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International Journal of Forecasting

journal homepage: www.elsevier.com/locate/ijforecast



GEFCom2012 hierarchical load forecasting: Gradient boosting machines and Gaussian processes



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ARTICLE INFO

Keywords: Load forecasting Gradient boosting machines Gaussian processes

ABSTRACT

This report discusses methods for forecasting hourly loads of a US utility as part of the load forecasting track of the Global Energy Forecasting Competition 2012 hosted on Kaggle. The methods described (gradient boosting machines and Gaussian processes) are generic machine learning/regression algorithms, and few domain-specific adjustments were made. Despite this, the algorithms were able to produce highly competitive predictions, which can hopefully inspire more refined techniques to compete with state-of-the-art load forecasting methodologies.

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1. Introduction

This report details the methods I used when competing in the load forecasting track of GEFCom2012. It is split into sections describing the various techniques used for forecasting temperatures and loads. Within each section, I have given the motivation for the particular choice of algorithm, discussed the way it was used and described how to replicate the results using the spreadsheets and scripts accompanying this report.²

I approached the competition in the spirit of a data mining competition. Consequently, some of the choices detailed below were based on intuition, in order to save time and focus on those aspects of the data which were most likely to give the greatest improvements in performance. Many of these choices could have been replaced by appropriate searches and cross validation; where more complex techniques would be required, I have briefly described how one could perform a more objective analysis.

My methodology for load backcasting/forecasting was to try different general purpose regression algorithms and then combine (average) the predictions. The final ensemble forecast comprised predictions from a gradient boosting machine (GBM), a Gaussian process (GP) regression, and the benchmark solution provided by the competition organisers (a linear model).

This paper is organised as follows. Section 2 discusses data cleansing, Section 3 is on temperature forecasting, Sections 4 and 5 introduce the GBM and GP forecasting methodologies respectively, and Section 6 discusses the way in which the final ensemble prediction was formed. A brief introduction to Gaussian processes is provided in the Appendix.

2. Data cleansing

A sensible first step in any prediction task is to look at your data, and in particular, to search for anomalies. This was performed for both the temperature and load data using the spreadsheets temp/temp.xlsx and load/load.xlsx, by plotting the data as time series and using various types of conditional formatting to do a visual search for irregularities.

This visual analysis revealed a large discontinuity in load series 10 and atypical dynamics in series 9 (see Fig. 1, and others for comparison). No other large anomalies were detected during the initial inspection of the data, and the smaller irregularities were not revisited because the

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¹ http://www.gefcom.org/.

² The source code is available at https://github.com/jamesrobertlloyd/GEFCOM2012/.

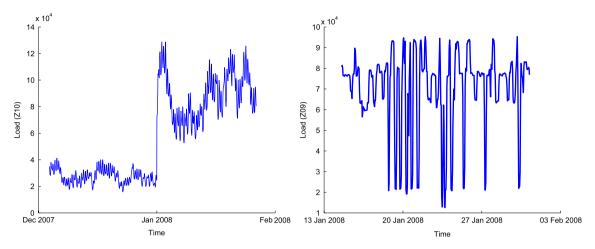


Fig. 1. Left: Raw data at zone 10, showing a large discontinuity. Right: Raw data at zone 9, showing atypical load dynamics.

algorithms detailed below performed acceptably well without requiring further data cleansing.

No adjustments were made for holidays or other irregular events such as black-outs. Ignoring them was a practical response to time constraints, rather than a design choice.

3. Temperature forecasting

3.1. Initial analysis and remarks

The error metric used in GEFCom2012 was heavily weighted towards times at which the temperatures were unknown (i.e., the load forecast rather than backcasts). Consequently, good temperature predictions seemed to be crucial for overall success.

When submitting a solution to Kaggle, the error metric was computed on 25% of the held out data and returned to the user. This allowed the user to optimise their temperature predictions by optimising the score of the resulting load predictions (i.e., computing load predictions based on different temperature predictions and selecting the temperature prediction with the highest corresponding load prediction score). Depending on the way in which the test dataset was split (the 25% test and 75% validation partition), this may have allowed users to come very close to knowing the true future temperatures.

I therefore used a flexible but simple method for forecasting temperatures that could be easily tuned. Fig. 2 shows data from temperature station 1 along with various curves which were used for prediction (described later). The black solid line is the raw data, which shows that temperatures follow a smooth trend, with a daily pattern of rising and falling temperatures. For the sake of simplicity, I modelled the smooth trend and the daily periodicity separately, and modelled each temperature station in isolation.

3.2. Methodology

The smooth trend was estimated within the data using a local linear regression (e.g., Hastie, Tibshirani, & Friedman, 2009, Chapter 6) with a bandwidth of one day. I assumed

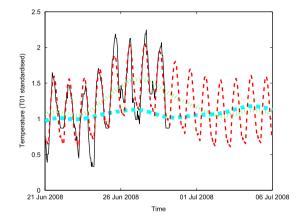


Fig. 2. Raw data at temperature station 1 (after removing the mean and scaling to have a unit standard deviation) (black solid line); the historic average of smoothed temperatures (blue dashed thick line); current and predicted smoothed temperatures (green dotted thick line); and final temperature predictions (red dashed line). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

that the smooth trend would probably return to the historical average smoothly. A suitable modelling technique that would give this type of prediction is Gaussian process regression (e.g., Rasmussen & Williams, 2006, or see the Appendix to this paper for a very brief introduction); the difference between the smoothed temperature and its historical average was regressed against time using a squared exponential kernel and zero mean function.

In Fig. 2, the thick blue dashed curve shows the historical average of smoothed temperatures, while the thick green dotted line shows the current smoothed temperature and prediction. The parameters of the GP model (length scale and scale factor of the squared exponential kernel) were tuned by hand, by initially choosing sensible values based on plots of the data, and then trying to optimise the public test score of the load predictions thus derived.

The difference between the temperature and the smoothed temperature was assumed to be a smooth periodic function with a period of one day. This modelling

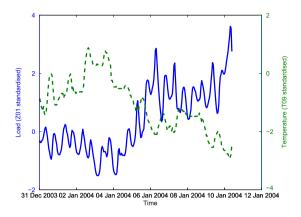


Fig. 3. Raw data at load zone 1 (after removing the mean and scaling to have a unit standard deviation) (blue solid line) and at temperature station 9 (after removing the mean and scaling to have a unit standard deviation) (green dashed). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article)

assumption was implemented using a Gaussian process with a periodic kernel (again regressing the difference against time). The parameters of the GP model were chosen by optimising the marginal likelihood of the model, given particular parameters, using optimisation methods supplied in the GPML toolbox.³ Only the last 250 data points (corresponding to approximately 10 days) were used to fit this part of the model, in order to capture the recent temperature dynamics.

3.3. Replication of the results

The spreadsheet and scripts used to manipulate the temperature data can be found on the IJF website (http://www.forecasters.org/ijf/). The MATLAB script makes use of the GPML toolbox. The temperature data were reshaped into a (time) × (temperature station) array using the spreadsheet temp.xlsx, and then saved in times_series_raw.csv. The method described above is implemented by the MATLAB script predict_temp.m, which saves the predicted time series in GP_pred_temp.csv, and the smoothing of these predictions in smooth_temp_GP.mat and smooth_temp_GP.csv.

3.4. Discussion

The red curve in Fig. 2 shows the results of the methodology when applied to temperature station 1. The fit to the data is far from perfect, but it has captured the broad features of the data. I am not familiar with the temperature/weather forecasting literature, but I am quite certain that far better methods do exist!

4. Gradient boosting machines

4.1. Initial analysis and remarks

Fig. 3 plots a subset of the data for loads in zone 1 and at temperature station 9. We can see that that the

load has a smoothly varying trend with roughly periodic daily deviations from this trend. The load also appears to be negatively correlated with the temperature in this region of data. It seems reasonable to assume that the load dynamics will be different on weekends compared to weekdays.

Based on these observations, I modelled loads as a function of time of the day, time within the week, temperatures, and smoothed temperatures (all stations). Each zone was modelled independently, for the sake of simplicity.

4.2. Methodology

A standard 'black-box' technique for learning an unknown regression function is that of using gradient boosting machines (GBM) (e.g., Hastie et al., 2009, Chapter 10). For each zone, I used all of the data to train a GBM and then used that to predict all of the outputs, i.e., I learned a global function for each zone.

To do this, I used a standard R implementation of GBM using most of the default settings. After some brief experimentation with parameter values, I used a shrinkage factor of 0.01, 10 000 trees, and an interaction depth of 3. I experimented with other parameter values, using the public test score as a guide, but nothing that I tried improved upon my initial guess, and therefore I did not expend much effort on trying to optimise the parameter values.

4.3. Replication of results

The scripts and data used can be found in the folder gbm. The load data were reshaped into a (time) × (load zone) array using the spreadsheet load.xlsx in the folder load. This was then concatenated with the temperature predictions and smoothed temperature predictions and saved in gbm_input.csv. The R script basic_gbm.R then performed the method described above to produce predictions, which are saved in gbm_output.csv.

4.4. Discussion

The time series for zone 10 had a very large discontinuity (see the left panel of Fig. 1). GBM was used as a global prediction method, which means it will have produced very bad predictions for zone 10. I later fixed this by modelling the loads either side of the discontinuity separately. Perversely, this resulted in a worse public test score. However, this change resulted in a much improved private test score; in hindsight, I should have opted for the more reasonable model!

5. Gaussian processes

5.1. Initial analysis and remarks

The observations made about the load data in Section 4.1 (i.e., smooth trends, near periodic variations, dependence on temperature) can be modelled using a

³ http://www.gaussianprocess.org/gpml/code/matlab/doc/.

⁴ http://cran.r-project.org/web/packages/gbm/index.html.

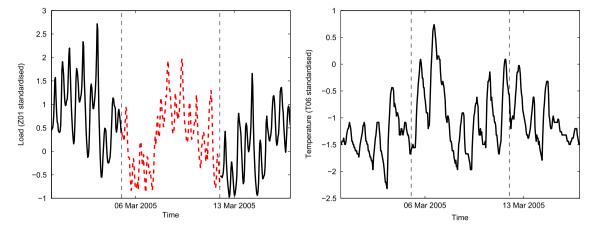


Fig. 4. Left: Raw data (after scaling and translation) (black solid line) and Gaussian process predictions (red dashed line) for zone 1. Right: The corresponding temperature time series used for prediction. Notice that the peak in temperature corresponds to a trough in the load predictions; i.e., the model has predicted a negative correlation between temperatures and loads. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Gaussian process regression. Specifying the kernel function of a Gaussian process allows one to encode these structural assumptions into a regression model. See the Appendix for a brief introduction to the effects of choosing different kernels.

5.2. Methodology

Three different kernel functions were used; one for backcasting, one for forecasting, and one for backcasting zone 9. The forms of the three kernels used were as follows⁵

$$SE_t + SE_S + SE_t \times SE_T \times PER_t$$
 (1)

$$SE_t + SE_t + PER_t \tag{2}$$

$$SE_t + SE_S + SE_T \times PER_t,$$
 (3)

where SE refers to a squared exponential kernel, PER is a periodic kernel, and the subscripts indicate the dimension which the kernel acts upon: (t)ime, (T)emperature or (S)moothed temperature. For backcasting, the model was applied to the 1000 surrounding data points; for forecasting, the last 500 data points were used. Only one temperature station was used in this method; for each backcasting/forecasting region, the marginal likelihood of the model was computed for each temperature station. Bayesian model averaging (e.g. Hoeting, Madigan, Raftery, & Volinsky, 1999) was then used to combine the predictions (in practice, this was usually numerically equivalent to selecting the model/temperature station with the highest marginal likelihood).

The kernel in Eq. (1) encodes the assumption that loads can be explained as a smoothly varying trend and an approximately periodic component. The smooth trend is the sum of a smooth function of smoothed temperature and a smooth function of time (to explain any deviations from

the trend implied by temperature). The periodic component can vary through time, and because it is multiplied by SE_t and SE_T , the shape of the periodicity will be more similar to recent times and points in time with similar temperatures. This kernel was used for backcasting all of the zones except for zone 9. An example of this kernel in action is shown in Fig. 4. The left plot shows the load data (black solid line) and the prediction (red dashed line). On the right is the temperature time series which resulted in the model with the highest marginal likelihood. Comparing the two plots, we can see that the deviations of the prediction from the trend through time correspond to fluctuations in the temperature time series.

The kernel in Eq. (2) encodes the assumption that loads can be explained as the sum of two smooth functions with different length scales and an exactly periodic smooth function. This simpler kernel was used for forecasting, since it gave more stable extrapolations of the data.

The kernel in Eq. (3) is a simpler version of that in Eq. (1) and is used for backcasting zone 9. The periodic component is now only similar to other times with similar temperatures. This prevented the predictions from being so greatly affected by the large isolated load fluctuations which are present in zone 9.

The forms and parameters of the kernel functions (see the accompanying code for all of the values) were chosen by trial and error (observing which kernels gave reasonable-looking predictions and computing public test scores).

5.3. Replication of results

The spreadsheet and scripts used can be found in the folder gp. The load data was reshaped into a (time) × (load zone) array using the spreadsheet load.xlsx in the folder load and then saved in load_input.csv, which encodes missing values as zeros. The outputs of the temperature prediction GP_pred_temp.csv and smooth_temp_GP.mat are used directly.

⁵ See the source code for parameter values.

The MATLAB script gp_elec.m performs the methodology described above, but saves the predictions to gp_pred.csv.

5.4. Discussion

Selecting the form and parameters of the kernels by hand requires a moderate degree of familiarity with Gaussian processes. The automatic selection of kernel functions is an active area of research; recent publications on the topic include the proposal of an automated search over a generative grammar of kernel expressions by Duvenaud, Lloyd, Grosse, Tenenbaum, and Ghahramani (2013), the use of deep neural networks to learn a kernel function by Salakhutdinov and Hinton (2008), and the development of a new class of kernels which are designed to have a good extrapolation performance by Wilson and Adams (2013). It is likely that better performances could have been achieved by larger and more principled searches over kernel functions.

6. Selecting the final ensemble

6.1. Remarks

The final prediction was formed as the ensemble (weighted average) of predictions from three separate methods: gradient boosting machines, a Gaussian process regression and the benchmark solution provided by the competition organisers (a linear model). Ensembling is a very powerful technique for combining predictions from separate models. If two predictions (viewed as random quantities) are statistically uncorrelated, then their average will have a lower variance than either one separately.

In practice, different algorithms are correlated, and ensembling highly correlated predictions will rarely lead to an improved performance. In particular, I also tried the random forest algorithm, but the predictions were too highly correlated with gradient boosting machines (they are both based on an ensemble of decision trees) to be a useful addition to the ensemble.

6.2. Methodology

The ensemble weights were chosen by hand, using the public test score as the metric to be optimised. The public test scores did not vary considerably once sensible parameters had been found, so more advanced techniques were not used to optimise the ensemble weights.

6.3. Replication of results

The spreadsheets which were used to manipulate the model output can be found in the folder ensemble. The spreadsheet sub_creator.xlsx was used to convert (time) × (load zone) arrays of model output into the required format for submission. The output of this spreadsheet was then copied into ensemble_creator.xlsx, which performs the averaging required to produce ensembles of the predictions.

6.4. Discussion

This method could have been been improved slightly by selecting the ensemble weights programmatically, to optimise some form of validation metric. One could also have tried to optimise the public test score directly. Since only two submissions could be tested per day, one would want to use an optimisation technique that made a very efficient use of the data (e.g. Osborne, Garnett, & Roberts, 2009; Snoek, Larochelle, & Adams, 2012).

Larger improvements could probably be achieved by considering a larger number of base predictions. It is also likely that the algorithms used by other competitors in GEFCom2012 would provide useful additions to the ensemble of predictions.

7. Conclusion

In this competition, I applied general purpose machine learning/regression algorithms and made few adjustments for the specific domain which the data arose from. Despite this, the resulting predictions were still highly competitive. It is hoped that this report shows that simple techniques can be very effective for predictive modelling, and can inspire practical techniques for load forecasting.

Acknowledgments

I would like to thank Alex Davies for guidance in the ways of data mining and David Duvenaud for advice on the practicalities of using Gaussian processes.

Appendix. A very brief introduction to Gaussian processes

For a much richer introduction, see Rasmussen and Williams (2006). A Gaussian process, $(f(x))_{x \in X}$, is a set of random variables, such that any finite collection has a jointly Gaussian distribution. A Gaussian process can be specified completely by a mean function m(x) and kernel function $\kappa(x, x')$ such that

$$Expectation(f(x)) = m(x) \tag{A.1}$$

Covariance(
$$f(x), f(x')$$
) = $\kappa(x, x')$. (A.2)

Gaussian processes can be used to specify a prior distribution on functions, and can then be used in a Bayesian analysis. They are nonparametric and can learn any function, given sufficient data.

The kernel function encodes the structure of a Gaussian process. The left plot in Fig. A.5 shows samples (random draws) from a Gaussian process distribution using squared exponential kernels; this function encodes an assumption of smoothness. Intuitively, these plots show the types of functions that can be learned most easily/quickly using Gaussian process regression. One parameter of a squared exponential kernel is a length scale, which controls how quickly the value of the Gaussian process varies. The blue

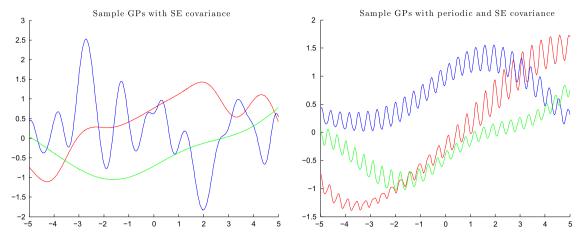


Fig. A.5. Left: Draws from a Gaussian process with a squared exponential kernel with differing length scales. Right: Draws using a squared exponential and periodic product kernel.

line in the left plot has a short length scale, which results in quick variations of the function. The green line has a long length scale, and consequently the Gaussian process is visually much smoother.

The right plot in Fig. A.5 shows samples from a Gaussian process with a more complicated kernel function. The kernel function is the product of a squared exponential kernel and a periodic kernel. This encodes the assumptions that the Gaussian process is roughly periodic, and that the shape of the periodicity changes smoothly.

By constructing more advanced kernel functions, one can specify more complex structures as desired. Kernel functions depend on parameters, and are typically chosen by maximising the marginal likelihood of the training data given the parameter choices (all of the gradients can be computed analytically). One can also perform a fully Bayesian analysis by integrating over the parameter values; this typically requires approximate inference techniques.

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