

Autoregressive Models

The *WaveNet* Architecture; with code*

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WaveNet*

Wavenet: A generative model for raw audio.

Aaron van den Oord, et al.

@deepmind, 2016

Contributions

- Generative model for wave-form forms
- Capable of capturing important audio structure at many time-scales
- Conditioning support

Led to the **most natural-sounding** speech/audio synthesis at the time.

*<https://arxiv.org/abs/1609.03499>

Content

This talk covers

- an introduction to autoregressive models and some of their limitations,
- the architectural ideas to overcome those limitations, and
- few of existing improvements.

This talk is not

- about audio/speech (we use time series / images instead),
- a comprehensive state-of-the-art presentation on generative models.

Accompanying code: <https://github.com/cheind/autoregressive>

Background

Generative Models

Generative models build a distribution over the data itself. Consider a set of random variables

$$\mathbf{X} = \{X_1, X_2, X_3\},$$

then a generative model estimates

$$p(\mathbf{X}).$$

Generative Model Applications

Given the joint distribution, we can carry out a number of tasks using our model

1. Generate novel data: $\mathbf{x} \sim p(\mathbf{X})$
2. Estimate density of observations: $p(\mathbf{X} = \mathbf{x})$
3. Perform conditional inference: $p(X_3 | X_2 = x_2, X_1 = x_1)$

In the experiments below we will also see how to use conditioning to perform MNIST classification.

Chain Rule of Probability

Allows us to break down $p(\mathbf{X})$ into a product of single-variable conditional distributions

$$\begin{aligned} p(\mathbf{X}) &= p(X_3 \mid X_2, X_1)p(X_2 \mid X_1)p(X_1) \\ &= p(X_1 \mid X_2, X_3)p(X_3 \mid X_2)p(X_2) \\ &\dots \end{aligned}$$

Autoregressive Models

Autoregressive Models

Given a set of (time-)ordered random variables $\mathbf{X} = \{X_1, X_2, X_3 \dots, X_T\}$, we represent their joint distribution as

$$\begin{aligned} p(\mathbf{X}) &= \prod_{i=1}^T p(X_i \mid \mathbf{X}_{j < i}) \\ &= p(X_1)p(X_2 \mid X_1)p(X_3 \mid X_2, X_1) \dots \end{aligned}$$

This induces a form of **causality**, as the distribution over a future variable depends on all previous observations. It also allows us to generate *new* data one sample point at a time (conditioned on all the previous ones).

Lagged Autoregressive Models

For computational reasons, one usually limits the number of past observations influencing future predictions. An autoregressive model of order/lag/receptive-field R is defined as

$$X_t \mid \mathbf{X}_{j < t} = \theta_0 + \sum_{i=1}^R \theta_i X_{t-i} + \epsilon_t,$$

where $\theta = \{\theta_0, \dots, \theta_R\}$ are the parameters of the model and ϵ_t is (white) noise.

Translation to Neural Networks

The definition of autoregressive models can be captured by a single fully connected neural layer

$$\begin{aligned} X_t \mid \mathbf{X}_{j < t} &= \theta_0 + \sum_{i=1}^R \theta_i X_{t-i} + \epsilon_t \\ &= \boldsymbol{\theta}^T \mathbf{h}_t + \epsilon_t, \end{aligned}$$

where $\boldsymbol{\theta} = (\theta_0 \quad \theta_1 \quad \dots \quad \theta_R)$ are the weights including the bias, and $\mathbf{h}_t = (1 \quad X_{t-1} \quad \dots \quad X_{t-R})$.

Deep models

For more model capacity, one might stack layers having multiple features, in which case we get something along the following line

$$\mathbf{H}_t^l = \sigma \left(\boldsymbol{\Theta}^l \mathbf{H}_t^{l-1} + \mathbf{E}_t^l \right),$$

where σ is a non-linearity and subscript l denotes the l -th layer.

Limitations

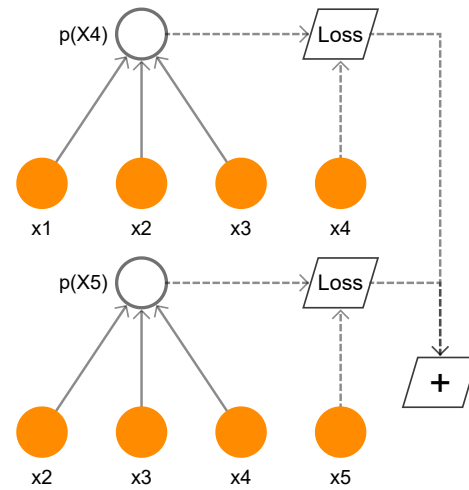
1. **Training** with linear layers is **inefficient** as autoregressive value needs to be computed for every possible window of size R .
2. The **number of weights** grows linearly with the receptive field of the model. For multi-time scale models (speech, audio) this becomes quickly an issue.

WaveNet

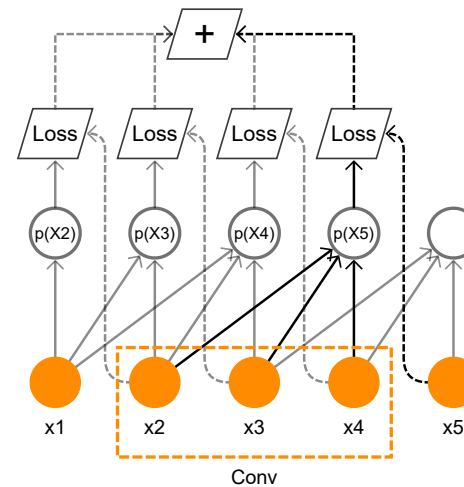
Convolutions: Improving Training Efficiency

Interpret $\mathbf{X}_t \mid \mathbf{X}_{j < t}$ in terms of convolution. Allows for a fully-convolutional computation of all \mathbf{X}_t in one sweep. Below illustration is for a model of $R = 3$.

Fully Connected Approach



Convolutional Approach

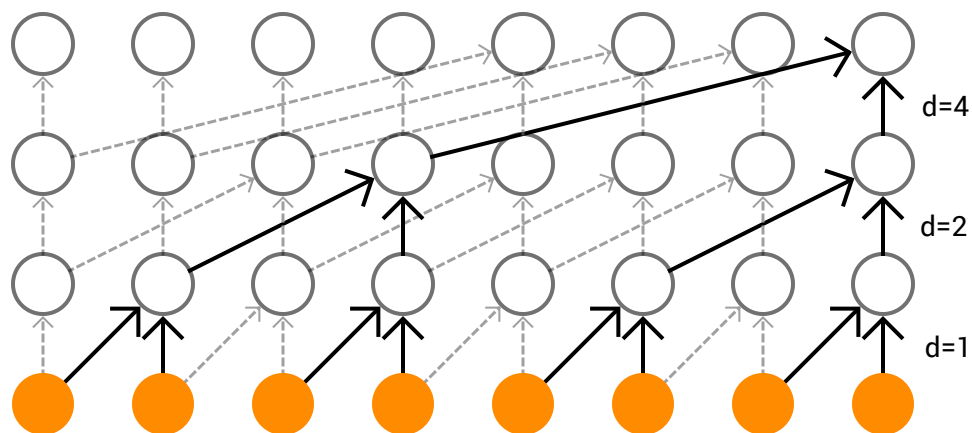


Need to be careful about (see Causal Padding slides)

- Ensure no data leakage happens (i.e input restricted to $\mathbf{x}_{j < t}$)
- How to handle variables X_t , where $t < R$

Dilated Convolutions: Exponential Receptive Fields

Receptive field of dilated convolutions grows exponentially while parameters increase only linearly. Figure below uses kernel size $K_i = 2$.



In general, each layer with dilation factor D_i and kernel size K_i adds

$$r_i = (K_i - 1)D_i$$

to the receptive field $R = \sum_i r_i + 1$.

Note, how each input (orange) within the receptive field is used exactly once.

Dilated Convolutions: Number of parameters

Assume kernel size $K_i = 2$ and a receptive field of $R = 512$. Then a vanilla convolution requires

$$R_{\text{vanilla}} = 512 \text{ parameters}$$

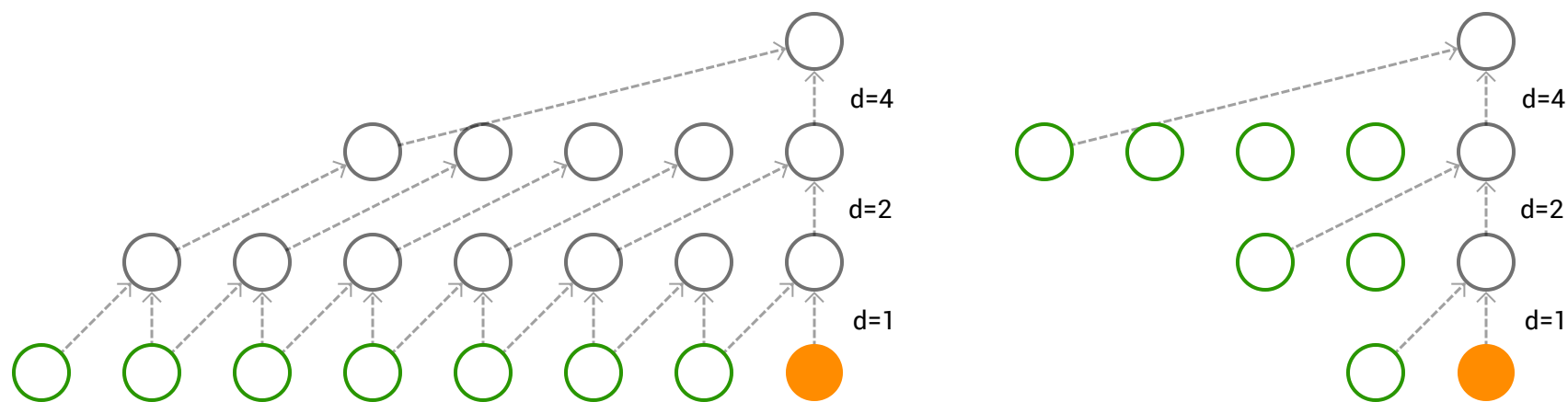
(without a bias), while a stacked dilated convolution requires

$$R_{\text{dilated}} = 2 * 9 = 18 \text{ parameters.}$$

Note: stacked dilated convolutions make use of all 512 inputs.

Causal Padding

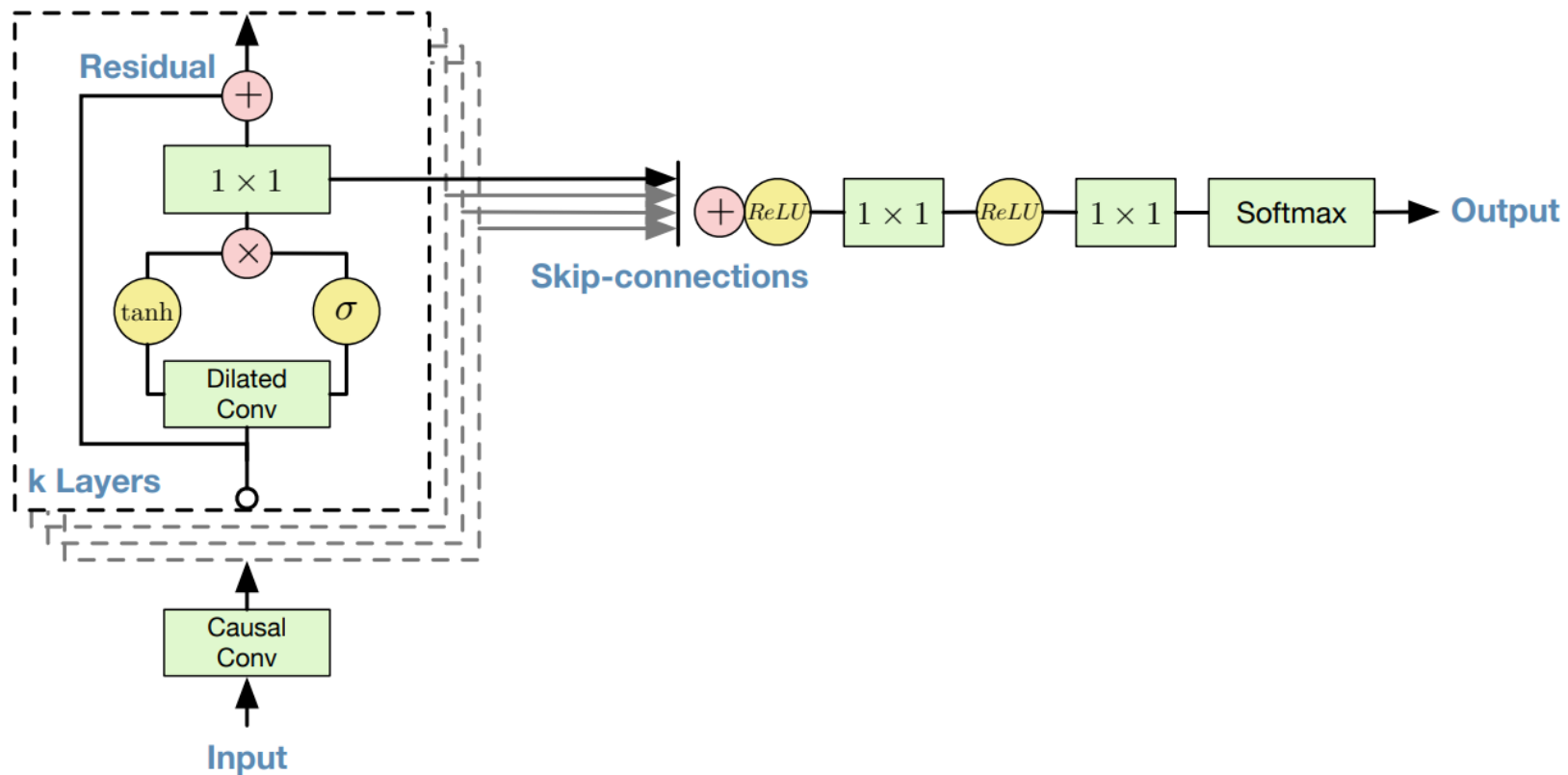
Causal padding (left-padding) ensures that convoluted features do not depend on future values and allows us to compute predictions for X_t , where $t < R$. Two possibilities: input-padding (left), layer-padding (right)



In general, a total of $P = R - 1$ padding values are required.

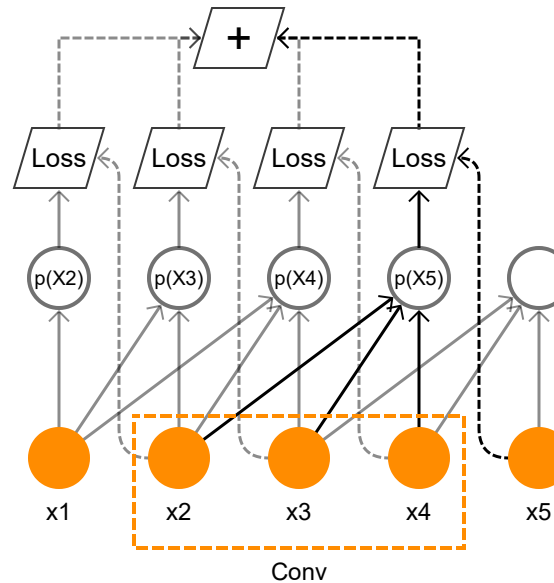
Full Architecture

WaveNet combines stacked dilated convolutions, causal padding and gated activation functions to predict a categorical distribution for $X_t | \mathbf{X}_{j < t}$ in parallel.



Training

Paper performs a one-step rolling origin training routine using cross entropy as loss function.

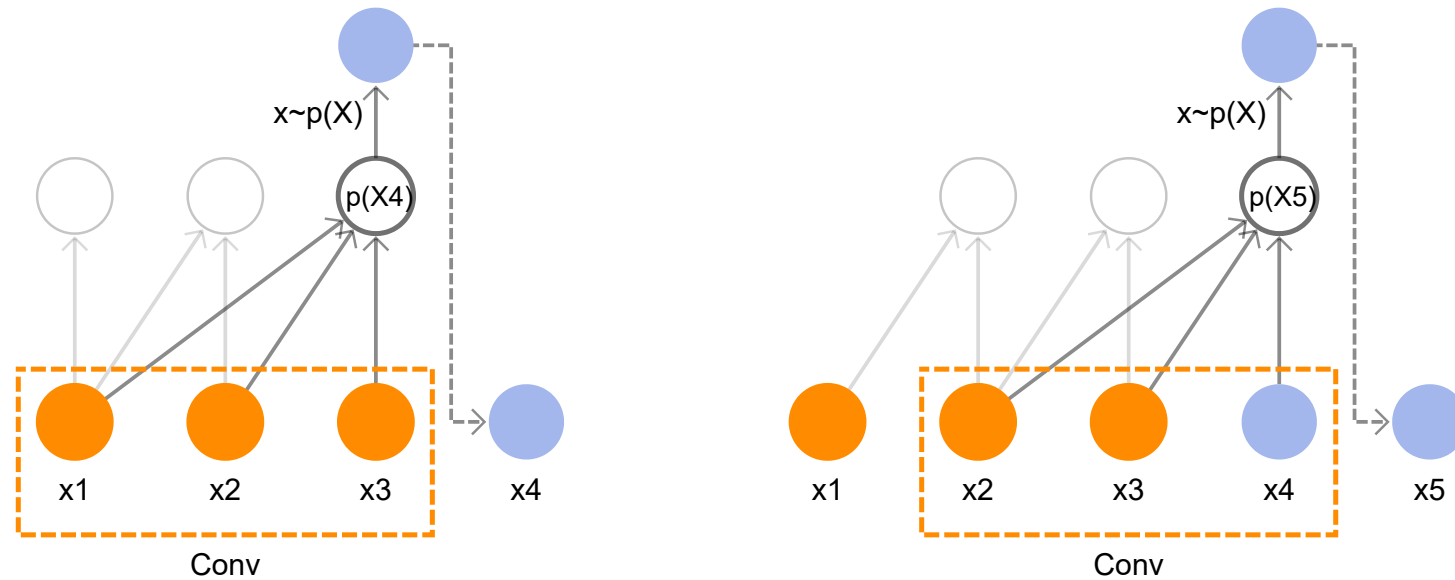


Raw audio data is quantized to 256 bins and one-hot encoded ($X_t \sim \text{Cat}(\pi_1, \dots, \pi_{256})$).

Side note: one-step loss does not account for generative n-step drift (which is probably ok for audio synthesis).

Data Generation

New data is generated one sample at a time. The figure below shows two steps for a model with $R = 3$



Remarks:

- Generation is inefficient - requires R inputs but uses only the last output.
- Generation involves sampling from the distribution.

Extensions

Conditional WaveNets*

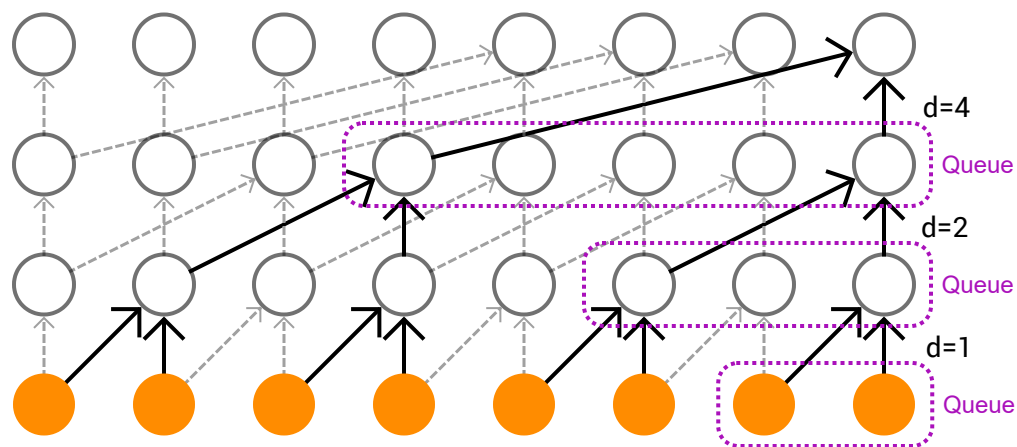
Condition the model on additional external input

$$\begin{aligned} p(\mathbf{X} \mid \mathbf{y}) &= \prod_{i=1}^T p(X_i \mid \mathbf{X}_{j < i}, \mathbf{y}) \\ &= p(X_1 \mid \mathbf{y}) p(X_2 \mid X_1, \mathbf{y}) p(X_3 \mid X_2, X_1, \mathbf{y}) \dots \end{aligned}$$

to change generative behavior. For example \mathbf{y} might represent speaker identity in which case the model would generate data wrt. the given speaker.

Faster Generation*

Relies on sparsity of access during computation. Introduce *queues* (i.e rolling buffers of size $r_i + 1$) to store intermediate outputs. During generation only use oldest in queue and update queue.



Similar to updates in recurrent neural nets.

*Fast WaveNet Generation Algorithm, Tom le Paine et al., 2016.

For even faster generation check Parallel WaveNet: Fast High-Fidelity Speech Synthesis, Aaron van den Oord et al., 2017.

Train Unrolling*

In training, WaveNet uses a one-step rolling-origin loss which can causes substantial drift.

Idea

A n-step loss would allow the model to correct its own drift.

I.e we want to apply n-step generation and backprop through all samples.

Issue

How to backprop through a random sample from a categorical distribution?

Fully Differentiable Train Unrolling

Reparametrization Idea

Note if $X_t \sim \mathcal{N}(\mu, \sigma)$, which we can express as $X_t \sim \mathcal{N}(0, 1)\sigma + \mu$.

Now $\frac{\partial}{\partial \mu}, \frac{\partial}{\partial \sigma}$ exist and randomness becomes an input (for which we do not require gradients).

Reparametrization of Categorical Distributions

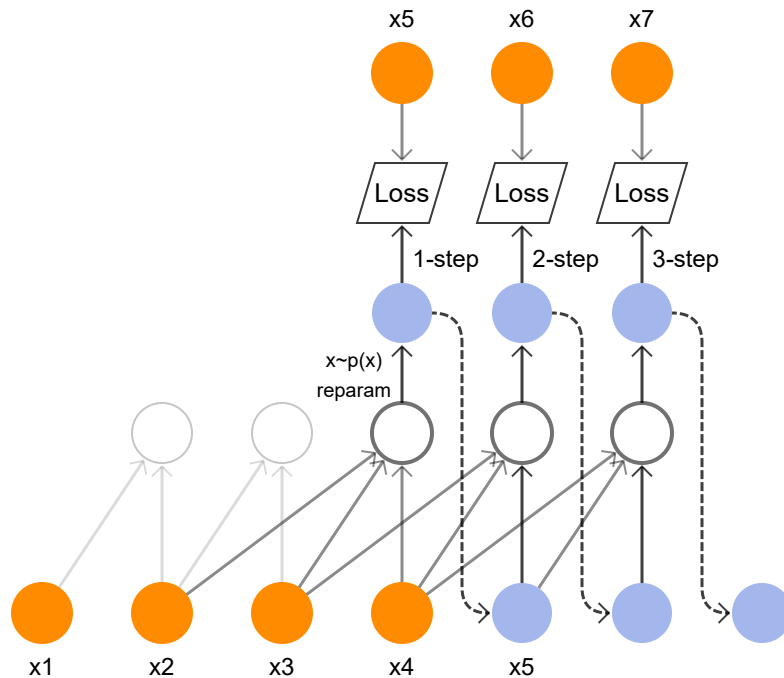
Similar reparametrization exists for $X_t \sim \text{Cat}(\pi_1, \dots, \pi_C)$ using Gumbel distribution*, which allows us to write

$$X_t \sim g(\text{Gumbel}(0, 1), \pi_1, \dots, \pi_C, \tau),$$

such that $\frac{\partial g}{\partial \pi_i}$ exists. Here τ is a temperature scaling parameter.

Fully Differentiable Train Unrolling

Forward pass



Backward pass

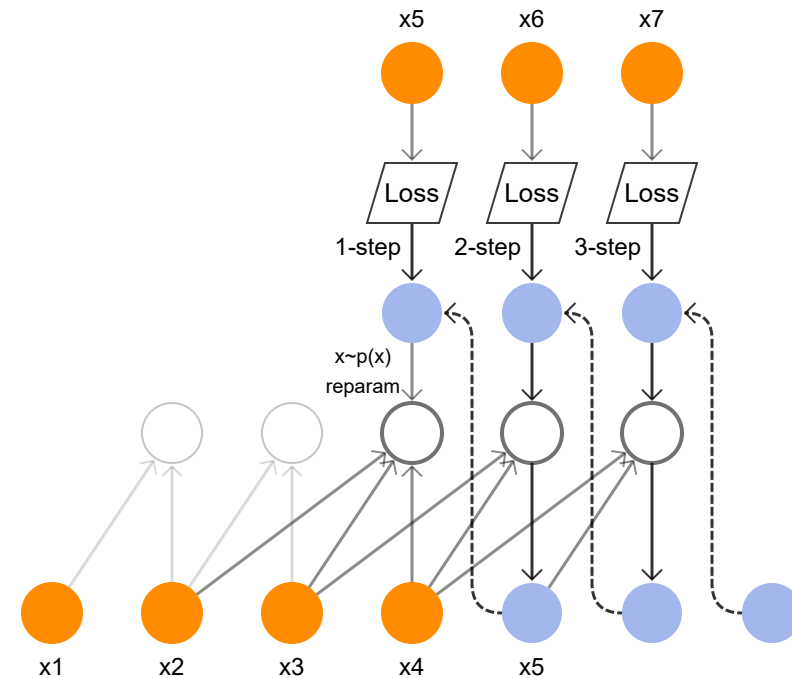
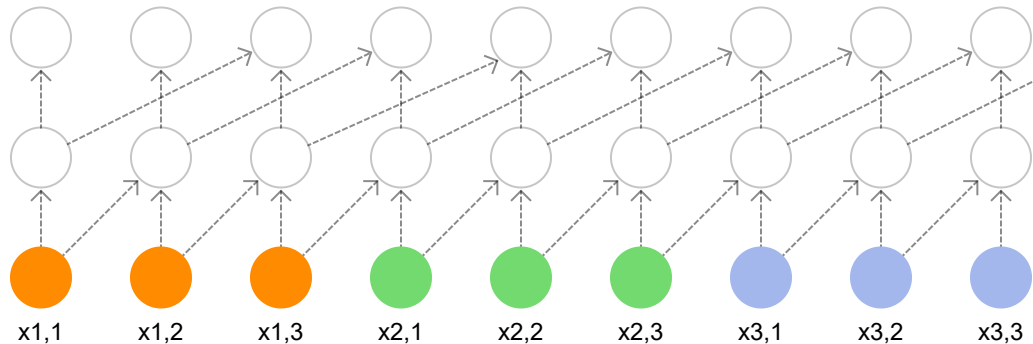
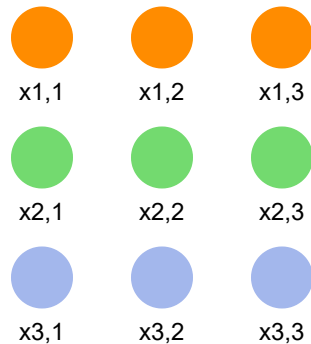


Image Domain

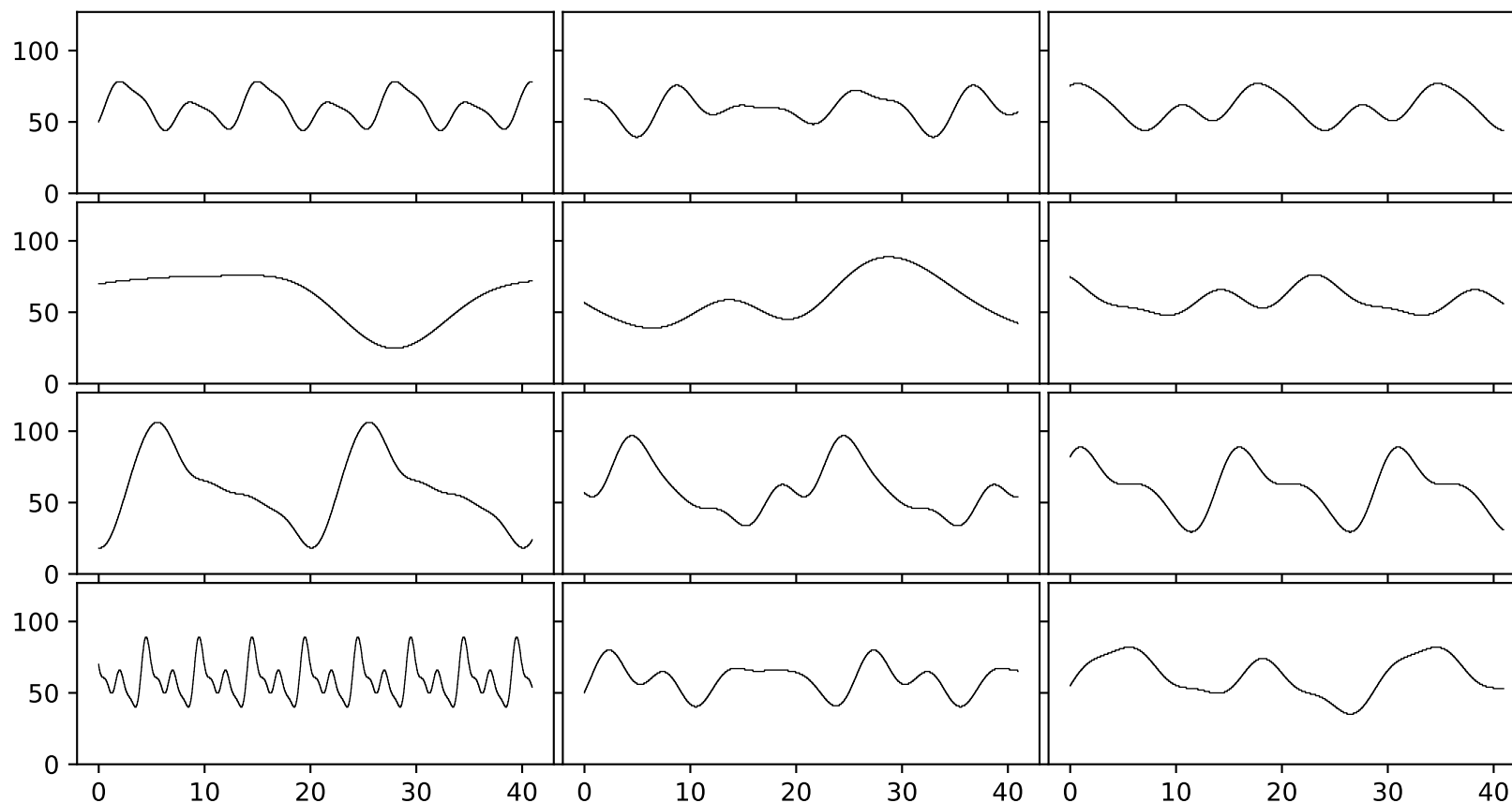
The WaveNet idea extends to 2D spatial domain*. In this library the most straightforward approach is chosen: unrolling the image to a 1D signal. A 3x3 image (left) is unrolled using scanline approach to a 1D signal (right), which can then be fed to a standard WaveNet.



1D Signal Experiments

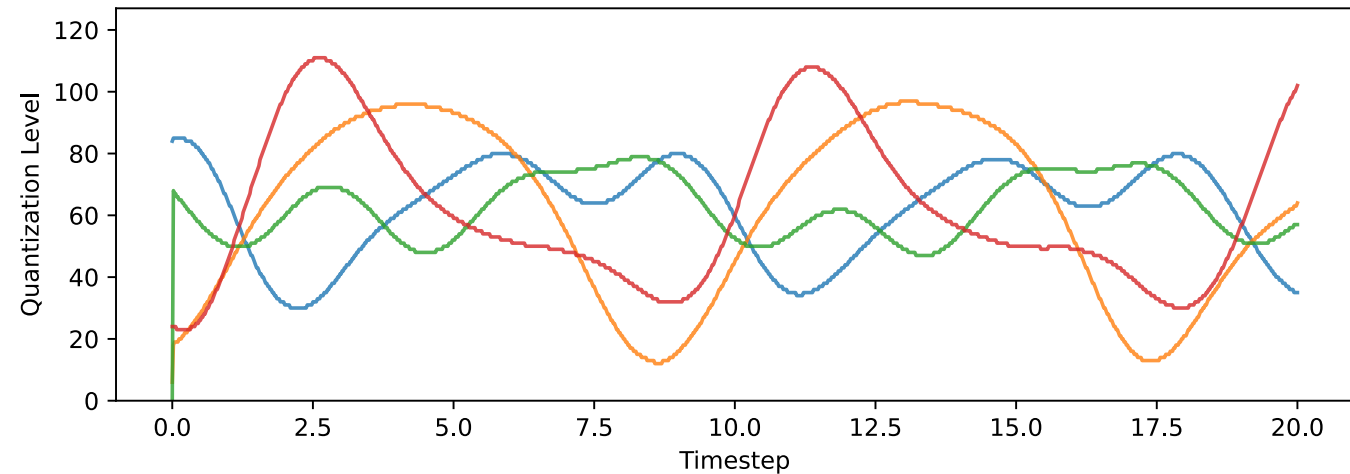
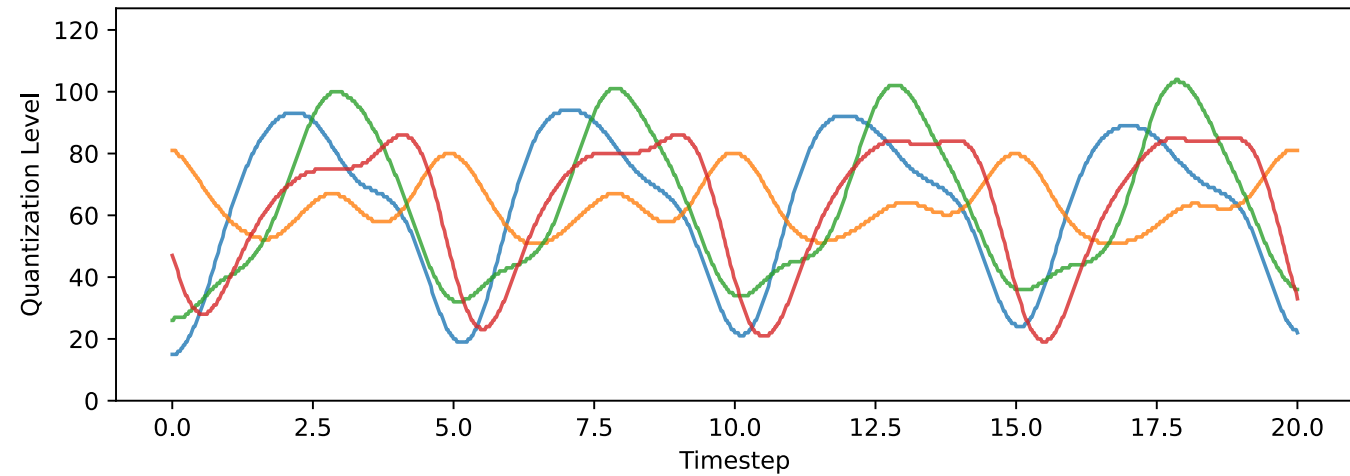
1D Signal Setup

Instead of audio waveforms as input, using a Fourier dataset with randomized coefficients, number of terms and periodicity (sampling: 50Hz, quantization: 127 bins, encoding one-hot, conditioned on periodicity between 5-10secs)



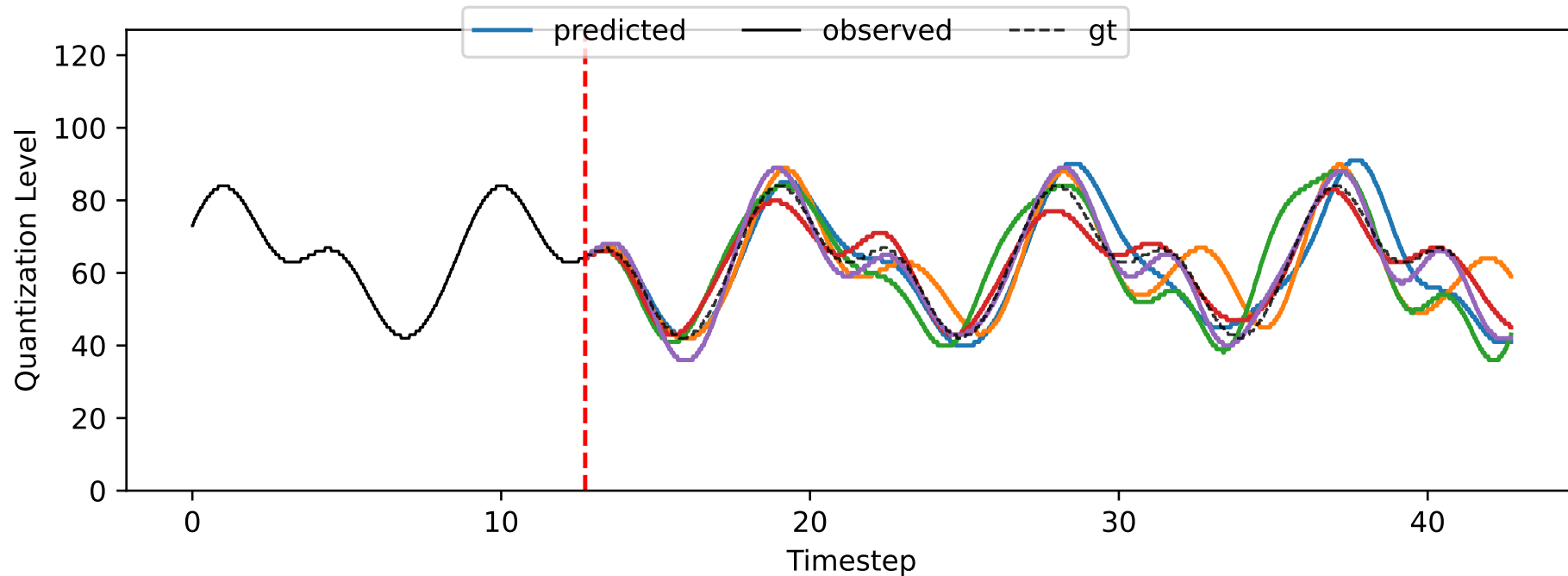
Sampling Results

The following diagrams show multiple samples $\mathbf{x} \sim p(\mathbf{X}|Y = \text{period})$: short periods (~5secs), longer periods (~10secs).



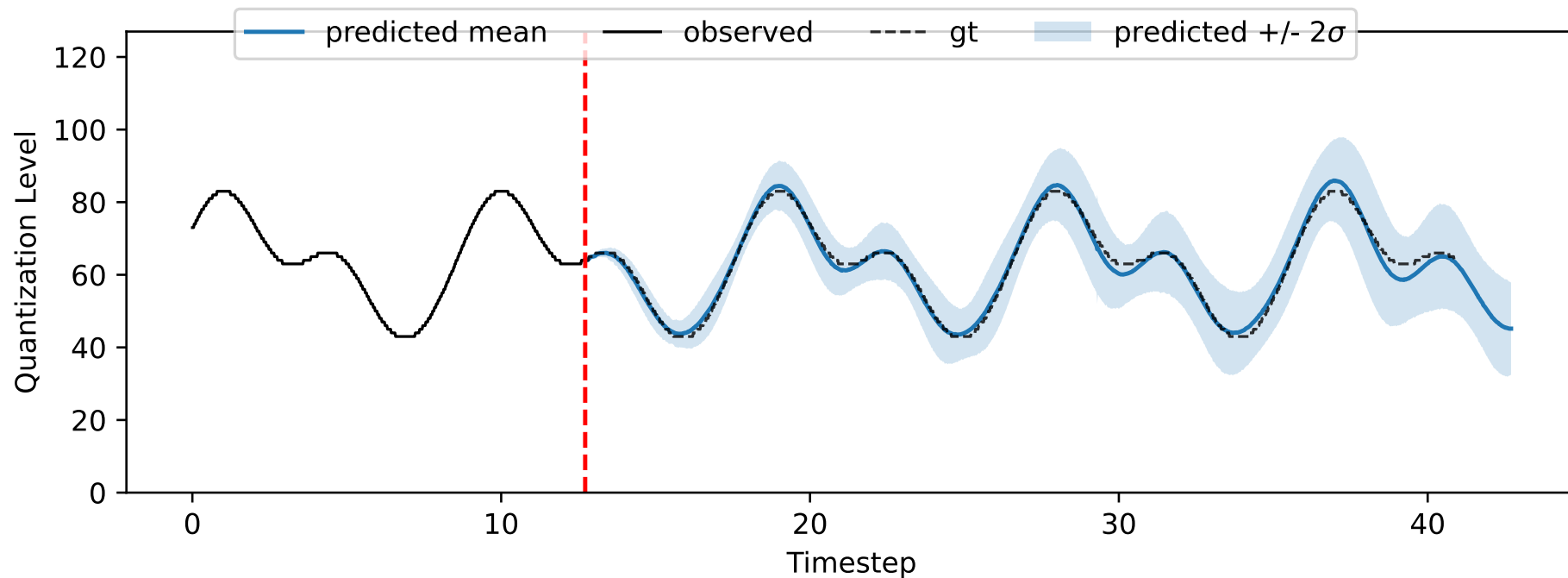
Prediction Results

In the following diagrams, multiple samples from the distribution $\mathbf{x} \sim p(\mathbf{X}_{>\text{obs}} | \mathbf{X}_{\leq \text{obs}}, Y)$ are shown. That is, the model predicts the future signal shape. Observe that for periodic signals, only little drift occurs as the horizon increases.



Prediction Results - Confidence Bounds

We can interpret each future trajectory as a sample from the distribution $\mathbf{x} \sim p(\mathbf{X}_{>\text{obs}} | \mathbf{X}_{\leq\text{obs}}, Y)$. Sampling enough trajectories, allows us to estimate confidence bounds of the model as shown below

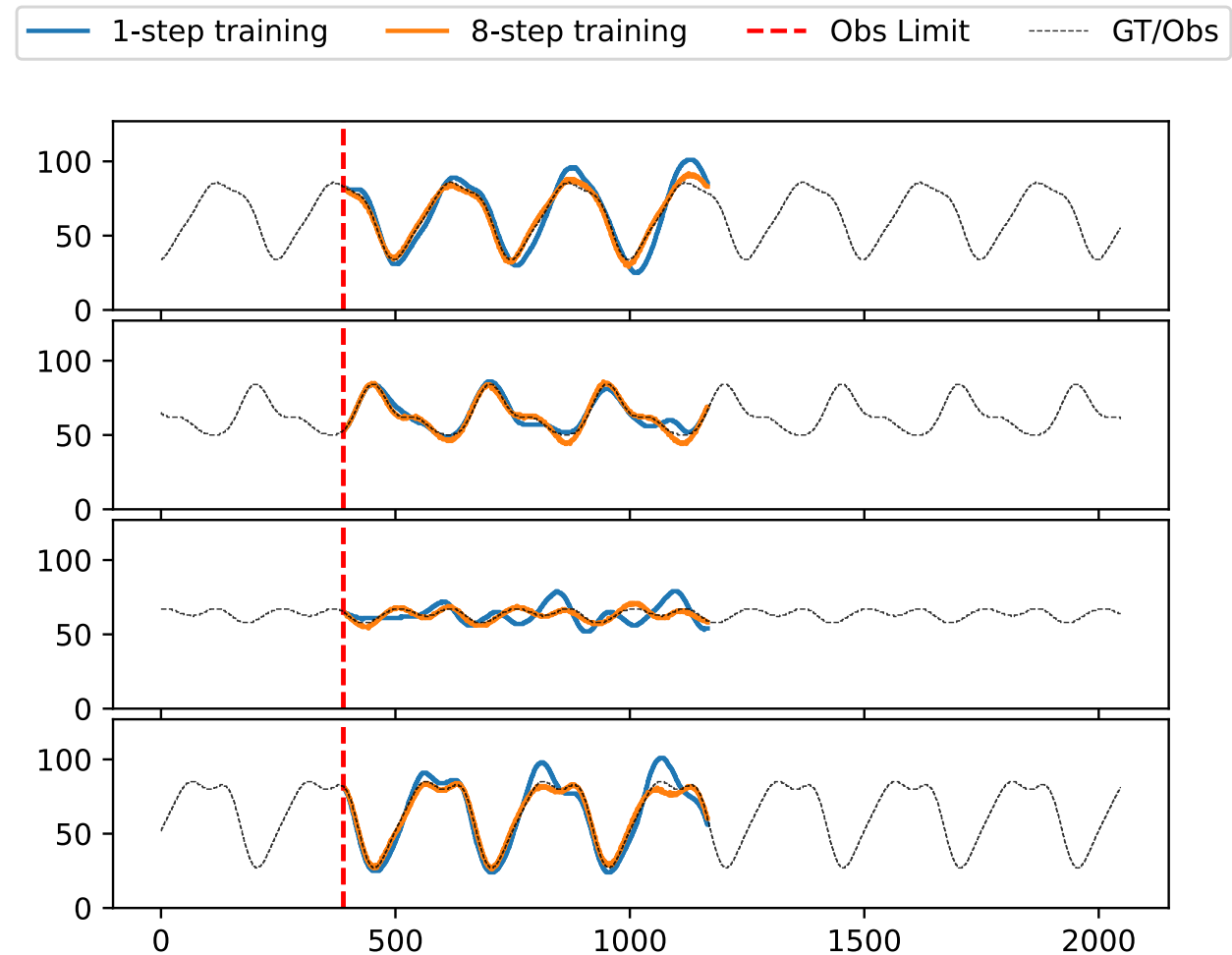


Train-Unrolling Results

N-step forecast comparison between two models trained with and without unrolling on Fourier-series dataset with up to 4 terms.

Conclusion

- (+) Decreases generative drift
- (+) Improves recreation of higher frequency patterns
- (-) Increases training time (rolling origin)
- (-) Sparser losses

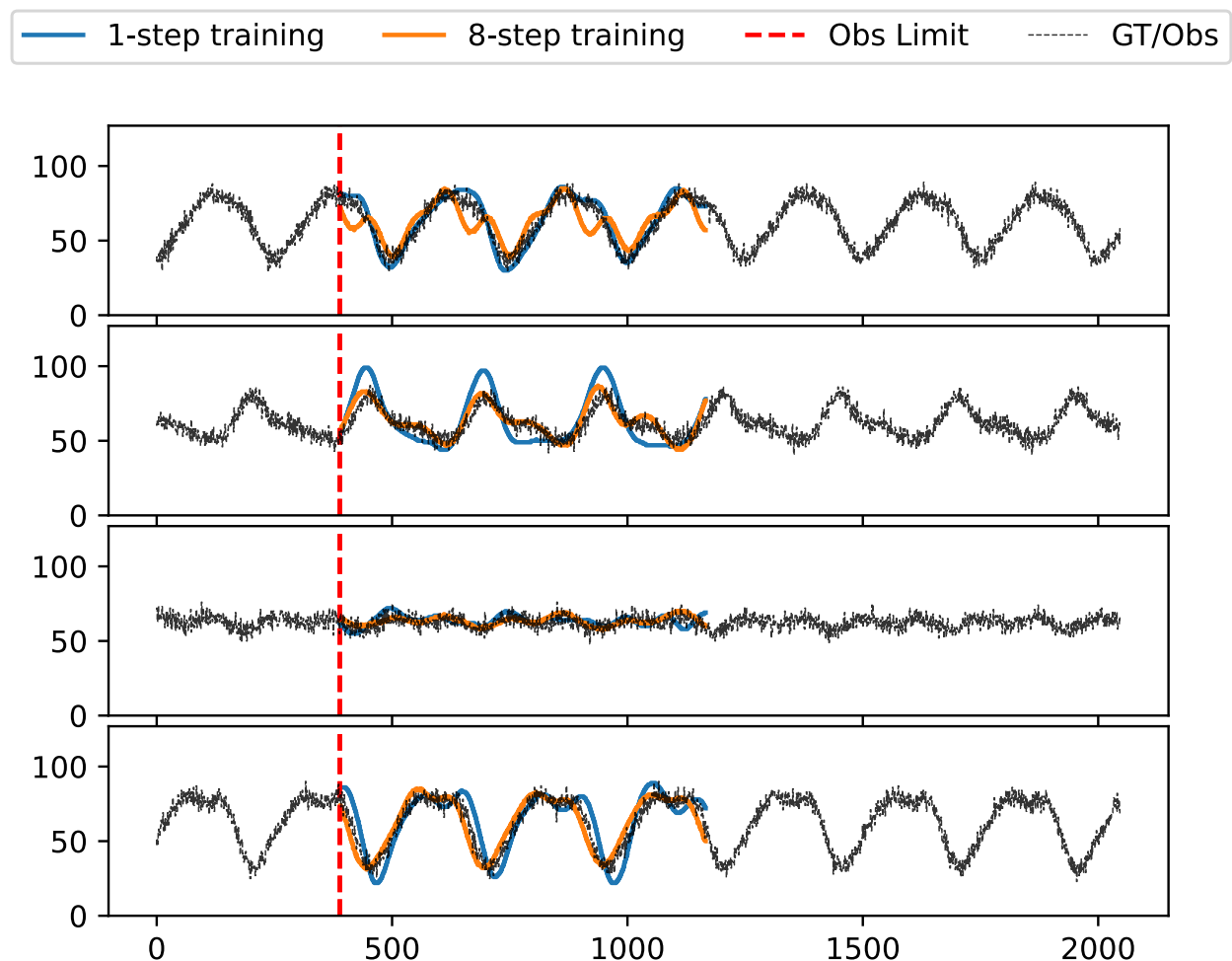


Noisy Train-Unrolling Results

N-step prediction based on noisy observations - comparison between two models trained with and without unrolling on a clean Fourier series dataset with up to 4 terms.

Conclusion

- (+) Both models capture global trends
- (-) Accuracy of both modes decreases

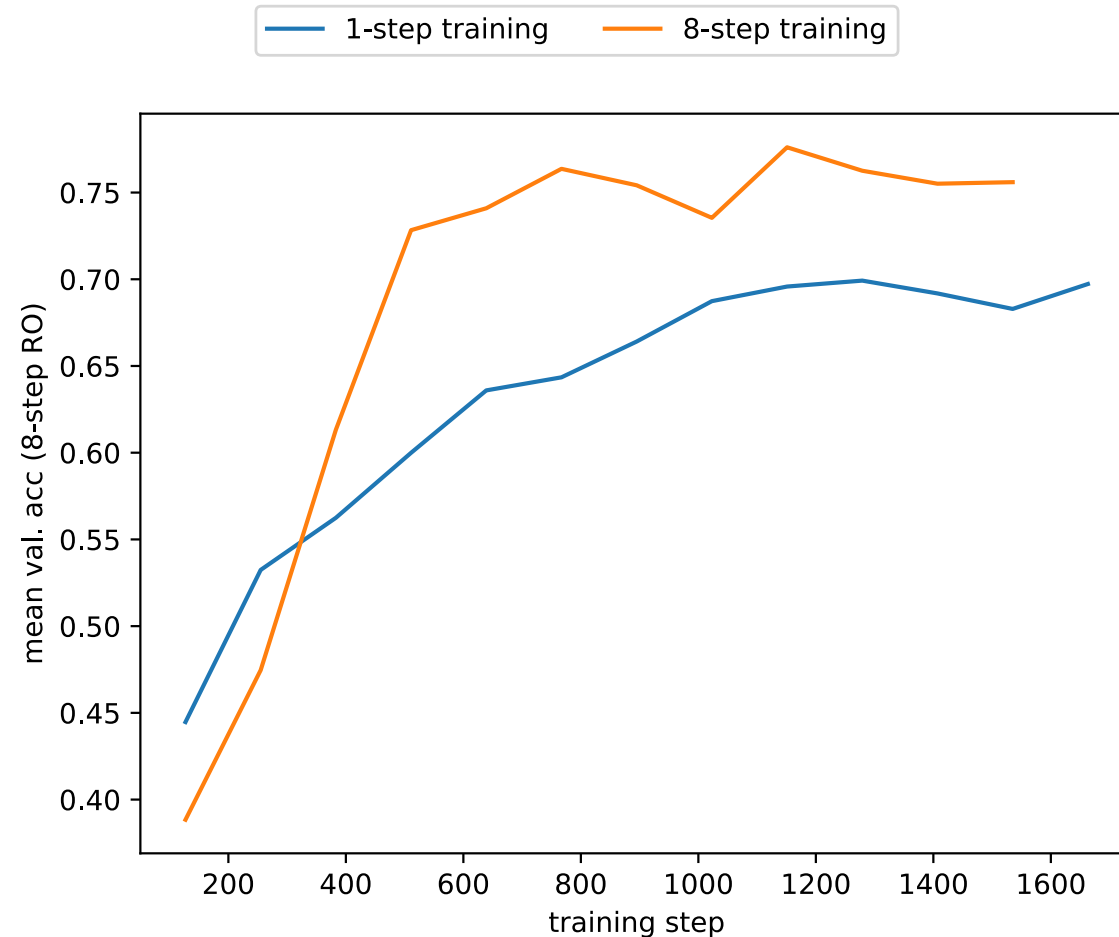


Train-Unrolling Validation Acc. Results

8-step rolling origin validation comparison between models trained with and without unrolling on Fourier-series dataset with up to 4 terms.

Conclusion

- (+) Generally higher validation acc. at earlier training epochs.
- (+) Similar picture if validation unrolling > train unrolling steps.

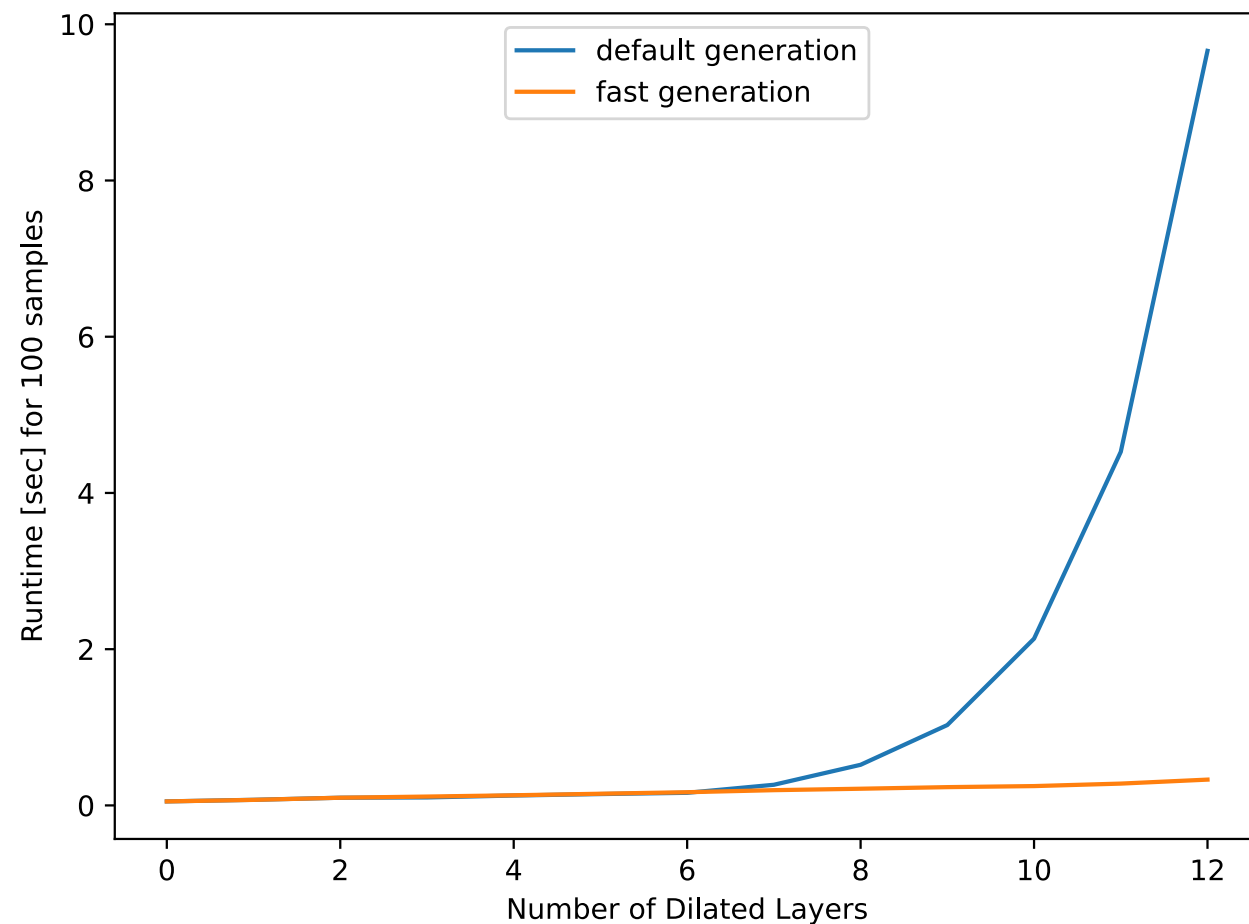


Runtime Performance Results

The plot to the left shows default (blue) and fast (orange) sample generation* using 64 wave-channels, 8 quantization levels and 32 batch-size.

Conclusion

- (+) Fast method avoids exponential inference time as layer depth increases.
- (-) Code overhead is considerable.



2D Image Experiments

2D Image Setup

We use the MNIST dataset, which consists of images taken from 10 digit classes (0..9).

Sampling: 28x28pixels, quantization: 256 bins / 2 bins, encoding one-hot.

Train/Val/Test splits as suggested.



MNIST Sampling Results

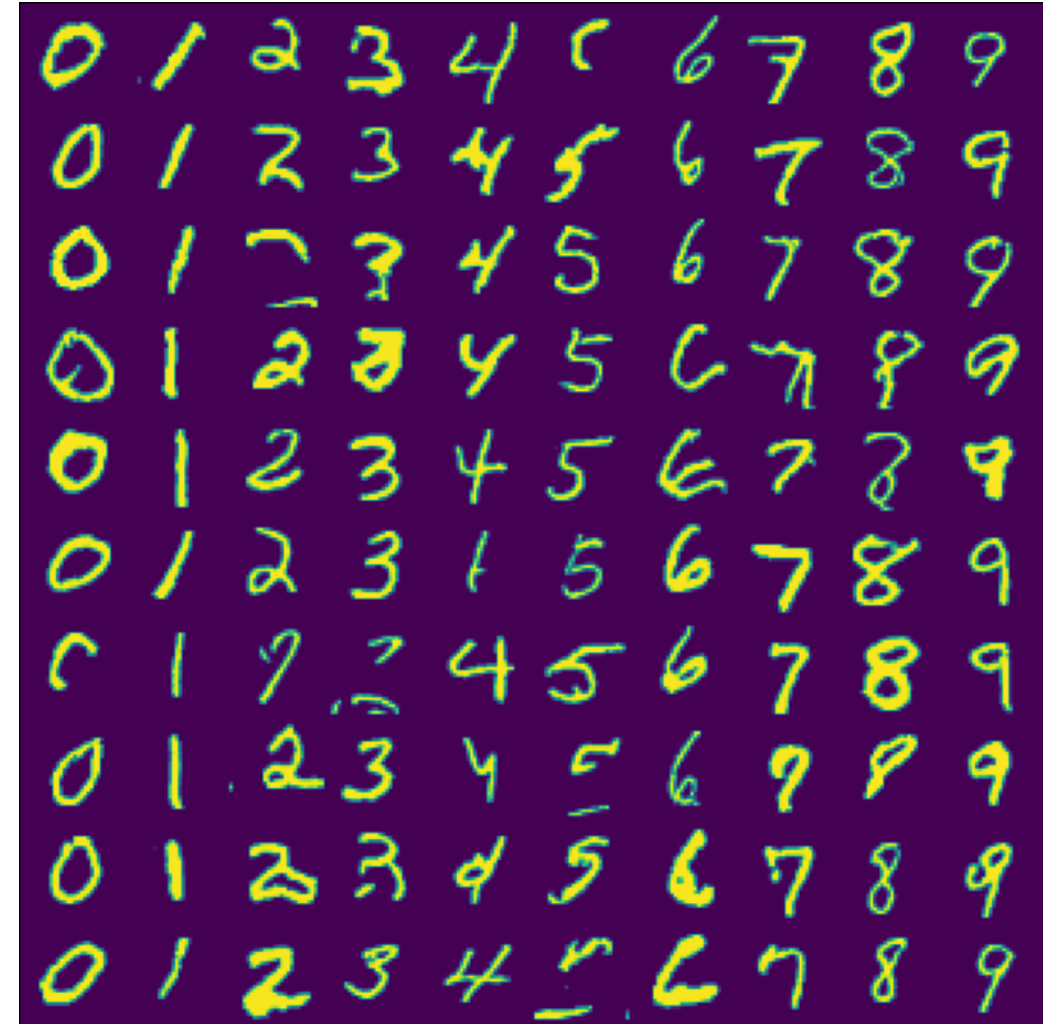
Samples drawn from $p(\mathbf{X} \mid Y)$, where \mathbf{X} is an MNIST 28x28 random variable and Y is the digit conditioned on. Quantization 256.

Note

- Almost all generated images contain human recognizable digits of the given target class.
- Fading effect to soften hard edges is captured by the model

Side note on Z-filling curves

- I played around with other z-filling curves for unrolling such as Peano curves, but the results have been considerably worse. I believe that's due to the effect that the distance to the north pixel varies across image columns.



MNIST Prediction Results

MNIST image reconstructions drawn from

$$p(X_{N+1}, \dots, X_T \mid X_1, \dots, X_N, Y),$$

where X_i denotes a random variable corresponding to the i -th (unrolled) MNIST 28x28 image pixel value and y is the digit class.

Top row: input images from the test set, of which the first 50% of all pixels are considered to be observed. Bottom rows: Predicted reconstructions.

Note

- Digit style is maintained during generation (thick strokes vs. thin strokes).
- Model capable of varying the global appearance (see second 7).
- Fading effect to soften hard edges is captured by the model.



MNIST Density Estimation Results

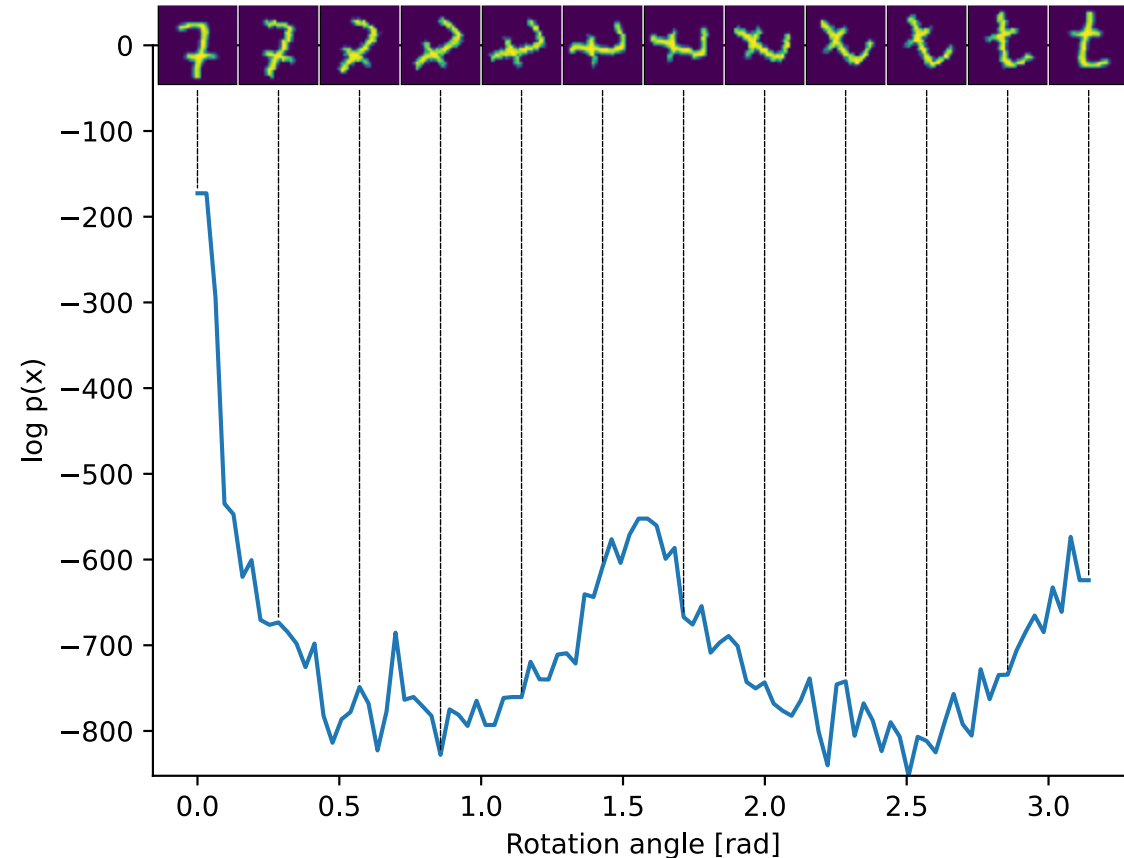
Assuming we know the class probabilities $p(Y) = \frac{1}{|Y|}$, we can compute the marginal image probability as follows

$$p(\mathbf{X} = \mathbf{x}) = \sum_{y_i=1}^Y p(\mathbf{X} = \mathbf{x} | Y = y_i) p(Y = y_i).$$

For computational reasons, we instead compute in the library

$$\log p(\mathbf{X} = \mathbf{x}) = \log \sum_{y_i=1}^Y \exp [\log p(\mathbf{X} = \mathbf{x} | Y = y_i) p(Y = y_i)].$$

The image on the right shows log probabilities as a single input image is incrementally rotated. Note, this is an unconditional log probability, which tells us whether the image is an inlier or outlier wrt. the model.



MNIST Classification Results

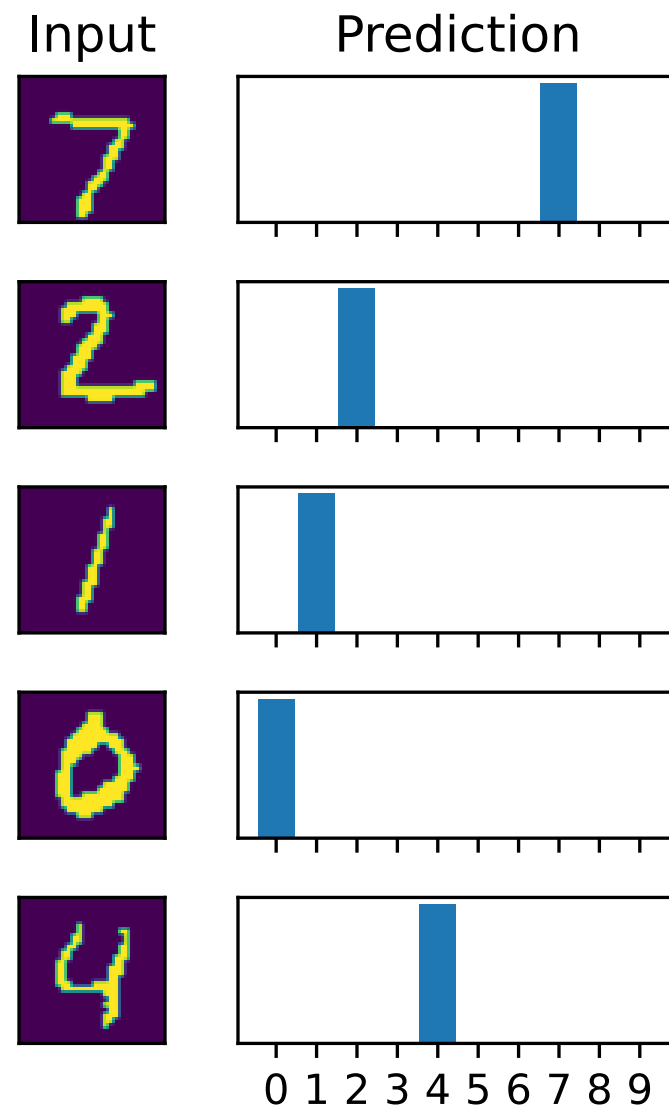
Given the class probabilities $p(Y)$, we compute from Bayes

$$p(Y|\mathbf{X} = \mathbf{x}) = \frac{p(\mathbf{X} = \mathbf{x}|Y)p(Y)}{p(\mathbf{X} = \mathbf{x})}.$$

A sample classification is shown on the right.

Accuracy

The 256 quantized model achieves an accuracy of 94% on MNIST test, while the binarized model yields a 98.7% accuracy score.



MNIST Progressive Classification Results

In this scenario, we consider pixels to become available incrementally over time and observe how $p(Y|\mathbf{X}_{0...H})$ evolves as H approaches $T=784$. The image below plots (from left to right) $p(Y|\mathbf{X}_{0...H})$ for $H=85$, $H=281$ and $H=589$.

