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Assessing Uncertainty in Space Weather Forecasting Using Quantile Regression and Complex Nonlinear Systems Identification Techniques

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***Abstract*— Space weather forecasting is of global interest, and its importance is well established in research community and recognized by government, industries and stockholders. Over the past years, many types of predictive models have been developed in the literature. There is a general agreement that forecasting models should not only provide point prediction but also inform the uncertainty associated with the prediction. This study presents a novel method bases on quantile regression and complex dynamic modelling for measuring uncertainties in space weather forecasting. The approach is implemented using Quantile regression and Nonlinear AutoRegressive Moving Average with Exogenous inputs (NARMAX) methods (for short the approach is called Q-NARMAX). The method is applied to Disturbance storm index (Dst) observations to examine its interpretability and capability for uncertainty analysis. Results show that the proposed Q-NARX model can produce excellent predictions of the Dst index, and meanwhile provides a measure for assessing the uncertainty in the forecast. The innovative integration of quantile regression, complex dynamic modelling and nonlinear system identification techniques enables the proposed work to have following attractive advantages and properties: 1) it can produce excellent prediction accuracy for space weather forecasting, 2) it uses transparent models to approximate (represent) black-box systems, enabling to interpret the dependent relationship between space weather indices (system outputs) and their drivers (system inputs), and 3) more importantly, it allows for uncertainty assessment and analysis of models and forecasts.**

Keywords—input/output systems, signals and systems, nonlinear system identification, data modeling, forecasting, prediction uncertainty, space weather.

I. Introduction

Space weather processes can cause adverse or even hazardous effects on the operation of modern technological systems, either space-based or ground-based. Space weather forecasting can help significantly mitigate space weather hazards [1]-[5]. Due to the huge complexity of the geospace evolution processes, it is nearly impossible to build comprehensive physical models of the geospace environment based on first principles, which can be used to forecast the space weather parameters [6][7]. However, the complementary data based or empirical approach, which treats the geospace as a black (or grey) box input-output system [8], provides attractive alternative tools that are able to make forecast of geomagnetic behaviours such as fluxes of energetic electrons in the radiation belts, TEC (total electron content), geomagnetic indices such as Dst (Ddisturbance storm index), Kp (a common index used to indicate the severity of the global magnetic disturbances in near-Earth space), AE (a geomagnetic index of the auroral electrojet, which characterizes the maximum range of excursion, both positive and negative, from quiet levels), and Sym-H (an index of storm time ring current intensity), among many others.

This paper restricts the attention to the case of magnetospheric space weather, where the Dst index has been developed to quantify middle latitude geomagnetic disturbances and is used to measure the strengths of such space weather hazards as geomagnetic storms [9], for example, for a great storm, Dst < -350 nT; for a severe storm, Dst is between -350 and -200 nT; for a strong one, it is between -200 and -100 nT; for a moderate one, it is between -100 and -50 nT, and for a weak one, it is between -50 and -30 nT [10]. Ring current, magnetopause current and other currents contribute to the evolution of Dst index.

Data-driven modelling has attracted increasing attention to space weather forecasts in recent years. Models used for Dst index prediction can be roughly categorized into two groups: transparent to end-user models and opaque to end-user models. Parametric models, such as NARMAX (Nonlinear AutoRegressive Moving Average with eXogenous inputs) methods [11]-[14], which were initially developed for solving complex control and systems engineering modelling problems, have found their way and successful applications in space weather forecast [15]-[20]. These models are transparent to end-users. Some neural network models, e.g. radial basis function networks [21]-[23] are partly transparent to end-users, but most neural network models, including classical artificial neural networks [24] and deep neural networks [25]-[27] are all opaque to end-users. It is worth mentioning that in the most recent few years there has been an explosive increase in publications on space weather forecast using deep learning or deep neural networks (see, e.g., the survey paper [27] and the references therein).

Over the past years, a variety of predictive models have been developed in the literature. There is now a general agreement that forecasting models should not only provide point predictions but also the uncertainty associated with the predictions. A number of approaches have been used to assess the accuracy of forecasting models, including correlation function, prediction efficiency, root mean square error, and many others (see e.g. [26][28]). However, for many of the developed data-based tools the assessment of forecast uncertainty is still an open question.

To help fill the gap between the demand of uncertainty assessment in space weather forecasting and the lack of the need, this study proposes a novel methodology based on Quantile regression and NARMAX methods, called Q-NARMAX models, which can be used to assess the uncertainty in space weather forecasting. To evaluate the performance of the proposed method, a case study is carried out by applying the method to Disturbance storm index (Dst) observations. Experimental results show that Q-NARMAX display excellent performance.

The proposed Q-NARMAX method has the following advantageous features: 1) It maintains all the attractive features of NARMAX, e.g., transparency, parsimony and interpretability; 2) The Q-NARMAX model parameters provide information on how the role of each regressor changes in each quantile of the distribution of the target signal (the system output); 3) Unlike a traditional deterministic model which can only produce a single point prediction for a given input sample, a Q-NARMAX model can produce many prediction points corresponding different quantiles of the model parameters. These multiple-point predictions can be used to measure the model uncertainty.

II. Methodology

A. A Brief Introduction to Quantile Regression

Least squares type methods play a key role in data modelling and analysis. In the sense of ordinary least squares, the regression model is designed to fit the mean value of the response data. To obtain a good model (e.g. unbiased estimates of model parameters), it requires that a number of conditions should be satisfied, these include: 1) the noise signal has mean zero and is uncorrelated with model regressors; 2) the noise has the same variance in all the observations; and 3) the observations (samples) of the regressors are independent and identically distributed. If one or more of these assumptions are violated, the resulting model may be biased and less reliable.

Quantile regression is an extension of the traditional ordinary least squares regression; it is used when the assumptions for ordinary least squares are not satisfied. Unlike ordinary least squares regression which attempts to fit the conditional mean of the target response data, quantile regression is designed to fit the conditional medians of the response values.

Let y be a response variable which depends on n predictors $x_1, x_2, \ldots, x_m$. The common regression representation that links the response to the potential predictors is:

$$y(k) = \beta_0 + \beta_1 x_1(k) + \beta_2 x_2(k) + \ldots + \beta_m x_m(k) + e(k) \quad (1)$$

where the β_i's, (i=0,1, …, m) are the regression coefficients, $\{x_i(k), y(k)\}$, with k=1,2,…, N, are measurements or samples, $e(k)$ is the model error of the kth sample. Let $\mathrm{x}_k = [1, x_1(k), \ldots, x_m(k)]^T$ and $\beta = [\beta_0, \beta_1 \ldots, \beta_m]^T$, the τth regression quantile is defined as any solution to the minimization problem [29]:

$$\min_{\beta} \left(\begin{array}{l} \sum_{k=1}^{N} [\tau \max[y(k) - \mathrm{x}^T(k)\beta, 0] \\ \quad + [(1-\tau)\max[\mathrm{x}_k^T\beta - y_k, 0)] \end{array} \right)$$

$$= \min_{\beta} \left(\begin{array}{l} \sum_{k \in \{j | y_j \geq \mathrm{x}_j^T \beta\}} \tau \, | \, y_k - \mathrm{x}_k^T \beta \, | + \\ + \sum_{k \in \{j | y_j < \mathrm{x}_j^T \beta\}} (1-\tau) \, | \, y_k - \mathrm{x}_k^T \beta \, | \end{array} \right) \quad (2)$$

For a given dataset, a group of regression models can be estimated using the quantile regression (2) by choosing different quantiles.

B. An Overview of NARMAX Methods

Assume the behaviour of a dynamical system output, y, is dependent on or correlated to a total of n inputs, $u_1, u_2, \ldots, u_n$. From systems engineering theory, the relationship between the output y and the input u can be represented by the following NARMAX model [11]:

$$\begin{array}{l} y(k) = f(y(k-s), y(k-s-1) \ldots, y(k-p), \\ \quad u_1(k-\tau), u_1(k-\tau-1), \ldots, u_1(k-q), \ldots, \\ \quad u_n(k-\tau), u_n(k-\tau+1), \ldots, u_n(k-q), \\ \quad e(k-1), \ldots, e(k-r) + e(k) \end{array} \quad (3)$$

where $u_1(k)$, $u_2(k)$,…, $u_n(k)$ are the values of the system inputs observed or measured at time instant k, $y(k)$ is the system output sequence, and $e(k)$ is noise sequence; p, q and r are the associated maximum time lags; s and τ are the time delays between the response and the model input variables, and usually s =1 and τ = 0 or τ = 1; $f(\cdot)$ is an unknown function that needs to be built from available training data. The noise signal $e(k)$ cannot be measured in real applications, but in practice it can be approximated using the model prediction error $\varepsilon(k) = y(k) - \hat{y}(k)$, where $\hat{y}(k)$ is the model prediction at time instant k. Note that the moving averaging (MA) elements, $e(k-1)$, $e(k-2)$, , …, $e(k-r)$, are mainly used for noise estimation and model refinement during the model building process, will be removed for later analysis and prediction purposes.

The nonlinear degree of a NARMAX model is determined by the highest order of all model terms. For example, the nonlinear degree of the model $y(k) = a_0 + a_1 y(k-1) + a_2 u(k-3)$ is 1, whereas the nonlinear degree of the two-term model $y(k) = a_1 y(k-1) + a_2 u(k-1) u^2(k-2)$ is 3.

In most applications, only a relatively small number of important model terms are needed in the final models. An efficient model structure detection method is highly needed to select the most significant model terms such as $y(k-1)$, $u(k-1)u^2(k-2)$.

When the NARMAX model (3) is applied to space weather forecasting, e.g., Dst index forecasting, the system output signal y is the Dst index, u_1, u_2,…, u_n can be a number of geomagnetic or solar wind parameters/indices such as Bst, Bx, By, Bz, V, solar wind density, and solar wind pressure.

The identification procedure of NARMAX models includes the following five steps:

1) Data acquisition and pre-processing (where necessary);
2) Design a sufficiently large dictionary, containing all candidate model terms of potentially important or useful, e.g., $y(k-1)$, $u_1(k-2)$, $u_2(k-5)u_3(k-2)$;
3) Apply model term selection and structure detection algorithms to select and determine the most important model terms;
4) Perform model validity test using nonlinear statistical tests; if the current model does not pass the statistical tests, then go back to the previous step to add new model terms and then update and refine the model until all tests are satisfied;
5) Model interpretation and application.

One of the most efficient model tern selection and structure detection algorithms is orthogonal least squares [11][30]. This study uses a forward regression with orthogonal least squares (FROLS) [31] algorithm, coupled with two metric indices, that is, error reduction ratio (ERR) and conditional entropy (CE) [32][33], to determine the NARMAX model structure.

The final identified model can be written in a linear-in-the-parameters form below:

$$y(k) = \beta_0 + \beta_1\phi_1(k) + \ldots + \beta_m\phi_m(k) \qquad (4)$$

where m is an integer representing the total number of model terms, $\phi_1(k),\ldots,\phi_m(k)$ are model terms, each of which is of a polynomial form such as $y(k-1)$, $u_1(k-1)$, $u_2(k-3)\times u_3(k-4)$.

C. Quantile NARMAX Models

This study innovatively combines quantile regression with NARMAX methods, aiming to exploit the power of NARMAX for nonlinear system identification and make use of the strength of quantile regression, so as to create a new modelling framework for better understanding, analyzing and forecasting dynamic space weather processes. The implementation procedure of Q-NARMAX is as follows:

1) Identify a NARMAX model; assume the model contains a total of m model terms, denoted by $\phi_1(k),\phi_2(k),\ldots,\phi_m(k)$, each term is formed by one or more candidate model input variables;
2) Choose a number of quantiles, τ_i (i =1, 2, …, I). For each of them, estimate a regression model of the form:

$$y^{(i)}(k) = \beta_0^{(i)} + \beta_1^{(i)}\phi_1(k) + \ldots + \beta_m^{(i)}\phi_m(k) \qquad (5)$$

3) Analyze the patterns of the m coefficients, and exploit and extract useful information from the coefficients;
4) Make prediction using each of these I quantile regression models;
5) The model prediction can be defined as an ensemble of the I prediction time series (e.g. weighted sum);
6) Define prediction uncertainty intervals using the I prediction time series.

III. A Case Study: Dst Index Prediction

In this section, the proposed Q-NARMAX method is applied to Dst index data. A total of five geomagnetic field and solar wind indices or factors are chosen to be the candidate drivers. These drivers are: solar wind speed, V (unit: km s^{-1}), solar wind density (Nsw, unit: cm^{-3}), solar wind pressure (Psw, unit: nPa), together with two derived variables: the root of Psw, that is $(Psw)^{1/2}$, and the toroidal magnetic field parameter, Bst (unit: nT). Some of these candidate drivers may not be important or useful for predicting the Dst index; we let the NARMAX method to detect and choose the most important ones and decide which ones should be included in the final models.

A. Data Used

The data measured in 2015 are used in this paper. Of the 8760 hourly recorded samples, the first 3624 (measured in the first 5 months) are used for model training, and the remaining 5136 samples are used for testing model performance. The measurements of these input and output variables are obtained from the OMNIweb and the NGDC website (see the Acknowledgment section for details).

B. The Identified NARMAX Model

This study concerned with 1-hour ahead prediction of Dst index. A total of five drivers (input variables) are considered, namely, u_1 = V, u_2 = Bst, u_3 = Nsw, u_4 = Psw, $u_5 = [\text{Psw}]^{1/2}$.

A total of 30 lagged candidate input variables are used to build the best model for estimating the value of Dst(k): V($k-d$), Bst($k-d$), Nsw($k-d$), Psw($k-d$), $[\text{Psw}(k-d)]^{1/2}$, with d =1, 2, …,6.

With the total of 30 candidate lagged input variables, using the FROLS+ERR+CE algorithm, together with the Bayesian information criterion (BIC), the identified model consisting of 7 regressors (model terms) is obtained as follows:

$$\left.\begin{aligned}\text{Dst}(k) &= \beta_1\phi_1(k) + \beta_2\phi_2(k) + \ldots + \beta_7\phi_7(k)\\ &= 3.9004 + 0.9152\text{Dst}(k-1)\\ &\quad -7.9257\text{V}(k-1) - 0.6187\text{Bst}(k-1)\\ &\quad -0.6046\,\text{Bst}(k-1)\sqrt{\text{Psw}(k-1)}\\ &\quad +0.5013\,\text{Bst}(k-3)\sqrt{\text{Psw}(k-1)}\\ &\quad -0.4387\text{V}(k-3)\text{Bst}(k-3)\sqrt{\text{Psw}(k-3)}\end{aligned}\right\} \qquad (6)$$

From (6), it can be noted that not all the initially selected 30 candidates are important for explaining the variation of the Dst index; those that are not or less important are not selected by the model selection algorithms. In this way, the obtained model is not only transparent but also parsimonious and sparse.

C. The Quantile-NARMAX Models

By setting the regression quantiles τ =0.1, 0.2, …, 0.9, the 7 model terms in (6) are used to build a total of 9 Q-NARMAX models of the form (5). In order to observe the change patterns of these 9 regressors and investigate how each of the regressors influences the variation of the Dst index, the plots of the 7 coefficients at the 9 quantiles are shown in Fig. 1.

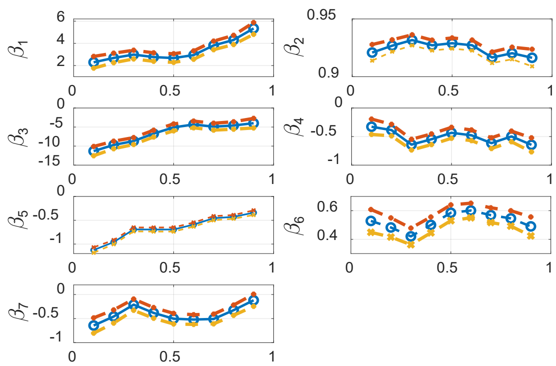

Fig. 1. Plots of the 7 Q-NARMAX model coefficients against the 9 regression quantiles (τ =0.1, 0.2, …, 0.9). The three horizontal parallel lines represent the model parameter estimates in the ordinary linear least squares sense, and the lower and upper 95% confidence intervals.

It can be observed from Fig. 1 that all the 7 Q-NARMAX coefficients vary with the change of the regression quantile τ. The change in a regression coefficient reflects the role or significance of the corresponding regressor (variable) in representing the variation of the Dst index at different quantiles.

For example, the second coefficient β_2 changes mildly with τ, and this has two implications: 1) the autoregressive variable, Dst(k−1) is important for predicting the variation in Dst(k) throughout all the quantiles, although the significance of the regression in predicting the response values in the lower and upper quantile bands is slightly different; 2) the regressor Dst(k−1) always makes "positive" contribution to the variation of Dst(k) in all the quantile bands. In other words, an increase in Dst(k−1) could very likely lead to an increase in Dst(k) and vice versa.

The pattern of the third and fifth coefficients, β_3 and β_5, are very similar, showing that the variable V(k−1) and the cross-product term Bst(k−1)[Psw(k−1)]$^{1/2}$ both make "negative" contribution to the increase/decrease of Dst(k): an increase in V(k−1) or Bst(k−1)[Psw(k−1)]$^{1/2}$ will lead to a decrease in Dst(k) and vice versa. An interesting finding is that their contributions are strong in low quantiles (corresponding severe and strong storms in this study) but gradually become weak in high quantile band (corresponding to weak or very weak storms).

The coefficients β_4, β_6 and β_7 show a common interesting pattern at $\tau = 0.3$ (roughly corresponding to Dst ≤ -20nT for the training data considered in this study); the reason behind this patter is not clear to us.

D. Prediction Confidence Interval

This section proposes an approach on how to establish a prediction uncertainty over a test dataset using the Q-NARMAX models.

The prediction confidence interval, over a test dataset, calculated from the nine Q-NARMAX models are as follows:

1) Separately perform prediction using each of the nine Q-NARMAX models;
2) Choose the prediction from the model at τ =0.1 as the lower bound, and the prediction of from the model at τ =0.9 as the upper bound, define the τ[0.1, 0.9] prediction confidence interval;
3) Compute the averaged prediction of the 9 prediction time series. Use the averaged quantile regression prediction as a reference for Dst index prediction.

As an example, the τ[0.1, 0.9] prediction confidence interval for the test period, days 172 – 175 of 2015, are shown in Fig. 2.

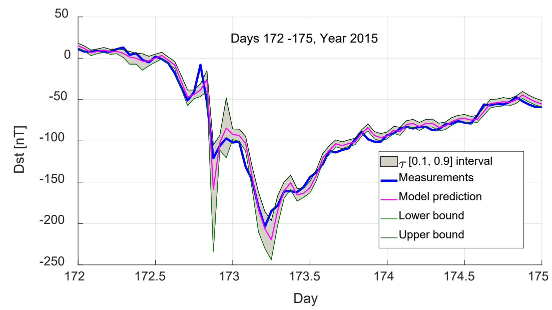

Fig. 2. The weighted model prediction and the τ[0.1, 0.9] prediction confidence interval, over the test period of days 172 – 175, 2015.

E. Prediction Performance Analysis

To evaluate the prediction performance of the proposed method, the averaged prediction values from the 9 Q-NARMAX models are compared with the corresponding measurements of Dst index. The following two common metrics are used to measure the prediction performance.

- R-squared coefficient (coefficient of determination).

$$R^2 = 1 - \frac{\sum_{y(k)\in\Gamma} [y(k) - \hat{y}(k)]^2}{\sum_{y(k)\in\Gamma} [y(k) - \bar{y}]^2} \quad (7)$$

- Mean Absolute Error

$$MAE = \frac{1}{K} \sum_{y(t)\in\Gamma} | y(t) - \hat{y}(t) | \quad (8)$$

- Root Mean Square Error

$$RMSE = \sqrt{\frac{1}{K} \sum_{y(k)\in\Gamma} [y(k) - \hat{y}(k)]^2} \quad (9)$$

where the symbol 'Γ' denote a test dataset consisting of a total of K samples, $y(k)$ is the measurements at the time instant k, $\hat{y}(k)$ represents the model prediction values, and $\bar{y}$ is the mean value. Note that there is certain equivalent between the coefficient of R-squared and other commonly used metrics, e.g., prediction efficiency (PE), variance of accounted for (VAF).

For the test period of days 172-175 of 2015 shown in Fig. 2, the values of R^2, MAE and RMSE are 0.9620, 6.4538 and 9.7783, respectively. These values confirm the excellent performance of the proposed Q-NARMAX method for strong and severe storm predictions.

Finally, for more information, the scatter plot between the model predictions and the true values, over the test period of days 172 – 175 of 2015, is shown in Fig. 3.

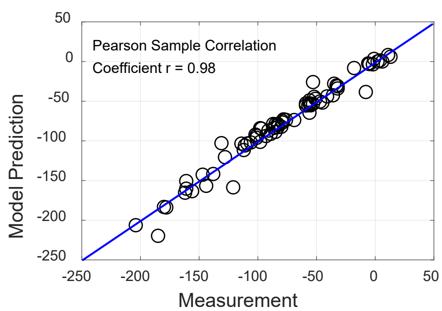

Fig. 3. The scatter plot between the model predictions and the true values, over the test period of days 172 – 175, 2015.

IV. Discussiosns

As mentioned earlier, the proposed method has several attractive features and advantages, for example: 1) the resulting models are transparent, parsimonious and simulatable; 2) using transparent models to approximate and represent black-box systems makes it easier to interpret the dependent relationship between space weather indices and their drivers; 3) the resulting models can be written down, so end-users can see how the desired response is related to the individual predictors and their interactions; and 4) model parameters are estimated using quantile regression algorithm, enabling the model to fit the conditional medians of the target response data, rather than the conditional mean of the data, as considered in traditional data based modelling approaches.

The last property above is useful for understanding and interpreting how the change of the system behaviour, at different quantiles of data distribution, is related to system input signals (drivers). It is also important and useful for assessing uncertainties in model based prediction. The proposed uncertainty evaluation procedure is as follows. Firstly, to identify a set of best model structures using nonlinear system identification techniques. Secondly, to estimate model parameters each of these model structures at a number of different quantiles of data distribution (say quantiles from 0.1 to 0.9. Thirdly, to make predictions using all the models with different quantiles. Finally, to ensemble the predictions form all the models, and calculate the quantile confidence intervals of interest and the mean or median of the prediction values.

Nevertheless, the overall performance of the proposed methods has not yet been comprehensively evaluated; more needs to be done to explore the advantages of the new method and to reveal its potential deficiencies and limitations as well. Based on our experience from the present work and our other related studies so far, we have the following comments on the implementation of the proposed method, its limitations, and potential improvements.

Implementation. The proposed method combines NARMAX modelling and quantile regression. The NARMAX method does not need a large number of samples to train models. More importantly, with the efficient forward regression with orthogonal least squares (FROLS) algorithm [34], the method can effectively solve the "$p >> n$ problem", where n is the number of observations and p is the number of predictors (regressors). As the resulting models are usually parsimonious, the quantile estimation procedure can usually be completed within a short time period. So, in comparison with other machine learning methods including deep learning approaches, the computational load is much smaller.

Limitations and improvements. Unlike linear regression where the dependent relationship between response and predictors can usually be easily recognized and interpreted, nonlinear dynamic quantile regression models are relatively difficult to explain due to the inclusion of interaction terms (regressors). Further work and investigations will be carried out to better explain the Q-NARMAX models and gain deep insight into the inhere associations of processes in space weather.

V. Conclusion

The paper introduced a novel nonlinear transparent, interpretable and parsimonious modelling method, called quantile-NARMAX (Q-NARMAX), which has several attractive features. In comparison to other predictive models, Q-NARMAX has several distinctive features, for example, the integration of quantile regression into the NARMAX modelling procedure enables to better explore the distribution of the target signals (response or output variables) at different quantiles and better represent the relationship between the input and output data using many quantile models rather than only a single model. This significantly improves the prediction robustness. Moreover, the predictions corresponding to different quantiles provide useful information for assessing the prediction uncertainty. Additionally, Q-NARMAX model parameters provide a useful indication of how each model term (regressor) affects the change of the system response in each quantile of the distribution of the output signal. The last feature here will be further explored in our future work.

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