Deep learning

10.2. Causal convolutions

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If we use an autoregressive model with a **masked input** as we saw in lecture 10.1. “Auto-regression”

$$f : \{0, 1\}^T \times \mathbb{R}^T \to \mathbb{R}^C$$

the input differs from a position to another.

During training, even though the full sequence is known, common computation is lost.

Notes

With the models we saw previously, the input differs from one position to another: when predicting a new component, both the mask and the value tensor are recomputed.
Consequently such a model does not leverage that most computation is shared between positions.
Classical autoregressive models used in practice rely on the structure of the model to ensure that the distribution predicted for a certain component of the signal only depends on the component predicted before, and can compute a loss on all the sequence component in one pass.
These structures are called “causal”, since only the “past” can influence the “future”.

Instead of predicting [the distribution of] one component, the model could predict [the distributions] at every position of the sequence, that is

$$f : \mathbb{R}^T \to \mathbb{R}^{T \times C}.$$

It can be used for synthesis with

$$\begin{aligned}
x_1 &\leftarrow \text{sample}\,(f_1(0, \dots, 0)) \\
x_2 &\leftarrow \text{sample}\,(f_2(x_1, 0, \dots, 0)) \\
x_3 &\leftarrow \text{sample}\,(f_3(x_1, x_2, 0, \dots, 0)) \\
&\dots \\
x_T &\leftarrow \text{sample}\,(f_T(x_1, x_2, \dots, x_{T-1}, 0))
\end{aligned}$$

where the 0s simply fill in for unknown values, and the mask is not needed.

If additionally, the model is such that "future values" do not influence the prediction at a certain time, that is

$$\forall t, x_1, \dots, x_t, \alpha_1, \dots, \alpha_{T-t}, \beta_1, \dots, \beta_{T-t},$$
$$f_{t+1}(x_1, \dots, x_t, \alpha_1, \dots, \alpha_{T-t}) = f_{t+1}(x_1, \dots, x_t, \beta_1, \dots, \beta_{T-t})$$

then, we have in particular

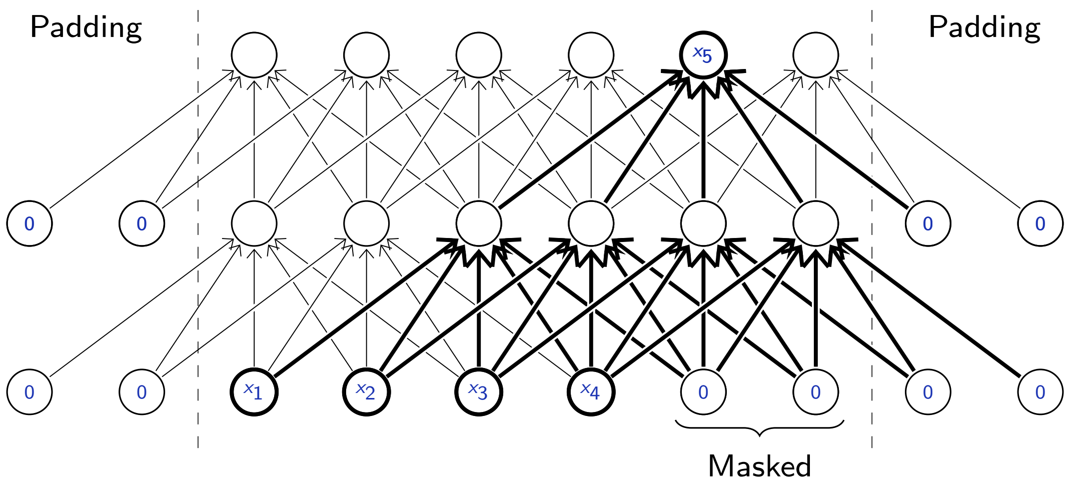
$$\begin{aligned}
f_1(0, \dots, 0) &= f_1(x_1, \dots, x_T) \\
f_2(x_1, 0, \dots, 0) &= f_2(x_1, \dots, x_T) \\
f_3(x_1, x_2, 0, \dots, 0) &= f_3(x_1, \dots, x_T) \\
&\dots \\
f_T(x_1, x_2, \dots, x_{T-1}, 0) &= f_T(x_1, \dots, x_T)
\end{aligned}$$

This provides a tremendous computational advantage during training, since all the $f_t(x_1, \dots, x_T)$ can be computed with a single forward pass:

$$\begin{aligned}\ell(f, x) &= \sum_t \ell(f_t(x_1, \dots, x_{t-1}, 0, \dots, 0), x_t) \\ &= \sum_t \ell(\underbrace{f_t(x_1, \dots, x_T)}_{f \text{ is computed once}}, x_t).\end{aligned}$$

Such models are referred to as **causal,** since the future cannot affect the past.

We can illustrate this with convolutional models. Standard convolutions let information flow "to the past," and masked input was a way to condition only on already generated values.



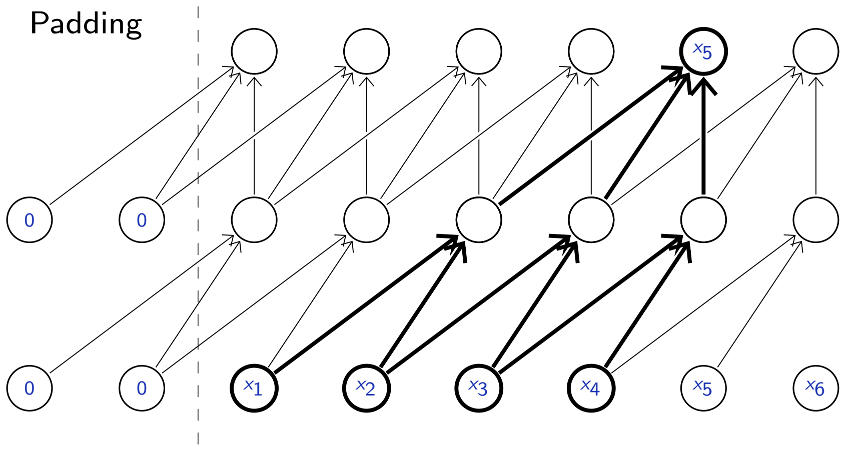
Notes

On this figure, the bottom row is the input sequence. Here we consider the prediction of x_5 based on (x_1, x_2, x_3, x_4).
A standard convolution with a filter of size $2n + 1$ takes as input n values around the location to predict:

- n values in the past,
- one at the current time step, and
- n values in the future.

To prevent "future" values to be taken into account in an autoregressive model, the current value and the future ones were zeroed.

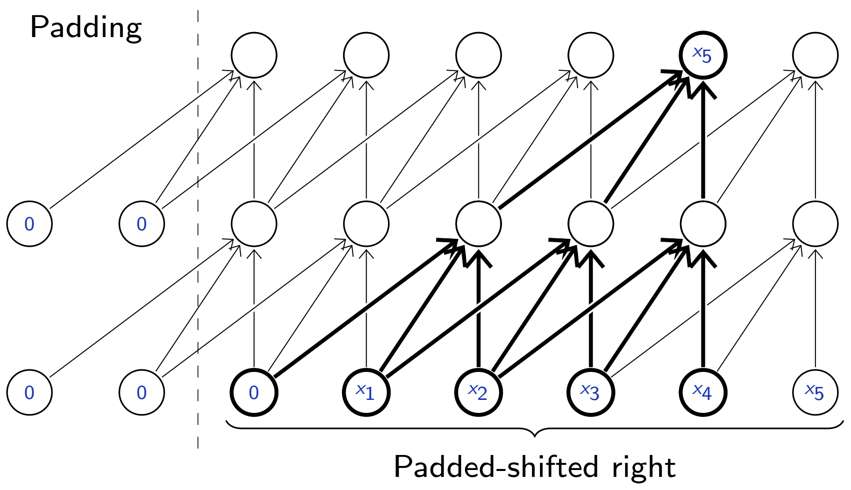
Such a model can be made **causal** with convolutions that let information flow only to the future, combined with a first convolution that hides the present.



Notes

Instead of using masks and zeroed values, the model can explicitly be made causal by using a first convolution that hides the current and future values, and all others that hide future values.

Another option for the first layer is to shift the input by one entry to hide the present.



PyTorch's convolutional layers do no accept asymmetric padding, but we can do it with `F.pad`, which even accepts negative padding to remove entries.

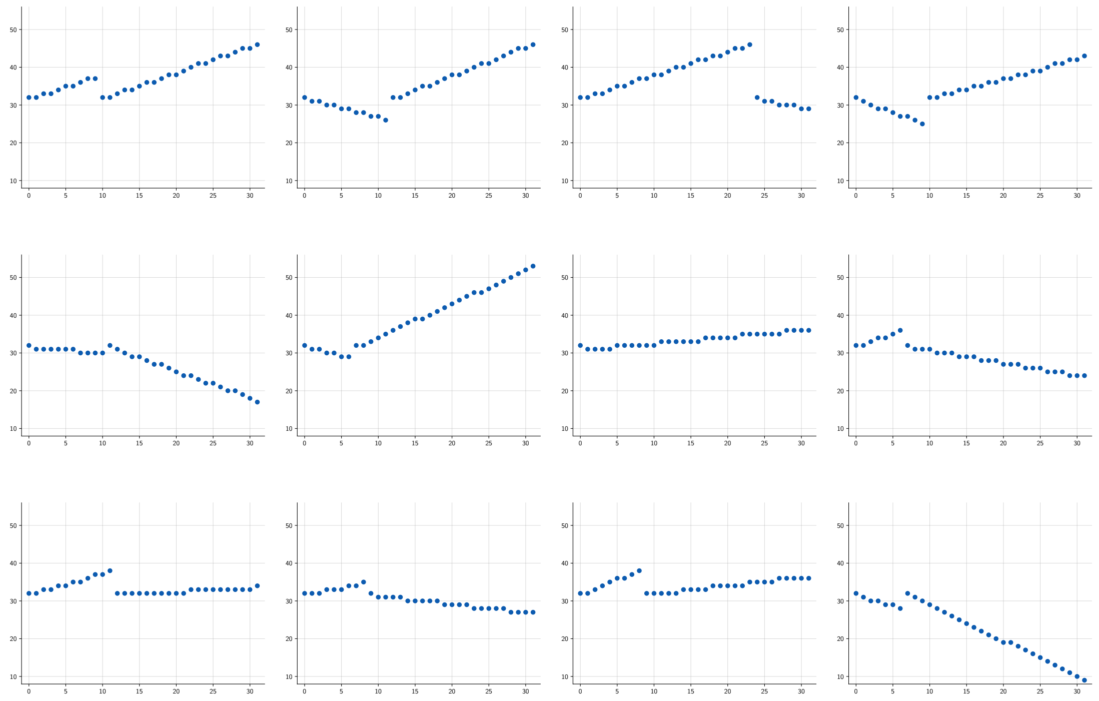
For a n-dim tensor, the padding specification is

$$(start_n, end_n, start_{n-1}, end_{n-1}, \dots, start_{n-k}, end_{n-k})$$

```
>>> x = torch.randint(10, (2, 1, 5))
>>> x
tensor([[[1, 6, 3, 9, 1]],
        [[4, 8, 2, 2, 9]]])
>>> F.pad(x, (-1, 1))
tensor([[[6, 3, 9, 1, 0]],
        [[8, 2, 2, 9, 0]]])
>>> F.pad(x, (0, 0, 2, 0))
tensor([[[0, 0, 0, 0, 0],
         [0, 0, 0, 0, 0],
         [1, 6, 3, 9, 1]],
        [[0, 0, 0, 0, 0],
         [0, 0, 0, 0, 0],
         [4, 8, 2, 2, 9]]])
```

Similar processing can be achieved with the modules `nn.ConstantPad1d`, `nn.ConstantPad2d`, or `nn.ConstantPad3d`.

Here some train sequences as in lecture 10.1. “Auto-regression”.



Model

```
class NetToy1d(nn.Module):
    def __init__(self, nb_classes, ks = 2, nc = 32):
        super().__init__()
        self.pad = (ks - 1, 0)
        self.conv0 = nn.Conv1d(1, nc, kernel_size = 1)
        self.conv1 = nn.Conv1d(nc, nc, kernel_size = ks)
        self.conv2 = nn.Conv1d(nc, nc, kernel_size = ks)
        self.conv3 = nn.Conv1d(nc, nc, kernel_size = ks)
        self.conv4 = nn.Conv1d(nc, nc, kernel_size = ks)
        self.conv5 = nn.Conv1d(nc, nb_classes, kernel_size = 1)

    def forward(self, x):
        x = F.relu(self.conv0(F.pad(x, (1, -1))))
        x = F.relu(self.conv1(F.pad(x, self.pad)))
        x = F.relu(self.conv2(F.pad(x, self.pad)))
        x = F.relu(self.conv3(F.pad(x, self.pad)))
        x = F.relu(self.conv4(F.pad(x, self.pad)))
        x = self.conv5(x)
        return x.permute(0, 2, 1).contiguous()
```

Notes

The model takes as input only one channel, the value tensor, and outputs the distribution over the classes.
The model is made causal using a negative padding `(1, -1)` on the input, which adds a zero on the left, and removes one value on the right.
The last convolution layer `conv5` uses a kernel of size 1 to convert the number of channels to the needed number of classes C.
The `permute` operation convert the batch tensor shape from $N \times C \times T$ to $N \times T \times C$ which is the format expected for sampling.

Training loop

```
for sequences in train_input.split(args.batch_size):
    input = (sequences - mean)/std

    output = model(input)

    loss = cross_entropy(
        output.view(-1, output.size(-1)),
        sequences.view(-1)
    )

    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
```

Notes

The cross-entropy loss is computed by reshaping the output to $NT \times C$ and the target to NT.

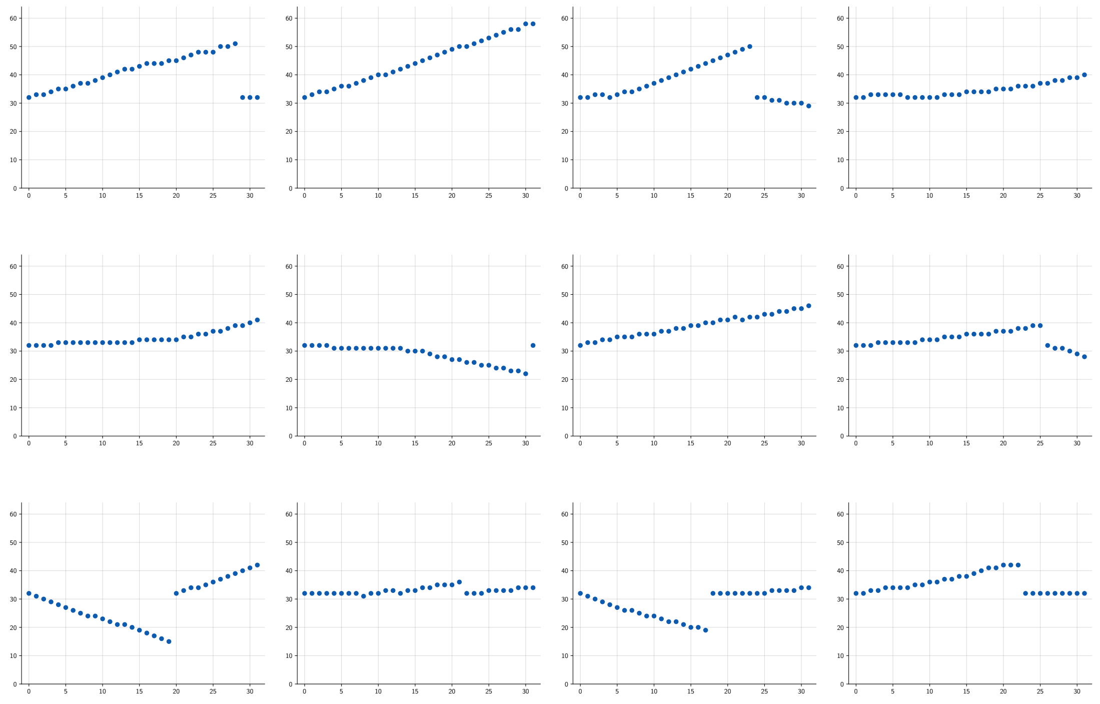
Synthesis

```
generated = train_input.new_zeros((48,) + train_input.size()[1:])

flat = generated.view(generated.size(0), -1)

for t in range(flat.size(1)):
    input = (generated.float() - mean) / std
    output = model(input)
    logits = output.view(flat.size() + (-1,))[:, t]
    dist = torch.distributions.categorical.Categorical(logits = logits)
    flat[:, t] = dist.sample()
```

Notes

For causal models, the sampling has also to be done in order, component by component. Even though the model outputs the distribution for the entire time steps at once, the only valid ones are those that follows immediately valid already generated values.
Here we generate a batch of 48 sequences in parallel.
The selection of distributions for position t is done with
`output.view(flat.size() + (-1,))[:, t]`.

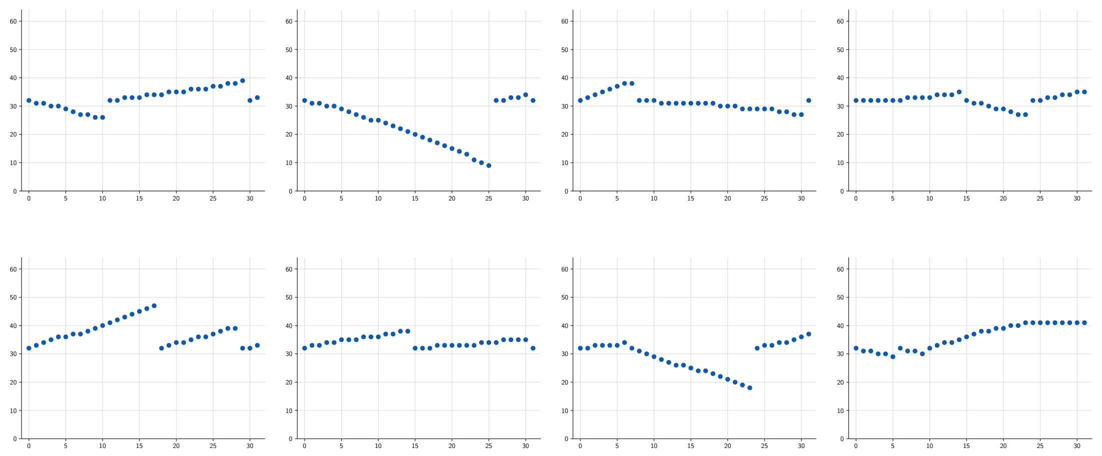
Some generated sequences



Notes

The generated sequences are generally satisfying
and have the expected structure.

The global structure may not be properly generated.



This can be fixed with **dilated convolutions** to have a larger context.

Notes

However, we may observe more than a single "cut" in a generated sequence, although training sequences only contain one.
This did not happen for the "masked" model of lecture 10.1. "Auto-regression". This pathological behavior is explained by the limited kernel size of the convolutions the prevent the model from looking at a context large enough. It cannot spot if a cut was already generated.

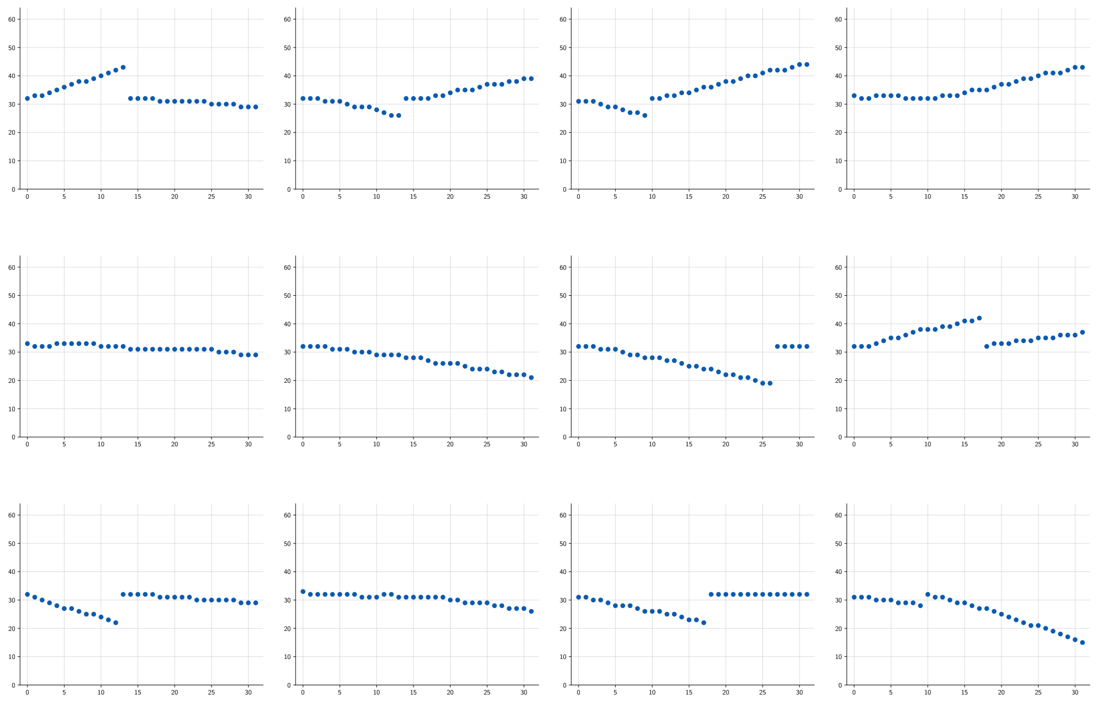
Model

```
class NetToy1dWithDilation(nn.Module):
    def __init__(self, nb_classes, ks = 2, nc = 32):
        super().__init__()
        self.conv0 = nn.Conv1d(1, nc, kernel_size = 1)
        self.pad1 = ((ks-1) * 2, 0)
        self.conv1 = nn.Conv1d(nc, nc, kernel_size = ks, dilation = 2)
        self.pad2 = ((ks-1) * 4, 0)
        self.conv2 = nn.Conv1d(nc, nc, kernel_size = ks, dilation = 4)
        self.pad3 = ((ks-1) * 8, 0)
        self.conv3 = nn.Conv1d(nc, nc, kernel_size = ks, dilation = 8)
        self.pad4 = ((ks-1) * 16, 0)
        self.conv4 = nn.Conv1d(nc, nc, kernel_size = ks, dilation = 16)
        self.conv5 = nn.Conv1d(nc, nb_classes, kernel_size = 1)

    def forward(self, x):
        x = F.relu(self.conv0(F.pad(x, (1, -1))))
        x = F.relu(self.conv1(F.pad(x, self.pad1)))
        x = F.relu(self.conv2(F.pad(x, self.pad2)))
        x = F.relu(self.conv3(F.pad(x, self.pad3)))
        x = F.relu(self.conv4(F.pad(x, self.pad4)))
        x = self.conv5(x)
        return x.permute(0, 2, 1).contiguous()
```

Notes

The context taken into account when generating a value can be increase with dilated convolutions (see lecture 4.4. "Convolutions"). The paddings to make the structure causal are adapted accordingly.

Some generated sequences



The WaveNet model proposed by Oord et al. (2016a) for voice synthesis relies in large part on such an architecture.

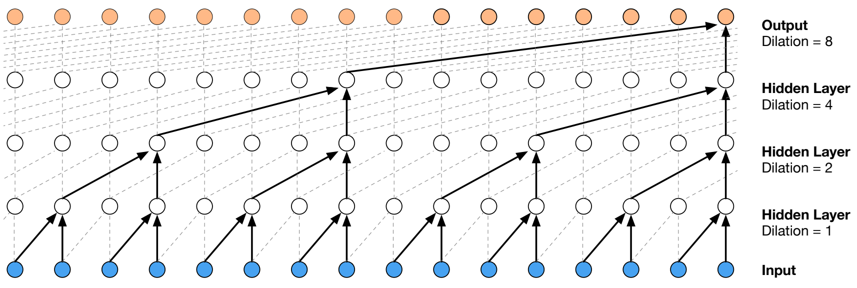


Figure 3: Visualization of a stack of *dilated* causal convolutional layers.

(Oord et al., 2016a)

Notes

The precursor of all the state-of-the-art methods for voice synthesis are based on autoregressive models with dilated convolutions (no recurrent networks as previously done).

Causal convolutions for images

The same mechanism can be implemented for images, using causal convolution:

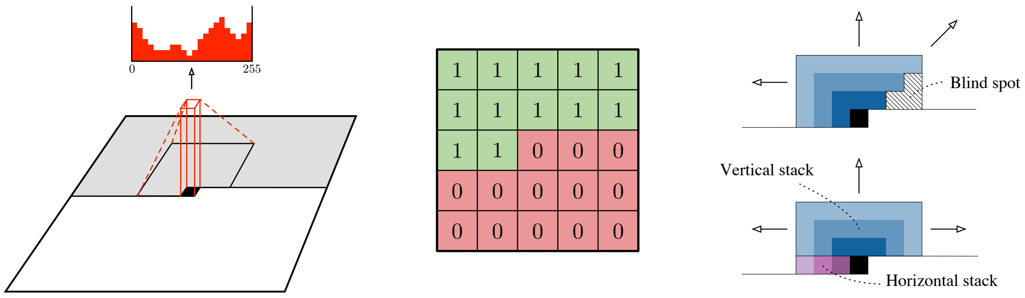


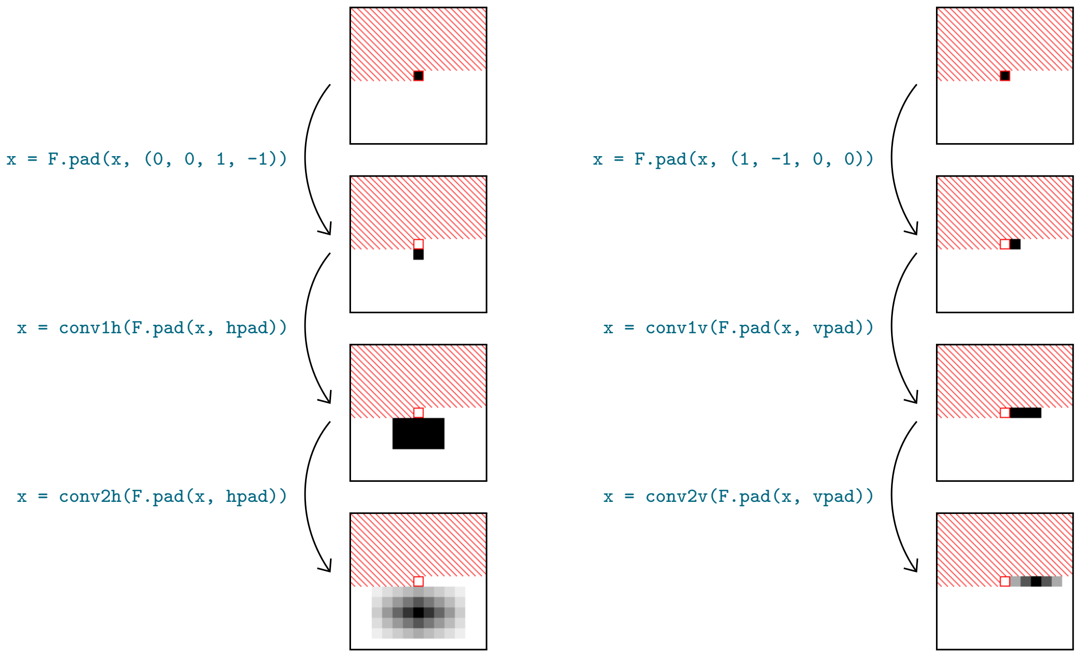
Figure 1: **Left**: A visualization of the PixelCNN that maps a neighborhood of pixels to prediction for the next pixel. To generate pixel x_i the model can only condition on the previously generated pixels $x_1, \dots x_{i-1}$. **Middle**: an example matrix that is used to mask the 5x5 filters to make sure the model cannot read pixels below (or strictly to the right) of the current pixel to make its predictions. **Right**: Top: PixelCNNs have a *blind spot* in the receptive field that can not be used to make predictions. Bottom: Two convolutional stacks (blue and purple) allow to capture the whole receptive field.

(Oord et al., 2016b)

Notes

(Oord et al., 2016b) propose 2D convolutions that respect the causal structure for the raster scan order. This is achieved by combining convolutions that look above the current point and strictly on its left.

```
ks = 5
hpad = (ks//2, ks//2, ks//2, 0)
conv1h = nn.Conv2d(1, 1, kernel_size = (ks//2+1, ks))
conv2h = nn.Conv2d(1, 1, kernel_size = (ks//2+1, ks))
vpad = (ks//2,     0,     0, 0)
conv1v = nn.Conv2d(1, 1, kernel_size = (1, ks//2+1))
conv2v = nn.Conv2d(1, 1, kernel_size = (1, ks//2+1))
```


x = F.pad(x, (0, 0, 1, -1))
x = conv1h(F.pad(x, hpad))
x = conv2h(F.pad(x, hpad))
x = F.pad(x, (1, -1, 0, 0))
x = conv1v(F.pad(x, vpad))
x = conv2v(F.pad(x, vpad))

Notes

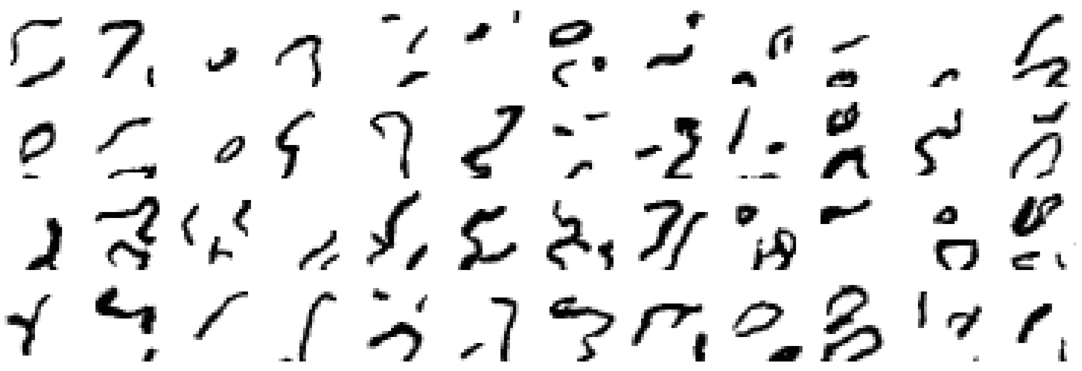
The shades of grays indicate how much the value at a given position is influenced by the value at the pixel framed in red.
On the left, we first shift the input signal downward by one row, and apply twice a padding to shift downward and a convolution with a centered rectangular kernel, resulting each time in a convolution by a shifted kernel downward.
On the right we first shift the signal to the right by one column, and then apply twice a padding to shift right and a convolution by a strip kernel, resulting each time in a convolution by a thin horizontal kernel shifted to the right.
This process assures that the value of the pixel framed in red influences only pixel strictly below or on the same row but strictly on its right.

```
class PixelCNN(nn.Module):
    def __init__(self, nb_classes, in_channels = 1, ks = 5):
        super().__init__()

        self.hpad = (ks//2, ks//2, ks//2, 0)
        self.vpad = (ks//2,     0,     0, 0)

        self.conv1h = nn.Conv2d(in_channels, 32, kernel_size = (ks//2+1, ks))
        self.conv2h = nn.Conv2d(32, 64, kernel_size = (ks//2+1, ks))
        self.conv1v = nn.Conv2d(in_channels, 32, kernel_size = (1, ks//2+1))
        self.conv2v = nn.Conv2d(32, 64, kernel_size = (1, ks//2+1))
        self.final1 = nn.Conv2d(128, 128, kernel_size = 1)
        self.final2 = nn.Conv2d(128, nb_classes, kernel_size = 1)

    def forward(self, x):
        xh = F.pad(x, (0, 0, 1, -1))
        xv = F.pad(x, (1, -1, 0, 0))
        xh = F.relu(self.conv1h(F.pad(xh, self.hpad)))
        xv = F.relu(self.conv1v(F.pad(xv, self.vpad)))
        xh = F.relu(self.conv2h(F.pad(xh, self.hpad)))
        xv = F.relu(self.conv2v(F.pad(xv, self.vpad)))
        x = F.relu(self.final1(torch.cat((xh, xv), 1)))
        x = self.final2(x)

        return x.permute(0, 2, 3, 1).contiguous()
```

Notes

The forward pass processes two tensors in parallel, one with the causal convolution propagating information down and the other with causal convolutions propagating it to the right. These two tensors are concatenated and processed through a 1×1 convolution to get 256 logits per locations.
The final step is to permute the dimensions from $N \times C \times H \times W$ to $N \times H \times W \times C$.

Some generated images



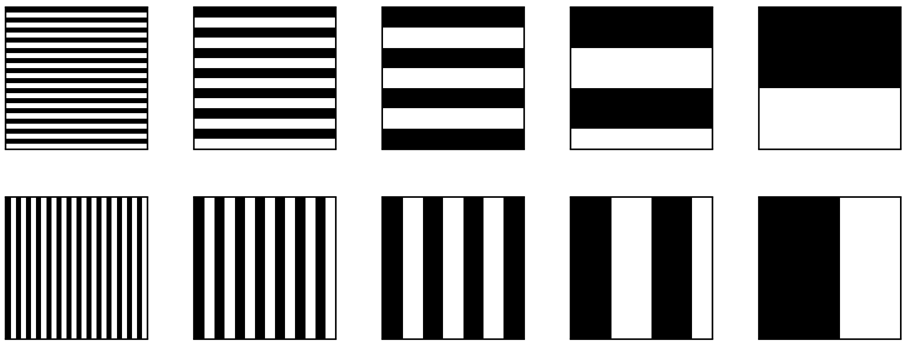
Notes

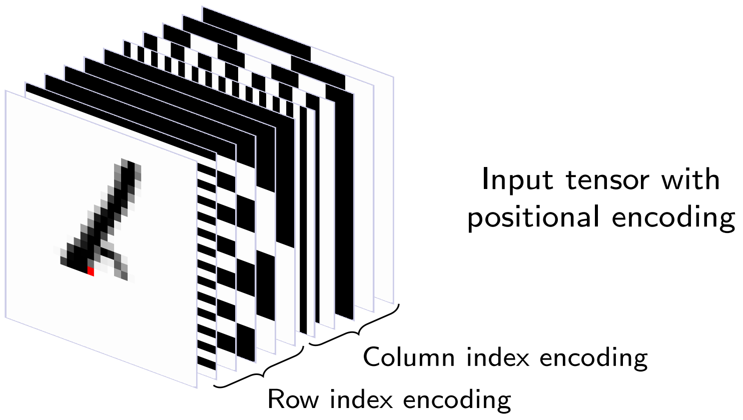
The synthesis process of 2D image here is exactly the same as for 1D sequences.
The generated images have some consistent characteristics: pieces of lines, rounded shapes, loops, white background.
The generation looks fine locally, but not globally. Since the model is fully convolutional, it has no way to make the prediction position-dependent. The generation process have no clue where it is in the image, and as result cannot behave differently at different locations.

Such a fully convolutional model has no way to make the prediction position-dependent, which results here in local consistency, but fragmentation.

A classical fix is to supplement the input with a **positional encoding,** that is a multi-channel input that provides full information about the location.

Here with a resolution of 28×28 we can encode the positions with 5 Boolean channels per coordinate.

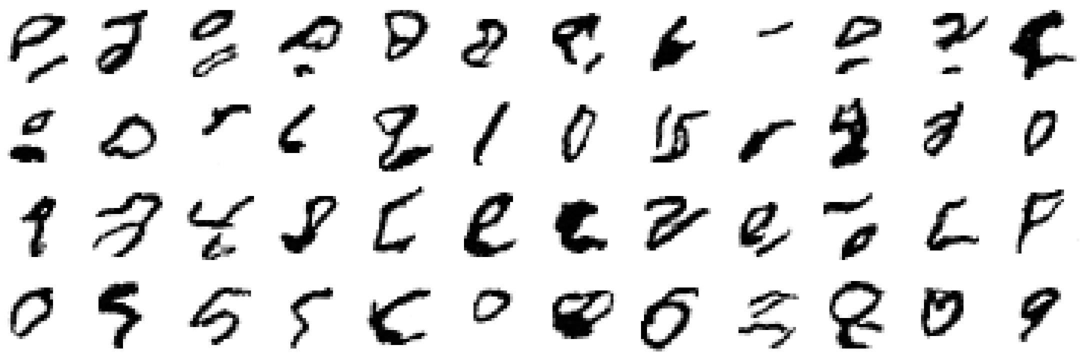




Notes

In addition to feeding the model with what has already been generated, we input ten additional channels which are the same for all the samples. Each pixel of the 28×28 image is associated with a unique set of Boolean values encoding its location in the image.

Some generated images



Notes

With the positional encoding, the synthesized results are more satisfying: there is no fragmentation anymore, and the overall shapes are more similar to that of actual MNIST samples.

References

A. Oord, S. Dieleman, H. Zen, K. Simonyan, O. Vinyals, A. Graves, N. Kalchbrenner, A. Senior, and K. Kavukcuoglu. **WaveNet: A generative model for raw audio**. CoRR, abs/1609.03499, 2016a.

A. Oord, N. Kalchbrenner, O. Vinyals, L. Espeholt, A. Graves, and K. Kavukcuoglu. **Conditional image generation with PixelCNN decoders**. CoRR, abs/1606.05328, 2016b.