Forecasting Across Time Series Databases using Long Short-Term Memory Networks on Groups of Similar Series

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Abstract

With the advent of Big Data, nowadays in many applications databases containing large quantities of similar time series are available. Forecasting time series in these domains with traditional univariate forecasting procedures leaves great potentials for producing accurate forecasts untapped. Recurrent neural networks, and in particular Long Short Term Memory (LSTM) networks, have proven recently that they are able to outperform state-of-the-art univariate time series forecasting methods in this context, when trained across all available time series. However, if the time series database is heterogeneous accuracy may degenerate, so that on the way towards fully automatic forecasting methods in this space, a notion of similarity between the time series needs to be built into the methods. To this end, we present a prediction model using LSTMs on subgroups of similar time series, which are identified by time series clustering techniques. The proposed methodology is able to consistently outperform the baseline LSTM model, and it achieves competitive results on benchmarking datasets, in particular outperforming all other methods on the CIF2016 dataset.

Keywords: Big data forecasting, RNN, LSTM, time series clustering, neural networks.

1. Introduction

Throughout the years, research in neural networks (NN) for univariate time series forecasting has received considerable attention. Recent developments have been mainly around preprocessing techniques such as deseasonalization and detrending to supplement the NN’s learning process, and novel NN architectures such as recurrent neural networks, echo state networks, generalized regression neural networks and ensemble architectures to uplift the constraints of the conventional NN architecture (Nelson et al., 1999; Zhang and Qi, 2005; Ilies et al., 2007; Rahman et al., 2016; Yan, 2012; Zimmermann et al., 2012).

However, in the time series forecasting community there has also been the long-standing consensus that simple methods will often outperform more sophisticated ones. This was a conclusion of the influential M3 forecasting competition held in 1999 (Makridakis and Hibon, 2000). So, complex methods are often viewed poorly in this field, and this has been especially true for NNs and other machine learning (ML) methods. In particular, NNs did not perform well in this competition and in subsequent competitions, e.g., more recently, in the NN3 and NN5 forecasting competitions, which were held specifically for ML methods. In the NN3 competition (Crone et al., 2011), only one participating ML method was able to outperform
damped trend exponential smoothing, and none of the methods was able to outperform the Theta method, which is equivalent to simple exponential smoothing with drift (Hyndman and Billah, 2003). Both these methods are relatively simple standard methods in time series forecasting.

The reasons for this under-performance of sophisticated methods can be attributed to individual series usually being too short to be modelled effectively using ML methods such as NNs. Simple methods have larger bias but smaller variance. As from short individual series the amount of information that can be extracted is limited, more complex methods that may have smaller bias will suffer from large variance, and finally end up performing worse (Zhang et al., 1998; Yan, 2012). Also, even if large amounts of data are available, the distant past is usually less useful for forecasting, as underlying patterns and relationships will have changed in the meantime. So, a common notion is that unless the underlying time series is very long and from a very stable system, NNs will not perform well, as they will not have enough data for learning or will not handle non-stationarity in the data adequately (Hyndman, 2016).

These problems preventing NNs from being successful in a univariate time series context do not simply vanish with the advent of “Big Data”, where ever increasing quantities of data are collected nowadays by many companies for the routine functioning of their businesses, for example server performance measures in computer centers, sales in retail of thousands of different products, measurements for predictive maintenance, smart meter data, etc. This is because in a time series context, availability of more data does not usually mean that the isolated series change or contain more data, e.g., that they are longer or have a higher sampling rate, as these are determined by the application and not by capturing and storage capabilities. Instead, it means that large quantities of related, similar series are available.

Therefore, forecasting time series in these domains with traditional univariate forecasting procedures leaves great potentials for producing more accurate forecasts untapped, as a separate model is built for each time series, and no information from other series is taken into account. On the other hand, in this situation now considerable more data is available, and using more complex models becomes feasible, when trained globally across all series.

Recurrent neural networks (RNNs), and in particular Long-short Term Memory (LSTM) networks have become increasingly popular to fill this gap. They are naturally suited for modelling problems that demand capturing dependency in span of contextual information, and are able to preserve knowledge as they progress through the subsequent time steps in the data. As a result, RNN architectures are heavily used in domains such as Natural Language Processing (Mikolov et al., 2010), machine translation (Sutskever et al., 2014), and speech recognition (Graves et al., 2013), and are also gaining popularity in time series research (Fei and Yeung, 2015; Pawlowski and Kurach, 2015; Lipton et al., 2015; Zimmermann et al., 2012). Recently, they have proven to be very competitive in the work of Smyl (2016) who presented an algorithm that was able to win the CIF2016 forecasting competition for monthly time series (ˇStˇepniˇcka and Burda, 2016), outperforming state-of-the-art univariate algorithms such as ETS (Hyndman et al., 2008), BaggedETS (Bergmeir et al., 2016), Theta (Hyndman and Billah, 2003), and ARIMA (Box et al., 2015).

When building such global models for a time series database, now the problem arises
that these global models are potentially trained across disparate series, which may deter the overall accuracy. We propose to overcome this shortcoming by building separate models for subgroups of time series. The grouping can be based on additional domain knowledge available, or, in the absence of such a natural grouping, we propose a fully automatic mechanism that works on time series databases in general, which accounts for the dissimilarities in a set of time series. In particular, we propose to augment the original LSTM forecasting framework developed by Smyl and Kuber (2016) with a time series clustering schema that improves the capability of the LSTM base algorithm by exploiting similarities between time series.

Specifically, our proposed method initially discovers clusters of similar series from the overall set of time series, as an augmentation step to exploit the similarity between time series. We propose a feature-based clustering approach using a set of interpretable features of a time series to obtain meaningful clusters. Firstly, we extract the respective features from a time series using the method proposed by Hyndman et al. (2015b). Then, the “Snob” clustering algorithm, a mixture model based on the Minimum Message Length concept (MML), introduced by Wallace and Dowel (2000), is applied to the extracted feature vector, to obtain the clusters. Once we distinguish the time series based on their feature properties, for each cluster of time series, we build a separate LSTM predictive model. Furthermore, as preprocessing steps, we apply a log transformation to the data, with the objective of stabilizing the variance of the time series, and we deseasonalize the time series using STL decomposition, following the assumption that NNs often have difficulties to model seasonality directly. Our results show that prior subgrouping of time series is able to consistently improve the performance of the baseline LSTM model.

The rest of the paper is organized as follows. In Section 2, we discuss the proposed methodology in detail. Section 3 presents the experimental setup and the results, and Section 4 concludes the paper.

2. Methods

In this section, we describe in detail the different parts of our proposed methodology. We first provide a brief introduction to our base algorithm, i.e., to RNNs and LSTMs. Afterwards, we explain our time series clustering method that is utilized to group sets of similar time series in the absence of other groupings. Finally, we discuss the classical time series preprocessing techniques used to supplement our forecasting framework. This includes a log transformation, STL decomposition, and a sliding window approach that structures the training data for our training algorithm, LSTM.

2.1. Recurrent Neural Networks

RNNs are a special type of artificial neural networks that account for the dependencies between data nodes (Elman, 1990). This qualifies the network to preserve the sequential information in an inner state, allowing them to persist the knowledge accrued from subsequent time steps. The past information is retained through a feedback loop topology, where as a part of input of the current step, the RNN uses output of the previous time step during its
network training. Figure 1 shows an example of a recurrent neural network unfolded in time, which unrolls the feedback loop to expand the complete sequence of the neural network in time.

![Figure 1: An unrolled recurrent neural network in time, with the shared weights of \( U \), \( V \), and \( W \).](image)

Here, \( x_t \) denotes the input at time step \( t \), \( s_t \) denotes the hidden state at time step \( t \), and \( o_t \) denotes the output at step \( t \). Moreover, \( s_t \) represents the “memory” of the network at time step \( t \), which is computed based on the current input \( x_t \) and the previous hidden state \( s_{t-1} \) at time step \( t-1 \). In other words, this is the overall knowledge and reasoning accumulated by the network based on the previous events of data. The hidden state \( s_t \) and output \( o_t \) at time step \( t \) can be formally defined by the following equations:

\[
\begin{align*}
    s_t &= f_\theta(Ux_t + Ws_{t-1}) \\
    o_t &= f_\alpha(Vs_t)
\end{align*}
\]

Generally, \( f_\theta \) is a non-linear function such as, e.g., \textit{tanh}, or \textit{rectified linear units} (ReLU; Le et al., 2015), whereas \( f_\alpha \) uses a linear function such as \textit{softmax} or \textit{sigmoid}. RNNs often use backpropagation through time (BPTT; Williams and Zipser, 1995) and real time recurrent learning (RTRL; Robinson and Fallside, 1987) as the learning algorithms. These are extensions of the backpropagation algorithm, which unrolls the network through time to propagate the error sequentially. Furthermore, unlike in vanilla NNs, which use different parameters at each layer, RNNs share the same set of weight parameters during the training process. This reduces the total number of parameters to be learned by the algorithm, decreasing the risk of over-fitting.

Even though RNN architectures are quite capable of capturing short-term dependencies in sequential data, they often have difficulties in learning long-term dependencies from distant past information. This is caused by the \textit{vanishing gradient problem} (Hochreiter, 1991).
Bengio et al. [1994], which is a well-known constraint in gradient based learning algorithms. Generally, gradient-based learning techniques determine the influence of a given input, based on the sensitivity of network parameters on the output. For example, as the length of a sequence grows, the corresponding error gradient is propagated through the network many steps. As a result, the gradient decays exponentially as it progresses through the chain, leaving small impact on the output from the initial elements of the sequence. This impedes the information retention ability of RNNs, while forgetting the impact from initial inputs to the network output.

2.2. Long Short-Term Memory Networks

LSTM networks were introduced by Hochreiter and Schmidhuber [1997], to address the long term memory shortage of vanilla RNNs. LSTM extends the RNN architecture by replacing the conventional perceptron architecture with a memory cell and a gating mechanism that regulates the information flow across the network. The gating mechanism is equipped with three units, namely: input, forget, and output gate. This mechanism cohesively determines which information to be persisted, how long it is to be persisted, and when it is to be read from the memory cell.

As a result, LSTMs are capable of retaining key information of input signals, and ignore the unnecessary parts. Also, the memory cell has a recurrently self-connected linear unit called “Constant Error Carousel” (CEC) that provides the short term memory storage for an extended period of time (Gers et al. 2000). Consequently, in contrast to vanilla RNNs, LSTMs preserve information and propagate errors for a much longer chain in the network. In fact, LSTMs possess the ability of remembering over 100 steps of a sequence (Längkvist et al. 2014). Figure 2 illustrates the basic structure of an LSTM memory block with a one cell architecture (following R2RT Blog 2016). In the figure, \( x_t \) denotes the input at time step \( t \), \( C_{t-1} \) and \( C_t \) denote the cell state at time steps \( t \) and \( (t-1) \), while \( h_t \) and \( h_{t-1} \) correspond to the output at time steps \( t \) and \( (t-1) \), respectively. The forget gate \( f_t \) takes \( x_t \) and \( h_{t-1} \) as inputs to determine which information to be retained in \( C_{t-1} \). Specifically, using a sigmoid layer, it squashes the output to a binary scale, for each value in \( C_{t-1} \); i.e., a “zero” output represents expunging a value from the memory cell, while a “one” represents retaining a value in the memory cell. Meanwhile, the input gate \( i_t \) is accompanied with a sigmoid layer that uses \( x_t \) and \( h_{t-1} \) to ascertain the values to be updated in \( C_t \). Additionally, a non-linear layer \( \phi \) (i.e., \( \tanh \)) is also introduced to generate a vector of candidate values, denoted as \( \tilde{C}_t \), to update the state of \( C_t \). The output gate \( o_t \), regulates the output values of an LSTM cell, based on the updated state of \( C_t \). Likewise as in the forget and input gates, the output gate deploys a sigmoid layer to filter the output. Correspondingly, the updated cell state \( C_t \) is fed into a \( \tanh \) layer, which scales down the vector to a value between (-1) and (+1). This is then multiplied by the output of the sigmoid layer to compute the final cell output \( h_t \) at time step \( t \). The aforementioned process can be formally defined by the
Figure 2: Basic architecture of an LSTM memory block with three gated layers: forget gate $f_t$, input gate $i_t$, and output gate $o_t$, controlling the activation of cells $c_{t-1}$ and $c_t$ following recursive equations:

$$
\begin{align*}
  f_t &= \sigma(W_{f}[h_{t-1}, x_t] + b_f) \\
  i_t &= \sigma(W_{i}[h_{t-1}, x_t] + b_i) \\
  \tilde{C}_t &= \tanh(W_{c}[h_{t-1}, x_t] + b_c) \\
  C_t &= f_t \odot C_{t-1} \oplus i_t \odot \tilde{C}_t \\
  o_t &= \sigma(W_{o}[h_{t-1}, x_t] + b_o) \\
  h_t &= o_t \odot \tanh(C_t)
\end{align*}
$$

Note that $W_f$, $W_i$, $W_c$, and $W_o$ represent the weight matrices of forget gate, input gate, memory cell state, and output gates respectively. Biases of the respective gates are $b_f$, $b_i$, $b_c$, and $b_o$.

Several variants to the originally proposed algorithm can be found in the literature. E.g., LSTM with “peephole connections,” introduced by [Gers et al. (2000)](Gers.et.al.2000), is one of the popular variants that allows LSTM gates to examine the state of their memory cell, before updating their states.

In this study, we use the Microsoft Cognitive Toolkit (CNTK), an open-source NN toolkit [Seide and Agarwal (2016)](Seide.Agarwal.2016), to implement the LSTM. As our base learning algorithm, we use an LSTM with peephole connections, which is followed by an affine neural layer (excluding the bias component) to project the LSTM cell output to the dimension of the intended forecast horizon. I.e., the dimension of this fully connected neural layer equals the size of the output window.
2.3. Time Series Clustering

Following Warren Liao (2005), we can distinguish three main approaches to time series clustering, namely algorithms that work directly with distances on raw data points (distance-based), indirectly with features extracted from the raw data (feature-based), or indirectly with models built from the raw data (model-based).

The performance of distance-based clustering approaches depends greatly on the particular distance metric used. However, defining an adequate distance measure for raw time series is a challenging task, and it has to consider noise, different length of the series, different dynamics, different scales, etc., and many of these measures mostly concentrate on the shape of the respective time series (Aghabozorgi et al., 2015). Often, they also may yield uninformative results and interpretability is limited (Wang et al., 2006).

So, in this work, we focus on feature-based clustering techniques, which, instead of capturing similarity of point values using a distance metric, use sets of global features obtained from a time series to summarize and describe the salient information of the time series. Feature-based approaches can be more interpretable and more resilient to missing data and noisy data (Wang et al., 2006). The feature-based clustering is comprised of two stages, namely a feature extraction phase and the clustering phase, for which standard clustering approaches can be used.

In terms of feature extraction, there is a lot of work present in the literature investigating the prospects of using features of a time series as a data-mining tool for extracting useful patterns from time series (Nanopoulos et al., 2001; Wang et al., 2006; Fulcher and Jones, 2014; Mörchen, 2003). The two main differences of approaches that we identify is to either extract as many features as possible or to use a limited set of carefully selected features that are interpretable and have a justification in the application case. Following the first approach, Fulcher and Jones (2014) introduce an automated feature construction process, using a large database of time series operations, which allows them to construct over 9000 different features, representing a wide range of properties of time series. As such a large amount of features seems not practical for our purpose, and limiting the amount of features is desirable, in our proposed framework we follow the second approach, and use a set of self-describable features proposed by Hyndman et al. (2015b) to obtain a meaningful division of clusters. These suggested features are designed to capture the majority of the dynamics that can be observed in time series common in many application cases, such as trends, seasonality, autocorrelation, etc. Table 1 summarizes the respective feature vector that is extracted from an individual time series. In our work, we use the implementation available in R, in the tsmeasures function from the anomalous-acm package (Hyndman et al., 2015b). Note that we discard the Season variable from the generated feature vector, since we deseasonalize the time series prior to training the LSTM.

The feature extraction phase is then followed by a clustering phase that discovers the optimal grouping between the time series by applying a conventional clustering algorithm to the extracted feature vector. Again, a host of different clustering methods exist, an overview gives Berkhin (2006). In this study, we use a Mixture Model algorithm called “Snob”, which is based on the MML concept, a Bayesian point estimation technique that accounts for the highest posterior probability distribution of each cluster (Wallace and Dowe, 2000). It is
| Feature    | Description                |
|------------|----------------------------|
| Mean       | Mean                       |
| Var        | Variance                   |
| ACF1       | First order of autocorrelation |
| Trend      | Strength of trend          |
| Linearity  | Strength of linearity      |
| Curvature  | Strength of curvature      |
| Season     | Strength of seasonality    |
| Peak       | Strength of peaks          |
| Trough     | Strength of trough         |
| Entropy    | Spectral entropy           |
| Lumpiness  | Changing variance in remainder |
| Spikiness  | Strength of spikiness      |
| Lshift     | Level shift using rolling window |
| Vchange    | Variance change            |
| Fspots     | Flat spots using disretization |
| Cpoints    | The number of crossing points |
| KLscore    | Kullback-Leibler score      |
| Change.idx | Index of the maximum KL score |

Table 1: Summary of features extracted from a time series, following [Hyndman et al., 2015b]

indifferent to scaling of the attributes and can handle attributes with different distributions and combinations of categorical and numerical attributes. As we only consider numerical attributes in this work, we limit Snob to normally distributed attributes so that it is a Gaussian Mixture Model. Then, the main advantage of Snob over other clustering algorithms (besides scale indifference) is that it is capable of discovering an optimal number of clusters autonomously without any manual intervention, i.e., the number of clusters doesn’t have to be specified in advance.

### 2.4 Time series decomposition

Early studies suggest that NNs are suitable to effectively model the underlying seasonality and cyclical patterns in time series due to their universal function approximation properties, i.e., their capacity to estimate linear and non-linear functions (Zaiyong Tang et al., 1991; Marseguerra et al., 1992).

However, more recently several studies argue that deseasonalizing data prior to modelling is necessary to produce accurate forecasts. In particular, Nelson et al., 1999 compare the forecasts generated from NNs trained with deseasonalized data and non-deseasonalized data, using 68 monthly time series from the M-competition (Makridakis et al., 1982). The results indicate that the NN trained with prior deseasonalization achieves better forecasting accuracy, in contrast to NNs trained with non-deseasonalized data. Similarly, using the NN5 competition data, Ben Taieb et al., 2011 empirically show that the resulting forecasts benefit from prior deseasonalization of the data. And Zhang and Qi, 2005 demonstrate that
NNs are not capable of effectively modelling trend or seasonality directly, and emphasize that the forecasting errors can be reduced by detrending or deseasonalization of the raw time series.

These findings are likely to be connected to limits in the availability of data, as outlined in the Introduction. However, as our method is intended to run also in situations where the overall amount of data is limited, we deseasonalize the time series in our work accordingly, to make best use of the available data. As the deseasonalization technique we use Seasonal and Trend decomposition using Loess (STL), as proposed by Cleveland et al. (1990), to divide a time series into trend, seasonal, and remainder components. Generally, STL is considered a robust method for decomposing time series. It consists of a sequence of applications of a loess smoother, making the decomposition computationally efficient, even for longer time series (Cleveland et al., 1990; Hyndman and Athanasopoulos, 2014).

As an example, Figure 3 illustrates the STL decomposition of series TS59 of the CIF2016 dataset. In R, STL is implemented in the stl function from the forecast package (Hyndman et al., 2015a; Khandakar and Hyndman, 2008). So, with the assumption of existence of seasonality in each time series, STL decomposition is used to decompose the log transformed time series into trend, seasonal, and remainder. Thereafter, the sum of trend and remainder is passed to the next step of data preprocessing.

Figure 3: STL decomposition into trend, seasonal part, and remainder, of the log transformed version of series TS59 of the CIF2016 dataset.
2.5. The Log transformation

In our proposed work, as a pre-processing step, each time series is transformed to a logarithmic scale before fed into the STL algorithm. Finally, in the post-processing stage, the corresponding forecasts are back-transformed into their actual scale, by taking the exponent of each generated output value. This is a popular transformation to stabilize the variance of a time series. Additionally, this is also necessary for our deseasonalization process by transforming the decomposition of a time series into additive, as STL decomposition is an additive decomposition method. To avoid problems for zero values, we use it in the following definition:

\[
w_t = \begin{cases} 
\log(y_t), & y_t > 0; \\
\log(y_t + 1), & y_t = 0;
\end{cases}
\]

For example, Figure 4 shows the original series and the log transformed version of Series TS59 of the CIF2016 dataset.

![Figure 4: Series TS59 of the CIF2016 dataset, which is a monthly time series. On left is the original series, right the log transformed version.](image)

2.6. Moving Window Approach

Usually, as a prerequisite, NNs expect a constant size of inputs for the learning procedure. We achieve this by transforming the time series into pairs of \textit{<input,output>} patches. To this end, we use a moving window approach that extracts features from a window of a constant size, covering the recent observations of the time series.
The proposed moving window approach follows the Multi-Input Multi-Output (MIMO) strategy of forecasting that models a multiple input and output mapping, while preserving the stochastic dependencies between predicted values. While RNNs can be operated with one input at a time, the internal state of the network then needs to memorize all relevant information. Using an input window relaxes this requirement and allows the network to also operate directly with lagged values as inputs. Furthermore, Ben Taieb et al. (2011) discuss the benefits of applying a MIMO strategy over a single-output forecasting strategy (recursive strategy) in multi-step forecasting. There, those authors highlight that accuracy of the latter approach is affected by its recursive nature, and errors are accumulated at each forecasting step in multi-step forecasting. Figure 5 illustrates the application of the MIMO strategy to a time series.

In this work, we apply the moving window method to the output generated by the STL procedure, i.e., namely to the sum of the trend and reminder of a time series. In detail, we use the moving window approach in the following way.

At first, a time series of length $tsLength$ is converted to patches of length $(outputSize + inputSize)$. In total, there are $(tsLength - outputSize - inputSize)$ such patches. Here, $outputSize$ refers to the length of the output window (i.e., the intended forecasting horizon), while $inputSize$ represents the length of the input window used in each frame. Figure 6 illustrates the procedure with an example of applying the moving window approach on the series TS59 of the CIF2016 dataset.

Also, as a local normalization step, the last value of the trend inside an input window (the corresponding trend component of the filled dot in Figure 6) is subtracted from each data point in the corresponding input and output windows. This local normalization process is performed in each window to supplement and stabilize the overall learning process of the LSTM. Then, the corresponding input and output windows are shifted forward by one step and the normalization process is repeated.

The training dataset is generated by iterating the above process until the last point of the input window is positioned at $(tsLength - outputSize - 1)$, i.e., the last output window of the series is reserved for validation and not used for training. For the validation, forecasts for this last output window are produced. Due to the recursive nature of the process, also for the validation we need to iterate through the whole time series (called the “warm-up” in this case), analogous to the training phase.
2.7. The overall procedure

To summarize, a scheme of the forecasting framework is given in Algorithm 1. If a partition of the time series is available in the form of additional knowledge, this partition can be considered. If no additional knowledge is present, we employ the following fully automatic procedure. As stated in Section 2.3, at first we use the “anomalous” feature extraction method from [Hyndman et al. (2015b)]. Then, an implementation of the Snob clustering algorithm is applied to the feature vector, to find the optimal grouping of time series ([Wallace and Dowe (2000)]). After discovering the clusters, for each cluster of time series, the following pre-processing steps are applied to generate input data for the LSTM training. First, we transform the time series to a logarithmic scale. Then, the series is decomposed into trend, seasonal part, and remainder using the \texttt{stl} function from the \texttt{forecast} package. As the \texttt{stl} function expects two full periods of data to be applicable, for shorter time series we omit deseasonalization and use directly the log transformed series as input. Afterwards, as stated in Section 2.6, the rolling window approach, along with a local normalization technique is applied to the sum of trend and remainder, to generate the training data. Thereafter, for each cluster, a separate LSTM model is trained, and used for prediction.

Figure 7 gives an illustration of the proposed forecasting framework. The overall model...
Algorithm 1 Generating target input files for LSTM

1: procedure lstmpreprocessing(ts, freq, input.win, output.win)
2: ts.features ← anomalous(ts, freq)
3: ts.clusters ← rsnob(ts.features)
4: for i : len(ts.clusters)
5: ts.log ← log(ts)
6: [trend, seasonal, remainder] ← stl(ts.log, freq)
7: ts.deseason ← [trend, remainder]
8: for i : [tsLength(ts.deseason)-output.win-1]
9: window.frame[i] ← rollWindow(ts.deseason, input.win, output.win)
10: normalize.series[i] ← normalize(window.frame[i])
11: [input, output] ← get(normalize.series[i])
12: end for
13: end for
14: return ts.series[input, output]
15: end procedure

is comprised of three components, namely: 1) the pre-processing layer which consists of a clustering phase and a log-transformation, deseasonalization, and a normalization phase, 2) the LSTM training layer which consists of an LSTM layer, followed by an affine neural layer (a fully connected layer), excluding the bias component, and 3) a post-processing layer which consists of a denormalization and a reseasonalization phase to ascertain the final forecasts.

3. Experimental study

In this section, we evaluate our procedure on two benchmark datasets, namely the CIF2016 and NN5 datasets. We describe the forecasting methods and error measures used to perform the experiments, and the results obtained.

3.1. Evaluation methodology

We use the publicly available datasets from the CIF2016 and NN5 forecasting competitions. These competitions were specifically organized to evaluate and compare the potential of machine learning techniques in handling large scale ex-ante forecasting. In fact, each dataset is comprised of similar time series, related to a certain domain. This is the main basis of using these specific public datasets, as they comply with our original hypothesis of exploiting the advantages of similar time series (unlike, e.g., the M3 competition data).

The CIF2016 competition dataset consists of monthly time series, composed of two different subgroups. On the one hand, series related to the banking industry, and on the other hand, artificially generated series [Stěpnička and Burda 2016]. Specifically, contestants were requested to submit 12-months-ahead forecasts for 57 time series, and 6-months-ahead forecasts for 15 time series, so for a total of 72 series. The CIF2016 attracted participants from numerous fields of Computational Intelligence (CI), such as artificial neural networks, fuzzy methods, support vector machines, decision and regression trees, etc.
The NN5 competition dataset contains 2 years of daily cash withdrawals at various automatic teller machines (ATMs) located in the UK (Crone, 2008). In detail, 111 time series of ATMs were made available during the competition, and the participants were asked to submit the forecasts for a prediction horizon of 56 days ahead. Moreover, the NN5 competition includes various challenges of a real-world forecasting task, such as multi-step ahead forecasting, outliers, missing values, and multiple seasonalities. Similar to the CIF2016, a variety of CI solutions were presented at the competition.

However, while primary means of ranking forecasting approaches of these competitions was among CI techniques, statistical and hybrid techniques were also permitted to submit their forecasting solutions. Therefore, we can straightforwardly evaluate our proposed approach against state-of-the-art statistical benchmarks such as ETS, ARIMA, Theta, etc.

To be able to compare our proposed approach against the participants’ forecasts of CIF2016 and NN5, we use the symmetric mean absolute percentage error (sMAPE) for evaluation, which is consistent with the evaluations in the competitions. The sMAPE is defined as:

\[ \text{sMAPE} = \frac{100\%}{n} \sum \left| \frac{\hat{y}_t - y_t}{y_t} \right| \]

We note that both these competitions only released the overall error metrics of the participating methods,
Table 2: Parameter grid used throughout the LSTM learning process. Here, n denotes the number of training examples in a training file. The range of values used in each parameter is represented by the respective Minimum and Maximum columns.

\[
sMAPE = \frac{200}{n} \sum_{t=1}^{n} \left( \frac{|F_t - A_t|}{|F_t| + |A_t|} \right).
\]

Here, \( A_t \) denotes the true value of the time series \( A \) at time \( t \), and \( F_t \) is the respective forecast.

3.2. Hyperparameter selection and compared methods

The LSTM has various hyper-parameters. We choose values for these parameters from a parameter grid using an additional validation set, i.e., we choose the configuration that performs best on the validation set respective to sMAPE. Table 2 shows the parameter grid that is used throughout the experiments, in the form of minimum and maximum values for each parameter.

Also, we need to choose adequate input and output window sizes throughout the experiments. The output window size is largely determined by the required forecast horizon. As a heuristic, the input window size is then chosen slightly larger than the output window size. Throughout our experiments, we use a factor of 1.25 here, i.e., \( \text{inputSize} = 1.25 \cdot \text{outputSize} \). I.e., for the NN5 dataset, as the forecasting horizon is 56, we use an \( \text{inputSize} \) of 70 and an \( \text{outputSize} \) of 56. As the CIF2016 dataset has two different target horizons and some very short series, choosing window sizes is more complicated here and differs among different models, as outlined in the following. In our experiments, we use the following variants of our proposed methodology and LSTM baseline:

**LSTM.Horizon** In the CIF2016 competition, additional knowledge was available in the form of 2 different required forecasting horizons. We use this additional knowledge to

but not the actual forecasts for each method on each time series, so that we are unable to perform statistical significance testing in this work.

\(^2\)More information about the respective hyper-parameters can be found on the CNTK web site Python API for CNTK [https://cntk.ai/pythondocs/cntk.html](https://cntk.ai/pythondocs/cntk.html)
group the time series accordingly. I.e., separate prediction models are generated for each group of time horizons, following the steps 5:16 of Algorithm 1. Also, some of the series with a required horizon of 6 are very short and consist only of 23 points. Following the above mentioned heuristic, we use an inputSize of 7 when the required outputSize is 6, and an inputSize of 15 when the required outputSize is 12.

**LSTM.Cluster** Our proposed method as illustrated in Algorithm 1. An individual prediction model is produced for each cluster obtained. Due to the peculiarities and short series within the CIF2016 dataset, we start with the same partition as for the LSTM.Horizon model in this case, and then apply the methodology only for the series with a target horizon of 12. This is mainly because the anomalous-acm package that we use to extract features uses internally an STL decomposition, and therefore needs 2 full periods of data, i.e., 24 data points in our case. So, as the clustering method is not applicable for some of the CIF2016 series, the LSTM.Cluster variant is only performed on 57 time series with 12 months of forecasting horizon. As a result, in addition to LSTM models that are generated for each cluster, a separate LSTM model is built for the remaining 15 time series with forecasting horizon of 6 months.

**LSTM.All** The baseline LSTM algorithm, where no subgrouping is performed but one model is generated globally across all time series in the dataset. Note that, as some series from the CIF2016 dataset are very short, we use here an inputSize of 7 throughout, and an outputSize of 12, both for target horizons 6 and 12.

### 3.3. Results of the experiments

Table 3 shows the original results for all methods that participated in the CIF2016 competition, along with our results for this dataset. We see that our proposed method, LSTM.Cluster variant, outperforms all other methods from the CIF2016 in terms of mean sMAPE, in particular the baseline LSTM.All variant. Furthermore, all LSTM variants outperform the ETS, BaggedETS, and Theta methods, which can be seen as the state of the art for forecasting monthly data.

However, the improvements of the LSTM.Cluster variant over the LSTM.Horizon variant, which groups the time series according to their respective forecasting horizon, are marginal, and not observable from the table. This may be attributed to the peculiarities of the CIF2016 dataset. The dataset contains 48 artificially generated time series that may not present useful cross-series information. This claim is strengthened by the fact that a univariate forecasting method, namely the BaggedETS submission to the competition, outperformed all other methods in this subset, in particular the LSTM methods (Stěpníčka and Burda, 2016). Therefore, in the absence of cross-series information in a set of time series, the LSTM may not reach its full potential, and the partition into two clusters according to the target horizon may already take into account all the structure in the dataset, in terms of similarities between series.

Regarding the NN5 forecasting competition data, Table 4 shows the original results for all methods that participated in the competition, along with our results. Note that the
proposed LSTM.Horizon variant is not benchmarked against the NN5 dataset, as no additional information is available in this case. It can be seen that the proposed LSTM.Cluster variant performs better than the LSTM.All variant, and reaches a 6th overall rank. Due to rich presence of cross-series information in the NN5 dataset, our proposed method, the LSTM.Cluster variant, is able to uplift the accuracy of the baseline LSTM model (LSTM.All) that generates only one model across all time series in the dataset.

4. Conclusions

Nowadays, large quantities of related and similar time series are available in many application cases. To exploit the similarities between multiple time series, recently methods to build global models across such time series databases have been introduced. One very
| Contender Name | Mean sMAPE |
|---------------|------------|
| Wildi         | 19.9       |
| Andrawis      | 20.4       |
| Vogel         | 20.5       |
| D’yakonov     | 20.6       |
| Noncheva      | 21.1       |
| **LSTM.Cluster** | **21.6**  |
| Rauch         | 21.7       |
| Luna          | 21.8       |
| Lagoo         | 21.9       |
| Wichard       | 22.1       |
| Gao           | 22.3       |
| **LSTM.All**  | **23.3**   |
| Puma-Villanueva | 23.7     |
| Autobox(Reilly) | 24.1     |
| Lewicke       | 24.5       |
| Brentnall     | 24.8       |
| Dang          | 25.3       |
| Pasero        | 25.3       |
| Adeodato      | 25.3       |
| undisclosed   | 26.8       |
| undisclosed   | 27.3       |
| Tung          | 28.1       |
| Naïve Seasonal | 28.8      |
| undisclosed   | 33.1       |
| undisclosed   | 36.3       |
| undisclosed   | 41.3       |
| undisclosed   | 45.4       |
| Naïve Level   | 48.4       |
| undisclosed   | 53.5       |

Table 4: Mean sMAPE results for the 111 daily series of the NN5, in ascending order.

promising approach in this space are Long Short-Term Memory networks, a special type of recurrent neural networks.

However, in the presence of disparate time series, the accuracy of such a model may degenerate, and accounting for the notion of similarity between the time series becomes necessary. Motivated by this need, we have proposed a forecasting framework that exploits the cross-series information in a set of time series by building separate models for subgroups of time series, specified by a systematic and automatic clustering methodology.

We have evaluated our proposed methodology on two benchmark competition datasets, and have achieved competitive results. On the CIF2016 dataset, our methods outperform all
the other methods from the competition, and in the NN5 competition dataset our method ranks 6th overall. The results indicate that the LSTM is a competitive method, effectively exploiting similarities of the time series and therewith being able to outperform state-of-the-art univariate forecasting methods. Subgrouping of similar time series with our proposed methodology can consistently augment the accuracy of this baseline LSTM model.

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