Deep Learning & Applied AI

Self-attention and transformers

Emanuele Rodolà
rodola@di.uniroma1.it

SAPIENZA
UNIVERSITÀ DI ROMA

2nd semester a.y. 2021/2022 · May 11, 2022

Sequential data

Example: numeric 1D sequential data (time series)

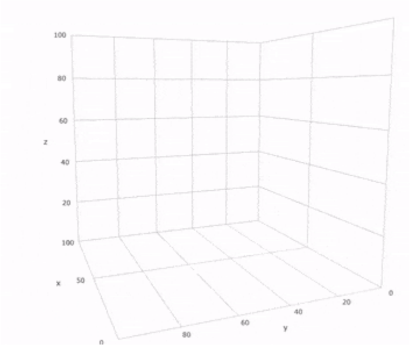
Sequential data

Example: numeric 1D sequential data (time series)

Prototypical task: predict the next numbers in the sequence

Sequential data

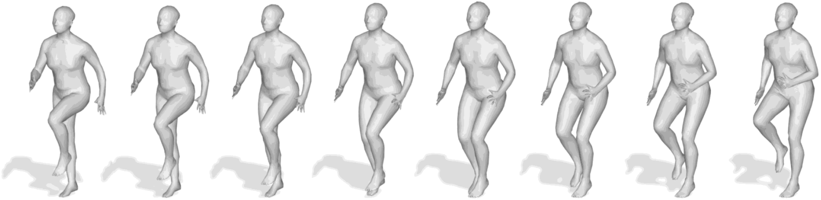
Example: Brownian motion of a particle in 3D space



Animation: Daniel Soper

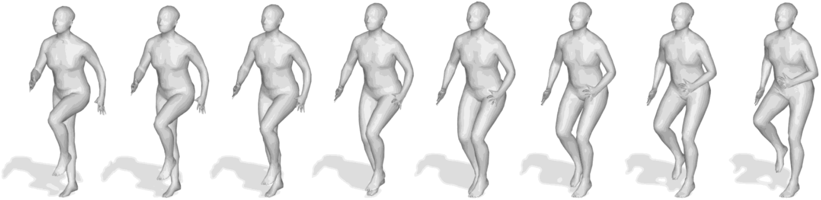
Sequential data

Example: 3D shape motions



Sequential data

Example: 3D shape motions



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

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

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

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.

Sequence-to-sequence model

Key property:

The same weights apply to sequences of different lengths.

If the output is another sequence, it's a sequence-to-sequence model.

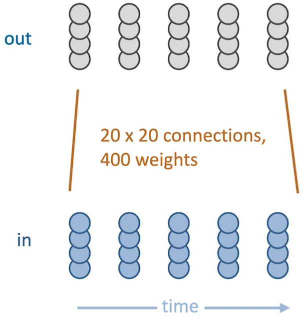
Sequence-to-sequence model

Key property:

The same weights apply to sequences of different lengths.

If the output is another sequence, it's a sequence-to-sequence model.

FC layer: **not** seq2seq



Figures: Peter Bloem

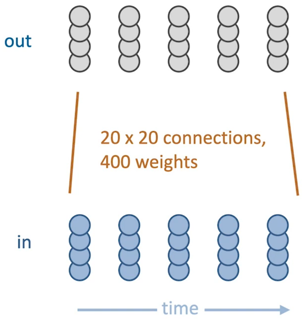
Sequence-to-sequence model

Key property:

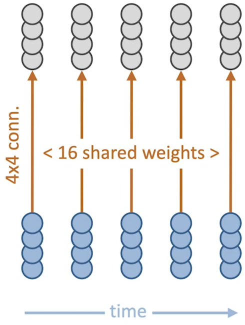
The same weights apply to sequences of different lengths.

If the output is another sequence, it's a sequence-to-sequence model.

FC layer: **not** seq2seq



One MLP per vector: seq2seq!



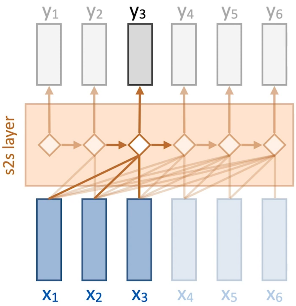
Figures: Peter Bloem

Causal vs. non-causal layers

S2S layers admit input and output with different lengths.

Causal vs. non-causal layers

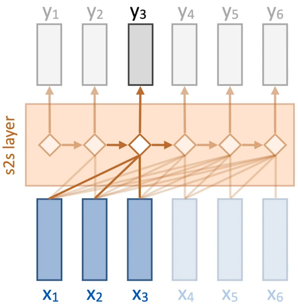
S2S layers admit input and output with different lengths.



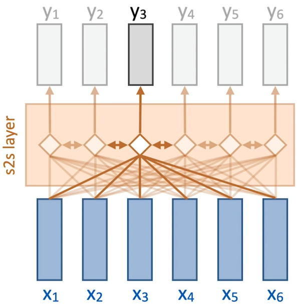
"causal" layer
can only look backward in time

Causal vs. non-causal layers

S2S layers admit input and output with different lengths.



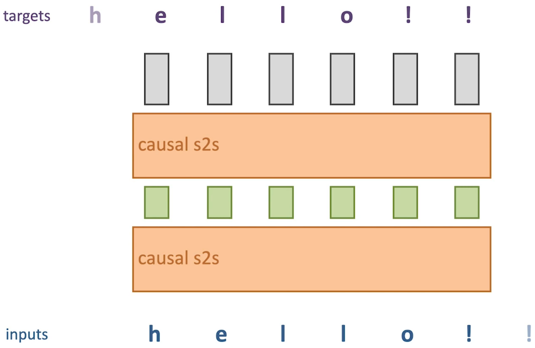
"causal" layer
can only look backward in time



"non-causal" layer
no restrictions

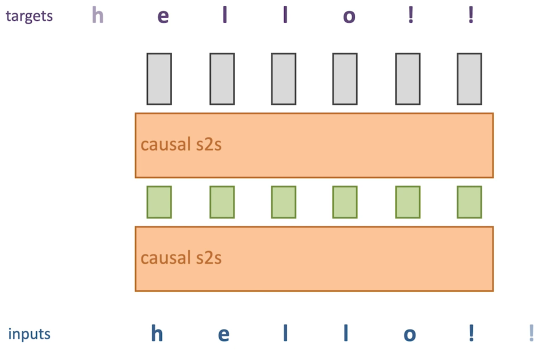
Autoregressive modeling

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



Autoregressive modeling

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



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 $[s_1, s_2, s_3, \ldots]$

Output: distribution $p(c \mid s_1, s_2, s_3, \ldots)$

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 $[s_1, s_2, s_3, \dots]$

Output: distribution $p(c \mid s_1, s_2, s_3, \dots)$

- Sample the output distribution
- Append the sampled symbol to the seed
- Iterate

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 $[s_1, s_2, s_3, \dots]$

Output: distribution $p(c \mid s_1, s_2, s_3, \dots)$

- Sample the output distribution
- Append the sampled symbol to the seed
- Iterate

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

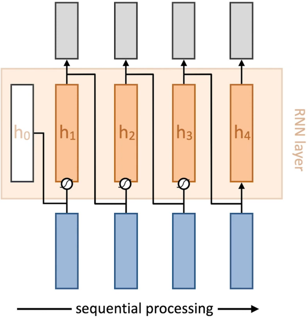
Sequence-to-sequence layers

How do we actually design a S2S layer?

Sequence-to-sequence layers

How do we actually design a S2S layer?

Many possible choices.



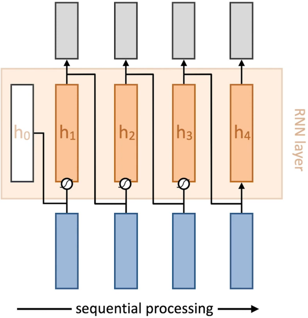
can look indefinitely far back in the sequence

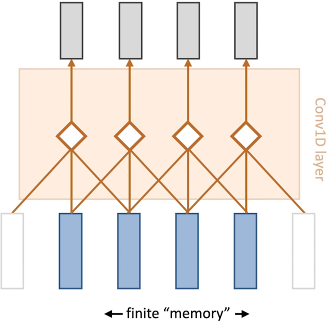
processing must be done sequentially

Sequence-to-sequence layers

How do we actually design a S2S layer?

Many possible choices.





can look indefinitely far back in the sequence
processing must be done sequentially

limited range backward or forward
parallel computation

Self-attention

Can we have both, parallel computation and long dependencies?

Self-attention

Can we have both, parallel computation and long dependencies?

Consider a linear model from input to output:

$$y_i = \sum_{ij} w_{ij} x_j$$

Self-attention

Can we have both, parallel computation and long dependencies?

Consider a linear model from input to output:

$$y_i = \sum_{ij} w_{ij} x_j$$

However, the w_{ij} are **not** trainable weights.

Self-attention

Can we have both, parallel computation and long dependencies?

Consider a linear model from input to output:

$$y_i = \sum_{ij} w_{ij} x_j$$

However, the w_{ij} are **not** trainable weights.

Instead, for a given position i, compute the correlations over all j:

$$w'_{ij} = x_i^\top x_j$$

Self-attention

Can we have both, parallel computation and long dependencies?

Consider a linear model from input to output:

$$y_i = \sum_{ij} w_{ij} x_j$$

However, the w_{ij} are **not** trainable weights.

Instead, for a given position i, compute the correlations over all j:

$$w'_{ij} = x_i^\top x_j$$

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

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

Self-attention

In matrix notation:

$$w'_{ij} = x_i^\top x_j \;\Rightarrow\; \mathbf{W}' = \mathbf{X}^\top \mathbf{X}$$

Self-attention

In matrix notation:

$$w'_{ij} = x_i^\top x_j \;\Rightarrow\; \mathbf{W}' = \mathbf{X}^\top \mathbf{X}$$

$$w_{ij} = \frac{e^{w'_{ij}}}{\sum_j e^{w'_{ij}}} \;\Rightarrow\; \mathbf{W} = \begin{pmatrix} \vdots \\ \mathrm{softmax}(-w'_{i:}-) \\ \vdots \end{pmatrix}$$

Self-attention

In matrix notation:

$$w'_{ij} = x_i^\top x_j \;\Rightarrow\; \mathbf{W}' = \mathbf{X}^\top \mathbf{X}$$

$$w_{ij} = \frac{e^{w'_{ij}}}{\sum_j e^{w'_{ij}}} \;\Rightarrow\; \mathbf{W} = \begin{pmatrix} \vdots \\ \mathrm{softmax}(-w'_{i:}-) \\ \vdots \end{pmatrix}$$

$$y_i = \sum_{ij} w_{ij} x_j \;\Rightarrow\; \mathbf{Y}^\top = \mathbf{W}\mathbf{X}^\top$$

Self-attention

In matrix notation:

$$w'_{ij} = x_i^\top x_j \;\Rightarrow\; \mathbf{W}' = \mathbf{X}^\top \mathbf{X}$$

$$w_{ij} = \frac{e^{w'_{ij}}}{\sum_j e^{w'_{ij}}} \;\Rightarrow\; \mathbf{W} = \begin{pmatrix} \vdots \\ \mathrm{softmax}(-w'_{i:}-) \\ \vdots \end{pmatrix}$$

$$y_i = \sum_{ij} w_{ij} x_j \;\Rightarrow\; \mathbf{Y}^\top = \mathbf{W}\mathbf{X}^\top$$

Matrix $\mathbf{W}$ is diagonally dominant, since typically $w'_{ii} \geq w'_{ij}$.

Self-attention

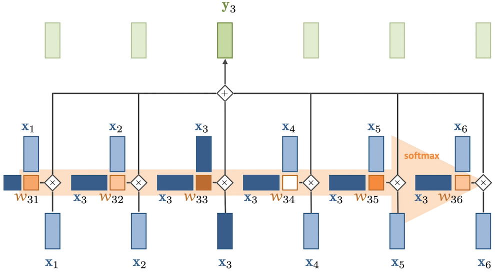
In matrix notation:

$$w'_{ij} = x_i^\top x_j \;\Rightarrow\; \mathbf{W}' = \mathbf{X}^\top \mathbf{X}$$

$$w_{ij} = \frac{e^{w'_{ij}}}{\sum_j e^{w'_{ij}}} \;\Rightarrow\; \mathbf{W} = \begin{pmatrix} \vdots \\ \mathrm{softmax}(-w'_{i:}-) \\ \vdots \end{pmatrix}$$

$$y_i = \sum_{ij} w_{ij} x_j \;\Rightarrow\; \mathbf{Y}^\top = \mathbf{W}\mathbf{X}^\top$$

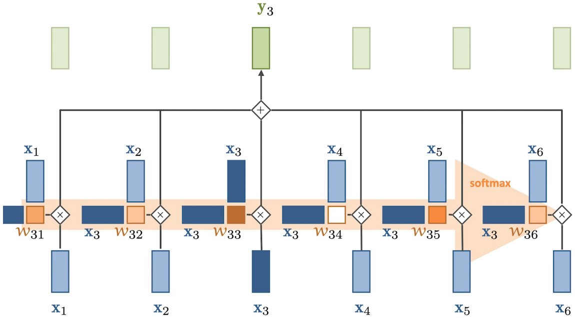
Matrix $\mathbf{W}$ is diagonally dominant, since typically $w'_{ii} \geq w'_{ij}$.



Self-attention

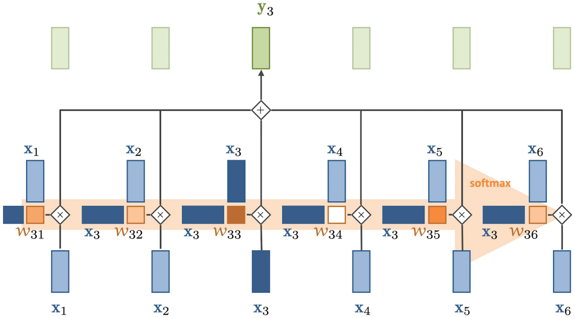
Self-attention is just a transformation. There are no trainable parameters.

However, the input may be the result of a learned transformation.



Self-attention

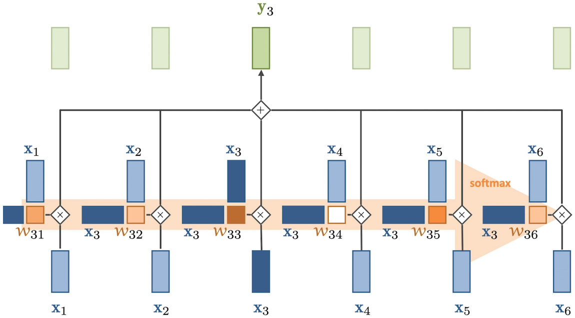
Self-attention is just a transformation. There are no trainable parameters. However, the input may be the result of a learned transformation.



Moreover, no temporal information is used. Sequences are seen as sets.

Self-attention

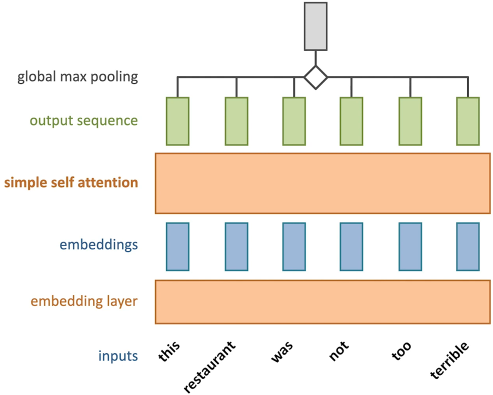
Self-attention is just a transformation. There are no trainable parameters.
However, the input may be the result of a learned transformation.



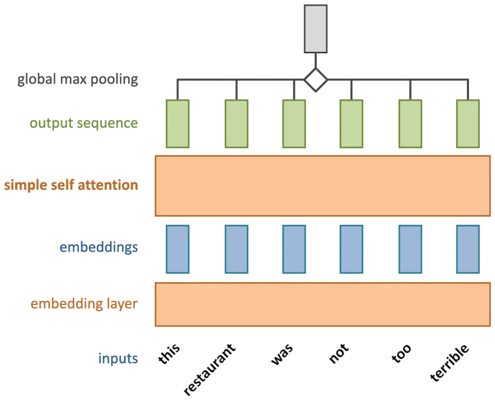
Moreover, no temporal information is used. Sequences are seen as sets.
Self-attention is permutation-equivariant:

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

Example


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

Example



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:

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

$$y_i = \sum_{ij} w_{ij} \underbrace{x_j}_{\text{value}}$$

Key, value, query

Each input vector plays three roles:

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

$$y_i = \sum_{ij} w_{ij} \underbrace{x_j}_{\text{value}}$$

We can now introduce trainable weights and biases:

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

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

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

Causal self-attention

If we need an auto-regressive model, we must avoid looking ahead.

Causal self-attention

If we need an auto-regressive model, we must avoid looking ahead.

We do this by only summing over the previous tokens in the sequence:

$$y_i = \sum_{ij} w_{ij} x_j$$

Causal self-attention

If we need an auto-regressive model, we must avoid looking ahead.

We do this by only summing over the previous tokens in the sequence:

$$y_i = \sum_{j \leq i} w_{ij} x_j$$

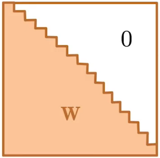
Causal self-attention

If we need an auto-regressive model, we must avoid looking ahead.

We do this by only summing over the previous tokens in the sequence:

$$y_i = \sum_{j \leq i} w_{ij} x_j$$

In matrix notation, we simply set:



This is also known as masking.

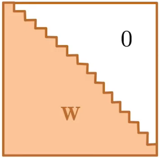
Causal self-attention

If we need an auto-regressive model, we must avoid looking ahead.

We do this by only summing over the previous tokens in the sequence:

$$y_i = \sum_{j \leq i} w_{ij} x_j$$

In matrix notation, we simply set:



This is also known as masking.

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

Position information

In some applications, the sequential structure is informative.

i.e., permutation-equivariance is not always desired.

Position information

In some applications, the sequential structure is informative.

i.e., permutation-equivariance is not always desired.

- Position embedding

  Learn a vector embedding for each position, sum it to the token

$$\boxed{\mathbf{1}} + \boxed{\mathbf{v}_1}\ , \ \boxed{\mathbf{2}} + \boxed{\mathbf{v}_2}\ , \ \boxed{\mathbf{3}} + \boxed{\mathbf{v}_3}\ , \ \ldots$$

Position information

In some applications, the sequential structure is informative.

i.e., permutation-equivariance is not always desired.

- Position embedding

  Learn a vector embedding for each position, sum it to the token

- Position encoding

  Define position embeddings a priori using some mathematical rule

$$\boxed{\mathbf{1}} + \boxed{\mathbf{v}_1}\ ,\ \boxed{\mathbf{2}} + \boxed{\mathbf{v}_2}\ ,\ \boxed{\mathbf{3}} + \boxed{\mathbf{v}_3}\ ,\ \dots$$

Position information

In some applications, the sequential structure is informative.

i.e., permutation-equivariance is not always desired.

- Position embedding

  Learn a vector embedding for each position, sum it to the token

- Position encoding

  Define position embeddings a priori using some mathematical rule

- Relative positions

  Embed/encode the relative rather than the absolute positions

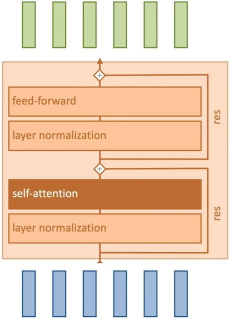
$$\boxed{\mathbf{1}} + \boxed{\mathbf{v}_1}\ ,\ \boxed{\mathbf{2}} + \boxed{\mathbf{v}_2}\ ,\ \boxed{\mathbf{3}} + \boxed{\mathbf{v}_3}\ ,\ \ldots$$

Transformers

A transformer is any model that primarily uses self-attention to propagate information across the basic tokens (e.g. vectors in a sequence, pixels in a grid, nodes in a graph, etc.).

Transformers

A transformer is any model that primarily uses self-attention to propagate information across the basic tokens (e.g. vectors in a sequence, pixels in a grid, nodes in a graph, etc.).

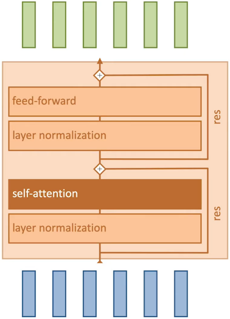


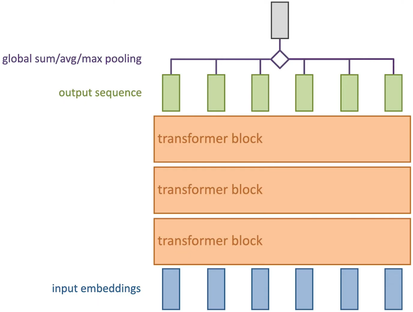
Transformers

A transformer is any model that primarily uses self-attention to propagate information across the basic tokens (e.g. vectors in a sequence, pixels in a grid, nodes in a graph, etc.).

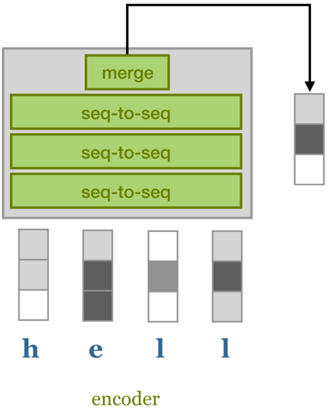
Main idea:

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

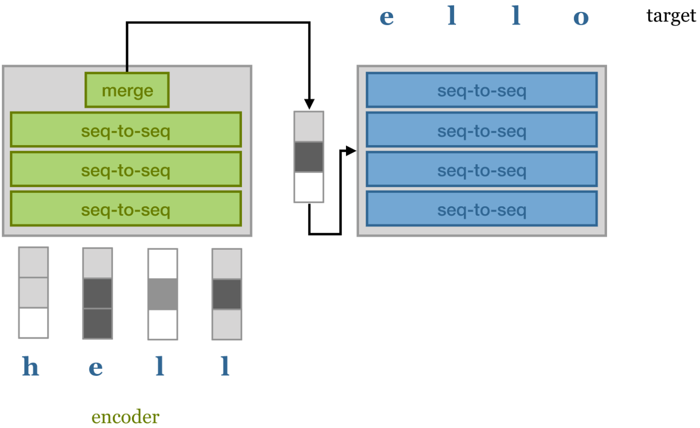




Encoder-decoder model



Encoder-decoder model



Encoder-decoder model