Deep learning

7.1. Transposed convolutions

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Constructing deep generative architectures requires layers to increase the signal dimension, the contrary of what we have done so far with feed-forward networks.

Some generative processes optimize the input, and as such rely on back-propagation to expend the signal from a low-dimension representation to the high-dimension signal space.

The same can be done in the forward pass with **transposed convolution layers** whose forward operation corresponds to a convolution layer’s backward pass.
Consider a 1d convolution with a kernel $\kappa$

$$
y_i = (x \odot \kappa)_i = \sum_a x_{i+a-1} \kappa_a = \sum_u x_u \kappa_{u-i+1}.
$$

We get

$$
\left[ \frac{\partial \ell}{\partial x} \right]_u = \frac{\partial \ell}{\partial x_u} = \sum_i \frac{\partial \ell}{\partial y_i} \frac{\partial y_i}{\partial x_u} = \sum_i \frac{\partial \ell}{\partial y_i} \kappa_{u-i+1}.
$$

which looks a lot like a standard convolution layer, except that the kernel coefficients are visited in reverse order.
This is actually the standard convolution operator from signal processing. If \( \ast \) denotes this operation, we have
\[
(x \ast \kappa)_i = \sum_a x_a \kappa_{i-a+1}.
\]

Coming back to the backward pass of the convolution layer, if

\[
y = x \otimes \kappa
\]

then
\[
\left[ \frac{\partial \ell}{\partial x} \right] = \left[ \frac{\partial \ell}{\partial y} \right] \ast \kappa.
\]
In the deep-learning field, since it corresponds to transposing the weight matrix of the equivalent fully-connected layer, it is called a transposed convolution.

\[
\begin{bmatrix}
\kappa_1 & \kappa_2 & \kappa_3 & 0 & 0 & 0 \\
0 & \kappa_1 & \kappa_2 & \kappa_3 & 0 & 0 \\
0 & 0 & \kappa_1 & \kappa_2 & \kappa_3 & 0 \\
0 & 0 & 0 & \kappa_1 & \kappa_2 & \kappa_3 \\
0 & 0 & 0 & 0 & \kappa_1 & \kappa_2 & \kappa_3
\end{bmatrix}^T
= 
\begin{bmatrix}
\kappa_1 & 0 & 0 & 0 & 0 \\
\kappa_2 & \kappa_1 & 0 & 0 & 0 \\
\kappa_3 & \kappa_2 & \kappa_1 & 0 \\
\kappa_3 & \kappa_2 & \kappa_1 & 0 \\
\kappa_3 & \kappa_2 & \kappa_1 & 0
\end{bmatrix}
\]

A convolution can be seen as a series of inner products, a transposed convolution can be seen as a weighted sum of translated kernels.
Convolution layer

Input

\[ \begin{array}{ccccccc}
1 & 4 & -1 & 0 & 2 & -2 & 1 & 3 & 3 & 1 \\
\end{array} \]

\[ W \]

\[ w \]

Output

\[ \begin{array}{cccc}
9 & 0 & 1 & 3 & -5 \\
\end{array} \]

\[ W - w + 1 \]
Transposed convolution layer

Input

\[
\begin{bmatrix}
  2 & 3 & 0 & -1 \\
\end{bmatrix}
\]

\[W\]

\[
\begin{bmatrix}
  1 & 2 & -1 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
  2 & 4 & -2 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
  3 & 6 & -3 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
  0 & 0 & 0 \\
\end{bmatrix}
\]

Output

\[
\begin{bmatrix}
  2 & 7 & 4 \\
\end{bmatrix}
\]

\[W + w - 1\]
F.conv_transpose1d implements the operation we just described. It takes as input a batch of multi-channel samples, and produces a batch of multi-channel samples.

```python
given
>>> x = torch.tensor([[0., 0., 1., 0., 0., 0., 0.]])
>>> k = torch.tensor([[1., 2., 3.]])
>>> F.conv1d(x, k)
tensor([[ 3., 2., 1., 0., 0.]])
```

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The class `nn.ConvTranspose1d` embeds that operation into a `nn.Module`.

```python
>>> x = torch.tensor([[1., 0., 0., 0., -1.]])
>>> m = nn.ConvTranspose1d(1, 1, kernel_size=3)
>>> with torch.autograd.no_grad():
...   m.bias.zero_()
...   m.weight.copy_(torch.tensor([1, 2, 1]))
...
Parameter containing:
tensor([0.], requires_grad=True)
Parameter containing:
tensor([[1., 2., 1.]], requires_grad=True)
>>> y = m(x)
>>> y
tensor([[1., 2., 1., 0., -1., -2., -1.]], grad_fn=<SqueezeBackward1>)
```
Transposed convolutions also have a dilation parameter that behaves as for convolution and expends the kernel size without increasing the number of parameters by making it sparse.

They also have a stride and padding parameters, however, due to the relation between convolutions and transposed convolutions:

⚠ While for convolutions stride and padding are defined in the input map, for transposed convolutions these parameters are defined in the output map, and the latter modulates a cropping operation.
Transposed convolution layer (stride = 2)

Input

\[
\begin{array}{ccc}
2 & 3 & 0 \\
\end{array}
\]

Output

\[
\begin{array}{cccc}
2 & 4 & 1 & 6 \\
\end{array}
\]

\[
\begin{array}{ccc}
1 & 2 & -1 \\
\end{array}
\]

\[
\begin{array}{ccc}
2 & 4 & -2 \\
\end{array}
\]

\[
\begin{array}{ccc}
3 & 6 & -3 \\
\end{array}
\]

\[
\begin{array}{ccc}
0 & 0 & 0 \\
\end{array}
\]

\[
\begin{array}{cccc}
2 & 4 & 1 & 6 \\
\end{array}
\]

\[
\begin{array}{ccc}
1 & 2 & -1 \\
\end{array}
\]

\[
\begin{array}{ccc}
2 & 4 & -2 \\
\end{array}
\]

\[
\begin{array}{ccc}
3 & 6 & -3 \\
\end{array}
\]

\[
\begin{array}{ccc}
0 & 0 & 0 \\
\end{array}
\]
The composition of a convolution and a transposed convolution of same parameters keep the signal size [roughly] unchanged.

A convolution with a stride greater than one may ignore parts of the signal. Its composition with the corresponding transposed convolution generates a map of the size of the observed area.

For instance, a 1d convolution of kernel size $w$ and stride $s$ composed with the transposed convolution of same parameters maintains the signal size $W$, only if

$$\exists q \in \mathbb{N}, \ W = w + s \cdot q.$$
It has been observed that transposed convolutions may create some grid-structure artifacts, since generated pixels are not all covered similarly.

For instance with a $4 \times 4$ kernel and stride 3
An alternative is to use an analytic up-scaling, implemented in the PyTorch functional `F.interpolate`.

```python
>>> x = torch.tensor([[1.0, 2.0], [3.0, 4.0]])
>>> F.interpolate(x, scale_factor = 3, mode = 'bilinear')
tensor([[1.0000, 1.0000, 1.3333, 1.6667, 2.0000, 2.0000],
        [1.0000, 1.0000, 1.3333, 1.6667, 2.0000, 2.0000],
        [1.6667, 1.6667, 2.0000, 2.3333, 2.6667, 2.6667],
        [2.3333, 2.3333, 2.6667, 3.0000, 3.3333, 3.3333],
        [3.0000, 3.0000, 3.3333, 3.6667, 4.0000, 4.0000],
        [3.0000, 3.0000, 3.3333, 3.6667, 4.0000, 4.0000]]))
```

```python
>>> F.interpolate(x, scale_factor = 3, mode = 'nearest')
tensor([[1.0, 1.0, 1.0, 2.0, 2.0, 2.0],
        [1.0, 1.0, 1.0, 2.0, 2.0, 2.0],
        [1.0, 1.0, 1.0, 2.0, 2.0, 2.0],
        [3.0, 3.0, 3.0, 4.0, 4.0, 4.0],
        [3.0, 3.0, 3.0, 4.0, 4.0, 4.0],
        [3.0, 3.0, 3.0, 4.0, 4.0, 4.0]])
```
Such module is usually combined with a convolution to learn local corrections to undesirable artifacts of the up-scaling.

In practice, a transposed convolution such as

\[
t\text{conv} = \text{nn.ConvTranspose2d}(\text{nic}, \text{noc},
\text{kernel\_size} = 3, \text{stride} = 2,
\text{padding} = 1, \text{output\_padding} = 1),
\]

\[y = t\text{conv}(x)\]

can be replaced by

\[
\text{conv} = \text{nn.Conv2d}(\text{nic}, \text{noc}, \text{kernel\_size} = 3, \text{padding} = 1)
\]

\[u = \text{F.interpolate}(x, \text{scale\_factor} = 2, \text{mode} = \text{bilinear}')
\]

\[y = \text{conv}(u)\]