Multi-variate Probabilistic Time Series Forecasting via Conditioned Normalizing Flows

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Abstract

Time series forecasting is often fundamental to scientific and engineering problems and enables decision making. With ever increasing data set sizes, a trivial solution to scale up predictions is to assume independence between interacting time series. However, modeling statistical dependencies can improve accuracy and enable analysis of interaction effects. Deep learning methods are well suited for this problem, but multi-variate models often assume a simple parametric distribution and do not scale to high dimensions. In this work we model the multi-variate temporal dynamics of time series via an autoregressive deep learning model, where the data distribution is represented by a conditioned normalizing flow. This combination retains the power of autoregressive models, such as good performance in extrapolation into the future, with the flexibility of flows as a general purpose high-dimensional distribution model, while remaining computationally tractable. We show that it improves over the state-of-the-art for standard metrics on many real-world data sets with several thousand interacting time-series.

1. Introduction

Classical time series forecasting methods such as those in (Hyndman & Athanasopoulos, 2018) typically provide univariate forecasts and require hand tuned features to model seasonality and other parameters. Time series models based on recurrent neural networks (RNN), like LSTM (Hochreiter & Schmidhuber, 1997), have become popular methods due to their end-to-end training, the ease of incorporating exogenous covariates, and their automatic feature extraction abilities, which are the hallmarks of deep learning. Forecasting outputs can either be points or probability distributions, in which case the forecasts typically come with uncertainty bounds.

The problem of modeling uncertainties in time series forecasting is of vital importance for assessing how much to trust the predictions for downstream tasks, such as anomaly detection or (business) decision making. Without probabilistic modeling, the importance of the forecast in regions of low noise (small variance around a mean value) versus a scenario with high noise cannot be distinguished. Hence, point estimation models ignore risk stemming from this noise, which would be of particular importance in some contexts such as making (business) decisions.

Finally, individual time series, in many cases, are statistically dependent on each other, and models need the capacity to adapt to this to improve forecast accuracy (Battaglia et al., 2018). For example, to model the demand for a retail article, it is important to not only model its sales dependent on its own past sales, but also to take into account the effect of interacting articles, which can lead to cannibalization effects in the case of article competition. As another example, consider traffic flow in a network of streets as measured by occupancy sensors. A disruption on one particular street will also ripple to occupancy sensors of nearby streets — a uni-variate model would arguably not be able to account for these effects.

In this work we propose an end-to-end trainable autoregressive deep learning model for probabilistic forecasting that explicitly models multi-variate time series and their temporal dynamics employing a normalizing flow architecture, like the Masked Autoregressive Flow (Papamakarios et al., 2017) or Real NVP (Dinh et al., 2017).

The main contributions of this paper are:

1. we propose a probabilistic method to model multi-variate time series, which is able to scale to thousands of time series and their interactions

2. we demonstrate that the model can uncover ground-truth dependency structure on toy data

3. the model establishes the new state-of-the-art on many real world data sets

The model further has the advantages that:
1. the underlying data distribution is modeled using a conditional normalizing flow, which enables adaptation to a broad class of underlying data distributions

2. it is highly efficient to train due to parallelization by using attention (Vaswani et al., 2017), unlike typical RNN-based time series models. Empirically, we observe an order of magnitude faster training times for Transformer-based models.

The paper first provides some background context in Section 2. We then cover related work in Section 3. Section 4 introduces our model and the experiments are detailed in Section 5. We conclude the paper with some discussion in Section 6.

2. Background

We briefly review the current time series forecasting landscape and present the building blocks of our method in this section.

2.1. Time Series Forecasting

Classical time series forecasting methods rely on the ARMA (see e.g. Box et al. 2015) method and its variants like ARIMA. Apart from the fact that these methods require manual feature engineering, they also suffer from the curse of dimensionality, require frequent re-training and are focused on model interpretability rather than test-set accuracy.

Deep learning models over the last years have shown impressive results over classical methods in many fields (Schmidhuber, 2015) like computer vision, speech recognition, natural language processing (NLP), and also time series forecasting, which is related to sequence modeling in NLP (Sutskever et al., 2014). Modern uni-variate point forecast methods like (e.g. an isotropic Gaussian) on the space $Z$ are transformed into some simple distribution $p_Z$ (e.g. an isotropic Gaussian) on the space $Z = R^D$. This mapping $f: X \rightarrow Z$, is composed of a sequence of bijections or invertible functions. Due to the change of variables formula we can express $p_X(x)$ by

$$p_X(x) = p_Z(z) \left| \det \left( \frac{\partial f(x)}{\partial x} \right) \right|,$$

where $\partial f(x)/\partial x$ is the Jacobian of $f$ at $x$. Normalizing flows have the property that the inverse $x = f^{-1}(z)$ is easy to evaluate and computing the Jacobian determinant takes $O(D)$ time.

The bijection introduced by Real NVP (Dinh et al., 2017) called the coupling layer satisfies the above two properties. It leaves part of its inputs unchanged and transforms the other part via functions of the un-transformed variables

$$y^1:D = x^1:D$$

$$y^{d+1:D} = x^{d+1:D} \odot \exp(s(x^{1:d})) + t(x^{1:d}),$$

where $\odot$ is an element wise product, $s$ is a scaling and $t$ a translation function from $R^d \rightarrow R^{D-d}$, given by neural networks. To model a nonlinear density map $f(x)$, a number of coupling layers $X \rightarrow Y_1 \rightarrow \cdots \rightarrow Y_{K-1} \rightarrow Z$ are composed together all the while alternating the dimensions which are unchanged and transformed. Via the change of variables formula the probability density function (PDF) of
the flow given a data point can be written as

\[
\log p_x(x) = \log p_Z(z) + \log |\det(\partial z/\partial x)| \\
= \log p_Z(z) + \sum_{i=1}^{K} \log |\det(\partial y_i/\partial y_{i-1})|.
\]

(1)

Note that the Jacobian for the Real NVP is a block-triangular matrix and thus the log-determinant simply becomes

\[
\log |\det(\partial y_i/\partial y_{i-1})| = \text{sum} \{\log |\text{diag}(\exp(s(y_{i-1}))|),
\]

(2)

where \text{sum}() is the sum over all the vector elements, \log() is the element-wise logarithm and \text{diag()} is the diagonal of the Jacobian. This model, parameterized by the weights of the scaling and translation neural networks \theta, is then trained via stochastic gradient descent (SGD) on training data points where for each batch \mathcal{D} we maximize the average log likelihood (1) given by

\[
\mathcal{L} = \frac{1}{|\mathcal{D}|} \sum_{x \in \mathcal{D}} \log p_X(x; \theta).
\]

In practice Batch Normalization (Ioffe & Szegedy, 2015) is applied, as a bijection, to outputs of successive coupling layers to stabilize training of normalizing flows. This bijection implements the normalization procedure using a weighted moving average of the layer’s mean and standard deviation values, which has to be adapted to either training or inference regimes.

The Real NVP approach can be generalized, resulting in Masked Autoregressive Flows (MAF, Papamakarios et al. 2017) where the transformation layer is built as an autoregressive neural network in the sense that it takes in some input \(x \in \mathbb{R}^D\) and outputs \(c_1, \ldots, c_D\) with the requirement that this transformation is invertible and any output \(c_i\) cannot depend on input dimensions \(x^{>i}\). The Jacobian of this transformation is triangular and thus the Jacobian determinant is tractable. Instead of using a RNN to share parameters across the \(D\) dimensions of \(x\) one avoids this sequential computation by using masking, giving the method its name. The inverse however, needed for generating samples, is sequential.

By realizing that the scaling and translation function approximators don’t need to be invertible, it is straightforward to implement conditioning of the PDF \(p_X(x|h)\) on some additional information \(h \in \mathbb{R}^H\): we concatenate \(h\) to the inputs of the scaling and translation function approximators of the coupling layers, i.e. \(s(\text{concat}(x^{1:d}, h))\) and \(t(\text{concat}(x^{1:d}, h))\) which are modified to map \(\mathbb{R}^{d+H} \rightarrow \mathbb{R}^{D-d}\). Another approach is to add a bias computed from \(h\) to every layer inside the \(s\) and \(t\) networks as proposed by (Korshunova et al., 2018). This does not change the log-determinant of the coupling layers given by (2). More importantly for us, for sequential data we can share parameters across the different conditioners by using RNNs in an autoregressive fashion.

For discrete data the distribution has differential entropy of negative infinity, which leads to arbitrary high likelihoods when training normalizing flow models, even on test data. To avoid this one can dequantize the data, often by adding Uniform[0, 1] noise. The log-likelihood of the continuous model is then lower-bounded by the log-likelihood of the discrete one as shown in Theis et al. (2016).

2.3. Self-attention

The self-attention based Transformer layer (Vaswani et al., 2017) has been used for sequence modeling with great success. The multi-head self-attention mechanism enables it to capture both long- and short-term dependencies in time series data. Essentially, the Transformer takes in a sequence \(X = [x_1, \ldots, x_t]^T \in \mathbb{R}^{t \times D}\), and the multi-head self-attention transforms this into \(H\) distinct query matrices \(Q_h = XW^Q_h\), key matrices \(K_h = XW^K_h\), and value matrices \(V_h = XW^V_h\) where the \(W^Q_h, W^K_h,\) and \(W^V_h\) are the learnable parameters. After these linear projections the scaled dot-product attention computes a sequence of vector outputs via:

\[
O_h = \text{Attention}(Q_h, K_h, V_h) \\
= \text{softmax} \left( \frac{Q_h K_h^T}{\sqrt{d_k}} \right) M V_h,
\]

where a mask \(M\) is applied to filter out right-ward attention (or future information leakage) by setting its upper-triangular elements to \(-\infty\) and we normalize by \(d_k\), the dimension of the \(W^K_h\) matrices. Afterwards all the \(H\) \(O_h\) outputs are concatenated and linearly projected again.

One typically uses the Transformer in an encoder-decoder setup, where some warm up time series is passed through the encoder and the decoder can be used to learn and autoregressively generate outputs.

3. Related Work

Related to this work are models that combine normalizing flows for sequential modeling in some way. Transformation Autoregressive Networks (TANs, Oliva et al. 2018) which model the density of a multi-variate variable \(x \in \mathbb{R}^D\) as \(D\) conditional distributions \(p_X(x^t | x^{t-1}, \ldots, x^1)\), where the conditioning is given by a mixture model coming from the state of a RNN, and is then transformed via a bijection. The PixelSNAIL (Chen et al., 2018) method also models the joint as a product of conditional distributions, optionally with some global conditioning, via causal convolutions and
We denote the entities of a multi-variate time series by \( x_t^i \in \mathbb{R} \) for \( i \in \{1, \ldots, D\} \) where \( t \) is the time index. Thus the multi-variate vector at time \( t \) is given by \( x_t \in \mathbb{R}^D \). In this paper, we investigate the effect of the time evolution and the output distribution module on both statistical accuracy and computation time. We find that an attention layer for time evolution together with an MAF output density model results in high forecasting accuracy. At the same time, attention results in orders of magnitudes faster training.

In the DeepAR model (Flunkert et al., 2017), the log-likelihood of each entity \( x_t^i \) at a time step \( t \in [1, t_0] \) is maximized given an individual time series’ history. This is done with respect to the parameters of the chosen distributional model (e.g. negative binomial for count data) via the state of a RNN derived from its previous time step \( x_{t-1}^i \) and its corresponding covariates \( c_{t-1}^i \). The emission distribution model, which is typically Gaussian for real-valued data or negative binomial for count data, is selected to best match the statistics of the time series and the network incorporates activation functions that satisfy the constraints of these distribution parameters, e.g. a \( \text{softplus()} \) for the scale parameter of the Gaussian.

A simple model for multi-variate real-valued data could use a factorizing distribution in the emissions. Shared parameters can then learn patterns across the individual time series through the temporal component — but the model falls short of capturing dependencies in the emissions of the model. For this, a full joint distribution at each time step must be modeled, for example by using a multivariate Gaussian model. However, modeling the full covariance matrix not only increases the number of parameters of the neural network by \( O(D^2) \), making learning difficult, but computing the loss becomes expensive when \( D \) is large. Further, statistical dependencies in the emissions would be limited to second-order effects. These models are referred to as Vec-LSTM in Salinas et al. (2019).

![Figure 1. RNN Conditioned Real NVP model schematic at time \( t \), consisting of \( K \) blocks of coupling layers and Batch Normalization, where in each coupling layer we condition \( x_t \) and its transformations on the state of a shared RNN from the previous time step \( x_{t-1} \) and its covariates \( c_{t-1} \) which are typically time dependent and time independent features.](image-url)

We wish to have a scalable model of \( D \) interacting time-series \( x_t \), and further to use a flexible distribution model on the emissions that allows to capture and represent higher order moments. To this end, we model the conditional joint distribution at time \( t \) of all time series \( p_X(x_t | h_t; \theta) \) with a flow, e.g. a Real NVP, conditioned on either the hidden state of a RNN at time \( t \) or an embedding of the time series up to \( t \) from an attention module. In the case of an autoregressive RNN (either a LSTM or a GRU; Chung et al. 2014), its hidden state \( h_t \) is updated given the previous time step observation \( x_{t-1} \) and its associated covariates \( c_{t-1} \) (as in...
This model is autoregressive since it consumes the observation of the last time step $x_{t-1}$ as well as the recurrent state $h_{t-1}$ to produce the state $h_t$ on which we condition the current observation.

To get a powerful emission distribution model, we stack $K$ layers of the flow model (Real NVP or MAF). Together with the RNN, we arrive at our model of the conditional distribution of the future of all time series, given its past $t \in [1, t_0 - 1]$ and all the covariates in $t \in [1, T]$. As the model is autoregressive it can be written as a product of factors

$$p_X(x_{t_0:T} | x_{1:t_0-1}, c_{1:T}) = \prod_{t=t_0}^T p_X(x_t | h_t; \theta),$$

where $\theta$ denotes the set of all parameters of both the flow and the RNN.

For modeling the time evolution, we also investigate using an attention module (Vaswani et al., 2017). This is used to compute an embedding of the time series up to $t$, which we will also call $h_t$ for simplicity. In this case, the training time series is split into a warm up or encoding portion $x_{1:t-1}$ and the output portion $x_{t:T}$. See Figure 2 for a schematic of the overall model in this case. In training, care has to be taken to prevent using information from future time points and to preserve the autoregressive property by utilizing a mask that reflects the causal direction of progressing time, i.e. to mask out future time points.

In real-world data the magnitudes of different time series can vary drastically. To normalize scales, we divide each individual time series by its mean before feeding it into the model. The outputs are then correspondingly multiplied with the same mean values to match the original scale. This rescaling technique simplifies the problem for the model, which is reflected in significantly improved empirical performance.

### 4.1. Training

Given data of $D$ time series, where at each time step we have $x_t \in \mathbb{R}^D$ and their associated covariates $c_t$, we maximize the log-likelihood given by (1) and (3)

$$\mathcal{L} = \frac{1}{|D|T} \sum_{x_{1:T} \in D} \sum_{t=1}^T \log p_X(x_t | h_t; \theta)$$

via SGD using Adam (Kingma & Ba, 2015) with respect to the parameters $\theta$ of the conditional flow and the RNN or Transformer. In practice, the time series $x_{1:T}$ in a batch $D$ is selected from a random time window of size $T$ within our training data, and the relative time steps are kept constant. This allows the model to learn to cold-start given only the covariates. This also increases the size of our training data when the training window size is not too large and allows us to trade-off computation time with memory consumption especially when $D$ or $T$ are large. Note that information about absolute time is only available to the RNN or Transformer via the covariates and not the relative position of $x_t$ in the training data.

The Transformer has computational complexity $O(T^2F)$ compared to a RNN which is $O(TF^2)$, where $F$ is the dimension of the hidden state and $T$ the time series length. This means for large multi-variate time series, i.e. $D > T$, and the assumption that the dimension of the hidden state grows proportional to the number of simultaneous time-series modeled, i.e. $F \propto D$, the Transformer flow model has smaller computational complexity. In addition, unlike the RNN, all the computation for training happens in parallel. The Transformer allows the model to access any part of the historic time series regardless of temporal distance and thus is able to generate better conditioning for the normalizing flow.

### 4.2. Covariates

We employ embeddings for categorical features (Charrington, 2018), which allows for relationships within a category, or its context, to be captured while training models. Combining these embeddings as features for time series forecasting yields powerful models like the first place winner of the Kaggle Taxi Trajectory Prediction challenge (De Brébisson et al., 2015). The covariates $c_t$ we use are composed

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1. https://www.kaggle.com/c/pkdd-15-predict-taxi-service-trajectory-i
of time-dependent (e.g. day of week, hour of day) and time-independent embeddings, if applicable, as well as lag features depending on the time frequency of the data set we are training on. All covariates must be known for the time periods we wish to forecast.

4.3. Inference

For inference we either obtain the hidden state \( \tilde{h}_{t_0+1} \) by passing a “warm up” time series \( x_{t_0:t} \) through the RNN or use the cold-start hidden state, i.e. we set \( h_{t_0+1} = h_0 \), and then by sampling a noise vector \( z_{t_1+1} \in \mathbb{R}^D \) from an isotropic Gaussian, go backward through the flow to obtain a sample of our time series for the next time step conditioned on this starting state \( x_{t_0+1} = f^{-1}(z_{t_1+1}|h_{t_0+1}) \). We then use this sample and its covariate to obtain the next conditioning state \( h_{t_2+2} \) via the RNN and repeat till our inference horizon. This process of sampling trajectories from some initial state can be repeated many times to obtain empirical quantiles of the uncertainty of our prediction for arbitrary long forecast horizons.

The attention model similarly uses a warm up time series \( x_{t_0:t} \) and covariates and passes them through the encoder and then uses the decoder to output the conditioning for sampling from the flow. This sample is then used again in the decoder to iteratively sample the next conditioning state, similar to the inference procedure in seq-to-seq models.

5. Experiments

Here we discuss a toy experiment sanity-checking our model as well as results on six real world data sets.

5.1. Simulated Flow in a System of Pipes

In this experiment, we check for some basic properties of our model by simulating flow of a liquid in a system of pipes with valves. See Figure 3 for a depiction of the system.

```
S0 V1 S1 V2 S2 S3
V1
V2
S0
S1
S2
S3
```

**Figure 3.** System of pipes with liquid flowing from left to right with sensors (S) and valves (V).

Liquid flows from left to right, where pressure at the first sensor in the system is given by \( S_0 = X + 3, X \sim \text{Gamma}(1, 0.2) \) in the shape/scale parameterization of the Gamma distribution. The valves are given by \( V_1, V_2 \sim \text{Beta}(0.5, 0.5) \), and we have

\[
S_i = \frac{V_i}{V_1 + V_2} S_0 + \epsilon_i
\]

for \( i \in \{1, 2\} \) and finally \( S_3 = S_1 + S_2 + \epsilon_3 \) with \( \epsilon_4 \sim \mathcal{N}(0, 0.1) \). With this simulation we check whether our model captures correlations in space and time. The correlation between \( S_1 \) and \( S_2 \) results from both having the same source, measured by \( S_0 \). This is reflected by \( \text{Cov}(S_1, S_2) > 0 \), which is captured by our model.

**Figure 4.** Covariance matrix for a fixed time point capturing the correlation between \( S_1 \) and \( S_2 \). Darker means higher positive values.

The cross-covariance structure between consecutive time points in ground truth and as captured by our trained model is depicted in Figure 5. It reflects the true flow of liquid in the system from \( S_0 \) at time \( t \) to \( S_1 \) and \( S_2 \) at time \( t + 1 \), on to \( S_3 \) at time \( t + 2 \).

**Figure 5.** Cross-covariance matrix between consecutive time points capturing true flow of liquid in the pipe system. Darker means higher positive values.

5.2. Real World Data Sets

For evaluation we compute the Continuous Ranked Probability Score (CRPS) (Matheson & Winkler, 1976) on each individual time series, as well as on the sum of all time series (the latter denoted by \( \text{CRPS}_{\text{sum}} \)). CRPS measures the compatibility of a cumulative distribution function \( F \) with an observation \( x \) as

\[
\text{CRPS}(F, x) = \int_{\mathbb{R}} (F(z) - I\{x \leq z\})^2 \, dz \quad (5)
\]

where \( I\{x \leq z\} \) is the indicator function which is one if \( x \leq z \) and zero otherwise. CRPS is a proper scoring function, hence CRPS attains its minimum when the predictive
We use batch sizes of \(100\) from (Salinas et al., 2019) and we used \(40\) train for a maximum of mean-scaled). Our model is trained on the training split of each data set, and for testing we use a rolling windows prediction starting series — both for the ground-truth data, and sampled data of the conditional distribution \((4)\) at each time point (Jordan et al., 2019). We take 100 samples to estimate the empirical CDF in practice. In comparison to log-likelihood, CRPS puts heavier penalty on the distribution tails (Gebetsberger et al., 2018). Finally, CRPS\(_{\text{sum}}\) is obtained by first summing across the \(D\) time-series — both for the ground-truth data, and sampled data (yielding \(\hat{F}_{\text{sum}}(t)\) for each time-point). The results are then averaged over the prediction horizon, i.e. formally

\[
\text{CRPS}_{\text{sum}} = \mathbb{E}_{t} \left[ \text{CRPS} \left( \hat{F}_{\text{sum}}(t), \sum_i x_i^t \right) \right].
\]

Our model is trained on the training split of each data set, and for testing we use a rolling windows prediction starting from the last point seen in the training data set and compare it to the test set.

We train on Exchange (Lai et al., 2018), Solar (Lai et al., 2018), Electricity\(^2\), Traffic\(^3\), Taxi\(^4\) and Wikipedia\(^5\) open data sets, preprocessed exactly as in (Salinas et al., 2019), with their properties listed in Table 2. Both Taxi and Wikipedia consist of count data and are thus dequantized before being fed to the flow (and mean-scaled).

We use batch sizes of 32, with 100 batches per epoch and train for a maximum of 40 epochs with a learning rate of \(1\text{e}^{-3}\). The LSTM/GRU hyperparameters were the ones from (Salinas et al., 2019) and we used \(K = 3\) or \(K = 5\) stacks of normalizing flow bijections. We sample 100 times to report the metrics on the test set. The Transformer uses \(H = 8\) heads and \(n = m = 3\) encoding and decoding layers and a dropout rate of 0.1. No extensive hyperparameter tuning was done. All the experiments run on a single Nvidia V-100 GPU.

We compare our method using GRU and two different normalizing flows (GRU-Real-NVP and GRU-MAF based on Real NVP and MAF, respectively) as well as a Transformer model with MAF (Transformer-MAF), with different RNN based methods and transformation schemes from (Salinas et al., 2019) and report the results in Table 1. Vec-LSTM-ind-scaling outputs the parameters of an independent normal distribution with mean-scaling. Vec-LSTM-lowrank-Copula parametrizes a low-rank plus diagonal covariance via Copula process. GP-scaling unrolls a LSTM with scaling on each individual time series before reconstructing the joint distribution. Similarly, GP-Copula unrolls a LSTM on each individual time series and then the joint emission distribution is given by a low-rank plus diagonal covariance Gaussian copula.

In Table 1 we observe that MAF with either RNN or self-attention mechanism for temporal conditioning achieves the state-of-the-art (to the best of our knowledge) CRPS\(_{\text{sum}}\) on all benchmarks. Moreover, bipartite flows with RNN either also outperform or are found to be competitive w.r.t. to the previous state-of-the-art results as listed in the first four columns of Table 1. Further analyses with other metrics (e.g. MSE) are reported in the Supplementary Material.

To assess how well our model captures dependencies in ex-

### Table 1. Test set CRPS\(_{\text{sum}}\) comparison (lower is better) of models from (Salinas et al., 2019) and our models GRU-Real-NVP, GRU-MAF and Transformer-MAF. The \(\mathbf{\text{\text{\textbf{n\ occurred}}}}\) best methods are in bold where the mean and standard errors are obtained by re-running each method three times.

| Data set       | Vec-LSTM ind-scaling | Vec-LSTM lowrank-Copula | GP scaling | GP Copula | GRU Real-NVP | GRU MAF | Transformer MAF |
|----------------|----------------------|-------------------------|------------|-----------|--------------|---------|-----------------|
| Exchange       | 0.008±0.001          | 0.007±0.000             | 0.009±0.000 | 0.007±0.000 | 0.0064±0.001 | 0.005±0.001 | 0.005±0.001     |
| Solar          | 0.391±0.017          | 0.319±0.011             | 0.368±0.012 | 0.337±0.024 | 0.331±0.02   | 0.315±0.023 | 0.301±0.014     |
| Electricity    | 0.025±0.001          | 0.064±0.008             | 0.022±0.000 | 0.024±0.002 | 0.024±0.001  | 0.0208±0.000 | 0.0207±0.000    |
| Traffic        | 0.087±0.041          | 0.103±0.006             | 0.079±0.000 | 0.078±0.002 | 0.078±0.001  | 0.069±0.002  | 0.056±0.001     |
| Taxi           | 0.506±0.005          | 0.326±0.007             | 0.183±0.305 | 0.208±0.183 | 0.175±0.001  | 0.161±0.002  | 0.179±0.002     |
| Wikipedia      | 0.133±0.002          | 0.241±0.033             | 1.483±1.034 | 0.086±0.004 | 0.078±0.001  | 0.067±0.001  | 0.063±0.003     |

### Table 2. Properties of the experiment data sets.

| DATA SET       | DIMENSION \(D\) | DOMAIN | FREQ. |
|----------------|-----------------|--------|-------|
| EXCHANGE       | 8               | \(\mathbb{R}^+\) | DAILY |
| SOLAR          | 137             | \(\mathbb{R}^+\) | HOURLY|
| ELECTRICITY    | 370             | \(\mathbb{R}^+\) | HOURLY|
| TRAFFIC        | 963             | (0, 1) | HOURLY|
| TAXI           | 1, 214          | N      | 30-MIN|
| WIKIPEDIA      | 2, 000          | N      | DAILY |
Figure 6. Analysis of the dependency structure extrapolation of the model. Left: Cross-covariance matrix computed from the test split of Traffic benchmark. Middle: Cross-covariance matrix computed from the mean of 100 sample trajectories drawn from the Transformer-MAF model’s extrapolation into the future (test split). Right: The absolute difference of the two matrices mostly shows small deviations between ground-truth and extrapolation.

6. Conclusion

We have presented a general method to model high-dimensional probabilistic multivariate time series via combining conditional normalizing flows with an autoregressive model, such as a recurrent neural network or an attention module. Autoregressive models have a long-standing reputation for working very well for time series forecasting, as they show good performance in extrapolation into the future. The flow model, on the other hand, does not assume any simple fixed distribution class, but instead can adapt to a broad range of high-dimensional data distributions. The combination hence combines the extrapolation power of the autoregressive model class with the density estimation flexibility of flows. Further, it is computationally efficient, without the need of resorting to approximations (e.g. low-rank approximations of a covariance structure). Analysis on six commonly used time series benchmarks establish the new state-of-the-art performance, without much hyperparameter tuning.

A natural way to improve the model is to incorporate a better underlying flow model. For example, Table 1 showed that swapping a Real NVP flow in for a MAF improved performance, which is a consequence of Real NVP lacking in density modeling performance compared to MAF. Likewise, we would expect other design choices of the flow model to improve performance, e.g. changes on the dequantization method, the specific affine coupling layer or more expressive conditioning, say via another Transformer. Recent improvements to flows, e.g. as proposed in the Flow++ paper (Ho et al., 2019), to obtain expressive bipartite flow models, or better flow models to handle discrete categorical data (Tran et al., 2019), are left as future work to assess their usefulness. To our knowledge, it is however still an open problem how to model discrete ordinal data via flows — which would best capture the nature of some data sets (e.g. sales data).

Also, we would expect improvements in the time evolution module to improve the time series forecasts. For example, recent improvements to the Transformer like the Reformer (Kitaev et al., 2020) could improve memory efficiency. We leave these improvements to future investigations.

Finally, real-world applications might require training on very large number of interacting time series $D$, such as e.g. in sales modeling in e-Commerce, where $D$ can be in the order of millions or more. Flows have been successfully applied to image modeling, which is comparable to the instantaneous dimensionality faced in this setting — but the memory requirement becomes infeasible for large time-series. In future work, we’ll investigate mechanisms for scalable training of time-series models, e.g. by subsampling time-series.
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