Probabilistic forecasting approaches for extreme NO₂ episodes: a comparison of models

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Abstract

High concentration episodes for NO₂ are increasingly dealt with by authorities through traffic restrictions which are activated when air quality deteriorates beyond certain thresholds. Foreseeing the probability that pollutant concentrations reach those thresholds becomes thus a necessity.

Probabilistic forecasting is a family of techniques that allow for the prediction of the expected distribution function instead of a single value. In the case of NO₂, it allows for the calculation of future chances of exceeding thresholds and to detect pollution peaks.

We thoroughly compared 10 state of the art probabilistic predictive models, using them to predict the distribution of NO₂ concentrations in a urban location for a set of forecasting horizons (up to 60 hours). Quantile gradient boosted trees shows the best performance, yielding the best results for both the expected value and the forecast full distribution. Furthermore, we show how this approach can be used to detect pollution peaks.

Keywords: probabilistic forecasting, air quality, quantile regression, nitrogen dioxide, Madrid

1. Introduction

Pollution has become a worrying issue in cities due to its adverse effects on health and the increase in pollutant concentrations, mainly due to human activity (traffic, heating systems...). In order to take preventive steps to maintain air quality, forecasting the evolution of pollution levels becomes a useful tool for decision makers: detecting pollution peaks beforehand could give cities enough time to take and communicate effective measures.

Multiple research papers have focused on this issue and have dealt with the prediction of air quality. Bai et al. [1] describes the state of the art in this exercise and collects a range of diverse solutions applied to this problem.

However, the prediction of the expected value of pollution concentrations through point-forecasting does not provide enough information about the likelihood of the pollutant levels reaching a certain threshold. Indeed, we have an estimate but we usually do not have a description of the confidence of the model nor the uncertainty in the predictions. Therefore, it is difficult to estimate the probability of the pollutant reaching above a certain threshold.

The reason this probability estimation is so important is because the measures taken by cities to limit pollution (for example, limiting traffic) impact the daily routines of citizens and prove themselves to be quite unpopular. Therefore, local governments need to have an estimation of the confidence in the prediction to safely engage in those preventive measures.

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As noted by Hothorn et al. [12], the real objective in a regression analysis is to find the full conditional distribution of the target variable: in our case, the distribution of the concentration of the pollutants. Indeed, this full distribution gives an idea of the uncertainty of our predictions and can be useful to forecast the probability of the signal being above a certain threshold. For example, in the city of Madrid, hourly NO$_2$ concentrations in the air are considered to be harmful from 180 $\mu$gm$^{-3}$.

Previous research on the same dataset has already shown the usefulness of probabilistic forecasting for NO$_2$ levels [16], establishing the advantages of the approach and focusing on 1 hour-ahead predictions with a single model (quantile random forests). We hereby extend that work by implementing other six models (quantile linear regression, quantile $k$-nearest neighbours, quantile gradient boosted trees, neural networks, distributional random forests, natural gradient boosting) and by using them for a wide set of forecasting horizons (up to 60 hours). Inspiration is drawn on some of the best approaches from the GEFCom forecasting competition [11, 18].

Furthermore, improving over these approaches, we also present a novel method to apply statistical inference to the output of the models. This method acknowledges the fact that the results show linear dependences between the predictors and the target, which slightly benefits linear models over nonlinear ones. By combining a linear model with nonlinear probabilistic modelling of its residuals we obtain optimized versions of the standard models.

Finally, in order to showcase one of the applications of probabilistic forecasts, we tackle the prediction of NO$_2$ peaks for the different horizons, and compare the performance of the proposed models on this task.

2. Probabilistic forecasting with quantile regression

The prediction from most regression models is a point estimate of the conditional mean of a dependent variable, or response, given a set of independent variables or predictors. However, the conditional mean does not provide a complete summary of the distribution, so in order to estimate the associated uncertainty, quantiles are in order. The 0.5 quantile (i.e., the median) can serve as a measure of the center, and the 0.9 quantile marks the value of the response below which reside the 90% of the predicted points. Recent advances in computing have inducted the development of regression models for predicting given quantiles of the conditional distribution. The technique is called quantile regression (QR) and was first proposed by Koenker in 1978 [15] based on the intuitions of the astronomer and polymath Rudjer Boscovich in the 18th century. Elaborating from the same concept of estimating conditional quantiles from different perspectives, several statistical and CI models that implement this technique have been developed: from the original linear proposal to multiple or additive regression, neural networks, support vector machines, random forests etc.

Quantile regression has gained an increasing attention from very different scientific disciplines [25], including financial and economic applications [3], medical applications [13], wind power forecasting [24], electric load forecasting [17], environmental modelling [5] and meteorological modelling [2] (these references are just examples and the list is not exhaustive). To our knowledge, despite its success in other areas, quantile regression has not been applied in the framework of air quality, with the exception of [20].

Thus, as we can estimate an arbitrary quantile and forecast its values, we can also estimate the full conditional distribution, which will entail us to the results presented in Section 4.

Among the growing array of methods that allow to estimate and forecast data-driven conditional quantiles, in this study we have chosen to compare linear regression, $k$-nearest neighbors, random forests and gradient boosted trees. We took the point-estimate version of those models and converted them to their quantile or probabilistic counterparts. We can therefore compare each model not only on the accuracy of their point estimation but on the confidence of each model.

We will compare the different algorithms through the RMSE, MAE and bias for the quantile 50 and the CRPS metric for the forecast distribution. As described by Gneiting et al. [10], CRPS is a measure of the squared difference between the forecast cumulative distribution function (CDF) and the empirical CDF of the observation.
3. Data description and experimental design

3.1. Nitrogen dioxide

The city of Madrid has an air quality monitoring system composed by 24 stations which capture hourly data for NO$_2$. For this study, we have selected one of the stations with higher average levels: Escuelas Aguirre station (code 28079008).

As we can see in 1, the shape of the histogram approaches the one from a lognormal distribution and therefore we transformed to the logarithm of the values. This has 2 positive effects: it reduces the tail of the distribution which will enable better quantile estimation and it reduces the skewness of the distribution which helps with linear models like the linear quantile regression.

The time series for this station consists of hourly measured values of the concentrations of NO$_2$ from 01/01/2013 to 30/11/2017. These values exhibit a clear intraday pattern, in which the higher values are located in two peaks around the morning and evening (with highest average value around 19h) while the nightly hours (from 00h to 05h) have lower average concentrations. Not only are the values higher at those hours, but also the variance is, as we can see in figure 1.

In order to analyze the seasonality of the signal, we extract the 5 main factors from the Fourier transform. Those correspond to the main repetitive patterns found on the series, and can be seen clearly from the first 3000 components. The series shows certain seasonality for 12-hour, 24-hour, one week (168-hour) and one year. Therefore, we will create, and use as inputs for the models, the output of periodic functions (cosine and sine) whose frequency is equal to the ones stated above. This will enable the machine learning models to learn the seasonality of our time series.

As is common when forecasting with machine learning models, we exploit the inertia of the modelled series by adding lagged variables to the inputs. Of course, in doing so, we are limited by the horizon of the prediction and by the ‘curse of dimensionality’, which implies keeping a limited number of features as input. In our case, the inertia of the series will be modeled by lagged values from the immediate past (hours before) and, based on the seasonal analysis: 1-5 hours before and every 11-13 hours up to 9 days before.

3.2. Ozone

The same station that records Nitrogen dioxide also records the levels of ozone (O$_3$). It is known that ozone and Nitrogen dioxide are related by chemical reactions occurring in the atmosphere in the presence of sunlight, especially of the UV spectrum. Thus, we will also add lagged values of O$_3$ as inputs to our models.
3.3. ECMWF numerical pollution prediction

The European Centre for Medium-Range Weather Forecasts (ECMWF) implements the Copernicus Atmosphere Monitoring Service. This service delivers a daily production of near-real-time European air quality analyses and forecasts with a multi-model ensemble system. Although these forecasts are a very good starting point, the resolution of the model is 10km and hence it is not expected to be capable of modelling the local urban effects of the NO$_2$ series under study.

3.4. Calendar Variables

As NO$_2$ levels are clearly be linked to human activity, we will also flag the hours belonging to a specific type of day. Days could be classified as bank holidays, heavy traffic days (for example, return from holidays), school holidays... We will also use as inputs to the models past values of this variables (1, 2 and 7 days before).

3.5. Experimental Design

As a summary, we use the following predictors: NO$_2$ measures lagged 1-5H and every 11-13H up to 9 days before, O$_3$ levels lagged every 24H up to 4 days before, calendar variables lagged 1, 2 and 7 days before, ECMWF predictions and seasonal features extracted from the Fourier analysis. This amounts to a total of 102 independent variables.

When performing the experiments, first we aligned and gathered all the hourly time series: NO$_2$, O$_3$, ECMWF and calendar variables. Then we transformed the signal levels and then we added the lagged values and a seasonal time series with the main periods of the NO$_2$ time series.

Once all this process is finalized, we train the following probabilistic models: quantile random forests (QRF), $k$-nearest neighbors (QKNN), quantile linear regression (QLR) and quantile gradient boosting (QGB). Figure 2 shows the data flow in the experimental design. All the hyperparameters of the models have been estimated through grid search on a validation set. In Section 3.6 we provide more information on each of the models.

Concerning cross-validation, there are several accepted methods to separate the train and test set which produce correct estimations of the error [4]: We can approximate the error of a model through a crossvalidated evaluation as long as we remove for each test set the correlated samples in the training dataset. We chose a cross validation with 5 splits for time execution reasons. We will always test with predictions done
at 10:00, as this is the time the forecast is done in the operational setting, as the data is first available at that time.

We want to forecast the full distribution of NO\textsubscript{2} levels for the next 60 hours and therefore we will train and evaluate the models for each hour (60 horizons).

After forecasting the quantiles, we will fit them to a normal distribution. Fitting a normal distribution to the predicted quantiles and then generating the percentiles for that fitted distribution has several advantages. It enables the calculation of more percentiles from a small number of them. It also helps estimating the upper tail of the distribution, in spite of the low probability for those values.

We will evaluate the predicted 50 percentile through standard evaluation metrics (RMSE and bias), and the predicted distribution through the continuous ranked probability score (CRPS).

We will perform this evaluation for each of the models and each of the horizons.

3.6. Probabilistic Models

As stated above, we will compare seven different probabilistic models, which are briefly described below for reference. We will provide alongside the models the abbreviation we will use for each of them throughout this article. Also we are adapting point-estimation algorithms to their probabilistic counterparts. This allows us to see the uncertainty these models have. Indeed, metrics like RMSE and Bias are linked to the confidence of the models for point estimation but the predicted CDF is much better at describing it. This also increases the interpretability of those models. Therefore the implementations we described can have applications beyond this forecast exercise.

3.6.1. Quantile linear regression (QLR)

As shown in [15], we can apply linear regression with a modified cost function in order to predict the quantiles of the dependent variable. Given a set of vectors \((x_i, y_i)\), in the usual point forecasting approach we are usually interested in the prediction \(\hat{y}(x) = \alpha_0 + \alpha_1 x\) which minimizes the mean squared error,

\[
E = \frac{1}{n} \sum_{i=1}^{n} \epsilon_i = \frac{1}{n} \sum_{i=1}^{n} [y_i - (\alpha_0 + \alpha_1 x)]^2.
\]

This prediction is the conditional sample mean of \(y\) given \(x\), that is, \(\hat{y}(x) = \hat{\alpha}_0 + \hat{\alpha}_1 x\), or the location of the conditional distribution. But we could be interested in estimating the conditional median (i.e., the 0.5 quantile) instead of the mean, in which case we should find the prediction \(\hat{y}(x)\) which minimizes the mean absolute error,

\[
E = \frac{1}{n} \sum_{i=1}^{n} \epsilon_i = \frac{1}{n} \sum_{i=1}^{n} |y_i - (\alpha_0 + \alpha_1 x)|.
\]

The fact is that, apart from the 0.5 quantile, it is possible to estimate any other given quantile \(\tau\). In that case, instead of (2), we could minimize

\[
E = \frac{1}{n} \sum_{i=1}^{n} f(y_i - (\alpha_0 + \alpha_1 x))
\]

where

\[
f(y - q) = \begin{cases} 
\tau(y - q) & \text{if } y \geq q \\
(1 - \tau)(q - y) & \text{if } y < q 
\end{cases}
\]

with \(\tau \in (0, 1)\). Equation (3) represents the median when \(\tau = 0.5\) and the \(\tau\)-th quantile in any other case.

We will train 5 linear regression models to predict 5 percentiles of the signal. As percentiles are calculated separately, we have the risk of quantile crossing. We will reorder the quantiles as explained in [6] to solve this problem.
3.6.2. Quantile \( k \)-nearest neighbors (QKNN)

We will use the probabilistic \( k \)-nearest neighbors algorithm as described in [19]. This algorithm is based on the standard \( k \) nearest neighbor, where instead of calculating the mean of the targets of the \( k \) nearest points to the input, it builds a distribution from the target of those neighbors.

3.6.3. Quantile random forests (QRF)

Quantile random forests create probabilistic predictions out of the original observations. They work like the usual random forest, except that, in each tree, leaves do not contain a single value as a prediction but the target observations from the training set belonging to that leaf.

Then predictions are calculated by selecting the leaves in each tree corresponding to the input features and combining the weighted histograms in each tree out of the target observations in those leaves. For more information refer to [21].

3.6.4. Quantile Gradient Boosted Trees (QGB)

Tree boosting [8] is a successful machine learning technique that consist on growing trees based on the compromise of a cost function and a regularization function. This cost function is usually used to forecast the mean of the signal. We will modify the cost function (in a similar way as in the quantile linear regression) to predict the quantiles of the target. Also, we will use the lightgbm implementation [14] which provides lower training times and higher accuracy.

We will train 5 gradient boosted trees models to predict 5 percentiles of the NO\(_2\) signal and we will solve quantile crossing with the technique explained in [6].

3.6.5. Multilayer Perceptron

We will also test a multilayer perceptron (MLP) [22] with 1 hidden layer. Like for quantile linear regression and quantile gradient boost, we will modify the cost function to predict the quantiles of the target.

We will therefore as well train 5 MLP to predict 5 percentiles of the NO\(_2\) signal and the whole distribution of the target.

3.6.6. Distributional Random Forests

Based on the idea of GAMLSS, Distributional Forests [23] extend the power of this semiparametric method by estimating the LSS (location, scale and shape) through the use of random forests, instead of using GAM’s. We will use the R implementation of this method from the package disttree.

3.6.7. NGBoost

NGBoost [7] uses the natural gradient instead of the standard gradient to build a boosted ensemble learner that predicts the parameters of the distribution of the target variable. Natural Gradients are presented as offering better stability and robustness than normal gradients.

3.6.8. Probabilistic forecast of linear regression residuals

We suspect there are high linear dependencies between the input predictors and the target. We will then experiment on combining 3 of the models: quantile random forest, quantile \( k \)-nearest neighbor and quantile gradient boost with a linear regression.

We decided to train a linear regressor which predicts the NO\(_2\) values and then use the QRF, QKNN and QGB models to predict the full distribution of the residuals of that linear regression. We abbreviate both models respectively with QRFL, QKNNL and QGBL.
Figure 3: Boxplot of continuous ranked probability score, root mean squared error and bias of the different models for all horizons.

Table 1: Error measures for the proposed models.

| method | CRPS (3.3) | RMSE (3.4) | bias (3.1) | time (3.3) | TP (3.4) | FP (3.4) | AUC (3.4) |
|--------|------------|------------|-------------|-------------|----------|----------|----------|
| NGB    | 10.0       | 19.4       | 4.6         | 997.6       | 4        | 3        | 0.28     |
| QKNNL  | 10.0       | 20.1       | 3.9         | 8.3         | 36       | 46       | 0.28     |
| DT     | 10.3       | 20.0       | 5.3         | 732.9       | 3        | 0        | 0.3      |
| QRFL   | 10.4       | 20.6       | 3.8         | 10.5        | 24       | 55       | 0.28     |
| QKNN   | 10.7       | 20.9       | 5.4         | 8.2         | 0        | 0        | 0.28     |
| MLP    | 10.8       | 20.6       | 4.5         | 232.9       | 131      | 219      | 0.28     |
| QLR    | 10.9       | 20.7       | 4.0         | 9.7         | 18       | 50       | 0.23     |
| QRF    | 12.2       | 22.8       | 7.5         | 30.8        | 0        | 0        | 0.3      |
| QGB    | 9.5        | 18.2       | 3.3         | 37.0        | 73       | 23       | 0.27     |
| QGBL   | 9.5        | 19.0       | 2.9         | 36.0        | 92       | 67       | 0.26     |

Figure 4: Average reliability and sharpness of the different models across all horizons. The dim blue lines correspond to the different horizons.
Figure 3 shows the different metrics for each model across all the horizons. First, we clearly see how quantile gradient boosted trees (QGB) outperforms the other models and displays better scores for all metrics. The additive nature of QGB is behind these results.

Quantile random forests and quantile k-nearest neighbors underperform compared to the other models, showing a bias which is clearly higher compared to the others. The main reason for this is the highly linear dependence of the data. This also explains then the good results of the linear model (QLR). However, the linear model underperforms when compared to other models, as it is not able to learn the non-linear relationships between the predictors and the target.

Regarding the models predicting the residuals of a linear regression, QKNNL and QRFL showcase good performance, which is surprising for QKNNL due to the simplicity of this model. On the other hand, QGBL brings no real benefit compared to QGB, as QGB can already integrate the linear component.

Distributional Forests (DT) and Natural gradient boosted trees (NGB) present good results but are still outperformed by QGB. Natural gradients bring no benefit in this case.

Finally, MLP has good bias results but underperforms against the other methods.

As stated earlier, the NO\textsubscript{2} levels follow a lognormal distribution and it seems that it is better modeled with a multiplicative model (different causes multiply the level of pollution), therefore the logarithm of the NO\textsubscript{2} levels are better forecast with an additive model. This is the reason why quantile gradient boosted trees outperform the other models: it can naturally add the nonlinear effects.

Table 1 displays the mean and standard deviation of CRPS of the different models. The table shows again the good performance of the quantile gradient boosted trees model for CRPS. The table also shows the training times of the different models. QGB appears as having a good compromise between low training times and metrics. QKNNL offers good performance with really low training times.

For probabilistic models, CRPS is a good summary of the performance of the models. Notwithstanding, the reliability and sharpness graphs are known to be useful at estimating how the observed values are positioned in the distributions. Figure 4 features the reliability and sharpness of the different models.

The sharpness curve shows that QRF and QKNN tend to underestimate the levels of NO\textsubscript{2}. This is clear in the sharpness curve for the upper percentiles. The observed values of those percentiles are usually noticeably higher than the forecast values. This means that, too many times, the observed values are in the upper percentiles of the distribution. This is also a consequence of the bias of both models.

For QRF and DT, we see few observations on the sides of the predicted distributions. This means the variance of the predicted variance is too high and the predictions have too much uncertainty.
Table 2: Average Rankings of the algorithms (Quade)

| Algorithm | Ranking                  |
|-----------|--------------------------|
| DT        | 4.86415525141552         |
| MLP       | 4.289954337899544       |
| NGB       | 6.81544901065449        |
| QGB       | 9.407153609071533       |
| QGBL      | 8.90677321156773        |
| QKNN      | 3.1086697108067         |
| QKNNL     | 5.12555707762557        |
| QLR       | 2.76255707762556        |
| QRF       | 1.448249619482494       |
| QRFL      | 5.3748097412480975      |

QGB and QLR forecast distributions seem more balanced but display high values at both sides of the sharpness curve. If we consider the distribution to be a gaussian distribution, this means the forecast distributions tend to have a too small standard deviation and are too narrow. Therefore, the forecast probability of some levels of NO$_2$ is too small compared to the observed one. QGBL and MLP also display this behaviour. As we are interested in predicting peaks of pollution, this is not detrimental.

In order to compare the result of the 10 methods, we will use advanced non parametric tests as described by Garca et al. [9]. The Quade test will calculate the rank of all the algorithms and then determine if they are significantly differently from the mean rank. We have 60 different datasets, each one corresponding to a horizon where we have performed a 5-fold crossvalidation and kept the mean of the results. The rank is calculated not only based on the results in the different datasets but also on the importance of the dataset (based on the variance of results). The result of the Quade Test rejects the null hypothesis that the methods have similar performance and we can use the ranks to classify the different methods. Table 2 shows the results of the Quade test.

4.1. Forecasting NO$_2$ concentration peaks

One of the applications of probabilistic forecasts is the estimation of the probability of the signal being above a certain threshold. In the case of NO$_2$ forecasting, this is especially useful when normative limits are established by authorities.

We evaluated the proposed models to check how good are they to detect those peaks. In Madrid, municipal regulations fix a threshold of 180 $\mu$gm$^{-3}$ to activate the first level of restrictive measures on traffic. Thus, we consider that a NO$_2$ peak is forecast when the probability of reaching above this limit is higher than 50%. It is important to note that this normative threshold lies around the 99.7 quantile of the NO$_2$ distribution, and thus it is safe to consider peaks as rare events. This fact of course implies that the possibility of using a classifier to predict peaks, with classes above or below the threshold, is not straightforward. Firstly, we would need a classifier per threshold, but more importantly, it would suffer from the fact that the training dataset would be highly imbalanced. A probabilistic model can learn from the predicted distribution even if the peak level has not been reached.

As noted before, there is usually a high cost on performing preventive measures against pollution. This has some consequences for the evaluation of our models. We must minimize the number of false positives and false negatives and thus secondary metrics like the ROC curve are not directly applicable as in this case, depending on the take of the decision makers, the cost of a false positive might be much higher than the cost of a false negative. Table 1 shows the true positives and false positives of each model. We see again the superior results of QGB against the other models as it has a good ratio of true positives against false positives. Finally, Area under curve ”AUC” seems to not be a good metric to compare the different models as the differences are not that high.

5. Conclusions

After extracting and processing the data from one of the pollution stations in Madrid, we have compared 10 different models to build a probabilistic forecast of the levels of NO$_2$ for up to 60 hours into the future.
We have evaluated our models through the forecast quantile 50 and the full forecast distribution.

We have observed a linear dependence between the target and the features. For this reason, the linear quantile regression has performed well compared to random forests and $k$-nearest neighbors. However, the multiplicative nature of the levels of NO$_2$ and the nonlinear dependence between target and features have lead to better results for the gradient boosted trees which has outperformed all the other models in all metrics.

However, we have shown how quantile random forest and quantile $k$-nearest neighbors could be used to improve the results of a linear model when nested to model the full distribution of the residuals of a linear regression. Those models, specially the $k$-nearest neighbor are easier to train, so they become worthy alternatives to the gradient boosted trees.

In sum, we have tested 10 alternative models to produce probabilistic forecasts for NO$_2$, and we have compared them through different metrics. Also, we have established how quantile gradient boosted trees are able to detect pollution peaks beforehand with few false positives.

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