If we use an autoregressive model with a masked input

\[ f : \{0, 1\}^T \times \mathbb{R}^T \rightarrow \mathbb{R}^C \]

the input differs from a position to another.

During training, even though the full input is known, common computation is lost.
We can avoid having the mask itself as input if the model predicts a distribution for every position of the sequence, that is
\[ f : \mathbb{R}^T \rightarrow \mathbb{R}^{T \times C}. \]

It can be used for synthesis with
\[
\begin{align*}
x_1 & \leftarrow \text{sample}(f_1(0, \ldots, 0)) \\
x_2 & \leftarrow \text{sample}(f_2(x_1, 0, \ldots, 0)) \\
x_3 & \leftarrow \text{sample}(f_3(x_1, x_2, 0, \ldots, 0)) \\
\vdots \\
x_T & \leftarrow \text{sample}(f_T(x_1, x_2, \ldots, x_{T-1}, 0))
\end{align*}
\]
where the 0s simply fill in for unknown values.

If additionally, the model is such that “future values” do not influence the prediction at a certain time, that is
\[
\forall t, x_1, \ldots, x_t, \alpha_1, \ldots, \alpha_{T-t}, \beta_1, \ldots, \beta_{T-t}, \\
f_{t+1}(x_1, \ldots, x_t, \alpha_1, \ldots, \alpha_{T-t}) = f_{t+1}(x_1, \ldots, x_t, \beta_1, \ldots, \beta_{T-t})
\]
then, we have in particular
\[
\begin{align*}
f_1(0, \ldots, 0) &= f_1(x_1, \ldots, x_T) \\
f_2(x_1, 0, \ldots, 0) &= f_2(x_1, \ldots, x_T) \\
f_3(x_1, x_2, 0, \ldots, 0) &= f_3(x_1, \ldots, x_T) \\
\vdots \\
f_T(x_1, x_2, \ldots, x_{T-1}, 0) &= f_T(x_1, \ldots, x_T)
\end{align*}
\]
Which provides a tremendous computational advantage during training, since

\[
\ell(f, x) = \sum_u \ell(f_u(x_1, \ldots, x_{u-1}, 0, \ldots, 0), x_u)
\]

\[
= \sum_u \ell(f_u(x_1, \ldots, x_T), x_u).
\]

Computed once

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.
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.

Another option for the first layer is to shift the input by one entry to hide the present.
PyTorch’s convolutional layers do not 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

\[(\text{start}_n, \text{end}_n, \text{start}_{n-1}, \text{end}_{n-1}, \ldots, \text{start}_{n-k}, \text{end}_{n-k})\]

```python
>>> 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`. 

Some train sequences
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()

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()
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()
The global structure may not be properly generated.

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

```python
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()
```
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)
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 \( x_1, \ldots, x_{i-1} \). **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)
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))

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()
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 $28 \times 28$ we can encode the positions with 5 Boolean channels per coordinate.
Row encoding

Column encoding

Input tensor with positional encoding

Some generated images
References
