Deep Learning & Applied AI

Self-attention and transformers

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Sequential data

Example: numeric 1D sequential data (time series)

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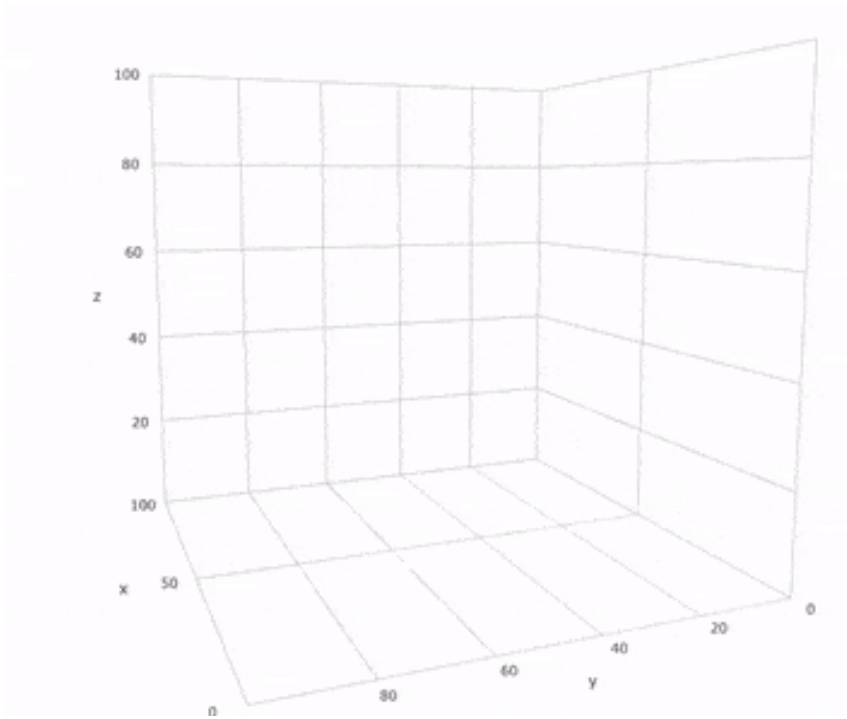
Prototypical task: predict the next numbers in the sequence

Sequential data

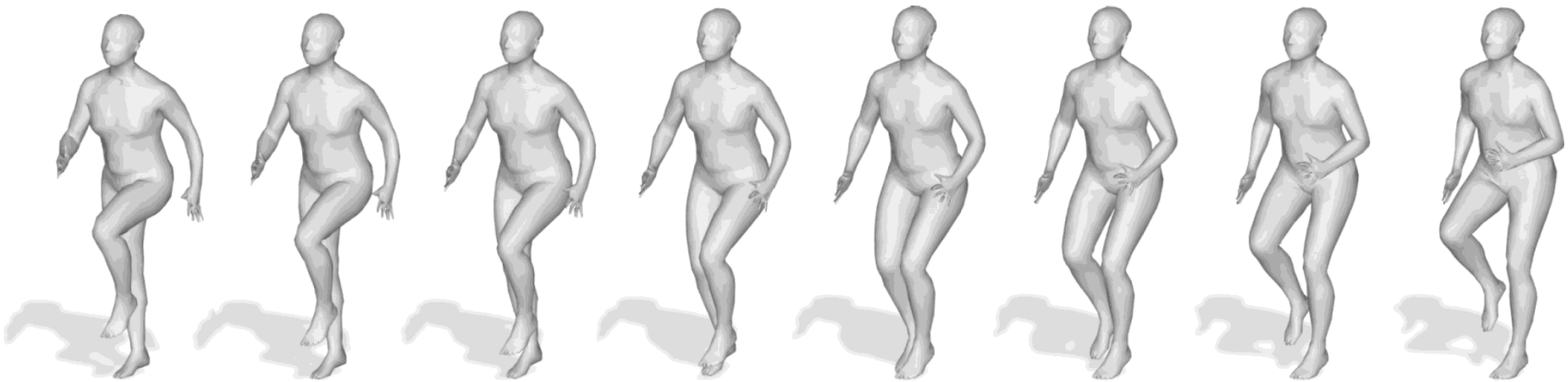
Example: Brownian motion of a particle in 3D space



Animation: Daniel Soper

Sequential data

Example: 3D shape motions



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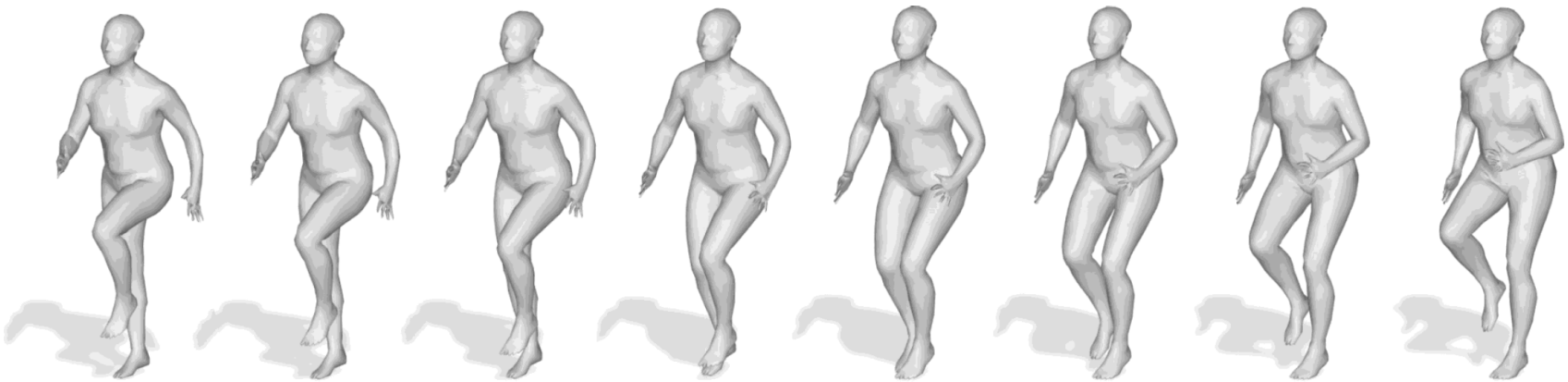

Prototypical task: classify the entire sequence (e.g. "running")

Sequential data

Example: Text (symbolic)

"the little brown fox"

the, little, brown, fox

t, h, e, , l, i, t, t, l, e, , b, r, o, w, n, , f, o, x

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Prototypical task: text translation (e.g. "茶色の小狐")

Sequence-to-sequence model

Key property:

The same weights apply to sequences of different lengths.

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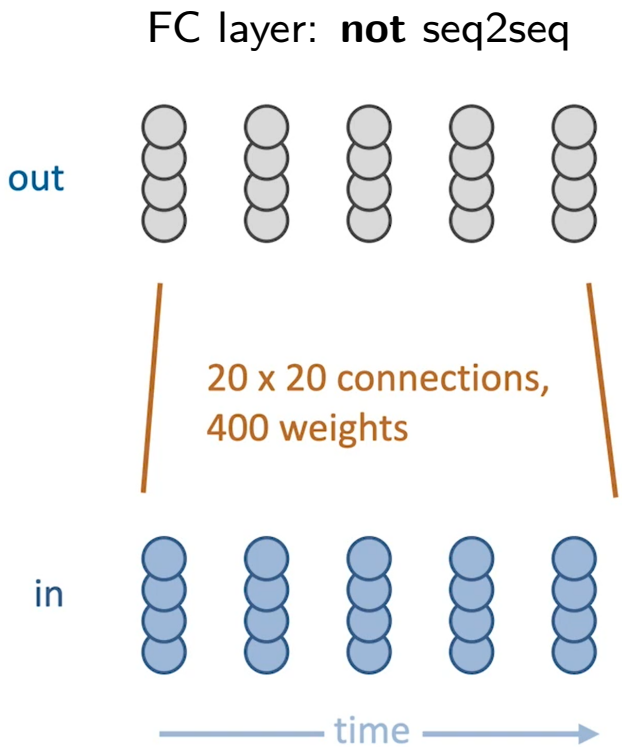

Figures: Peter Bloem

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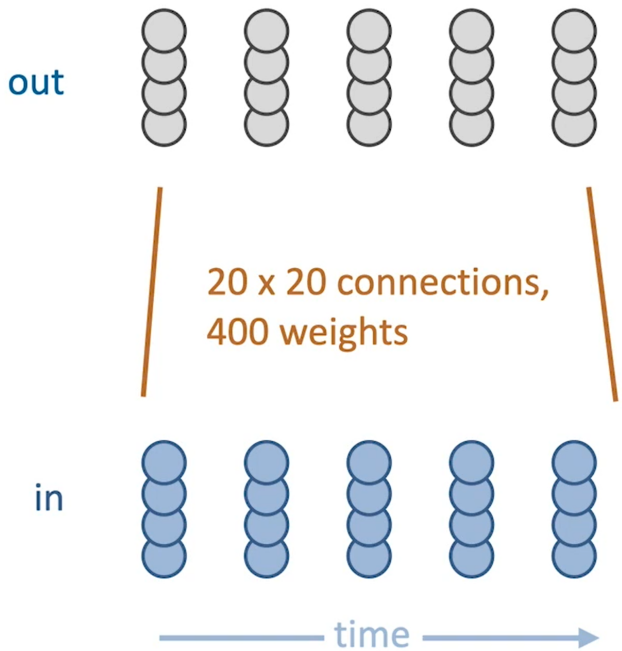
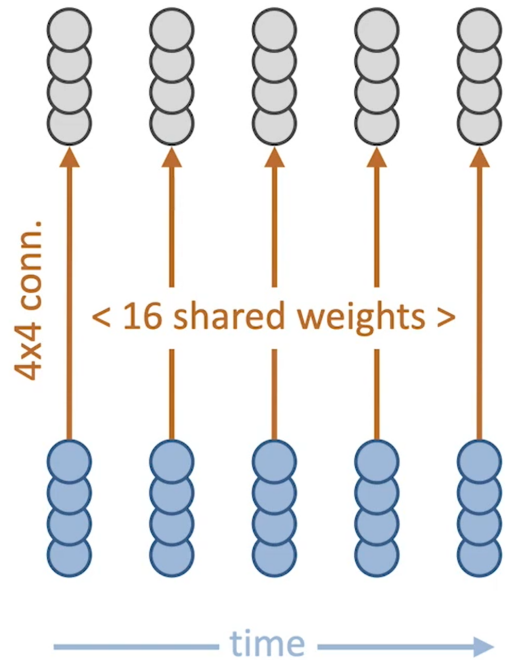
FC layer: **not** seq2seq



One MLP per vector: seq2seq!



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Causal vs. non-causal layers

S2S layers admit input and output with different lengths.

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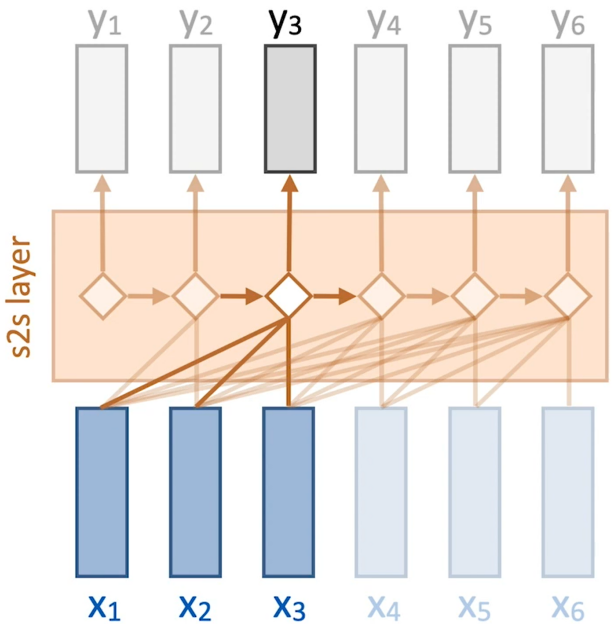

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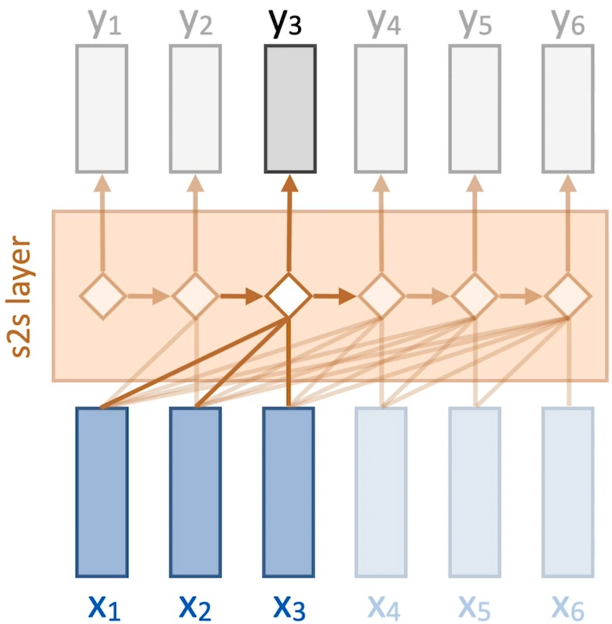

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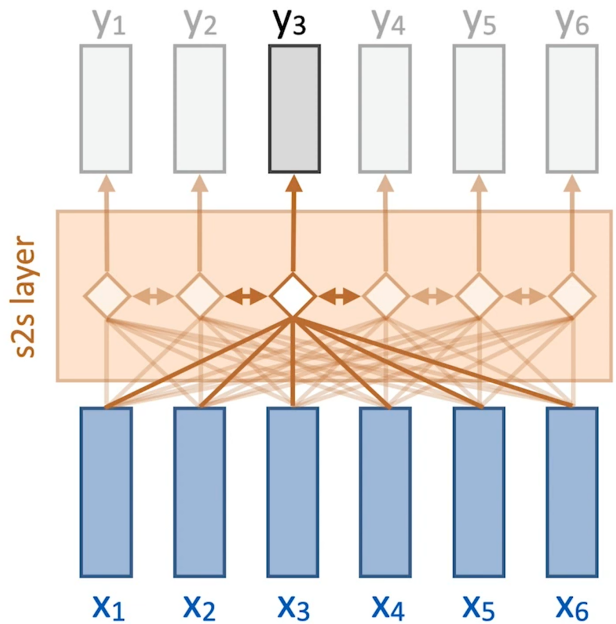
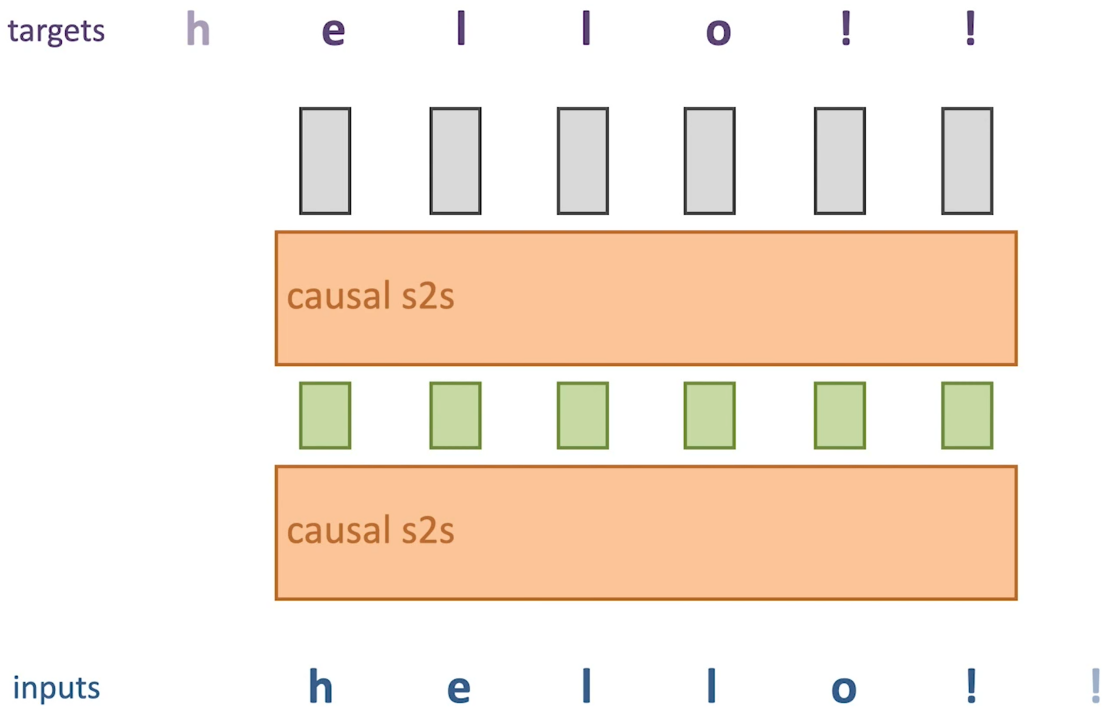


"non-causal" layer
no restrictions

Autoregressive modeling

Given an unlabeled dataset of sequences, take a subsequence and train to predict the next character:



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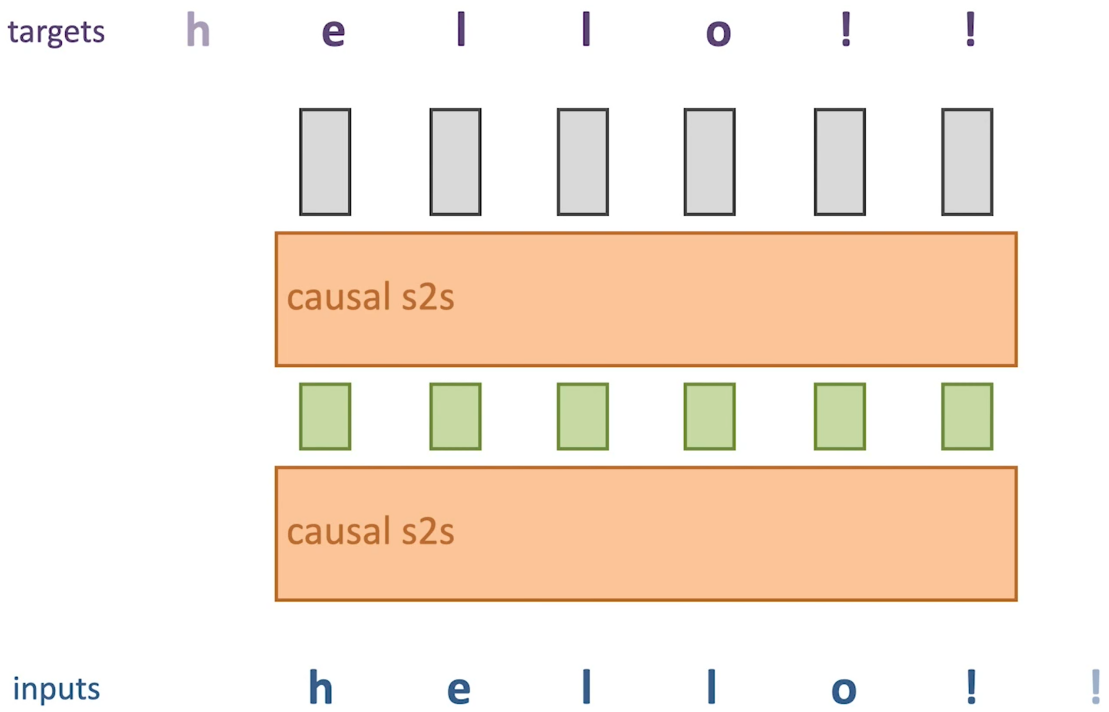

Since causal layers are used, the model can not "cheat" by looking ahead in the sequence.

Autoregressive modeling

The model outputs, for each token, a probability distribution over the set of symbols (e.g. over the letters of the alphabet).

Once trained, one can generate sequences by sequential sampling:

Input: seed $[s_1, s_2, s_3, \dots]$

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"I like to eat hot $\underbrace{\text{dogs}}_{80\%}$ $\underbrace{\text{pancakes}}_{20\%}$"

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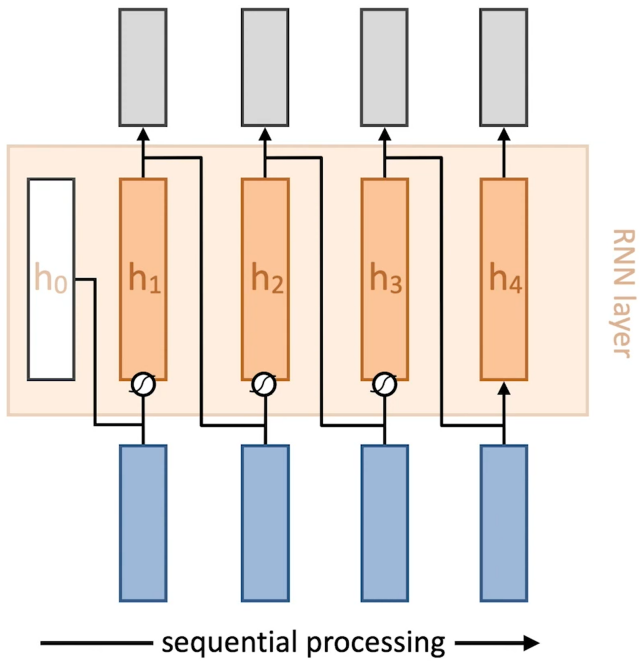

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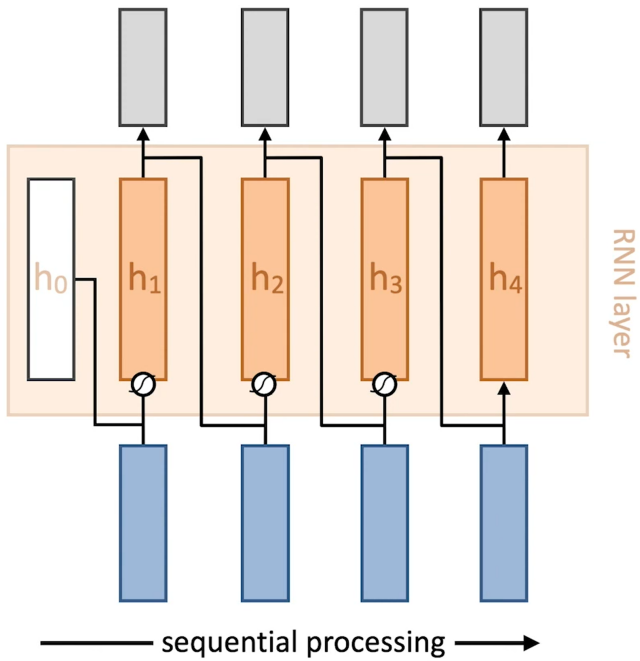

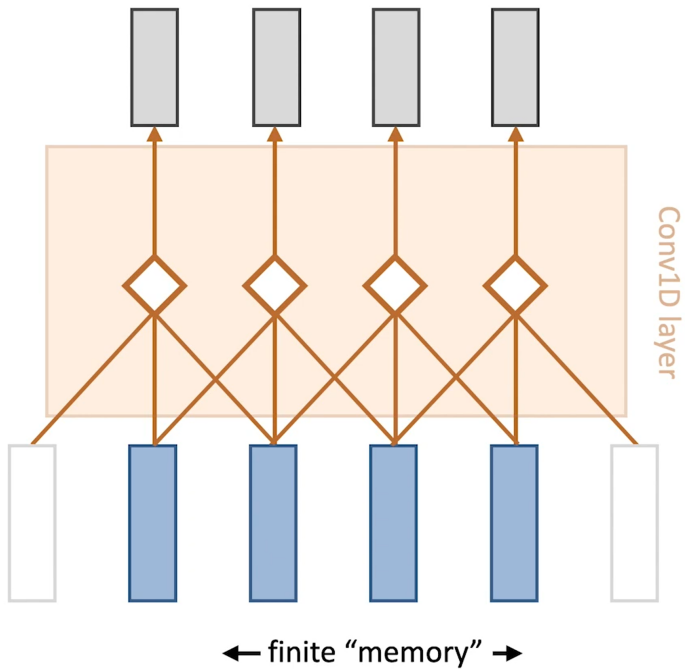

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limited range backward or forward

parallel computation

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Can we have both, parallel computation and long dependencies?

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and transform them so that each $w_{ij} > 0$ and $\sum_j w_{ij} = 1$:

$$w_{ij} = \frac{e^{w'_{ij}}}{\sum_j e^{w'_{ij}}}$$

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In matrix notation:

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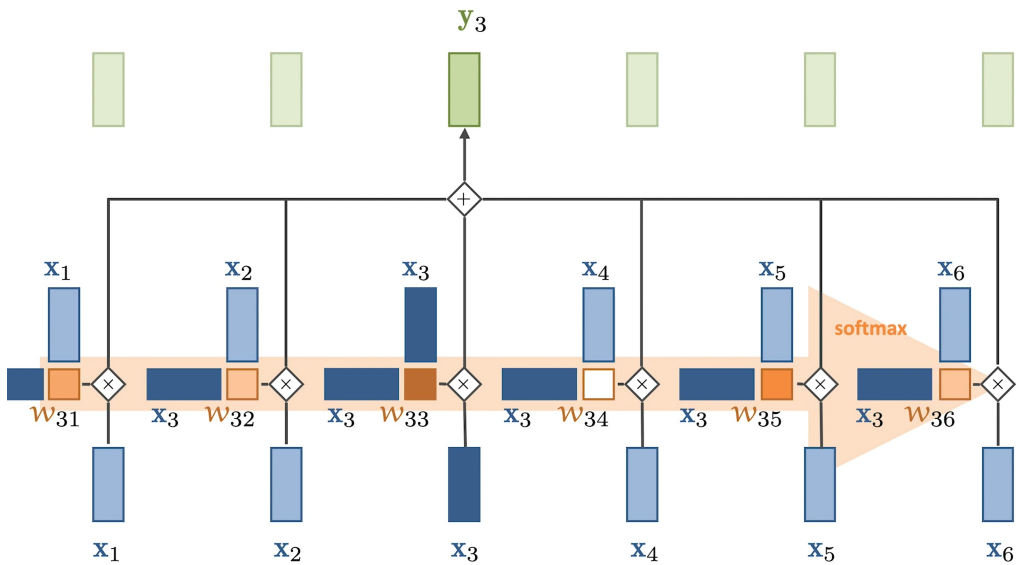

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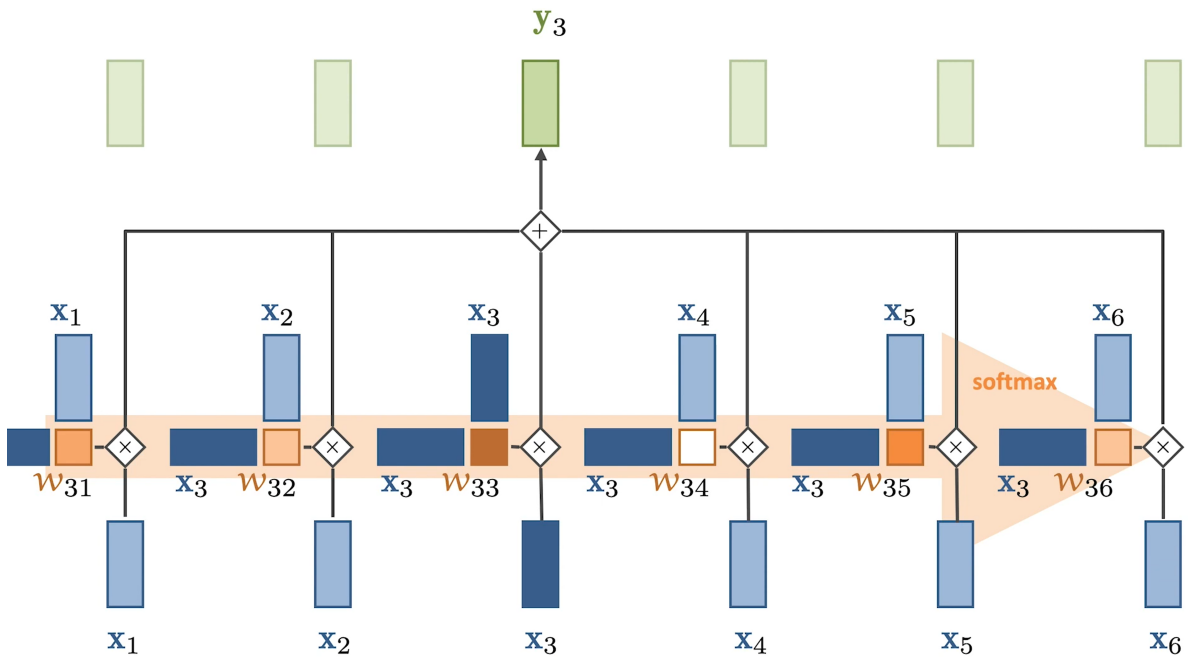
Self-attention is just a transformation. There are no trainable parameters. However, the input may be the result of a learned transformation.



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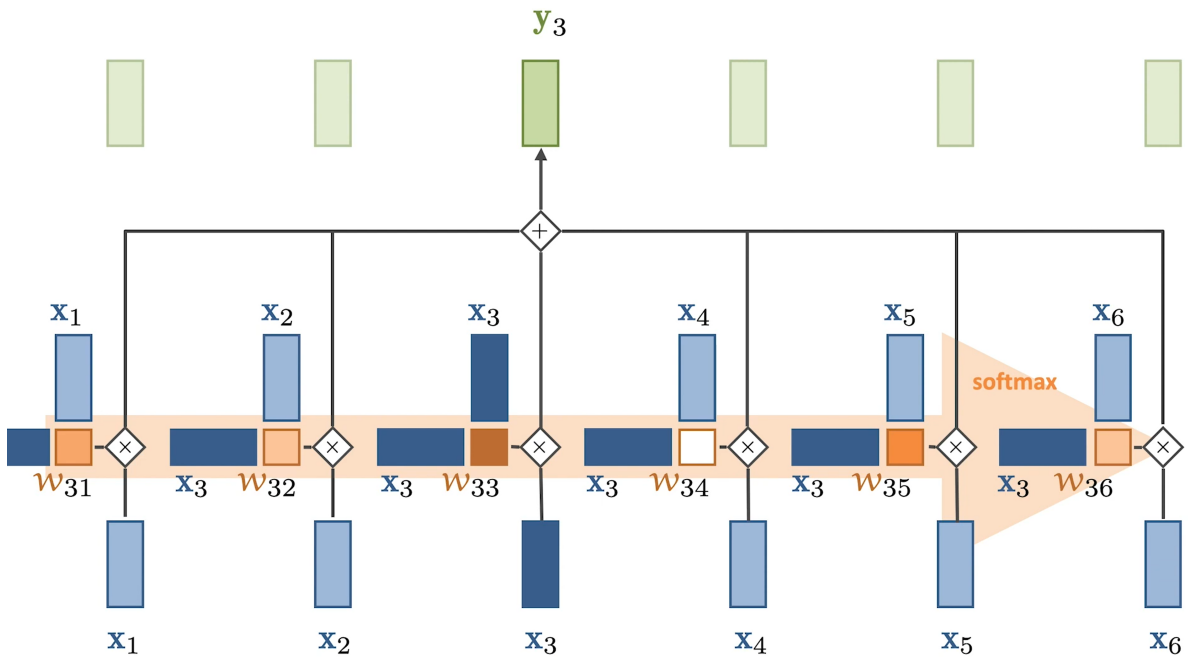

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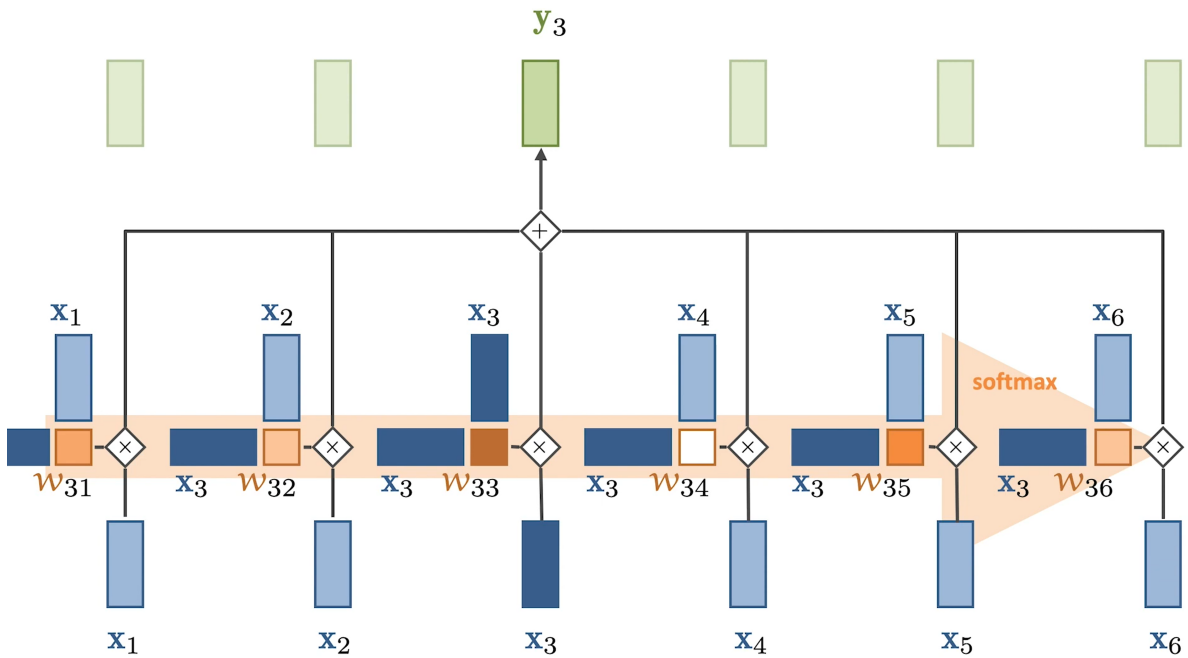

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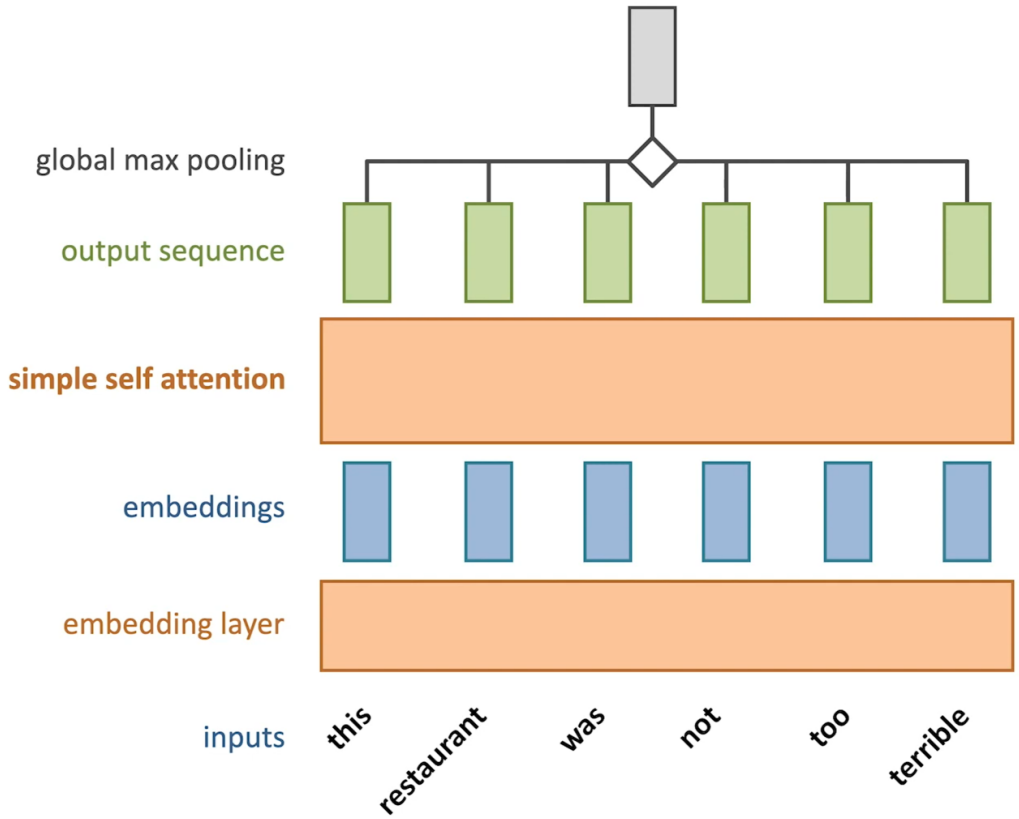
Self-attention is permutation-equivariant:

$$\pi(\mathrm{sa}(\mathbf{x})) = \mathrm{sa}(\pi(\mathbf{x}))$$

Example


global max pooling
output sequence
simple self attention
embeddings
embedding layer
inputs
this
restaurant
was
not
too
terrible

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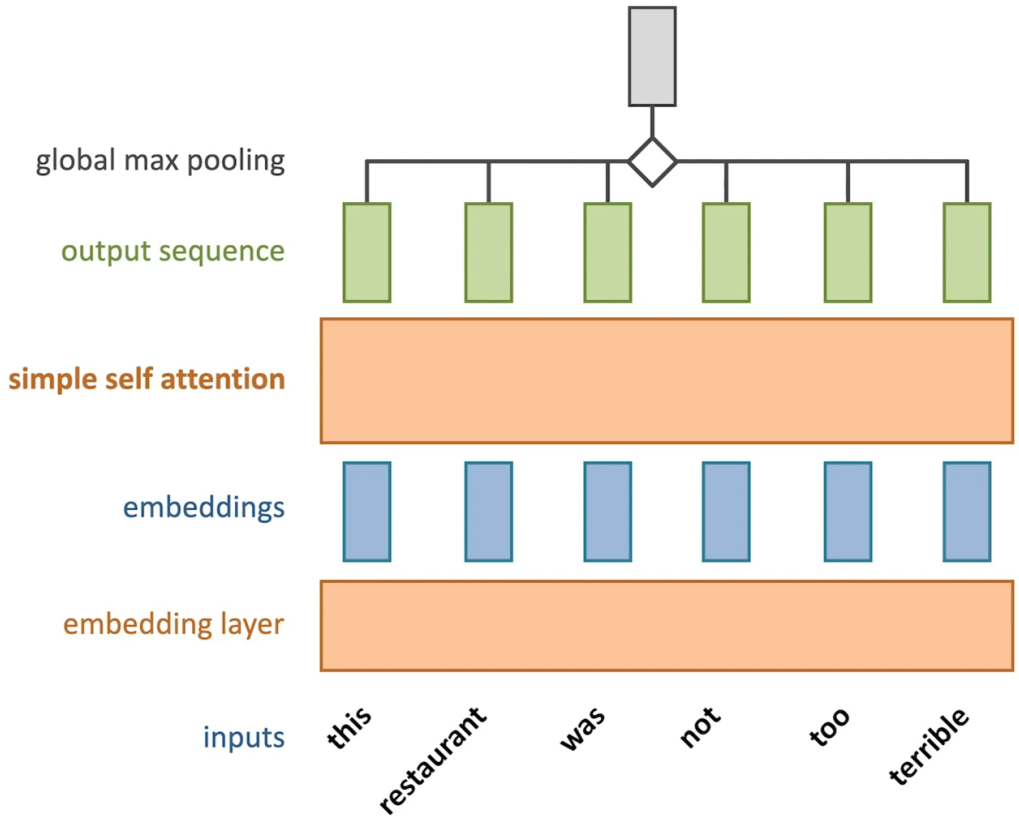

The word "not" directly affects "terrible"

i.e., the dot product $x_{\text{not}}{}^{\top} x_{\text{terrible}}$ should be large.

Key, value, query

Each input vector plays three roles:

$$w'_{ij} = \underbrace{x_i^\top}_{\text{query}} \underbrace{x_j}_{\text{key}}$$

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We can now introduce trainable weights and biases:

$$w'_{ij} = q_i^\top k_j$$

$$y_i = \sum_j w_{ij} v_j$$

where $q = Qx + b$ (and similarly for k and v).

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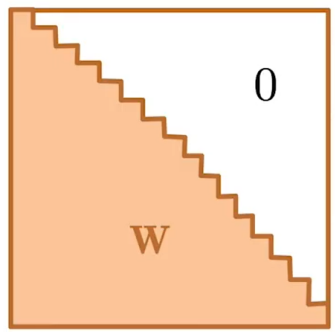

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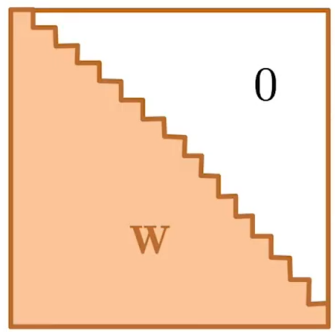

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Other priors can be encoded by enforcing a structure on $\mathbf{W}$.

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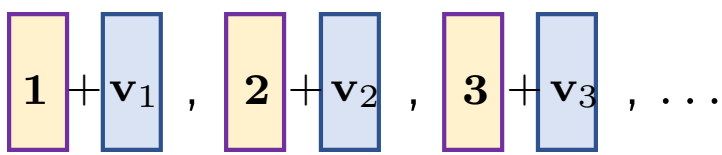

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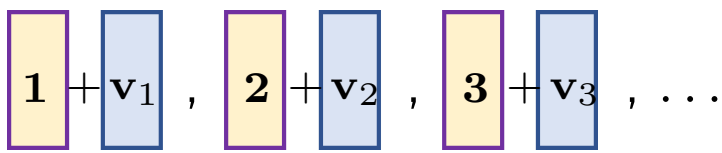

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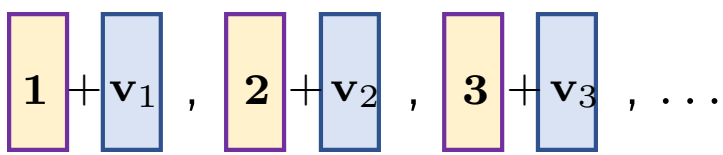
- Relative positions

  Embed/encode the relative rather than the absolute positions



Transformers

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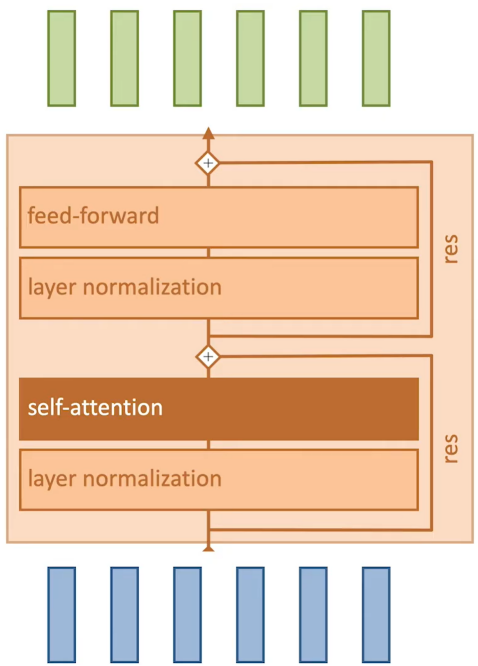

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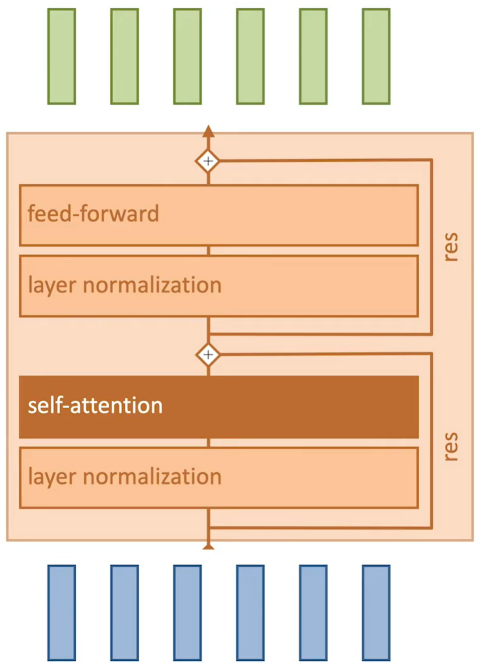
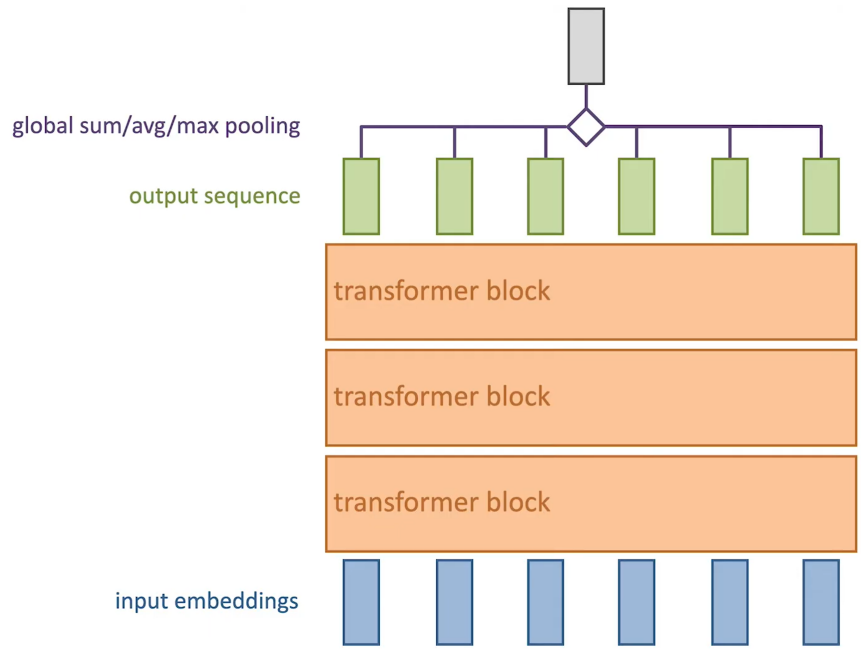
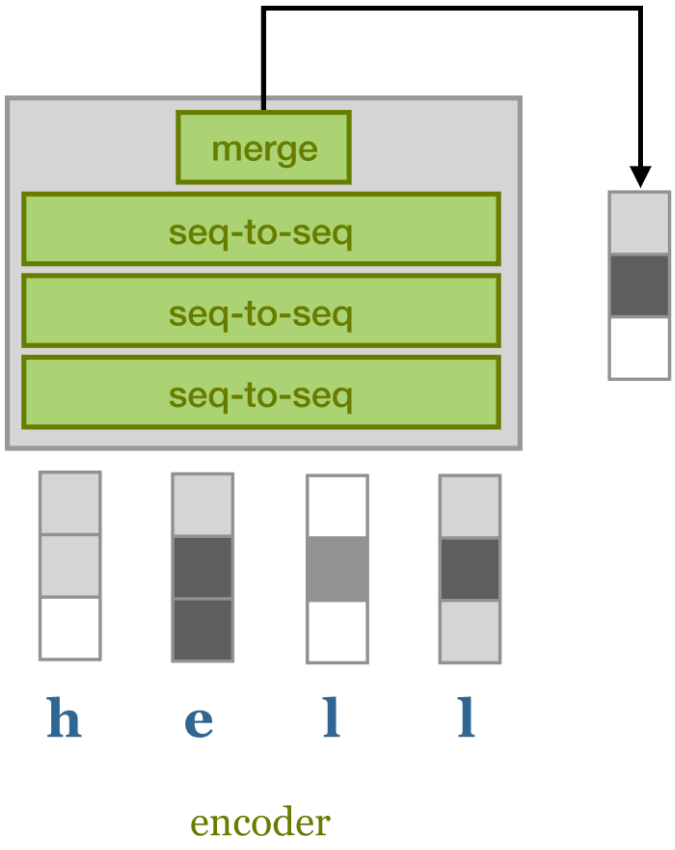
Main idea:

Define a generic transformer block, and compose it several times.





Encoder-decoder model



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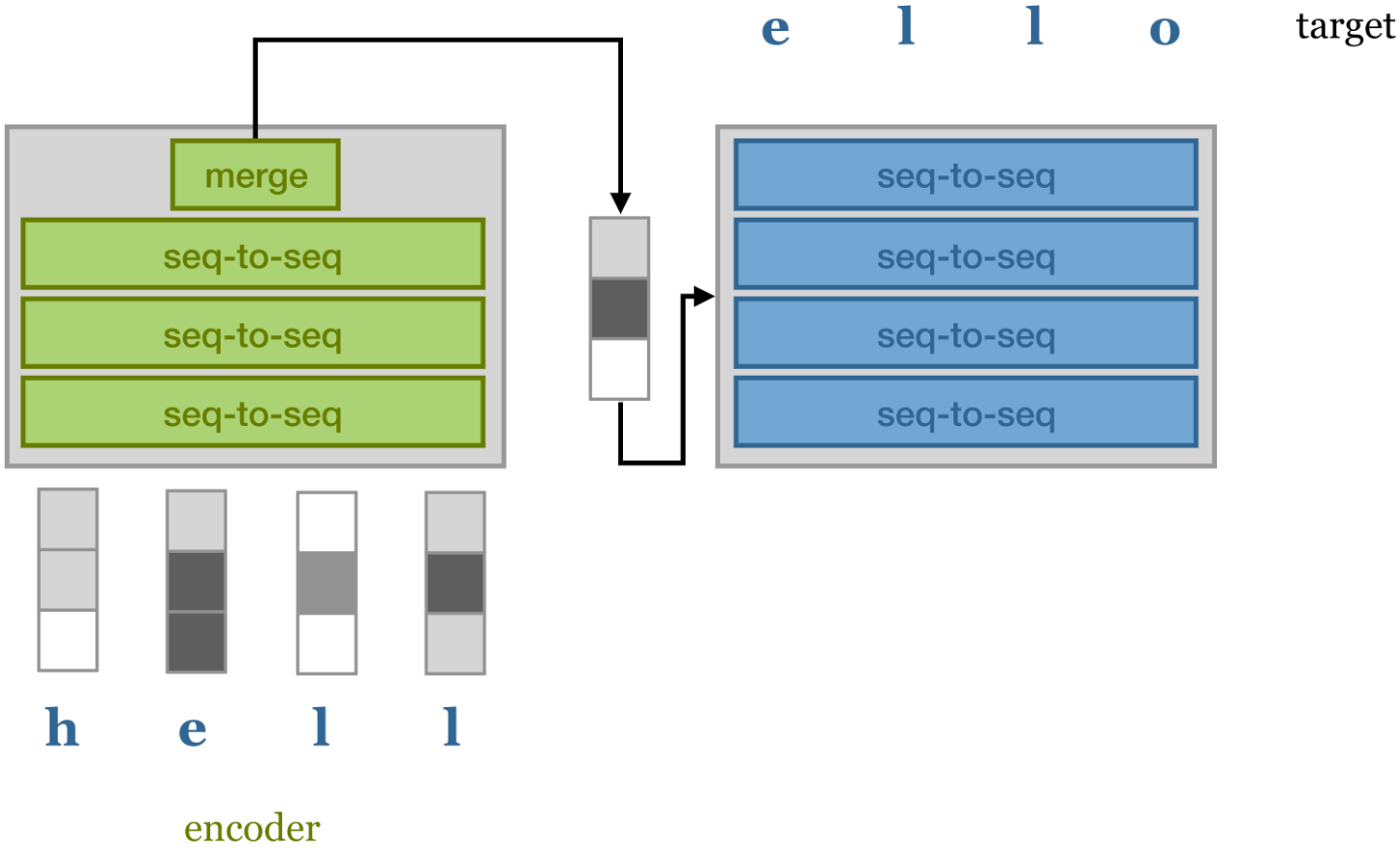

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