Multivariate Time Series Forecasting with NBEATS

Thesis Defence

Philip Kurzendörfer

Supervisors
Lars Schmidt-Thieme
Rafael Rêgo Drumond

University of Hildesheim, ISMLL

January 25, 2022

Outline

Introduction

- Predicting the future relevant task
- e.g. in business world: Optimize decision making
- Real-world applications often require the forecasting of multiple related time series
- Relevance in demand forecasting or stock price forecasting.
- Capturing dynamics between time series

Introduction

- N-BEATS published in ICLR 2020
- State-of-art in univariate time series forecasting (M3, M4, TOURISM) [7]
- Normalizing flow conditioned on transformer model [8]
- Published in ICLR 2021
- State-of-art in multivariate time series forecasting on data sets used in this thesis

Introduction

Research Question

- If and how N-BEATS can be extended for multivariate time series (M-N-BEATS)

Contributions

(i) Naive approach of multivariate N-BEATS

(ii) Next, M-N-BEATS, adjusts vanilla N-BEATS architecture at block level

(iii) M-N-BEATS is combined with a normalizing flow model

Related Work

Univariate Time Series Forecasting

Classical Statistical Approaches

- Based on exponential smoothing and moving averages
- AR, MA, ARMA, ARIMA, VAR

Hybrid Approaches

- Statistical + machine learning
- Ensebmles
- For example LSTM stack with a classical Holt-Winters statistical model [4]

Pure Machine Learning Approaches

- N-BEATS
- LSTM, CONV, Transformer etc.

Related Work

Univariate Time Series Forecasting

Where is machine learning so far (Univariate TS)

- LSTM+Holt-Winters won M4 challenge in 2020 [10]
- Best "pure" machine learning method was on rank 23 out of 60 [6]
- N-BEATS achieves better results than winner of M3 and M4 challenges

Related Work

Notation and Problem Formulation I

- Time series $\mathbf{x} \in \mathbb{R}^S$
- $\mathbf{x} = (x_1, x_2, \cdots, x_S)^T$
- Equally spaced time series
- Forecasts of the next consecutive H future values $\mathbf{y} \in \mathbb{R}^H$
- $\mathbf{y} = (y_1, y_2, \cdots, y_H)^T$

Related Work

Notation and Problem Formulation II

- Multivariate time series $\mathbf{X} \in \mathbb{R}^{S \times D}$
- $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_S)^T$
- $\mathbf{x}_i$ is a D-dimensional vector
- Forecast the next H consecutive future values $\mathbf{Y} = (\mathbf{y}_1, \mathbf{y}_2, \cdots, \mathbf{y}_T)^T$
- $\widehat{\mathbf{Y}} \in \mathbb{R}^{H \times D}$, $\widehat{\mathbf{Y}} = (\widehat{\mathbf{y}}_1, \widehat{\mathbf{y}}_2, \cdots, \widehat{\mathbf{y}}_H)^T$

Related Work

N-BEATS

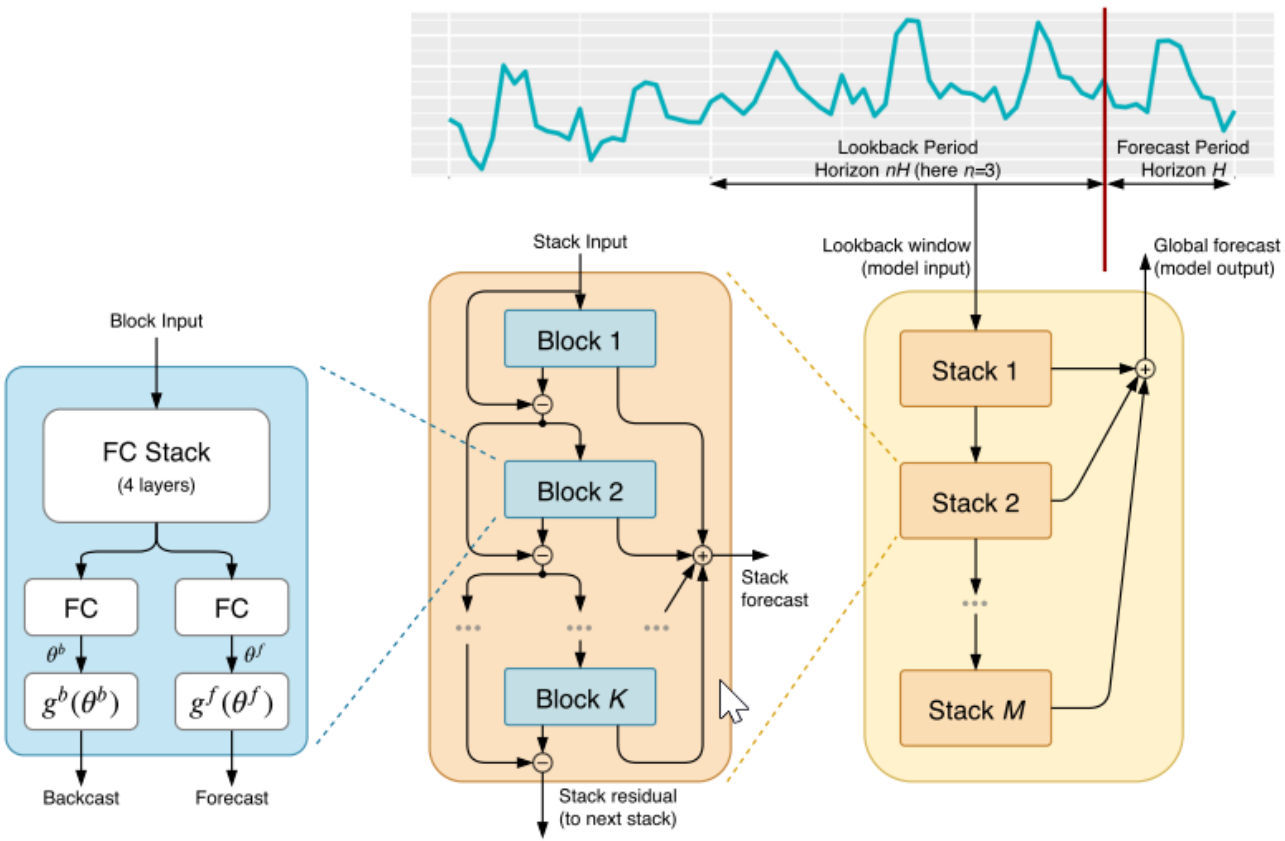


Figure 1: N-BEATS architecture.
source: [7].

Related Work

N-BEATS

Given block ℓ

- Basis parameters $\boldsymbol{\theta}_\ell^b$ and $\boldsymbol{\theta}_\ell^f$
- Using the basis function g
- Forecast $\widehat{\mathbf{y}}_\ell = g_\ell^f\left(\theta_\ell^f\right)$
- Backcast $\widehat{\mathbf{x}}_\ell = g_\ell^b\left(\theta_\ell^b\right)$

Related Work

N-BEATS

Basis function g is given by

$$g_\ell^f\left(\theta_\ell^f\right) = \widehat{\mathbf{y}}_\ell = \mathbf{V}_\ell^f \boldsymbol{\theta}_\ell^f, \quad g_\ell^b\left(\theta_\ell^b\right) = \widehat{\mathbf{x}}_\ell = \mathbf{V}_\ell^b \theta_\ell^b \tag{1}$$

with the basis $\mathbf{V}_\ell^f \in \mathbb{R}^{H \times dim(\theta^f)}$ and $\mathbf{V}_\ell^b \in \mathbb{R}^{S \times dim(\theta^b)}$.

Related Work

N-BEATS

- Basis vectors $\mathbf{V}$ can be learnable parameters (generic variant)
- Can be fixed introducing an inductive bias (interpretable variant)
- Standard basis

Related Work

N-BEATS

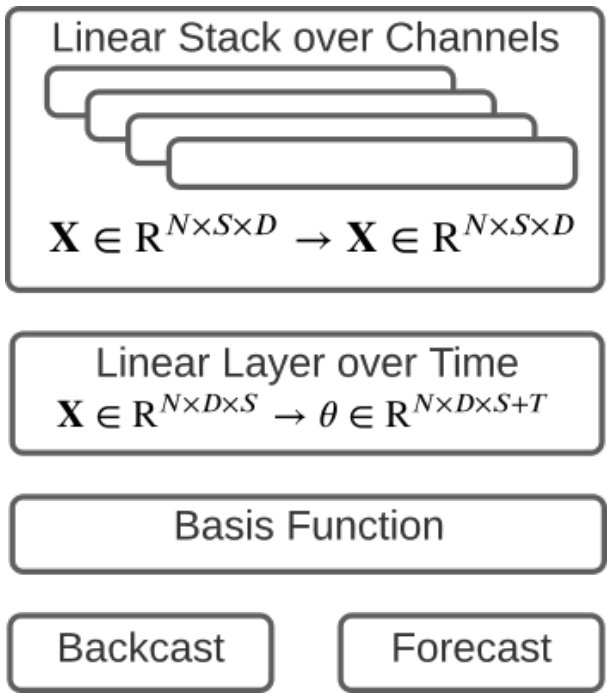
Blocks are connected with so called Doubly residual connections defined by

$$\mathbf{x}_\ell = \mathbf{x}_{\ell-1} - \widehat{\mathbf{x}}_{\ell-1}, \quad \widehat{\mathbf{y}} = \sum_\ell \widehat{\mathbf{y}}_\ell \tag{2}$$

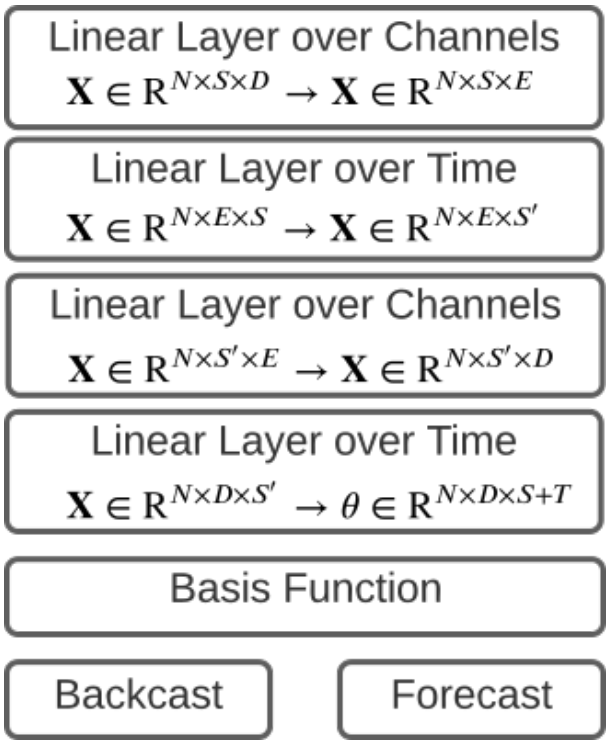
- $\mathbf{x}_\ell$ block input of block ℓ
- $\mathbf{x}_{\ell-1}$ block input of block $\ell - 1$
- $\widehat{\mathbf{x}}_{\ell-1}$ is the block forecast block $\ell - 1$

Methodology

M-N-BEATS Blocks



(a) *Simple Block*, N is the batch size, S is the sequence length and D is the number of time series.

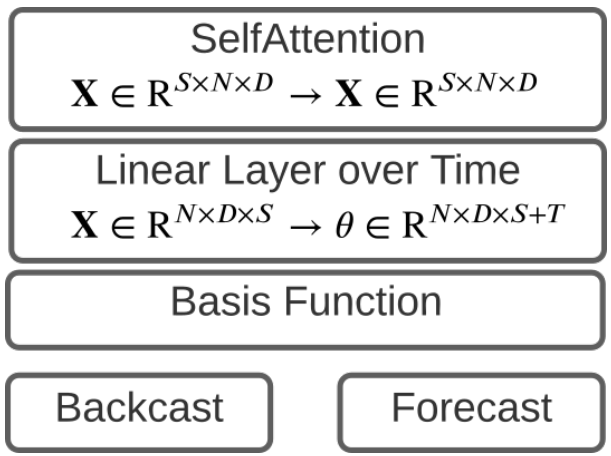


(b) *Linear Block*, N is the batch size, S is the sequence length and D is the number of time series.

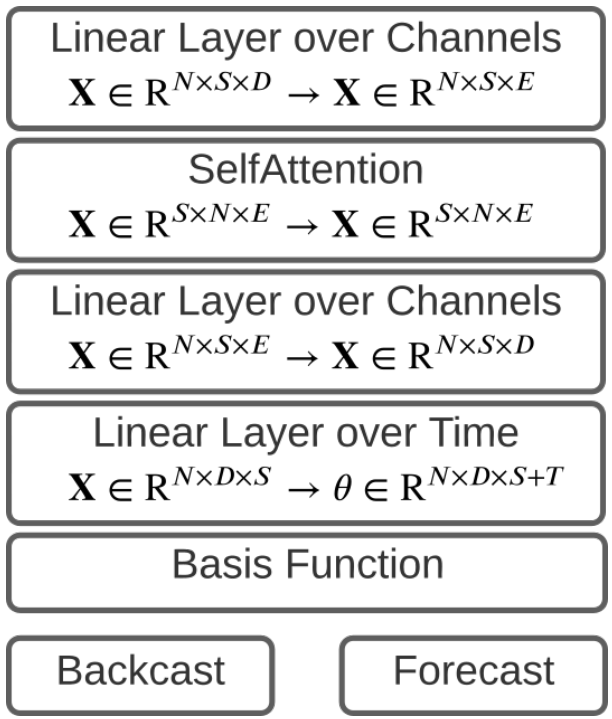
Figure 2: Multivariate N-BEATS blocks using linear layers.

Methodology

M-N-BEATS Blocks



(a) *Attention Block*, N is the batch size, S is the sequence length and D is the number of time series.

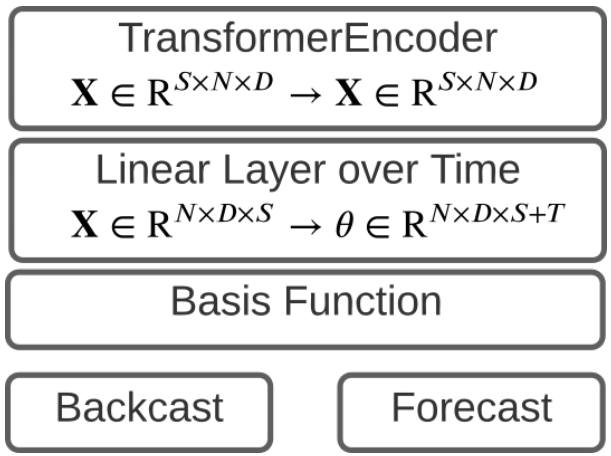


(b) *Linear Attention Block*, N is the batch size, S is the sequence length and D is the number of time series.

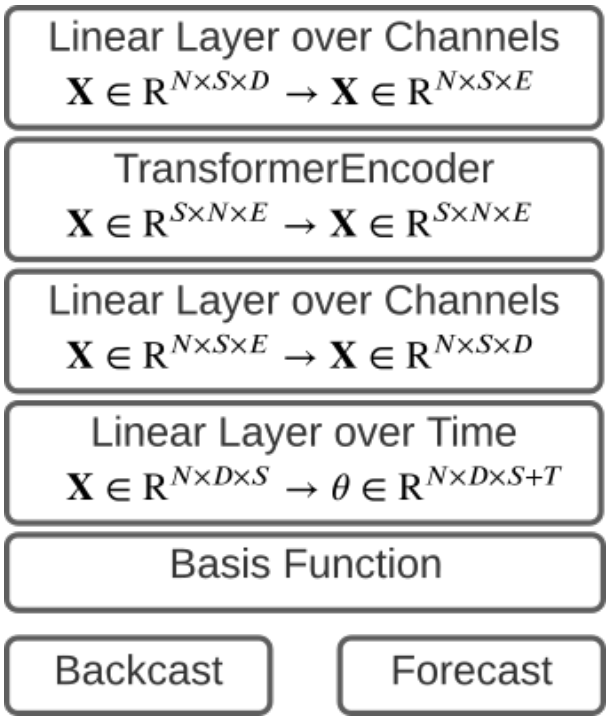
Figure 3: Multivariate N-BEATS blocks using attention module.

Methodology

M-N-BEATS Blocks



(a) *Transformer Block*, N is the batch size, S is the sequence length and D is the number of time series.

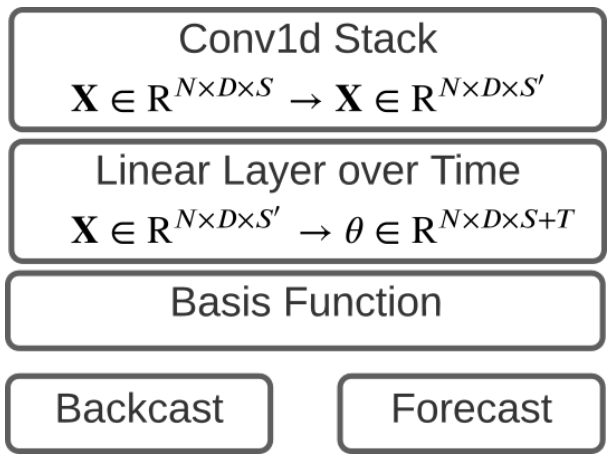


(b) *Linear Transformer Block*, N is the batch size, S is the sequence length and D is the number of time series.

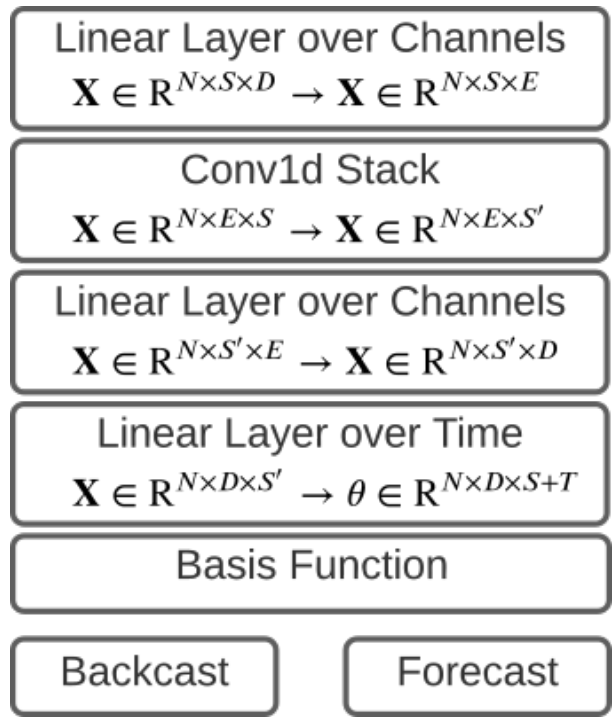
Figure 4: Multivariate N-BEATS blocks using transformer encoder layer.

Methodology

M-N-BEATS Blocks



(a) *Conv Block*, N is the batch size, S is the sequence length and D is the number of time series.



(b) *Linear Conv Block*, N is the batch size, S is the sequence length and D is the number of time series.

Figure 5: Multivariate N-BEATS blocks using convolutional layers.

Methodology

Normalizing Flow

- RV Z with simple base distribution $p_{\mathcal{Z}}$
- Transform the simple distribution into a more complex target distribution $p_{\mathcal{X}}$
- Mapping $f : \mathcal{X} \mapsto \mathcal{Z}$
- $z = f(x) = f_K \circ \ldots \circ f_2 \circ f_1(x)$
- f is a composition of bijections or invertible functions (transformations)
- for any x there is exactly one z that could have been sampled to produce x
- By applying $\mathbf{x} = f^{-1}(\mathbf{z})$
- should be easy to compute

Methodology

Normalizing Flow

- Apply change of variable formula
- Target distribution of X can be expressed in terms of the known base distribution $p_{\mathcal{Z}}$ and the Jacobian matrix of $f(\mathbf{x})$

$$p_{\mathcal{X}}(\mathbf{x}) = p_{\mathcal{Z}}(\mathbf{z}) \left| \det \left(\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right) \right| = p_{\mathcal{Z}}(\mathbf{z}) \left| \det \left(\frac{\partial f^{-1}(\mathbf{z})}{\partial \mathbf{z}} \right) \right|^{-1} \quad (3)$$

Methodology

Normalizing Flow

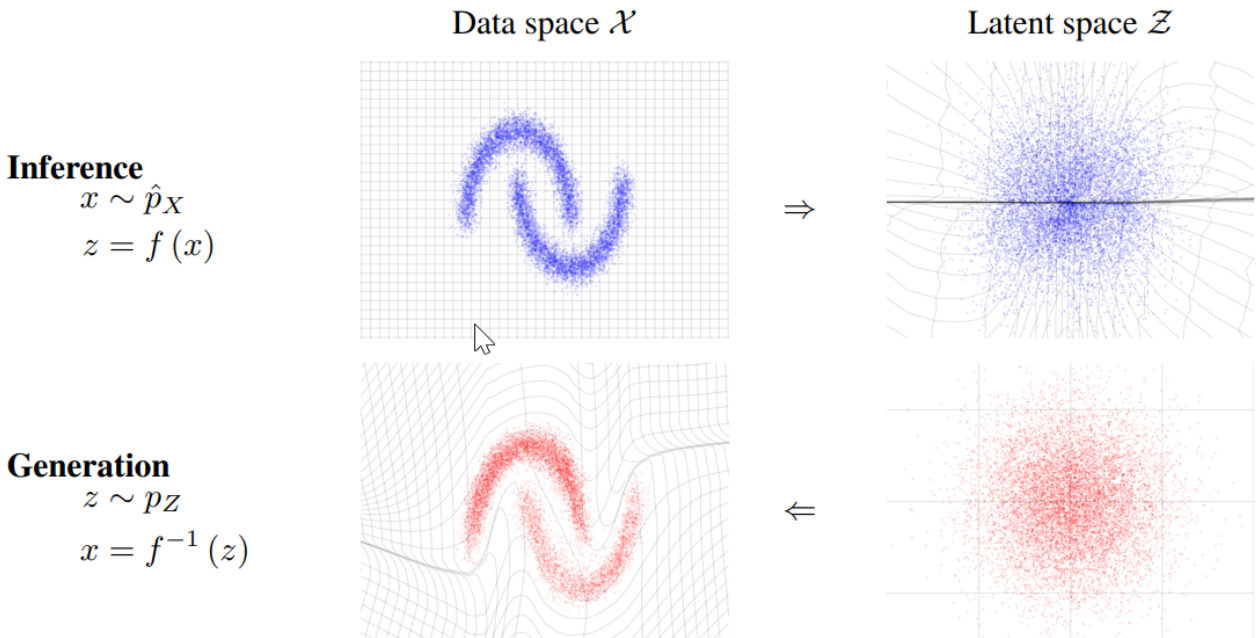


Figure 6: Normalizing Flow, RealNVP mapping learned on toy dataset. Source: [1].

Experiments

Proposed Models and Baselines

- N-BEATS-Naive
- M-N-BEATS
- M-N-BEATS-Flow
- Transformer+Flow [8]
- LSTM+Flow [8]
- GP-Copula [9]

Experiments

Loss Functions

sMAPE for single time series

$$\text{sMAPE} = \frac{200}{H} \sum_{i=1}^{H} \frac{|y_{T+i} - \widehat{y}_{T+i}|}{|y_{T+i}| + |\widehat{y}_{T+i}|} \tag{4}$$

- y_{T+i} is the target value
- $\widehat{y}_{T+i}$ is the forecast for a single time step of a single time series
- For multivariate time series, mean of sMAPE of all channels

Experiments

Loss Functions

M-N-BEATS-Flow

- Maximize the average log likelihood

$$\mathcal{L} = \frac{1}{|\mathcal{D}|\,T} \sum_{\mathbf{x}_{1:T} \in \mathcal{D}} \sum_{t=1}^{T} \log p_{\mathcal{X}} \left(\mathbf{x}_t \mid \mathbf{h}_t; \theta \right) \tag{5}$$

Experiments

Metrics

- Mean Squared Error (MSE)
- Continuous Ranked Probability Score ($CRPS$)
- $CRPS_{sum}$

$$MSE(\mathbf{Y}, \widehat{\mathbf{Y}}) = \left\| \mathbf{Y} - \widehat{\mathbf{Y}} \right\|_F^2 \tag{6}$$

where $\|\cdot\|_F$ is the Frobenius norm.

Experiments

Metrics

CRPS for a given fixed data point x at time step t is given as

$$\mathrm{CRPS}(F, x) = \int_{\mathbb{R}} (F(z) - \mathbb{I}\{x \leq z\})^2 \, \mathrm{d}z \tag{7}$$

- $\mathbb{I}\{x \leq z\})^2$ is 1 if $x \leq z$ and 0 otherwise
- Measures how good the approximated distribution compares to the data using the CDF F
- Forecast CDF can be approximated with empirical CDF

$$F(z) = \mathbf{P}[X \leq z] \qquad \hat{F}(z) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}\{X_i \leq z\} \tag{8}$$

Experiments

Metrics

$CRPS_{sum}$ for a single time step t is given by

$$\mathrm{CRPS}_{\mathrm{sum}} = \mathbb{E}_t \left[\mathrm{CRPS} \left(\hat{F}_{\mathrm{sum}}(t), \sum_{i=0}^{D} x_t^i \right) \right] \tag{9}$$

- $\hat{F}_{\mathrm{sum}}(t)$ is computed by summing up the individual $\hat{F}$ over all D time series

Experiments

Data Sets

Table 4.1: Data Set Description

DATA SET	DIMENSION D	DOMAIN	FREQ.	TOTAL TIME STEPS	PREDICTION LENGTH
Exchange	8	$\mathbb{R}^+$	DAILY	6, 071	30
Solar	137	$\mathbb{R}^+$	HOURLY	7, 009	24
Electricity	370	$\mathbb{R}^+$	HOURLY	5, 790	24
Traffic	963	(0, 1)	HOURLY	10, 413	24

Source: [Rasul et al., 2021], [Salinas et al., 2019]

Experiments

Data Pipeline

Additional features

- Static features (Channel index as embedding, repeated along time)
- Time dependent features (**day of week**)
- Lagged time series

Experiments

Data Pipeline

Scaling

- Magnitudes of time series differ strongly
- Divide each time series by its training window mean
- Target divided by the same factor
- After training for data generation, the output distribution is multiplied by the same factor.

Experiments

Data Pipeline

Train test split and sampling

- Official train test splits are available
- The training set is split into train and validation set (70%)

Experiments

N-BEATS-Naive

- Flattening the multivariate input into a very long one-dimensional vector
- Apply vanilla N-BEATS
- Mean Results of 10 runs are reported
- Results are not competitive (see Appendix)

Experiments

N-BEATS-Naive

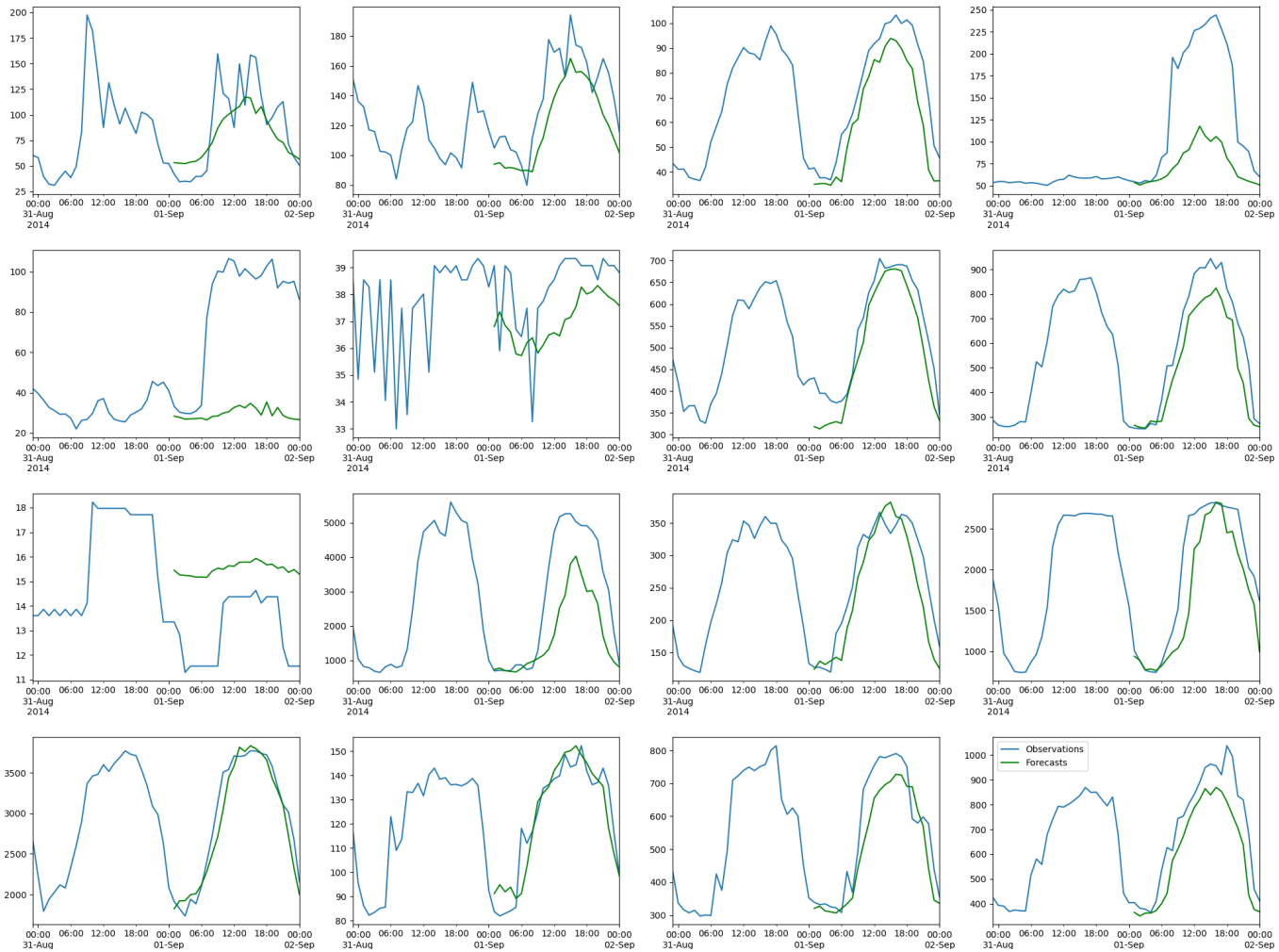


Figure 7: Forecasts produced by N-BEATS-Naive on the *Electricity* data set, only the forecasts of a single run are plotted.

Experiments

Hyperparameter Search

- M-N-BEATS
- M-N-BEATS-Flow
- Linear-Attention Block
- Linear-Transformer Block

Learning Rate	[0.0001, 0.00001]
Number of Blocks	[3, 5, 10]
Attention Heads	[4, 8]
Attention Embedding Size	[32, 64, 28]
Flow Type	[RealNVP, MAF]

Table 1: Hyperparameter Grid. Flow Type only applies for M-N-BEATS-Flow. The same grid has been applied for each data set independently.

Experiments

Main Results

- Best Model from HP-search is trained 10 times
- Average and standard deviation metrics on test set are reported
- For M-N-BEATS and M-N-BEATS-Flow, linear-transformer-block performed better

Experiments

Main Results Baseline Comparison

MSE

Data Set	GP-Copula	LSTM-RealNVP	LSTM-MAF	Transformer-MAF	M-N-BEATS-Flow (Transformer)
Electricity	240,000±55,000	250,000	**180,000**	200,000	**155,810±26,344**
Traffic	0.00069±0.000022	0.00069	**0.00049**	0.00050	**0.00045±0.0000**
Solar	980±52	**910**	980	930	**925±41**
Exchange	**0.00017±0.000016**	0.00024	0.00038	0.00034	**0.000174±0.0000**

Table 2: *MSE* for baseline methods, M-N-BEATS-Flow with *Linear-Transformer-Block*. For methods proposed in this thesis mean and standard deviation of 10 runs is reported. Results for GP-Copula are taken from [9], mean and standard deviation of 3 runs are reported. For models proposed in [8] results were taken from the paper, mean and standard deviation of a single run are reported. Two best methods are in bold.

Experiments

Main Results Baseline Comparison

CRPS

Data Set	GP-Copula	LSTM-RealNVP	LSTM-MAF	Transformer-MAF	M-N-BEATS-Flow (Transformer)
Electricity	0.056±0.002	0.059±0.001	**0.051±0.000**	0.052±0.000	**0.0511±0.0019**
Traffic	0.133±0.001	0.172±0.001	0.124±0.002	0.134±0.001	**0.1148±0.0039**
Solar	0.371±0.022	**0.365±0.02**	0.378±0.032	**0.368±0.001**	0.3829±0.0104
Exchange	**0.008±0.000**	0.010±0.001	0.012±0.003	0.012±0.003	**0.0092±0.0001**

Table 3: *CRPS* for baseline methods, M-N-BEATS-Flow with *Linear-Transformer-Block*. For methods proposed in this thesis mean and standard deviation of 10 runs is reported. Results for GP-Copula are taken from [9], mean and standard deviation of 3 runs are reported. For models proposed in [8] results were taken from the paper, mean and standard deviation of a single run are reported. Two best methods are in bold.

Experiments

Main Results Baseline Comparison

$CRPS_{sum}$

Data Set	GP-Copula	LSTM-RealNVP	LSTM-MAF	Transformer-MAF	M-N-BEATS-Flow (Transformer)
Electricity	0.024±0.002	0.024±0.001	**0.0208±0.000**	**0.0207±0.000**	0.0223±0.0021
Traffic	0.078±0.002	0.078±0.001	0.069±0.002	**0.056±0.001**	**0.0485±0.0049**
Solar	0.337±0.024	0.331±0.02	**0.315±0.023**	**0.301±0.014**	0.3289±0.0124
Exchange	0.007±0.000	0.0064±0.003	**0.005±0.003**	**0.005±0.003**	0.0062±0.0001

Table 4: $CRPS_{sum}$ for baseline methods, M-N-BEATS-Flow with *Linear-Transformer-Block*. For methods proposed in this thesis mean and standard deviation of 10 runs is reported. Results for GP-Copula are taken from [9], mean and standard deviation of 3 runs are reported. For models proposed in [8] results were taken from the paper, mean and standard deviation of a single run are reported. Two best methods are in bold.

Experiments

Forecast Plots

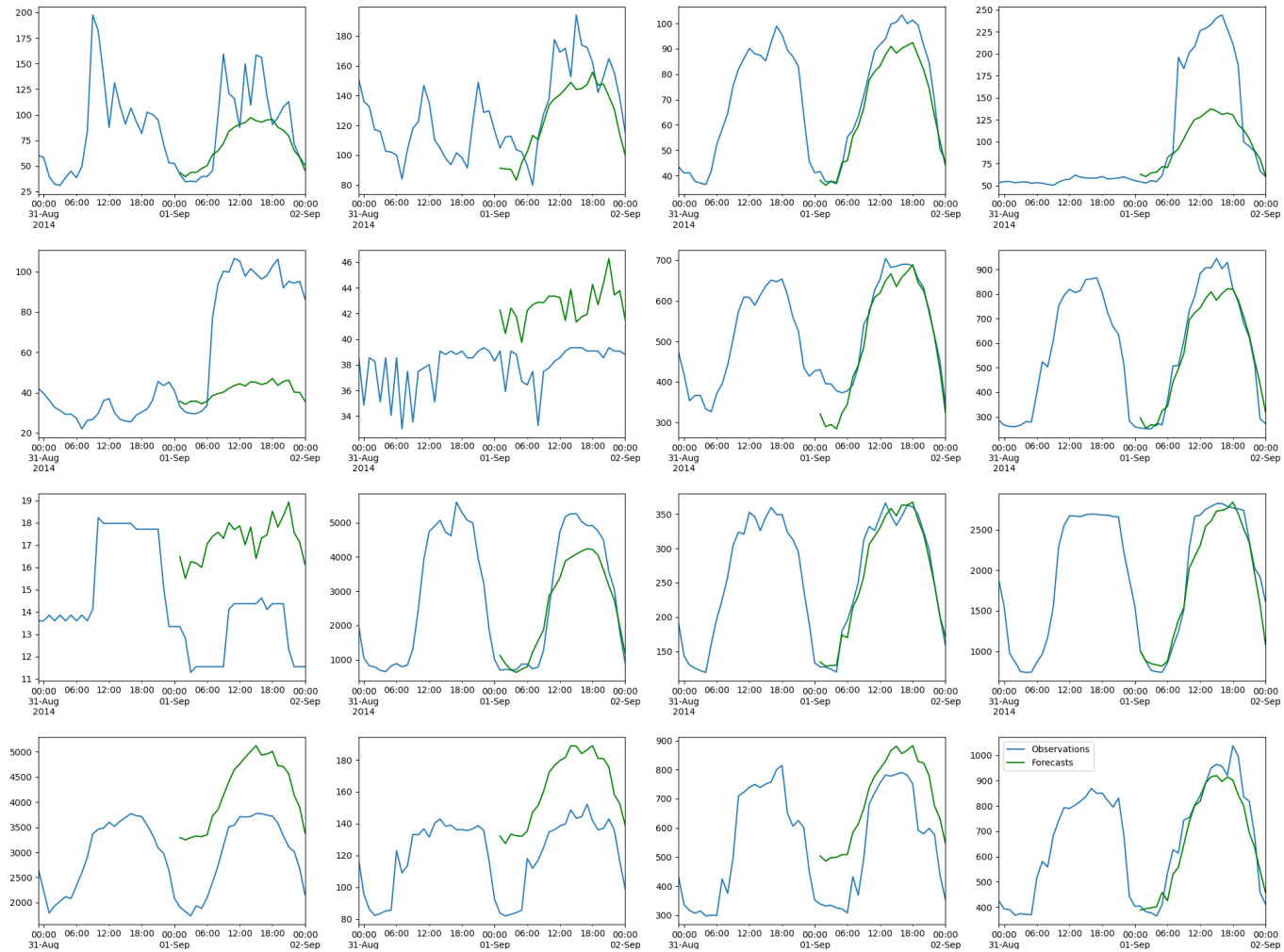


Figure 8: Forecasts produced by M-N-BEATS with *Linear-Transformer-Block* on the *Electricity* data set, only the forecasts of a single run are plotted.

Experiments

Forecast Plots

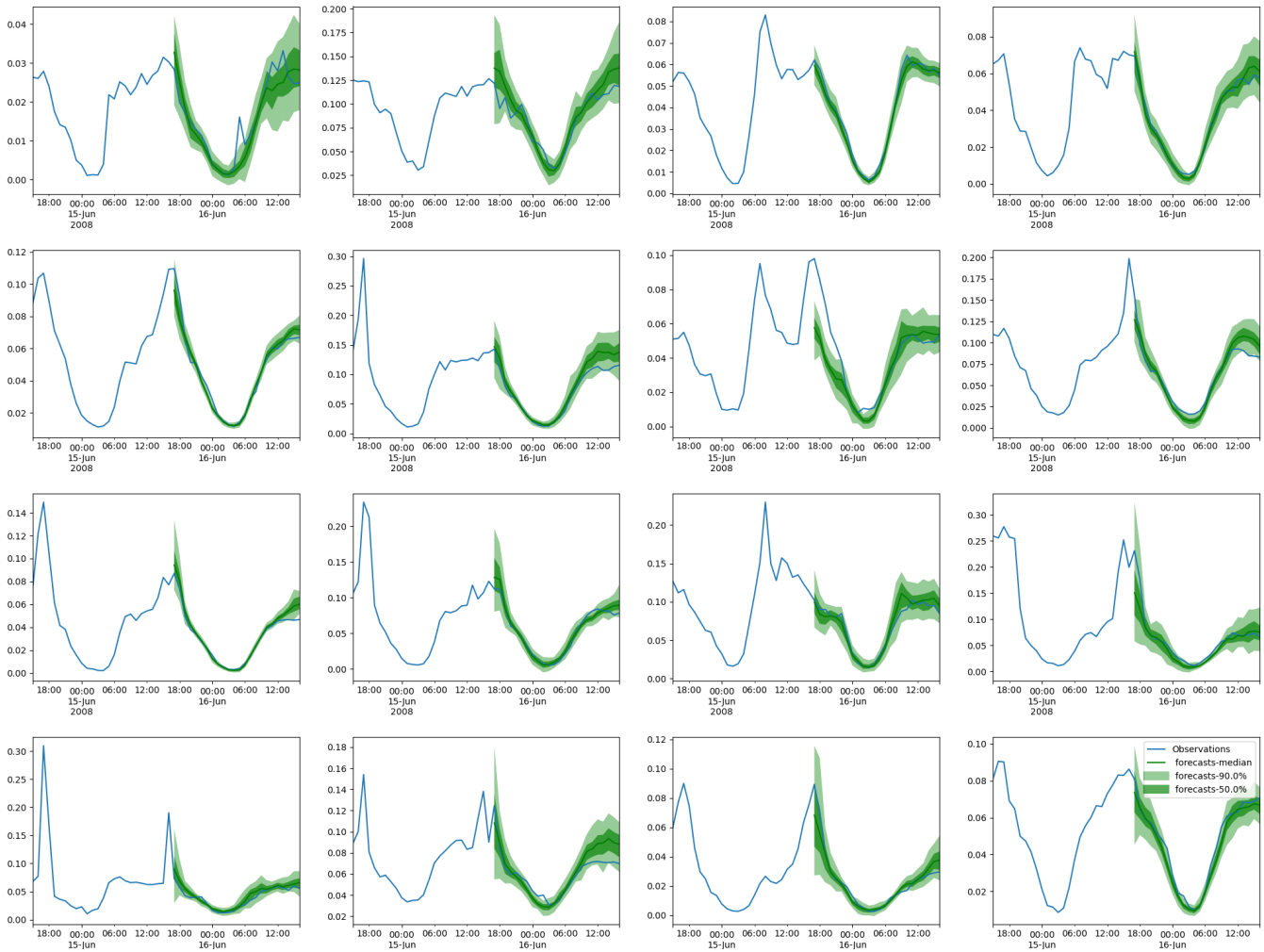


Figure 9: Forecasts produced by M-N-BEATS-Flow with *Linear-Transformer-Block* on the *Traffic* data set, only the forecasts of a single run are plotted.

Experiments

Further Experiments Results

Further Experiments

- Other Block types
- Same hyperparameters as with *linear-transformer-block*

MSE

Data Set	Simple-Block	Linear-Block	Conv-Block	Linear-Conv-Block
Electricity	253864±181095	**162721±13712**	339995±253724	**135090±10410**
Traffic	0.0007±0.0003	**0.000435±0.00002**	None	0.0005±0.0001
Solar	925±68	**746±47**	1014±72	**815±61**
Exchange Rate	0.00018±0.0000	**0.00016±0.0000**	0.00034±0.0000	0.00019±0.0000

Table 5: *MSE* for M-N-BEATS-Flow with other blocks, mean and standard deviation of 10 runs. Scores in bold beat the baseline models in table 2.

Experiments

Further Experiments Results

CRPS

Data Set	Simple-Block	Linear-Block	Conv-Block	Linear-Conv-Block
Electricity	0.0617±0.0235	0.052±0.0008	0.0617±0.0127	**0.0495±0.0006**
Traffic	0.1932±0.1072	**0.1117±0.0078**	None	0.1278±0.0264
Solar	0.3717±0.0129	**0.3348±0.0114**	0.3934±0.0153	**0.3591±0.0168**
Exchange Rate	0.0092±0.0002	0.0089±0.0004	0.0108±0.0008	0.0094±0.0005

Table 6: *CRPS* for M-N-BEATS-Flow with other blocks, mean and standard deviation of 10 runs. Scores in bold beat the baseline models in table 3.

Experiments

Further Experiments Results

$CRPS_{sum}$

Data Set	Simple-Block	Linear-Block	Conv-Block	Linear-Conv-Block
Electricity	0.0321±0.0252	**0.0206±0.0014**	0.0314±0.0132	**0.0203±0.0011**
Traffic	0.1351±0.1047	**0.0451±0.0102**	None	0.0653±0.0285
Solar	0.3154±0.0173	**0.2737±0.0143**	0.3475±0.0211	0.3028±0.0217
Exchange Rate	0.0062±0.0003	0.0059±0.0003	0.0074±0.0014	0.0064±0.0006

Table 7: $CRPS_{sum}$ for M-N-BEATS-Flow with other blocks, mean and standard deviation of 10 runs. Scores in bold beat the baseline models in table 4.

Experiments

Forecast Plots

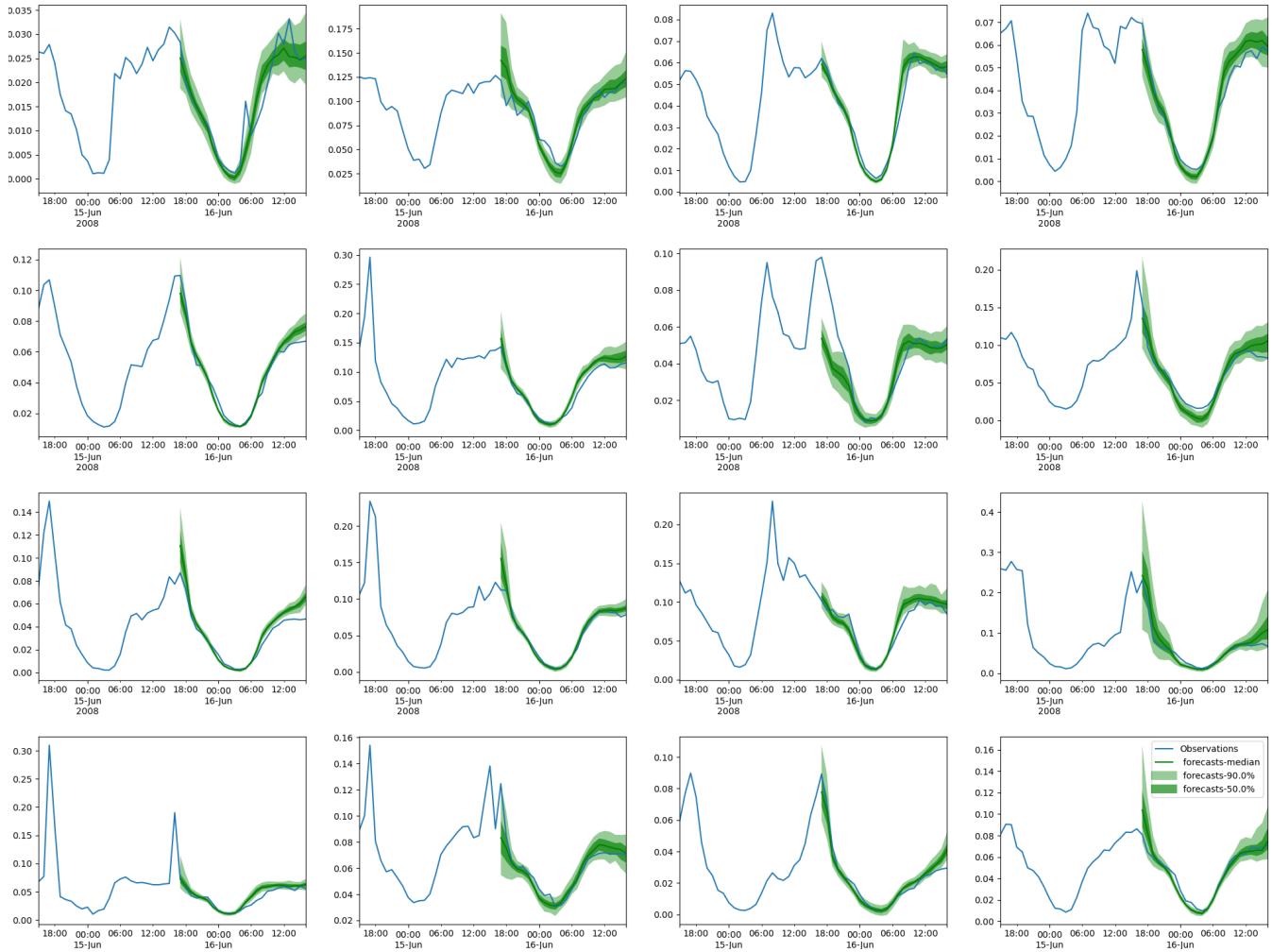


Figure 10: Forecasts produced by M-N-BEATS-Flow with *Linear-Block* on the *Traffic* data set, only the forecasts of a single run are plotted.

Conclusion

- Naive approach and M-N-BEATS not competitive
- By N-BEATS design due to residual connections model size explodes for high dimensional data
- Combine M-N-BEATS + normalizing flow
- competitive results
- Linear-Block performed very well on all data sets and outperformed all baselines
- This is likely to show the effectiveness of normalizing flows

References I

[1] Laurent Dinh, Jascha Sohl-Dickstein, and Samy Bengio. "Density estimation using Real NVP". In: *CoRR* abs/1605.08803 (2016). arXiv: 1605.08803. URL: http://arxiv.org/abs/1605.08803.

[2] Dheeru Dua and Casey Graff. *UCI Machine Learning Repository*. 2017. URL: http://archive.ics.uci.edu/ml.

[3] Cheng Guo and Felix Berkhahn. "Entity Embeddings of Categorical Variables". In: *CoRR* abs/1604.06737 (2016). arXiv: 1604.06737. URL: http://arxiv.org/abs/1604.06737.

References II

[4] Charles C. Holt. "Forecasting seasonals and trends by exponentially weighted moving averages". In: *International Journal of Forecasting* 20.1 (2004), pp. 5–10. ISSN: 0169-2070. DOI: https://doi.org/10.1016/j.ijforecast.2003.09.015. URL: https://www.sciencedirect.com/science/article/pii/S0169207003001134.

[5] Guokun Lai et al. "Modeling Long- and Short-Term Temporal Patterns with Deep Neural Networks". In: *The 41st International ACM SIGIR Conference on Research amp; Development in Information Retrieval*. SIGIR '18. Ann Arbor, MI, USA: Association for Computing Machinery, 2018, pp. 95–104. ISBN: 9781450356572. DOI: 10.1145/3209978.3210006. URL: https://doi.org/10.1145/3209978.3210006.

References III

[6] Spyros Makridakis, Evangelos Spiliotis, and Vassilios Assimakopoulos. "The M4 Competition: Results, findings, conclusion and way forward". In: *International Journal of Forecasting* 34.4 (2018), pp. 802–808. ISSN: 0169-2070. DOI: https://doi.org/10.1016/j.ijforecast.2018.06.001. URL: https://www.sciencedirect.com/science/article/pii/S0169207018300785.

[7] Boris N Oreshkin et al. "N-BEATS: Neural basis expansion analysis for interpretable time series forecasting". In: *arXiv preprint arXiv:1905.10437* (2019).

[8] Kashif Rasul et al. "Multivariate Probabilistic Time Series Forecasting via Conditioned Normalizing Flows". In: *International Conference on Learning Representations*. 2021. URL: https://openreview.net/forum?id=WiGQBFuVRv.

References IV

[9] David Salinas et al. "High-Dimensional Multivariate Forecasting with Low-Rank Gaussian Copula Processes". In: *NeurIPS*. 2019.

[10] Slawek Smyl. "A hybrid method of exponential smoothing and recurrent neural networks for time series forecasting". In: *International Journal of Forecasting* 36.1 (2020), pp. 75–85.

[11] Ashish Vaswani et al. "Attention is all you need". In: *arXiv preprint arXiv:1706.03762* (2017).

APPENDIX

N-BEATS

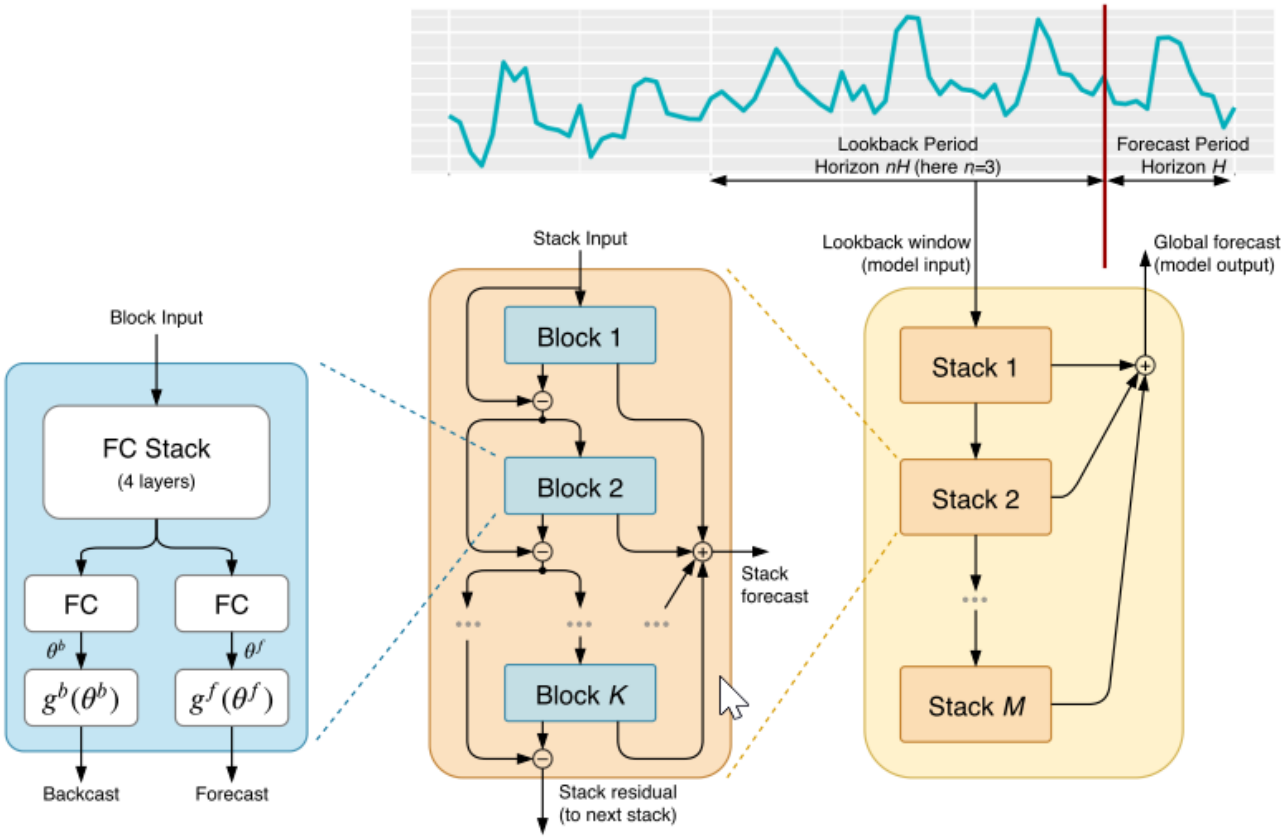


Figure 11: N-BEATS architecture. Illustration of the N-BEATS architecture, index ℓ was dropped for simplicity.
source: [7].

Appendix

N-BEATS

Stack of linear Layers

$$\mathbf{h}_{\ell,1} = \text{ReLu}\left(\mathbf{W}_{\ell,1}\mathbf{x}_{\ell} + \mathbf{b}_{\ell,1}\right) \tag{10}$$

$$\mathbf{h}_{\ell,2} = \text{ReLu}\left(\mathbf{W}_{\ell,2}\mathbf{h}_{\ell,1} + \mathbf{b}_{\ell,2}\right) \tag{11}$$

$$\mathbf{h}_{\ell,3} = \text{ReLu}\left(\mathbf{W}_{\ell,3}\mathbf{h}_{\ell,2} + \mathbf{b}_{\ell,3}\right) \tag{12}$$

$$\mathbf{h}_{\ell,4} = \text{ReLu}\left(\mathbf{W}_{\ell,4}\mathbf{h}_{\ell,3} + \mathbf{b}_{\ell,4}\right) \tag{13}$$

where $\mathbf{x}_{\ell}$ is the block input and $\mathbf{W}_{\ell}$ and $\mathbf{b}_{\ell}$ are weights and bias of the layers.

Appendix

N-BEATS

Basis vectors trend block

Given a time vector $\mathbf{t} = [0, 1, 2, \ldots, H-2, H-1]^T / H$, the basis function is given by

$$\widehat{\mathbf{y}}_{s,\ell} = \sum_{i=0}^{p} \theta^f_{s,\ell,i} t^i. \tag{14}$$

or

$$\widehat{\mathbf{y}}^{tr}_{s,\ell} = \mathbf{T}\theta^f_{s,\ell} \tag{15}$$

with the basis $\mathbf{T} = [\mathbf{1}, \mathbf{t}, \ldots, \mathbf{t}^p]$. The *tr* superscript in $\widehat{\mathbf{y}}^{tr}_{s,\ell}$ indicates that the block returns a forecast of the trend. For the backcast, the time vector is $\mathbf{t} = [0, 1, 2, \ldots, S-2, S-1]^T / S$ where S is the sequence length of the input time series. The number of basis parameters is $dim(\theta^f) = p + 1$ for the forecast and $dim(\theta^b) = p + 1$ for the backcast.

Appendix

N-BEATS

Basis vectors seasonality block

$$\widehat{\mathbf{y}}_{s,\ell} = \sum_{i=0}^{\lfloor H/2-1 \rfloor} \theta^{f}_{s,\ell,i} \cos(2\pi i t) + \theta^{f}_{s,\ell,i+\lfloor H/2 \rfloor} \sin(2\pi i t) \tag{16}$$

which can be written in matrix form as

$$\widehat{\mathbf{y}}^{\text{seas}}_{s,\ell} = \mathbf{S}\theta^{f}_{s,\ell} \tag{17}$$

with

$$\mathbf{S} = [\mathbf{1}, \cos(2\pi \mathbf{t}), \dots \cos(2\pi \lfloor H/2-1 \rfloor \mathbf{t})), \sin(2\pi \mathbf{t}), \dots, \sin(2\pi \lfloor H/2-1 \rfloor \mathbf{t}))] \tag{18}$$

The number of basis parameters is $dim(\theta^{f}) = H$ for the forecast branch and $dim(\theta^{b}) = H$ for the backcast branch.

Methodology

M-N-BEATS Blocks

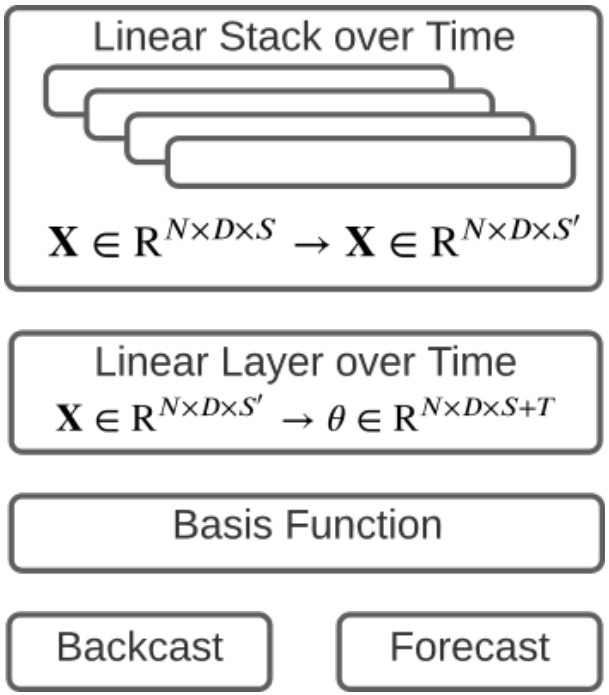


Figure 12: Univariate N-BEATS block. Vanilla N-BEATS block when applied to multivariate time series data applies the model identically to each time series.

Methodology

Transformer encoder layer

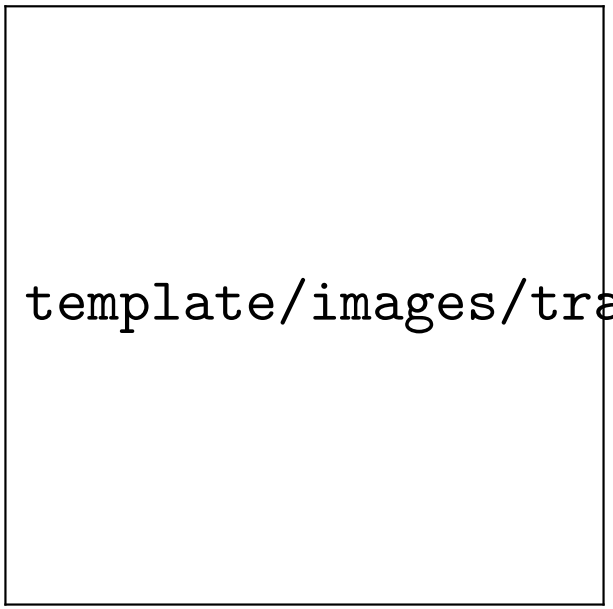


Figure 13: Transformer encoder layer. Source: [11].

Experiments

Metrics

- Mean Squared Error (MSE)
- Continuous Ranked Probability Score ($CRPS$)
- $CRPS_{sum}$

- MSE for M-N-BEATS
- MSE, $CRPS$, $CRPS_{sum}$ for M-N-BEATS-Flow

$$MSE(\mathbf{Y}, \widehat{\mathbf{Y}}) = \left\| \mathbf{Y} - \widehat{\mathbf{Y}} \right\|_F^2 \tag{19}$$

where $\|\cdot\|_F$ is the Frobenius norm.

Experiments

Metrics

CRPS

- *CRPS* score is computed for each time series
- Measures how good the approximated distribution compares to the data using the CDF F
- CDF for the predictive target distribution $F(z) = \mathbf{P}[X \leq z]$
- Measures the probability that the normalizing flow samples a x smaller than z

Experiments

Metrics

CRPS for a given fixed data point at time step t is given as

$$\text{CRPS}(F, x) = \int_{\mathbb{R}} (F(z) - \mathbb{I}\{x \leq z\})^2 \, \mathrm{d}z \tag{20}$$

- x is a single data point (one time step of one channel)
- $\mathbb{I}\{x \leq z\})^2$ is 1 if $x \leq z$ and 0 otherwise
- Final score is the mean over the *CRPS* score of all data points and channels

Experiments

Metrics

- CDF $F(z) = \mathbf{P}[X \leq z]$ for a certain value of z can be approximated using the empirical CDF

$$\hat{F}(z) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}\{X_i \leq z\} \tag{21}$$

- n is the number of samples generated from the model using $X_i \sim F$
- In [8] 100 samples were used to compute the empirical CDF
- Lower values of *CRPS* are better

Experiments

Metrics

$CRPS_{sum}$ for a single time step t is given by

$$\mathrm{CRPS}_{\mathrm{sum}} = \mathbb{E}_t \left[\mathrm{CRPS} \left(\hat{F}_{\mathrm{sum}}(t), \sum_{i=0}^{D} x_t^i \right) \right] \tag{22}$$

- $\hat{F}_{\mathrm{sum}}(t)$ is computed by summing up the individual $\hat{F}$ over all D time series
- The final score is obtained by taking the mean of the $CRPS_{sum}$ of all time steps

Experiments

Data Sets

- Exchange rate: daily exchange rate between 8 currencies as used in [5]
- Solar: hourly photo-voltaic production of 137 stations in Alabama State used in [5]
- Electricity: hourly time series of the electricity consumption of 370 customers [2]
- Traffic: hourly occupancy rate, between 0 and 1, of 963 San Francisco car lanes [2]

Source: [9]

Experiments

Data Sets

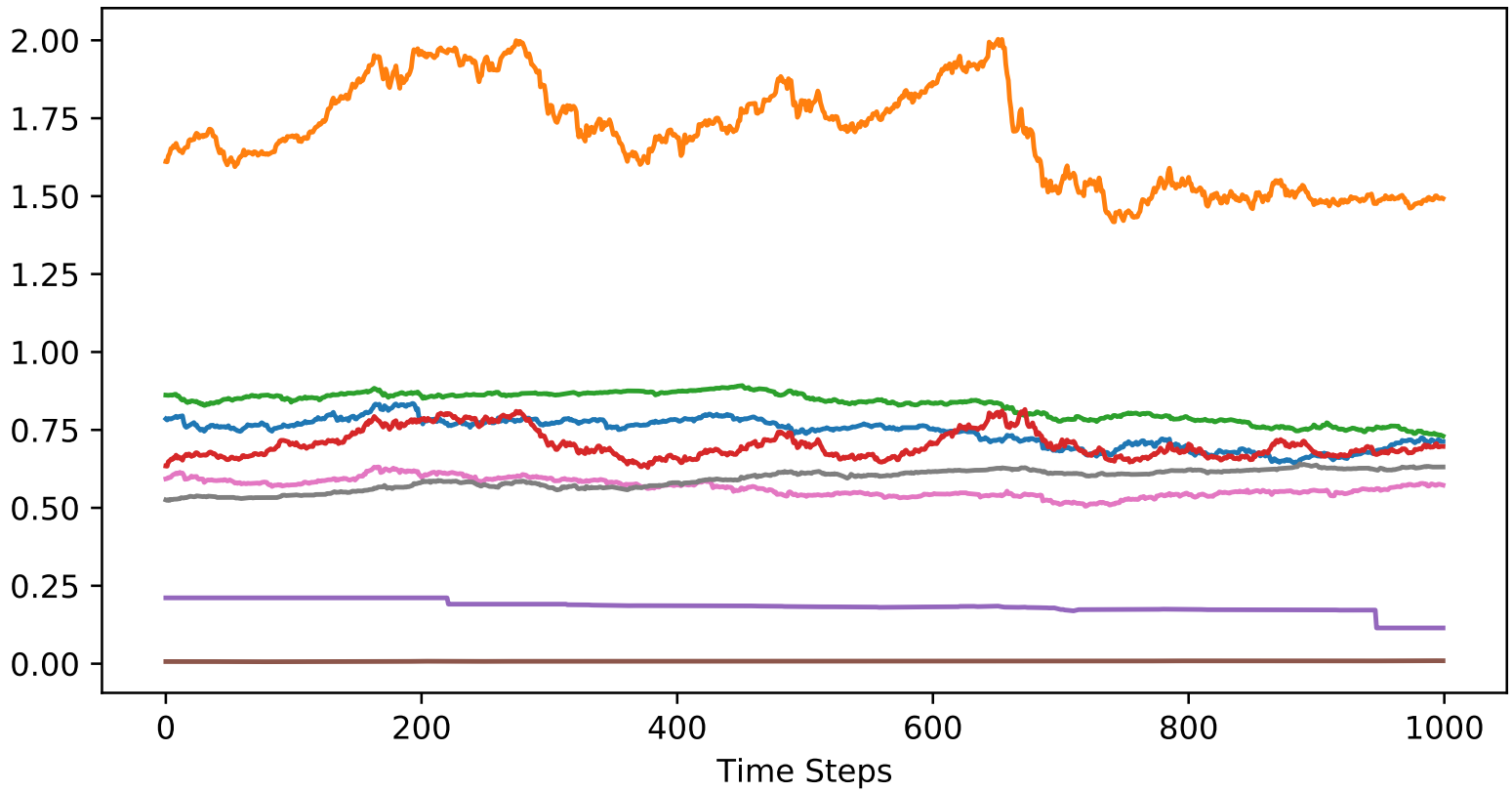


Figure 14: Exchange data set. The first 1000 time steps of the all time series in the *Exchange Rate* data set.

Experiments

Data Sets

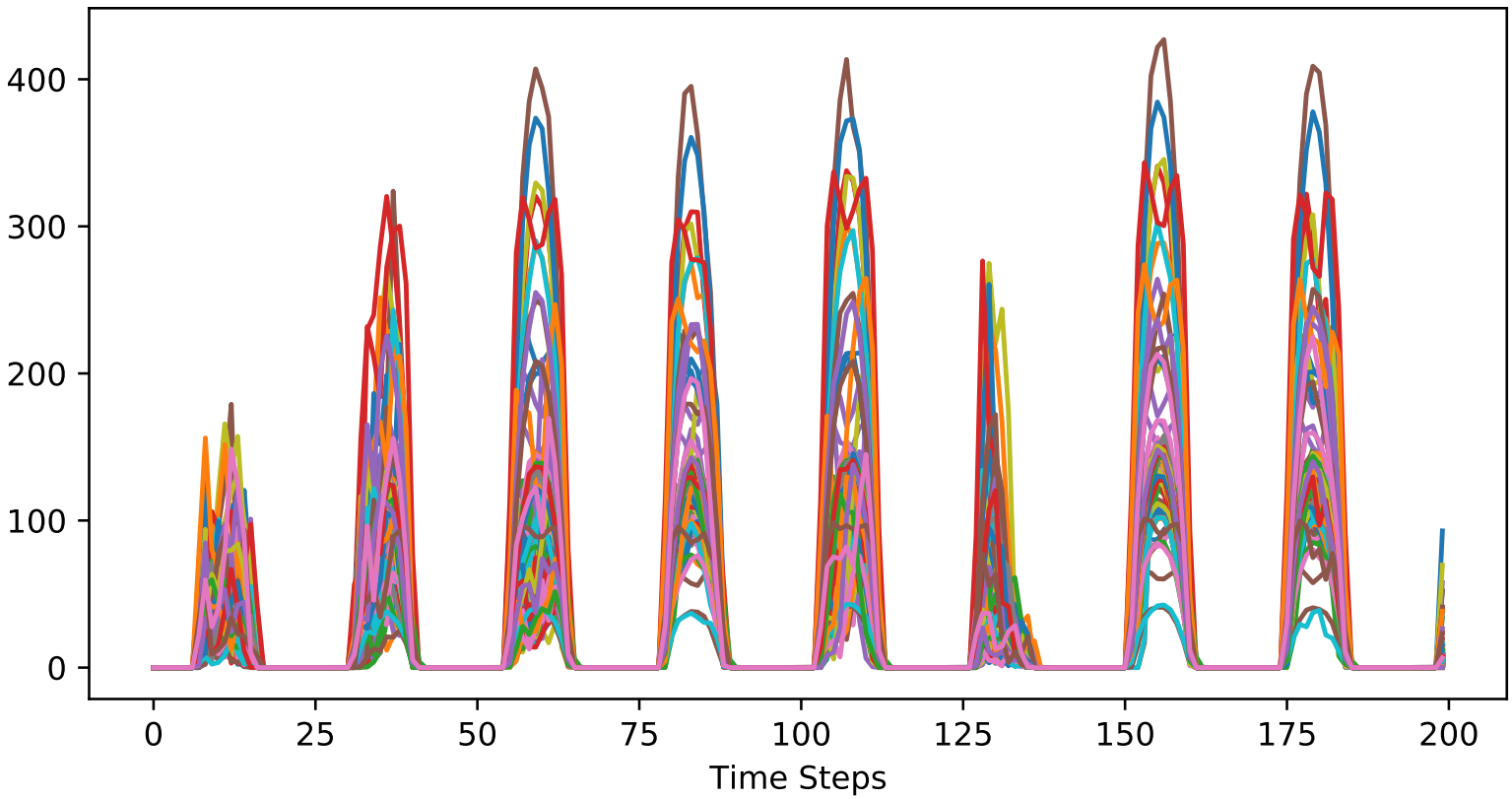


Figure 15: Solar data set. The first 200 time steps of the all time series in the *Solar* data set.

Experiments

Data Sets

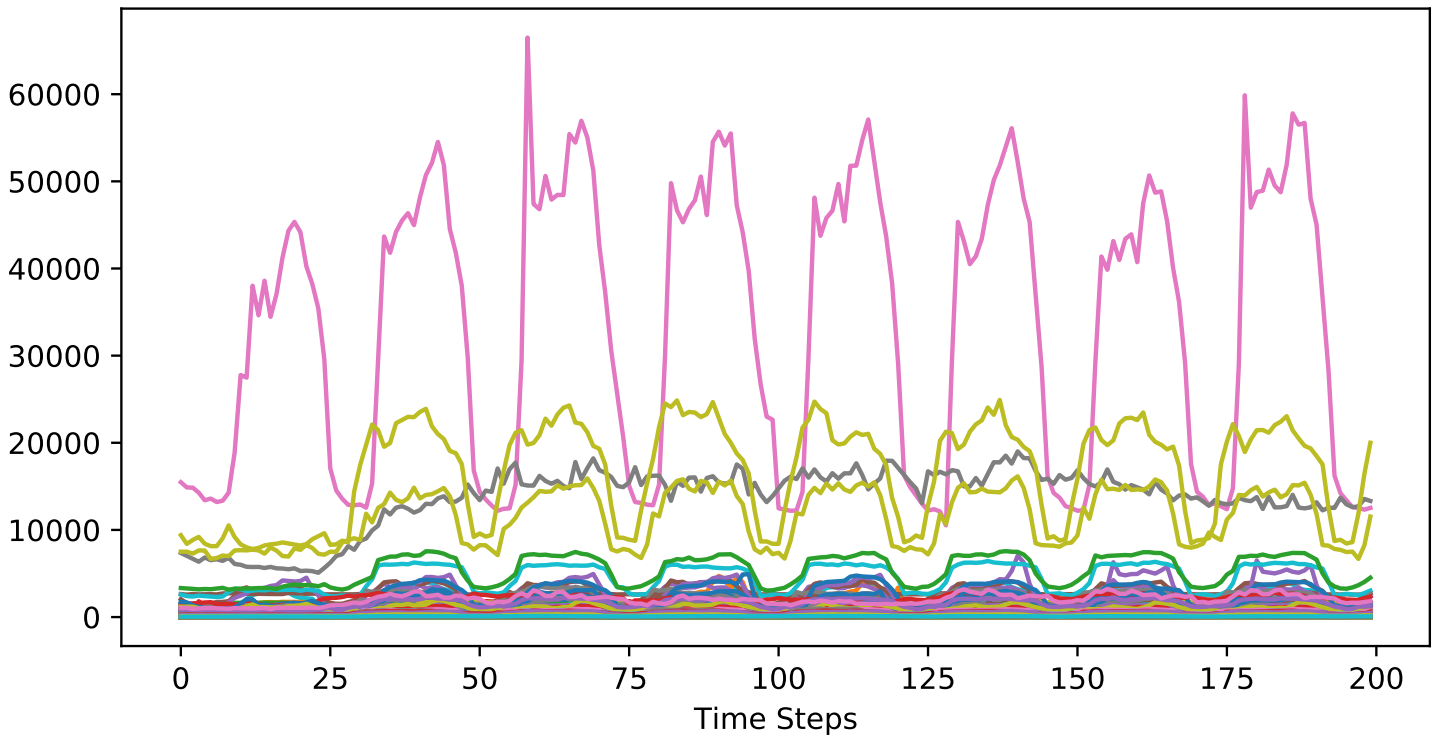


Figure 16: Electricity data set. The first 200 time steps of the all time series in the *Electricity* data set.

Experiments

Data Sets

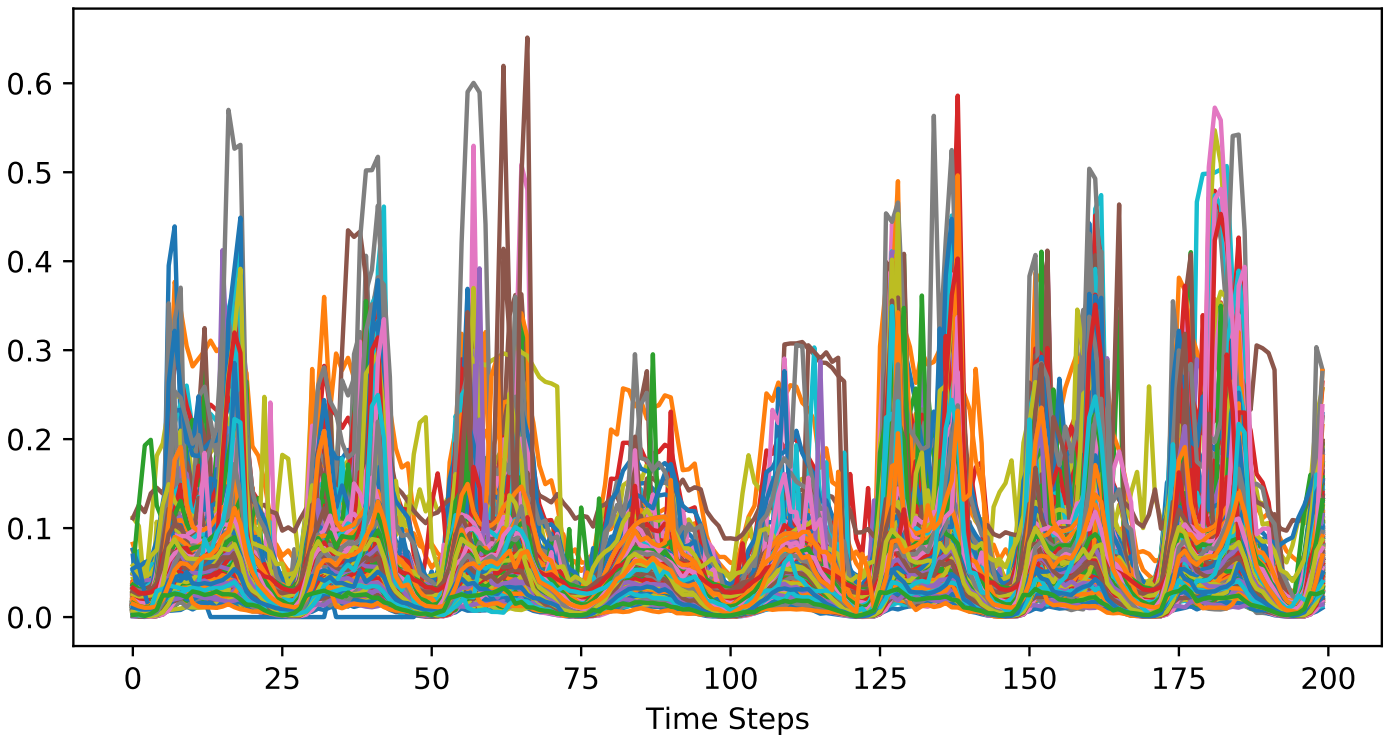


Figure 17: Traffic data set. The first 200 time steps of the all time series in the *Traffic* data set.

Experiments

Data Pipeline

Static features

- Channel index is used as categorical variable and an entity embedding like proposed in [3] is applied

Time dependent features

- Sinus cosinus from time features like **day of week** or **hour of day**

Lagged time series

- Lags are applied according to the data set's frequency
- 1, 24 and 168 for hourly time series
- 1, 2 For daily time series (*Exchange*, only business days)

Experiments

Data Pipeline

Scaling

- Magnitudes of time series differ strongly
- Divide each time series by its training window mean
- Target divided by the same factor
- After training for data generation, the output distribution is multiplied by the same factor.

Example time dependent features

- Time features for *hour* and *dayofweek*
- 0 to 23, 0 to 6
- 2 features are computed for a single time step

The time features for a single time step are computed by

$$\sin(\text{dayofweek} \times 2.0 \times \pi / S), \qquad \cos(\text{dayofweek} \times 2.0 \times \pi / S) \quad (23)$$

$$\sin(\text{hour} \times 2.0 \times \pi / S), \qquad \cos(\text{hour} \times 2.0 \times \pi / S) \quad (24)$$

Experiments

Data Pipeline

- For hourly data, *hour* and *dayofweek* time features are used (*Traffic*, *Solar* and *Electricity*)
- For dailiy data, *dayofweek* and *dayofyear* (*Exchange*)
- Fourier time features are $(N \times S \times 4)$
- time dependent features since they vary over time.

Experiments

N-BEATS-Naive Results

Data Set	**M-N-BEATS-Naive**
Electricity	5005447±2500474
Traffic	0.00088±0.0000
Solar	8842±9854
Exchange Rate	0.00037±0.0000

Table 8: *MSE* for N-BEATS-Naive, mean and standard deviation of 10 runs are reported.

Experiments

Hyperparameter Search

Max Learning Rate	0.001
Batches per Epoch	100
Epochs	25
Batch Size	64
p (Dropout)	0.5
Weight Decay	0.01

Table 9: Fixed hyperparameters for M-N-BEATS and M-N-BEATS-Flow.

Experiments

Hyperparameter Search Results M-N-BEATS

Learning Rate	Block Type	N Blocks	N Heads	Embedding Size	MSE
0.000010	*Linear-Transformer-Block*	10	4	32	794697
0.000010	*Linear-Attention-Block*	10	8	32	940344
0.000010	*Linear-Attention-Block*	10	8	128	944887
0.000010	*Linear-Transformer-Block*	10	8	32	963443
0.000010	*Linear-Transformer-Block*	3	4	128	974484

Table 10: Grid search best 5 combinations for M-N-BEATS on *Electricity* data set. *N Heads* is number of attention heads, *Embedding Size* is the attention embedding size and *N Blocks* is the number of blocks.

Experiments

Hyperparameter Search Results M-N-BEATS

Learning Rate	Block Type	N Blocks	N Heads	Embedding Size	MSE
0.000100	*Linear-Transformer-Block*	3	8	64	0.000837
0.000100	*Linear-Transformer-Block*	5	8	64	0.001060
0.000010	*Linear-Attention-Block*	3	4	128	0.001088
0.000010	*Linear-Transformer-Block*	10	8	128	0.001097
0.000010	*Linear-Transformer-Block*	3	8	128	0.001112

Table 11: Grid search best 5 combinations for M-N-BEATS on *Traffic* data set. *N Heads* is number of attention heads, *Embedding Size* is the attention embedding size and *N Blocks* is the number of blocks.

Experiments

Hyperparameter Search Results M-N-BEATS

Learning Rate	Block Type	N Blocks	N Heads	Embedding Size	MSE
0.000100	*Linear-Attention-Block*	5	4	128	6051.420232
0.000010	*Linear-Attention-Block*	10	4	128	6778.967792
0.000010	*Linear-Transformer-Block*	3	8	64	6788.116120
0.000100	*Linear-Transformer-Block*	3	8	32	6788.814785
0.000010	*Linear-Attention-Block*	10	8	128	6796.519731

Table 12: Grid search best 5 combinations for M-N-BEATS on *solar* data set. *N Heads* is number of attention heads, *Embedding Size* is the attention embedding size and *N Blocks* is the number of blocks.

Experiments

Hyperparameter Search Results M-N-BEATS

Learning Rate	Block Type	N Blocks	N Heads	Embedding Size	MSE
0.000010	*Linear-Attention-Block*	5	8	32	0.001
0.000100	*Linear-Attention-Block*	5	4	64	0.0011
0.000100	*Linear-Attention-Block*	3	8	32	0.0011
0.000010	*Linear-Attention-Block*	10	4	128	0.0011
0.000100	*Linear-Attention-Block*	3	4	64	0.0012

Table 13: Grid search best 5 combinations for M-N-BEATS on *Exchange Rate* data set. *N Heads* is number of attention heads, *Embedding Size* is the attention embedding size and *N Blocks* is the number of blocks.

Experiments

Hyperparameter Search Results M-N-BEATS-Flow

Learning Rate	Block Type	N Blocks	N Heads	Embedding Size	Flow Type	MSE
0.000010	*Linear-Transformer-Block*	3	8	128	RealNVP	295682
0.000010	*Linear-Transformer-Block*	10	4	128	MAF	307175
0.000010	*Linear-Transformer-Block*	5	4	32	RealNVP	312071
0.000100	*Linear-Transformer-Block*	10	4	64	MAF	326673
0.000010	*Linear-Transformer-Block*	3	8	32	RealNVP	340831

Table 14: Grid search best 5 combinations for M-N-BEATS-Flow on *Electricity* data set. *N Heads* is number of attention heads, *Embedding Size* is the attention embedding size and *N Blocks* is the number of blocks.

Experiments

Hyperparameter Search Results M-N-BEATS-Flow

Learning Rate	Block Type	N Blocks	N Heads	Embedding Size	Flow Type	MSE
0.000010	*Linear-Attention-Block*	10	8	128	RealNVP	0.00066
0.000010	*Linear-Transformer-Block*	5	4	128	MAF	0.00068
0.000010	*Linear-Attention-Block*	10	4	64	RealNVP	0.00069
0.000100	*Linear-Transformer-Block*	3	8	128	MAF	0.00076
0.000100	*Linear-Attention-Block*	10	8	64	MAF	0.00077

Table 15: Grid search best 5 combinations for M-N-BEATS-Flow on *Traffic* data set. *N Heads* is number of attention heads, *Embedding Size* is the attention embedding size and *N Blocks* is the number of blocks.

Experiments

Hyperparameter Search Results M-N-BEATS-Flow

Learning Rate	Block Type	N Blocks	N Heads	Embedding Size	Flow Type	MSE
0.000010	*Linear-Attention-Block*	5	4	32	RealNVP	309
0.000100	*Linear-Attention-Block*	3	4	64	RealNVP	319
0.000010	*Linear-Attention-Block*	10	8	32	RealNVP	320
0.000100	*Linear-Transformer-Block*	10	4	32	RealNVP	327
0.000100	*Linear-Transformer-Block*	5	8	128	MAF	327

Table 16: Grid search best 5 combinations for M-N-BEATS-Flow on *Solar* data set. *N Heads* is number of attention heads, *Embedding Size* is the attention embedding size and *N Blocks* is the number of blocks.

Experiments

Hyperparameter Search Results M-N-BEATS-Flow

Learning Rate	Block Type	N Blocks	N Heads	Embedding Size	Flow Type	MSE
0.000100	*Linear-Transformer-Block*	10	4	64	RealNVP	0.00036
0.000010	*Linear-Transformer-Block*	10	4	32	RealNVP	0.00047
0.000010	*Linear-Transformer-Block*	3	4	64	MAF	0.00050
0.000100	*Linear-Attention-Block*	10	8	128	RealNVP	0.00052
0.000010	*Linear-Attention-Block*	3	8	32	RealNVP	0.00052

Table 17: Grid search best 5 combinations for M-N-BEATS-Flow on *Exchange Rate* data set. *N Heads* is number of attention heads, *Embedding Size* is the attention embedding size and *N Blocks* is the number of blocks.

M-N-BEATS MSE

Data Set	Linear-Attention-Block	Linear-Transformer-Block
Electricity	1865557±2686855	1110571±797587
Traffic	0.0019±0.0000	0.0017±0.0000
Solar	25157±55542	4384±417
Exchange Rate	0.00037±0.00001	0.00030±0.00006

Table 18: *MSE* for M-N-BEATS with *Linear-Transformer-Block* and *Linear-Attention-Block* , mean and standard deviation of 10 runs. Scores in bold beat the baseline models in table 2.

M-N-BEATS-Flow MSE

Data Set	Linear-Attention-Block	Linear-Transformer-Block
Electricity	6085982±3535539	**155810±26344**
Traffic	0.00089±0.0008	**0.00045±0.0000**
Solar	1329±803	925±41
Exchange Rate	0.000174±0.0000	0.000174±0.0000

Table 19: *MSE* for M-N-BEATS-Flow with *Linear-Transformer-Block* and *Linear-Attention-Block* , mean and standard deviation of 10 runs. Scores in bold beat the baseline models in table 2.

M-N-BEATS-Flow CRPS

Data Set	Linear-Attention-Block	Linear-Transformer-Block
Electricity	0.2247±0.1013	0.0511±0.0019
Traffic	0.2202±0.1767	**0.1148±0.0039**
Solar	0.4686±0.1780	0.3829±0.0104
Exchange Rate	0.0092±0.0002	0.0092±0.0001

Table 20: *CRPS* for M-N-BEATS-Flow with *Linear-Transformer-Block* and *Linear-Attention-Block* , mean and standard deviation of 10 runs. Scores in bold beat the baseline models in table 3.

M-N-BEATS-Flow $CRPS_{sum}$

Data Set	Linear-Attention-Block	Linear-Transformer-Block
Electricity	0.2172±0.1129	0.0223±0.0021
Traffic	0.1776±0.2012	**0.0485±0.0049**
Solar	0.4183±0.1948	0.3289±0.0124
Exchange Rate	0.0061±0.0001	0.0062±0.0001

Table 21: $CRPS_{sum}$ for M-N-BEATS-Flow with *Linear-Transformer-Block* and *Linear-Attention-Block* , mean and standard deviation of 10 runs. Scores in bold beat the baseline models in table 4.

Experiments

Forecast Plots

Figure 18: Forecasts produced by M-N-BEATS with *Linear-Transformer-Block* on the *Solar* data set, only the forecasts of a single run are plotted.

Experiments

Forecast Plots

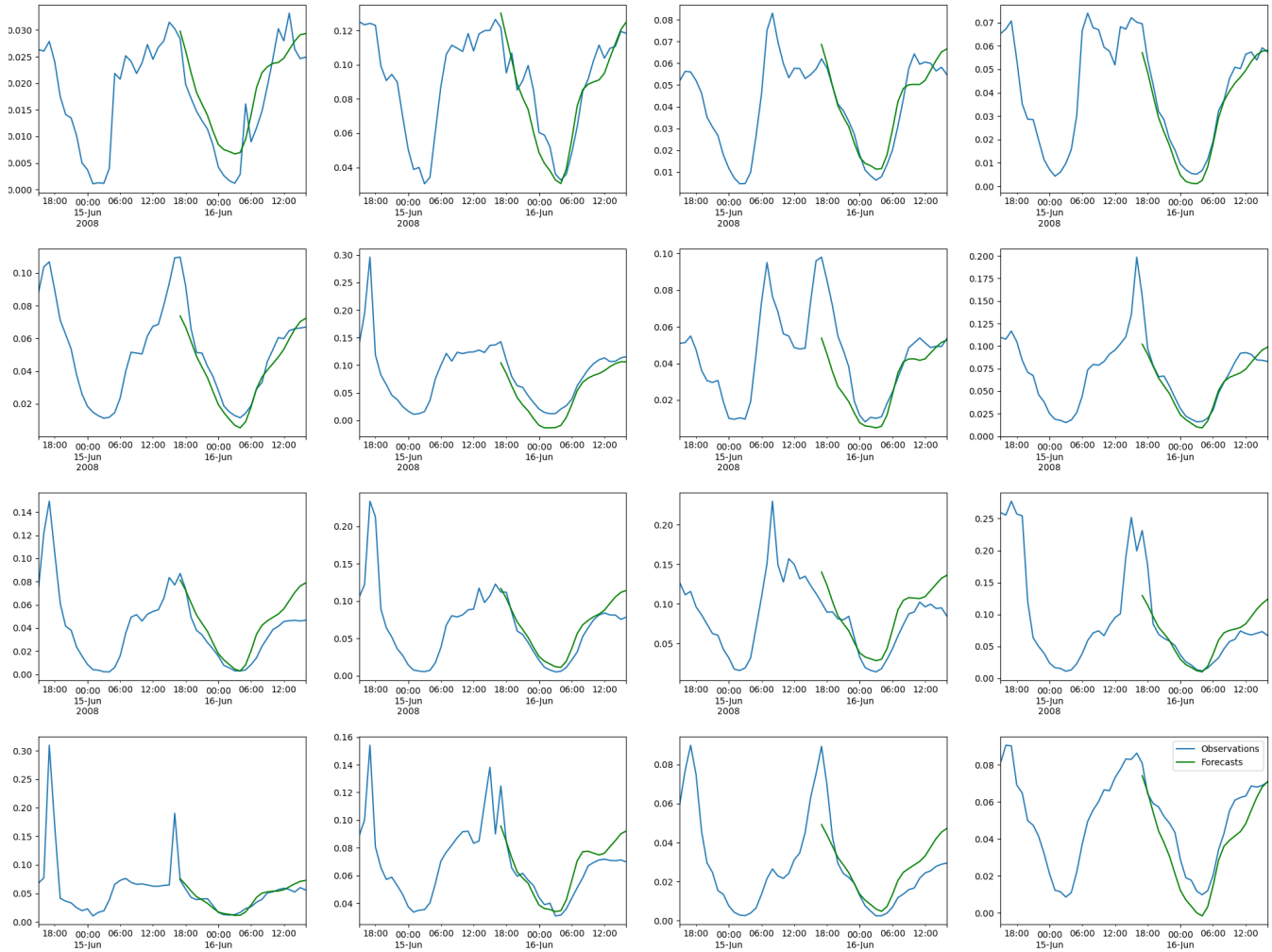


Figure 19: Forecasts produced by M-N-BEATS with *Linear-Transformer-Block* on the *Traffic* data set, only the forecasts of a single run are plotted.

Experiments

Forecast Plots

Figure 20: Forecasts produced by M-N-BEATS with *Linear-Transformer-Block* on the *Exchange Rate* data set, only the forecasts of a single run are plotted.

Experiments

Forecast Plots

Experiments

Forecast Plots

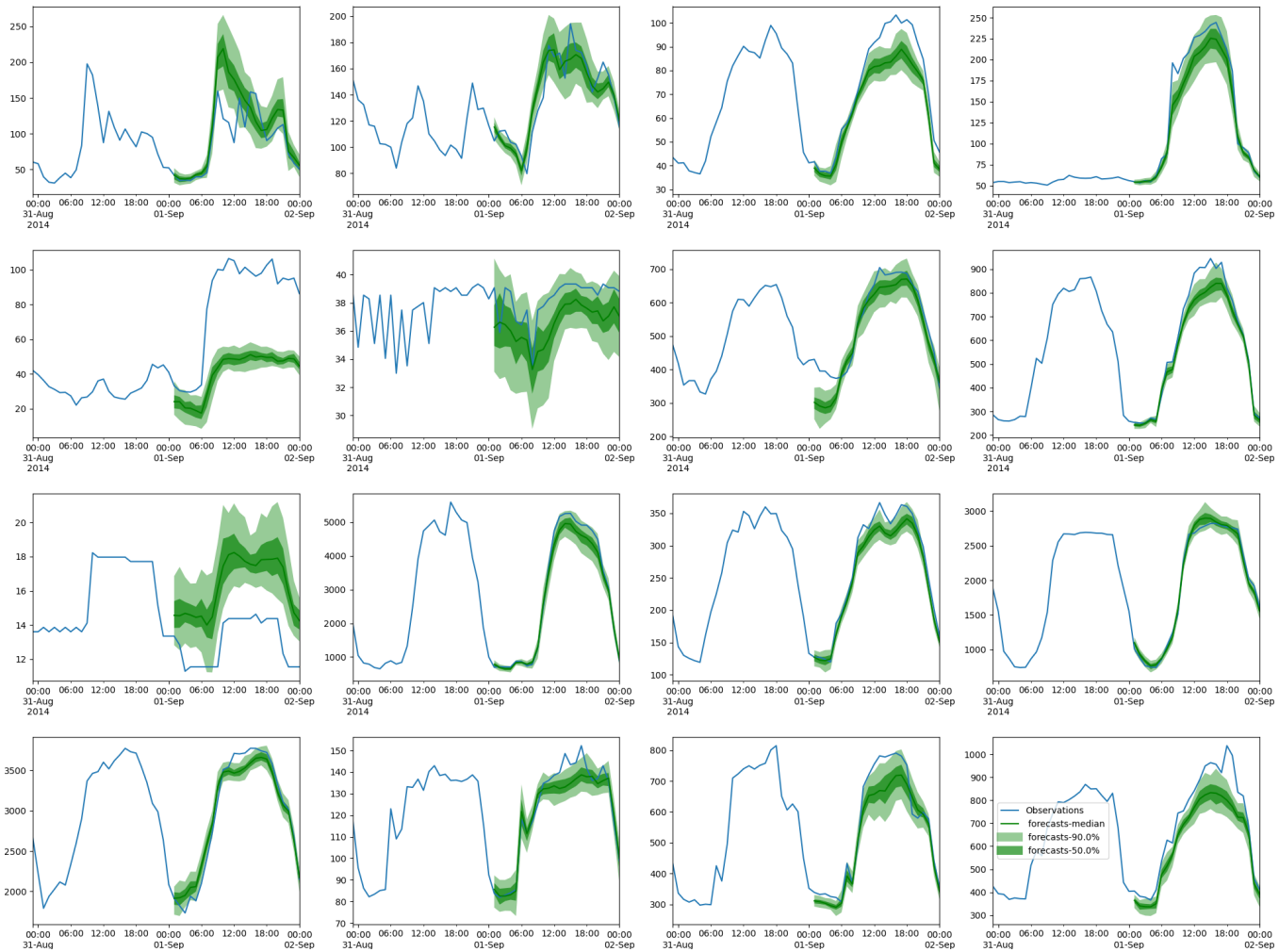


Figure 21: Forecasts produced by M-N-BEATS-Flow with *Linear-Transformer-Block* on the *Electricity* data set, only the forecasts of a single run are plotted.

Experiments

Forecast Plots

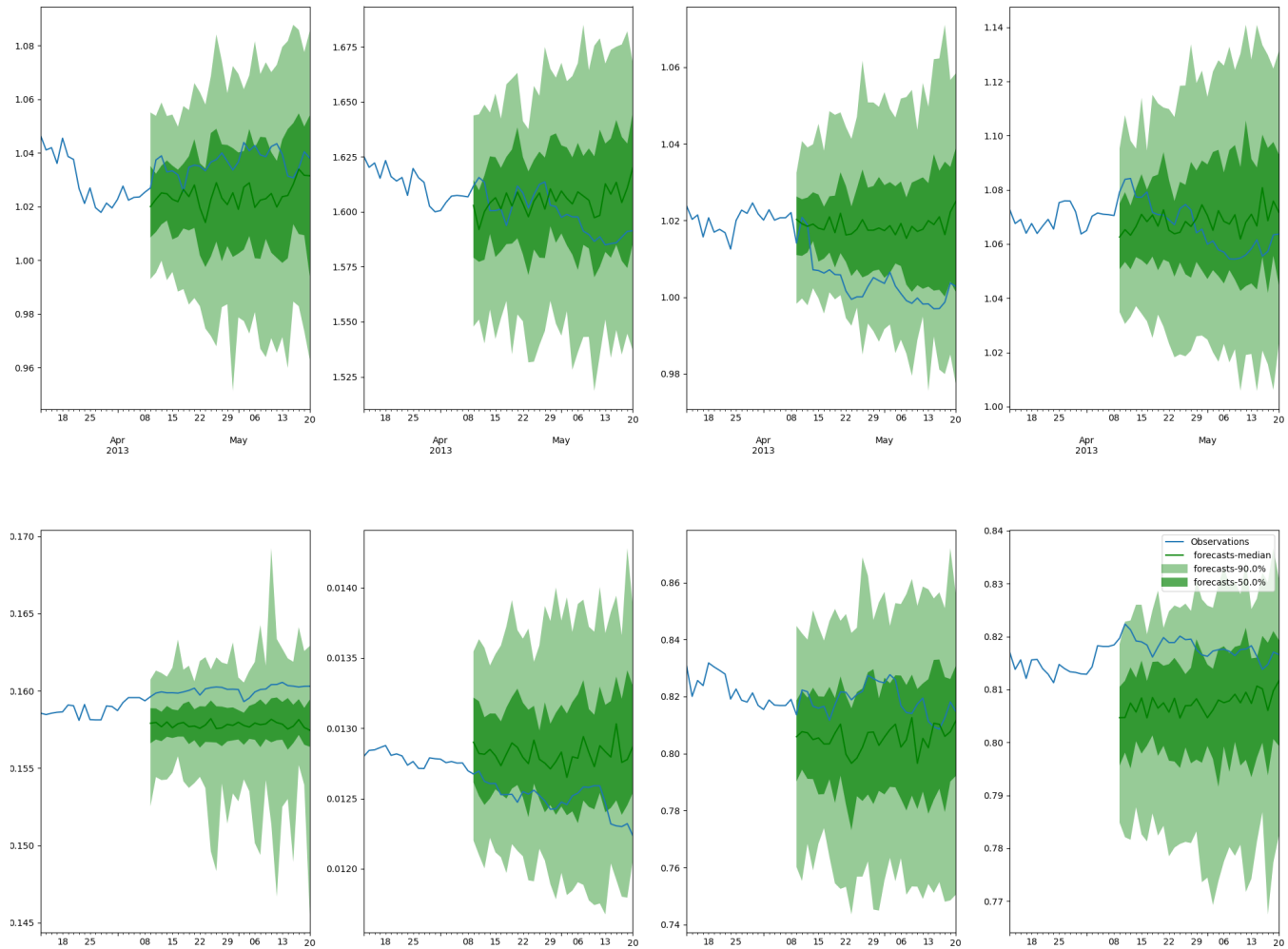


Figure 22: Forecasts produced by M-N-BEATS-Flow with *Linear-Transformer-Block* on the *Exchange Rate* data set, only the forecasts of a single run are plotted.

Experiments

Forecast Plots

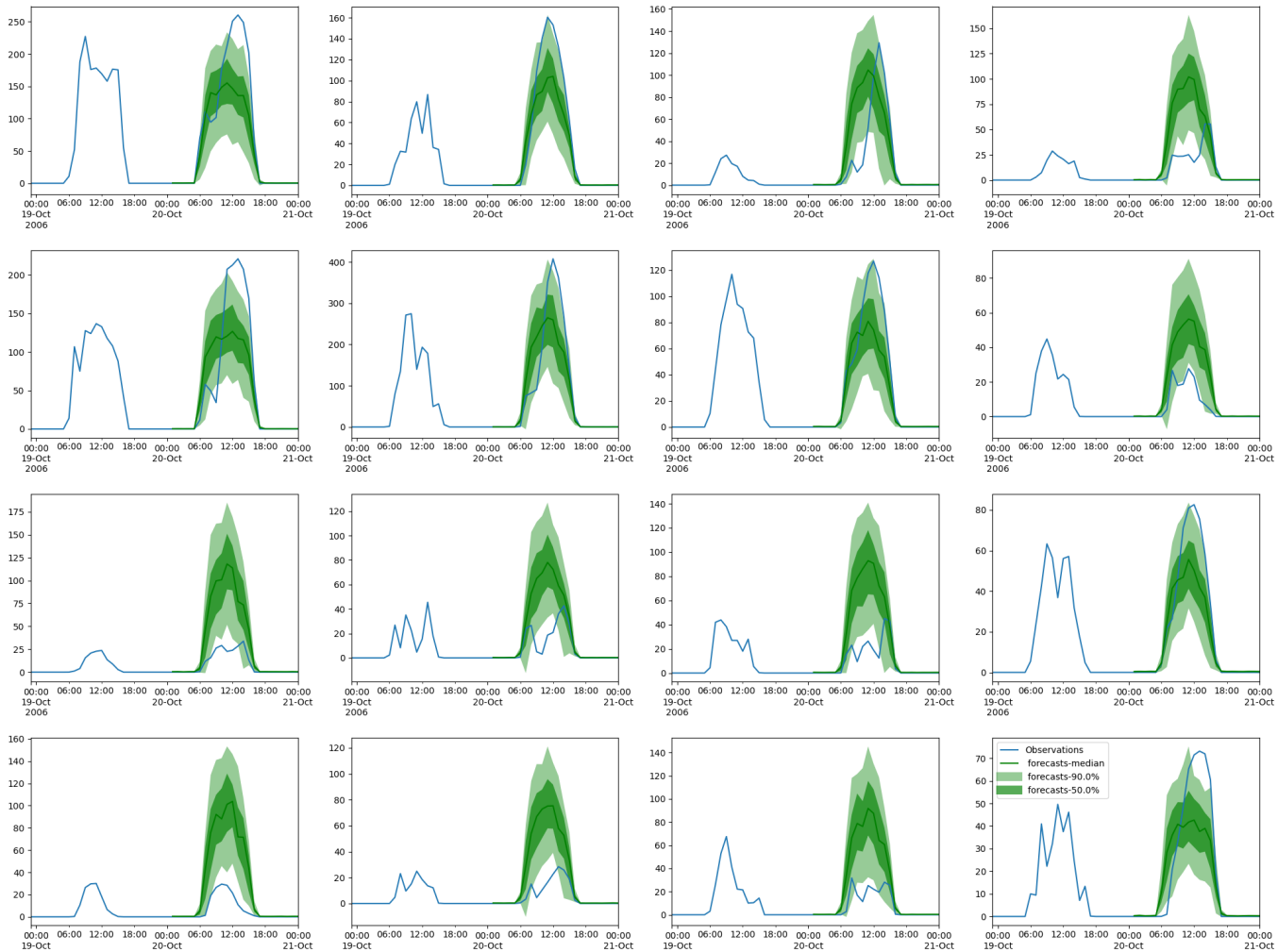


Figure 23: Forecasts produced by M-N-BEATS-Flow with *Linear-Transformer-Block* on the *Solar* data set, only the forecasts of a single run are plotted.

Experiments

Forecast Plots

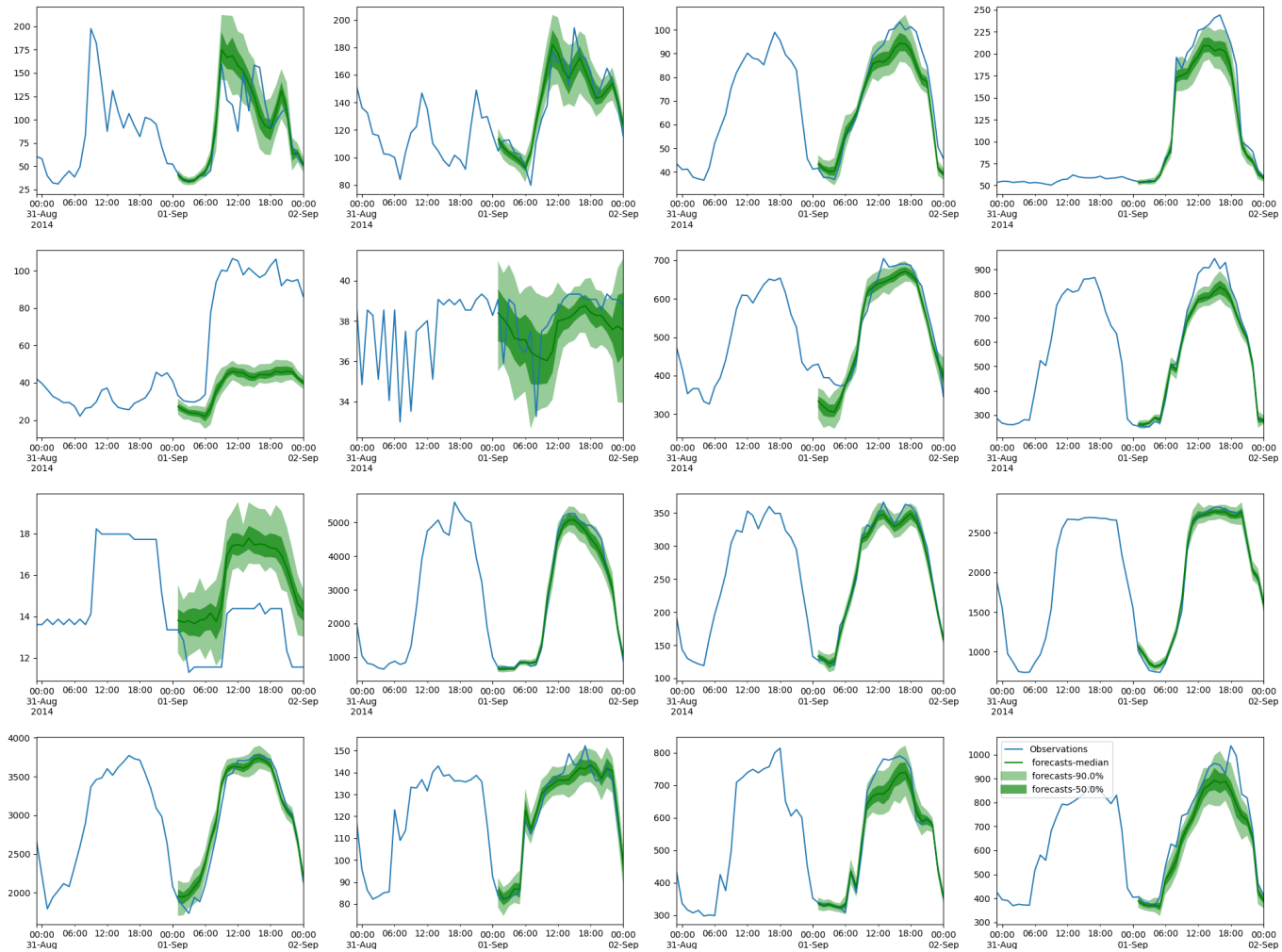


Figure 24: Forecasts produced by M-N-BEATS-Flow with *Linear-Block* on the *Electricity* data set, only the forecasts of a single run are plotted.

Experiments

Forecast Plots

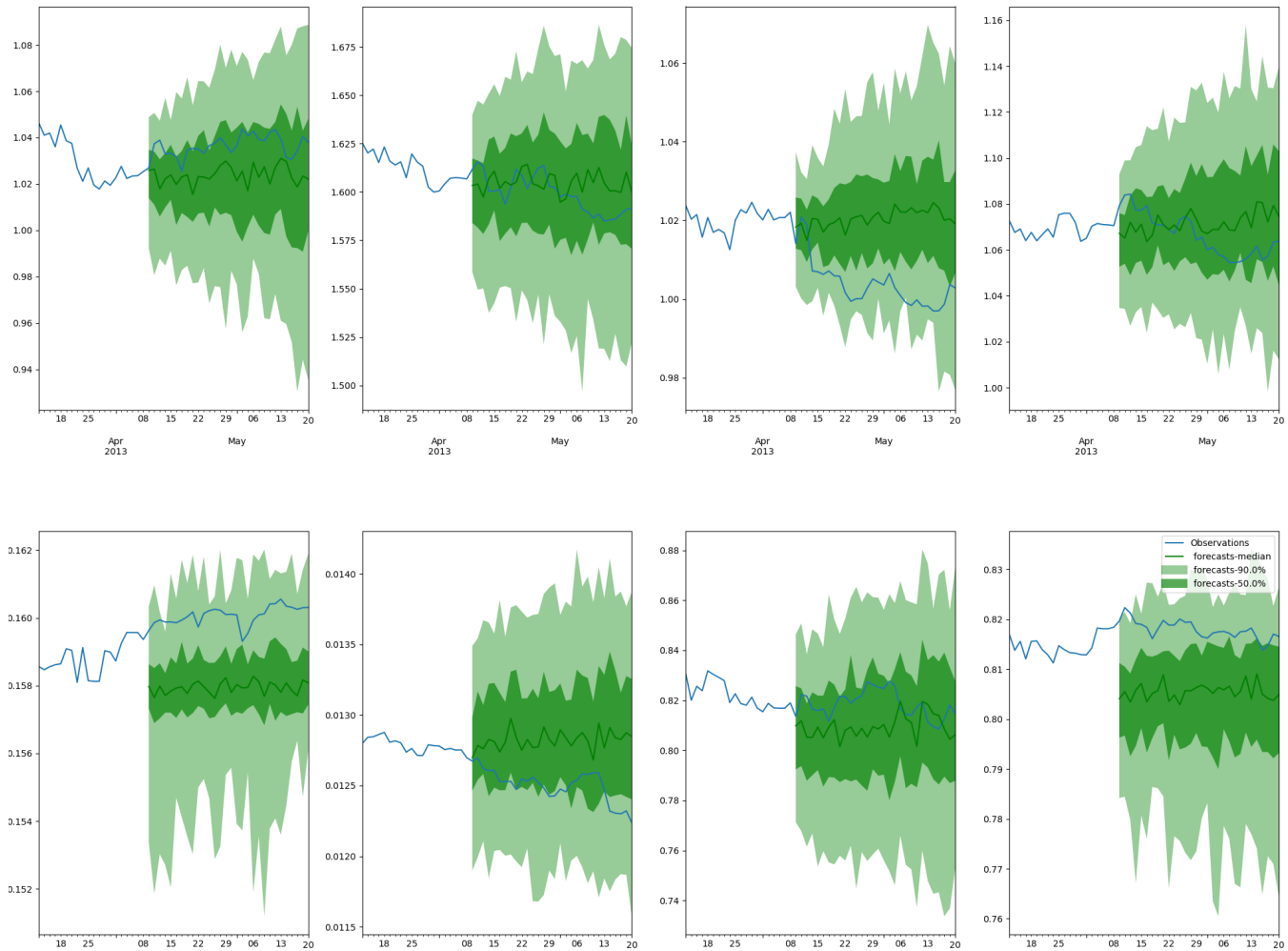


Figure 25: Forecasts produced by M-N-BEATS-Flow with *Linear-Block* on the *Exchange Rate* data set, only the forecasts of a single run are plotted.

Experiments

Forecast Plots

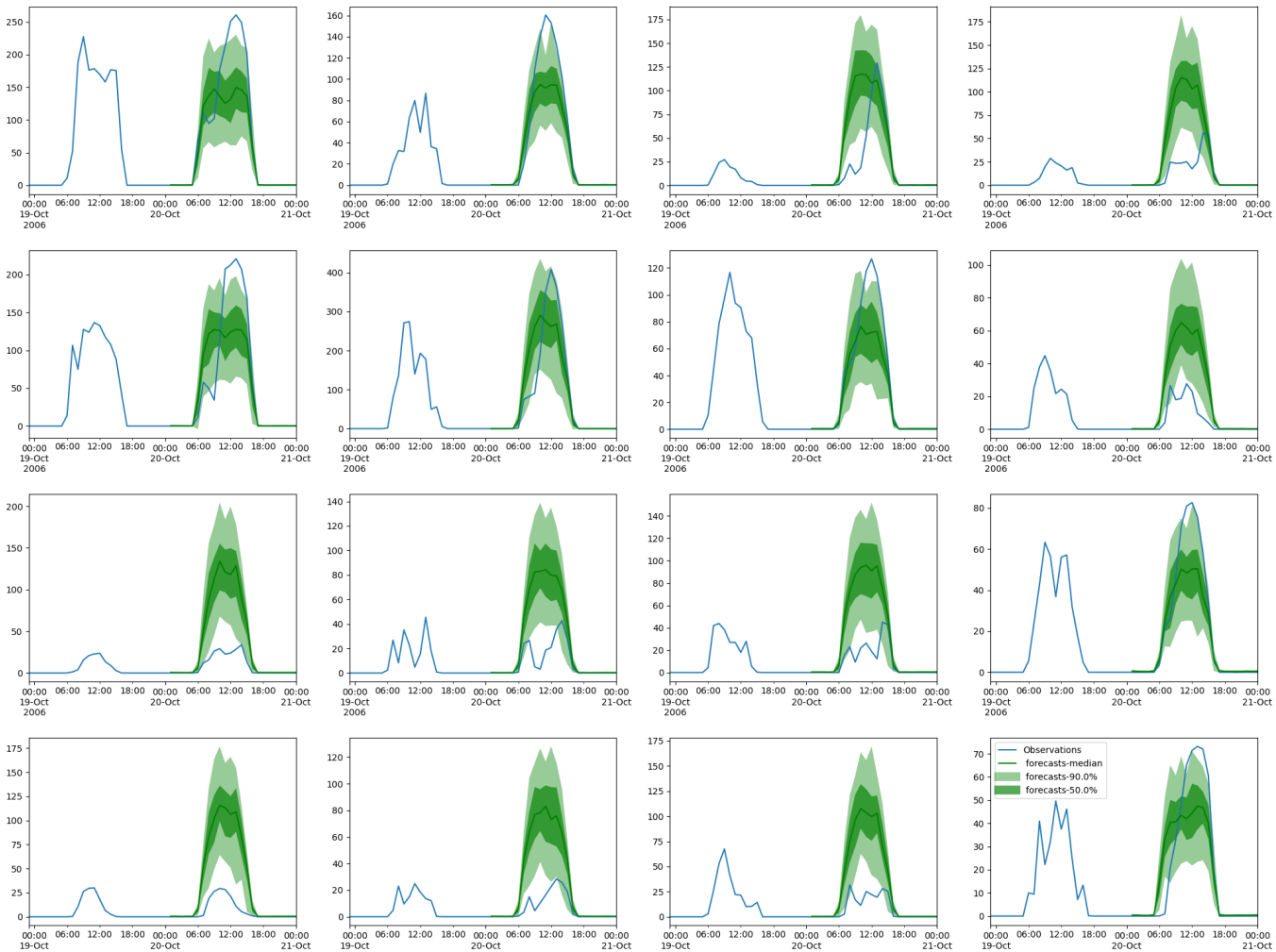


Figure 26: Forecasts produced by M-N-BEATS-Flow with *Linear-Block* on the *Solar* data set, only the forecasts of a single run are plotted.

Experiments

Forecast Plots

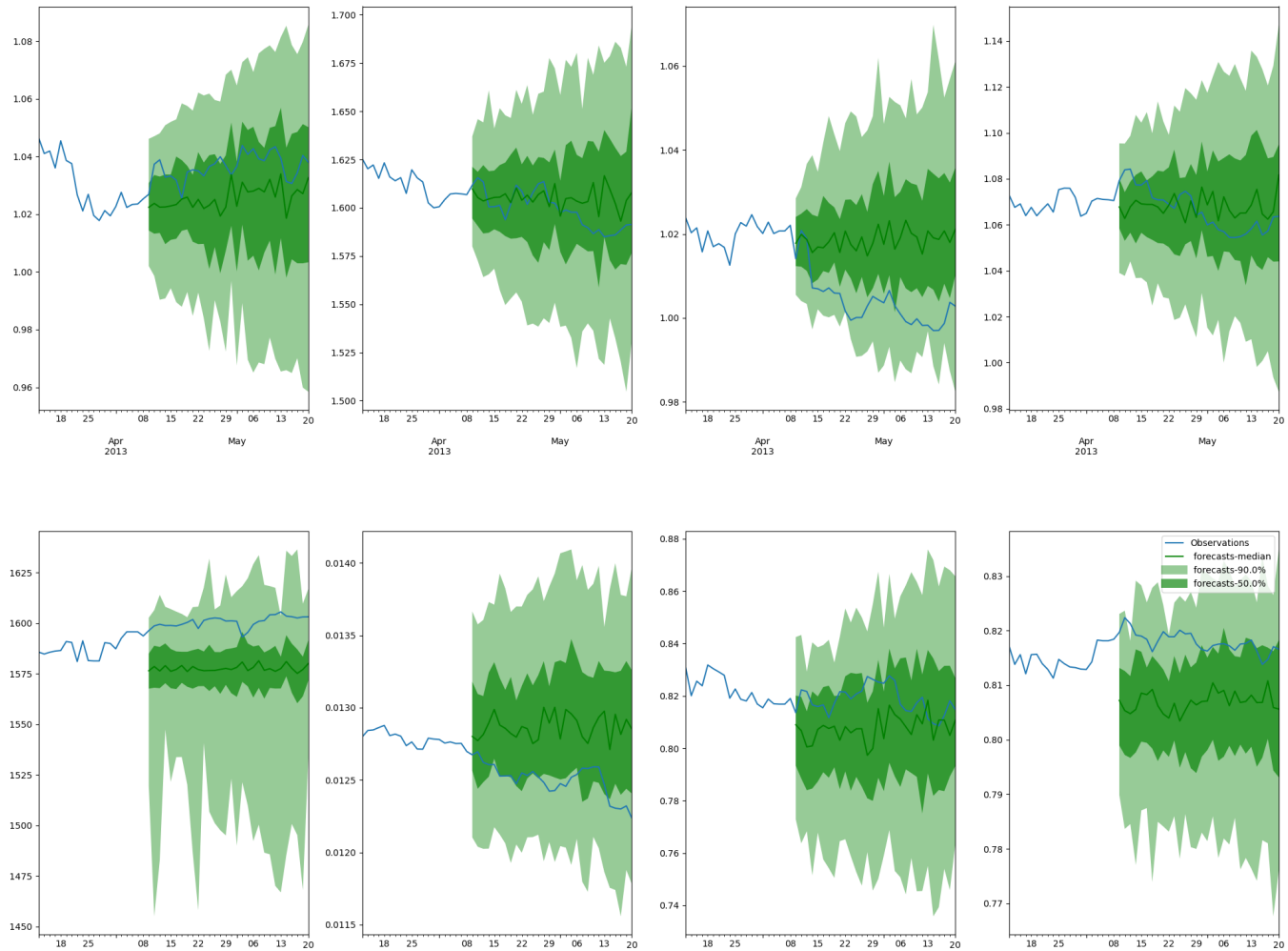


Figure 27: Forecasts produced by M-N-BEATS-Flow with *Linear-Conv-Block* on the *Exchange Rate* data set, only the forecasts of a single run are plotted.

Experiments

Forecast Plots

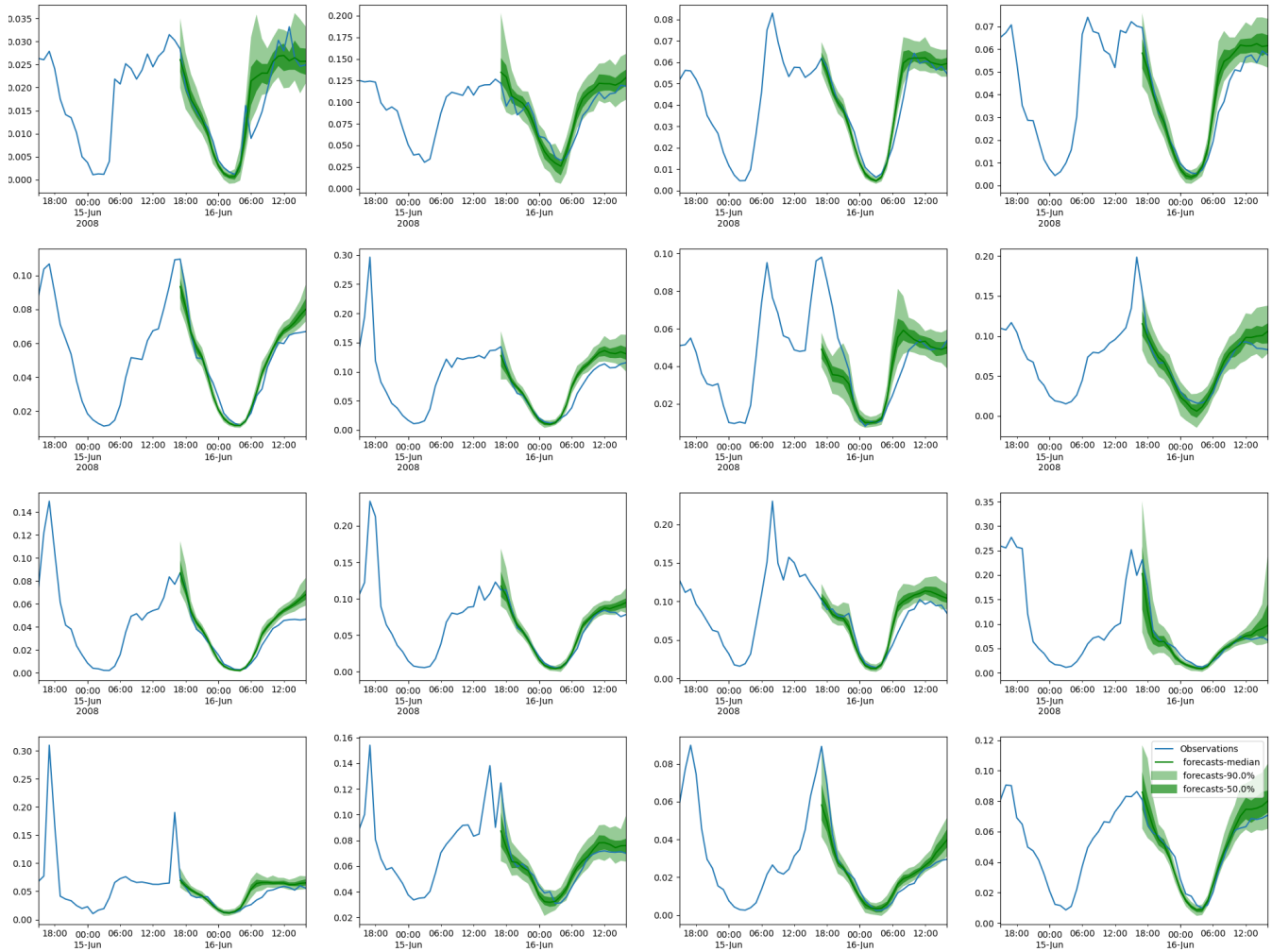


Figure 28: Forecasts produced by M-N-BEATS-Flow with *Linear-Conv-Block* on the *Traffic* data set, only the forecasts of a single run are plotted.

Experiments

Forecast Plots

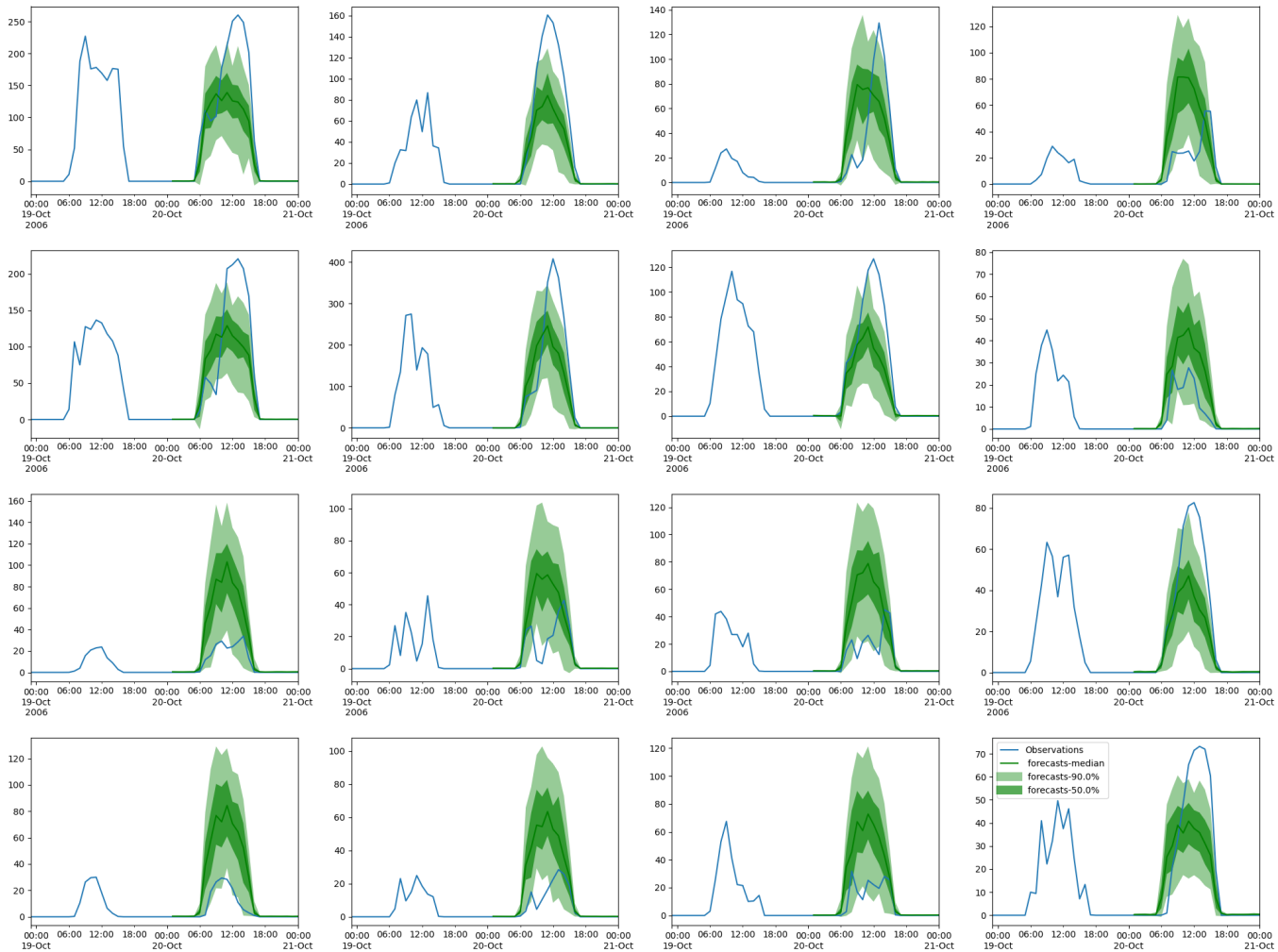


Figure 29: Forecasts produced by M-N-BEATS-Flow with *Linear-Conv-Block* on the *Solar* data set, only the forecasts of a single run are plotted.

Experiments

Forecast Plots

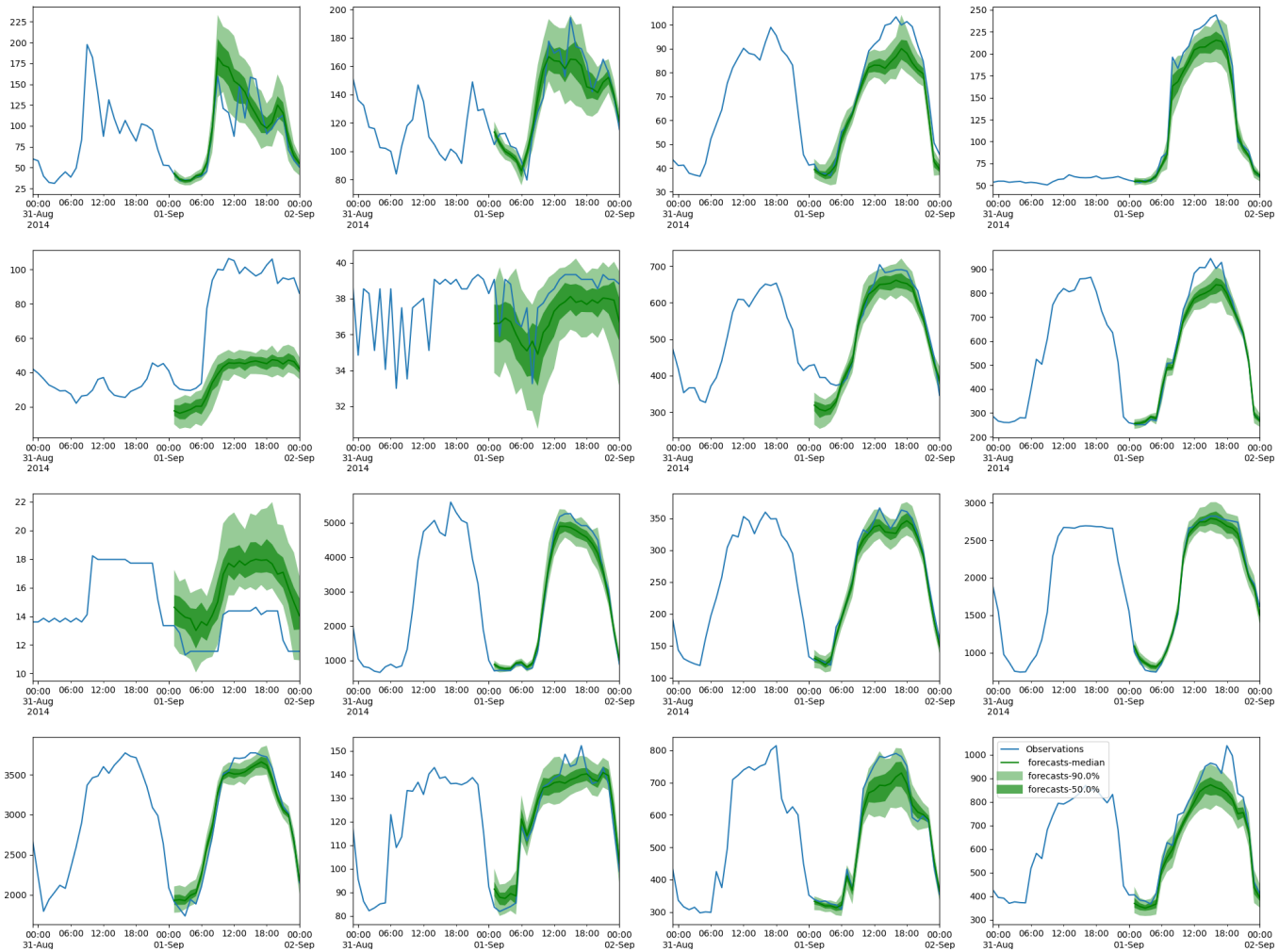


Figure 30: Forecasts produced by M-N-BEATS-Flow with *Linear-Conv-Block* on the *Electricity* data set, only the forecasts of a single run are plotted.

Experiments

Forecast Plots

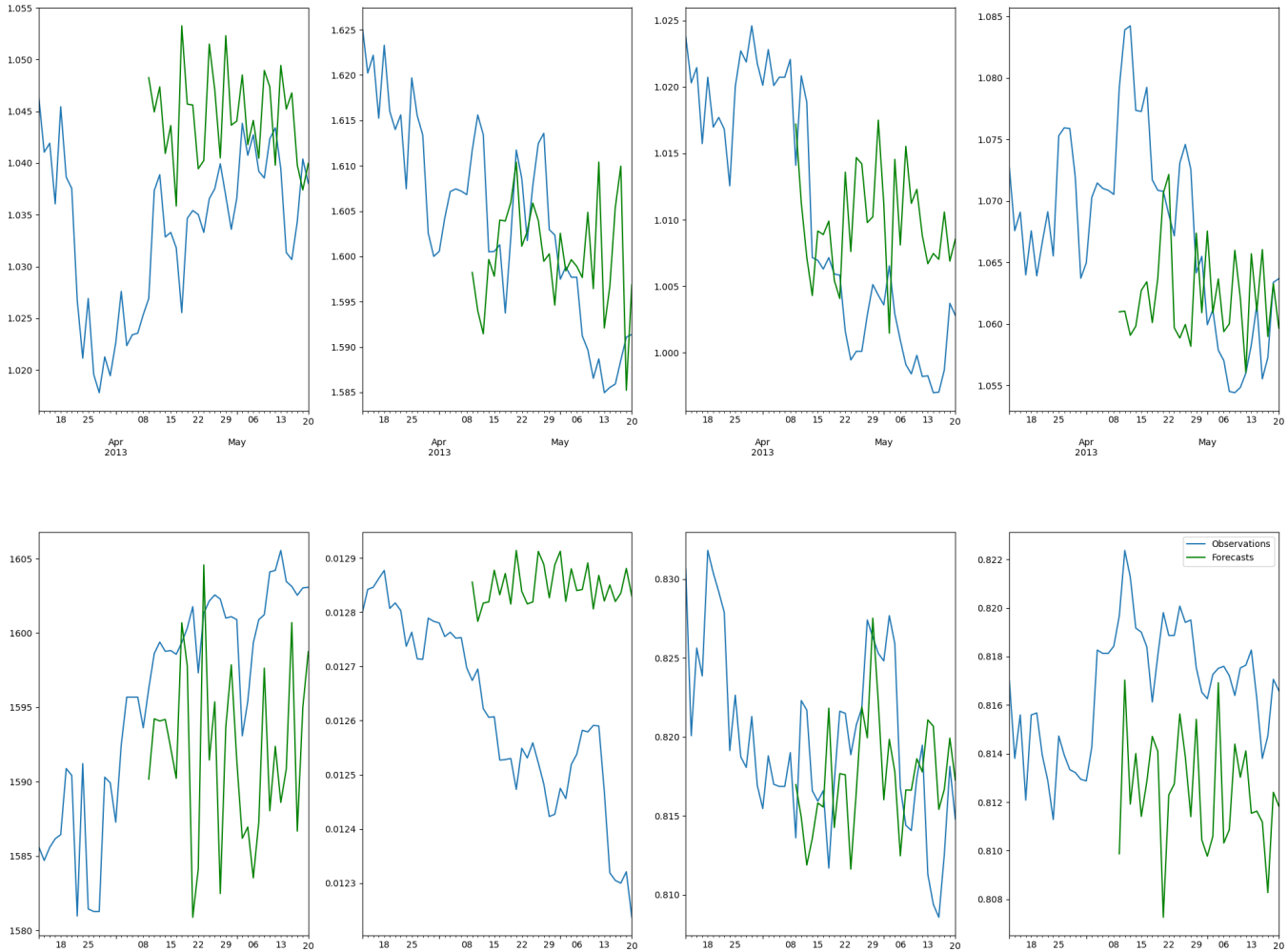


Figure 31: Forecasts produced by N-BEATS-Naive on the *Exchange Rate* data set, only the forecasts of a single run are plotted.

Experiments

Forecast Plots

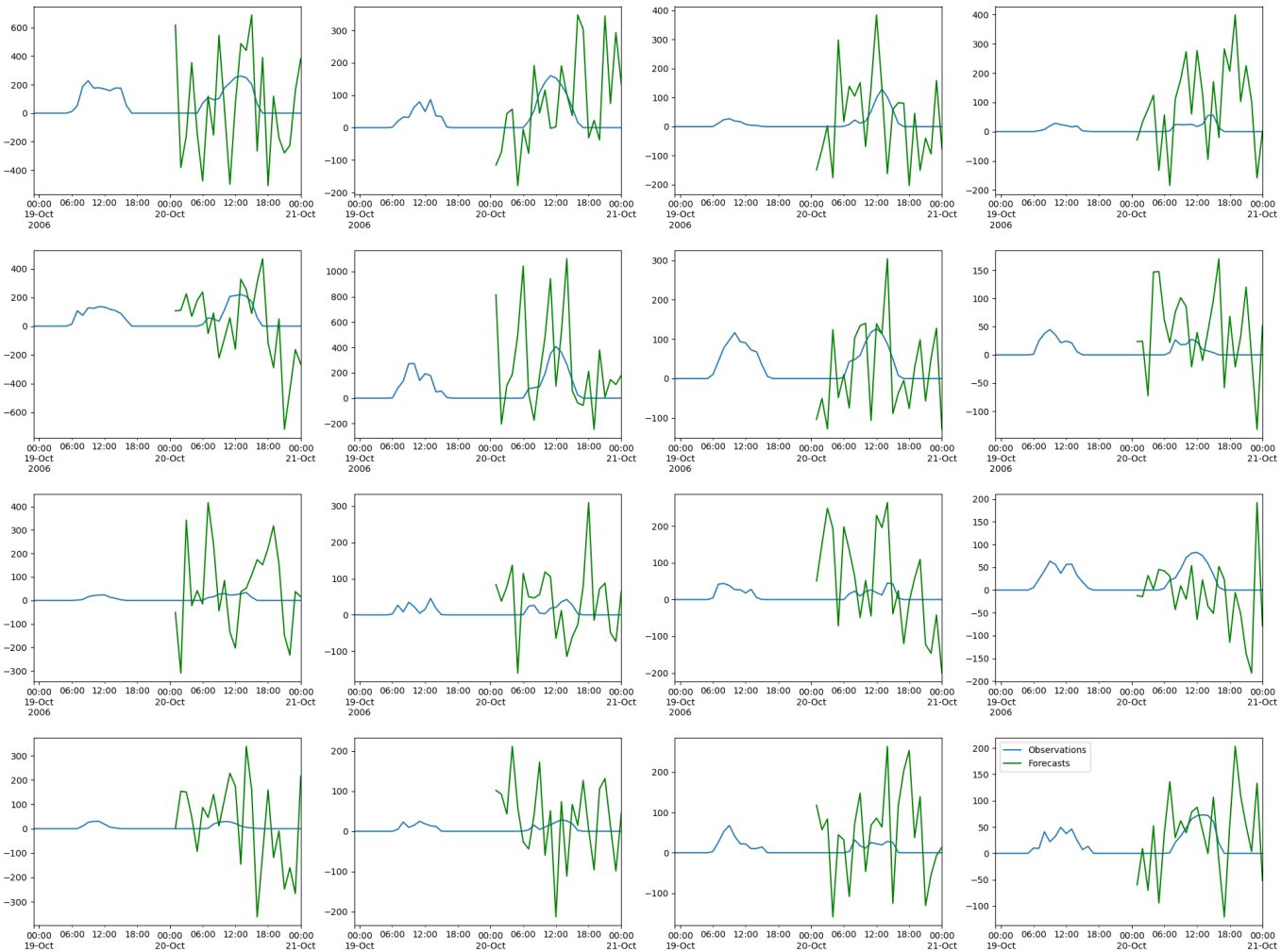


Figure 32: Forecasts produced by N-BEATS-Naive on the *Solar* data set, only the forecasts of a single run are plotted.

Experiments

N-BEATS-Naive

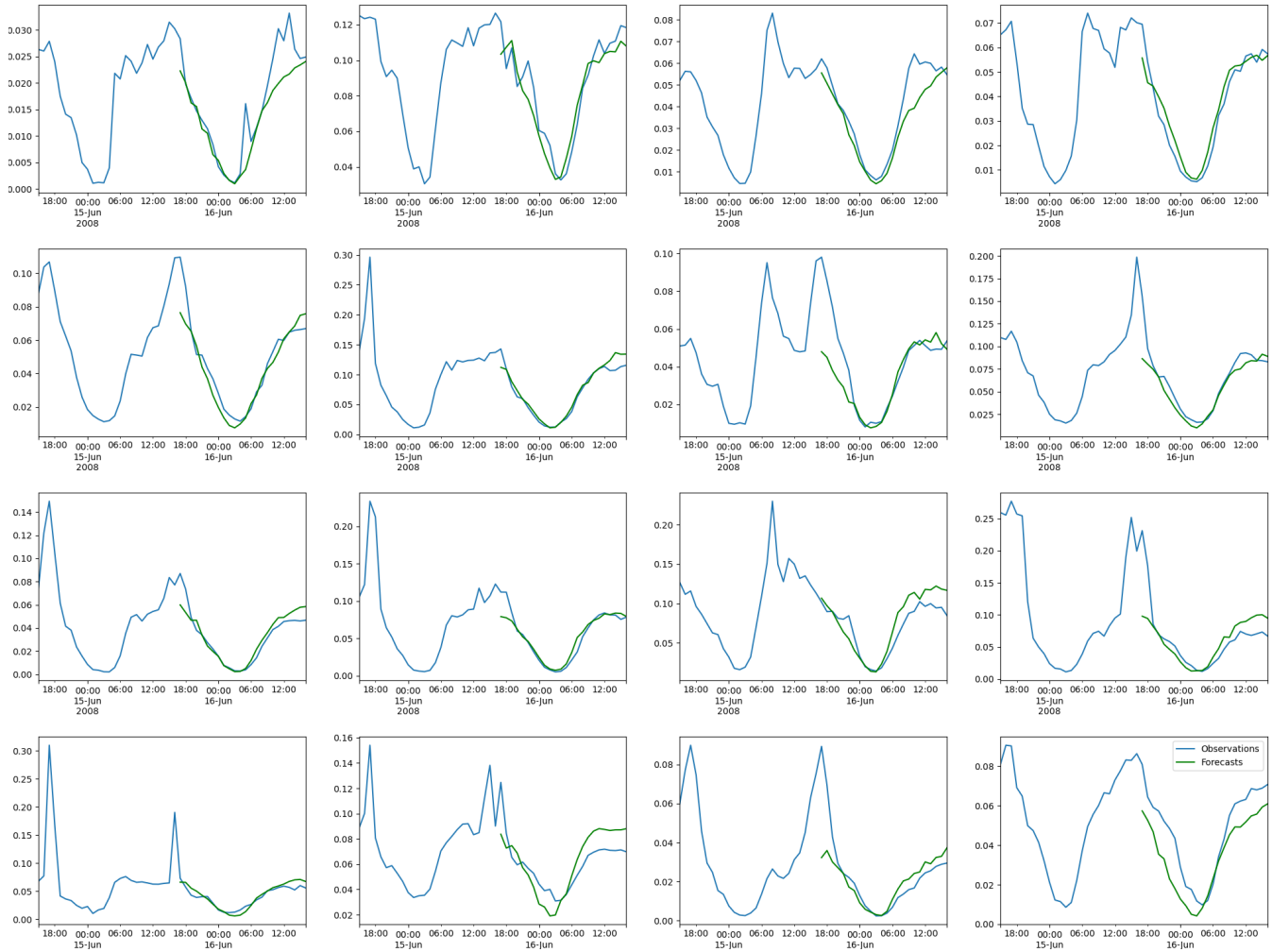


Figure 33: Forecasts produced by N-BEATS-Naive on the *Traffic* data set, only the forecasts of a single run are plotted.

Experiments

Learning Curves

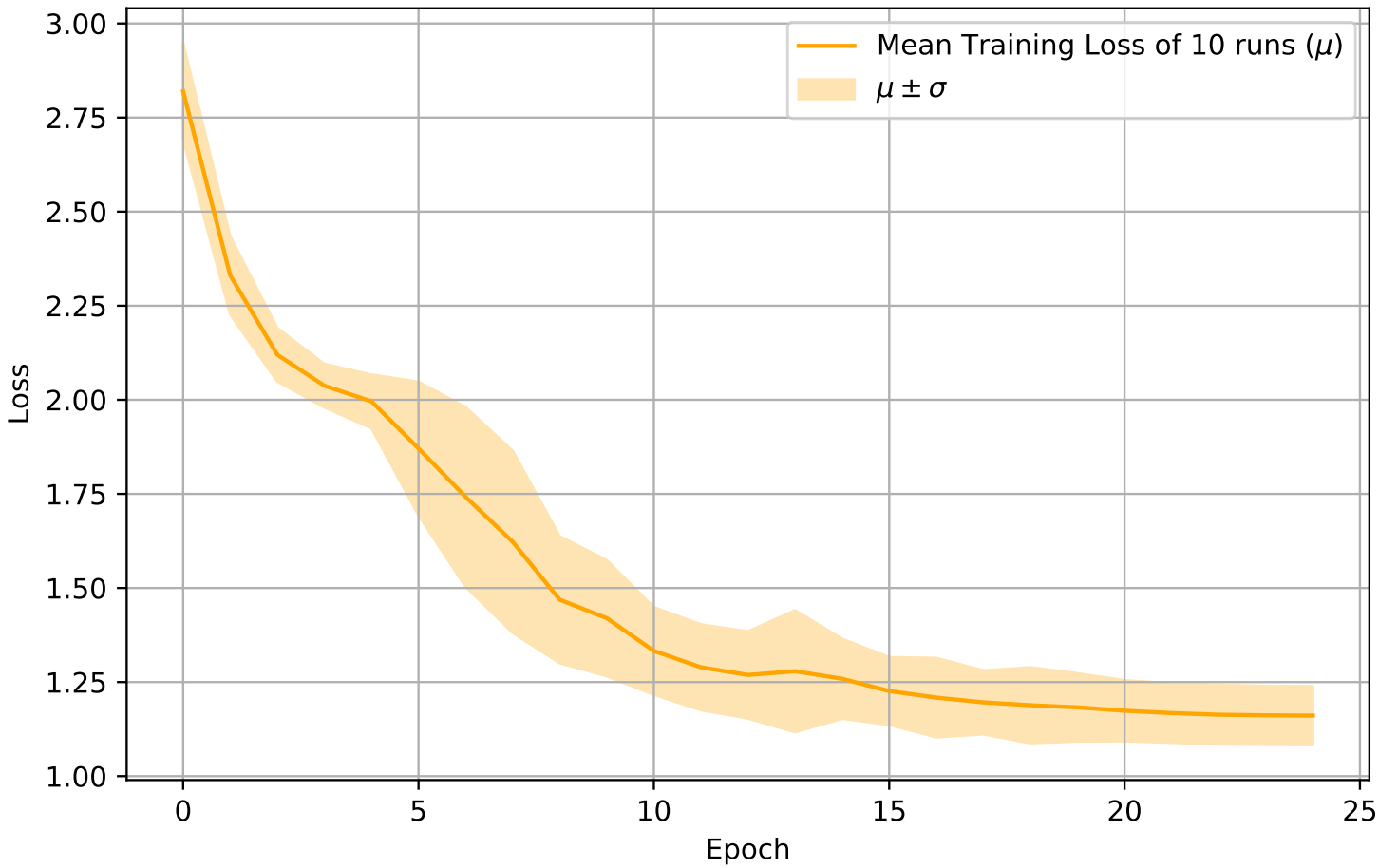


Figure 34: Learning curves for M-N-BEATS on *Electricity* data set. Mean plus minus one standard deviation is plotted.

Experiments

Learning Curves

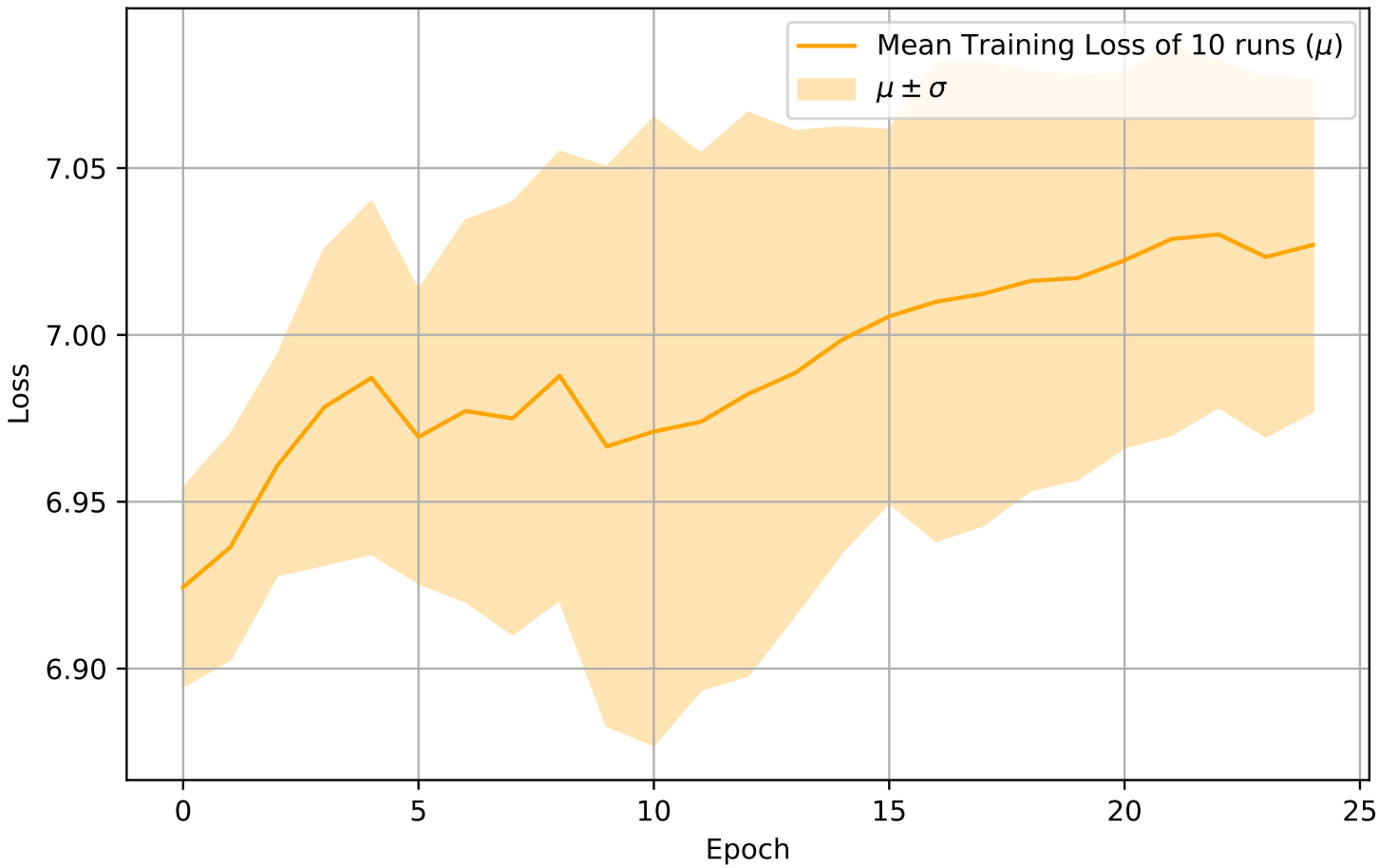


Figure 35: Learning curves for M-N-BEATS on *Solar* data set. Mean plus minus one standard deviation is plotted.

Experiments

Learning Curves

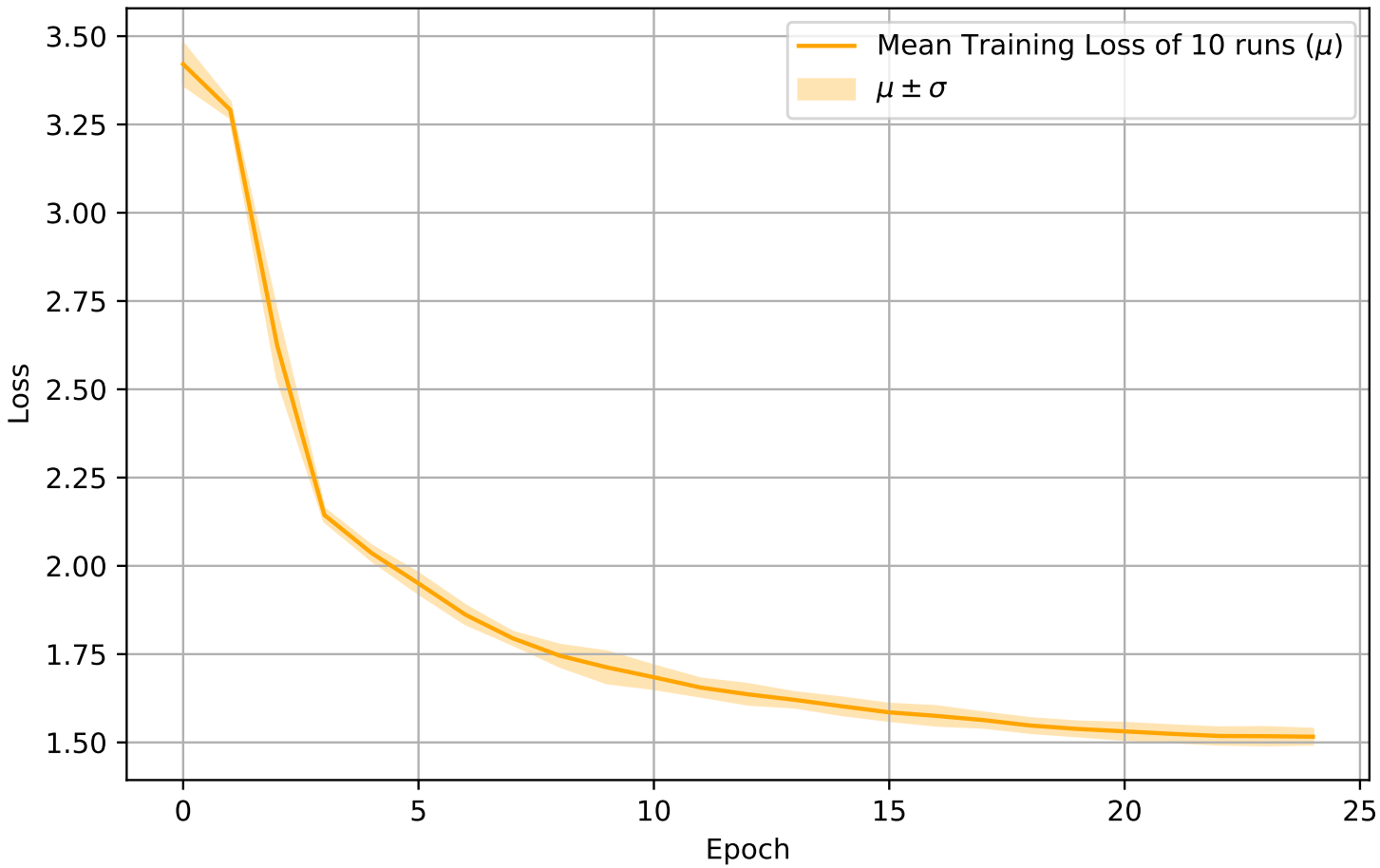


Figure 36: Learning curves for M-N-BEATS on *Traffic* data set. Mean plus minus one standard deviation is plotted.

Experiments

Learning Curves

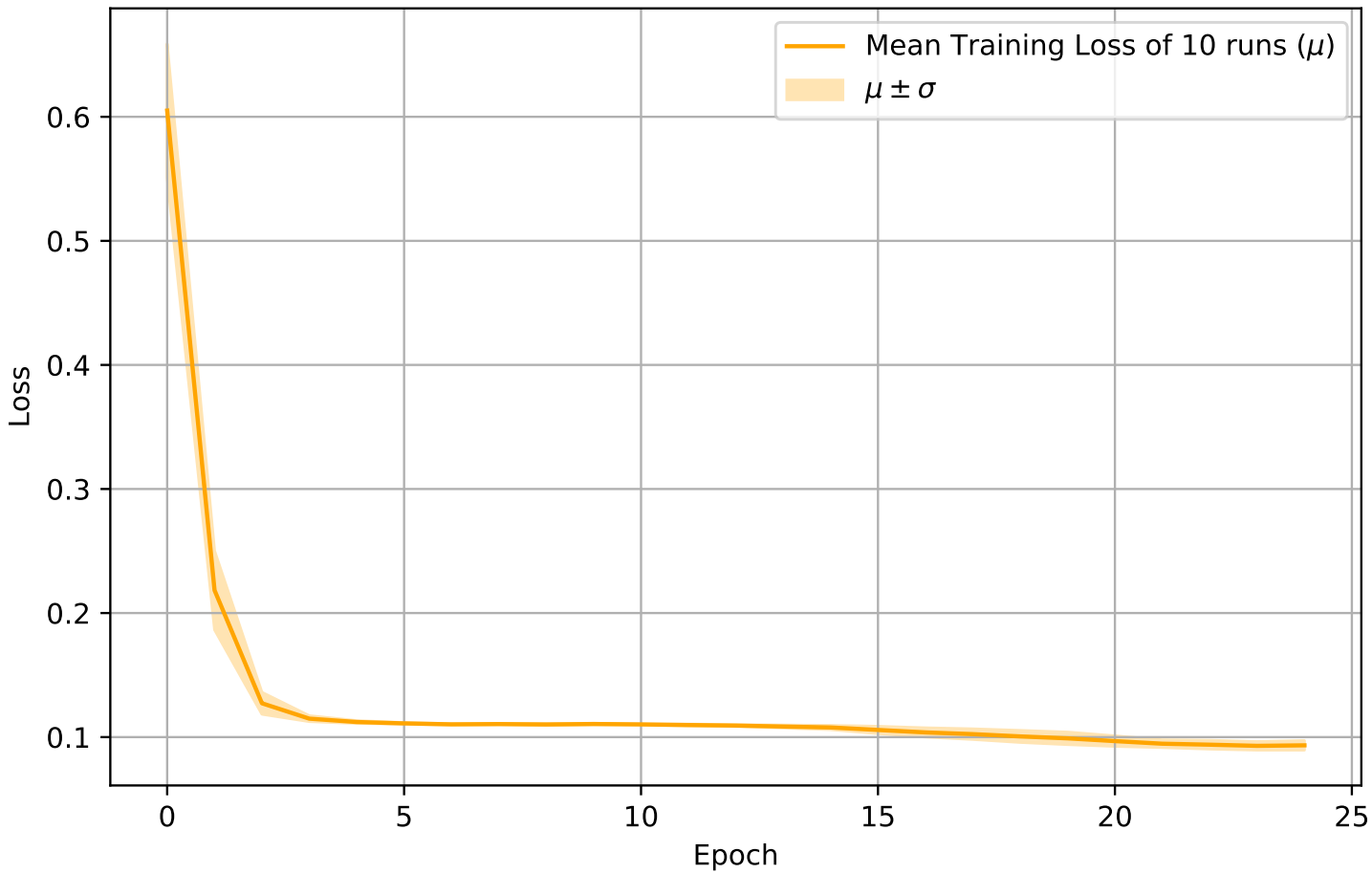


Figure 37: Learning curves for M-N-BEATS on *Exchange Rate* data set. Mean plus minus one standard deviation is plotted.

Experiments

Learning Curves

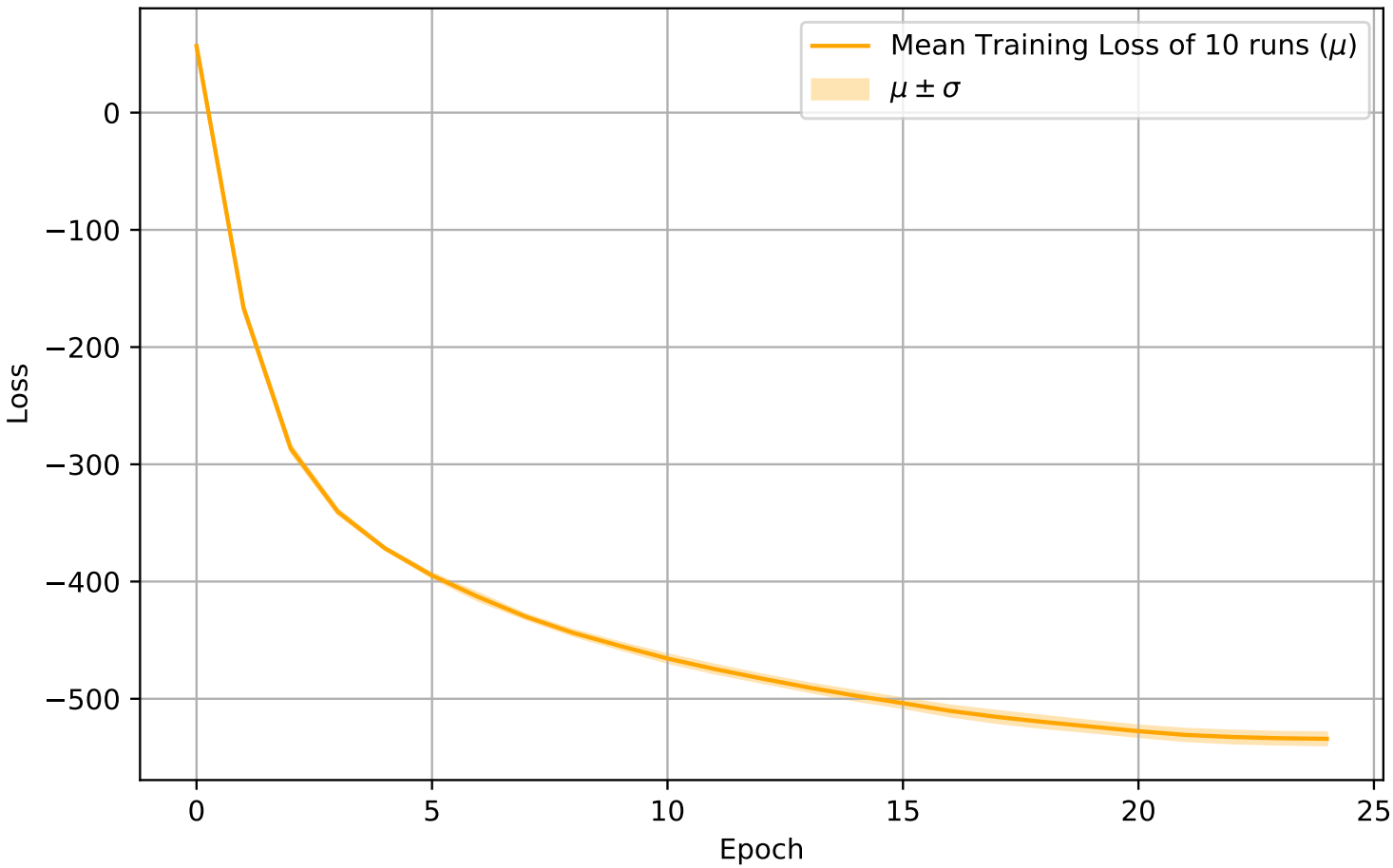


Figure 38: Learning curves for M-N-BEATS-Flow on *Electricity* data set. Mean plus minus one standard deviation is plotted.

Experiments

Learning Curves

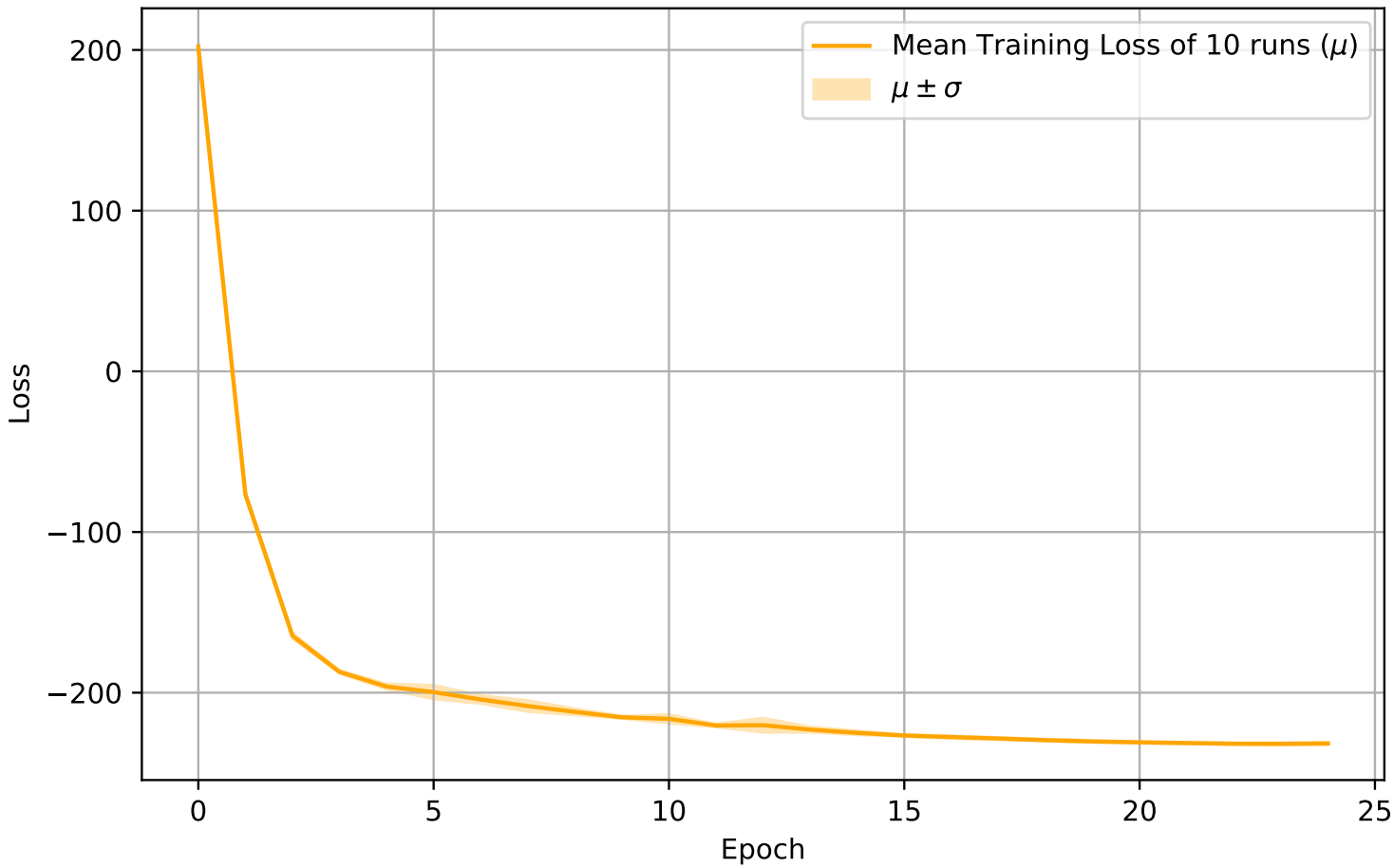


Figure 39: Learning curves for M-N-BEATS-Flow on *Solar* data set. Mean plus minus one standard deviation is plotted.

Experiments

Learning Curves

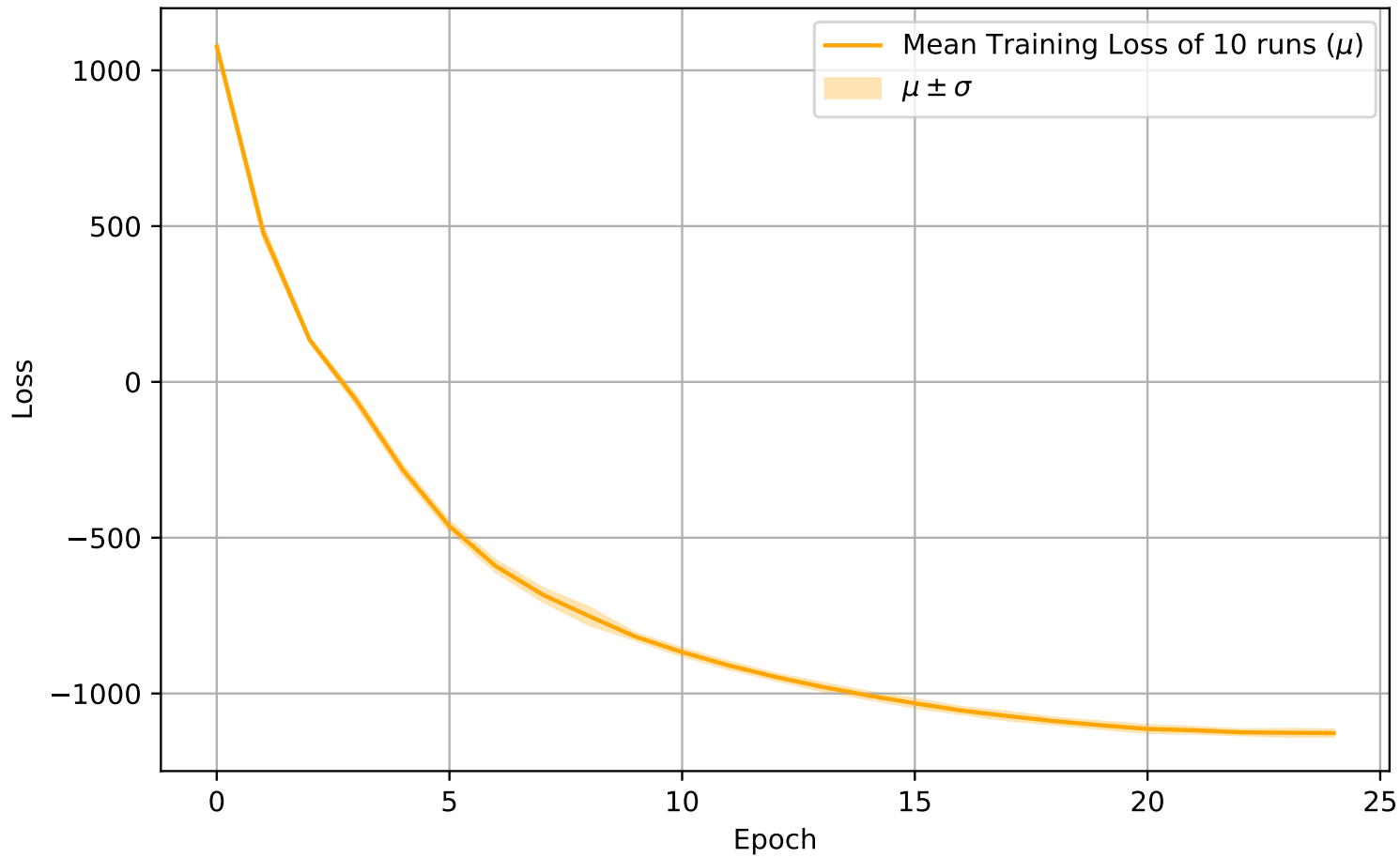


Figure 40: Learning curves for M-N-BEATS-Flow on *Traffic* data set. Mean plus minus one standard deviation is plotted.

Experiments

Learning Curves

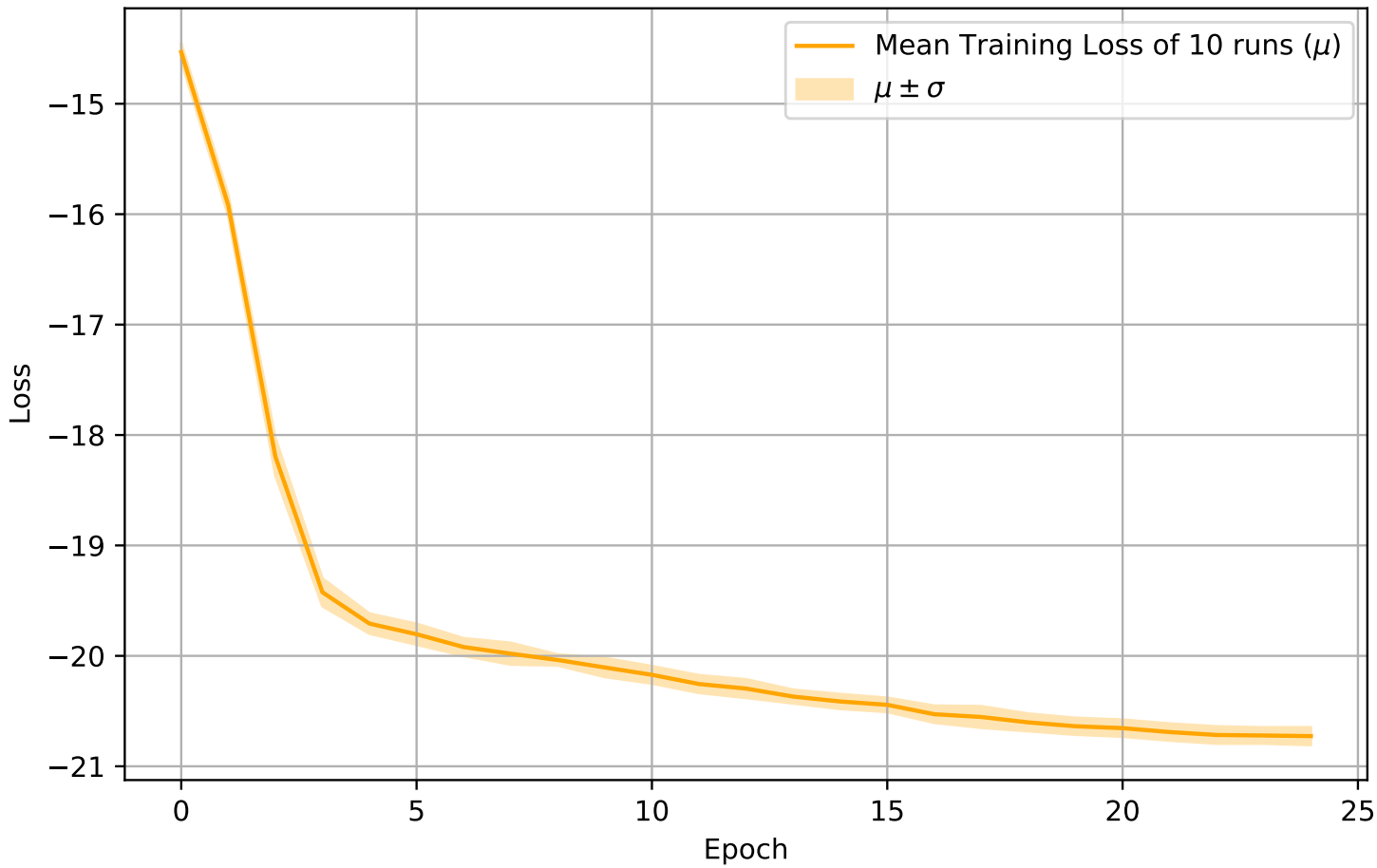


Figure 41: Learning curves for M-N-BEATS-Flow on *Exchange Rate* data set. Mean plus minus one standard deviation is plotted.