The Annotated Transformer

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```
from IPython.display import Image
Image(filename='images/aiayn.png')
```

Attention Is All You Need

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Abstract

The dominant sequence transduction models are based on complex recurrent or convolutional neural networks that include an encoder and a decoder. The best performing models also connect the encoder and decoder through an attention mechanism. We propose a new simple network architecture, the Transformer, based solely on attention mechanisms, dispensing with recurrence and convolutions entirely. Experiments on two machine translation tasks show these models to be superior in quality while being more parallelizable and requiring significantly less time to train. Our model achieves 28.4 BLEU on the WMT 2014 English-to-German translation task, improving over the existing best results, including ensembles, by over 2 BLEU. On the WMT 2014 English-to-French translation task, our model establishes a new single-model state-of-the-art BLEU score of 41.8 after training for 3.5 days on eight GPUs, a small fraction of the training costs of the best models from the literature. We show that the Transformer generalizes well to other tasks by applying it successfully to English constituency parsing both with large and limited training data.

The Transformer from "Attention is All You Need" has been on a lot of people's minds over the last year. Besides producing major improvements in translation quality, it provides a new architecture for many other NLP tasks. The paper itself is very clearly written, but the conventional wisdom has been that it is quite difficult to implement correctly.

In this post I present an "annotated" version of the paper in the form of a line-by-line implementation. I have reordered and deleted some sections from the original paper and added comments throughout. This document itself is a working notebook, and should be a completely usable implementation. In total there are 400 lines of library code which can process 27,000 tokens per second on 4 GPUs.

To follow along you will first need to install PyTorch. The complete notebook is also available on github or on Google Colab with free GPUs.

Note this is merely a starting point for researchers and interested developers. The code here is based heavily on our OpenNMT packages. (If helpful feel free to cite.) For other full-sevice implementations of the model check-out Tensor2Tensor (tensorflow) and Sockeye (mxnet).

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Prelims

```
# !pip install http://download.pytorch.org/whl/cu80/torch-0.3.0.post4-cp36-cp36m-linux_x86_64.whl numpy matplotlib spacy torchtext seaborn
```

```
import numpy as np
import torch
import torch.nn as nn
import torch.nn.functional as F
import math, copy, time
from torch.autograd import Variable
import matplotlib.pyplot as plt
import seaborn
seaborn.set_context(context="talk")
%matplotlib inline
```

Table of Contents

Background

The goal of reducing sequential computation also forms the foundation of the Extended Neural GPU, ByteNet and ConvS2S, all of which use convolutional neural networks as basic building block, computing hidden representations in parallel for all input and output positions. In these models, the number of operations required to relate signals from two arbitrary input or output positions grows in the distance between positions, linearly for ConvS2S and logarithmically for ByteNet. This makes it more difficult to learn dependencies between distant positions. In the Transformer this is reduced to a constant number of operations, albeit at the cost of reduced effective resolution due to averaging attention-weighted positions, an effect we counteract with Multi-Head Attention.

Self-attention, sometimes called intra-attention is an attention mechanism relating different positions of a single sequence in order to compute a representation of the sequence. Self-attention has been used successfully in a variety of tasks including reading comprehension, abstractive summarization, textual entailment and learning task-independent sentence representations. End- to-end memory networks are based on a recurrent attention mechanism instead of sequencealigned recurrence and have been shown to perform well on simple- language question answering and language modeling tasks.

To the best of our knowledge, however, the Transformer is the first transduction model relying entirely on self-attention to compute representations of its input and output without using sequence aligned RNNs or convolution.

Model Architecture

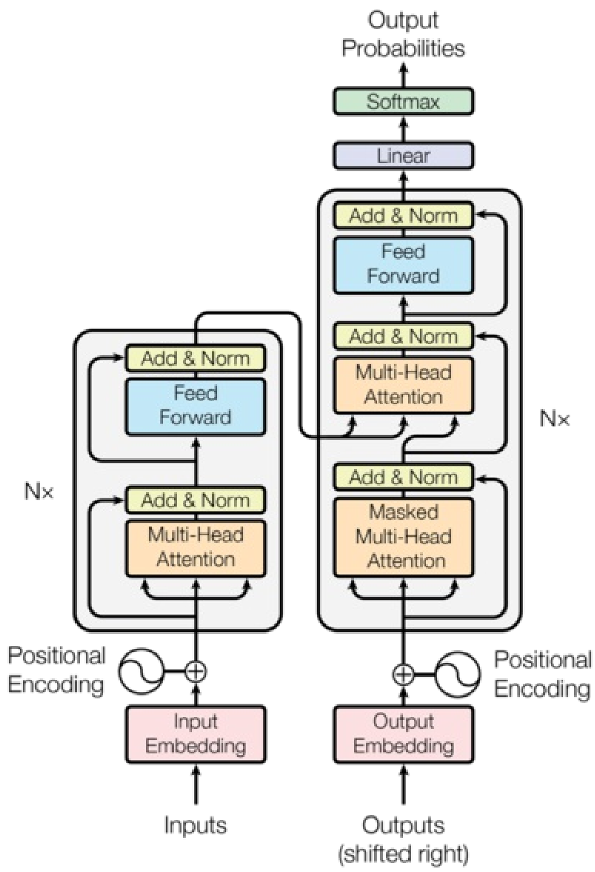
Most competitive neural sequence transduction models have an encoder-decoder structure (cite). Here, the encoder maps an input sequence of symbol representations $(x_1, \ldots, x_n)$ to a sequence of continuous representations $\mathbf{z} = (z_1, \ldots, z_n)$. Given $\mathbf{z}$, the decoder then generates an output sequence $(y_1, \ldots, y_m)$ of symbols one element at a time. At each step the model is auto-regressive (cite), consuming the previously generated symbols as additional input when generating the next.

```
class EncoderDecoder(nn.Module):
    """
    A standard Encoder-Decoder architecture. Base for this and many
    other models.
    """
    def __init__(self, encoder, decoder, src_embed, tgt_embed, generator):
        super(EncoderDecoder, self).__init__()
        self.encoder = encoder
        self.decoder = decoder
        self.src_embed = src_embed
        self.tgt_embed = tgt_embed
        self.generator = generator

    def forward(self, src, tgt, src_mask, tgt_mask):
        "Take in and process masked src and target sequences."
        return self.decode(self.encode(src, src_mask), src_mask,
                           tgt, tgt_mask)

    def encode(self, src, src_mask):
        return self.encoder(self.src_embed(src), src_mask)

    def decode(self, memory, src_mask, tgt, tgt_mask):
        return self.decoder(self.tgt_embed(tgt), memory, src_mask, tgt_mask)
```

```
class Generator(nn.Module):
    "Define standard linear + softmax generation step."
    def __init__(self, d_model, vocab):
        super(Generator, self).__init__()
        self.proj = nn.Linear(d_model, vocab)

    def forward(self, x):
        return F.log_softmax(self.proj(x), dim=-1)
```

The Transformer follows this overall architecture using stacked self-attention and point-wise, fully connected layers for both the encoder and decoder, shown in the left and right halves of Figure 1, respectively.

```
Image(filename='images/ModalNet-21.png')
```



Encoder and Decoder Stacks

Encoder

The encoder is composed of a stack of $N = 6$ identical layers.

```
def clones(module, N):
    "Produce N identical layers."
    return nn.ModuleList([copy.deepcopy(module) for _ in range(N)])
```

```
class Encoder(nn.Module):
    "Core encoder is a stack of N layers"
    def __init__(self, layer, N):
        super(Encoder, self).__init__()
        self.layers = clones(layer, N)
        self.norm = LayerNorm(layer.size)

    def forward(self, x, mask):
        "Pass the input (and mask) through each layer in turn."
        for layer in self.layers:
            x = layer(x, mask)
        return self.norm(x)
```

We employ a residual connection (cite) around each of the two sub-layers, followed by layer normalization (cite).

```
class LayerNorm(nn.Module):
    "Construct a layernorm module (See citation for details)."
    def __init__(self, features, eps=1e-6):
        super(LayerNorm, self).__init__()
        self.a_2 = nn.Parameter(torch.ones(features))
        self.b_2 = nn.Parameter(torch.zeros(features))
        self.eps = eps

    def forward(self, x):
        mean = x.mean(-1, keepdim=True)
        std = x.std(-1, keepdim=True)
        return self.a_2 * (x - mean) / (std + self.eps) + self.b_2
```

That is, the output of each sub-layer is $\mathrm{LayerNorm}(x + \mathrm{Sublayer}(x))$, where $\mathrm{Sublayer}(x)$ is the function implemented by the sub-layer itself. We apply dropout (cite) to the output of each sub-layer, before it is added to the sub-layer input and normalized.

To facilitate these residual connections, all sub-layers in the model, as well as the embedding layers, produce outputs of dimension $d_{\text{model}} = 512$.

```
class SublayerConnection(nn.Module):
    """
    A residual connection followed by a layer norm.
    Note for code simplicity the norm is first as opposed to last.
    """
    def __init__(self, size, dropout):
        super(SublayerConnection, self).__init__()
        self.norm = LayerNorm(size)
        self.dropout = nn.Dropout(dropout)

    def forward(self, x, sublayer):
        "Apply residual connection to any sublayer with the same size."
        return x + self.dropout(sublayer(self.norm(x)))
```

Each layer has two sub-layers. The first is a multi-head self-attention mechanism, and the second is a simple, position-wise fully connected feed-forward network.

```
class EncoderLayer(nn.Module):
    "Encoder is made up of self-attn and feed forward (defined below)"
    def __init__(self, size, self_attn, feed_forward, dropout):
        super(EncoderLayer, self).__init__()
        self.self_attn = self_attn
        self.feed_forward = feed_forward
        self.sublayer = clones(SublayerConnection(size, dropout), 2)
        self.size = size

    def forward(self, x, mask):
        "Follow Figure 1 (left) for connections."
        x = self.sublayer[0](x, lambda x: self.self_attn(x, x, x, mask))
        return self.sublayer[1](x, self.feed_forward)
```

Decoder

The decoder is also composed of a stack of $N = 6$ identical layers.

```
class Decoder(nn.Module):
    "Generic N layer decoder with masking."
    def __init__(self, layer, N):
        super(Decoder, self).__init__()
        self.layers = clones(layer, N)
        self.norm = LayerNorm(layer.size)

    def forward(self, x, memory, src_mask, tgt_mask):
        for layer in self.layers:
            x = layer(x, memory, src_mask, tgt_mask)
        return self.norm(x)
```

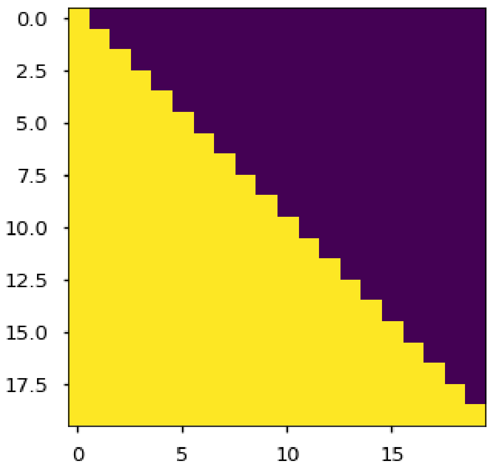
In addition to the two sub-layers in each encoder layer, the decoder inserts a third sub-layer, which performs multi-head attention over the output of the encoder stack. Similar to the encoder, we employ residual connections around each of the sub-layers, followed by layer normalization.

```
class DecoderLayer(nn.Module):
    "Decoder is made of self-attn, src-attn, and feed forward (defined below)"
    def __init__(self, size, self_attn, src_attn, feed_forward, dropout):
        super(DecoderLayer, self).__init__()
        self.size = size
        self.self_attn = self_attn
        self.src_attn = src_attn
        self.feed_forward = feed_forward
        self.sublayer = clones(SublayerConnection(size, dropout), 3)

    def forward(self, x, memory, src_mask, tgt_mask):
        "Follow Figure 1 (right) for connections."
        m = memory
        x = self.sublayer[0](x, lambda x: self.self_attn(x, x, x, tgt_mask))
        x = self.sublayer[1](x, lambda x: self.src_attn(x, m, m, src_mask))
        return self.sublayer[2](x, self.feed_forward)
```

We also modify the self-attention sub-layer in the decoder stack to prevent positions from attending to subsequent positions. This masking, combined with fact that the output embeddings are offset by one position, ensures that the predictions for position i can depend only on the known outputs at positions less than i.

```
def subsequent_mask(size):
    "Mask out subsequent positions."
    attn_shape = (1, size, size)
    subsequent_mask = np.triu(np.ones(attn_shape), k=1).astype('uint8')
    return torch.from_numpy(subsequent_mask) == 0
```

```
plt.figure(figsize=(5,5))
plt.imshow(subsequent_mask(20)[0])
None
```

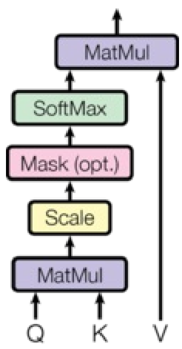


Attention

An attention function can be described as mapping a query and a set of key-value pairs to an output, where the query, keys, values, and output are all vectors. The output is computed as a weighted sum of the values, where the weight assigned to each value is computed by a compatibility function of the query with the corresponding key.

We call our particular attention “Scaled Dot-Product Attention”. The input consists of queries and keys of dimension d_k, and values of dimension d_v. We compute the dot products of the query with all keys, divide each by $\sqrt{d_k}$, and apply a softmax function to obtain the weights on the values.

```
Image(filename='images/ModalNet-19.png')
```



In practice, we compute the attention function on a set of queries simultaneously, packed together into a matrix Q. The keys and values are also packed together into matrices K and V. We compute the matrix of outputs as:

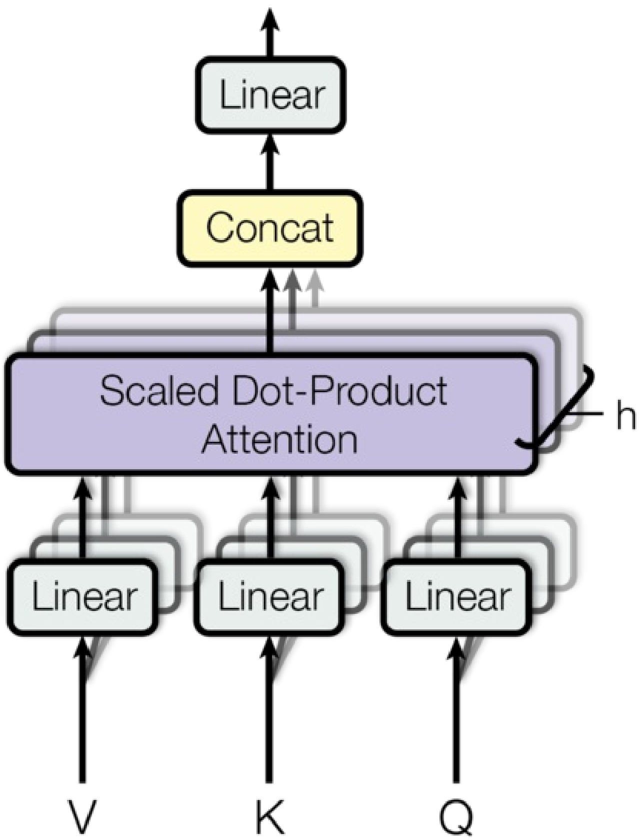
$$\mathrm{Attention}(Q, K, V) = \mathrm{softmax}(\frac{QK^T}{\sqrt{d_k}})V$$

```
def attention(query, key, value, mask=None, dropout=None):
    "Compute 'Scaled Dot Product Attention'"
    d_k = query.size(-1)
    scores = torch.matmul(query, key.transpose(-2, -1)) \
             / math.sqrt(d_k)
    if mask is not None:
        scores = scores.masked_fill(mask == 0, -1e9)
    p_attn = F.softmax(scores, dim = -1)
    if dropout is not None:
        p_attn = dropout(p_attn)
    return torch.matmul(p_attn, value), p_attn
```

The two most commonly used attention functions are additive attention (cite), and dot-product (multiplicative) attention. Dot-product attention is identical to our algorithm, except for the scaling factor of $\frac{1}{\sqrt{d_k}}$. Additive attention computes the compatibility function using a feed-forward network with a single hidden layer. While the two are similar in theoretical complexity, dot-product attention is much faster and more space-efficient in practice, since it can be implemented using highly optimized matrix multiplication code.

While for small values of d_k the two mechanisms perform similarly, additive attention outperforms dot product attention without scaling for larger values of d_k (cite). We suspect that for large values of d_k, the dot products grow large in magnitude, pushing the softmax function into regions where it has extremely small gradients (To illustrate why the dot products get large, assume that the components of q and k are independent random variables with mean 0 and variance 1. Then their dot product, $q \cdot k = \sum_{i=1}^{d_k} q_i k_i$, has mean 0 and variance d_k.). To counteract this effect, we scale the dot products by $\frac{1}{\sqrt{d_k}}$.

```
Image(filename='images/ModalNet-20.png')
```



Multi-head attention allows the model to jointly attend to information from different representation subspaces at different positions. With a single attention head, averaging inhibits this. $\mathrm{MultiHead}(Q, K, V) = \mathrm{Concat}(\mathrm{head}_1, \ldots, \mathrm{head}_h)W^O$ where $\mathrm{head}_i = \mathrm{Attention}(QW_i^Q, KW_i^K, VW_i^V)$

Where the projections are parameter matrices $W_i^Q \in \mathbb{R}^{d_{\text{model}} \times d_k}$, $W_i^K \in \mathbb{R}^{d_{\text{model}} \times d_k}$, $W_i^V \in \mathbb{R}^{d_{\text{model}} \times d_v}$ and $W^O \in \mathbb{R}^{hd_v \times d_{\text{model}}}$. In this work we employ $h = 8$ parallel attention layers, or heads. For each of these we use $d_k = d_v = d_{\text{model}}/h = 64$. Due to the reduced dimension of each head, the total computational cost is similar to that of single-head attention with full dimensionality.

```python
class MultiHeadedAttention(nn.Module):
    def __init__(self, h, d_model, dropout=0.1):
        "Take in model size and number of heads."
        super(MultiHeadedAttention, self).__init__()
        assert d_model % h == 0
        # We assume d_v always equals d_k
        self.d_k = d_model // h
        self.h = h
        self.linears = clones(nn.Linear(d_model, d_model), 4)
        self.attn = None
        self.dropout = nn.Dropout(p=dropout)

    def forward(self, query, key, value, mask=None):
        "Implements Figure 2"
        if mask is not None:
            # Same mask applied to all h heads.
            mask = mask.unsqueeze(1)
        nbatches = query.size(0)

        # 1) Do all the linear projections in batch from d_model => h x d_k
        query, key, value = \
            [l(x).view(nbatches, -1, self.h, self.d_k).transpose(1, 2)
             for l, x in zip(self.linears, (query, key, value))]

        # 2) Apply attention on all the projected vectors in batch.
        x, self.attn = attention(query, key, value, mask=mask,
                                 dropout=self.dropout)

        # 3) "Concat" using a view and apply a final linear.
        x = x.transpose(1, 2).contiguous() \
             .view(nbatches, -1, self.h * self.d_k)
        return self.linears[-1](x)
```

Applications of Attention in our Model

The Transformer uses multi-head attention in three different ways: 1) In “encoder-decoder attention” layers, the queries come from the previous decoder layer, and the memory keys and values come from the output of the encoder. This allows every position in the decoder to attend over all positions in the input sequence. This mimics the typical encoder-decoder attention mechanisms in sequence-to-sequence models such as (cite).

2) The encoder contains self-attention layers. In a self-attention layer all of the keys, values and queries come from the same place, in this case, the output of the previous layer in the encoder. Each position in the encoder can attend to all positions in the previous layer of the encoder.

3) Similarly, self-attention layers in the decoder allow each position in the decoder to attend to all positions in the decoder up to and including that position. We need to prevent leftward information flow in the decoder to preserve the auto-regressive property. We implement this inside of scaled dot- product attention by masking out (setting to $-\infty$) all values in the input of the softmax which correspond to illegal connections.

Position-wise Feed-Forward Networks

In addition to attention sub-layers, each of the layers in our encoder and decoder contains a fully connected feed-forward network, which is applied to each position separately and identically. This consists of two linear transformations with a ReLU activation in between.

$$\mathrm{FFN}(x) = \max(0, xW_1 + b_1)W_2 + b_2$$

While the linear transformations are the same across different positions, they use different parameters from layer to layer. Another way of describing this is as two convolutions with kernel size 1. The dimensionality of input and output is $d_{\text{model}} = 512$, and the inner-layer has dimensionality $d_{ff} = 2048$.

```python
class PositionwiseFeedForward(nn.Module):
    "Implements FFN equation."
    def __init__(self, d_model, d_ff, dropout=0.1):
        super(PositionwiseFeedForward, self).__init__()
        self.w_1 = nn.Linear(d_model, d_ff)
        self.w_2 = nn.Linear(d_ff, d_model)
        self.dropout = nn.Dropout(dropout)

    def forward(self, x):
        return self.w_2(self.dropout(F.relu(self.w_1(x))))
```

Embeddings and Softmax

Similarly to other sequence transduction models, we use learned embeddings to convert the input tokens and output tokens to vectors of dimension d_{model}. We also use the usual learned linear transformation and softmax function to convert the decoder output to predicted next-token probabilities. In our model, we share the same weight matrix between the two embedding layers and the pre-softmax linear transformation, similar to (cite). In the embedding layers, we multiply those weights by $\sqrt{d_{\text{model}}}$.

```
class Embeddings(nn.Module):
    def __init__(self, d_model, vocab):
        super(Embeddings, self).__init__()
        self.lut = nn.Embedding(vocab, d_model)
        self.d_model = d_model

    def forward(self, x):
        return self.lut(x) * math.sqrt(self.d_model)
```

Positional Encoding

Since our model contains no recurrence and no convolution, in order for the model to make use of the order of the sequence, we must inject some information about the relative or absolute position of the tokens in the sequence. To this end, we add "positional encodings" to the input embeddings at the bottoms of the encoder and decoder stacks. The positional encodings have the same dimension d_{model} as the embeddings, so that the two can be summed. There are many choices of positional encodings, learned and fixed (cite).

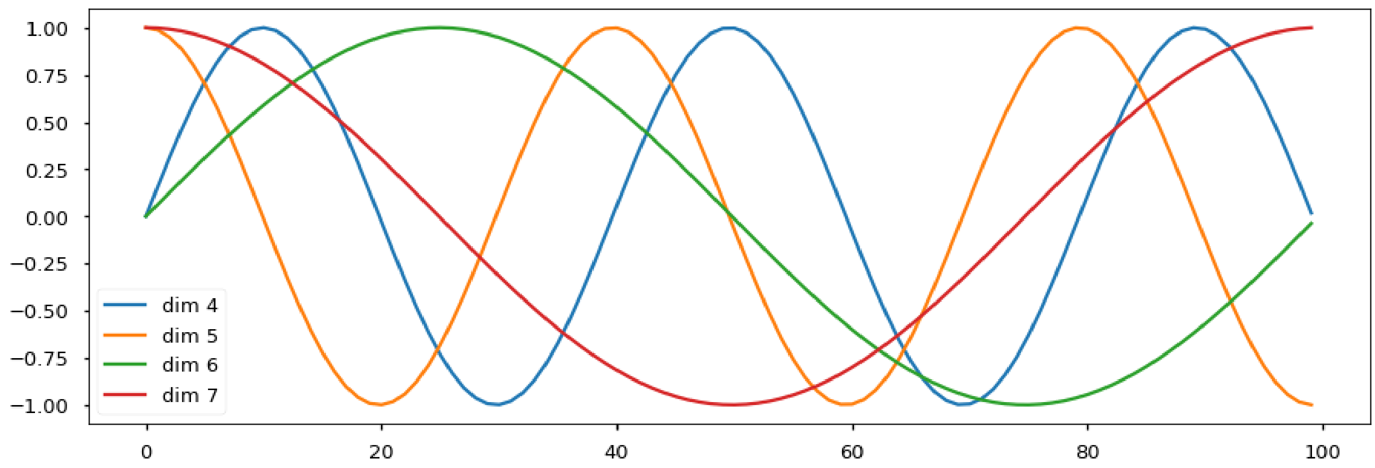
In this work, we use sine and cosine functions of different frequencies: $PE_{(pos,2i)} = sin(pos/10000^{2i/d_{\text{model}}})$

$PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{\text{model}}})$ where pos is the position and i is the dimension. That is, each dimension of the positional encoding corresponds to a sinusoid. The wavelengths form a geometric progression from 2π to $10000 \cdot 2\pi$. We chose this function because we hypothesized it would allow the model to easily learn to attend by relative positions, since for any fixed offset k, PE_{pos+k} can be represented as a linear function of PE_{pos}.

In addition, we apply dropout to the sums of the embeddings and the positional encodings in both the encoder and decoder stacks. For the base model, we use a rate of $P_{drop} = 0.1$.

```
class PositionalEncoding(nn.Module):
    "Implement the PE function."
    def __init__(self, d_model, dropout, max_len=5000):
        super(PositionalEncoding, self).__init__()
        self.dropout = nn.Dropout(p=dropout)

        # Compute the positional encodings once in log space.
        pe = torch.zeros(max_len, d_model)
        position = torch.arange(0, max_len).unsqueeze(1)
        div_term = torch.exp(torch.arange(0, d_model, 2) *
                             -(math.log(10000.0) / d_model))
        pe[:, 0::2] = torch.sin(position * div_term)
        pe[:, 1::2] = torch.cos(position * div_term)
        pe = pe.unsqueeze(0)
        self.register_buffer('pe', pe)

    def forward(self, x):
        x = x + Variable(self.pe[:, :x.size(1)],
                         requires_grad=False)
        return self.dropout(x)
```

```
plt.figure(figsize=(15, 5))
pe = PositionalEncoding(20, 0)
y = pe.forward(Variable(torch.zeros(1, 100, 20)))
plt.plot(np.arange(100), y[0, :, 4:8].data.numpy())
plt.legend(["dim %d"%p for p in [4,5,6,7]])
None
```



We also experimented with using learned positional embeddings (cite) instead, and found that the two versions produced nearly identical results. We chose the sinusoidal version because it may allow the model to extrapolate to sequence lengths longer than the ones encountered during training.

Full Model

```python
def make_model(src_vocab, tgt_vocab, N=6,
               d_model=512, d_ff=2048, h=8, dropout=0.1):
    "Helper: Construct a model from hyperparameters."
    c = copy.deepcopy
    attn = MultiHeadedAttention(h, d_model)
    ff = PositionwiseFeedForward(d_model, d_ff, dropout)
    position = PositionalEncoding(d_model, dropout)
    model = EncoderDecoder(
        Encoder(EncoderLayer(d_model, c(attn), c(ff), dropout), N),
        Decoder(DecoderLayer(d_model, c(attn), c(attn),
                             c(ff), dropout), N),
        nn.Sequential(Embeddings(d_model, src_vocab), c(position)),
        nn.Sequential(Embeddings(d_model, tgt_vocab), c(position)),
        Generator(d_model, tgt_vocab))

    # This was important from their code.
    # Initialize parameters with Glorot / fan_avg.
    for p in model.parameters():
        if p.dim() > 1:
            nn.init.xavier_uniform(p)
    return model
```

```python
# Small example model.
tmp_model = make_model(10, 10, 2)
None
```

Training

This section describes the training regime for our models.

Batches and Masking

```
class Batch:
    "Object for holding a batch of data with mask during training."
    def __init__(self, src, trg=None, pad=0):
        self.src = src
        self.src_mask = (src != pad).unsqueeze(-2)
        if trg is not None:
            self.trg = trg[:, :-1]
            self.trg_y = trg[:, 1:]
            self.trg_mask = \
                self.make_std_mask(self.trg, pad)
            self.ntokens = (self.trg_y != pad).data.sum()

    @staticmethod
    def make_std_mask(tgt, pad):
        "Create a mask to hide padding and future words."
        tgt_mask = (tgt != pad).unsqueeze(-2)
        tgt_mask = tgt_mask & Variable(
            subsequent_mask(tgt.size(-1)).type_as(tgt_mask.data))
        return tgt_mask
```

Training Loop

```
def run_epoch(data_iter, model, loss_compute):
    "Standard Training and Logging Function"
    start = time.time()
    total_tokens = 0
    total_loss = 0
    tokens = 0
    for i, batch in enumerate(data_iter):
        out = model.forward(batch.src, batch.trg,
                            batch.src_mask, batch.trg_mask)
        loss = loss_compute(out, batch.trg_y, batch.ntokens)
        total_loss += loss
        total_tokens += batch.ntokens
        tokens += batch.ntokens
        if i % 50 == 1:
            elapsed = time.time() - start
            print("Epoch Step: %d Loss: %f Tokens per Sec: %f" %
                    (i, loss / batch.ntokens, tokens / elapsed))
            start = time.time()
            tokens = 0
    return total_loss / total_tokens
```

Training Data and Batching

We trained on the standard WMT 2014 English-German dataset consisting of about 4.5 million sentence pairs. Sentences were encoded using byte-pair encoding, which has a shared source-target vocabulary of about 37000 tokens. For English- French, we used the significantly larger WMT 2014 English-French dataset consisting of 36M sentences and split tokens into a 32000 word-piece vocabulary.

Sentence pairs were batched together by approximate sequence length. Each training batch contained a set of sentence pairs containing approximately 25000 source tokens and 25000 target tokens.

```
global max_src_in_batch, max_tgt_in_batch
def batch_size_fn(new, count, sofar):
    "Keep augmenting batch and calculate total number of tokens + padding."
    global max_src_in_batch, max_tgt_in_batch
    if count == 1:
        max_src_in_batch = 0
        max_tgt_in_batch = 0
    max_src_in_batch = max(max_src_in_batch,  len(new.src))
    max_tgt_in_batch = max(max_tgt_in_batch,  len(new.trg) + 2)
    src_elements = count * max_src_in_batch
    tgt_elements = count * max_tgt_in_batch
    return max(src_elements, tgt_elements)
```

Hardware and Schedule

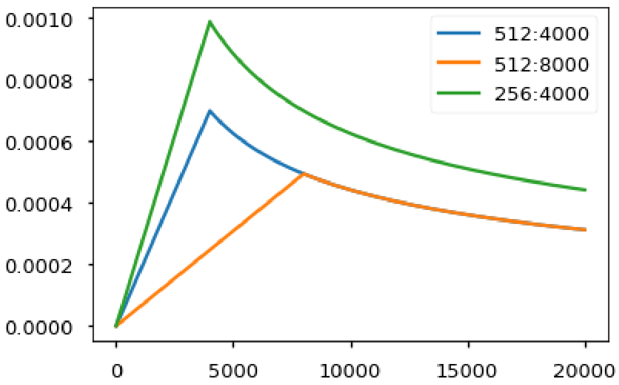
We trained our models on one machine with 8 NVIDIA P100 GPUs. For our base models using the hyperparameters described throughout the paper, each training step took about 0.4 seconds. We trained the base models for a total of 100,000 steps or 12 hours. For our big models, step time was 1.0 seconds. The big models were trained for 300,000 steps (3.5 days).

Optimizer

We used the Adam optimizer (cite) with $\beta_1 = 0.9$, $\beta_2 = 0.98$ and $\epsilon = 10^{-9}$. We varied the learning rate over the course of training, according to the formula: $lrate = d_{\text{model}}^{-0.5} \cdot \min(step\_num^{-0.5}, step\_num \cdot warmup\_steps^{-1.5})$ This corresponds to increasing the learning rate linearly for the first $warmup_steps$ training steps, and decreasing it thereafter proportionally to the inverse square root of the step number. We used $warmup_steps = 4000$.

```
class NoamOpt:
    "Optim wrapper that implements rate."
    def __init__(self, model_size, factor, warmup, optimizer):
        self.optimizer = optimizer
        self._step = 0
        self.warmup = warmup
        self.factor = factor
        self.model_size = model_size
        self._rate = 0

    def step(self):
        "Update parameters and rate"
        self._step += 1
        rate = self.rate()
        for p in self.optimizer.param_groups:
            p['lr'] = rate
        self._rate = rate
        self.optimizer.step()

    def rate(self, step = None):
        "Implement `lrate` above"
        if step is None:
            step = self._step
        return self.factor * \
            (self.model_size ** (-0.5) *
            min(step ** (-0.5), step * self.warmup ** (-1.5)))

def get_std_opt(model):
    return NoamOpt(model.src_embed[0].d_model, 2, 4000,
            torch.optim.Adam(model.parameters(), lr=0, betas=(0.9, 0.98), eps=1e-9))
```

```
# Three settings of the lrate hyperparameters.
opts = [NoamOpt(512, 1, 4000, None),
        NoamOpt(512, 1, 8000, None),
        NoamOpt(256, 1, 4000, None)]
plt.plot(np.arange(1, 20000), [[opt.rate(i) for opt in opts] for i in range(1, 20000)])
plt.legend(["512:4000", "512:8000", "256:4000"])
None
```



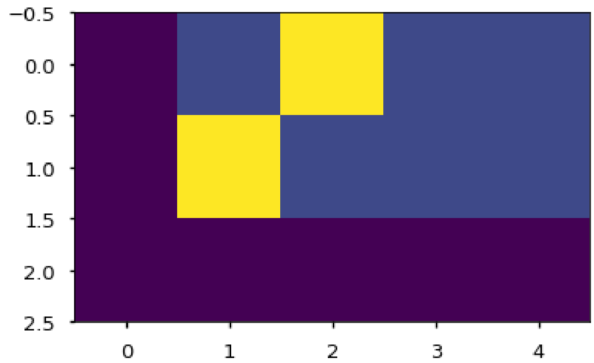
Regularization

Label Smoothing

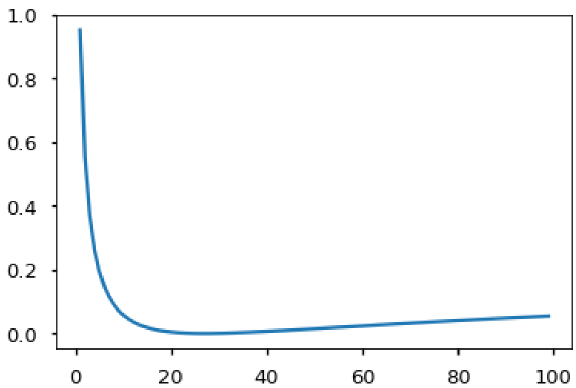
During training, we employed label smoothing of value $\epsilon_{ls} = 0.1$ (cite). This hurts perplexity, as the model learns to be more unsure, but improves accuracy and BLEU score.

```
class LabelSmoothing(nn.Module):
    "Implement label smoothing."
    def __init__(self, size, padding_idx, smoothing=0.0):
        super(LabelSmoothing, self).__init__()
        self.criterion = nn.KLDivLoss(size_average=False)
        self.padding_idx = padding_idx
        self.confidence = 1.0 - smoothing
        self.smoothing = smoothing
        self.size = size
        self.true_dist = None

    def forward(self, x, target):
        assert x.size(1) == self.size
        true_dist = x.data.clone()
        true_dist.fill_(self.smoothing / (self.size - 2))
        true_dist.scatter_(1, target.data.unsqueeze(1), self.confidence)
        true_dist[:, self.padding_idx] = 0
        mask = torch.nonzero(target.data == self.padding_idx)
        if mask.dim() > 0:
            true_dist.index_fill_(0, mask.squeeze(), 0.0)
        self.true_dist = true_dist
        return self.criterion(x, Variable(true_dist, requires_grad=False))
```

```python
# Example of label smoothing.
crit = LabelSmoothing(5, 0, 0.4)
predict = torch.FloatTensor([[0, 0.2, 0.7, 0.1, 0],
                             [0, 0.2, 0.7, 0.1, 0],
                             [0, 0.2, 0.7, 0.1, 0]])
v = crit(Variable(predict.log()),
         Variable(torch.LongTensor([2, 1, 0])))

# Show the target distributions expected by the system.
plt.imshow(crit.true_dist)
None
```




```python
crit = LabelSmoothing(5, 0, 0.1)
def loss(x):
    d = x + 3 * 1
    predict = torch.FloatTensor([[0, x / d, 1 / d, 1 / d, 1 / d],
                                 ])
    #print(predict)
    return crit(Variable(predict.log()),
                Variable(torch.LongTensor([1]))).data[0]
plt.plot(np.arange(1, 100), [loss(x) for x in range(1, 100)])
None
```



A First Example

Synthetic Data

```
def data_gen(V, batch, nbatches):
    "Generate random data for a src-tgt copy task."
    for i in range(nbatches):
        data = torch.from_numpy(np.random.randint(1, V, size=(batch, 10)))
        data[:, 0] = 1
        src = Variable(data, requires_grad=False)
        tgt = Variable(data, requires_grad=False)
        yield Batch(src, tgt, 0)
```

Loss Computation

```
class SimpleLossCompute:
    "A simple loss compute and train function."
    def __init__(self, generator, criterion, opt=None):
        self.generator = generator
        self.criterion = criterion
        self.opt = opt

    def __call__(self, x, y, norm):
        x = self.generator(x)
        loss = self.criterion(x.contiguous().view(-1, x.size(-1)),
                              y.contiguous().view(-1)) / norm
        loss.backward()
        if self.opt is not None:
            self.opt.step()
            self.opt.optimizer.zero_grad()
        return loss.data[0] * norm
```

Greedy Decoding

```
# Train the simple copy task.
V = 11
criterion = LabelSmoothing(size=V, padding_idx=0, smoothing=0.0)
model = make_model(V, V, N=2)
model_opt = NoamOpt(model.src_embed[0].d_model, 1, 400,
        torch.optim.Adam(model.parameters(), lr=0, betas=(0.9, 0.98), eps=1e-9))

for epoch in range(10):
    model.train()
    run_epoch(data_gen(V, 30, 20), model,
              SimpleLossCompute(model.generator, criterion, model_opt))
    model.eval()
    print(run_epoch(data_gen(V, 30, 5), model,
                    SimpleLossCompute(model.generator, criterion, None)))
```

```
Epoch Step: 1 Loss: 3.023465 Tokens per Sec: 403.074173
Epoch Step: 1 Loss: 1.920030 Tokens per Sec: 641.689380
1.9274832487106324
Epoch Step: 1 Loss: 1.940011 Tokens per Sec: 432.003378
Epoch Step: 1 Loss: 1.699767 Tokens per Sec: 641.979665
1.657595729827881
Epoch Step: 1 Loss: 1.860276 Tokens per Sec: 433.320240
Epoch Step: 1 Loss: 1.546011 Tokens per Sec: 640.537198
1.4888023376464843
Epoch Step: 1 Loss: 1.682198 Tokens per Sec: 432.092305
Epoch Step: 1 Loss: 1.313169 Tokens per Sec: 639.441857
1.3485562801361084
Epoch Step: 1 Loss: 1.278768 Tokens per Sec: 433.568756
Epoch Step: 1 Loss: 1.062384 Tokens per Sec: 642.542067
0.9853351473808288
Epoch Step: 1 Loss: 1.269471 Tokens per Sec: 433.388727
Epoch Step: 1 Loss: 0.590709 Tokens per Sec: 642.862135
0.5686767101287842
Epoch Step: 1 Loss: 0.997076 Tokens per Sec: 433.009746
Epoch Step: 1 Loss: 0.343118 Tokens per Sec: 642.288427
0.34273059368133546
Epoch Step: 1 Loss: 0.459483 Tokens per Sec: 434.594030
Epoch Step: 1 Loss: 0.290385 Tokens per Sec: 642.519464
0.2612409472465515
Epoch Step: 1 Loss: 1.031042 Tokens per Sec: 434.557008
Epoch Step: 1 Loss: 0.437069 Tokens per Sec: 643.630322
0.4323212027549744
Epoch Step: 1 Loss: 0.617165 Tokens per Sec: 436.652626
Epoch Step: 1 Loss: 0.258793 Tokens per Sec: 644.372296
0.27331129014492034
```

```
def greedy_decode(model, src, src_mask, max_len, start_symbol):
    memory = model.encode(src, src_mask)
    ys = torch.ones(1, 1).fill_(start_symbol).type_as(src.data)
    for i in range(max_len-1):
        out = model.decode(memory, src_mask,
                           Variable(ys),
                           Variable(subsequent_mask(ys.size(1))
                                    .type_as(src.data)))
        prob = model.generator(out[:, -1])
        _, next_word = torch.max(prob, dim = 1)
        next_word = next_word.data[0]
        ys = torch.cat([ys,
                        torch.ones(1, 1).type_as(src.data).fill_(next_word)], dim=1)
    return ys

model.eval()
src = Variable(torch.LongTensor([[1,2,3,4,5,6,7,8,9,10]]) )
src_mask = Variable(torch.ones(1, 1, 10) )
print(greedy_decode(model, src, src_mask, max_len=10, start_symbol=1))
```

```
    1     2     3     4     5     6     7     8     9    10
[torch.LongTensor of size 1x10]
```

A Real World Example

```
#!pip install torchtext spacy
#!python -m spacy download en
#!python -m spacy download de
```

Data Loading

```
# For data loading.
from torchtext import data, datasets

if True:
    import spacy
    spacy_de = spacy.load('de')
    spacy_en = spacy.load('en')

    def tokenize_de(text):
        return [tok.text for tok in spacy_de.tokenizer(text)]

    def tokenize_en(text):
        return [tok.text for tok in spacy_en.tokenizer(text)]

    BOS_WORD = '<s>'
    EOS_WORD = '</s>'
    BLANK_WORD = "<blank>"
    SRC = data.Field(tokenize=tokenize_de, pad_token=BLANK_WORD)
    TGT = data.Field(tokenize=tokenize_en, init_token = BOS_WORD,
                     eos_token = EOS_WORD, pad_token=BLANK_WORD)

    MAX_LEN = 100
    train, val, test = datasets.IWSLT.splits(
        exts=('.de', '.en'), fields=(SRC, TGT),
        filter_pred=lambda x: len(vars(x)['src']) <= MAX_LEN and
            len(vars(x)['trg']) <= MAX_LEN)
    MIN_FREQ = 2
    SRC.build_vocab(train.src, min_freq=MIN_FREQ)
    TGT.build_vocab(train.trg, min_freq=MIN_FREQ)
```

Iterators

```
class MyIterator(data.Iterator):
    def create_batches(self):
        if self.train:
            def pool(d, random_shuffler):
                for p in data.batch(d, self.batch_size * 100):
                    p_batch = data.batch(
                        sorted(p, key=self.sort_key),
                        self.batch_size, self.batch_size_fn)
                    for b in random_shuffler(list(p_batch)):
                        yield b
            self.batches = pool(self.data(), self.random_shuffler)

        else:
            self.batches = []
            for b in data.batch(self.data(), self.batch_size,
                                          self.batch_size_fn):
                self.batches.append(sorted(b, key=self.sort_key))

def rebatch(pad_idx, batch):
    "Fix order in torchtext to match ours"
    src, trg = batch.src.transpose(0, 1), batch.trg.transpose(0, 1)
    return Batch(src, trg, pad_idx)
```

Multi-GPU Training

- replicate - split modules onto different gpus.
- scatter - split batches onto different gpus
- parallel_apply - apply module to batches on different gpus
- gather - pull scattered data back onto one gpu.
- nn.DataParallel - a special module wrapper that calls these all before evaluating.

```python
# Skip if not interested in multigpu.
class MultiGPULossCompute:
    "A multi-gpu loss compute and train function."
    def __init__(self, generator, criterion, devices, opt=None, chunk_size=5):
        # Send out to different gpus.
        self.generator = generator
        self.criterion = nn.parallel.replicate(criterion,
                                               devices=devices)
        self.opt = opt
        self.devices = devices
        self.chunk_size = chunk_size

    def __call__(self, out, targets, normalize):
        total = 0.0
        generator = nn.parallel.replicate(self.generator,
                                          devices=self.devices)
        out_scatter = nn.parallel.scatter(out,
                                          target_gpus=self.devices)
        out_grad = [[] for _ in out_scatter]
        targets = nn.parallel.scatter(targets,
                                      target_gpus=self.devices)

        # Divide generating into chunks.
        chunk_size = self.chunk_size
        for i in range(0, out_scatter[0].size(1), chunk_size):
            # Predict distributions
            out_column = [[Variable(o[:, i:i+chunk_size].data,
                                    requires_grad=self.opt is not None)]
                          for o in out_scatter]
            gen = nn.parallel.parallel_apply(generator, out_column)

            # Compute loss.
            y = [(g.contiguous().view(-1, g.size(-1)),
                  t[:, i:i+chunk_size].contiguous().view(-1))
                 for g, t in zip(gen, targets)]
            loss = nn.parallel.parallel_apply(self.criterion, y)

            # Sum and normalize loss
            l = nn.parallel.gather(loss,
                                   target_device=self.devices[0])
            l = l.sum()[0] / normalize
            total += l.data[0]

            # Backprop loss to output of transformer
            if self.opt is not None:
                l.backward()
                for j, l in enumerate(loss):
                    out_grad[j].append(out_column[j][0].grad.data.clone())

        # Backprop all loss through transformer.
        if self.opt is not None:
            out_grad = [Variable(torch.cat(og, dim=1)) for og in out_grad]
            o1 = out
            o2 = nn.parallel.gather(out_grad,
                                    target_device=self.devices[0])
            o1.backward(gradient=o2)
            self.opt.step()
            self.opt.optimizer.zero_grad()
        return total * normalize
```

```
# GPUs to use
devices = [0, 1, 2, 3]
if True:
    pad_idx = TGT.vocab.stoi["<blank>"]
    model = make_model(len(SRC.vocab), len(TGT.vocab), N=6)
    model.cuda()
    criterion = LabelSmoothing(size=len(TGT.vocab), padding_idx=pad_idx, smoothing=0.1)
    criterion.cuda()
    BATCH_SIZE = 12000
    train_iter = MyIterator(train, batch_size=BATCH_SIZE, device=0,
                            repeat=False, sort_key=lambda x: (len(x.src), len(x.trg)),
                            batch_size_fn=batch_size_fn, train=True)
    valid_iter = MyIterator(val, batch_size=BATCH_SIZE, device=0,
                            repeat=False, sort_key=lambda x: (len(x.src), len(x.trg)),
                            batch_size_fn=batch_size_fn, train=False)
    model_par = nn.DataParallel(model, device_ids=devices)
None
```

Training the System

```
#!wget https://s3.amazonaws.com/opennmt-models/iwslt.pt
```

```
if False:
    model_opt = NoamOpt(model.src_embed[0].d_model, 1, 2000,
            torch.optim.Adam(model.parameters(), lr=0, betas=(0.9, 0.98), eps=1e-9))
    for epoch in range(10):
        model_par.train()
        run_epoch((rebatch(pad_idx, b) for b in train_iter),
                  model_par,
                  MultiGPULossCompute(model.generator, criterion,
                                      devices=devices, opt=model_opt))
        model_par.eval()
        loss = run_epoch((rebatch(pad_idx, b) for b in valid_iter),
                         model_par,
                         MultiGPULossCompute(model.generator, criterion,
                         devices=devices, opt=None))
        print(loss)
else:
    model = torch.load("iwslt.pt")
```

```
for i, batch in enumerate(valid_iter):
    src = batch.src.transpose(0, 1)[:1]
    src_mask = (src != SRC.vocab.stoi["<blank>"]).unsqueeze(-2)
    out = greedy_decode(model, src, src_mask,
                        max_len=60, start_symbol=TGT.vocab.stoi["<s>"])
    print("Translation:", end="\t")
    for i in range(1, out.size(1)):
        sym = TGT.vocab.itos[out[0, i]]
        if sym == "</s>": break
        print(sym, end =" ")
    print()
    print("Target:", end="\t")
    for i in range(1, batch.trg.size(0)):
        sym = TGT.vocab.itos[batch.trg.data[i, 0]]
        if sym == "</s>": break
        print(sym, end =" ")
    print()
    break
```

```
Translation: <unk> <unk> . In my language , that means , thank you very much .
Gold: <unk> <unk> . It means in my language , thank you very much .
```

Additional Components: BPE, Search, Averaging

_Die _Protokoll datei _kann _ heimlich _per _E - Mail _oder _FTP _an _einen _bestimmte n _Empfänger _gesendet _werden .

```
if False:
    model.src_embed[0].lut.weight = model.tgt_embeddings[0].lut.weight
    model.generator.lut.weight = model.tgt_embed[0].lut.weight
```

```
def average(model, models):
    "Average models into model"
    for ps in zip(*[m.params() for m in [model] + models]):
        p[0].copy_(torch.sum(*ps[1:]) / len(ps[1:]))
```

Results

On the WMT 2014 English-to-German translation task, the big transformer model (Transformer (big) in Table 2) outperforms the best previously reported models (including ensembles) by more than 2.0 BLEU, establishing a new state-of-the-art BLEU score of 28.4. The configuration of this model is listed in the bottom line of Table 3. Training took 3.5 days on 8 P100 GPUs. Even our base model surpasses all previously published models and ensembles, at a fraction of the training cost of any of the competitive models.

On the WMT 2014 English-to-French translation task, our big model achieves a BLEU score of 41.0, outperforming all of the previously published single models, at less than 1/4 the training cost of the previous state-of-the-art model. The Transformer (big) model trained for English-to-French used dropout rate Pdrop = 0.1, instead of 0.3.

```
Image(filename="images/results.png")
```

Table 2: The Transformer achieves better BLEU scores than previous state-of-the-art models on the English-to-German and English-to-French newstest2014 tests at a fraction of the training cost.

Model	BLEU		Training Cost (FLOPs)	
	EN-DE	EN-FR	EN-DE	EN-FR
ByteNet [18]	23.75			
Deep-Att + PosUnk [39]		39.2		$1.0 \cdot 10^{20}$
GNMT + RL [38]	24.6	39.92	$2.3 \cdot 10^{19}$	$1.4 \cdot 10^{20}$
ConvS2S [9]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$
MoE [32]	26.03	40.56	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$
Deep-Att + PosUnk Ensemble [39]		40.4		$8.0 \cdot 10^{20}$
GNMT + RL Ensemble [38]	26.30	41.16	$1.8 \cdot 10^{20}$	$1.1 \cdot 10^{21}$
ConvS2S Ensemble [9]	26.36	**41.29**	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$
Transformer (base model)	27.3	38.1	$\mathbf{3.3 \cdot 10^{18}}$	
Transformer (big)	**28.4**	**41.8**	$2.3 \cdot 10^{19}$	

```
!wget https://s3.amazonaws.com/opennmt-models/en-de-model.pt
```

```
model, SRC, TGT = torch.load("en-de-model.pt")
```

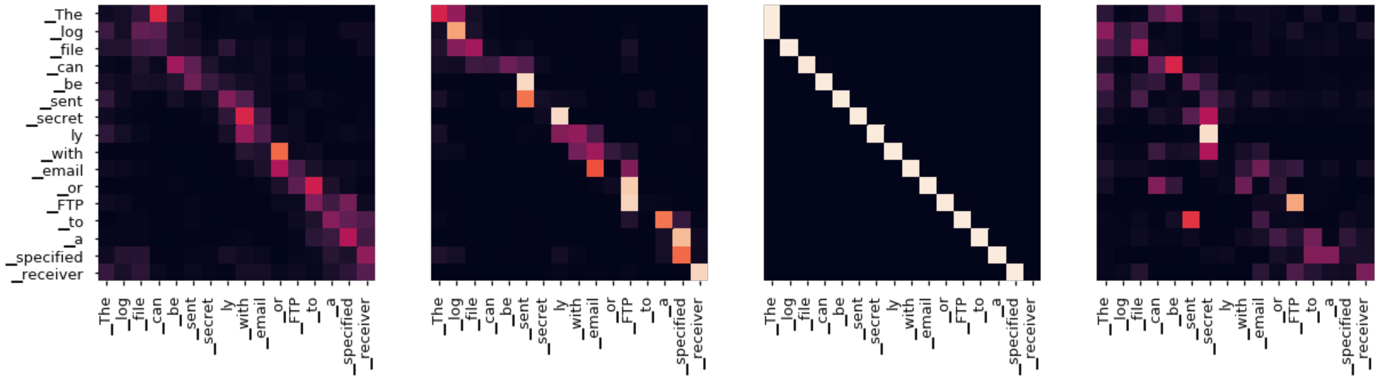
```
model.eval()
sent = "▁The ▁log ▁file ▁can ▁be ▁sent ▁secret ly ▁with ▁email ▁or ▁FTP ▁to ▁a ▁specified ▁receiver".split()
src = torch.LongTensor([[SRC.stoi[w] for w in sent]])
src = Variable(src)
src_mask = (src != SRC.stoi["<blank>"]).unsqueeze(-2)
out = greedy_decode(model, src, src_mask,
                    max_len=60, start_symbol=TGT.stoi["<s>"])
print("Translation:", end="\t")
trans = "<s> "
for i in range(1, out.size(1)):
    sym = TGT.itos[out[0, i]]
    if sym == "</s>": break
    trans += sym + " "
print(trans)
```

```
Translation: <s> ▁Die ▁Protokoll datei ▁kann ▁ heimlich ▁per ▁E - Mail ▁oder ▁FTP ▁an ▁einen ▁bestimmte n ▁Empfänger ▁gesendet ▁werden .
```

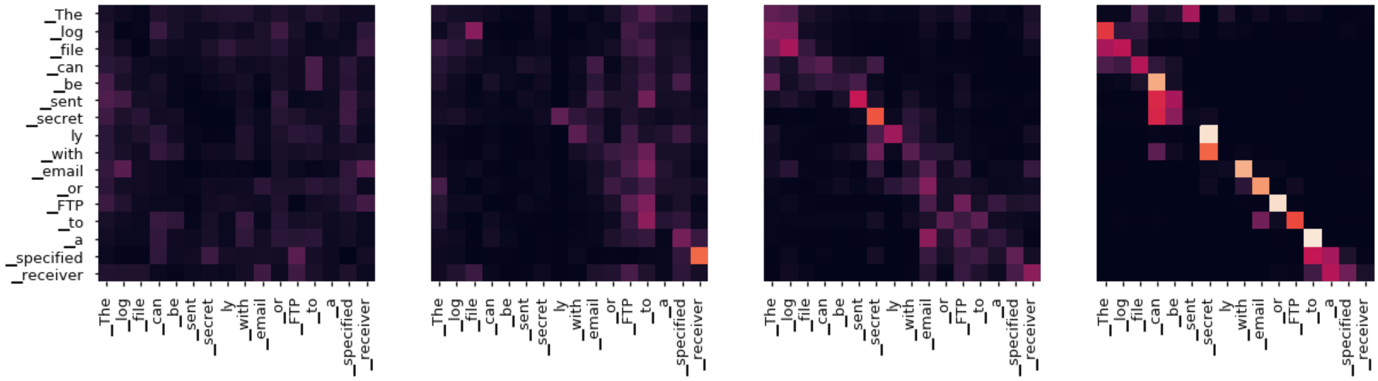
Attention Visualization

```
tgt_sent = trans.split()
def draw(data, x, y, ax):
    seaborn.heatmap(data,
                    xticklabels=x, square=True, yticklabels=y, vmin=0.0, vmax=1.0,
                    cbar=False, ax=ax)

for layer in range(1, 6, 2):
    fig, axs = plt.subplots(1,4, figsize=(20, 10))
    print("Encoder Layer", layer+1)
    for h in range(4):
        draw(model.encoder.layers[layer].self_attn.attn[0, h].data,
            sent, sent if h ==0 else [], ax=axs[h])
    plt.show()

for layer in range(1, 6, 2):
    fig, axs = plt.subplots(1,4, figsize=(20, 10))
    print("Decoder Self Layer", layer+1)
    for h in range(4):
        draw(model.decoder.layers[layer].self_attn.attn[0, h].data[:len(tgt_sent), :len(tgt_sent)],
            tgt_sent, tgt_sent if h ==0 else [], ax=axs[h])
    plt.show()
    print("Decoder Src Layer", layer+1)
    fig, axs = plt.subplots(1,4, figsize=(20, 10))
    for h in range(4):
        draw(model.decoder.layers[layer].self_attn.attn[0, h].data[:len(tgt_sent), :len(sent)],
            sent, tgt_sent if h ==0 else [], ax=axs[h])
    plt.show()
```

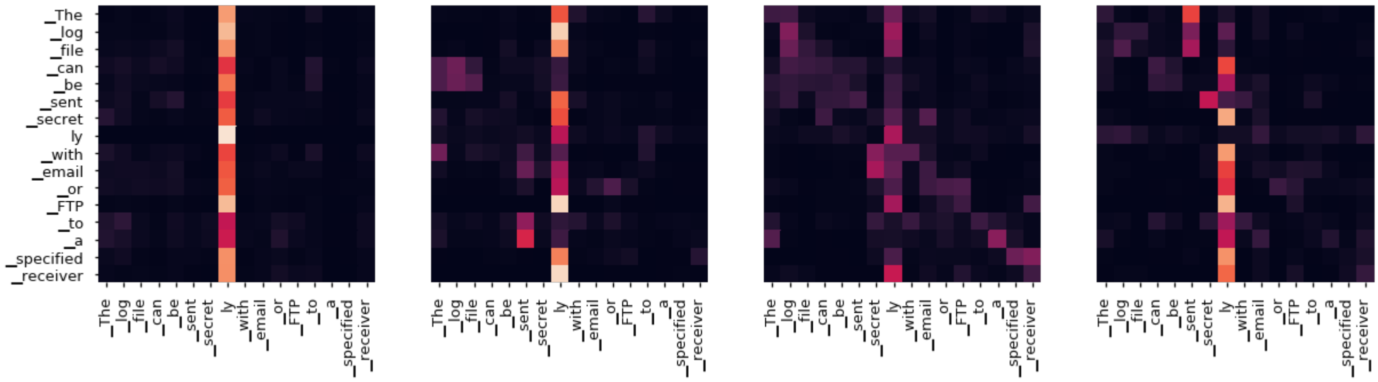
```
Encoder Layer 2
```



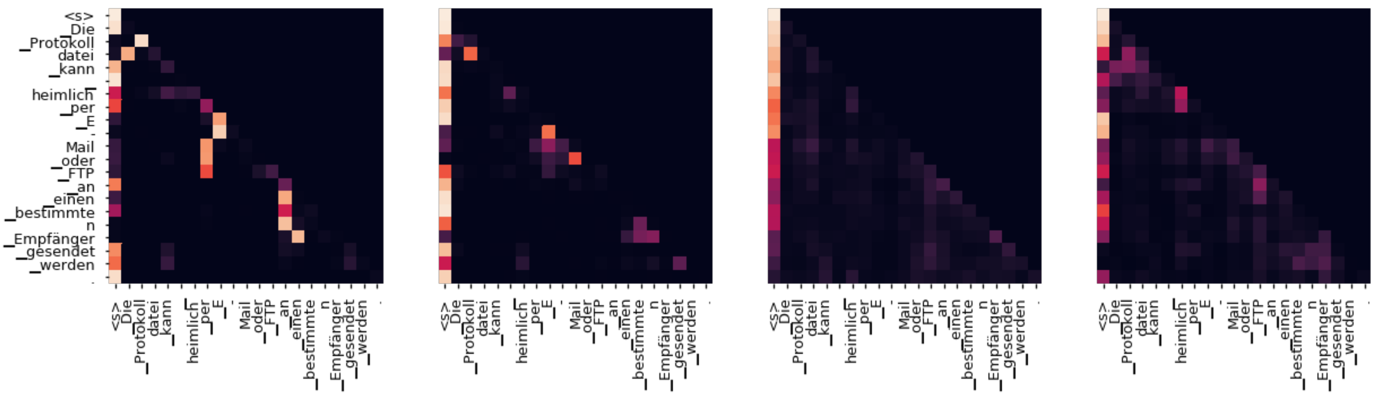
Encoder Layer 4



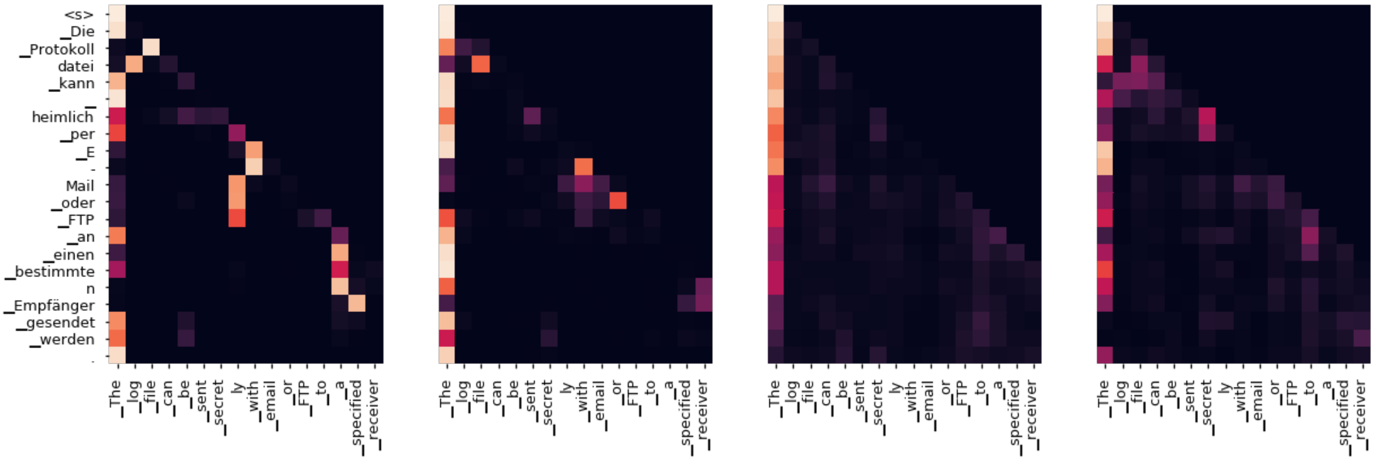
Encoder Layer 6



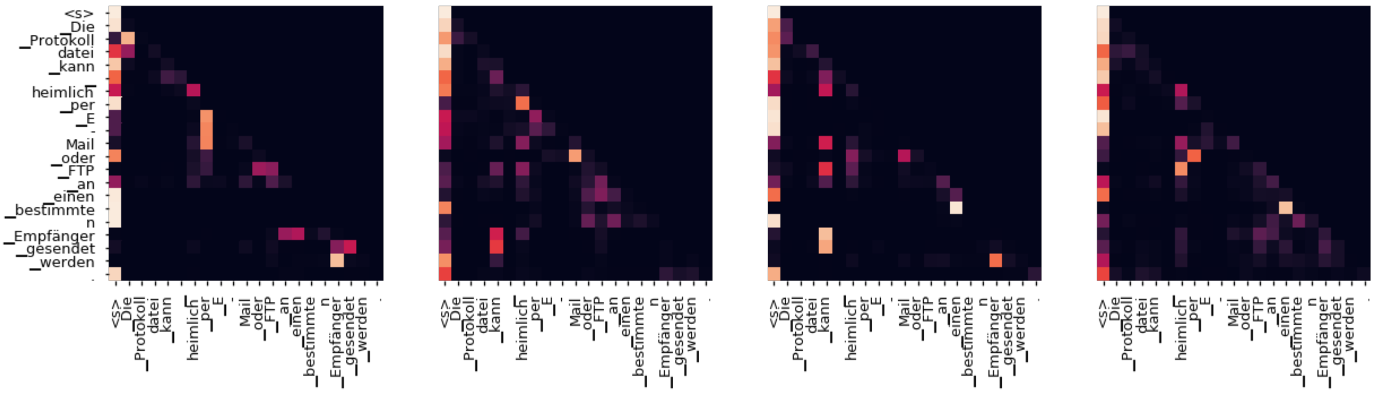
Decoder Self Layer 2



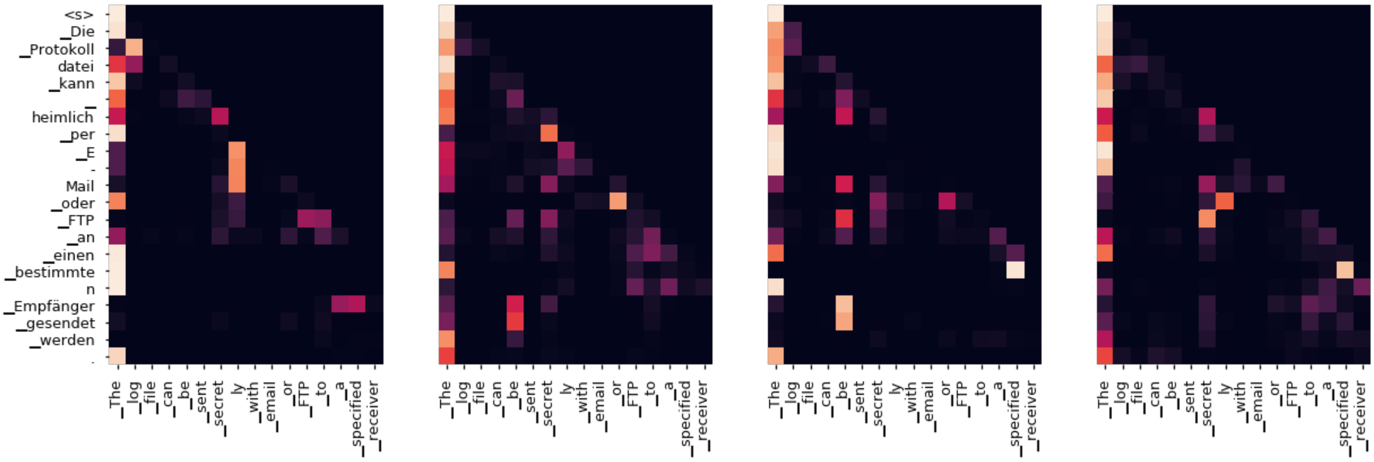
Decoder Src Layer 2



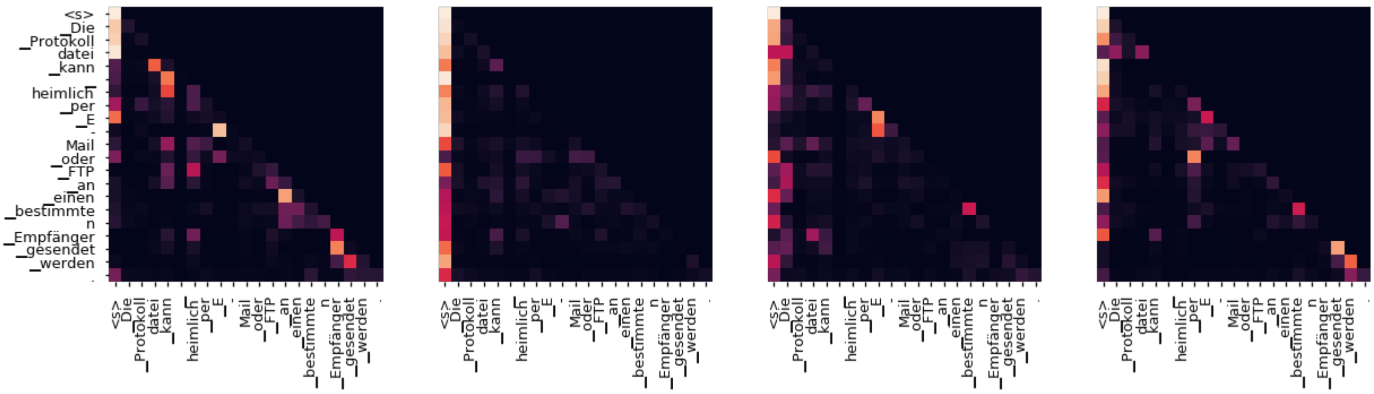
Decoder Self Layer 4



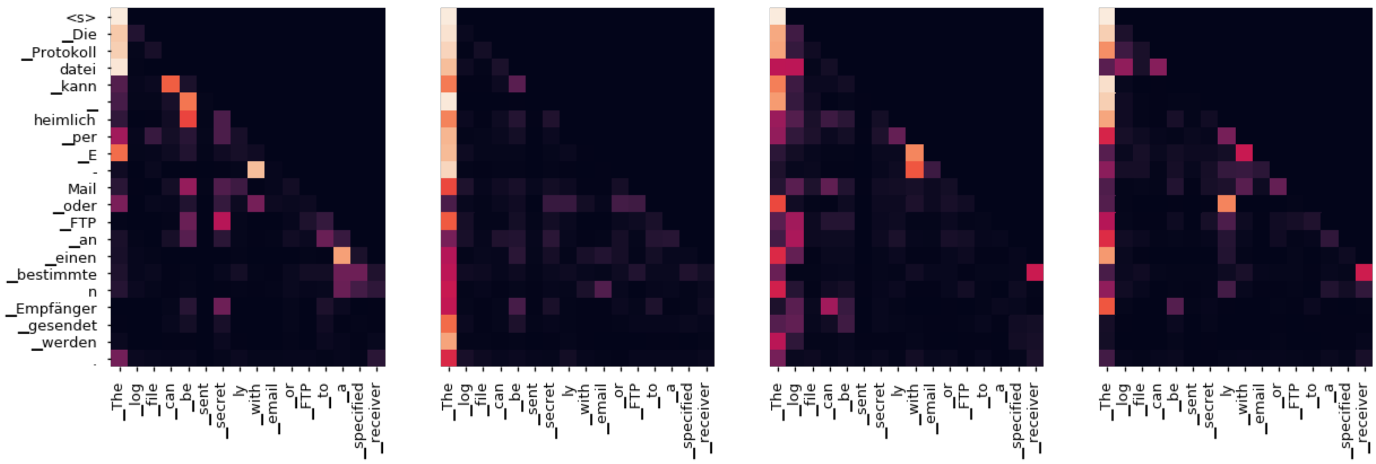
Decoder Src Layer 4



Decoder Self Layer 6



Decoder Src Layer 6



Conclusion

```
@inproceedings{opennmt,
  author    = {Guillaume Klein and
               Yoon Kim and
               Yuntian Deng and
               Jean Senellart and
               Alexander M. Rush},
  title     = {OpenNMT: Open-Source Toolkit for Neural Machine Translation},
  booktitle = {Proc. ACL},
  year      = {2017},
  url       = {https://doi.org/10.18653/v1/P17-4012},
  doi       = {10.18653/v1/P17-4012}
}
```

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