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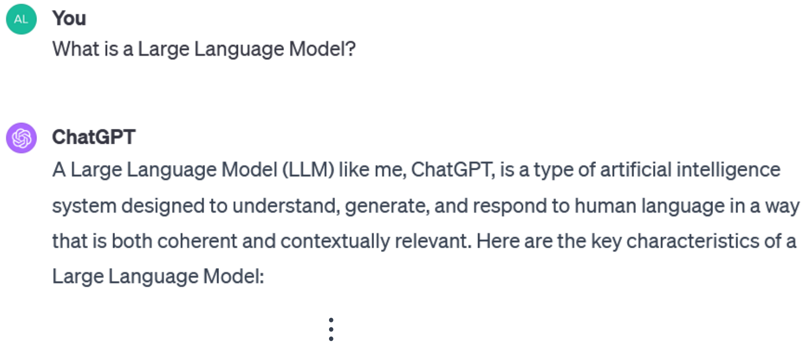
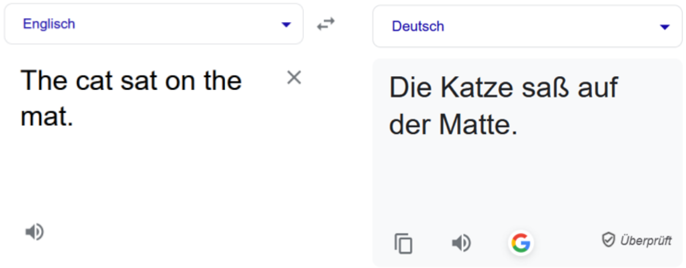
Transformer Network Encoders

An overview

What are Transformer Networks?

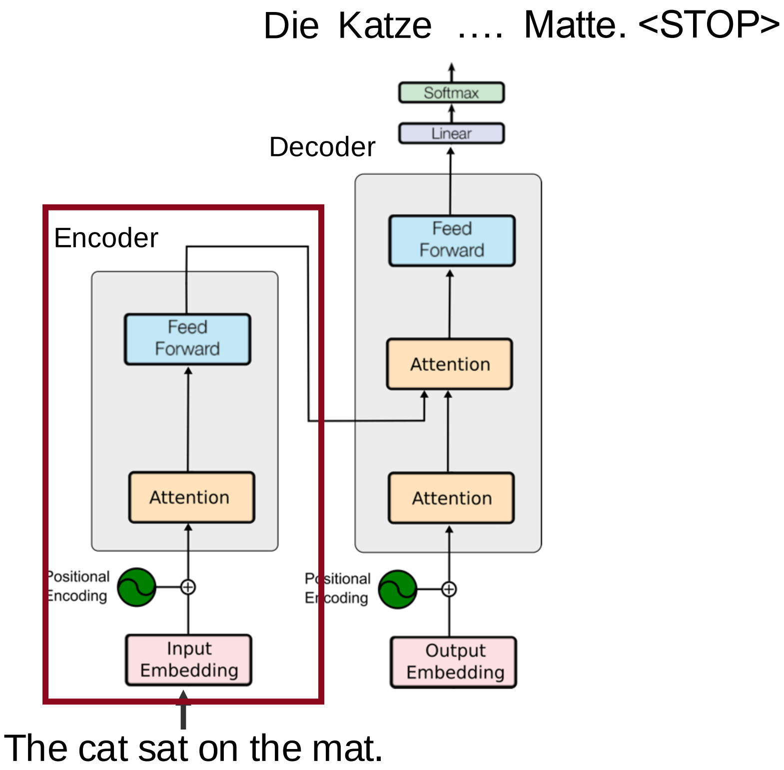
- Transformer Networks are a type of neural network architecture designed to handle sequential data
- Examples:
  - Chatbots
  - Translator





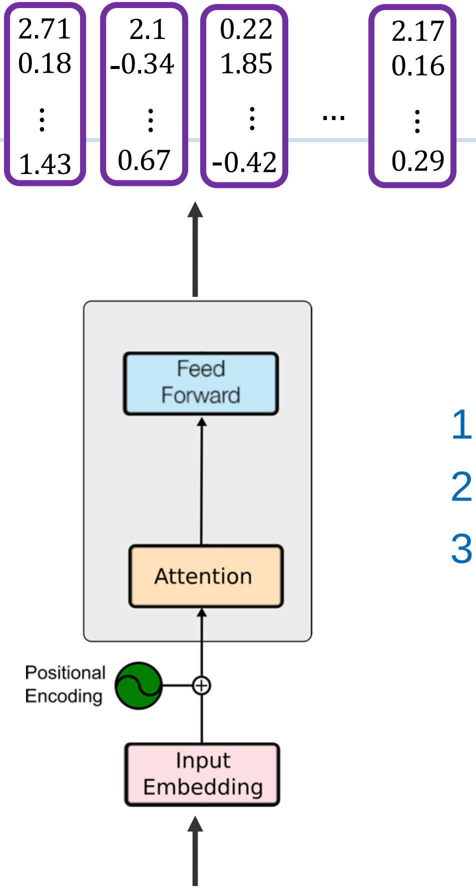
Transformer Network Architecture

- Transformer Network
  - Encoder: Encodes the input sequence into numerical vectors
  - Decoder: Uses the numerically encoded input sequence as its input and produces an output sequence.



Modified figure from: Vaswani, A., et al. (2017). Attention is all you need. *Adv. Neural Inf. Process. Syst.*, *30*.

Encoder



The cat sat on the mat.

1. Input Embedding & Positional Encoding
2. Attention
3. Feed Forward Neural Network

Modified figure from: Vaswani, A., et al. (2017). Attention is all you need. *Adv. Neural Inf. Process. Syst.*, *30*.

Input Embedding

- For every word, we have a specific vector representing this word

„The“ →

→ $\begin{pmatrix} 0.17 \\ 0.32 \\ \vdots \\ 0.25 \end{pmatrix} = \vec{w}_1 \in \mathbb{R}^d$

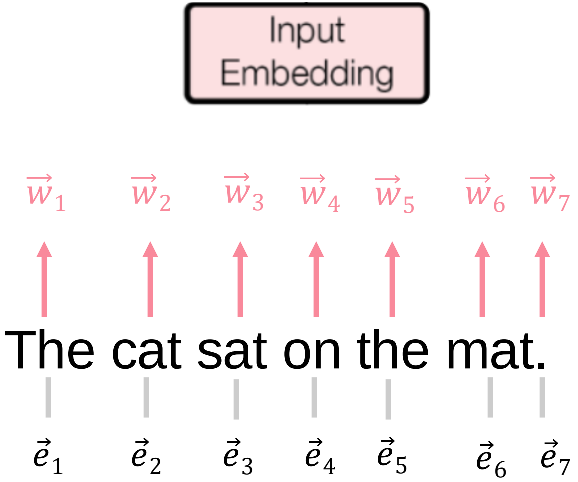
„cat“ →

→ $\begin{pmatrix} 0.40 \\ -0.21 \\ \vdots \\ 0.53 \end{pmatrix} = \vec{w}_2$

⋮ ⋮ ⋮

„.“ →

→ $\begin{pmatrix} -1.22 \\ 0.76 \\ \vdots \\ -2.19 \end{pmatrix} = \vec{w}_7$

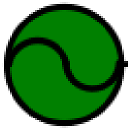


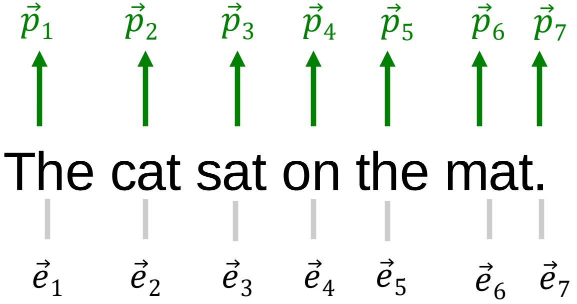
Positional Encoding

Positional Encoding:

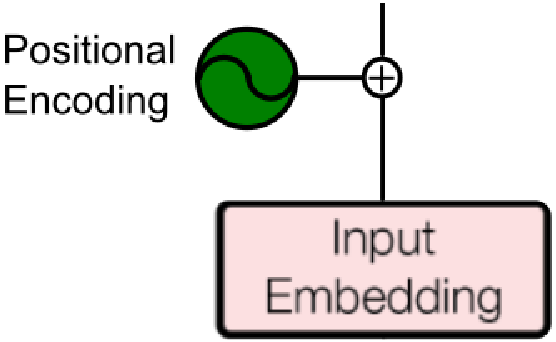
$$\vec{p}_1 = \boxed{\begin{matrix} 0.00 \\ 0.84 \\ \vdots \\ 0.14 \end{matrix}} \quad \vec{p}_2 = \boxed{\begin{matrix} 1.00 \\ 0.54 \\ \vdots \\ \text{-}0.99 \end{matrix}} \quad \dots \quad \vec{p}_7 = \boxed{\begin{matrix} 0.00 \\ 1.00 \\ \vdots \\ 0.96 \end{matrix}} \in \mathbb{R}^{\mathrm{d}}$$

- The same positional encoding is used for every input sequence!

Positional Encoding 



Input Embedding & Positional Encoding



$$\vec{e}_1 = \begin{pmatrix} 0.00 + 0.17 \\ 0.84 + 0.32 \\ \vdots \\ 0.14 + 0.25 \end{pmatrix} \quad \cdots \quad \cdots \quad \cdots \quad \vec{e}_7 = \begin{pmatrix} 0.00 - 1.22 \\ 1.00 + 0.76 \\ \vdots \\ 0.96 - 2.19 \end{pmatrix} \in \mathbb{R}^{d}$$

$$= \quad = \quad = \quad \quad \quad \quad =$$

$$\vec{p}_1 \quad \vec{p}_2 \quad \vec{p}_3 \quad \vec{p}_4 \quad \vec{p}_5 \quad \vec{p}_6 \quad \vec{p}_7$$

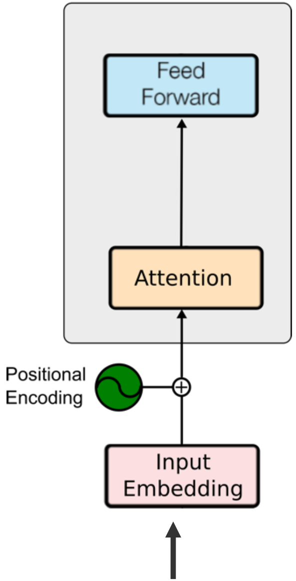
$$+ \quad + \quad + \quad + \quad + \quad + \quad +$$

$$\vec{w}_1 \quad \vec{w}_2 \quad \vec{w}_3 \quad \vec{w}_4 \quad \vec{w}_5 \quad \vec{w}_6 \quad \vec{w}_7$$

The cat sat on the mat.

$$\vec{e}_1 \quad \vec{e}_2 \quad \vec{e}_3 \quad \vec{e}_4 \quad \vec{e}_5 \quad \vec{e}_6 \quad \vec{e}_7$$

Encoder



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1. Input Embedding & Positional Encoding
2. Attention
3. Feed Forward Neural Network

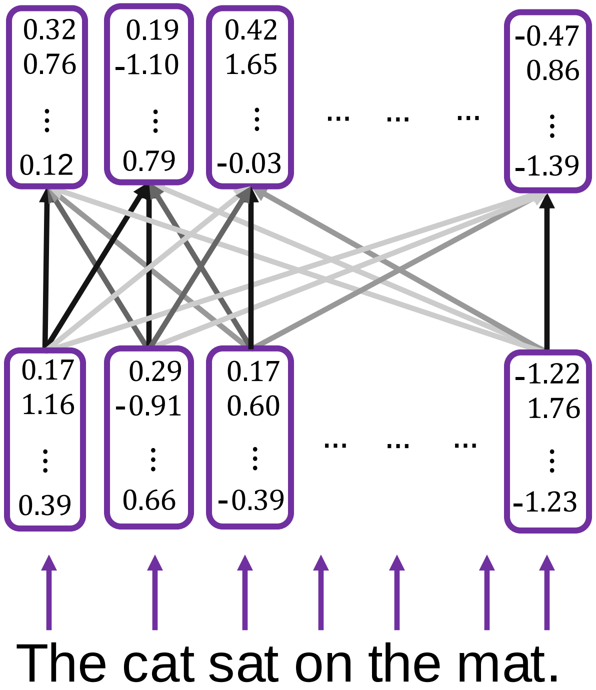
Attention

$$Attention(\vec{e}_i, K, V) = softmax\left(\frac{\vec{e}_i^{\,T} \cdot K}{\sqrt{d}}\right) \cdot V^T$$

$$K = (\vec{e}_1, \vec{e}_2, \dots, \vec{e}_7), \qquad V^T = \begin{pmatrix} \vec{e}_1 \\ \vec{e}_2 \\ \vdots \\ \vec{e}_7 \end{pmatrix}$$

<u>**Example for $i = 1$:**</u>

$$\vec{e}_1 = 0.45 \cdot \vec{e}_1 + 0.25 \cdot \vec{e}_2 + 0.14 \cdot \vec{e}_3 + 0.05 \cdot \vec{e}_4 + 0.03 \cdot \vec{e}_5 + 0.06 \cdot \vec{e}_6 + 0.02 \cdot \vec{e}_7$$



Attention

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$$Attention(\vec{e}_i, K, V) = softmax(\frac{\vec{e}_i^{\,T} \cdot K}{\sqrt{d}}) \cdot \mathrm{V}^{\mathrm{T}}$$

$$K = (\vec{e}_1, \vec{e}_2, \ldots, \vec{e}_7), \qquad V^T = \begin{pmatrix} \vec{e}_1^{\,T} \\ \vec{e}_2^{\,T} \\ \vdots \\ \vec{e}_7^{\,T} \end{pmatrix}$$

Example for $i = 2$:

$$Attention(\vec{e}_2, K, V)$$

1. $\vec{e}_i^{\,T} \cdot K = \vec{e}_2^{\,T} \cdot K =$

$$= (\vec{e}_2^{\,T} \cdot \vec{e}_1, \vec{e}_2^{\,T} \cdot \vec{e}_2, \ldots, \vec{e}_2^{\,T} \cdot \vec{e}_7)$$

$$= (23.2, 70.8, 33.7, 5.7, -12.4, 27.8, -22.4)$$

2. $\frac{\vec{e}_i^{\,T} \cdot K}{\sqrt{d}} = (0.8, 2.6, 1.2, 0.2, -0.4, 1.0, -0.8)$

3. $softmax(\frac{\vec{e}_i^{\,T} \cdot K}{\sqrt{d}}) = (0.1, 0.55, 0.14, 0.05, 0.03, 0.12, 0.02)$

4. $softmax(\frac{\vec{e}_i^{\,T} \cdot K}{\sqrt{d}}) \cdot \mathrm{V}^{\mathrm{T}} = (0.1 \cdot \vec{e}_1 + 0.55 \cdot \vec{e}_2 + 0.14 \cdot \vec{e}_3 + 0.05 \cdot \vec{e}_4 + 0.03 \cdot \vec{e}_5 + 0.12 \cdot \vec{e}_6 + 0.02 \cdot \vec{e}_7)^T$

$$\vec{e}_1 = \begin{pmatrix} 0.7 \\ 0.4 \\ \vdots \\ 2.1 \end{pmatrix} \quad \vec{e}_2 = \begin{pmatrix} 0.2 \\ -0.9 \\ \vdots \\ 0.6 \end{pmatrix} \quad \vec{e}_3 = \begin{pmatrix} 0.1 \\ 0.6 \\ \vdots \\ -0.3 \end{pmatrix} \quad \ldots \quad \ldots \quad \ldots \quad \vec{e}_7 = \begin{pmatrix} -0.1 \\ 0.8 \\ \vdots \\ -1.6 \end{pmatrix}$$

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Attention (2)

$$Attention(\vec{e}_i, K, V) = softmax\left(\frac{\vec{e}_i^{\,T} \cdot K}{\sqrt{d}}\right) \cdot \mathrm{V}^{\mathrm{T}}$$

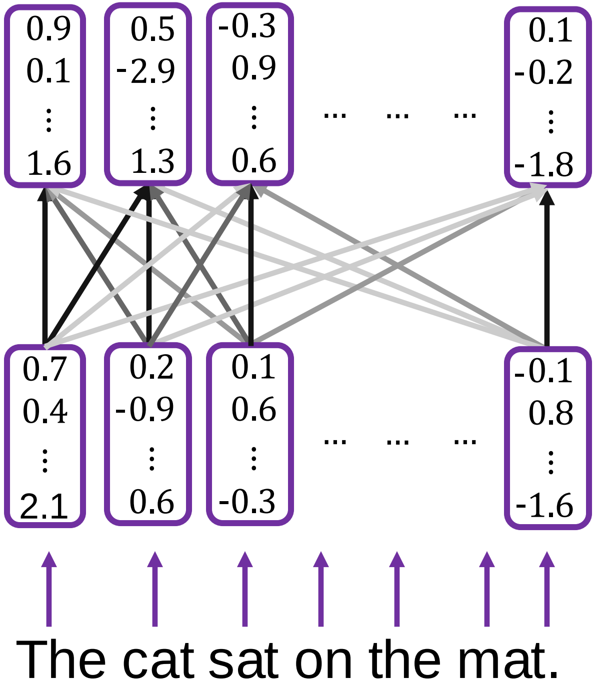
$$Attention(W_E \cdot \vec{e}_i, W_K \cdot K, W_V \cdot V)$$

$$= Attention\left(\vec{\tilde{e}}_i, \tilde{K}, \tilde{V}\right)$$

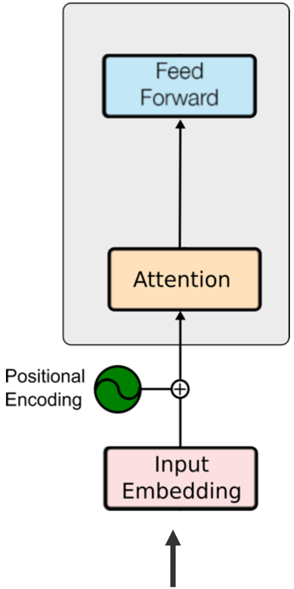
$$\tilde{K} = W_K \cdot K = (WK \cdot \vec{e}_1, W_K \cdot \vec{e}_2, \ldots, W_K \cdot \vec{e}_7),$$

$$\tilde{V} = WV \cdot V = (WV \cdot \vec{e}_1, \; WV \cdot \vec{e}_2, \ldots, W_V \cdot \vec{e}_7)$$

$$softmax(\vec{x})_j = \frac{e^{x_j}}{\sum_{k=1}^{n} e^{x_k}}, \quad \vec{x} \in \mathbb{R}^{\mathrm{N}}$$



Encoder



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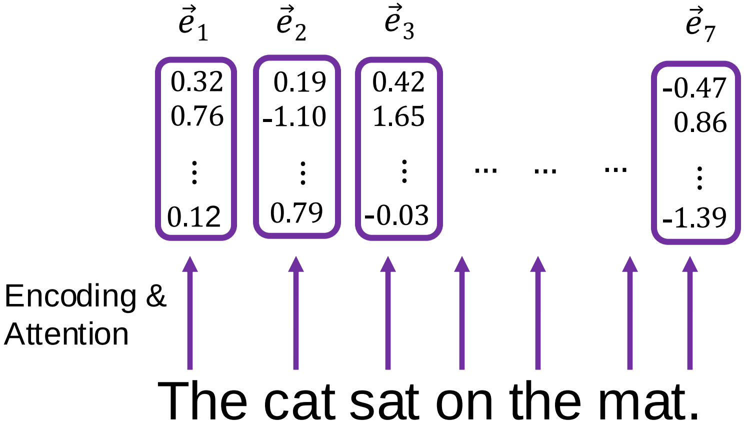
Feed Forward Neural Network

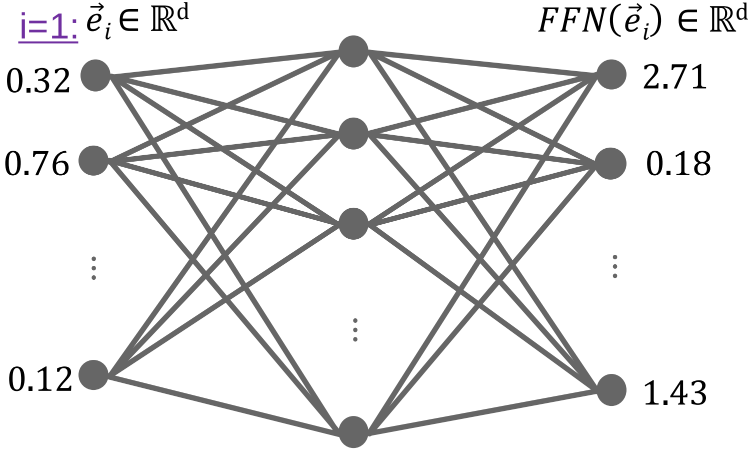
- Mapping through Encoding and Attention:



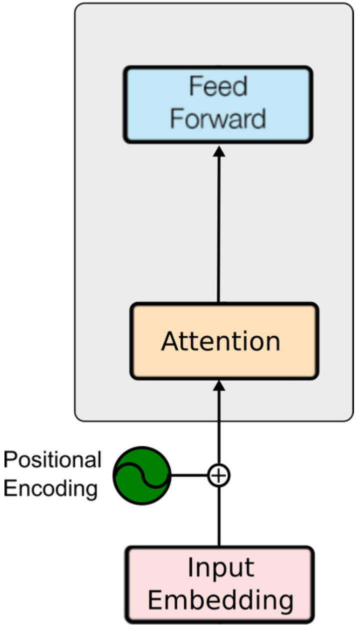
- Feed Forward Neural Network:

Feed Forward

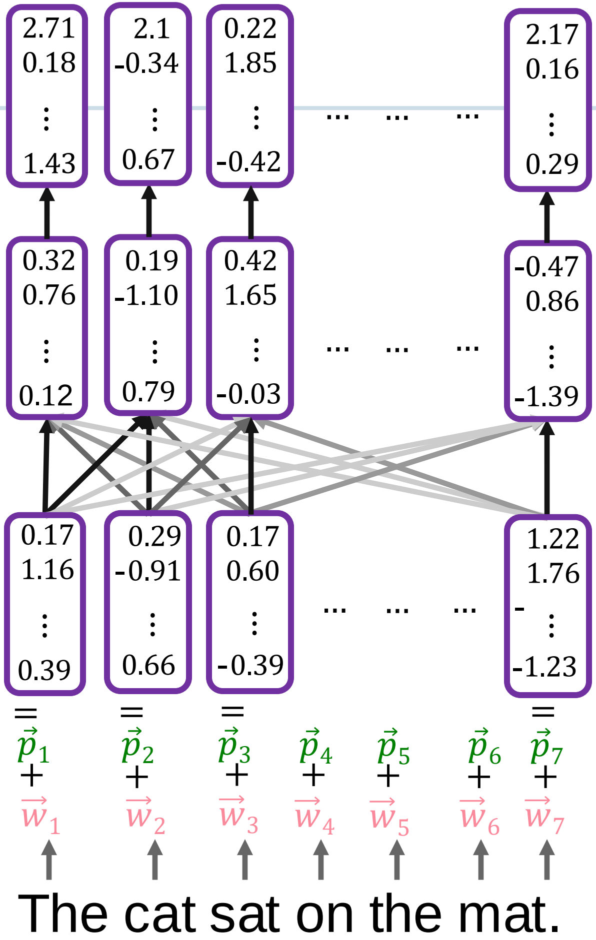
$$FFN(\vec{e}_i) = W_2 \cdot \mathrm{ReLU}(W_1 \cdot \vec{e}_i + \vec{b_1}) + \vec{b_2}$$



Encoder



Feed Forward
Attention
Positional Encoding
Input Embedding



2.71 0.18 ⋮ 1.43
2.1 -0.34 ⋮ 0.67
0.22 1.85 ⋮ -0.42
2.17 0.16 ⋮ 0.29
0.32 0.76 ⋮ 0.12
0.19 -1.10 ⋮ 0.79
0.42 1.65 ⋮ -0.03
-0.47 0.86 ⋮ -1.39
0.17 1.16 ⋮ 0.39
0.29 -0.91 ⋮ 0.66
0.17 0.60 ⋮ -0.39
1.22 1.76 ⋮ -1.23
$\vec{p}_1 + \vec{w}_1$
$\vec{p}_2 + \vec{w}_2$
$\vec{p}_3 + \vec{w}_3$
$\vec{p}_4 + \vec{w}_4$
$\vec{p}_5 + \vec{w}_5$
$\vec{p}_6 + \vec{w}_6$
$\vec{p}_7 + \vec{w}_7$
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Applying Encoders to Protein Sequences