Chapter 9. Part II

Sequence-to-Sequence

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Summary

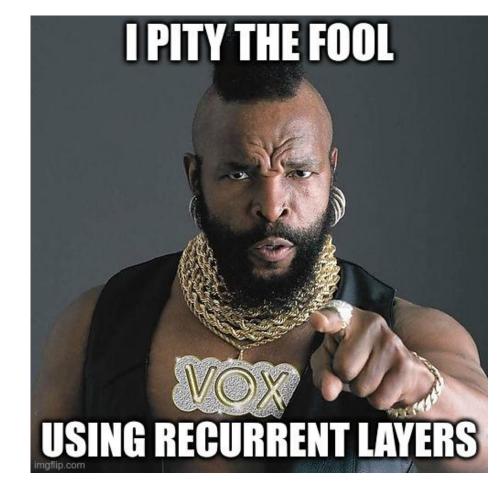
- I) Self-Attention
- II) Target mask
- III) Positional encoding

Self-Attention

"What if we replaced the recurrent layer with an attention mechanism?

This is the main proposal of the famous paper 'Attention Is All You Need' by Vaswani, A., et al.

The recurrent layer in the encoder received the source sequence and generated hidden states one by one. But we don't need to generate hidden states in this manner. We can use a separate attention mechanism to replace the encoder (and, wait, the decoder too!)."



Encoder

An encoder using self-attention!

Each context vector produced by the self-attention mechanism passes through a feed-forward network to generate a 'hidden state' as output.

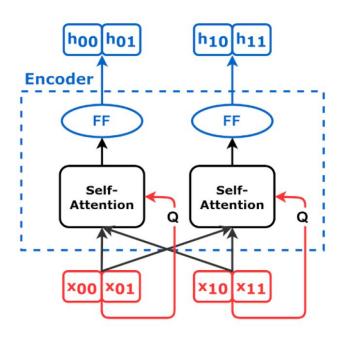
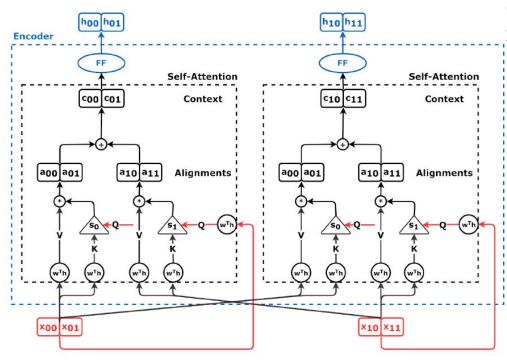


Figure 1 - Encoder with self-attention (simplified)

Encoder



Hidden states (h00, h01); Values (V), Query (Q); Keys (K); Data points (x00, x01, x10, x11)

$$\alpha_{00}, \alpha_{01} = \operatorname{softmax}(\frac{Q_0 \cdot K_0}{\sqrt{2}}, \frac{Q_0 \cdot K_1}{\sqrt{2}})$$

$$\operatorname{context\ vector}_0 = \alpha_{00} V_0 + \alpha_{01} V_1$$

Equation 1 - Context vector for first input (x_0)

$$\alpha_{10}, \alpha_{11} = \operatorname{softmax}(\frac{Q_1 \cdot K_0}{\sqrt{2}}, \frac{Q_1 \cdot K_1}{\sqrt{2}})$$

$$\operatorname{context} \ \operatorname{vector}_1 = \alpha_{10} V_0 + \alpha_{11} V_1$$

Equation 2 - Context vector for second input (x₁)

Figure 2 - Encoder with self-attention

Encoder

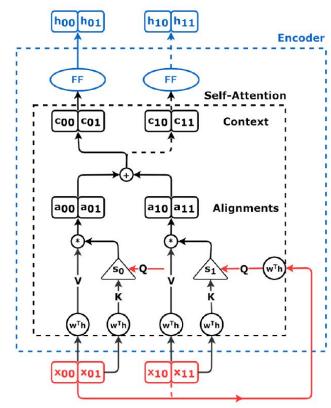
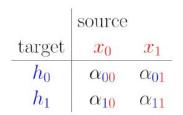


Figure 3 - only one selfattention mechanism, assuming it will be fed a different "query" (Q) every time.



Equation 3 - Attention scores

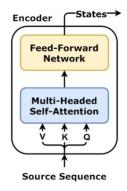


Figure 4 - Encoder with self-attention (diagram)

Encoder + Self-Attention

```
class EncoderSelfAttn(nn.Module):
    # Classe que implementa um Codificador com Auto-Atenção (Self-Attention)
    def init (self, n heads, d model, ff units, n features=None):
        # Método de inicialização do modelo
        # n heads: número de cabeças de atenção (multi-head attention)
        # d model: dimensionalidade do modelo
       # ff units: número de unidades na camada feed-forward
       # n features: número de características (features) de entrada, se aplicável
       super(). init () # Inicializa a classe pai nn.Module
       self.n heads = n heads # Armazena o número de cabecas de atenção
        self.d model = d model # Armazena a dimensionalidade do modelo
       self.ff units = ff units # Armazena o número de unidades na feed-forward
       self.n features = n features # Armazena o número de características (opcional)
       # Define a camada de Auto-Atenção com múltiplas cabeças (multi-head self-attention)
        self.self attn heads = MultiHeadAttention(n heads, d model, input dim=n features)
       # Define a rede feed-forward usando nn.Sequential
       self.ffn = nn.Sequential(
           nn.Linear(d model, ff units), # Primeira camada linear: reduz a dimensão de d model para ff units
            nn.ReLU(), # Função de ativação ReLU
           nn.Linear(ff units, d model), # Segunda camada linear: retorna à dimensão original d model
   def forward(self, query, mask=None):
        # Método de passagem à frente (forward) do modelo
       # query: entrada do modelo, geralmente o tensor de embeddings
       # mask: máscara opcional para o mecanismo de atenção (usada para ignorar certos elementos)
       # Inicializa as chaves para a atenção com base na entrada (query)
        self.self attn heads.init keys(query)
       # Executa a camada de atenção e obtém o resultado
        att = self.self attn heads(query, mask)
       # Passa o resultado da atenção pela rede feed-forward
       out = self.ffn(att)
       # Retorna o resultado final
        return out
```

Create an encoder and feed it with a source sequence:

Output:

Produced a sequence of states that will be the input to the cross-attention mechanism used by the decoder.

Cross-Attention

In the figure, self-attention as the encoder, cross-attention on top of it, and the modifications in the decoder.

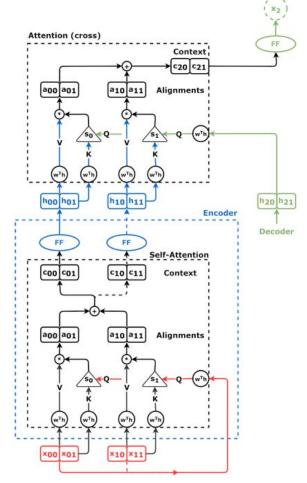


Figure 5 - Encoder with self- and cross-attentions



Decoder + Self-Attention

Encoder vs Decoder (self-attention):

- <u>Encoder: Feed-forward network self-attention.</u>
- Decoder: Feed-forward network cross-attention, maps the decoder output and produces predictions.

```
class DecoderSelfAttn(nn.Module):
   # Classe que implementa um Decodificador com Auto-Atenção e Atenção Cruzada (Self-Attention + Cross-Attention)
   def init (self, n heads, d model, ff units, n features=None):
       # Método de inicialização do modelo
       super(). init () # Inicializa a classe pai nn.Module
        self.n heads = n heads # Armazena o número de cabeças de atenção
        self.d model = d model # Armazena a dimensionalidade do modelo
        self.ff units = ff units # Armazena o número de unidades na feed-forward
        self.n features = d model if n features is None else n features # Define n features; se não for especificado, usa d model como padrão
       # Define a camada de Auto-Atenção (Self-Attention) com múltiplas cabecas
        self.self attn heads = MultiHeadAttention(n heads, d model, input dim=self.n features)
       # Define a camada de Atenção Cruzada (Cross-Attention) para conectar a entrada do decodificador com a saída do codificador
        self.cross attn heads = MultiHeadAttention(n heads, d model)
       # Define a rede feed-forward usando nn.Sequential
        self.ffn = nn.Sequential(
           nn.Linear(d model, ff units), # Primeira camada linear: reduz a dimensão de d model para ff units
                                          # Função de ativação ReLU
            nn.Linear(ff units, self.n features), # Segunda camada linear: retorna à dimensão original (ou n features)
    def init kevs(self, states):
       # Método para inicializar as chaves na atenção cruzada com base nos estados do codificador
       self.cross attn heads.init keys(states)
   def forward(self, query, source mask=None, target mask=None):
       # Método de passagem à frente (forward) do modelo
       # Inicializa as chaves para a auto-atenção com base na entrada (query)
        self.self attn heads.init keys(query)
       # Executa a auto-atenção (Self-Attention) no próprio decodificador
       att1 = self.self attn heads(query, target mask)
       # Executa a atenção cruzada (Cross-Attention), ligando a saída da auto-atenção aos estados do codificador
        att2 = self.cross attn heads(att1, source mask)
       # Passa o resultado da atenção cruzada pela rede feed-forward
       out = self.ffn(att2)
       return out
```

Decoder

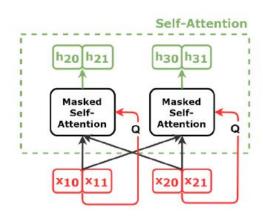


Figure 6 - Decoder with self-attention (simplified)

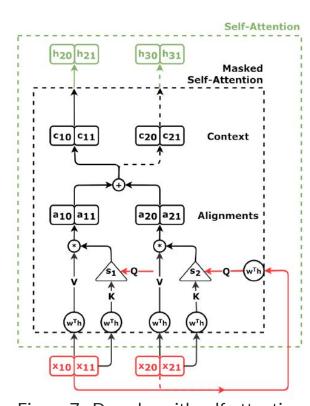


Figure 7 - Decoder with self-attention

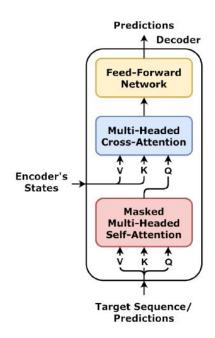


Figure 8 - Decoder with self- and cross-attentions (diagram) 10

Subsequent Inputs and Teacher Forcing

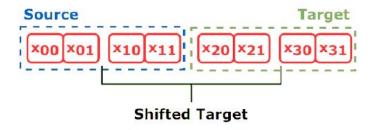


Figure 9 - Shifted target sequence



One of the advantages of self-attention over recurrent layers is that the operations can be parallelized. There is no longer a need to do anything sequentially, including teacher forcing. This means that we are using the entire target sequence shifted at once as the 'query' input to the decoder.

Attention Scores

To understand the problem, let's look at the context vector that will result in the first 'hidden state' produced by the decoder, which, in turn, will lead to the first prediction:

$$\alpha_{21}, \alpha_{22} = \operatorname{softmax}(\frac{Q_1 \cdot K_1}{\sqrt{2}}, \frac{Q_1 \cdot K_2}{\sqrt{2}})$$

$$\operatorname{context\ vector}_2 = \alpha_{21}V_1 + \alpha_{22}V_2$$

Equation 4 - Context vector for the first target

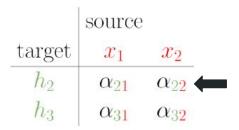
The problem is that it is using a 'key' (K2) and a 'value' (V2) that are transformations of the data point it is trying to predict.

In other words, the model is being allowed to cheat by peeking into the future because we are giving it all the data points in the target sequence, except for the last one.

Target Mask (Training)

The purpose of the target mask is to zero out the attention scores for 'future' data points.





Equation 6 - Decoder's attention scores

	source	
target	x_1	x_2
h_2	α_{21}	0
h_3	$lpha_{31}$	$lpha_{32}$

Equation 7 - Decoder's (masked) attention scores

Target Mask

Subsequent Mask

```
subsequent_mask(2) # 1, L, L
```

Output

In practice:

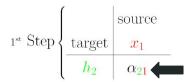
Output

Target Mask (Evaluation/Prediction)

```
inputs = source_seq[:, -1:]
trg_masks = subsequent_mask(1)
out = decself(inputs, trg_masks)
out
```

Output

```
tensor([[[0.4132, 0.3728]]], grad_fn=<AddBackward0>)
```

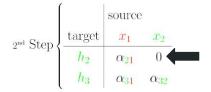


Equation 8 - Decoder's (masked) attention scores for the first target

```
inputs = torch.cat([inputs, out[:, -1:, :]], dim=-2)
inputs
```

Output

```
tensor([[[-1.0000, 1.0000], [ 0.4132, 0.3728]]], grad_fn=<CatBackward>)
```



Equation 9 - Decoder's (masked) attention scores for the second target

Target Mask (Evaluation/Prediction)



The decoder with self-attention expects the complete sequence as the 'query', then we concatenate the prediction with the previous 'query'.







Predicted coordinates of both x_2 and x_3 :

```
trg_masks = subsequent_mask(2)
out = decself(inputs, trg_masks)
out
```

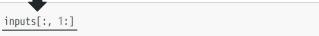
Output

Concatenating prediction to sequence:

```
inputs = torch.cat([inputs, out[:, -1:, :]], dim=-2)
inputs
```

Output

Decoder predictions:



Output

Encoder + Decoder + Self-Attention

The encoder and decoder come together again, each using self-attention to calculate their corresponding 'hidden states'.

In addition to using masked self-attention, the decoder uses cross-attention to make predictions.

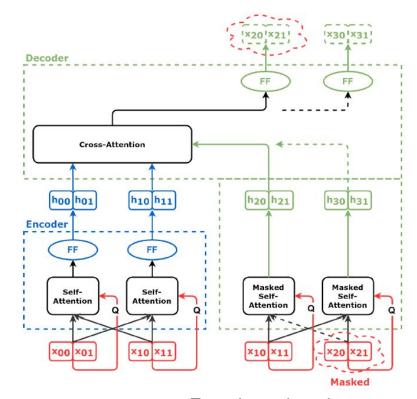
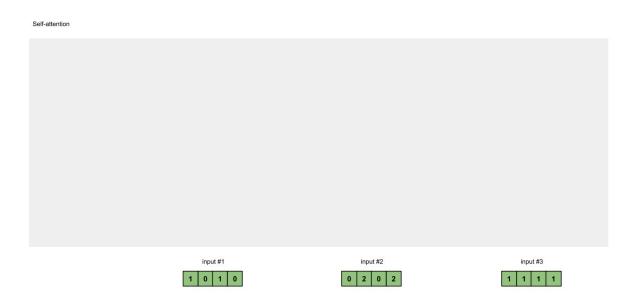


Figure 10 - Encoder + decoder + attention (simplified)

Self-Attention



Model Configuration & Training

Model Configuration

Model Training

```
1 sbs_seq_selfattn = StepByStep(model, loss, optimizer)
2 sbs_seq_selfattn.set_loaders(train_loader, test_loader)
3 sbs_seq_selfattn.train(100)
```

```
fig = sbs_seq_selfattn.plot_losses() # graph of losses
```



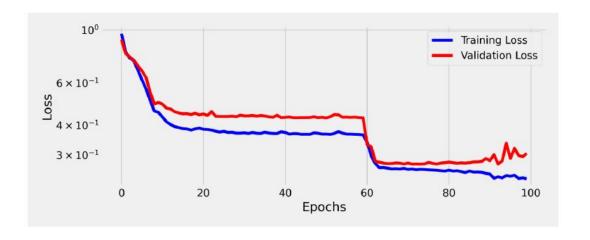


Figure 12 - Losses-encoder + decoder + self-attention

Visualizing Predictions

fig = sequence_pred(sbs_seq_selfattn, full_test, test_directions)

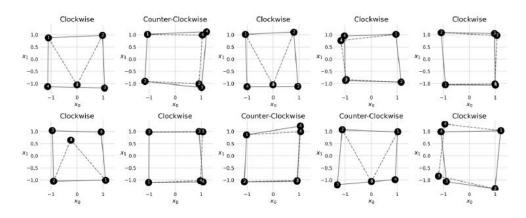
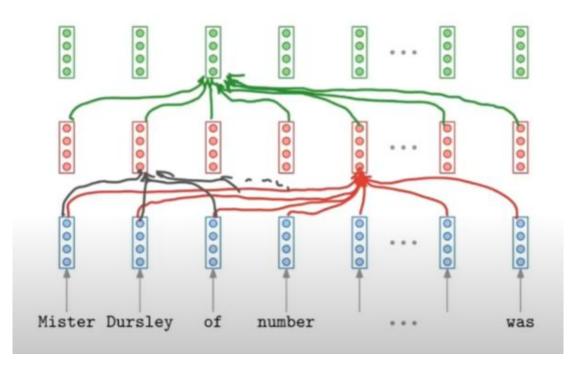


Figure 13 - Predictions-encoder + decoder + self-attention







- Order

Position	0	1	2	3	4	5	6	7
(Pos mod 4)/4	0.00	0.25	0.50	0.75	0.00	0.25	0.50	0.75
(Pos mod 5)/5	0.00	0.20	0.40	0.60	0.80	0.00	0.20	0.40
(Pos mod 7)/7	0.00	0.14	0.29	0.43	0.57	0.71	0.86	0.00

Figure 9.41 - Combining results for different modules

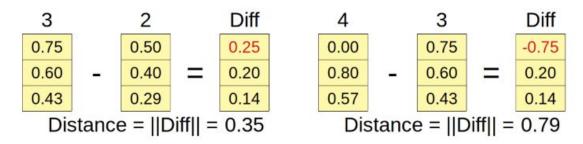


Figure 9.42 - Inconsistent distances

Position	0	1	2	3	4	5	6	7
sine (base 4)	0.00	1.00	0.00	-1.00	0.00	1.00	0.00	-1.00
cosine (base 4)	1.00	0.00	-1.00	0.00	1.00	0.00	-1.00	0.00
sine (base 5)	0.00	0.95	0.59	-0.59	-0.95	0.00	0.95	0.59
cosine (base 5)	1.00	0.31	-0.81	-0.81	0.31	1.00	0.31	-0.81
sine (base 7)	0.00	0.78	0.97	0.43	-0.43	-0.97	-0.78	0.00
cosine (base 7)	1.00	0.62	-0.22	-0.90	-0.90	-0.22	0.62	1.00

$$PE_{\text{pos, }2d} = \sin\left(\frac{1}{10000^{\frac{2d}{d_{\text{model}}}}}\text{pos}\right)$$

$$PE_{\text{pos, }2d+1} = \cos\left(\frac{1}{10000^{\frac{2d}{d_{\text{model}}}}}\text{pos}\right)$$

Figure 9.46 - Consistent distances

```
max len = 10
d \mod el = 8
position = torch.arange(0, max_len).float().unsqueeze(1)
angular_speed = torch.exp(
  torch.arange(0, d_model, 2).float() * (-np.log(10000.0) / d_model)
encoding = torch.zeros(max_len, d_model)
encoding[:, 0::2] = torch.sin(angular_speed * position)
encoding[:, 1::2] = torch.cos(angular_speed * position)
```

```
np.round(encoding[0:4], 4) # first four positions
```

Output

```
tensor([[ 0.0000, 1.0000, 0.0000, 1.0000, 0.0000, 1.0000,
0.0000, 1.0000],
       [ 0.8415, 0.5403, 0.0998, 0.9950, 0.0100, 1.0000,
0.0010, 1.00001,
       [ 0.9093, -0.4161, 0.1987, 0.9801, 0.0200, 0.9998,
0.0020, 1.0000],
       [ 0.1411, -0.9900, 0.2955, 0.9553, 0.0300, 0.9996,
0.0030, 1.0000]])
```

```
class PositionalEncoding(nn.Module):
   def __init__(self, max_len, d_model):
        super().__init__()
        self.d model = d model
        pe = torch.zeros(max_len, d_model)
        position = torch.arange(0, max_len).float().unsqueeze(1)
        angular_speed = torch.exp(
           torch.arange(0, d_model, 2).float() *
            (-np.log(10000.0) / d_model)
        # even dimensions
       pe[:, 0::2] = torch.sin(position * angular_speed)
       # odd dimensions
        pe[:, 1::2] = torch.cos(position * angular_speed)
        self.register buffer('pe', pe.unsqueeze(0))
   def forward(self, x):
       # x is N, L, D
       # pe is 1, maxlen, D
        scaled_x = x * np.sqrt(self.d_model)
        encoded = scaled_x + self.pe[:, :x.size(1), :]
        return encoded
```

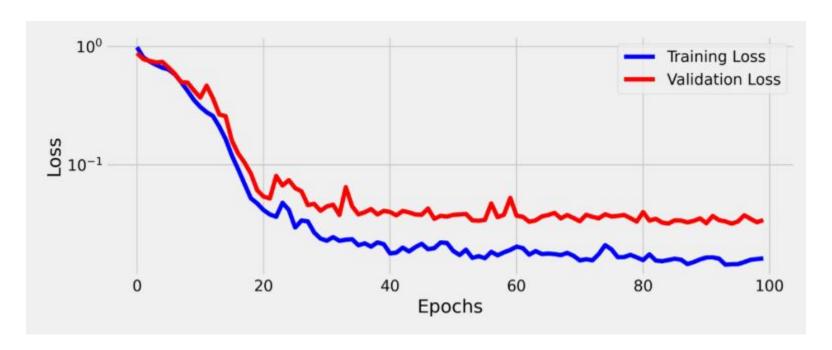
ENCODER + DECODER + PE

```
class DecoderPe(nn.Module):
class EncoderPe(nn.Module):
                                                                def init (self, n heads, d model, ff units,
   def __init__(self, n_heads, d_model, ff_units,
                                                                             n features=None, max len=100):
                 n features=None, max len=100):
                                                                    super(). init ()
        super(). init ()
                                                                    pe_dim = d_model if n_features is None else n_features
                                                                    self.pe = PositionalEncoding(max_len, pe_dim)
        pe_dim = d_model if n_features is None else n_feat
                                                                    self.layer = DecoderSelfAttn(n heads, d model,
        self.pe = PositionalEncoding(max_len, pe_dim)
                                                                                                 ff units, n features)
        self.layer = EncoderSelfAttn(n_heads, d_model,
                                      ff units, n features)
                                                                def init_keys(self, states):
                                                                    self.layer.init_keys(states)
   def forward(self, query, mask=None):
                                                                def forward(self, query, source_mask=None, target_mask=None):
        query_pe = self.pe(query)
                                                                    query pe = self.pe(query)
        out = self.layer(query_pe, mask)
                                                                    out = self.layer(query pe, source mask, target mask)
        return out
                                                                    return out
```

Model Configuration & Training

```
torch.manual seed(43)
encpe = EncoderPe(n_heads=3, d_model=2, ff_units=10, n_features=2)
decpe = DecoderPe(n_heads=3, d_model=2, ff_units=10, n_features=2)
model = EncoderDecoderSelfAttn(encpe, decpe,
                                 input len=2, target len=2)
loss = nn.MSELoss()
optimizer = optim.Adam(model.parameters(), lr=0.01)
     1 sbs_seq_selfattnpe = StepByStep(model, loss, optimizer)
    2 sbs_seq_selfattnpe.set_loaders(train_loader, test_loader)
     3 sbs_seq_selfattnpe.train(100)
    fig = sbs_seq_selfattnpe.plot_losses()
```

Losses



ENCODER+DECODER+PE

Losses

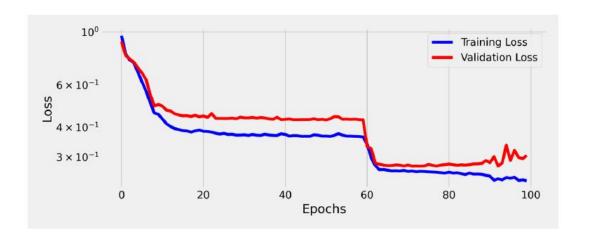
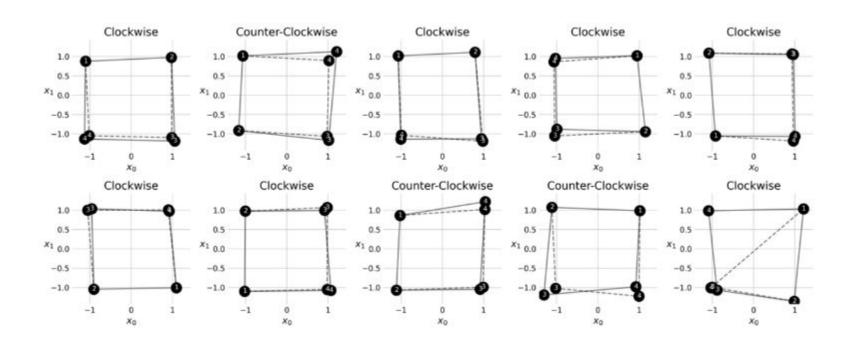


Figure 12 - Losses-encoder + decoder + self-attention

Visualizing Predictions



Model assembly

```
class EncoderDecoderSelfAttn(nn.Module):
   def init (self, encoder, decoder, input len, target len):
        super(). init ()
        self.encoder = encoder
        self.decoder = decoder
        self.input len = input len
        self.target len = target len
        self.trg masks = self.subsequent mask(self.target len)
    @staticmethod
    def subsequent_mask(size):
        attn shape = (1, size, size)
        subsequent_mask = (
           1 - torch.triu(torch.ones(attn_shape), diagonal=1)
        ).bool()
        return subsequent mask
```

Model assembly

```
def predict(self, source_seq, source_mask):
    # Decodes / generates a sequence using one input
    # at a time - used in EVAL mode
    inputs = source_seq[:, -1:]
    for i in range(self.target_len):
        out = self.decode(inputs,
                          source mask,
                          self.trg masks[:, :i+1, :i+1])
        out = torch.cat([inputs, out[:, -1:, :]], dim=-2)
        inputs = out.detach()
    outputs = inputs[:, 1:, :]
    return outputs
def forward(self, X, source_mask=None):
    # Sends the mask to the same device as the inputs
    self.trg masks = self.trg masks.type as(X).bool()
    # Slices the input to get source sequence
    source_seq = X[:, :self.input_len, :]
    # Encodes source sequence AND initializes decoder
    self.encode(source seg, source mask)
    if self.training:
        # Slices the input to get the shifted target seg
        shifted_target_seq = X[:, self.input_len-1:-1, :]
        # Decodes using the mask to prevent cheating
        outputs = self.decode(shifted_target_seq,
                              source mask,
```

```
self.trg_masks)
else:
    # Decodes using its own predictions
    outputs = self.predict(source_seq, source_mask)
return outputs
```

Model assembly

```
class PositionalEncoding(nn.Module):
    def __init__(self, max_len, d_model):
        super(). init_()
        self.d model = d model
        pe = torch.zeros(max len, d model)
        position = torch.arange(0, max_len).float().unsqueeze(1)
        angular speed = torch.exp(
            torch.arange(0, d_model, 2).float() *
            (-np.log(10000.0) / d_model)
        # even dimensions
        pe[:, 0::2] = torch.sin(position * angular_speed)
        # odd dimensions
        pe[:, 1::2] = torch.cos(position * angular_speed)
        self.register_buffer('pe', pe.unsqueeze(0))
    def forward(self, x):
        # x is N, L, D
        # pe is 1, maxlen, D
        scaled_x = x * np.sqrt(self.d_model)
        encoded = scaled_x + self.pe[:, :x.size(1), :]
        return encoded
```

```
class EncoderPe(nn.Module):
    def __init__(self, n_heads, d_model, ff_units,
                 n features=None, max len=100):
        super(). init ()
        pe_dim = d_model if n_features is None else n_features
        self.pe = PositionalEncoding(max_len, pe_dim)
        self.layer = EncoderSelfAttn(n heads, d model,
                                     ff units, n features)
    def forward(self, query, mask=None):
        query pe = self.pe(query)
        out = self.layer(query_pe, mask)
        return out
class DecoderPe(nn.Module):
    def __init__(self, n_heads, d_model, ff_units,
                 n features=None, max len=100):
        super(). init ()
        pe dim = d model if n features is None else n features
        self.pe = PositionalEncoding(max_len, pe_dim)
        self.layer = DecoderSelfAttn(n_heads, d_model,
                                     ff units, n features)
    def init keys(self, states):
        self.layer.init keys(states)
    def forward(self, query, source_mask=None, target_mask=None):
        query_pe = self.pe(query)
        out = self.layer(query_pe, source_mask, target_mask)
        return out
```

References

GODOY, Daniel Voigt. *Deep Learning with PyTorch Step-by-Step: A Beginner's Guide.* Leanpub, 2022. Disponível em: https://leanpub.com/deep-learning-with-pytorch-step-by-step.