |
| XGB-Theta-bc-t         | 0.906  | 1.009     | 0.976   | 1.006  | 1.04  | 0.998  | 0.971 |

**Notes:** Rows show forecasters described in table 4. Columns show M4 data sets grouped by sampling frequency.

### Table 7: Performance of tuned machine learning models (OWA)

|                        | Yearly | Quarterly | Monthly | Weekly | Daily | Hourly | Total |
|------------------------|--------|-----------|---------|--------|-------|--------|-------|
| RF-s                   | 0.967  | 1.014     | 0.994   | 1.015  | 1.078 | 0.493  | 0.994 |
| RF-t-s                 | 1.005  | 1.070     | 1.057   | 0.967  | 1.087 | 0.683  | 1.047 |
| XGB-s                  | 1.022  | 1.091     | 1.118   | 1.113  | 1.149 | 0.496  | 1.088 |
| XGB-t-s                | 1.038  | 1.144     | 1.170   | 1.031  | 1.179 | 0.746  | 1.131 |
| KNN-s                  | 1.086  | 1.171     | 1.257   | 1.218  | 1.338 | 0.544  | 1.197 |
| KNN-t-s                | 1.062  | 1.185     | 1.276   | 1.147  | 1.331 | 0.751  | 1.205 |
| LR-s                   | -      | 1.037     | 2.160   | 0.964  | 1.070 | 0.501  | -     |
| LR-t-s                 | -      | -         | 1.876   | 0.889  | 1.089 | 0.670  | -     |

**Notes:** Rows show forecasters described in table 4. Columns show M4 data sets grouped by sampling frequency. We exclude LR model results when generated forecasts were unstable/exploding, likely due the little available data and linear extrapolation.
6 Conclusion

We presented sktime’s new forecasting framework, the first open-source framework for forecasting that integrates with existing machine learning toolboxes, like scikit-learn, and allows to easily build, tune and evaluate composite machine learning models. We discussed key features of sktime’s forecasting API, including composite models familiar from scikit-learn, but also novel meta-forecasters for reduction and detrending.

In addition, we replicated and extended the M4 forecasting study. Replicating the M4 study allowed us to test our model implementations, and validate published results. We found no or small differences for the naïve and statistical forecasting algorithms, and larger improvements for the machine learning algorithms.

Extending the M4 study allowed us to highlight the usefulness of sktime and to further investigate the potential of univariate machine learning models for forecasting. sktime allows to easily build, tune and evaluate machine learning models. In particular, we found that pure machine learning approaches like reduction, pipelining and tuning can achieve competitive forecasting performance on the hourly data sets, outperforming the statistical algorithms and coming close to the best M4 models. In addition, we found that hybrid approaches using residual boosting of statistical methods can help improve their forecasting performance.

With sktime, we hope to further advance toolbox capabilities for time series analysis and to enable researchers and practitioners to rapidly and systematically explore the potential of machine learning approaches. In future work, we want to further develop sktime by adding full support for:

- Time series regression algorithms, refactoring existing time series classification algorithm as well as adding bespoke time series regressors,
- Exogenous, multivariate time series, extending bespoke algorithms and adding modular composition techniques specifically for multivariate series,
- Prediction intervals and probabilistic forecasting.

In addition, we hope to develop new frameworks for related learning tasks, including multivariate/panel forecasting and time series annotation (e.g. segmentation and outlier detection). We are looking for new contributors, and contributors can help improve and maintain existing functionality or lead the development of new frameworks.
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Authors’ contributions

ML made key contributions to architecture and design, including composition and reduction interfaces. ML is one of sktime’s lead developers, having contributed to almost all parts of it, including the overall toolbox architecture, the time series classification framework, and specific algorithms. ML drafted and wrote most of this manuscript. He wrote the code to replicate and extend the M4 study.

FK conceived the project and architectural outlines, including taxonomy of learning tasks, composition approaches and reduction relations. FK further made key contributions to architecture and design, and contributed to writing of this manuscript.
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Appendix

Table 8: The number of M4 series per sampling frequency and domain

|          | Demographic | Finance | Industry | Macro | Micro | Other | Total |
|----------|-------------|---------|----------|-------|-------|-------|-------|
| Yearly   | 1088        | 6519    | 3716     | 3903  | 6538  | 1236  | 23000 |
| Quarterly| 1858        | 5305    | 4637     | 5315  | 6020  | 865   | 24000 |
| Monthly  | 5728        | 10987   | 10017    | 10016 | 10975 | 277   | 48000 |
| Weekly   | 24          | 164     | 6        | 41    | 112   | 12    | 359   |
| Daily    | 10          | 1559    | 422      | 127   | 1476  | 633   | 4227  |
| Hourly   | 0           | 0       | 0        | 0     | 0     | 0     | 0     |
| Total    | 8708        | 24534   | 18798    | 19402 | 25121 | 3437  | 100000|

*Notes*: Rows show M4 data sets grouped by sampling frequency. Columns show M4 data sets grouped by domains. Values show the number of available series.

Table 9: Summary statistics of the length of time series in the training set

|          | Mean | Std  | Min | 25%  | 50%  | 75%  | Max  |
|----------|------|------|-----|------|------|------|------|
| Yearly   | 31.3 | 24.5 | 13  | 20   | 29   | 40   | 835  |
| Quarterly| 92.3 | 51.1 | 16  | 62   | 88   | 115  | 866  |
| Monthly  | 216.3| 137.4| 42  | 82   | 202  | 306  | 2794 |
| Weekly   | 1022.0| 707.1| 80  | 379  | 934  | 1603 | 2597 |
| Daily    | 2357.4| 1756.6| 93  | 323  | 2940 | 4197 | 9919 |
| Hourly   | 853.9 | 127.9| 700 | 700  | 960  | 960  | 960  |
| Total    | 240.0 | 592.3| 13  | 49   | 97   | 234  | 9919 |

*Notes*: Rows show M4 data sets grouped by sampling frequency. Columns show summary statistics of the distribution of the length of the training series.
Notes: The forecasters are described in detail in the original M4 study [80]. We follow the categorisation of the M4 study here for consistency, but more fruitful categorisations have been proposed by [90].
Table 12: OWA percentage difference between replicated and published results

|         | Yearly | Quarterly | Monthly | Weekly | Daily | Hourly |
|---------|--------|-----------|---------|--------|-------|--------|
| Naïve   | 0.000  | 0.000     | 0.000   | 0.000  | 0.000 | 0.000  |
| Naïve2  | 0.000  | 0.000     | 0.000   | 0.000  | 0.000 | 0.000  |
| sNaïve  | 0.000  | 0.000     | 0.000   | 0.000  | 0.000 | 0.000  |
| SES     | −0.006 | 0.042     | 0.027   | −0.003 | 0.007 | 0.000  |
| Holt    | 4.782  | −0.812    | 3.382   | −2.568 | 0.244 | −4.048 |
| Damped  | 2.594  | −0.753    | 0.751   | −1.729 | 0.926 | −0.984 |
| Com     | 2.179  | −0.524    | 1.100   | −1.646 | 0.416 | −3.256 |
| ARIMA   | 0.909  | 3.984     | 1.727   | −5.082 | 3.502 | 0.053  |
| Theta   | −2.267 | −0.541    | −0.031  | 0.081  | 0.008 | 0.053  |
| Theta-bc| −1.416 | −0.542    | −0.147  | −0.372 | 0.008 | −0.308 |
| MLP     | −13.251| −27.165   | −34.713 | −71.246| 66.951| −7.691 |
| RNN     | −23.582| −31.657   | −30.563 | −32.746| −34.685| −16.490|

Notes: Rows show forecasters described in table 10. Columns show M4 data sets grouped by sampling frequency. Values show the percentage difference between replicated and published OW A values relative to the published values. Negative values indicate that replicated results are lower/better than published ones.

Table 13: sMAPE difference between published and replicated results

|         | Yearly | Quarterly | Monthly | Weekly | Daily | Hourly |
|---------|--------|-----------|---------|--------|-------|--------|
| Naïve   | −0.0   | ± 0.0     | 0.0     | ± 0.0  | 0.0   | ± 0.0  |
| Naïve2  | −0.0   | ± 0.0     | 0.0     | ± 0.0  | 0.0   | ± 0.0  |
| sNaïve  | −0.0   | ± 0.0     | 0.0     | ± 0.0  | 0.0   | ± 0.0  |
| SES     | −0.001 | ± 0.006   | 0.007   | ± 0.004| 0.002 | ± 0.001|
| Holt    | 0.665  | ± 0.083   | −0.167  | ± 0.034| 0.580 | ± 0.044|
| Damped  | 0.241  | ± 0.056   | −0.105  | ± 0.023| 0.001 | ± 0.020|
| Com     | 0.246  | ± 0.042   | −0.063  | ± 0.016| 0.151 | ± 0.016|
| ARIMA   | 0.245  | ± 0.058   | 0.477   | ± 0.038| 0.325 | ± 0.035|
| Theta   | −0.221 | ± 0.017   | 0.005   | ± 0.007| 0.010 | ± 0.004|
| Theta-bc| −0.127 | ± 0.017   | −0.010  | ± 0.005| −0.012 | ± 0.004|
| MLP     | −2.598 | ± 0.048   | −4.460  | ± 0.062| −6.708 | ± 0.062|
| RNN     | −5.091 | ± 0.091   | −4.994  | ± 0.073| −7.413 | ± 0.089|

Notes: Rows show forecasters described in table 10. Columns show M4 data sets grouped by sampling frequency. Values show the difference between replicated and published mean sMAPE values, together with the standard error of the difference in means between paired samples. Values in bold indicate that the difference is statistically significant at the 95% level based on a two-sided paired t-test. Negative values indicate that replicated results are lower than published ones.

Table 14: MASE difference between published and replicated results

|         | Yearly | Quarterly | Monthly | Weekly | Daily | Hourly |
|---------|--------|-----------|---------|--------|-------|--------|
| Naïve   | 0.0    | ± 0.0     | 0.0     | ± 0.0  | 0.0   | ± 0.0  |
| Naïve2  | 0.0    | ± 0.0     | 0.0     | ± 0.0  | 0.0   | ± 0.0  |
| sNaïve  | 0.0    | ± 0.0     | 0.0     | ± 0.0  | 0.0   | ± 0.0  |
| SES     | −0.0   | ± 0.0     | 0.0     | ± 0.0  | 0.0   | ± 0.0  |
| Holt    | 0.198  | ± 0.012   | 0.00    | ± 0.02 | 0.028 | ± 0.002|
| Damped  | 0.125  | ± 0.008   | −0.005  | ± 0.002| 0.015 | ± 0.005|
| Com     | 0.090  | ± 0.006   | −0.005  | ± 0.001| 0.010 | ± 0.002|
| ARIMA   | 0.005  | ± 0.010   | 0.039   | ± 0.003| −0.009 | ± 0.002|
| Theta   | −0.103 | ± 0.002   | −0.014  | ± 0.000| −0.001 | ± 0.001|
| Theta-bc| −0.058 | ± 0.005   | −0.012  | ± 0.001| −0.002 | ± 0.000|
| MLP     | −0.725 | ± 0.027   | −0.699  | ± 0.019| −0.796 | ± 0.045|
| RNN     | −1.213 | ± 0.028   | −0.688  | ± 0.008| −0.485 | ± 0.005|

Notes: Rows show forecasters described in table 10. Columns show M4 data sets grouped by sampling frequency. Values show the difference between replicated and published mean MASE values, together with the standard error of the difference in means between paired samples. Values in bold indicate that the difference is statistically significant at the 95% level based on a two-sided paired t-test. Negative values indicate that replicated results are lower than published ones.
Table 15: Tabular regression algorithms used to extend the M4 study

| Name      | Description               | Hyper-parameters       |
|-----------|---------------------------|------------------------|
| LR        | Linear regression         | fit_intercept=True     |
| KNN       | K-nearest neighbours      | n_neighbors=1          |
| RF        | Random forest             | n_estimators=500       |
| XGB       | Gradient boosted trees    | n_estimators=500       |

Notes: For all algorithms except XGB, we use scikit-learn. For XGB, we use xgboost [77]. For all other hyper-parameters, we use the packages’ default settings.

Table 16: Complete results (sMAPE)

| Forecaster       | Yearly | Quarterly | Monthly | Weekly | Daily | Hourly |
|------------------|--------|-----------|---------|--------|-------|--------|
| Theta-bc         | 0.132  | 0.101     | 0.13    | 0.091  | 0.03  | 0.182  |
| Theta            | 0.144  | 0.103     | 0.13    | 0.091  | 0.031 | 0.181  |
| Com              | 0.151  | 0.101     | 0.136   | 0.088  | 0.03  | 0.217  |
| RF-Theta-bc-t    | 0.146  | 0.108     | 0.135   | 0.09   | 0.031 | 0.181  |
| Damped           | 0.154  | 0.101     | 0.135   | 0.088  | 0.031 | 0.191  |
| RF-Theta-bc      | 0.147  | 0.11      | 0.135   | 0.098  | 0.031 | 0.181  |
| ARIMA            | 0.154  | 0.109     | 0.138   | 0.087  | 0.031 | 0.137  |
| SES              | 0.164  | 0.106     | 0.136   | 0.09   | 0.03  | 0.181  |
| XGB-Theta-bc-t   | 0.153  | 0.115     | 0.142   | 0.095  | 0.031 | 0.183  |
| XGB-Theta-bc     | 0.154  | 0.117     | 0.141   | 0.108  | 0.032 | 0.182  |
| Naïve2           | 0.163  | 0.11     | 0.144   | 0.092  | 0.03  | 0.184  |
| KNN-Theta-bc     | 0.155  | 0.12      | 0.148   | 0.111  | 0.032 | 0.193  |
| KNN-Theta-bc-t   | 0.155  | 0.12      | 0.149   | 0.102  | 0.032 | 0.194  |
| RF-s             | 0.167  | 0.117     | 0.149   | 0.093  | 0.033 | 0.11   |
| RF               | 0.167  | 0.118     | 0.15    | 0.093  | 0.033 | 0.137  |
| Holt             | 0.17   | 0.107     | 0.154   | 0.094  | 0.031 | 0.28   |
| Naïve            | 0.163  | 0.116     | 0.153   | 0.092  | 0.03  | 0.137  |
| sNaïve           | 0.163  | 0.125     | 0.16    | 0.092  | 0.033 | 0.137  |
| RF-t-s           | 0.173  | 0.123     | 0.16    | 0.09   | 0.033 | 0.158  |
| RNN              | 0.173  | 0.12      | 0.166   | 0.113  | 0.04  | 0.133  |
| XGB-s            | 0.177  | 0.126     | 0.172   | 0.102  | 0.035 | 0.143  |
| XGB              | 0.177  | 0.127     | 0.173   | 0.102  | 0.035 | 0.143  |
| LR-s             | -      | 0.122     | 0.178   | 0.095  | 0.033 | 0.112  |
| LR               | -      | 0.122     | 0.178   | 0.095  | 0.033 | 0.163  |
| XGB-t-s          | 0.18   | 0.132     | 0.181   | 0.095  | 0.036 | 0.172  |
| MLP              | 0.192  | 0.14      | 0.176   | 0.101  | 0.036 | 0.132  |
| KNN-t-s          | 0.184  | 0.137     | 0.197   | 0.105  | 0.041 | 0.163  |
| KNN-s            | 0.188  | 0.135     | 0.198   | 0.112  | 0.041 | 0.12   |
| KNN              | 0.188  | 0.136     | 0.199   | 0.112  | 0.041 | 0.146  |
| LR-t-s           | -      | 0.186     | 0.086   | 0.034  | 0.168  |

Notes: Rows show forecasters described in table 4. Columns show M4 data sets grouped by sampling frequency. We exclude LR model results when generated forecasts were instable/exploding, likely due the little available data and linear extrapolation.
Table 17: Complete results (MASE)

| Forecasters | Yearly | Quarterly | Monthly | Weekly | Daily | Hourly |
|-------------|--------|-----------|---------|--------|-------|--------|
| Theta-bc    | 2.951  | 1.186     | 0.964   | 2.582  | 3.252 | 2.465  |
| Theta       | 3.279  | 1.218     | 0.968   | 2.637  | 3.261 | 2.457  |
| RF-Theta-bc-t| 3.246  | 1.229     | 0.985   | 2.592  | 3.257 | 2.363  |
| ARIMA       | 3.407  | 1.204     | 0.939   | 2.27   | 3.244 | 0.981  |
| RF-Theta-bc | 3.282  | 1.253     | 0.984   | 2.27   | 3.18  | 2.365  |
| Com         | 3.371  | 1.168     | 0.976   | 2.386  | 3.213 | 4.383  |
| Damped      | 3.504  | 1.168     | 0.987   | 2.334  | 3.262 | 2.922  |
| XGB-Theta-bc-t| 3.392  | 1.338     | 1.025   | 3.127  | 3.309 | 2.837  |
| XGB-Theta-bc-t| 3.476  | 1.332     | 1.032   | 2.713  | 3.446 | 2.398  |
| KNN-Theta-bc-t| 3.394  | 1.366     | 1.069   | 3.01   | 3.365 | 2.52   |
| KNN-Theta-bc-t| 3.396  | 1.368     | 1.083   | 2.842  | 3.4   | 2.529  |
| RF-s        | 3.639  | 1.327     | 1.016   | 2.809  | 3.523 | 0.93   |
| RF          | 3.64   | 1.341     | 1.037   | 2.823  | 3.521 | 1.032  |
| Holt        | 3.748  | 1.198     | 1.038   | 2.381  | 3.23  | 8.988  |
| RF-t-s      | 3.779  | 1.399     | 1.068   | 2.639  | 3.553 | 1.212  |
| SES         | 3.98   | 1.34      | 1.02    | 2.684  | 3.281 | 2.385  |
| RNN         | 3.733  | 1.329     | 1.116   | 3.139  | 3.962 | 2.408  |
| Naïve2      | 3.974  | 1.371     | 1.063   | 2.777  | 3.278 | 2.395  |
| XGB-s       | 3.814  | 1.42      | 1.113   | 3.091  | 3.754 | 0.954  |
| XGB         | 3.814  | 1.431     | 1.129   | 3.091  | 3.754 | 1.063  |
| XGB-t-s     | 3.883  | 1.493     | 1.154   | 2.857  | 3.847 | 1.335  |
| Naïve       | 3.974  | 1.477     | 1.205   | 2.777  | 3.278 | 11.608 |
| sNaïve      | 3.974  | 1.602     | 1.26    | 2.777  | 3.278 | 1.193  |
| MLP         | 4.221  | 1.615     | 1.129   | 2.694  | 3.763 | 2.35   |
| KNN-s       | 4.072  | 1.524     | 1.217   | 3.378  | 4.38  | 1.044  |
| KNN-t-s     | 3.977  | 1.543     | 1.261   | 3.192  | 4.355 | 1.471  |
| KNN         | 4.072  | 1.534     | 1.239   | 3.378  | 4.38  | 1.112  |
| LR-s        | -      | 1.319     | 3.284   | 2.467  | 3.442 | 0.934  |
| LR          | -      | 1.327     | 3.301   | 2.467  | 3.442 | 1.001  |
| LR-t-s      | -      | -         | 2.618   | 2.338  | 3.518 | 1.027  |

Notes: Rows show forecasters described in table [4]. Columns show M4 data sets grouped by sampling frequency. We exclude LR model results when generated forecasts were instable/exploding, likely due to the little available data and linear extrapolation.
| Model                | Yearly | Quarterly | Monthly | Weekly | Daily | Hourly |
|----------------------|--------|-----------|---------|--------|-------|--------|
| Theta-bc             | 0.776  | 0.893     | **0.904** | 0.964  | 0.996 | 1.009  |
| Theta                | 0.852  | 0.912     | 0.906   | 0.972  | 0.999 | 1.006  |
| Com                  | 0.886  | **0.885** | 0.93    | 0.911  | **0.982** | 1.506  |
| RF-Theta-bc-t        | 0.854  | 0.938     | 0.933   | 0.959  | 0.999 | 0.987  |
| Damped               | 0.913  | 0.886     | 0.931   | 0.901  | 1.006 | 1.13   |
| ARIMA                | 0.9    | 0.934     | 0.919   | **0.885** | 1.008 | 0.577  |
| RF-Theta-bc          | 0.864  | 0.957     | 0.932   | 1.052  | 0.988 | 0.985  |
| XGB-Theta-bc         | 0.898  | 1.017     | 0.971   | 1.153  | 1.023 | 0.993  |
| SES                  | 1.002  | 0.97      | 0.952   | 0.975  | 1.0   | 0.99   |
| XGB-Theta-bc-t       | 0.906  | 1.009     | 0.976   | 1.006  | 1.04  | 0.998  |
| RF-s                 | 0.967  | 1.014     | 0.994   | 1.015  | 1.078 | **0.493** |
| Holt                 | 0.992  | 0.924     | 1.021   | 0.941  | 0.997 | 2.637  |
| KNN-Theta-bc         | 0.901  | 1.045     | 1.016   | 1.149  | 1.037 | 1.052  |
| Naïve2               | 1.0    | 1.0       | 1.0     | 1.0    | 1.0   | 1.0    |
| KNN-Theta-bc-t       | 0.902  | 1.045     | 1.025   | 1.067  | 1.042 | 1.055  |
| RF                   | 0.967  | 1.025     | 1.008   | 1.016  | 1.077 | 0.587  |
| RF-t-s               | 1.005  | 1.07      | 1.057   | 0.967  | 1.087 | 0.683  |
| RNN                  | 0.999  | 1.031     | 1.102   | 1.18   | 1.26  | 0.865  |
| Naïve                | 1.0    | 1.066     | 1.095   | 1.0    | 1.0   | 3.593  |
| XGB-s                | 1.022  | 1.091     | 1.118   | 1.113  | 1.149 | 0.496  |
| XGB                  | 1.022  | 1.097     | 1.129   | 1.113  | 1.149 | 0.611  |
| sNaïve               | 1.0    | 1.153     | 1.146   | 1.0    | 1.0   | 0.628  |
| XGB-t-s              | 1.038  | 1.144     | 1.17    | 1.031  | 1.179 | 0.746  |
| MLP                  | 1.117  | 1.226     | 1.142   | 1.037  | 1.16  | 0.85   |
| KNN-s                | 1.086  | 1.171     | 1.257   | 1.218  | 1.338 | 0.544  |
| KNN-t-s              | 1.062  | 1.185     | 1.276   | 1.147  | 1.331 | 0.751  |
| KNN                  | 1.086  | 1.177     | 1.272   | 1.218  | 1.338 | 0.63   |
| LR-s                 | -      | 1.037     | 2.16    | 0.964  | 1.07  | 0.501  |
| LR                   | -      | 1.039     | 2.169   | 0.964  | 1.07  | 0.654  |
| LR-t-s               | -      | -         | 1.876   | 0.889  | 1.089 | 0.67   |

Notes: Rows show forecasters described in table 4. Columns show M4 data sets grouped by sampling frequency. We exclude LR model results when generated forecasts were unstable/exploding, likely due to the little available data and linear extrapolation.
Table 19: Summary results of new machine learning models

| Model                  | sMAPE  | MASE  | OWA    | Running time (min) |
|------------------------|--------|-------|--------|--------------------|
| Theta-bc               | 11.95  | 1.58  | 0.88   | 8.1                |
| Theta                  | 12.26  | 1.67  | 0.9    | 6.27               |
| Com                    | 12.66  | 1.68  | 0.91   | 69.47              |
| RF-Theta-bc-t         | 12.67  | 1.67  | 0.91   | 14539.77           |
| Damped                 | 12.69  | 1.71  | 0.92   | 53.45              |
| ARIMA                  | 12.99  | 1.67  | 0.92   | 14992.88           |
| RF-Theta-bc            | 12.76  | 1.68  | 0.92   | 69.47              |
| XGB-Theta-bc           | 13.35  | 1.75  | 0.96   | 122.94             |
| SES                    | 13.09  | 1.88  | 0.97   | 5.9                |
| XGB-Theta-bc-t        | 13.37  | 1.78  | 0.97   | 1826.44            |
| RF-s                   | 14.00  | 1.81  | 0.99   | 1168.56            |
| Holt                   | 14.16  | 1.83  | 0.99   | 11.72              |
| KNN-Theta-bc           | 13.81  | 1.78  | 0.99   | 64.36              |
| Naïve2                 | 13.56  | 1.91  | 1.0    | 3.66               |
| KNN-Theta-bc-t        | 13.84  | 1.79  | 1.0    | 656.04             |
| RF                     | 14.09  | 1.82  | 1.0    | 1163.64            |
| RF-t-s                 | 14.86  | 1.88  | 1.04   | 14165.87           |
| RNN                    | 15.12  | 1.90  | 1.06   | 38941.68           |
| Naïve                  | 14.20  | 2.04  | 1.07   | 1.04               |
| XGB-s                  | 15.57  | 1.92  | 1.09   | 116.95             |
| XGB                    | 15.64  | 1.93  | 1.09   | 115.76             |
| sNaïve                 | 14.65  | 2.05  | 1.10   | 1.03               |
| XGB-t-s                | 16.24  | 1.98  | 1.13   | 1718.15            |
| MLP                    | 16.48  | 2.07  | 1.16   | 157.88             |
| KNN-s                  | 17.31  | 2.08  | 1.19   | 58.71              |
| KNN-t-s                | 17.25  | 2.09  | 1.20   | 634.12             |
| KNN                    | 17.40  | 2.10  | 1.20   | 56.99              |
| LR-s                   | -      | -     | -      | 55.36              |
| LR                     | -      | -     | -      | 53.37              |
| LR-t-s                 | -      | -     | -      | 590.87             |

Notes: Rows show forecasters described in table 4. Columns show aggregate values for sMAPE, MASE and OWA metrics, as well as the total running time in minutes scaled to the number of CPUs used in the original M4 study, as described in section 5. We exclude LR model results when generated forecasts were unstable/exploding, likely due to little available data and linear extrapolation.