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 $\mathbf{X} = \{X_1, X_2, X_3..., X_T\}$, we represent their joint distribution as

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

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

Translation to Neural Networks

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

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

where $\theta = \begin{pmatrix} \theta_0 & \theta_1 & \dots & \theta_R \end{pmatrix}$ are the weights including the bias, and $\mathbf{h}_t = \begin{pmatrix} 1 & X_{t-1} & \dots & X_{t-R} \end{pmatrix}$.

Deep models

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

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

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

Limitations

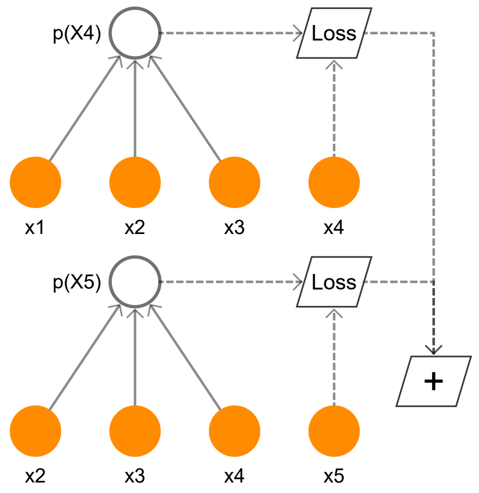
1. **Training** with linear layers is **inefficient** as autoregressive value needs to be computed for every possible window of size R.
2. The **number of weights** grows linearily with the receptive field of the model. For multi-time scale models (speech, audio) this becomes quickly an issue.

WaveNet

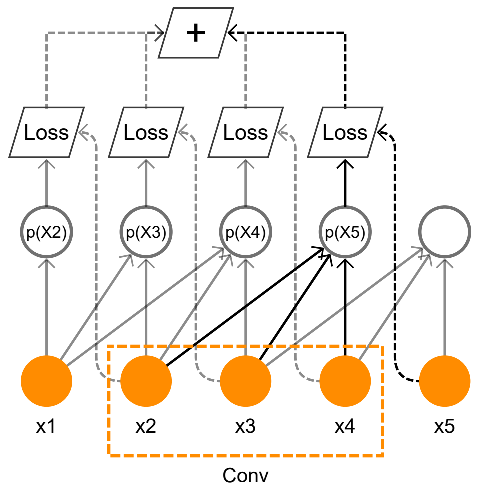
Convolutions: Improving Training Efficiency

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

Fully Connected Approach



Convolutional Approach

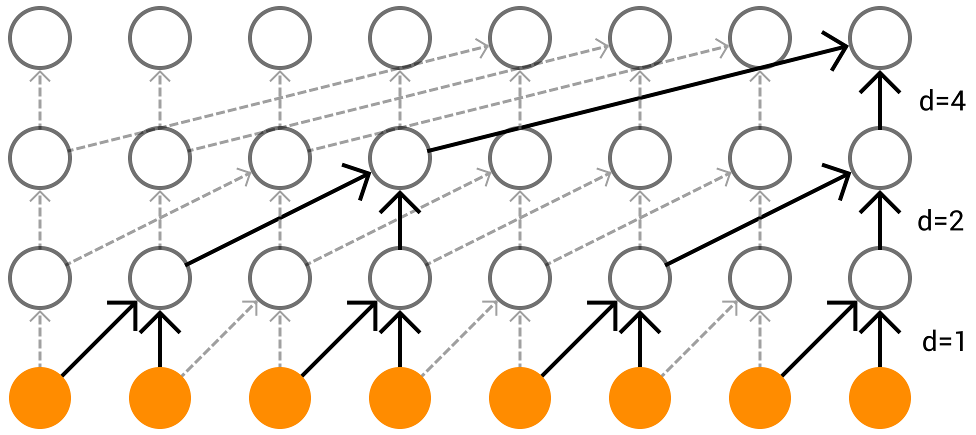


Need to be careful about (see Causal Padding slides)

- 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

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

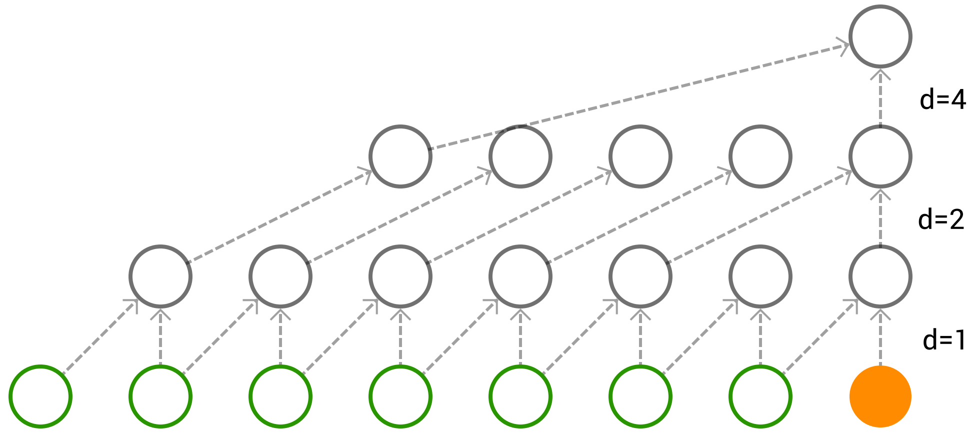
(without a bias), while a stacked dilated convolution requires

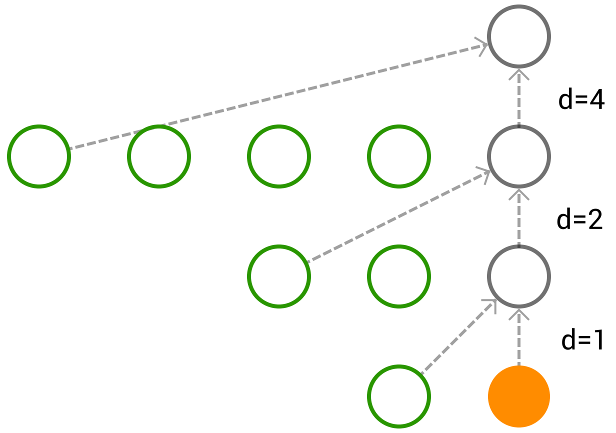
$$R_{\text{dilated}} = 2 * 9 = 18 \text{ parameters.}$$

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)



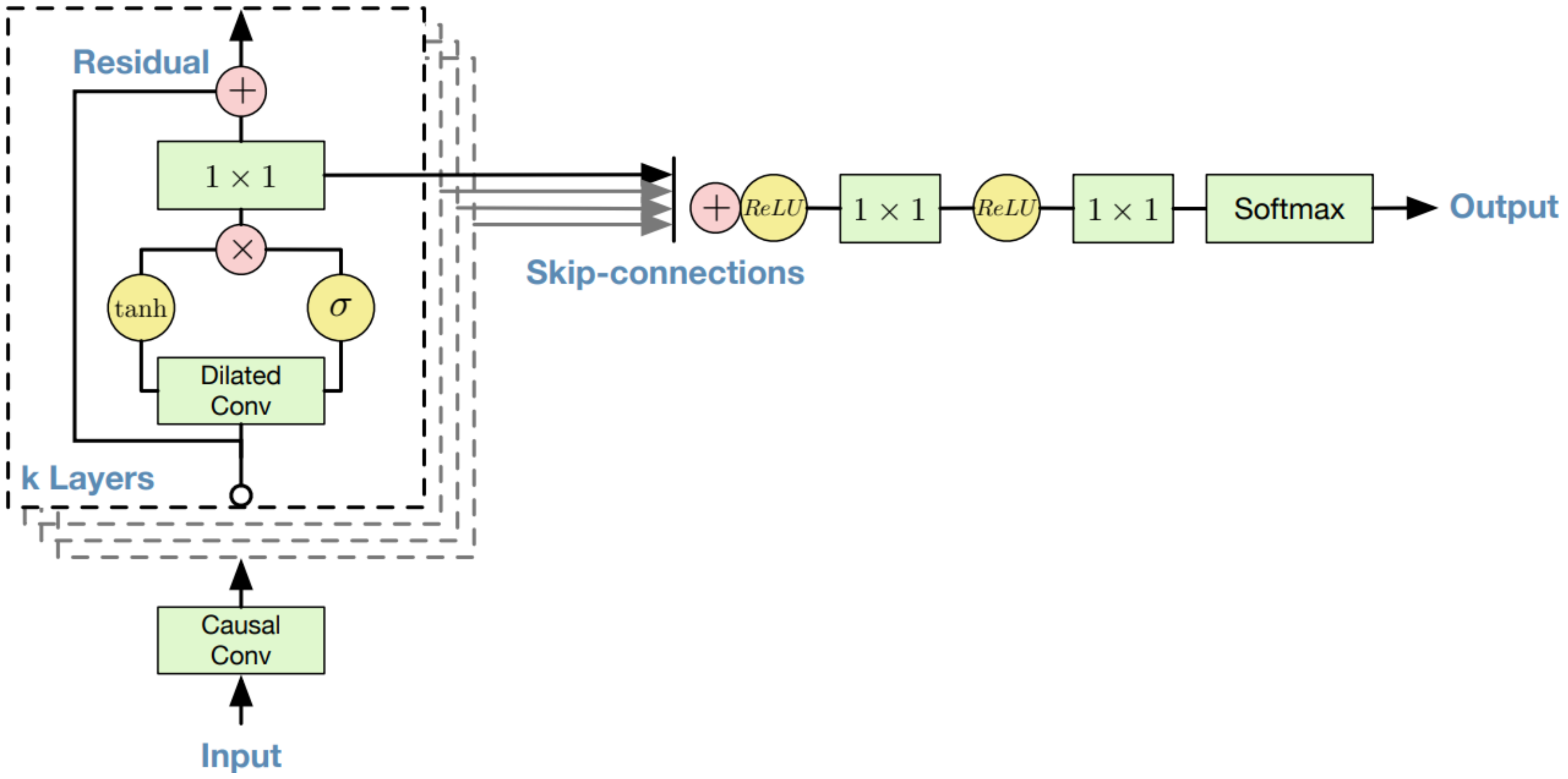


In general, a total of $P = R - 1$ padding values are required.

Autoregressive library uses layer-padding, WaveNet paper suggest input padding.

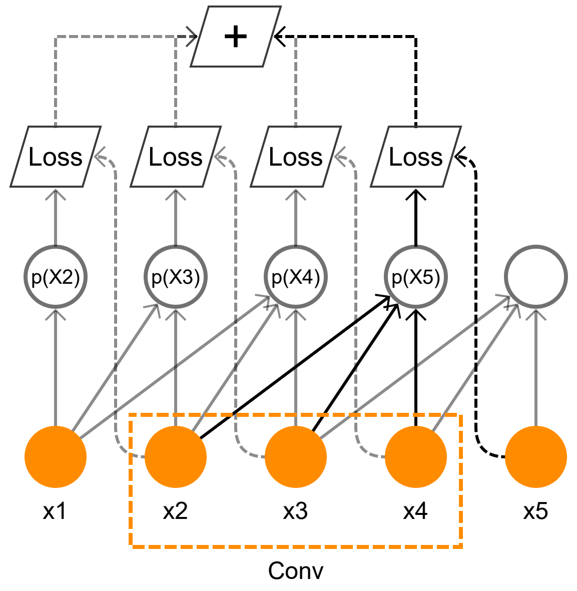
Full Architecture

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.

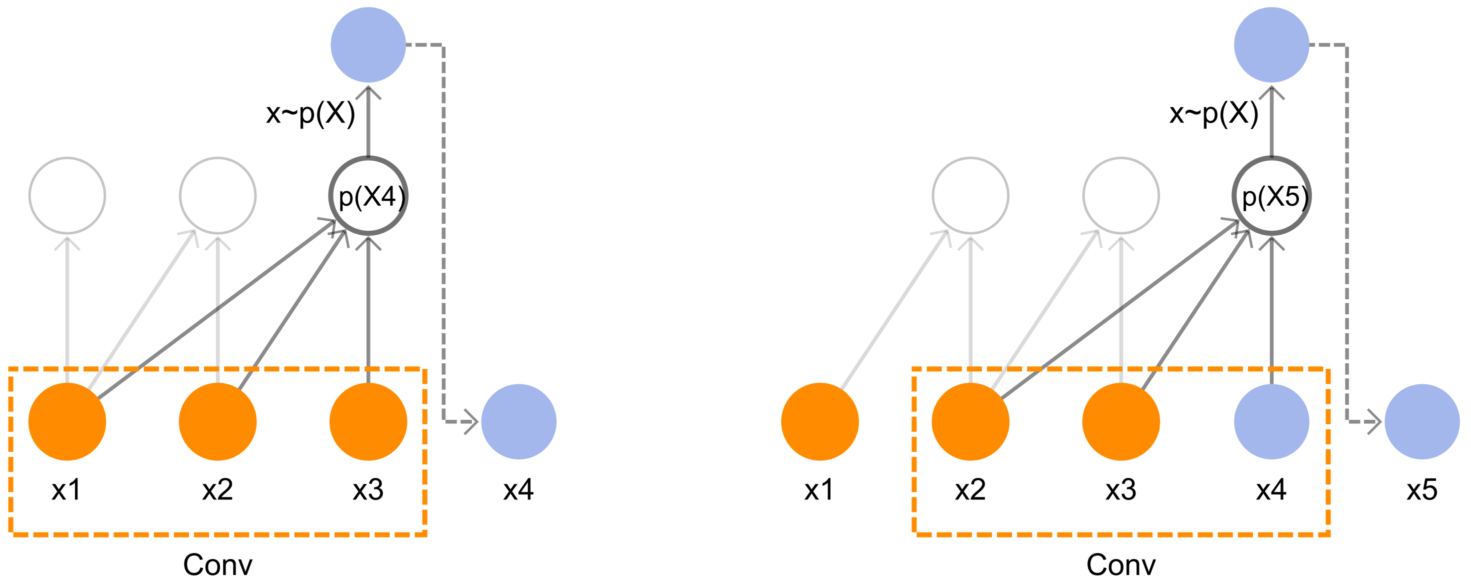


Raw audio data is quantized to 256 bins and one-hot encoded ($X_t \sim Cat(\pi_1, \ldots, \pi_{256})$).

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

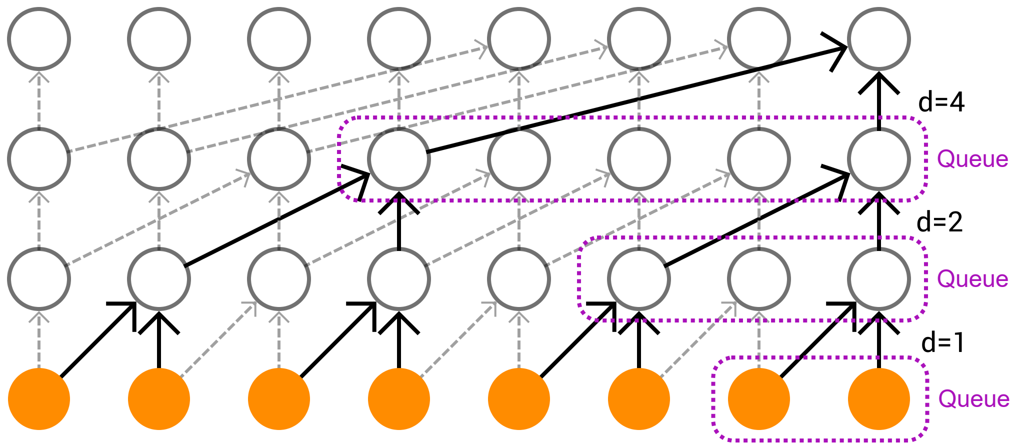
$$\begin{aligned} p(\mathbf{X} \mid \mathbf{y}) &= \prod_{i=1}^{T} p(X_i \mid \mathbf{X}_{j<i}, \mathbf{y}) \\ &= p(X_1 \mid \mathbf{y}) p(X_2 \mid X_1, \mathbf{y}) p(X_3 \mid X_2, X_1, \mathbf{y}) \ldots . \end{aligned}$$

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

*Wavenet: A generative model for raw audio, Aaron van den Oord, et al., 2016

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?

*TBD, Christoph Heindl, 2021 (unpublished)

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 $X_t \sim \mathcal{C}at(\pi_1, \ldots, \pi_C)$ using Gumbel distribution*, which allows us to write

$$X_t \sim g(Gumbel(0,1), \pi_1, \ldots, \pi_C, \tau),$$

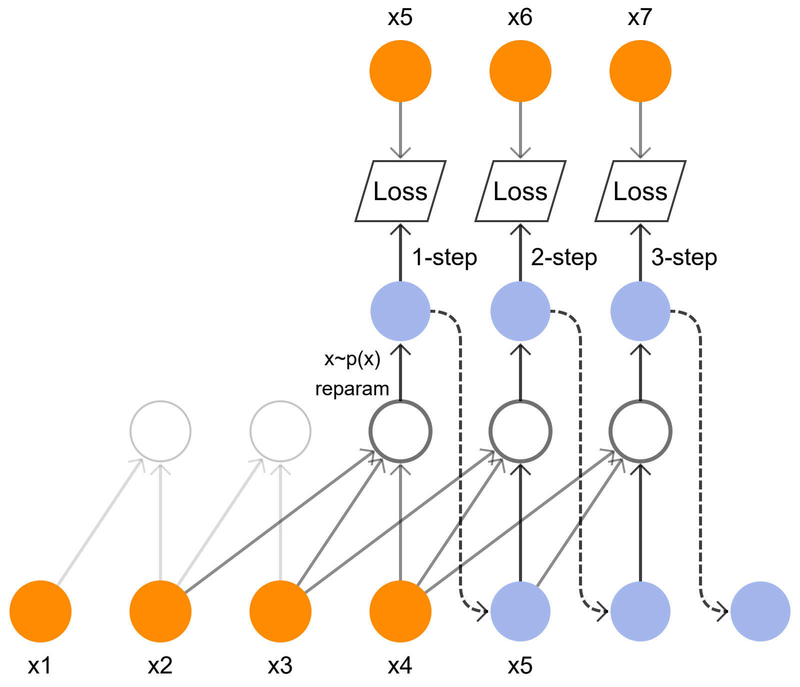
such that $\frac{\partial g}{\partial \pi_i}$ exists. Here τ is a temperature scaling parameter.

Categorical Reparameterization with Gumbel-Softmax, Eric Jang et al., 2017

The Concrete Distribution: A Continuous Relaxation of Discrete Random Variables, C. Maddison et al., 2017 -

Fully Differentiable Train Unrolling

Forward pass



Backward pass

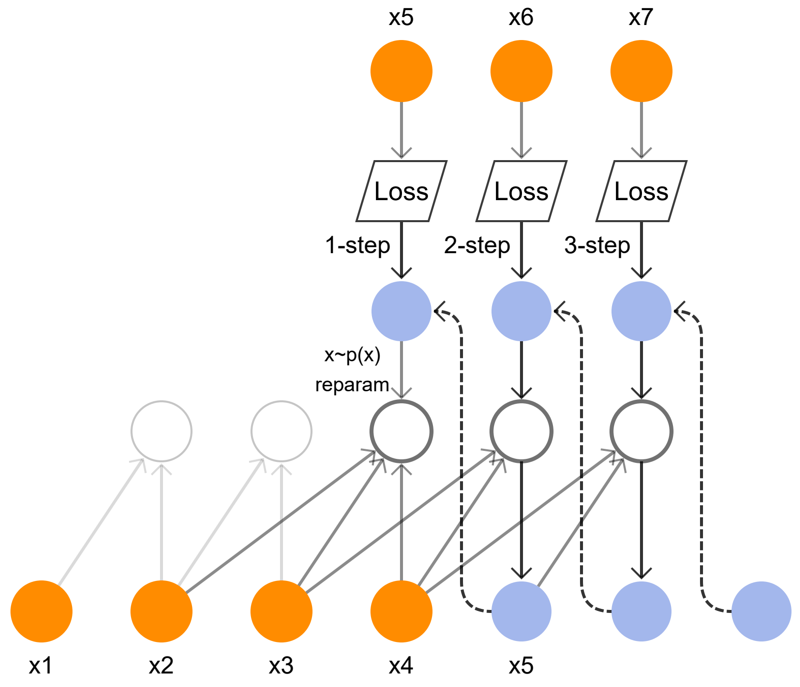
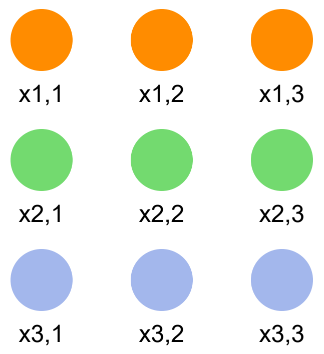
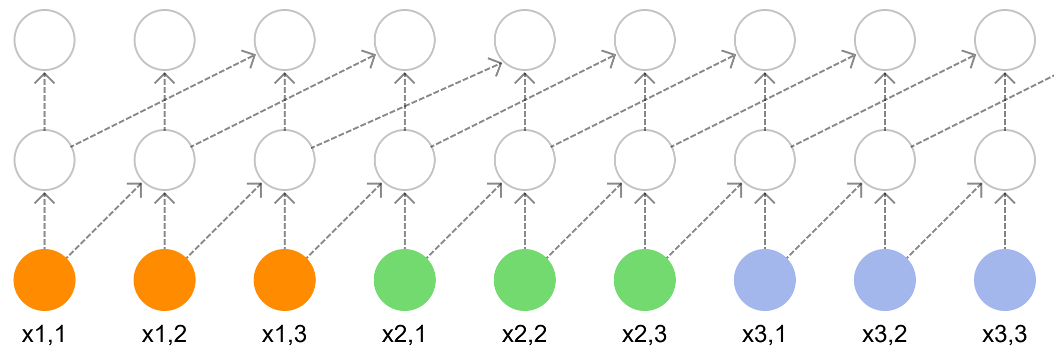


Image Domain

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.

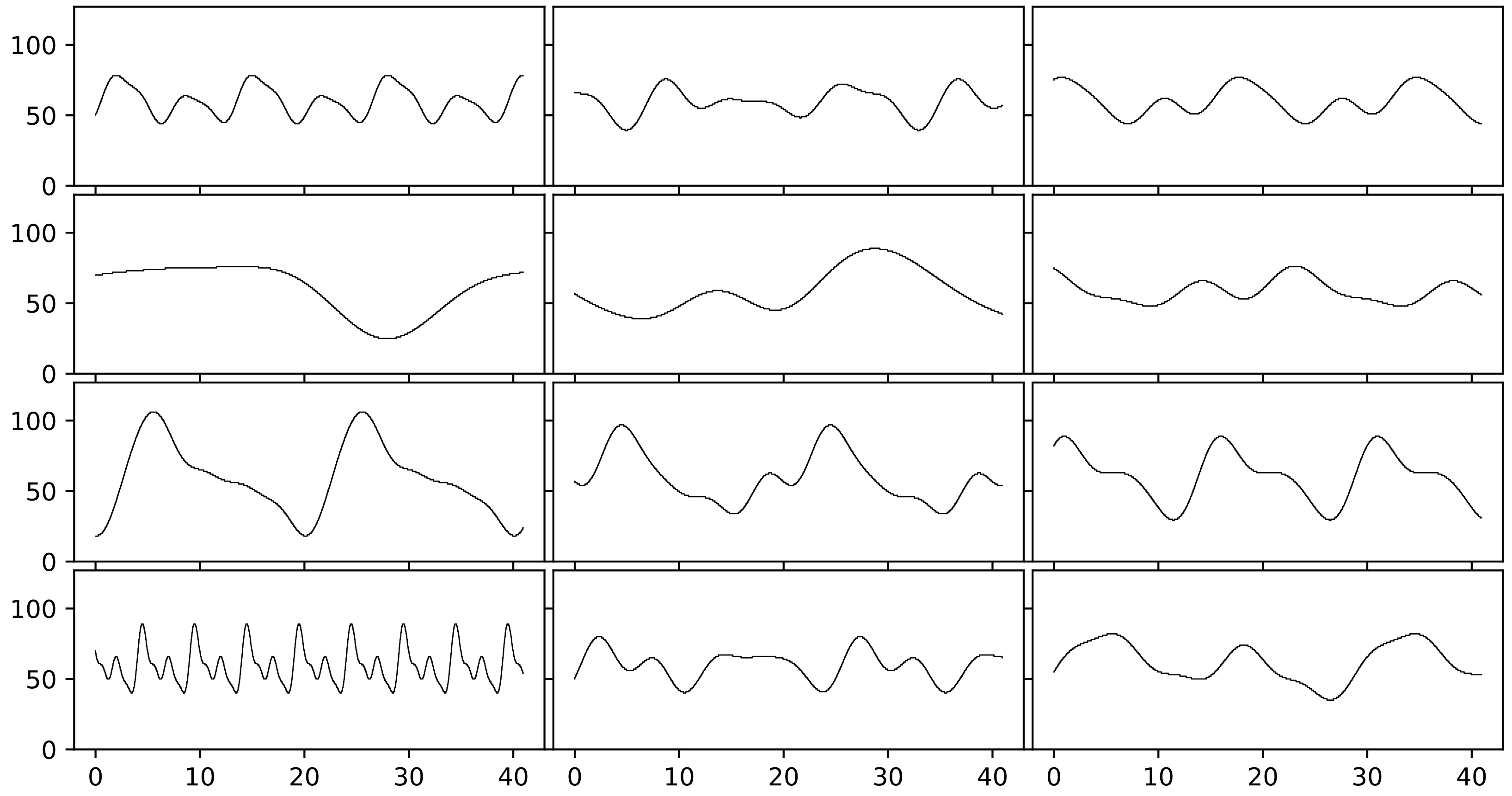




1D Signal Experiments

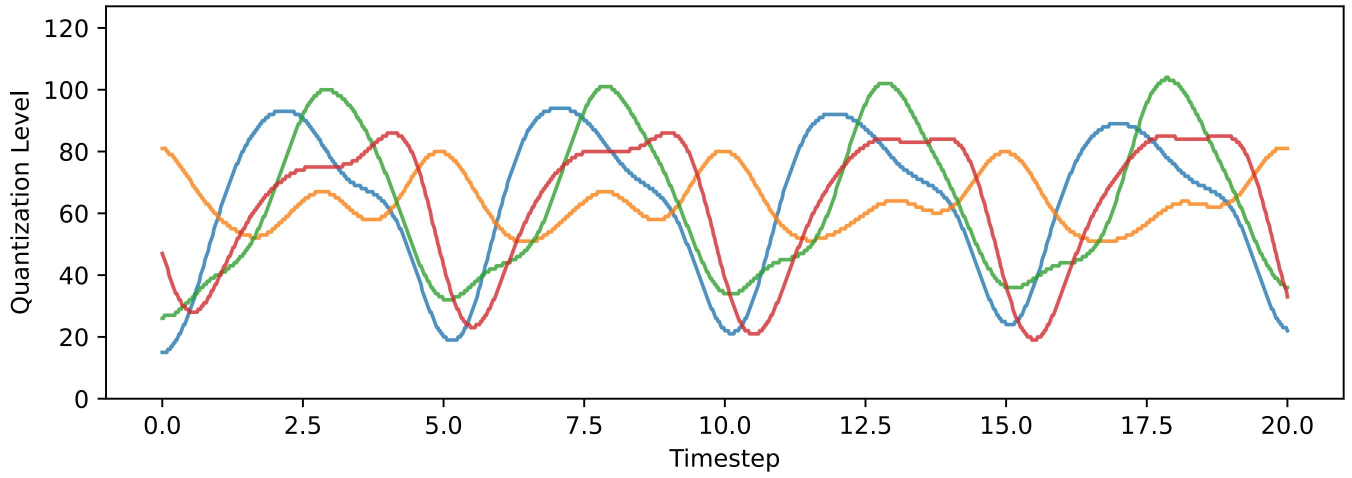
1D Signal Setup

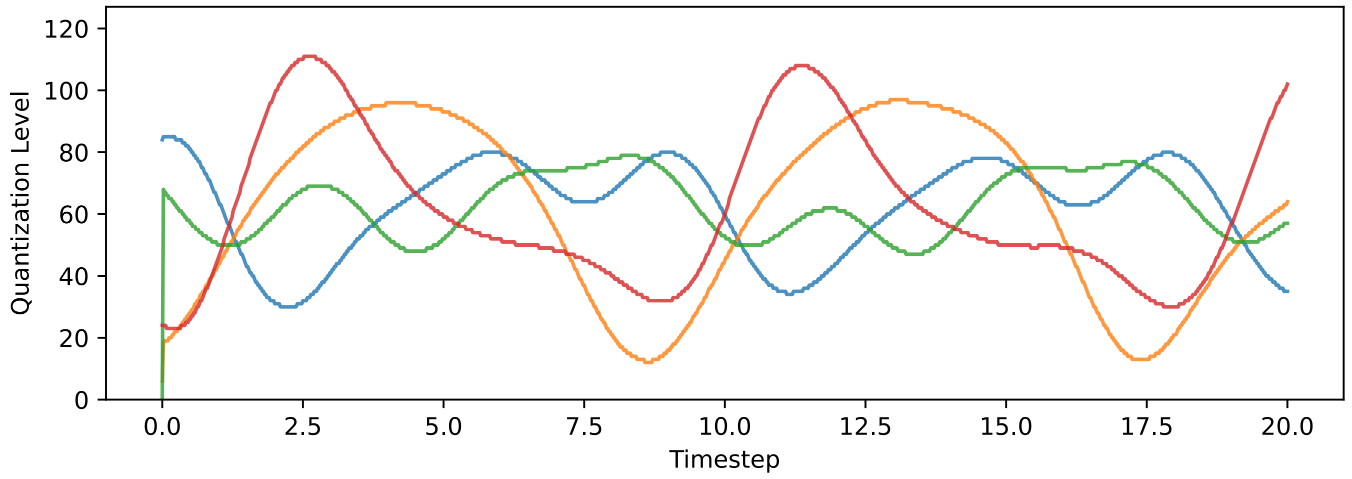
Instead of audio waveforms as input, using a Fourier dataset with randomized coefficients, number of terms and periodicity (sampling: 50Hz, quantization: 127 bins, encoding one-hot, conditioned on periodicity between 5-10secs)



Sampling Results

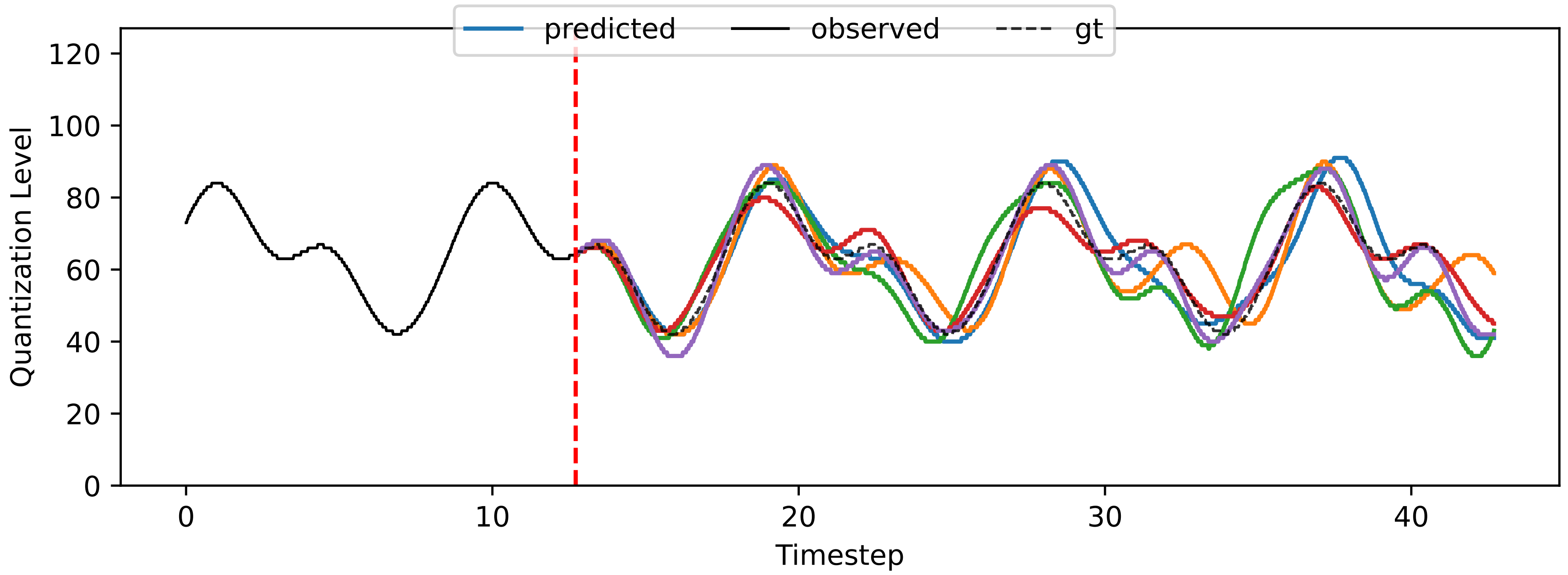
The following diagrams show multiple samples $\mathbf{x} \sim p(\mathbf{X}|Y = \text{period})$: short periods (~5secs), longer periods (~10secs).





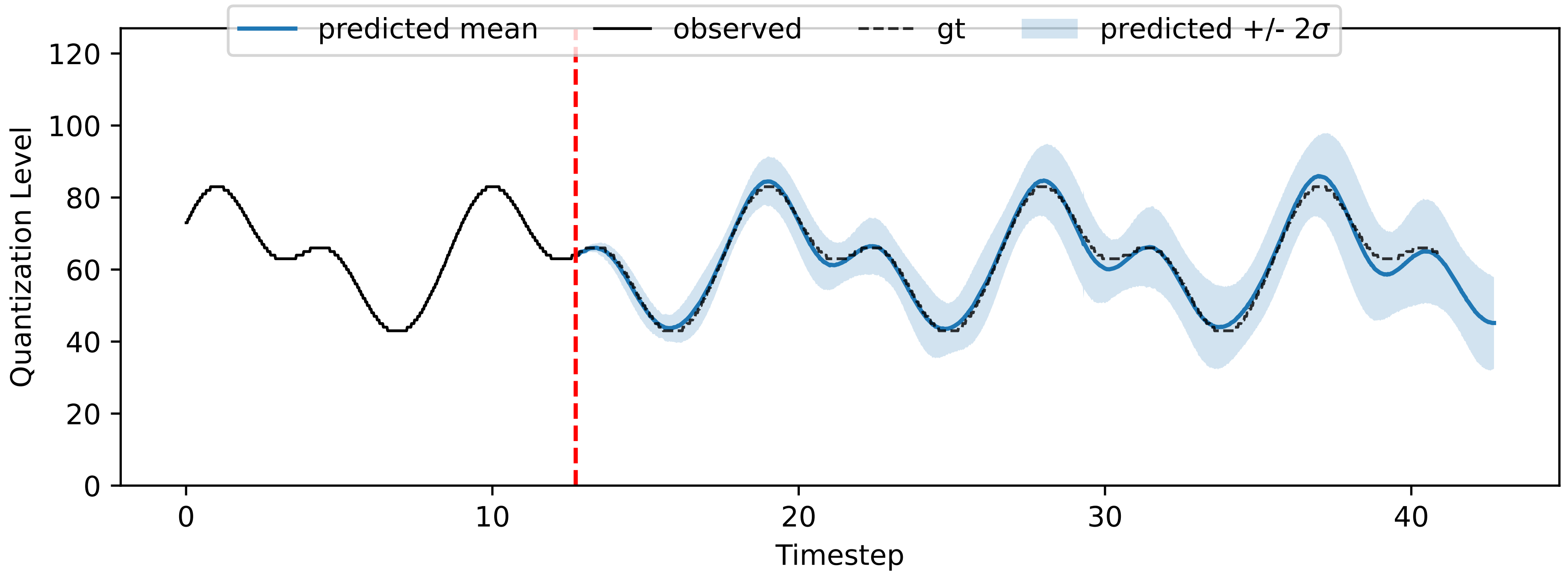
Prediction Results

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.



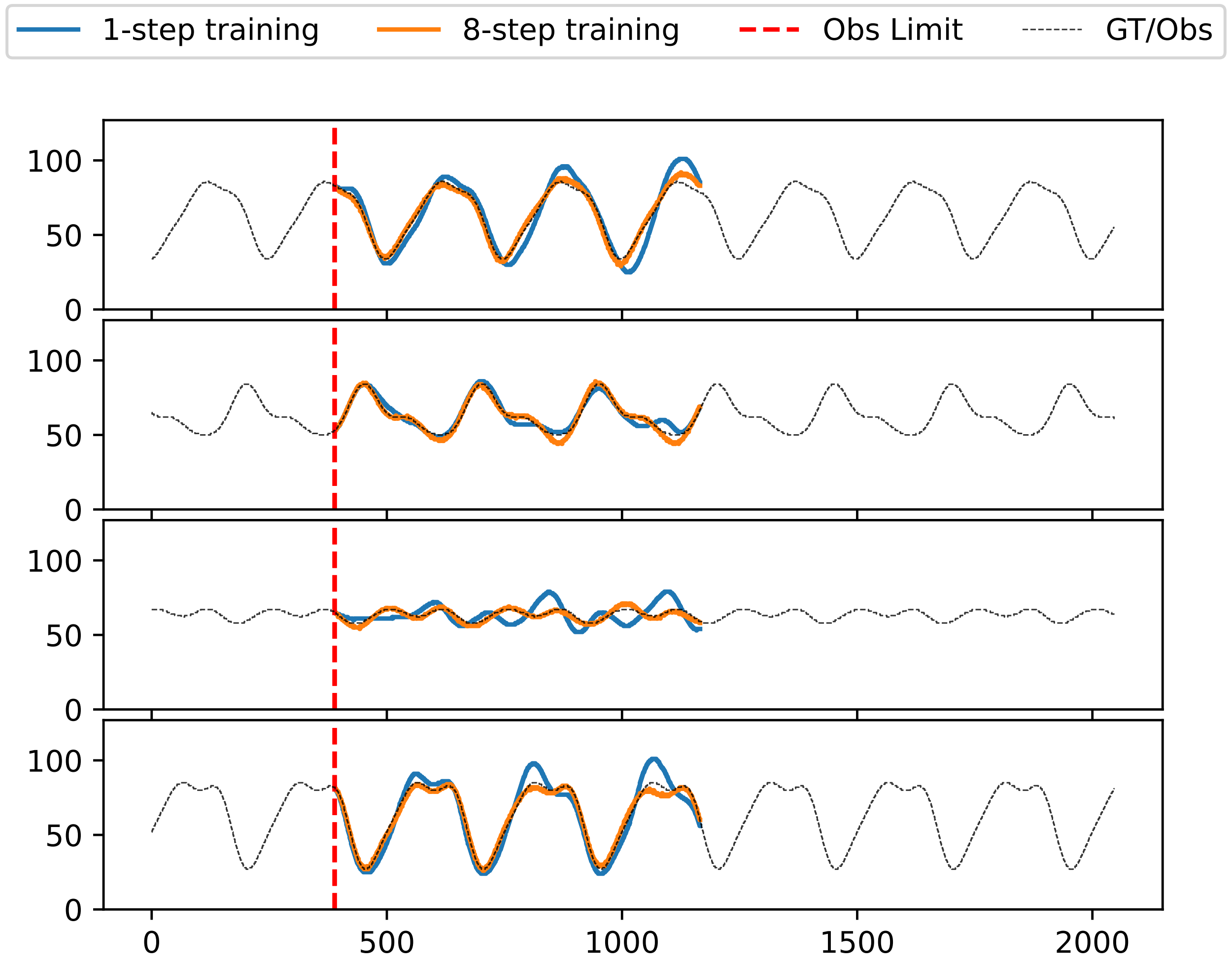
Prediction Results - Confidence Bounds

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)

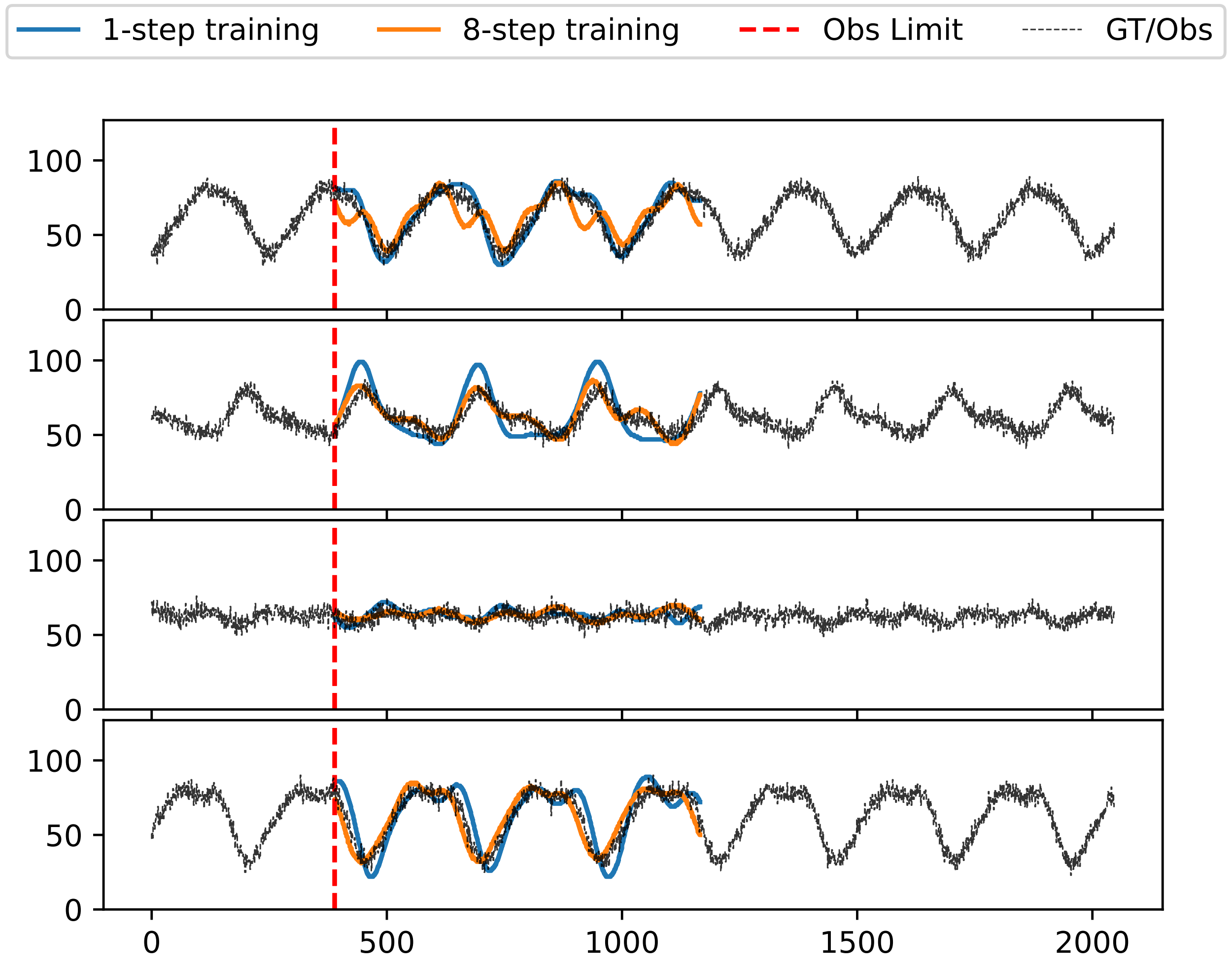
(-) Sparser losses

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

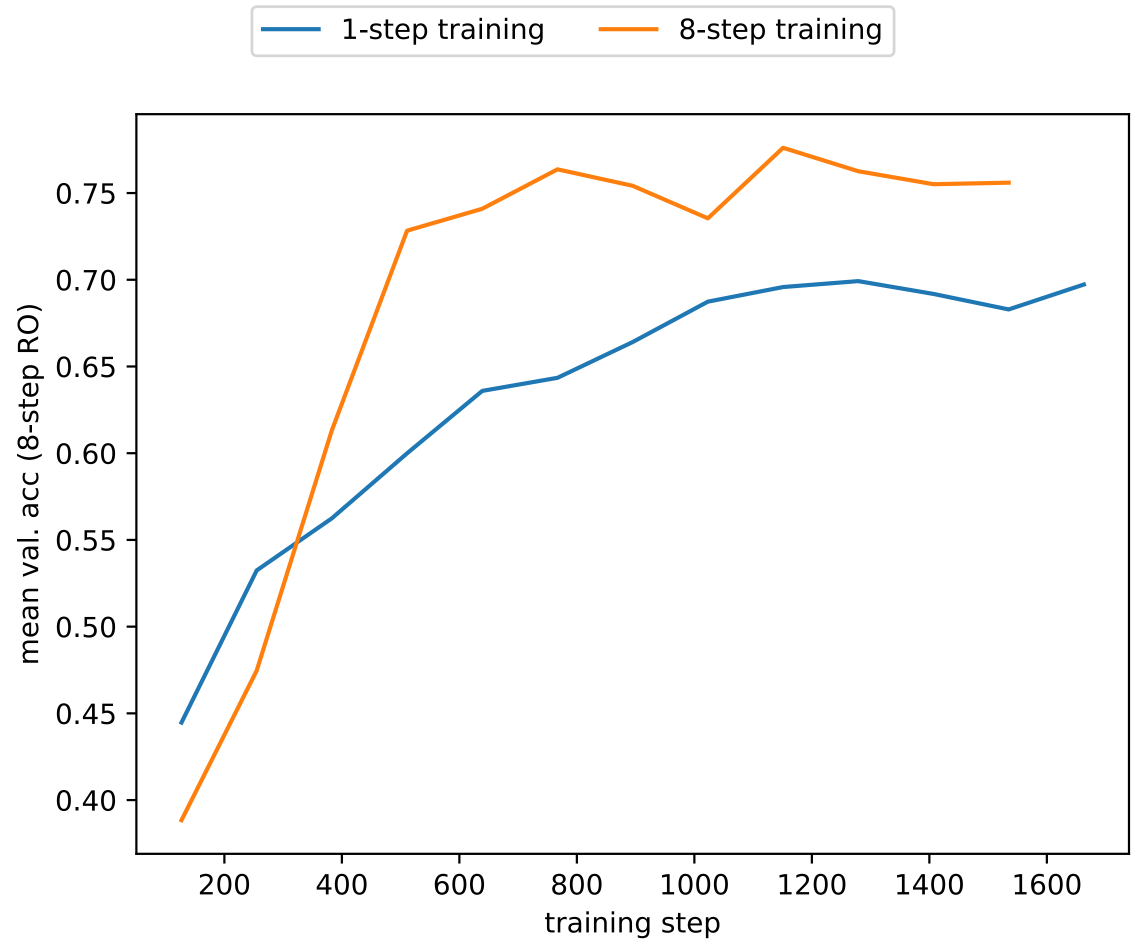


Train-Unrolling Validation Acc. Results

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.

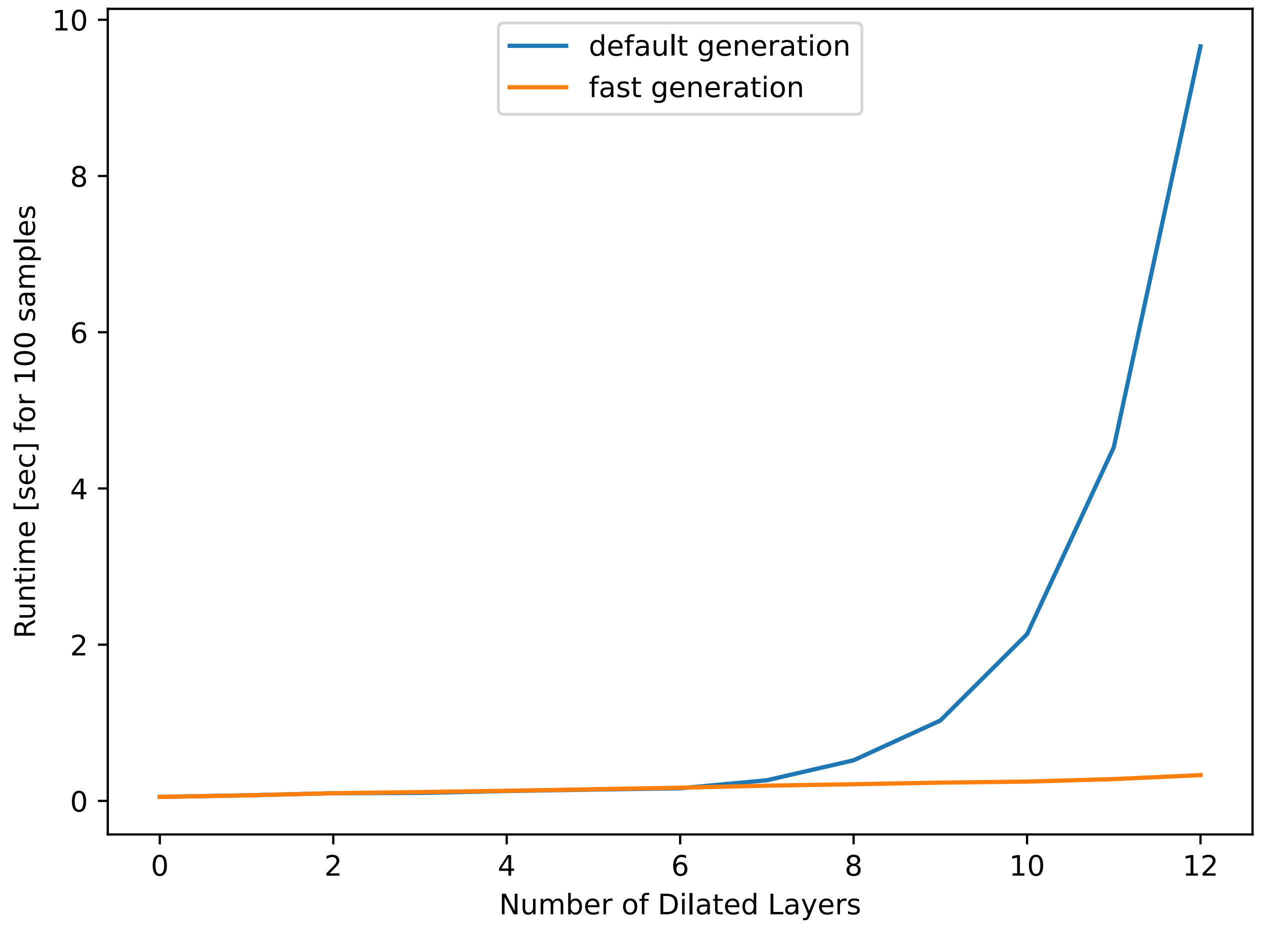


Runtime Performance Results

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.



*Performed on a 1080 Ti

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

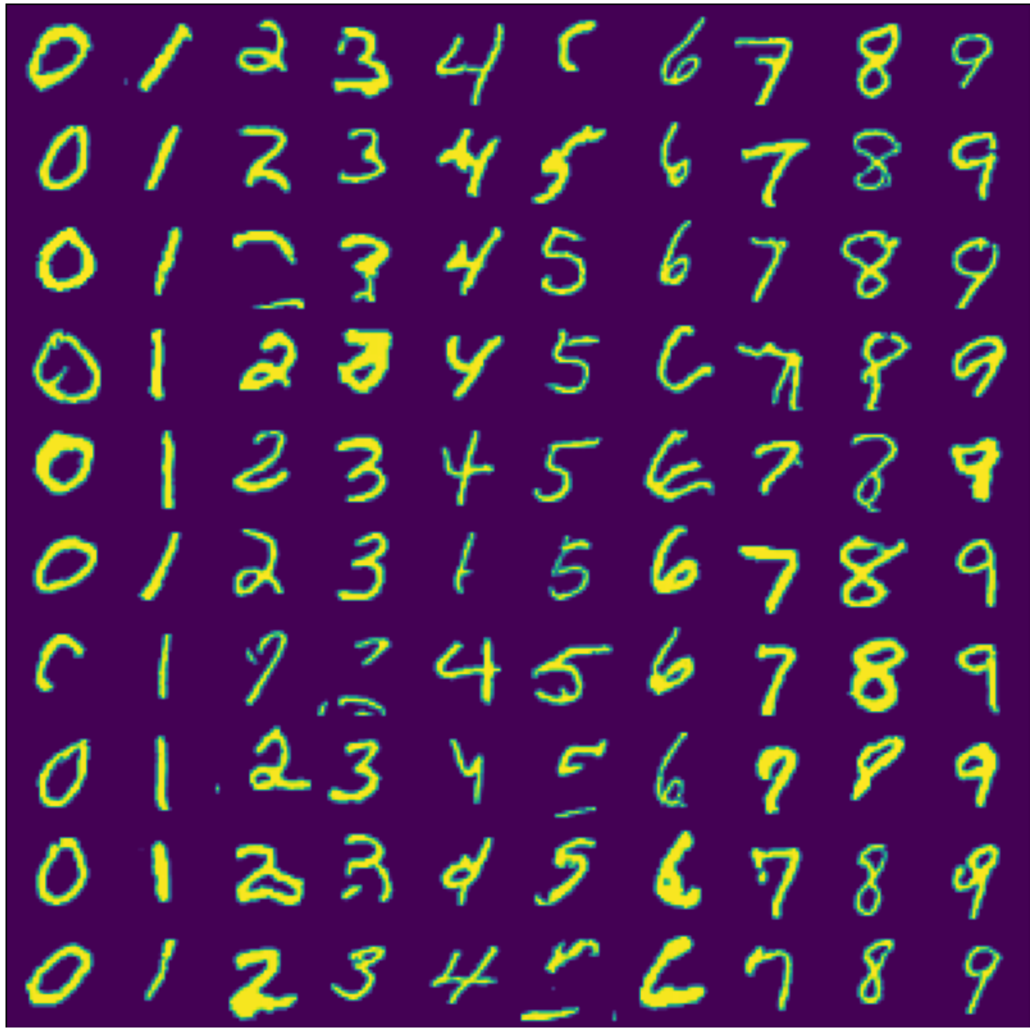
Samples drawn from $p(\mathbf{X} \mid Y)$, where $\mathbf{X}$ is an MNIST 28x28 random variable and Y is the digit conditioned on. Quantization 256.

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 Completion Results

MNIST image reconstructions drawn from

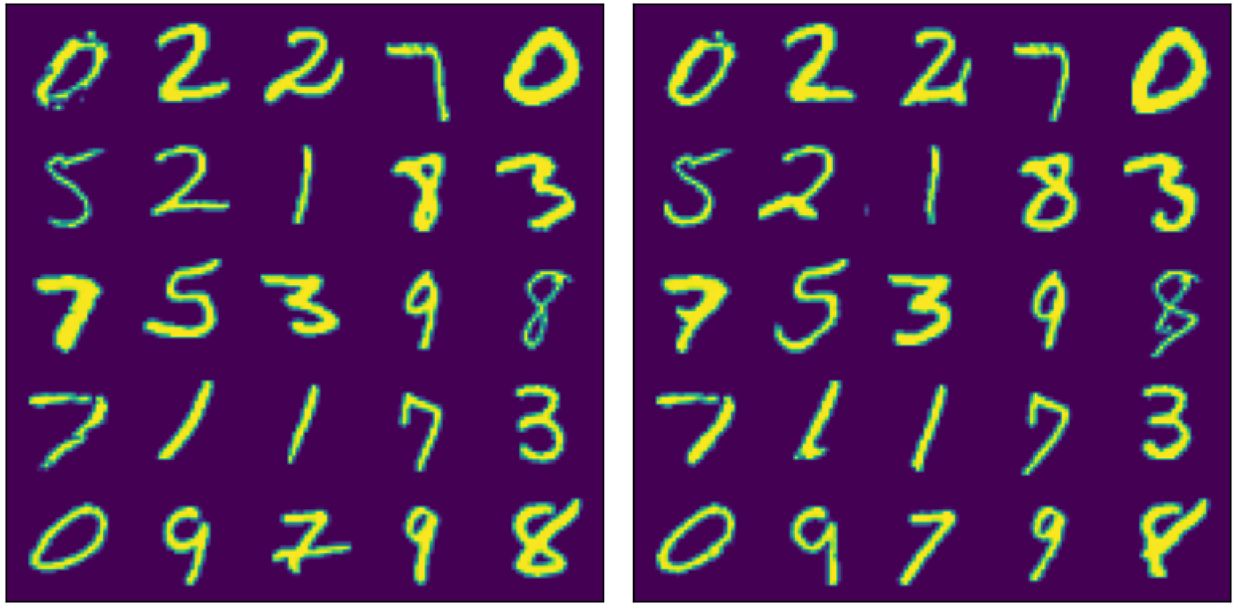
$$p(X_{N+1}, \ldots, X_T \mid X_1, \ldots, X_N, Y),$$

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

Left: original images, Right: reconstructed image after observing N=392 (first image half). Images are from the test set.

Note

- Digit style is maintained during generation (thick strokes vs. thin strokes)
- 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

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

For MNIST images the average $\log p(\mathbf{X} = \mathbf{x})$ is -60.7, whereas random images range around -1300.0.

MNIST Classification Results

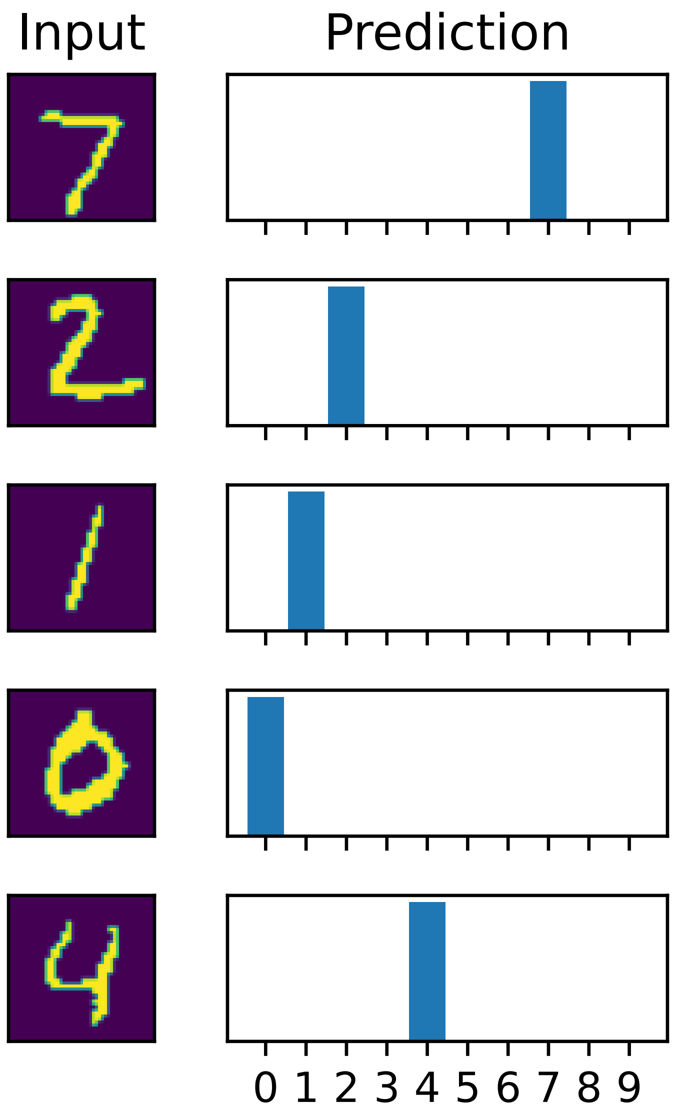
Given the class probabilities $p(Y)$, we compute from Bayes

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

A sample classification is shown on the right.

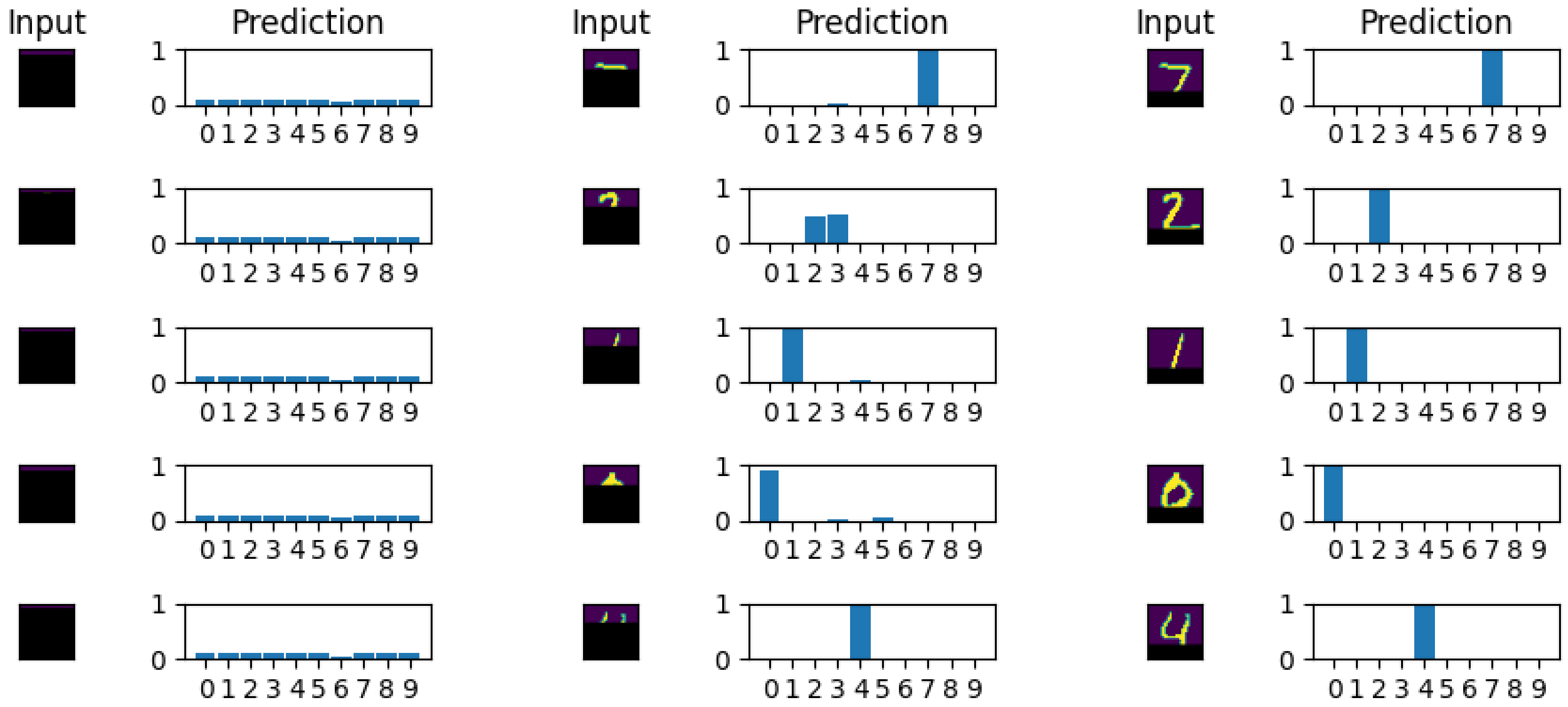
Accuracy

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 $p(Y|\mathbf{X}_{0\ldots H})$ evolves as H approaches T=784. The image below plots (from left to right) $p(Y|\mathbf{X}_{0\ldots H})$ for H=85, H=281 and H=589.



See https://media.giphy.com/media/TsM2qbgxGwi3QPrlkk/giphy.gif for an animated version