Structural combination of neural network models

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***Abstract*—Forecasts combinations normally use point forecasts that were obtained from different models or sources ([1], [2], [3]). This paper explores the incorporation of internal structure parameters of feed-forward neural network (NN) models as an approach to combine their forecasts via ensembles. First, the generated NN models that could be part of the ensembles are subject to a clustering algorithm that uses the structure parameters and, from each of the clusters obtained, a small set of models is selected and their forecasts are combined in a two-stage procedure. Secondly, in an alternative and simpler implementation, a subset of the generated NN models is selected by using several reference points in the model structure parameter space. The choice of the reference points is optimised through a genetic algorithm and the models selected are averaged. Hourly electricity demand time series is used to assess multi-step ahead forecasting performance for up to a 12 hours horizon. Results are compared against several statistical benchmarks, the average of the individual forecasts and the best models in the ensembles. Results show that the cluster-based (CB) structural combinations do better than the genetic algorithm (GA) structural combinations in outperforming the average forecast, which is the traditional point forecast from an ensemble.**

I. Introduction

The term ensemble originated in climate modelling, where scientists distinguish different types of uncertainty, as [4] described. *Structural uncertainty* refers to uncertainty about the form that the modelling equations should take; *parametric uncertainty* is about the values that should be assigned to parameters within a set of modelling equations and *initial condition uncertainty*, which refers to the difficulty in measuring all the required variables needed in models.

Ensembles were adopted in NNs by [5], and came to mean the use of several models, constructed with differences in one or more of their design parameters. They used ensembles of NNs for classification. In this seminal research only synthetic data were used, and superiority of the ensemble was reported in comparison to individual models. Since this research, NN ensembles have evolved from the use of simple sets of models to the collective evolution of them through sophisticated computational intelligence techniques.

Ensembles involve three main tasks, as depicted in Figure 1: generation, pruning and combination. Generation involves the creation of different models. Pruning comprises a selection of them, and is optional ([6]). The final stage performs the combination of forecasts. Other factors to be considered are: the type of model to ensemble, how the individual models are produced, the level of automation of the process and the way combinations are made. Therefore the construction of ensembles is far more complex than the construction of a single model.

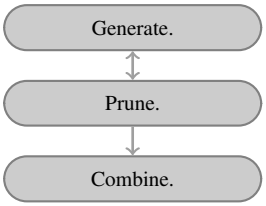


Fig. 1. General steps in ensemble generation.

There are sequential approaches where the generation of models is followed by a pruning stage and finished with a combination stage (see for example [7]). But in other approaches this sequence is not entirely observed: the evolution (or generation) of the individual models can be done in parallel, so that the information from the training stage can be shared, and used to modify the collective estimation of parameters ([8] ,[9]).

The type of model used and the generation process are interrelated. The most common types of models in the literature are feed-forward NNs (e.g. [5] , [10]), although Radial Basis Functions ([11], [12]), Elman recurrent network and Hopfield ([12]), Deep belief network ([13]) and Abductive networks ([14]) can also be found.

Once the type of model is chosen, a question arises about how to specify the individual models. In the case of feed-forward NN, the creation of a single model for forecasting requires several parameters, which can be determined by trial and error, heuristic rules or systematic approaches. For example, [15] conducted model selection with strategies based on sequential statistical tests, information criteria and cross validation. [16] and [17] use design of experiments to identify an appropriate network configuration. [18] emphasised input selection, as part of model specification, and proposed a methodology for seasonal components. Nevertheless, no universal guideline exists on how to select the appropriate model ([19]).

In ensemble construction, once the characteristics of the models are established, variety is usually introduced by modifying initial random weights ([20]), or by randomising training

samples ([7], [21]). The randomisation of the feature space ([9]) could count both as a strategy for model variation and as a strategy for model specification.

In the final block in Figure 1, models are combined to produce the output of the ensemble. The methods that have been proposed in the literature (focusing on forecasting rather than on classification) include: a gating network ([22]), a simple or weighted average ([8], [12], [23], [24]), a nonlinear average through another NN ([23]), a feed-forward NN ([25], [26]), a Radial Basis Function ([11]), the median of forecasts ([10], [20]) and the mode ([19]). It can be seen that the complexity and effectiveness of the ensembling approaches are only partially related to the combining procedure at the end of the process, as there are other steps involved.

In the energy forecasting area the use of NN ensembles is common. [27] and [28] forecasted hourly electricity demand and gas consumption, respectively, by using feed-forward NNs. Forecasts were combined through the average, recursive least squares, fuzzy logic, feed-forward NN, functional link NN, a partition of the temperature space (an external variable), a linear programming algorithm and a mixture of local experts. The best performance was obtained with a NN as a combination mechanism.

[29] forecasted hourly and peak load (with data from two US utilities) for the next 24 and 120 hours with a small ensemble of NNs. K-nearest neighbour was used to select training sets. NNs were trained in parallel with an iterative approach, feeding back averaged forecasts as inputs for subsequent forecast horizons. Results were competitive when compared with usual forecast error measures in similar utilities and previous publications .

[30] used NNs to produce load forecasts from 1 to 10 days ahead based on ensembles of weather forecasts. Comparisons were made with uni-variate benchmarks and point forecasts from individual models. For ten lead times, the mean of the load scenarios built with weather variables was a more accurate forecast than that produced by the non-ensemble based procedure. This research combines the use of ensemble weather forecasts with an ensemble of rather low complexity NNs leading to a improvements in forecast accuracy. Variety in the data is not needed as different scenarios are used as inputs.

Further research involving combination of forecasts produced with different types of NNs include [10], [13], [14], [26], [31], [32] and [33]. In general, there is limited research on forecast combination approaches that consider the internal characteristics of the models involved. [21] suggested this direction, by considering clustering of structural parameters to summarise models based on such clusters. This line of thought can be further explored, in terms of the clustering techniques and the kind of time series to be considered.

This paper proposes one form of structural combination, implemented in two ways: one with a recursive partitioning of the weights space of NNs to then select models to combine, and another with a Genetic Algorithm which searches for reference points in such parameter space to select models to combine. The next sections describe the method and illustrate their use in forecasting electricity demand from Rio de Janeiro 12 hours ahead.

II. Methodology

The most common types of NN models in the literature of ensemble development are feed-forward NNs (see for example [5] and [10]). Such NNs are common in forecasting ([34], [18]) and, specifically, in the electricity sector (i.e. [27], [29], [14]). Multi-layer perceptrons are the most frequently applied ([34]) and, therefore, are adopted here.

Figure 2 describes the modelling process. A base NN structure, which has been selected through a preliminary process (such as a sensitivity analysis or a heuristic approach, e.g. [17]), is used to fit the time series with different models. Parameter diversity can be introduced through various mechanisms, one of which is the randomisation of input-output patterns for the neural networks, which is adopted here and is described in the next subsection. Once the ensemble is generated, the models are subject to a combination procedure involving the structure, as described below, and, finally, forecasts are produced and their uncertainty assessed.

The modelling process depends on specific design decisions. The combination algorithm, the forecast stage, the uncertainty assessment and the multi-step ahead forecast approach used to fit the individual models can influence each other. In an iterative approach, where a network produces forecasts for all horizons, the modelling process leads to a single ensemble that forecasts different horizons.

A. Randomisation of input-output patterns

The pre-processing stage uses randomisation of input-output data patterns during the training period. This mechanism facilitates the creation of diverse NN models (with different parameter sets), thus facilitating the identification of different clusters of models in the parameter space.

B. Structural Combination based on Clustering

When the structural combination stage in Figure 2 is implemented through clustering, the combination becomes a mechanism that looks into the structure of models and finds groups in the space defined by such structure. An algorithm based on fuzzy C-means was chosen, which incorporates concepts from fuzzy systems.

Fuzzy C-Means is an algorithm that partitions a collection of vectors into c fuzzy groups and finds a cluster centre in each group such that a cost function of dissimilarity is minimised (see [35]). The choice of a fuzzy C-means oriented approach is due to its use of a degree of membership of elements to clusters (between 0 and 1), instead of a binary membership (0 or 1, equivalent to *non-member* and *member* in K-means). Therefore, a NN model can belong to several clusters with different degrees of belongingness that are defined by grades between 0 and 1 ([35, p. 426]).

However, C-means produces non-deterministic partitions or clusters. A variant of the algorithm was therefore adopted here,

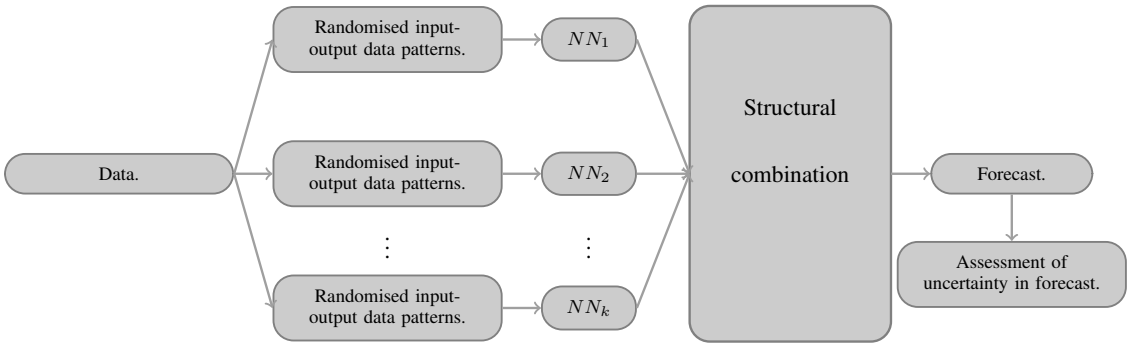


Fig. 2. Modelling process.

based on [36], which uses a recursive partitioning of the model space that helps in producing a deterministic partition. The next sub-section describes the model in detail.

C. The forecasting model

The clustering-based algorithm (CB) uses structure information of models and produces forecasts based on the data and this information. It creates partitions in the parameter space of the NNs and centres of such regions are used as cluster centres. When the individual NN models are used to issue forecasts in an iterative manner, the clustering procedure takes into account the in-sample one-step-ahead forecasts produced by NNs in order to calculate the loss function, which is to be minimised. The forecast for each horizon h is calculated based on the forecasts made by the clustered NNs for the respective horizon, as follows:

$$\hat{y}_h = \sum_{i=1}^{n} \phi_i \hat{y}_{C_i,h} \tag{1}$$

Where $\hat{y}_{C_i,h}$ is the forecast from cluster i for horizon h:

$$\hat{y}_{C_i,h} = \alpha_0 + \alpha_1 M_{i_1}(h) + \alpha_2 M_{i_2}(h) + \ldots + \alpha_L M_{i_L}(h) \tag{2}$$

$M_{i_1}(h), M_{i_2}(h), \ldots$ are forecasts for step ahead h from models selected within cluster i.

The coefficients ϕ_k are calculated as an average of the normalised weights of vectors (models in vectorial form):

$$\phi_k = \frac{\sum_{i=1}^{N_k} w_k}{N_k} \tag{3}$$

where N_k is the number of models in cluster k.

$$w_i(v) = \frac{u_i(v)}{\sum_{j=1}^{n} u_j(v)} \tag{4}$$

$$u_i(v) = e^{-\frac{D_i^2(v)}{\sum_{j=1}^{n} D_j^2(v)}} \tag{5}$$

$u_i(v)$ is the membership of v to cluster i (v is a model represented in the form of a vector). The squared distance between v and the i-th centre is divided by the sum of squared distances from v to all centres. Subsequently, an exponential transformation is taken so that the membership of a model to a cluster decreases as long as its distance from the centre increases. Consequently, there is always a degree of membership, however small, of every vector to every cluster.

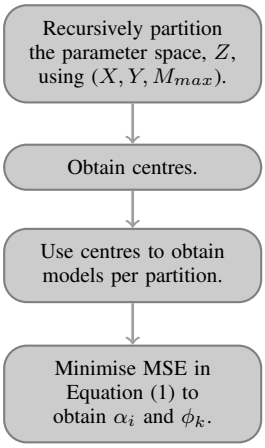


Fig. 3. Clustering Scheme.

The partitioning routine, in Figure 3, which is used to build the clusters, recursively splits the parameter space of models in two steps. A forward step, which grows partitions in the form of a tree and a backward step, which prunes those regions that do not improve fit function (MSE).

X is the set of input variables, including lagged values of the dependent variable, Y is the one step ahead forecast for the independent variable. The recursive partitioning uses internally a matrix Z, where every row represents a model (a NN) in the parameter space, which has already been trained with the X, Y data set. M_{max} is the maximum number of clusters allowed.

In the first step of Figure 3, a procedure $regressByCluster(X, Y, B)$ is internally used, which performs an OLS regression of Y on X in a per-cluster manner, with B containing the definitions of the regions or clusters. This gives initial estimates of α and ϕ that are then updated in the last stage of Figure 3.

The regions, B, are defined in the form of base functions:

$$B_m(\mathbf{Z}) = \prod_{k=1}^{K_m} H\left(s_{km} \cdot \left(z_{v(k,m)} - t_{km}\right)\right) \tag{6}$$

$$H(\eta) = \begin{cases} 1 \text{ if } \eta \geq 0 \\ 0 \text{ otherwise} \end{cases} \quad (7)$$

For a vector z, the function $B_m(z)$ establishes if z belongs to the m-th region. If so, the function takes the value 1. If z does not belong to the region, the function would have the value 0. K_m is the number of partitions in the space that define the region. s_{km} is a constant that takes the values 1 or -1, signalling if the partition is to the right or to the left of the value t_{km}. The variable z_v is the dimension, in the space of parameters, in which a partition is made.

Both the individual NNs and the CB algorithms were implemented in Matlab® 2010 using its neural networks toolbox.

D. Structural combination based on genetic algorithms

The cluster-based implementation described in the previous subsection creates clusters that serve to extract and combine models. A simplified implementation was conducted by using genetic algorithms. Again, X is the set of input variables, including lagged values of the dependent variable, Y is the one step ahead forecast for the independent variable and Z is a matrix where every row represents a model (a neural network) in the parameter space, which has already been trained with the X, Y data set.

A series of reference points in the parameter space is generated. From each point, $\mathbf{P_i}$, a number of NN models is selected, having the smallest euclidean distance to it. The forecast produced by this combination (y_{Avg}) is calculated as the average forecast of all models selected from all reference points (5 models are selected from each point, as specified in Table I). The routine optimises through a genetic algorithm the set of reference points such that the MSE of the y_{Avg} in-sample one-step-ahead point forecasts is minimised.

A GA combination can be viewed as a structurally informed average: it selects models based on closeness around different points in the parameter space and then performs an average. The algorithm is run over the same NN pool used to perform the structural combination proposed in previous subsections. It was implemented in Matlab® 2010 using *ga* routine, setting a maximum number of generations to 3000.

III. Study with an electricity demand time-series

A time series of electricity demand was used to asses the performance of CB and GA structural combination approaches. The series contains hourly observations in Rio de Janeiro covering the period from Sunday 5 May 1996 to Saturday 30 November 1996 (Figure 4). It has been used by [37] to evaluate the performance of various uni-variate models, including a NN, which was implemented according to [38].

The direct approach of fitting different NNs for different forecast horizons led to a performance markedly different from results obtained by [37]. In their study, the authors fitted a NN with input lags 1, 2, 24, 25, 48, 72, 96, 120, 144, 168, 192, 216, 240, 264, 312, 336 and forecasted the differences in an iterative manner. Further experiments with this setting provided better results than the direct approach and therefore it was adopted for the present study.

A preliminary analysis suggested that an NN architecture with 16 inputs (corresponding to all lags considered) and 2 neurons would be the best choice. Such architecture is used here with the CB and GA procedures described above to test the structural combination of forecasts. Due to the existence of extreme values in the out-of-sample performance of NNs, the ensemble to perform the combination was built with the over-produce and choose approach ([6]): 150 NNs where generated and 50 selected. The forecast performance for $h = 12$ was assessed with a rolling window in the in-sample period and the best models were used to conduct the structural combination. The configurations of the individual NNs and combination algorithms is summarised in Table I.

Results are compared with those obtained by [37] with a Holt-Winters-Taylor (HWT) exponential smoothing method and a NN. Comparisons are made by using MSE and MAPE error metrics.

TABLE I
STUDY CONFIGURATION.

Individual NN configuration.	
Factor	**Values**
Num. inputs	$1, \ldots, 16$, being 16 the number of lags.
Num. hidden layers	1
Num. hidden units	2
Activation function for hidden nodes	Tangent Sigmoid
Activation function for the output node	Linear
Initial values for the weights	Values in the range [-2 2] established by the Nguyen-Widrow algorithm
Training algorithm	Backpropagation with Levenberg-Marquardt optimisation and Bayesian regularization
Data normalisation	Yes
Init. Combination coefficient (μ)	0.001
Sample size	5040
Data config. for training, testing and validation	$Ntr = 3024$, $Nva = 336$ $Nte = 1680$
Extreme values treated	No.
Forecast approach	Iterative
Combination configuration.	
Num. of models	50
Num. Max. clusters	2, 4, 8
Models per cluster	5
Final combination	Linear
Randomised input-output patterns	Yes
Structural content	All synaptic weights in each NN.

Figure 5 shows the out-of-sample MAPE for the different CB models and the selected benchmarks and Figure 6 provides a ranking of models and the percentage differences in performance with respect to the average forecast of all NN models. While the rankings comprise all models and benchmarks, the

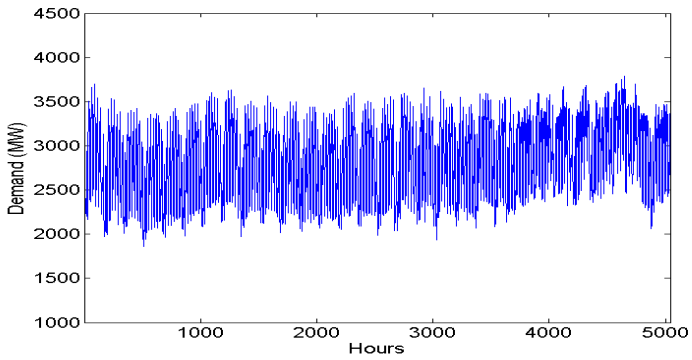


Fig. 4. Hourly electricity demand in Rio de Janeiro for Sunday, 5 May 1996 to Saturday, 30 November 1996. Original Series.

percentage differences are calculated only for models derived from the NNs produced in the study. Table II provides sample coefficients for CB models. The assessment of uncertainty in forecasts, by using forecast intervals, is provided in Figure 7 (only CB models are considered).

TABLE II
COEFFICIENTS FOR STRUCTURAL COMBINATION OF NN FOR RIO DE JANEIRO ELECTRICITY DEMAND SERIES.

CB2						
α_1	24.9383	0.38	0.4028	0.0896	-0.0942	0.2126
Φ	1					
CB4						
α_1	25.3822	0.7965	-1.7627	1.1277	0.2929	-0.4866
α_2	26.3815	-1.0451	3.2846	0.5185	1.8219	1.4281
α_3	28.9069	0.5246	-2.3253	0.5201	0.8754	0.2391
Φ	0.3984	0.1786	0.4233			
CB8						
α_1	24.9104	1.4617	-5.6481	2.2431	0.3346	0.1906
α_2	26.1478	1.7667	6.8272	0.5522	3.0498	1.7813
α_3	27.6467	-2.071	1.087	0.9352	0.0621	0.3737
α_4	21.5636	-2.3524	0.62	-0.3881	1.4783	-1.4435
α_5	29.9801	-6.0529	1.2764	2.8328	0.9112	1.7857
Φ	0.2199	0.1086	0.2297	0.2243	0.2169	

α_i are the coefficients applied to point-forecasts from models in cluster i and Φ are the weights applied to the outputs from clusters. The α in the first column ($\alpha_{i,0}$) is the intercept of the linear combination. The $\alpha_{i,j}$, for $j > 0$, in the remaining columns, are applied to point forecasts.

IV. DISCUSSION

It is noticeable that not only the best performing NNs for the electricity demand series are simple in terms neurons, but also the best performing CB models are the simplest. For example, CB2, with a maximum of 2 clusters, was able to consistently outperform the average forecast from the NNs. The need for structural simplicity in the case of the electricity demand series is manifested both at single model and at ensemble level.

This time series required a sensible selection of inputs in the early stages of the study, so as to capture the regularities in the series, in accord with [18]. However, this also implies that the the statistical benchmarks are very well suited to the data, and thus the NN models and ensembles had difficulty in outperforming the well specified models. It thus appears that faced with regular data, it pays off to invest time and effort in the selection of inputs and use a well-specified model that address these regularities to forecast the series.

Larger structural representations of models can be used. However, their complexity could create challenging features to perform structural combinations. A proper balance between dimension reduction and the use of a sufficiently rich structural representation would be needed to achieve practical computing times.

Replacing the randomisation of the training set by a bootstrap strategy to create the individuals models that participate in the clustering algorithm, would move the approach in the direction of bagging. The GA combination can also benefit from such modification and these are potential research avenues for future research.

V. CONCLUSION

This paper presents a novel forecasting combination approach that involves the creation of ensembles of NNs and the combination of a subset of them based on parameters from their structure. The first implementation of the proposed combination approach is based on clustering algorithms, which groups together models that share a measure of similarity (in this case, a measure of distance in the parameter space of models). The second implementation uses genetic algorithms to select models by using reference points (analogous to cluster centres) in the parameter space and can be seen as a structurally informed average of forecasts. Different levels in the number of clusters were used to assess the combinations.

For the double-seasonal time series considered here the CB tend to do better in relation to the simple average combination. Furthermore, there is no marked superiority of structural combinations over individual models. In spite of this, CB shows better performance than GA with respect to the best models.

CB and GA structural combinations were outperformed by the chosen statistical benchmark. HWT exponential smoothing models are better equipped to capture the regularities in these time series and are more adaptive to changes in the data than NNs. Consequently, the potential structural combinations of these models should be investigated, as they may be more

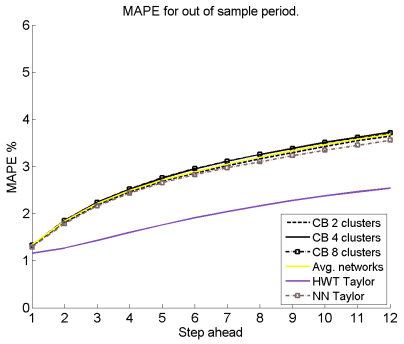
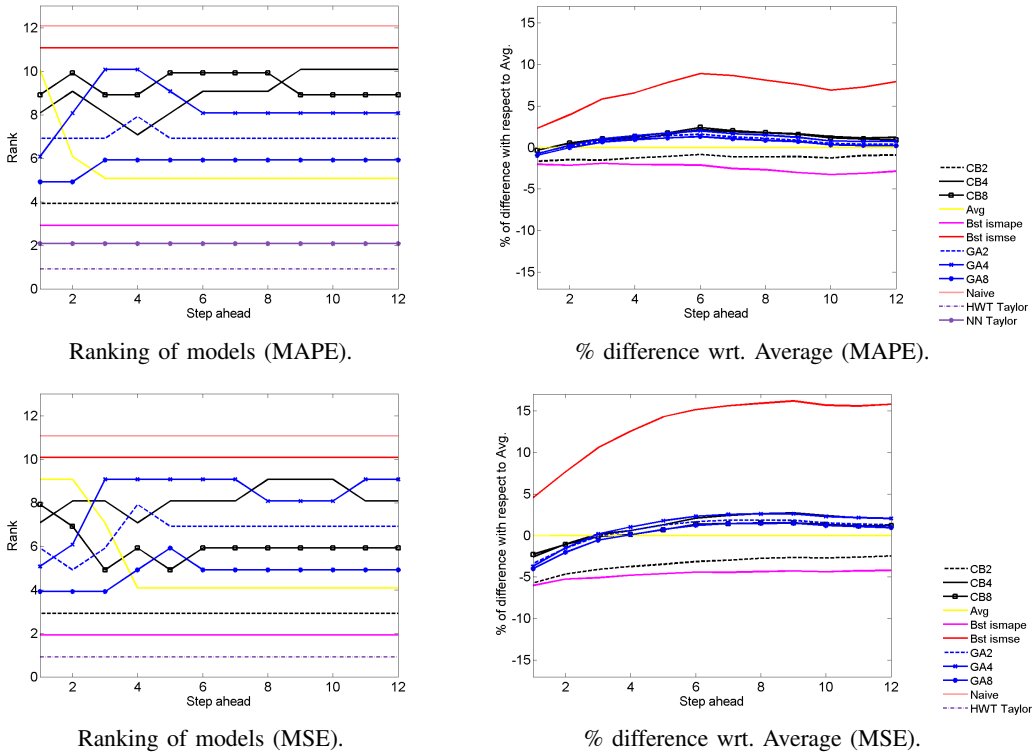


Fig. 5. Out-of-sample MAPE for Rio de Janeiro electricity demand series.



Ranking of models (MAPE). % difference wrt. Average (MAPE).

Ranking of models (MSE). % difference wrt. Average (MSE).

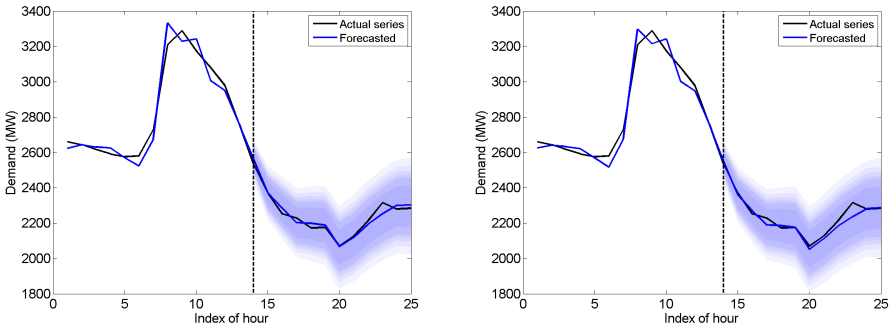
Fig. 6. Comparison by forecast horizon. Best model is in rank 1. % differences with respect to the average are negative when there is improvement over the average benchmark. CB2 stands for a cluster-based combination with a maximum of 2 clusters. GA2 stands for a genetic-algorithm based combination with 2 reference points. Bst. ismape denotes the NN in the study with the lowest in-sample MAPE. Bst. ismse denotes the NN with the lowest in-sample MSE. HWT Taylor and NN Taylor denote results from [37].

attractive in the case of double-seasonal time series data. Nonetheless, it is noteworthy that HWT has an in-built error correction mechanism, which is not present in the NNs. Given changes in the data pattern within the out-of-sample period, as observed in this time series, structural combinations of recursive neural networks become an attractive avenue for research.

Based on these findings, future research could investigate the behaviour of a structural combination approach when models of different nature are combined. If, for example, instead of using single single unit models (statistical or computational intelligence model), bundles of the form $B_i =< ARIMA, NN >$ are formed, the structural combination of such bundles could potentially improve performance, when dealing with complex forecasting problems.

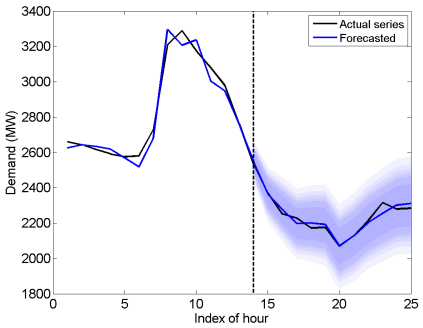
Other forms of structural representation can be envisaged, while taking care of keeping a reasonable computing cost. Changes in the generation of individual models could lead to approaches closer to bagging, thus facilitating the exploration of research avenues that could improve forecasting performance.

Additionally, the better performance obtained with an iterative multi-step-ahead forecasting approach, when compared to a direct approach, in the case of electricity demand time



(a) $MaxC = 2$ clusters.

(b) $MaxC = 4$ clusters.



(c) $MaxC = 8$ clusters.

Fig. 7. Forecast intervals for Rio electricity demand time series.

The graphs cover the period for $t - 12 \leq t \leq t + H$ where t is the last observation of the in-sample period and $H = 12$ is the number of forecast horizons. The shades, from lighter to darker, correspond to α levels 0.95, 0.90, 0.85, 0.80, 0.75 and 0.60.

series, suggests that an extension of the present research could investigate how the chosen multi-step-ahead forecast approach affects the performance of structural combination.

Overall, the exploration of structural combination of forecasts, and its implementation in two forms, open the possibility to investigate new forms of ensembles, specially when relationships between components in the individual models can be clearly distinguished.

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