Deep learning

13.2. Attention Mechanisms

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The most classical version of attention is a context-attention with a dot-product for attention function, as used by Vaswani et al. (2017) for their transformer models. We will come back to them.

Using the terminology of Graves et al. (2014), attention is an averaging of **values** associated to **keys** matching a **query**. Hence the keys used for computing attention and the values to average are different quantities.

Given a query sequence $Q \in \mathbb{R}^{T \times D}$, a key sequence $K \in \mathbb{R}^{T' \times D}$, and a value sequence $V \in \mathbb{R}^{T' \times D'}$, compute an attention matrix $A \in \mathbb{R}^{T \times T'}$ by matching Qs to Ks, and weight V with it to get the result sequence $Y \in \mathbb{R}^{T \times D'}$.

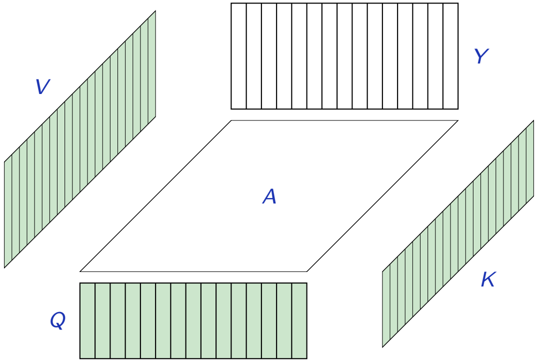
$$
\begin{aligned}
\forall i, A_i &= \operatorname{softmax}\left(\frac{KQ_i}{\sqrt{D}}\right) \\
Y_i &= V^\top A_i,
\end{aligned}
$$

or

$$
\begin{aligned}
A &= \operatorname{softmax}_{row}\left(\frac{QK^\top}{\sqrt{D}}\right) \\
Y &= AV.
\end{aligned}
$$

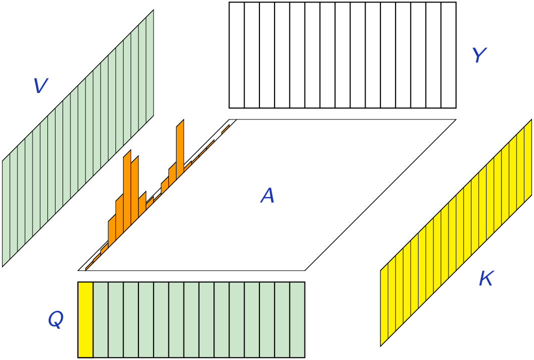
The queries and keys have the same dimension D, and there are as many keys T' as there are values. The result Y has as many rows T as there are queries, and they are of same dimension D' as the values.

[Tensors are depicted here transposed for ease of representation.]



[Tensors are depicted here transposed for ease of representation.]

$$A_i = \text{softmax}\left(\frac{KQ_i}{\sqrt{D}}\right)$$



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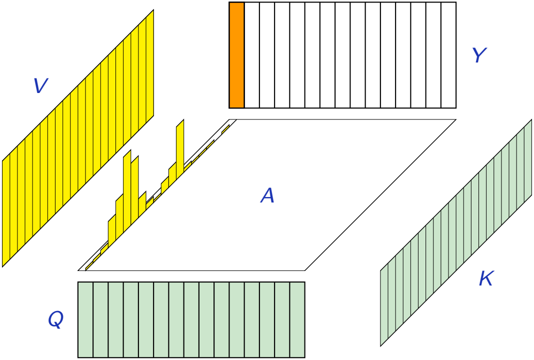
$$Y_i = V^\top A_i$$



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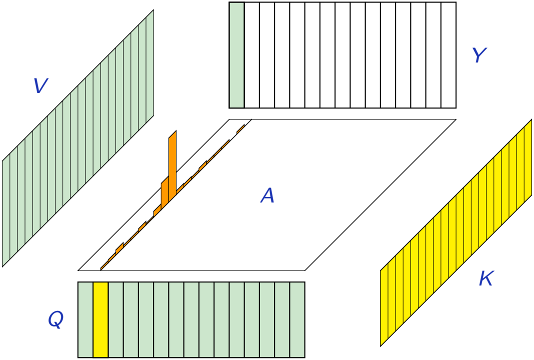

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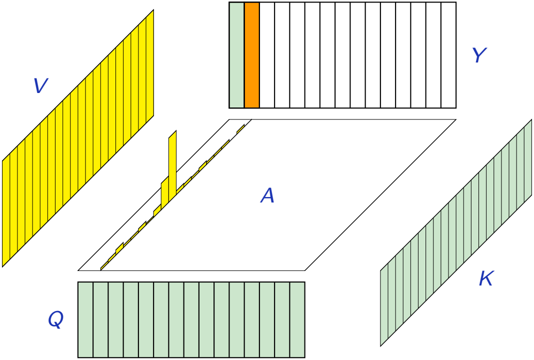

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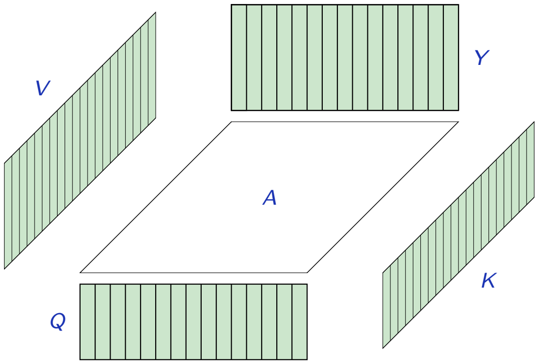
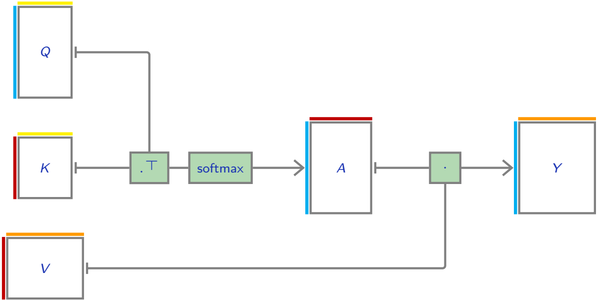


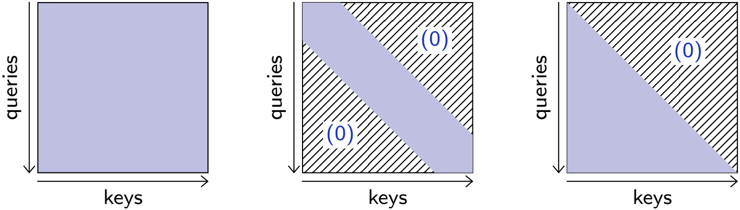


$$A = \text{softmax}_{row}\left(\frac{QK^\top}{\sqrt{D}}\right)$$

$$Y = AV.$$

Standard attention

It may be useful to mask the attention matrix, for instance in the case of self-attention, for computational reasons, or to make the model causal for auto-regression.



Full attention	Local attention	Causal attention
	$|i-j| > \Delta \Rightarrow A_{i,j} = 0$	$j > i \Rightarrow A_{i,j} = 0$

Attention layers

A standard attention layer takes as input two sequences X and X' and computes the tensors K, V, and Q as per-row linear functions.

$$Q = X {W^Q}^\top$$

$$K = X' {W^K}^\top$$

$$V = X' {W^V}^\top$$

$$A = \mathrm{softmax}_{row}\left(\frac{QK^\top}{\sqrt{D}}\right)$$

$$Y = AV$$

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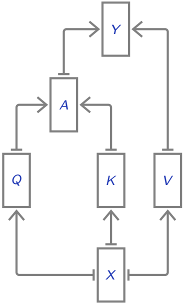

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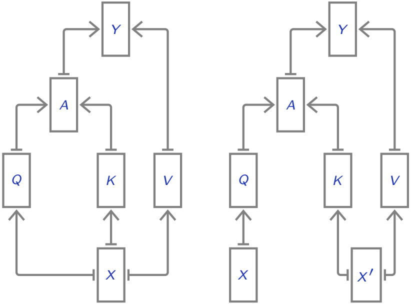

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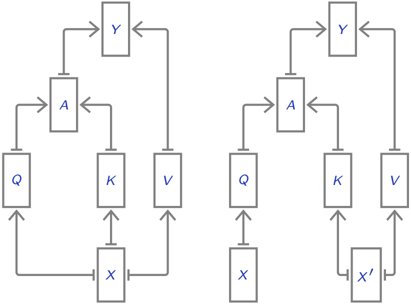

When $X = X'$, this is **self attention**, otherwise it is **cross attention.**

Multi-head attention combines several such operations in parallel, and Y is the concatenation of the results along the feature dimension to which is applied one more linear transformation.

Given a permutation σ and a $2d$ tensor X, let us use the following notation for the permutation of the rows: $\sigma(X)_i = X_{\sigma(i)}$.

The standard attention operation is **invariant to a permutation of the keys and values:**

$$Y(Q, \sigma(K), \sigma(V)) = Y(Q, K, V),$$

and **equivariant to a permutation of the queries**, that is the resulting tensor is permuted similarly:

$$Y(\sigma(Q), K, V) = \sigma(Y(Q, K, V)).$$

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Consequently self attention and cross attention are equivariant to permutations of X, and cross attention is invariant to permutations of X'.

To illustrate the behavior of such an attention layer, we consider a toy sequence-to-sequence problem with sequences composed of two triangular and two rectangular patterns.

The target averages the heights in each **pair of shapes**.

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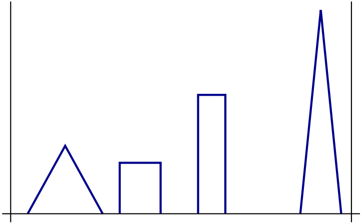
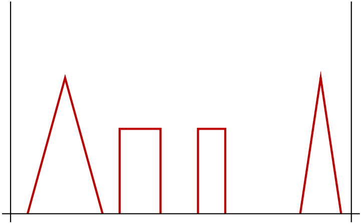


Input



Target

To illustrate the behavior of such an attention layer, we consider a toy sequence-to-sequence problem with sequences composed of two triangular and two rectangular patterns.

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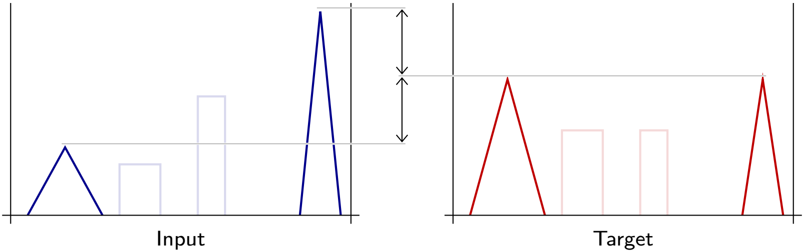

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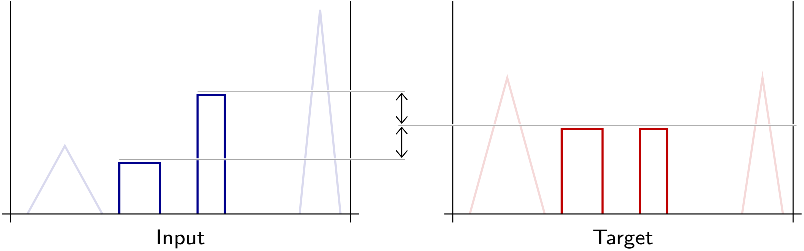

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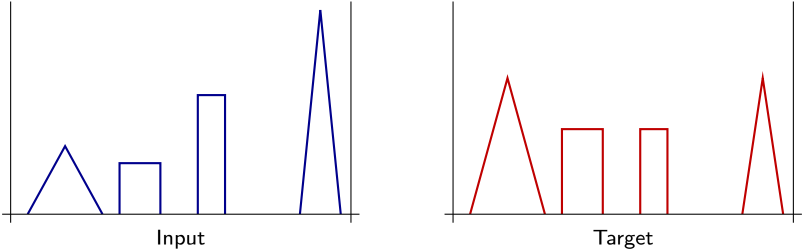
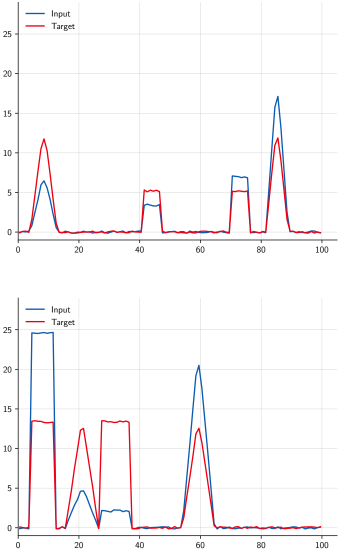


Some training examples.

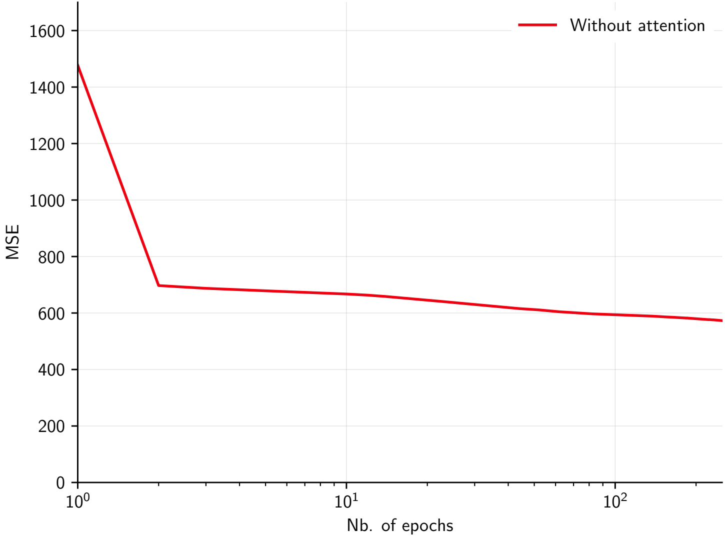


We test first a 1d convolutional network, with no attention mechanism.

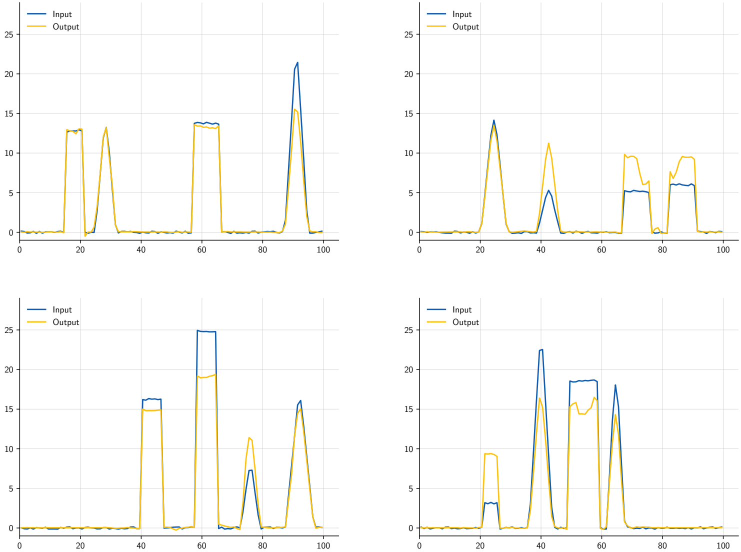
```
Sequential(
  (0): Conv1d(1, 64, kernel_size=(5,), stride=(1,), padding=(2,))
  (1): ReLU()
  (2): Conv1d(64, 64, kernel_size=(5,), stride=(1,), padding=(2,))
  (3): ReLU()
  (4): Conv1d(64, 64, kernel_size=(5,), stride=(1,), padding=(2,))
  (5): ReLU()
  (6): Conv1d(64, 64, kernel_size=(5,), stride=(1,), padding=(2,))
  (7): ReLU()
  (8): Conv1d(64, 1, kernel_size=(5,), stride=(1,), padding=(2,))
)

nb_parameters 62337
```

Training is done with the MSE loss and Adam.

```
batch_size = 100

optimizer = torch.optim.Adam(model.parameters(), lr = 1e-3)
mse_loss = nn.MSELoss()


mu, std = train_input.mean(), train_input.std()

for e in range(args.nb_epochs):

    for input, targets in zip(train_input.split(batch_size),
                              train_targets.split(batch_size)):


        output = model((input - mu) / std)
        loss = mse_loss(output, targets)

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



Without attention
1600
1400
1200
1000
800
600
400
200
0
MSE
10^0
10^1
10^2
Nb. of epochs


Input
Output
25
20
15
10
5
0
0
20
40
60
80
100
Input
Output
25
20
15
10
5
0
0
20
40
60
80
100
Input
Output
25
20
15
10
5
0
0
20
40
60
80
100
Input
Output
25
20
15
10
5
0
0
20
40
60
80
100

The poor performance of this model is not surprising given its inability to transport information from "far away" in the signal. Using more layers, global channel averaging, or fully connected layers could possibly solve the problem.

However it is more natural to equip the model with the ability to combine information from parts of the signal that it actively identifies as relevant.

This is exactly what an attention layer would do.

We implement our own self attention layer with tensors $N \times C \times T$ so that the products by W_Q, W_K, and W_V can be implemented as convolutions.

To compute $QK^\top$ and AV we need a batch matrix product, which is provided by `torch.matmul()`.

```
>>> a = torch.rand(11, 9, 2, 3)
>>> b = torch.rand(11, 9, 3, 4)
>>> m = a.matmul(b)
>>> m.size()
torch.Size([11, 9, 2, 4])
>>>
>>> m[7, 1]
tensor([[0.8839, 1.0253, 0.7473, 1.1397],
        [0.4966, 0.5515, 0.4631, 0.6616]])
>>> a[7, 1].mm(b[7, 1])
tensor([[0.8839, 1.0253, 0.7473, 1.1397],
        [0.4966, 0.5515, 0.4631, 0.6616]])
>>>
>>> m[3, 0]
tensor([[0.6906, 0.7657, 0.9310, 0.7547],
        [0.6259, 0.5570, 1.1012, 1.2319]])
>>> a[3, 0].mm(b[3, 0])
tensor([[0.6906, 0.7657, 0.9310, 0.7547],
        [0.6259, 0.5570, 1.1012, 1.2319]])
```

```python
class SelfAttentionLayer(nn.Module):
    def __init__(self, in_dim, out_dim, key_dim):
        super().__init__()
        self.conv_Q = nn.Conv1d(in_dim, key_dim, kernel_size = 1, bias = False)
        self.conv_K = nn.Conv1d(in_dim, key_dim, kernel_size = 1, bias = False)
        self.conv_V = nn.Conv1d(in_dim, out_dim, kernel_size = 1, bias = False)

    def forward(self, x):
        Q = self.conv_Q(x)
        K = self.conv_K(x)
        V = self.conv_V(x)
        A = Q.transpose(1, 2).matmul(K).softmax(2)
        y = A.matmul(V.transpose(1, 2)).transpose(1, 2)
        return y
```

Note that for simplicity it is single-head attention, and the $1/\sqrt{D}$ is missing.

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The computation of the attention matrix A and the layer's output Y could also be expressed somehow more clearly with Einstein summations (see lecture 1.5. "High dimension tensors") as

```
A = torch.einsum('nct,ncs->nts', Q, K).softmax(2)
y = torch.einsum('nts,ncs->nct', A, V)
```

```
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  (3): ReLU()
  (4): SelfAttentionLayer(in_dim=64, out_dim=64, key_dim=64)
  (5): Conv1d(64, 64, kernel_size=(5,), stride=(1,), padding=(2,))
  (6): ReLU()
  (7): Conv1d(64, 1, kernel_size=(5,), stride=(1,), padding=(2,))
)

nb_parameters 54081
```
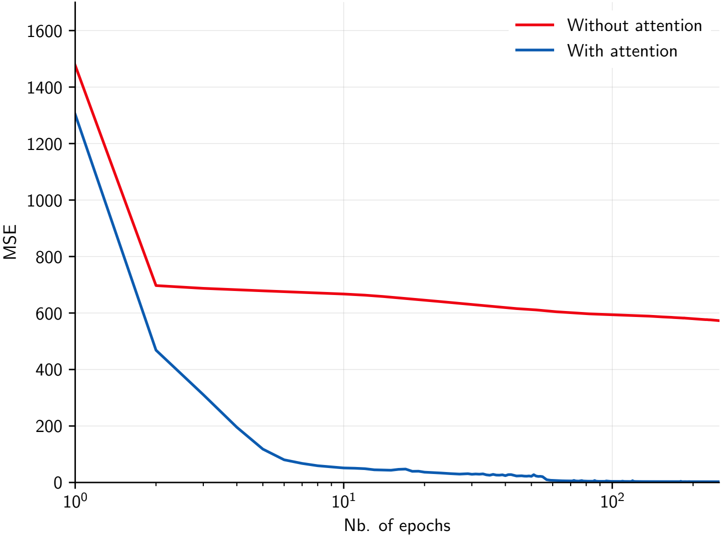
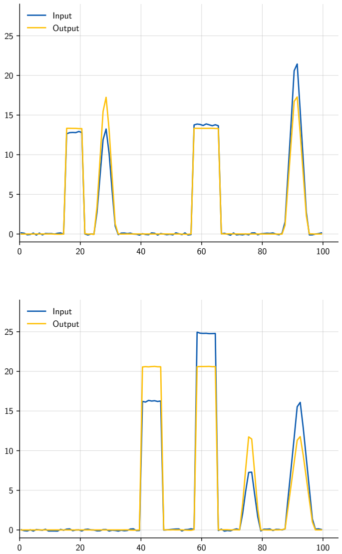
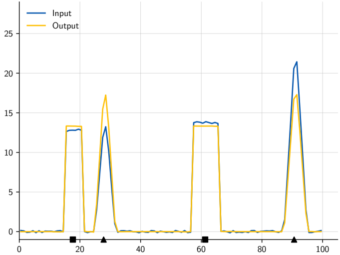
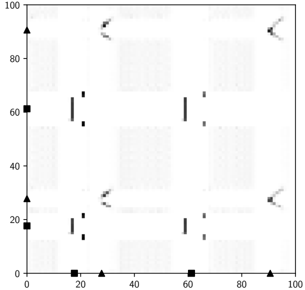
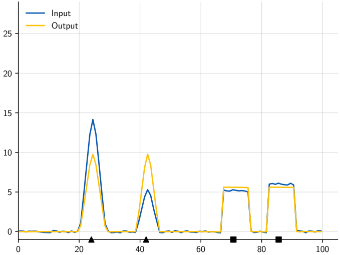


Without attention
With attention
1600
1400
1200
1000
800
600
400
200
0
MSE
10^0
10^1
10^2
Nb. of epochs

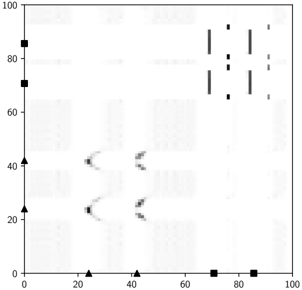

Input
Output
0
5
10
15
20
25
0
20
40
60
80
100


Input
Output
25
20
15
10
5
0
0
20
40
60
80
100

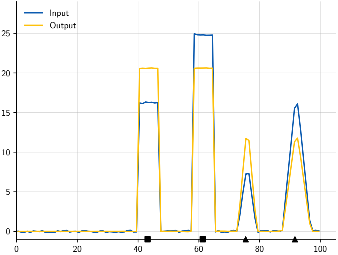

100
80
60
40
20
0
0
20
40
60
80
100

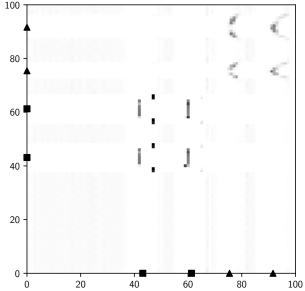


Input
Output
25
20
15
10
5
0
0
20
40
60
80
100



100
80
60
40
20
0
0
20
40
60
80
100


Input
Output
0
5
10
15
20
25
0
20
40
60
80
100


0
20
40
60
80
100
0
20
40
60
80
100

Because it is invariant to a permutation of the keys and values, such an attention layer disregards the absolute location of the values.

Our toy problem does not require to take into account the positioning in the tensor. We can modify it with a target where the pairs to average are the two rightmost and leftmost shapes.

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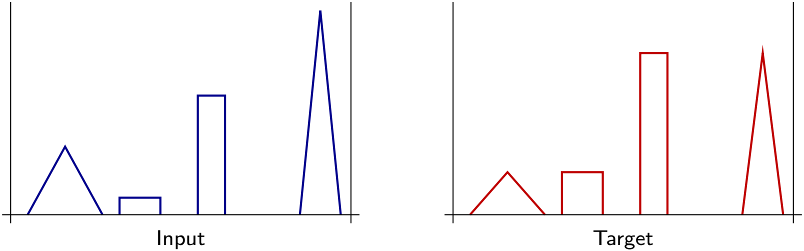

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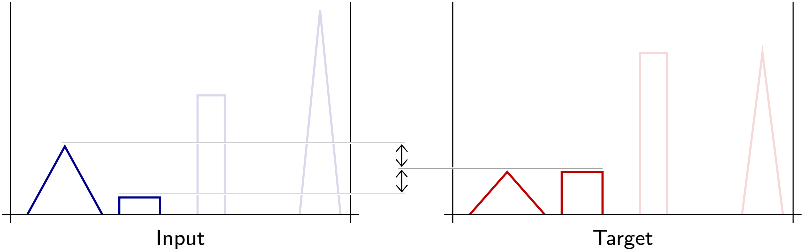

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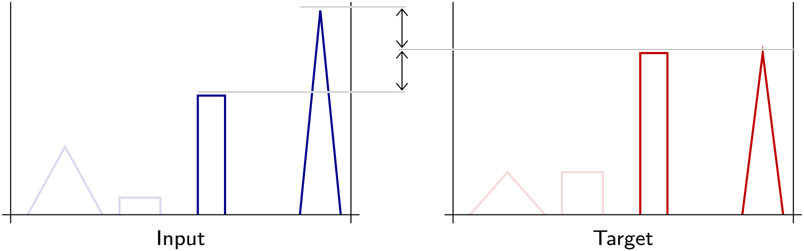

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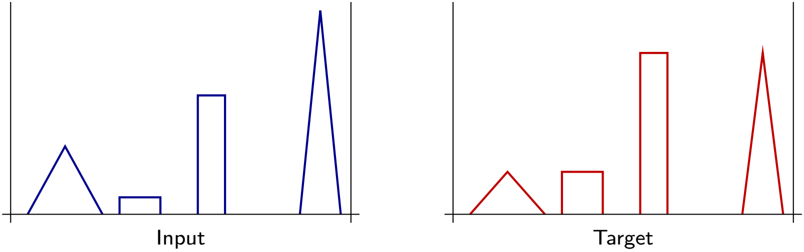
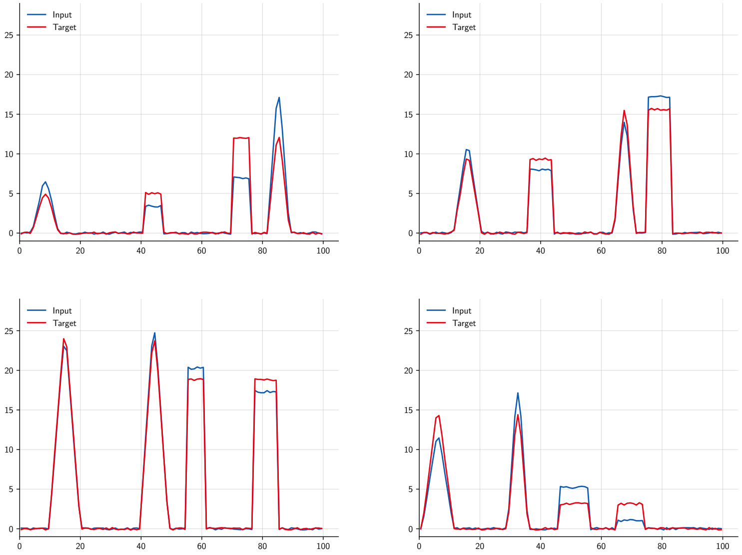
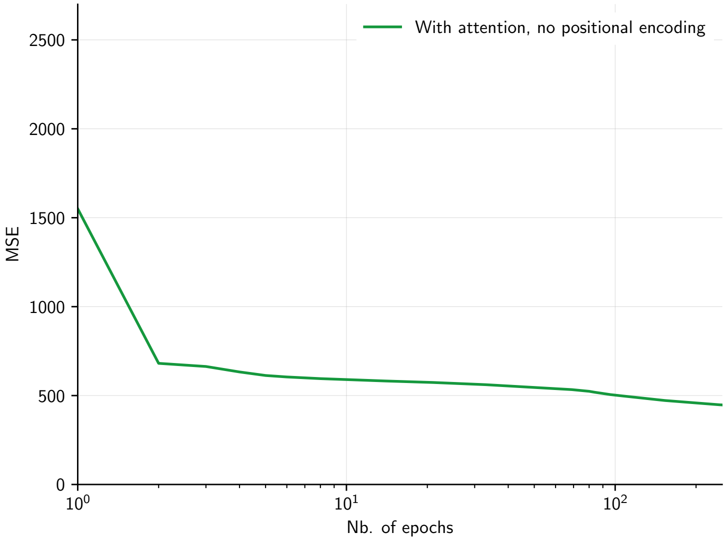
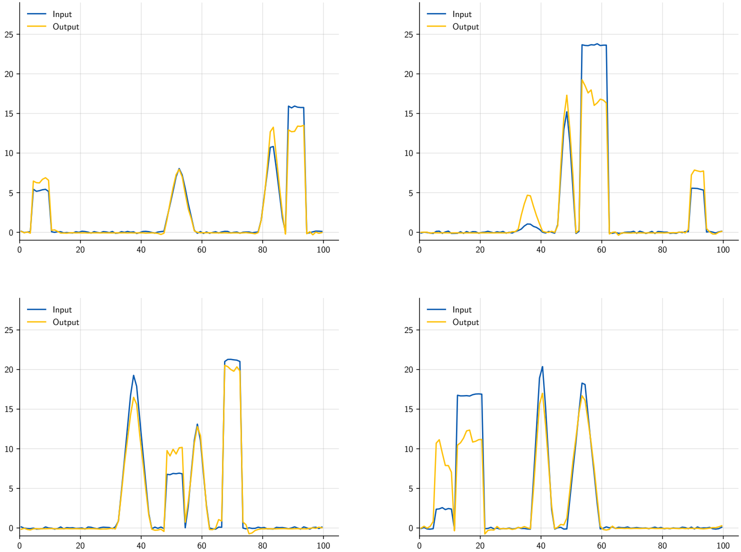


Some training examples.





With attention, no positional encoding
MSE
2500
2000
1500
1000
500
0
10^0
10^1
10^2
Nb. of epochs


Input
Output
25
20
15
10
5
0
0
20
40
60
80
100

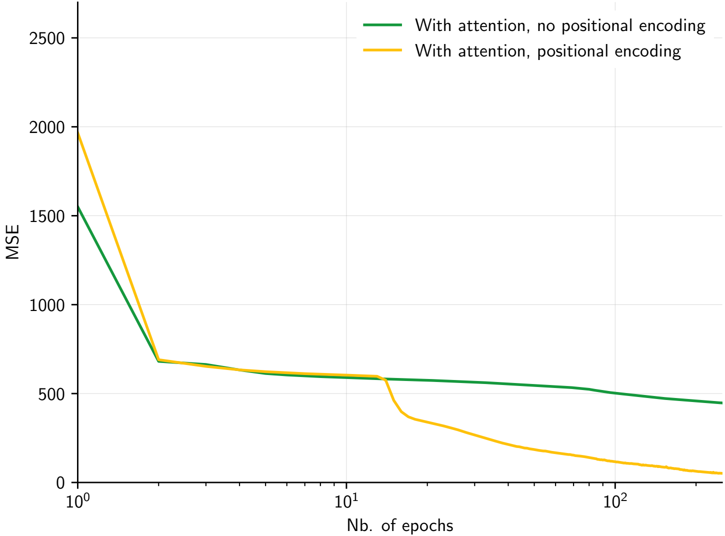
The poor performance of this model is not surprising given its inability to take into account positions in the attention layer.

We can fix this by providing to the model a **positional encoding**.

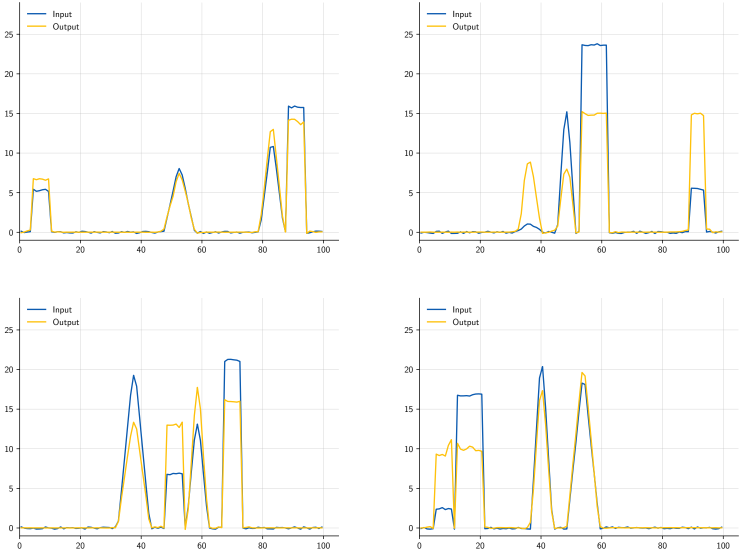
```
>>> len = 20
>>> c = math.ceil(math.log(len) / math.log(2.0))
>>> o = 2**torch.arange(c).unsqueeze(1)
>>> pe = (torch.arange(len).unsqueeze(0).div(o, rounding_mode = 'floor')) % 2
>>> pe
tensor([[0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1],
        [0, 0, 1, 1, 0, 0, 1, 1, 0, 0, 1, 1, 0, 0, 1, 1, 0, 0, 1, 1],
        [0, 0, 0, 0, 1, 1, 1, 1, 0, 0, 0, 0, 1, 1, 1, 1, 0, 0, 0, 0],
        [0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 0, 0, 0, 0],
        [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1]])
```

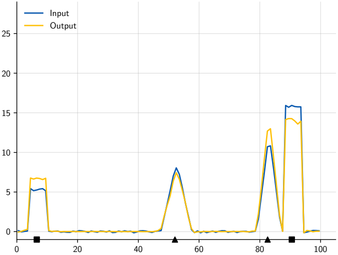
Such a tensor can simply be channel-concatenated to the input batch:

```
>>> pe = pe[None].float()
>>> input = torch.cat((input, pe.expand(input.size(0), -1, -1)), 1)
```

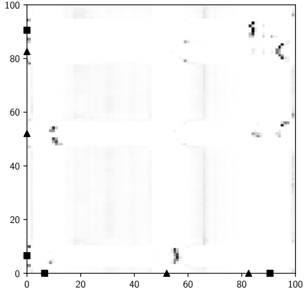


With attention, no positional encoding
With attention, positional encoding
MSE
2500
2000
1500
1000
500
0
10^0
10^1
10^2
Nb. of epochs

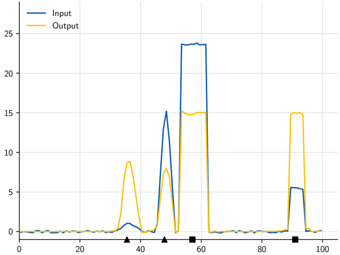

Input
Output

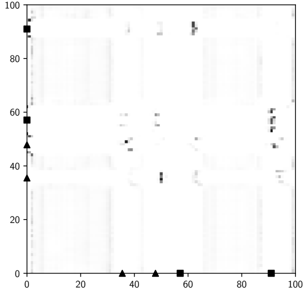


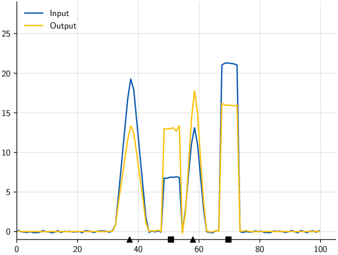
Input
Output
25
20
15
10
5
0
0
20
40
60
80
100

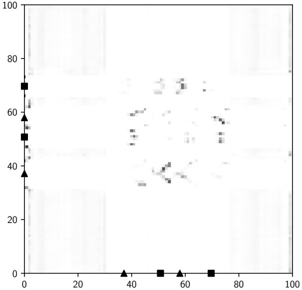


100
80
60
40
20
0
0
20
40
60
80
100


Input
Output




Input
Output



The end

References

A. Graves, G. Wayne, and I. Danihelka. **Neural turing machines**. CoRR, abs/1410.5401, 2014.

A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. Gomez, L. Kaiser, and I. Polosukhin. **Attention is all you need**. CoRR, abs/1706.03762, 2017.