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Mathematical Optimization for Analyzing and Forecasting Nonlinear Network Time Series

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Abstract. This work presents an innovative short to mid-term forecasting model that analyzes nonlinear complex spatial and temporal dynamics in energy networks under demand and supply balance constraints using Network Nonlinear Time Series (TS) and Mathematical Programming (MP) approach. We address three challenges simultaneously, namely, the adjacency matrix is unknown; the total amount in the network has to be balanced; dependence is unnecessarily linear. We use a nonparametric approach to handle the nonlinearity and estimate the adjacency matrix under the sparsity assumption. The estimation is conducted with the Mathematical Optimisation method. We illustrate the accuracy and effectiveness of the model on the example of the natural gas transmission network of one of the largest transmission system operators (TSOs) in Germany, Open Grid Europe. The obtained results show that, especially for shorter forecasting horizons, proposed method outperforms all considered benchmark models, improving the average nMAPE for 5.1% and average RMSE for 79.6% compared to the second-best model. The model is capable to capture the nonlinear dependencies in the complex spatial-temporal network dynamics and benefits from both sparsity assumption and the demand and supply balance constraint.

Keywords: nonlinear time series, mathematical optimization, energy networks

1 Introduction

Since the EU introduced market regulations in 2005, the natural gas market is becoming increasingly competitive, moving towards short-term planning, e.g., day-ahead contracts, making the control of natural gas transmission networks even more challenging. The main task of TSOs is to fulfill all transport demands, ensuring the security of supply safely and efficiently. Since gas in the pipes travels relatively slow with an average velocity of approximately 25km/h [5], a high-precision short and mid-term forecast of supplies and demands is essential for the efficient and safe operation of the complex natural gas transmission networks and distribution systems.

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MODAL [6] with one of Germany’s largest transmission system operators, Open Grid Europe (OGE) [1]. Together with our industry partner, we develop a Network AutoRegressive Nonlinear model with a Balance constraint (NAR-NLB) model. The primary purpose of the proposed model is to provide a comprehensive understanding of the network dynamic and compute high-precision, multi-step, hourly forecasts for supply and demand nodes in the gas network. The focus is on forecasting shorter horizons (up to 8 hours is the most relevant horizon in practice) to support the daily operations of the gas network. The results are used for optimizing gas transport, for example, routing the gas with compressors or valves and finding the optimal settings for these elements [9].

2 Methodology

Let N denote the number of nodes in a large-scale complex gas transmission network, and $y_{t,i}$ is the continuous response collected from node i at time point t with $0 \leq t \leq T$ and $1 \leq i \leq N$. In the network, N nodes are connected with pipelines but the flow connection is unknown. At any time point t , the total sum of gas in-flow and out-flow in the network equals zero. To capture the network effect of the N different nodes, we propose the NAR-NLB model, where the total gas in-flows and out-flows need to be balanced. Without loss of generality, we assume the demeaned process for the gas network and write the model without the intercept term. The NAR-NLB model with lag 1 is defined as:

$$y_{t,i} = g_i\left(\sum_{j=1}^N y_{t-1,j} b_{j,i}\right) + \epsilon_{t,i}, \quad i, j = 1, \dots, N, \quad (1)$$

$$s.t. \quad \sum_{i=1}^N g_i\left(\sum_{j=1}^N y_{t-1,j} b_{j,i}\right) = 0 \text{ for all } t = 1, \dots, T,$$

where $g(\cdot)$ is an unknown link function which is assumed to be smooth. $\epsilon_{t,i}$ is a strong white noise with zero mean and finite second moment $E\|\epsilon_{t,i}\|^2 < \infty$. When $j = i$, $b_{j,i}$ controls the autoregressive dependence. When $j \neq i$, the parameter $b_{j,i}$ tells us how the j -th node influences the i -th node; that is, the network influence of the past value of the j -th node on the current value of the i -th node. If $b_{j,i} = 0$ for all the $i = 1, \dots, N$ and $i \neq j$, then the j -th node has no effect in the network. In (1), the constraint is imposed to the forecast of gas flows denoted as $\sum_{j=1}^N g(y_{t-1,j} b_{j,i})$ for a balanced demand and supply.

The model can be represented in a matrix form:

$$Y = g(ZB) + E, \quad (2)$$

$$s.t. \quad g(ZB)1_N = 0,$$

where Y is a $T \times N$ matrix of the observed gas flow values. Let $y_t = (y_{t,1}, \dots, y_{t,N})$ denote the gas values for all nodes at time point t , we then have $Y = (y_1, \dots, y_T)^T$. Z is a $T \times N$ matrix containing the past values of Y . Similarly, we have $Z =$

$(z_1, \dots, z_T)^\top$. The parameter matrix B is a $N \times N$ matrix with unknown parameters $b_{j,i}$. Given the autoregressive dependence reflected by $b_{i,i}$ for $i = 1, \dots, N$ in the diagonal elements of B , let the non-diagonal elements of matrix B define the *weighted adjacency matrix*. The column vector $B_i = (b_{1,i}, \dots, b_{N,i})^\top$ of the weighted adjacency matrix represents the influence of other nodes in the network on the future value of the i -th node. The weighted adjacency matrix is assumed to be sparse. There is, however, no prior knowledge of the sparse structure in terms of location and number of significant elements. Finally, 1_N is a unit vector and E is a $T \times N$ matrix of white noise errors.

Next, we show the estimation of the unknown nonlinear function and parametric coefficients with mathematical programming (MP). In semiparametric models, as in (1), it is popular to approximate the unknown nonlinear functions using the spline smoothing approach, see [2]. We apply this technique for estimating the nonlinear link function $g(\cdot)$ for a given parameter value B using B-splines, or so-called basis splines [3]. We estimate the unknown coefficient matrix by applying the feature selection technique developed by [4] for the weighted adjacency matrix, with additional balance constraints for the demand and supply as follows.

$$\begin{aligned}
 & \min_B \sum_{t=1}^T \sum_{i=1}^N (y_{t,i} - Z_t B_i)^2 \\
 & \text{s.t.} \quad \|B_i\|_0 \leq L \quad \text{for } i = 1, \dots, N \\
 & \quad \sum_{i=1}^N Z_t B_i = 0, \quad \text{for } t = 1, \dots, T
 \end{aligned} \tag{3}$$

where the upper bound L for l_0 -norm of a column vector B_i given by

$$\sum_{j=1}^N 1(b_{j,i} \neq 0)$$

ensures the number of nonzeros in B_i to be less than integer L , where $j \neq i$ and $1(\cdot)$ denotes the indicator function. We use the estimated coefficient matrix \hat{B}_i for $i = 1, \dots, N$ to approximate the unknown nonlinear function $g(\cdot)$ using the B-spline interpolation [2]. To estimate the function, the B-spline requires the hyperparameters such as knots, spline coefficients, and degree of a spline.

$$B_{k,m}(\theta) = \frac{\theta - \theta_k}{\theta_{k+m} - \theta_k} B_{k,m-1}(\theta) + \frac{\theta_{k+m+1} - \theta}{\theta_{k+m+1} - \theta_{k+1}} B_{k+1,m-1}(\theta), \tag{4}$$

$$B_{k,0}(\theta) = \begin{cases} 1, & \text{if } \theta_k \leq \theta < \theta_{k+1} \\ 0, & \text{otherwise} \end{cases} .$$

Finally, we estimate the B-spline coefficients $\alpha_{k,i}$ with MP.

$$\min_{\alpha_{k,i}} \sum_{t=1}^T \sum_{i=1}^N (y_{t,i} - \sum_{j=1}^N \sum_{k=0}^{P_k} \alpha_{k,i} B_{k,m}(Z_t \hat{B}_i))^2, \quad i = 1, \dots, N, \tag{5}$$

3 Experimental setup

In this paper, we study the nonlinear dependencies and dynamic patterns of natural gas flows in the high-pressure gas pipeline network of OGE [1]. The

dataset consists of demand and supply nodes with an hourly time resolution for a period of one year. To demonstrate the effectiveness of the proposed model, we consider a small network of one supply (S1) and four demand nodes (D1-D4). Figure 1 illustrates the temporal dependence among the five observed nodes. As it can be seen in the diagonal, there is a strong positive autocorrelation of each node with its own past values, while off the diagonal, the cross-correlations represent the dynamic temporal dependency among different nodes.

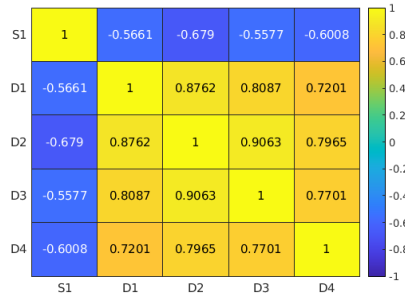


Fig. 1: Sample cross-correlation heatmap for one supply and four demand nodes in gas network.

We calculate an out-of-sample forecast in real time starting from 05:00 and predict 1 to 24 hours ahead forecast. Multi-step forecasts are made for the next day, for a total of 3 months. We use the training-validation technique to choose optimal hyperparameters in the NAR-NLB model for the sparsity estimation, spline order and number of knots. With the chosen parameters, we estimate the weighted adjacency matrix B at each point by training the model on the past seven days of balanced network data. With a rolling window size of 168 hours (i.e., seven days), we move forward one period at a time to update the sparse adjacency matrix and then forecast until we reach the end of the sample.

In order to evaluate the quality of the obtained results, we compare the performance of NAR-NLB model with well-known benchmarks: Baseline forecast (repeating value for the same hour of the previous day) and ARIMA as well as with Network Autoregressive Linear model with Balance constraint (NAR-LB) proposed by Zakiyeva and Petkovic in [8]. We determine the best ARIMA models for a univariate time series of five considered nodes according to an Akaike information criterion (AIC) using 28 days of the rolling window. The setup for NAR-LB model is identical to the proposed model. The performance of NAR-NLB model is measured and quantified by calculating the forecast accuracy for individual nodes, as well as the mean for the entire network. We use mean daily root mean squared error (RMSE) and mean daily normalized mean absolute percentage error (nMAPE) defined as:

$$RMSE = \frac{\sum_{d \in D_{test}} \sqrt{\frac{1}{H} \sum_{h=0}^{H-1} (q_{d,h} - \hat{q}_{d,h})^2}}{|D_{test}|},$$

$$nMAPE = \frac{\sum_{d \in D_{test}} \left(\frac{100\%}{H} \sum_{h=0}^{H-1} \left| \frac{q_{d,h} - \hat{q}_{d,h}}{\max(q)} \right| \right)}{|D_{test}|},$$

where $q_{d,h}$ and $\hat{q}_{d,h}$ are the real and forecasted values of the natural gas flows on day d and hour h while H is a forecasting horizon.

4 Results

We demonstrate the multistep-ahead out-of-sample forecasting results in a balanced network. Table 1 shows an average $RMSE$ and $nMAPE$ for three different forecasting horizons (1h, 12h and 24h ahead) comparing to the alternative models for five gas nodes of the balanced network. The results show that NAR-NLB consistently outperforms all benchmark models. It can be noted that the difference is the smallest between NAR-LB and NAR-NLB models, which strongly indicates that using the network dynamic information as well as balancing constraint benefits the forecasting accuracy.

For shorter horizon, the NAR-NLB performs as the most accurate forecast model with the smallest forecast errors. This illustrates that modeling the nonlinear network dynamics improves the average forecast errors of the NAR-LB model from RMSE 6.294 and nMAPE 13.4% to RMSE 4.293 and nMAPE 1%. The difference in prediction performance with NAR-NLB is most significant for the shorter horizons, where nMAPE is improved for 5.1% and RMSE for 79.6% compared to the second best alternative model (ARIMA). As for the longer horizons (12h), NAR-NLB performs similar to NAR-LB model with the improvement of nMAPE by 1.4%. Similarly, for 24 hours ahead forecast, NAR-NLB provides similar second-best accurate prediction as the BAS with a difference of nMAPE around 0.01%. Note that for calculating multi-step ahead forecast we are using recursive strategy, which can lead to accumulation of errors for longer horizons. The obtained results clearly show that proposed model benefits from modeling nonlinear temporal dependencies in the network.

H	RMSE				nMAPE			
	NAR-NLB	BAS	ARIMA	NAR-LB	NAR-NLB	BAS	ARIMA	NAR-LB
1	4.293	46.178	21.049	6.294	1%	14.3%	6.1%	13.4%
12	3.804	48.002	50.585	42.671	8.5%	13.1%	12.1%	9.9%
24	60.268	48.494	69.978	68.420	13.2%	13.1%	15.77%	14.2%

Table 1: Comparison of the NAR-NLB model and the alternative time series models on multi step-ahead gas flow forecasts at five nodes in a balanced network.

By taking into account both nonlinear dynamics and sparse dependent structure, the NAR-NLB model provides superior performance compared to the three

alternative predictive models. The NAR-NLB is able to capture the nonlinear dependencies in the complex spatial-temporal network dynamics. It improves out-of-sample forecast accuracy of individual nodes and consequently, there are fewer balancing errors in the network. Furthermore, the estimated adjacency matrix in NAR-NLB provides additional information on the cross-dependencies between the nodes, which shows the influential nodes that drive the network dynamics. In summary, it is useful to introduce both the nonlinearity and sparsity assumption together with the demand and supply balance constraint for accurate and stable forecasts in energy networks.

5 Conclusion

In this paper, we propose a network autoregression nonlinear model with balance constraint for robust short to mid-term forecasting and analyzing nonlinear complex spatial and temporal dynamics in energy networks under demand and supply constraints. The results show that the proposed model consistently outperforms the alternative models, improving the nMAPE by up to 5.1% compared to the second-best benchmark model, benefiting from modeling nonlinear dependencies between different nodes in the network and from implying balancing constraints on demand and supply.

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