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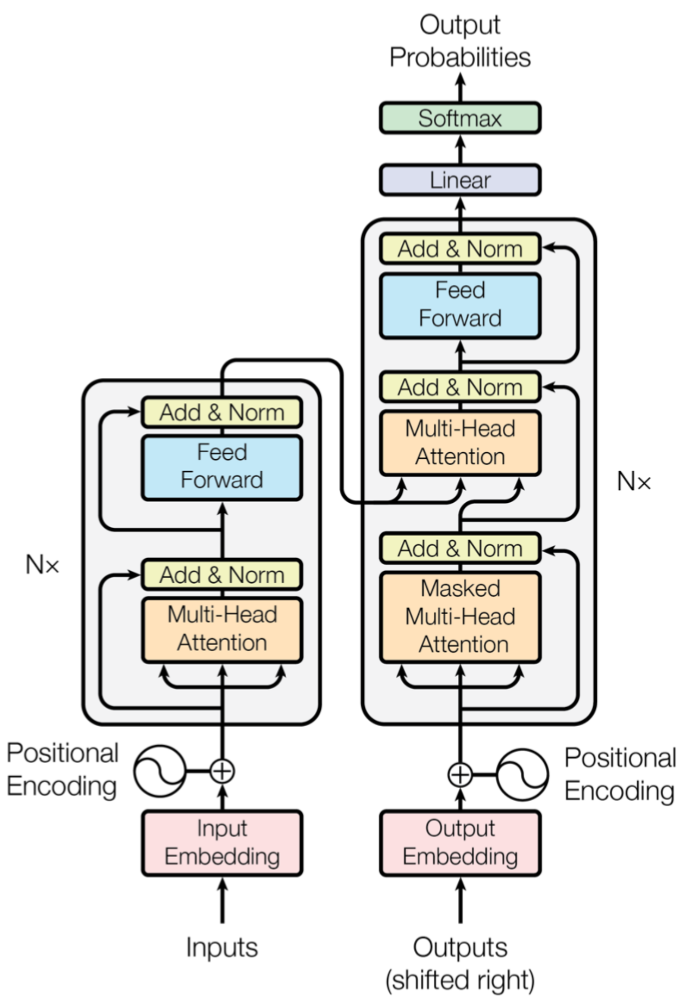
Transformer通用特征提取器



1 输入序列、目标序列与输出序列

输入序列$inputs = \left(i_1, i_2, \cdots, i_p, \cdots, i_N\right)$，其中$i_p \in \mathbb{N}^*$为输入符号表中的序号。
目标序列$targets = \left(t_1, t_2, \cdots, t_q, \cdots, t_M\right)$，其中$t_q \in \mathbb{N}^*$为目标符号表中的序号。

$$outputs\_probabilities = Transformer(inputs, targets)$$

其中，$outputs_probabilities = \left(o_1, o_2, \cdots, o_q, \cdots, o_M\right)$为预测序列，$o_q \in \mathbb{N}^*$为目标符号表中的序号。

在自然语言处理任务中，当输入序列与目标序列中的元素较多，通常以句子为单位划分为若干个对应的“输入-目标”子序列进行学习。

2 词嵌入与位置编码

2.1 输入序列词嵌入与位置编码

输入序列词嵌入$Embedding(inputs) \in \mathbb{R}^{N \times d_{model}}$，其中，$N$为输入序列长度，$d_{model}$为词嵌入维度。

输入序列位置编码$Pos_Enc(inputs_position) \in \mathbb{R}^{N \times d_{model}}$，
其中，$inputs_position = (1, 2, \cdots, p, \cdots, N)$为输入序列中输入符号对应的位置序号；

$$Pos\_Enc_{(pos,2i)} = \sin\left(pos/10000^{2i/d_{model}}\right)$$
$$Pos\_Enc_{(pos,2i+1)} = \cos\left(pos/10000^{2i/d_{model}}\right)$$

其中，$pos \in inputs\_position, i \in (0, 1, \cdots, d_{model}/2)$。

2.2 目标序列词嵌入与位置编码

目标序列词嵌入$Embedding(targets) \in \mathbb{R}^{M \times d_{model}}$，其中$M$为目标序列长度，$d_{model}$为词嵌入维度。

目标序列位置编码$Pos_Enc(targets_position) \in \mathbb{R}^{M \times d_{model}}$，
其中，$targets_position = (1, 2, \cdots, q, \cdots, M)$为目标序列的位置序号。

3 编码器Encoder

3.1 编码器结构

编码器结构：

$$\begin{aligned} e_0 &= Embedding(inputs) + Pos\_Enc(inputs\_position) \\ e_l &= EncoderLayer(e_{l-1}), l \in [1, n] \end{aligned}$$

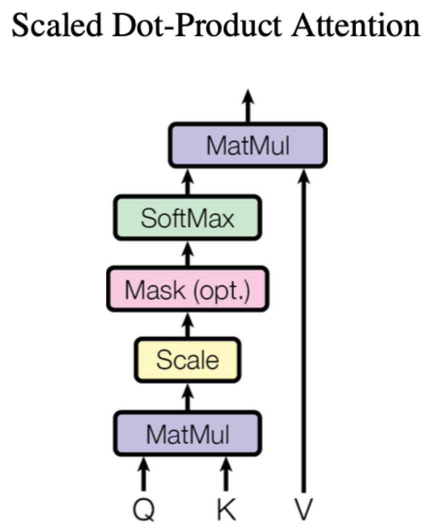
其中，$e_0 \in \mathbb{R}^{N \times d_{model}}$为编码器输入，$EncoderLayer(\cdot)$为编码器层，$n$为层数，$e_l \in \mathbb{R}^{N \times d_{model}}$为第$l$层编码器层输出。

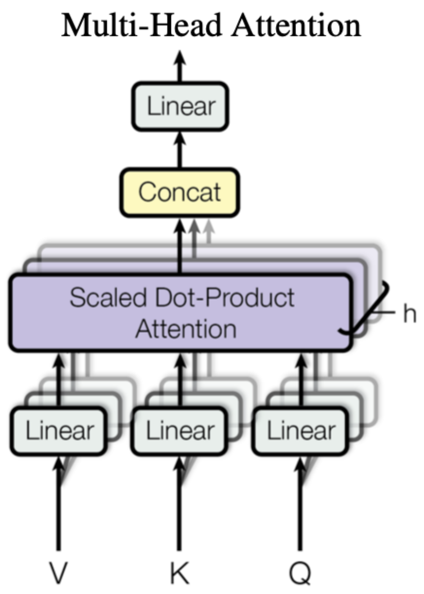
编码器层EncoderLayer：

$$\begin{aligned} e_{mid} &= LayerNorm(e_{in} + MultiHeadAttention(e_{in})) \\ e_{out} &= LayerNorm(e_{mid} + FFN(e_{mid})) \end{aligned}$$

其中，$e_{in} \in \mathbb{R}^{N \times d_{model}}$为编码器层输入，$e_{out} \in \mathbb{R}^{N \times d_{model}}$为编码器层输出，$MultiHeadAttention(\cdot)$为多头注意力机制，$FFN(\cdot)$为前馈神经网络，$LayerNorm(\cdot)$为层归一化。

3.2 多头注意力机制与缩放点积





输入向量序列$e_{in} = (e_{in1}, e_{in2}, \cdots, e_{inN}) \in \mathbb{R}^{N \times d_{model}}$，分别得到查询向量序列$Q = e_{in}$，键向量序列$K = e_{in}$，值向量序列$V = e_{in}$。

多头注意力机制

$$MultiHeadAttention(e_{in}) = MultiHead(Q, K, V) = Concat(head_1, \cdots, head_h)W^O$$

其中，多头输出$head_i = Attention\left(QW_i^Q, KW_i^K, VW_i^V\right)$，可学习的参数矩阵$W_i^Q \in \mathbb{R}^{d_{model} \times d_k}, W_i^K \in \mathbb{R}^{d_{model} \times d_k}, W_i^V \in \mathbb{R}^{d_{model} \times d_v}, W^O \in \mathbb{R}^{hd_v \times d_{model}}$

使用缩放点积作为打分函数的自注意力机制

$$Attention\left(QW_i^Q, KW_i^K, VW_i^V\right) = softmax\left(\frac{QW_i^Q\left(KW_i^K\right)^\top}{\sqrt{d_k}}\right)VW_i^V$$

3.3 编码器pad掩码

$$enc\_pad\_mask_j = \left(e_{j1}, e_{j2}, \cdots, e_{jp}, \cdots, e_{jN}\right)$$

其中，

$$e_{jp} = \begin{cases} True, & i_p = 0 \\ False, & i_p \neq 0 \end{cases} \quad j = 1, 2, \cdots, N$$

$enc\_pad\_mask \in \mathbb{R}^{N \times N}$，$i_p$为输入序列$inputs$对应位置序号。

3.4 前馈神经网络

$$\begin{aligned} FFN(e_{mid}) &= ReLU(e_{mid}W_1 + b_1)W_2 + b_2 \\ &= \max(0, e_{mid}W_1 + b_1)W_2 + b_2 \end{aligned}$$

其中，参数矩阵$W_1 \in \mathbb{R}^{d_{model} \times d_{ff}}, W_2 \in \mathbb{R}^{d_{ff} \times d_{model}}$，偏置$b_1 \in \mathbb{R}^{d_{ff}}, b_2 \in \mathbb{R}^{d_{model}}$。

4 解码器Decoder

4.1 解码器结构

$$\begin{aligned} d_0 &= Embedding(targets) + Pos\_Enc(targets\_position) \\ d_l &= DecoderLayer(d_{l-1}), l \in [1, n] \\ outputs\_probabilities &= softmax(d_nW) \end{aligned}$$

其中，$d_0 \in \mathbb{R}^{M \times d_{model}}$为解码器输入，$DecoderLayer(\cdot)$为解码器层，$n$为层数，$d_l \in \mathbb{R}^{M \times d_{model}}$为第$l$层解码器层输出，$W \in \mathbb{R}^{M \times tgt_vocab_size}$输入输出参数矩阵，$softmax(\cdot)$为softmax层。

解码器层DecoderLayer：

$$\begin{aligned} d_{mid1} &= LayerNorm\left(d_{in} + MaskedMultiHeadAttention\left(d_{in}\right)\right) \\ d_{mid2} &= LayerNorm\left(d_{mid1} + MultiHeadAttention\left(d_{mid1}, e_{out}\right)\right) \\ d_{out} &= LayerNorm\left(d_{mid2} + FFN\left(d_{mid2}\right)\right) \end{aligned}$$

其中，$d_{in} \in \mathbb{R}^{M \times d_{model}}$为解码器层输入，$d_{out} \in \mathbb{R}^{M \times d_{model}}$为解码器层输出，$MultiHeadAttention(\cdot)$为多头注意力机制，$FFN(\cdot)$为前馈神经网络，$LayerNorm(\cdot)$为层归一化。

4.2 解码器pad掩码、解码器sequence掩码和编码器解码器pad掩码

解码器pad掩码

$$dec\_pad\_mask_j = \left(d_{j1}, d_{j2}, \cdots, d_{jq}, \cdots, d_{jM}\right)$$

其中，

$$d_{jq} = \begin{cases} True, & t_q = 0 \\ False, & t_q \neq 0 \end{cases} \quad j = 1, 2, \cdots, M$$

$dec\_pad\_mask \in \mathbb{R}^{M \times M}$，$t_q$为目标序列$targets$对应位置序号。

解码器sequence掩码

$$dec\_sequence\_mask_j = \left(s_{j1}, s_{j2}, \cdots, s_{jl}, \cdots, s_{jM}\right)$$

其中，

$$s_{jl} = \begin{cases} 0, & j \geq l \\ 1, & j < l \end{cases} \quad j = 1, 2, \cdots, M$$

$dec\_sequence\_mask \in \mathbb{R}^{M \times M}$，为非零元素为1的上三角矩阵。

解码器掩码

$$dec\_mask = dec\_pad\_mask + dec\_sequence\_mask$$

编码器解码器pad掩码

$$dec\_enc\_pad\_mask_j = \left(de_{j1}, de_{j2}, \cdots, de_{jp}, \cdots, de_{jN}\right)$$

其中，

$$de_{jp} = \begin{cases} True, & i_p = 0 \\ False, & i_p \neq 0 \end{cases} \quad j = 1, 2, \cdots, M$$

$dec\_enc\_pad\_mask \in \mathbb{R}^{M \times N}$，$i_p$为输入序列$inputs$对应位置序号。

5 代码实现

5.1 数据处理

In [3]:

```python
import numpy as np
import torch
import torch.nn as nn
import torch.optim as optim
from torch.autograd import Variable
import matplotlib.pyplot as plt

dtype = torch.FloatTensor

sentences = ['ich mochte ein bier P', 'S i want a beer', 'i want a beer E']
src_vocab = {'P' : 0, 'ich' : 1, 'mochte' : 2, 'ein' : 3, 'bier' : 4}
src_vocab_size = len(src_vocab)

tgt_vocab = {'P' : 0, 'i' : 1, 'want' : 2, 'a' : 3, 'beer' : 4, 'S' : 5, 'E' : 6}
number_dict = {i: w for i, w in enumerate(tgt_vocab)}
tgt_vocab_size = len(tgt_vocab)

src_len = 5
tgt_len = 5

d_model = 512
d_ff = 2048
d_k = d_v = 64
n_layers = 6
n_heads = 8

def make_batch(sentences):
    input_batch = [[src_vocab[w] for w in sentences[0].split()]]
    output_batch = [[tgt_vocab[w] for w in sentences[1].split()]]
    target_batch = [[tgt_vocab[w] for w in sentences[2].split()]]
    return Variable(torch.LongTensor(input_batch)), Variable(torch.LongTensor(output_batch
```

executed in 9ms, finished 17:19:54 2020-04-23

In [4]:

```python
make_batch(sentences)
```

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Out[4]:

```
(tensor([[1, 2, 3, 4, 0]]),
 tensor([[5, 1, 2, 3, 4]]),
 tensor([[1, 2, 3, 4, 6]]))
```

5.2 Transformer定义

In [5]:

```python
class Transformer(nn.Module):
    def __init__(self):
        super(Transformer, self).__init__()
        self.encoder = Encoder()
        self.decoder = Decoder()
        self.projection = nn.Linear(d_model, tgt_vocab_size, bias=False)
    def forward(self, enc_inputs, dec_inputs):
        enc_outputs, enc_self_attns = self.encoder(enc_inputs)
        dec_outputs, dec_self_attns, dec_enc_attns = self.decoder(dec_inputs, enc_inputs,
        dec_logits = self.projection(dec_outputs) # dec_logits : [batch_size x src_vocab_s
        return dec_logits.view(-1, dec_logits.size(-1)), enc_self_attns, dec_self_attns, d
```

executed in 7ms, finished 17:19:56 2020-04-23

5.3 编码器定义

In [6]:

```
class Encoder(nn.Module):
    def __init__(self):
        super(Encoder, self).__init__()
        self.src_emb = nn.Embedding(src_vocab_size, d_model)
        self.pos_emb = nn.Embedding.from_pretrained(get_sinusoid_encoding_table(src_len+1,
        self.layers = nn.ModuleList([EncoderLayer() for _ in range(n_layers)])

    def forward(self, enc_inputs): # enc_inputs : [batch_size x source_len]
        enc_outputs = self.src_emb(enc_inputs) + self.pos_emb(torch.LongTensor([[1,2,3,4,0
        enc_self_attn_mask = get_attn_pad_mask(enc_inputs, enc_inputs)
        enc_self_attns = []
        for layer in self.layers:
            enc_outputs, enc_self_attn = layer(enc_outputs, enc_self_attn_mask)
            enc_self_attns.append(enc_self_attn)
        return enc_outputs, enc_self_attns

class EncoderLayer(nn.Module):
    def __init__(self):
        super(EncoderLayer, self).__init__()
        self.enc_self_attn = MultiHeadAttention()
        self.pos_ffn = PoswiseFeedForwardNet()

    def forward(self, enc_inputs, enc_self_attn_mask):
        enc_outputs, attn = self.enc_self_attn(enc_inputs, enc_inputs, enc_inputs, enc_sel
        enc_outputs = self.pos_ffn(enc_outputs) # enc_outputs: [batch_size x len_q x d_moc
        return enc_outputs, attn

```

executed in 9ms, finished 17:19:58 2020-04-23

5.4 解码器定义

In [7]:

```
class Decoder(nn.Module):
    def __init__(self):
        super(Decoder, self).__init__()
        self.tgt_emb = nn.Embedding(tgt_vocab_size, d_model)
        self.pos_emb = nn.Embedding.from_pretrained(get_sinusoid_encoding_table(tgt_len+1,
        self.layers = nn.ModuleList([DecoderLayer() for _ in range(n_layers)])

    def forward(self, dec_inputs, enc_inputs, enc_outputs): # dec_inputs : [batch_size x t
        dec_outputs = self.tgt_emb(dec_inputs) + self.pos_emb(torch.LongTensor([[5,1,2,3,4
        dec_self_attn_pad_mask = get_attn_pad_mask(dec_inputs, dec_inputs)
        dec_self_attn_subsequent_mask = get_attn_subsequent_mask(dec_inputs)
        dec_self_attn_mask = torch.gt((dec_self_attn_pad_mask + dec_self_attn_subsequent_m

        dec_enc_attn_mask = get_attn_pad_mask(dec_inputs, enc_inputs)

        dec_self_attns, dec_enc_attns = [], []
        for layer in self.layers:
            dec_outputs, dec_self_attn, dec_enc_attn = layer(dec_outputs, enc_outputs, dec
            dec_self_attns.append(dec_self_attn)
            dec_enc_attns.append(dec_enc_attn)
        return dec_outputs, dec_self_attns, dec_enc_attns

class DecoderLayer(nn.Module):
    def __init__(self):
        super(DecoderLayer, self).__init__()
        self.dec_self_attn = MultiHeadAttention()
        self.dec_enc_attn = MultiHeadAttention()
        self.pos_ffn = PoswiseFeedForwardNet()

    def forward(self, dec_inputs, enc_outputs, dec_self_attn_mask, dec_enc_attn_mask):
        dec_outputs, dec_self_attn = self.dec_self_attn(dec_inputs, dec_inputs, dec_inputs
        dec_outputs, dec_enc_attn = self.dec_enc_attn(dec_outputs, enc_outputs, enc_output
        dec_outputs = self.pos_ffn(dec_outputs)
        return dec_outputs, dec_self_attn, dec_enc_attn

```

executed in 11ms, finished 17:20:00 2020-04-23

5.5 缩放点积多头注意力机制与前馈神经网络

In [8]:

```
class MultiHeadAttention(nn.Module):
    def __init__(self):
        super(MultiHeadAttention, self).__init__()
        self.W_Q = nn.Linear(d_model, d_k * n_heads)
        self.W_K = nn.Linear(d_model, d_k * n_heads)
        self.W_V = nn.Linear(d_model, d_v * n_heads)

    def forward(self, Q, K, V, attn_mask):
        # q: [batch_size x len_q x d_model], k: [batch_size x len_k x d_model], v: [batch_
        residual, batch_size = Q, Q.size(0)
        # (B, S, D) -proj-> (B, S, D) -split-> (B, S, H, W) -trans-> (B, H, S, W)
        q_s = self.W_Q(Q).view(batch_size, -1, n_heads, d_k).transpose(1,2)  # q_s: [batch
        k_s = self.W_K(K).view(batch_size, -1, n_heads, d_k).transpose(1,2)  # k_s: [batch
        v_s = self.W_V(V).view(batch_size, -1, n_heads, d_v).transpose(1,2)  # v_s: [batch

        attn_mask = attn_mask.unsqueeze(1).repeat(1, n_heads, 1, 1) # attn_mask : [batch_s

        # context: [batch_size x n_heads x len_q x d_v], attn: [batch_size x n_heads x len
        context, attn = ScaledDotProductAttention()(q_s, k_s, v_s, attn_mask)
        context = context.transpose(1, 2).contiguous().view(batch_size, -1, n_heads * d_v)
        output = nn.Linear(n_heads * d_v, d_model)(context)
        return nn.LayerNorm(d_model)(output + residual), attn # output: [batch_size x len_

class ScaledDotProductAttention(nn.Module):
    def __init__(self):
        super(ScaledDotProductAttention, self).__init__()

    def forward(self, Q, K, V, attn_mask):
        scores = torch.matmul(Q, K.transpose(-1, -2)) / np.sqrt(d_k) # scores : [batch_siz
        scores.masked_fill_(attn_mask, -1e9) # Fills elements of self tensor with value wh
        attn = nn.Softmax(dim=-1)(scores)
        context = torch.matmul(attn, V)
        return context, attn

class PoswiseFeedForwardNet(nn.Module):
    def __init__(self):
        super(PoswiseFeedForwardNet, self).__init__()
        self.conv1 = nn.Conv1d(in_channels=d_model, out_channels=d_ff, kernel_size=1)
        self.conv2 = nn.Conv1d(in_channels=d_ff, out_channels=d_model, kernel_size=1)

    def forward(self, inputs):
        residual = inputs # inputs : [batch_size, len_q, d_model]
        output = nn.ReLU()(self.conv1(inputs.transpose(1, 2)))
        output = self.conv2(output).transpose(1, 2)
        return nn.LayerNorm(d_model)(output + residual)

```

executed in 15ms, finished 17:20:02 2020-04-23

5.6 掩码与位置编码

In [9]:

```python
def get_sinusoid_encoding_table(n_position, d_model):
    def cal_angle(position, hid_idx):
        return position / np.power(10000, 2 * (hid_idx // 2) / d_model)
    def get_posi_angle_vec(position):
        return [cal_angle(position, hid_j) for hid_j in range(d_model)]

    sinusoid_table = np.array([get_posi_angle_vec(pos_i) for pos_i in range(n_position)])
    sinusoid_table[:, 0::2] = np.sin(sinusoid_table[:, 0::2])  # dim 2i
    sinusoid_table[:, 1::2] = np.cos(sinusoid_table[:, 1::2])  # dim 2i+1
    return torch.FloatTensor(sinusoid_table)

def get_attn_pad_mask(seq_q, seq_k):
    batch_size, len_q = seq_q.size()
    batch_size, len_k = seq_k.size()
    # eq(zero) is PAD token
    pad_attn_mask = seq_k.data.eq(0).unsqueeze(1)  # batch_size x 1 x len_k(=len_q), one i
    return pad_attn_mask.expand(batch_size, len_q, len_k)  # batch_size x len_q x len_k

def get_attn_subsequent_mask(seq):
    attn_shape = [seq.size(0), seq.size(1), seq.size(1)]
    subsequent_mask = np.triu(np.ones(attn_shape), k=1)
    subsequent_mask = torch.from_numpy(subsequent_mask).byte()
    return subsequent_mask

```

executed in 11ms, finished 17:20:03 2020-04-23

5.7 模型训练与验证

In [10]:

```python
model = Transformer()

criterion = nn.CrossEntropyLoss()
optimizer = optim.Adam(model.parameters(), lr=0.001)

for epoch in range(20):
    optimizer.zero_grad()
    enc_inputs, dec_inputs, target_batch = make_batch(sentences)
    outputs, enc_self_attns, dec_self_attns, dec_enc_attns = model(enc_inputs, dec_inputs)
    loss = criterion(outputs, target_batch.contiguous().view(-1))
    print('Epoch:', '%04d' % (epoch + 1), 'cost =', '{:.6f}'.format(loss))
    loss.backward()
    optimizer.step()

```

executed in 7.39s, finished 17:20:12 2020-04-23

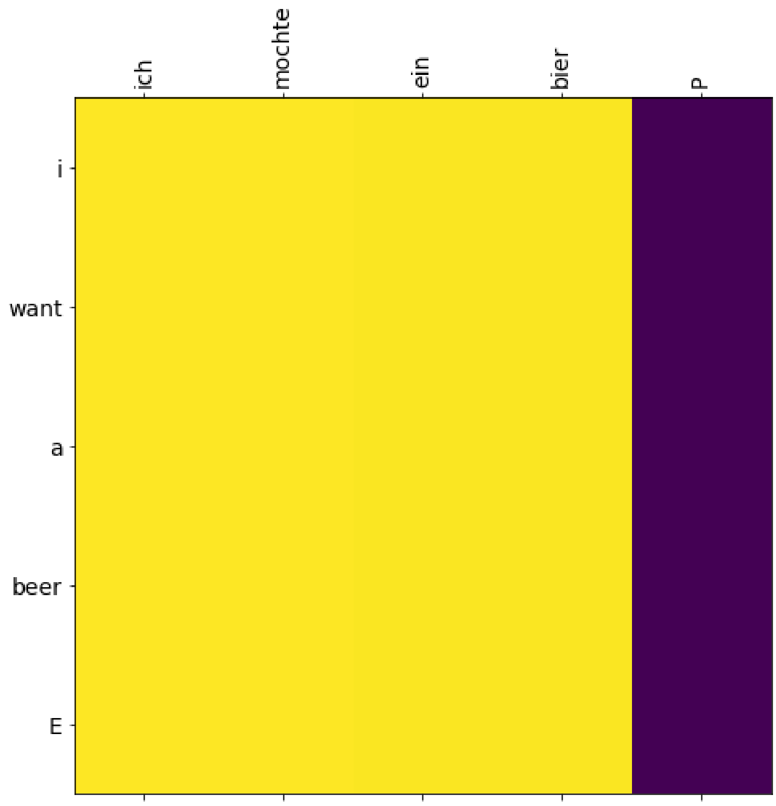
```
Epoch: 0001 cost = 1.946148
Epoch: 0002 cost = 0.061065
Epoch: 0003 cost = 0.061755
Epoch: 0004 cost = 0.040034
Epoch: 0005 cost = 0.030705
Epoch: 0006 cost = 0.001976
Epoch: 0007 cost = 0.001366
Epoch: 0008 cost = 0.001905
Epoch: 0009 cost = 0.003293
Epoch: 0010 cost = 0.004082
Epoch: 0011 cost = 0.000338
Epoch: 0012 cost = 0.002591
Epoch: 0013 cost = 0.005281
Epoch: 0014 cost = 0.000948
Epoch: 0015 cost = 0.000256
Epoch: 0016 cost = 0.000409
Epoch: 0017 cost = 0.000859
Epoch: 0018 cost = 0.024325
Epoch: 0019 cost = 0.007099
Epoch: 0020 cost = 0.020045
```

In [11]:

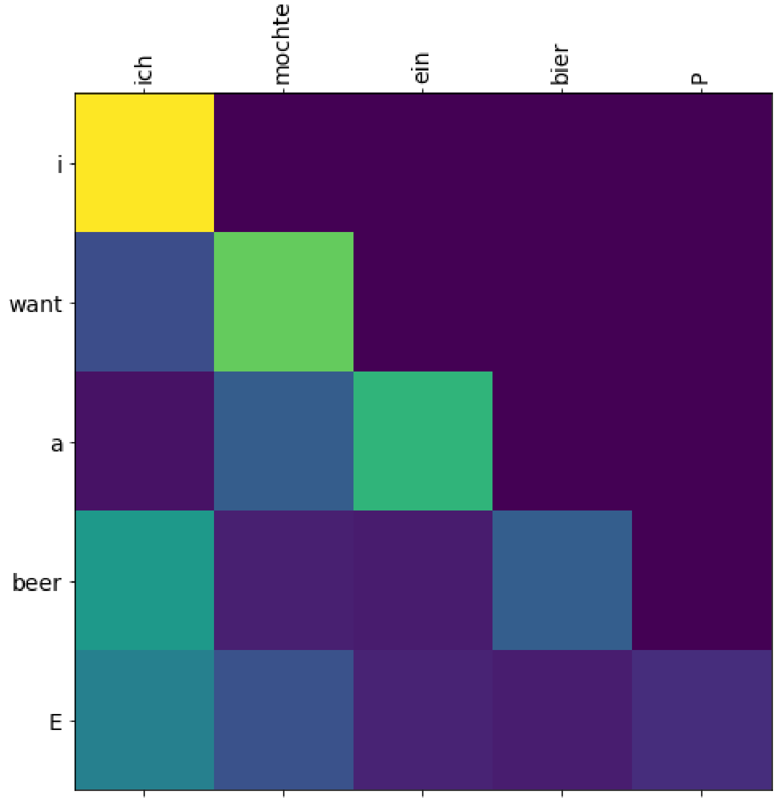
```python
def showgraph(attn):
    attn = attn[-1].squeeze(0)[0]
    attn = attn.squeeze(0).data.numpy()
    fig = plt.figure(figsize=(n_heads, n_heads)) # [n_heads, n_heads]
    ax = fig.add_subplot(1, 1, 1)
    ax.matshow(attn, cmap='viridis')
    ax.set_xticklabels(['']+sentences[0].split(), fontdict={'fontsize': 14}, rotation=90)
    ax.set_yticklabels(['']+sentences[2].split(), fontdict={'fontsize': 14})
    plt.show()

predict, _, _, _ = model(enc_inputs, dec_inputs)

predict = predict.data.max(1, keepdim=True)[1]
print(sentences[0], '->', [number_dict[n.item()] for n in predict.squeeze()])

print('first head of last state enc_self_attns')
showgraph(enc_self_attns)

print('first head of last state dec_self_attns')
showgraph(dec_self_attns)

print('first head of last state dec_enc_attns')
showgraph(dec_enc_attns)

```

executed in 635ms, finished 17:20:13 2020-04-23

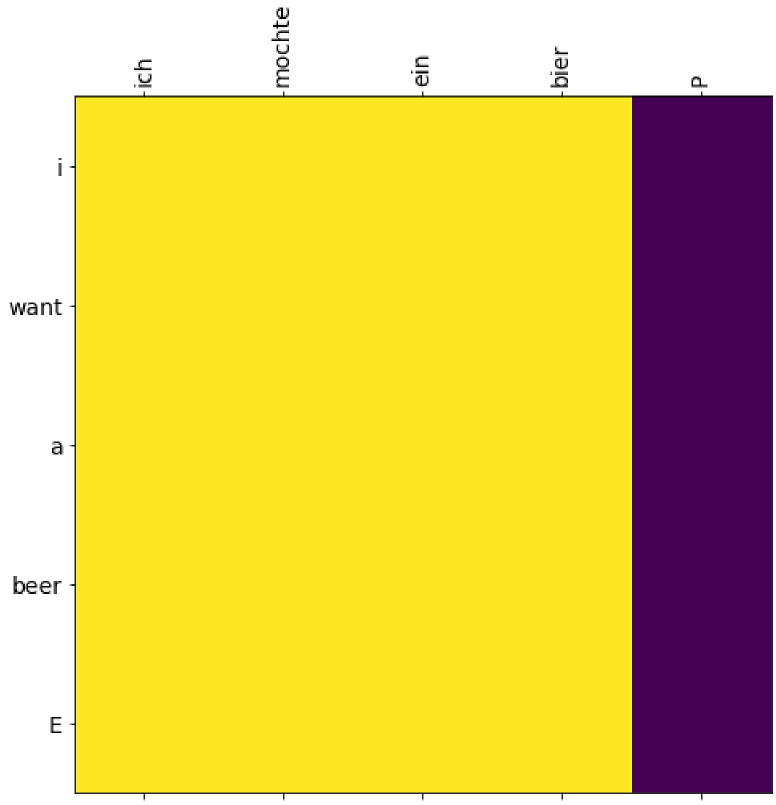
```
ich mochte ein bier P -> ['i', 'want', 'a', 'beer', 'E']
first head of last state enc_self_attns
```




```
first head of last state dec_self_attns
```



first head of last state dec_enc_attns



In [ ]:
```
1
```