安徽大学
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《自然语言处理》论文阅读报告

Transformer & BERT

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1 Transformer [1]

1.1 算法设计背景

在自然语言处理领域，传统循环神经网络（RNN）及其变体（如 LSTM、GRU）因顺序处理特性，难以捕捉长距离依赖且训练效率低。卷积神经网络（CNN）虽擅长局部特征提取，但建模长距离依赖能力不足。为突破这些限制，”Attention is All You Need” 提出 Transformer 架构，基于自注意力机制实现高效并行计算与长距离依赖建模，为 NLP 任务带来新范式。

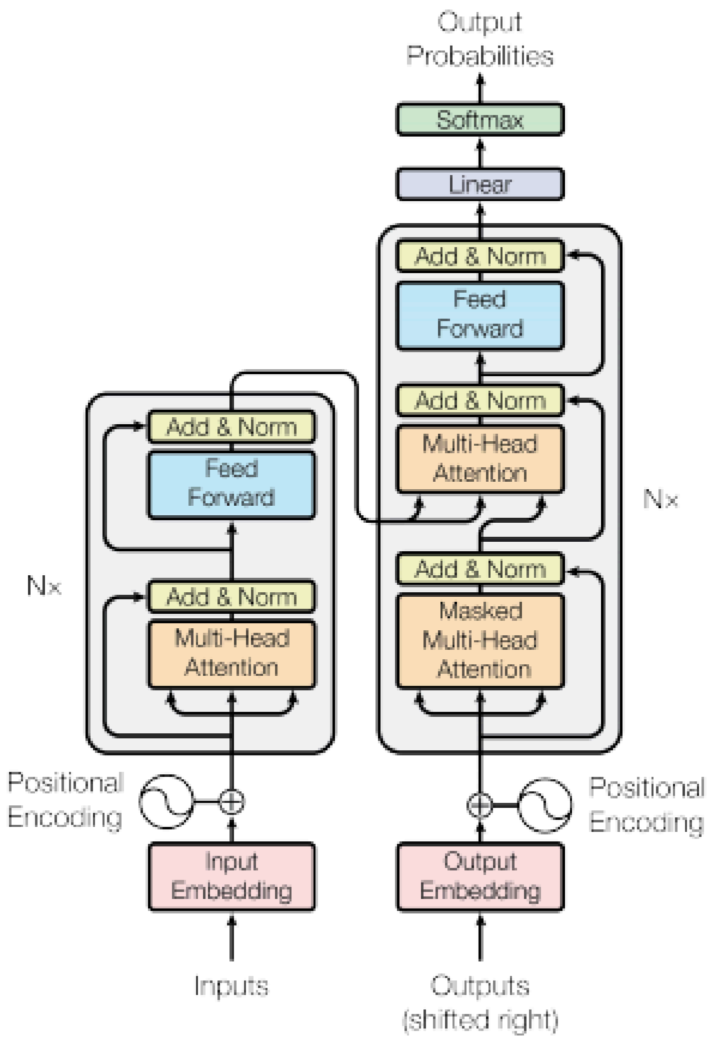

Figure 1: The Transformer - model architecture.

图 1: Transformer 模型主图

1.2 算法核心架构

1.2.1 Encoder 与 Decoder 结构

Encoder 由 $N = 6$ 个相同层堆叠而成，每层包含多头自注意力（Multi-head Self-Attention）和前馈神经网络（Feed-Forward Network），辅以残差连接（Residual Connection）和层归一化（LayerNorm）。其核心功能是将输入序列编码为高维特征向量，捕捉全局语义依赖。

Decoder 同样包含 $N = 6$ 个层，除与 Encoder 相同的两个子层外，新增针对 Encoder 输出的多头注意力层，用于跨模态信息交互。此外，Decoder 采用遮蔽自注意力（Masked Self-Attention）避免未来信息泄露，确保自回归生成的正确性，适用于序列生成任务如机器翻译。

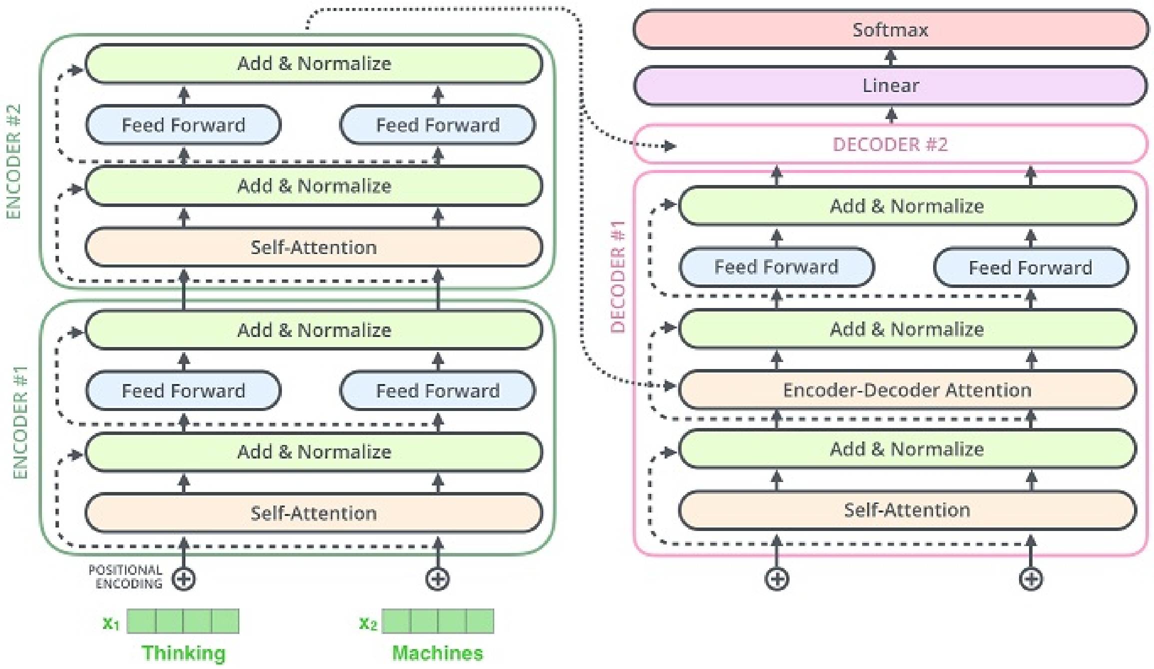

图 2: 编码器-解码器机制 [2]

1.2.2 自注意力机制（Self-Attention）

传统 RNN 的顺序计算导致长距离依赖建模困难，而 Self-Attention 通过 Query-Key-Value 机制，允许每个位置直接关联序列中所有位置，计算复杂度为 $O(n^2 d)$。相比 RNN，其优势在于：1）并行化计算大幅提升训练速度；2）直接建模任意位置依赖，解决长距离梯度消失问题；3）计算效率在序列长度 n 小于模型维度 d 时更优。

1.2.3 多头注意力（Multi-head Attention）

通过 h 组独立的线性变换将输入投影到不同子空间（$d_k = d_v = d_{\text{model}}/h$），并行计算注意力后拼接输出。该设计使模型能从多个子空间捕捉多样化语义关系，避免单头注意力的信息局限，例如不同头可分别关注语法结构与语义依赖，提升模型表示能力。

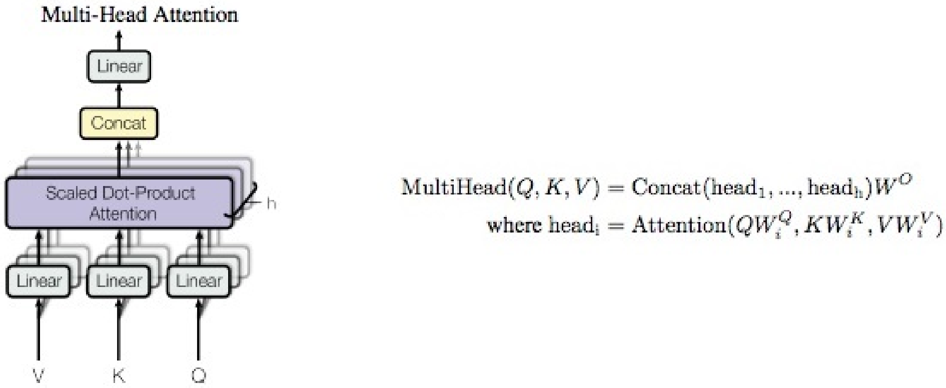

图 3: 多头注意力机制

1.2.4 位置编码（Position Encoding）

由于 Transformer 不包含递归结构，需显式编码位置信息。论文采用正弦余弦函数生成位置编码：

$$PE_{(pos,2i)} = \sin(pos/10000^{2i/d_{\text{model}}}), \quad PE_{(pos,2i+1)} = \cos(pos/10000^{2i/d_{\text{model}}})$$

其中 pos 为位置，i 为维度索引。位置编码与词嵌入相加后输入模型，确保模型能区分序列顺序，弥补非递归架构的位置感知缺陷。最终采用正弦以推广更长序列。

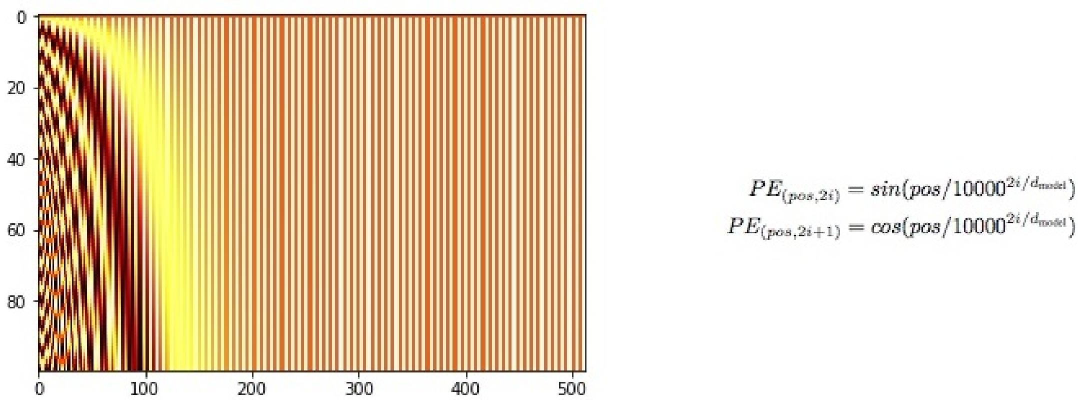

图 4: 位置编码

1.3 关键技术细节

1.3.1 Scaled Dot-Product Attention

公式为：

$$\text{Attention}(Q, K, V) = \text{Softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

其中 Q（Query）、K（Key）、V（Value）由输入经线性变换得到。除以 $\sqrt{d_k}$ 是为避免高维下点积过大导致 Softmax 梯度消失，通过缩放使梯度保持合理范围，提升训练稳定性。

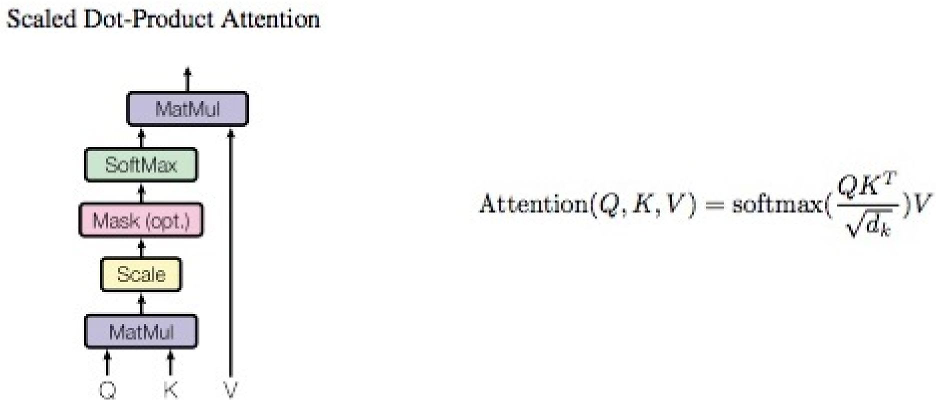

图 5: 缩放点积注意力

1.3.2 前馈神经网络（Feed-Forward Network，FNN）

在 Transformer 的编码器与解码器结构中，每层均包含一个全连接前馈神经网络（FNN），其核心作用是为模型引入非线性变换能力以学习更复杂的特征表示。该网络对序列中的每个位置独立执行相同操作，具体由两个线性层和中间的 ReLU 激活函数构成，数学表达式为：

$$\text{FFN}(x) = (\text{ReLU}(xW_1 + b_1))W_2 + b_2$$

其中，$x \in R^{d_{\text{model}}}$ 为输入向量，$W_1 \in R^{d_{\text{model}} \times d_{ff}}$ 和 $W_2 \in R^{d_{ff} \times d_{\text{model}}}$ 是可学习的权重矩阵，$b_1 \in R^{d_{ff}}$ 和 $b_2 \in R^{d_{\text{model}}}$ 为偏置项。这一操作等价于两次内核大小为 1 的一维卷积：首先将维度从 $d_{\text{model}} = 512$ 提升至 $d_{ff} = 2048$，经 ReLU 激活后再降回 d_{model}，在保持序列长度不变的前提下完成非线性变换。FNN 的设计兼具位置独立性（对每个位置应用相同变换以确保平移不变性）、参数分层性（不同层使用独立参数而同一层内位置共享参数，平衡表达能力与计算效率）及非线性增强特性（通过 ReLU 捕捉特征间复杂交互，弥补自注意力机制的线性本质缺陷），与多头自注意力层协同工作：前者负责建模全局依赖，后者实现局部特征的非线性转换，共同构成 Transformer 高效处理序列数据的核心单元。注：这里使用的是 ReLU 激活函数，但是后续的 Transformer 的工作包括后面的 BERT 都采用了 GeLU。

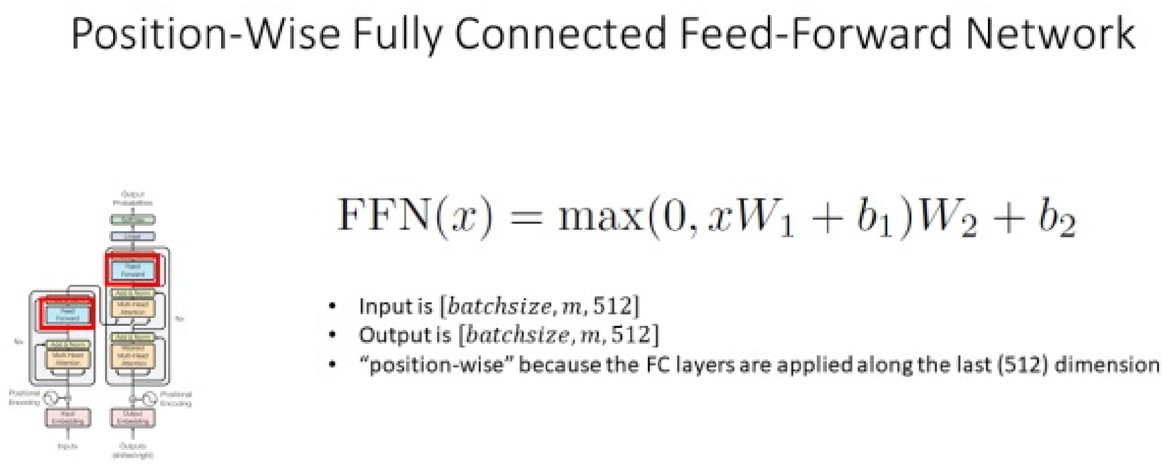

图 6: 前馈神经网络

1.3.3 残差连接与层归一化

残差连接(x+Sublayer(x))解决深层网络梯度消失问题,允许模型训练更深架构;层归一化(LayerNorm)对每个样本的隐藏层输出归一化,加速收敛并提升训练稳定性,二者结合是 Transformer 高效训练的关键。

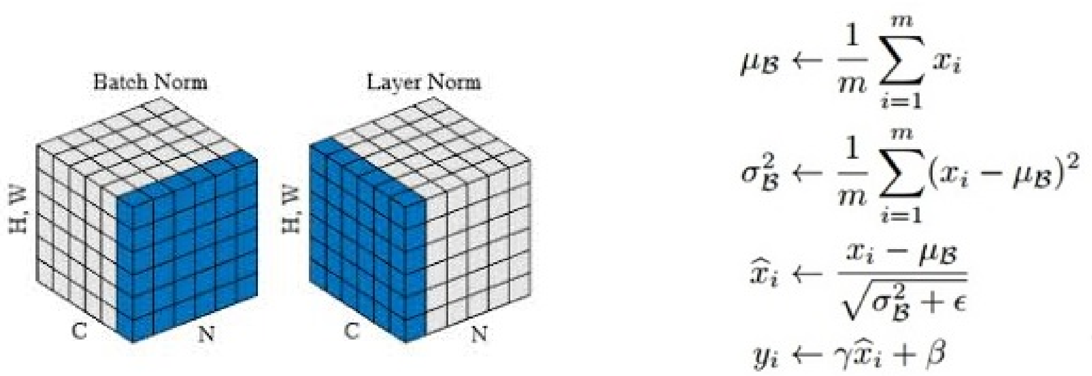

图 7: 层归一化

1.4 实验验证与优化

1.4.1 任务与性能

在 WMT 2014 英德/英法翻译任务中,Transformer 分别取得 28.4 BLEU 和 41.8 BLEU 的单模型最优结果,训练时间仅为传统模型的 1/4。通过消融实验证明,多头注意力($h = 8$)、位置编

码、层归一化等组件对性能提升至关重要。

1.4.2 训练技巧

采用学习率预热（Warm-up）策略：前 4000 步线性提升学习率，之后按公式

$$\mathrm{lrate} = d_{\mathrm{model}}^{-0.5} \cdot \min(\mathrm{step\_num}^{-0.5}, \mathrm{step\_num} \cdot \mathrm{warmup\_steps}^{-1.5})$$

衰减，平衡初期收敛速度与后期稳定性。标签平滑（Label Smoothing, $\epsilon_{ls} = 0.1$）通过软化真实标签分布，减少模型过拟合，提升泛化能力。

2 BERT [3]

2.1 预训练模型设计背景

现有预训练模型如 ELMo（双向 LSTM 拼接）和 GPT（单向 Transformer Decoder）在上下文利用上存在局限：ELMo 的双向性为浅层拼接，GPT 仅能处理单向上下文。BERT 通过深层双向 Transformer Encoder 与创新预训练任务，实现对上下文的深度融合，为下游任务提供更强语义表示。

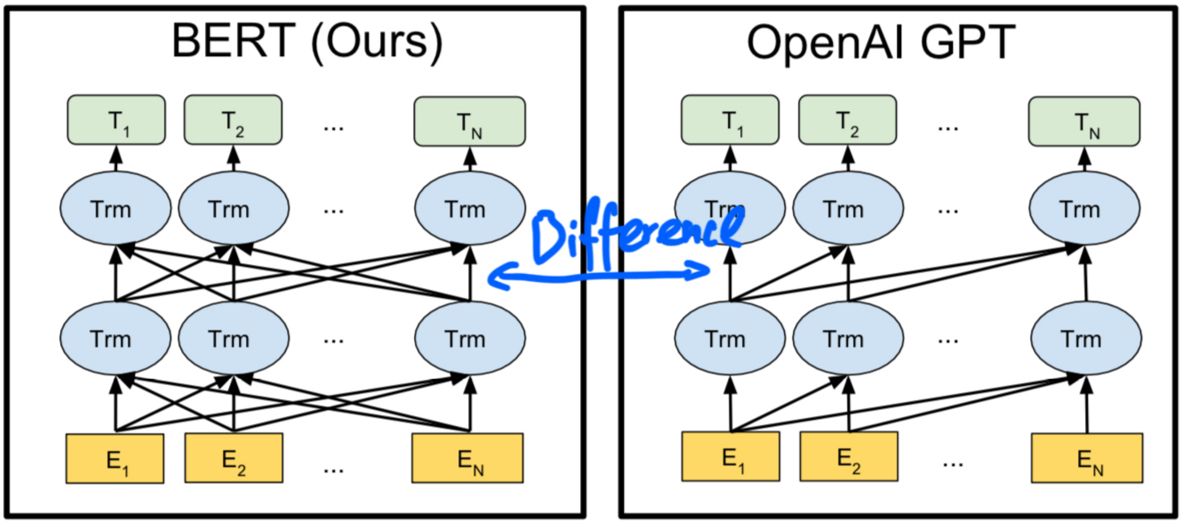

图 8: BERT 核心贡献，其实就是双向模型，这在之后的 NLP 和 CV 基础模型中被广泛考虑

2.2 输入表示与架构

2.2.1 三元嵌入结构

输入表示由三部分组成：1）词嵌入（Token Embeddings）采用 WordPiece 分词，30k 词汇表；2）位置嵌入（Position Embeddings）编码序列顺序；3）句子嵌入（Segment Embeddings）区分双句子输入（A/B 句），通过相加形成最终输入向量：$E = E_{\mathrm{token}} + E_{\mathrm{position}} + E_{\mathrm{segment}}$。

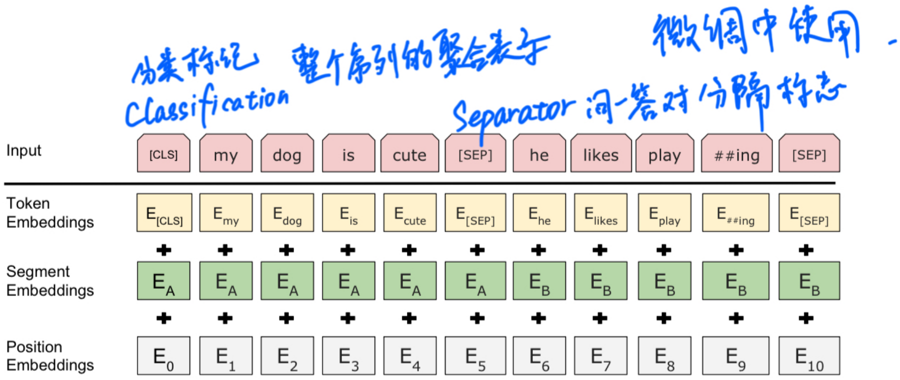

Figure 2: BERT input representation. The input embeddings are the sum of the token embeddings, the segmentation embeddings and the position embeddings.

图 9: BERT 输入表示

2.2.2 基于 Transformer Encoder

BERT 仅使用 Transformer 的 Encoder 部分，分为 BASE（L=12, H=768, A=12, 110M 参数）和 LARGE（L=24, H=1024, A=16, 340M 参数）两种配置。深层自注意力机制允许每个 token 同时关注上下文，实现真正的双向语义建模。

2.3 预训练任务设计

2.3.1 掩码语言模型（MLM）

随机选择 15% 的 Token 进行处理：80% 替换为 [MASK]，10% 替换为随机词，10% 保留原词。该策略迫使模型依赖上下文预测词汇，避免 [MASK] 标记在微调阶段的分布偏移，同时增强模型对噪声输入的鲁棒性。例如，输入”my dog is [MASK]” 时，模型需通过”my dog is” 预测出”cute”。

2.3.2 下一句预测（NSP）

构造 50% 正样本（B 为 A 的下一句）和 50% 负样本（B 为随机句子），训练模型判断句子对的连贯性。该任务提升模型对句子级关系的理解，对自然语言推理（NLI）、问答（QA）等需要跨句推理的任务至关重要，消融实验显示 NSP 可提升 MNLI 任务 4.6% 准确率。

2.4 训练与微调策略

2.4.1 数据与资源需求

预训练数据包含 BooksCorpus（800M 词）和 English Wikipedia（2500M 词），大规模语料确保模型捕捉丰富语言模式。训练使用 16/64 TPU 芯片，1M 步训练（约 4 天），巨大的参数量（340M）和计算量需求源于深层架构与复杂预训练任务。

2.4.2 下游任务微调

针对不同任务调整输入输出：1）分类任务使用 [CLS] 标记的输出向量；2）序列标注任务利用每个 Token 的隐藏层输出；3）问答任务通过起始/结束位置概率预测答案跨度。微调时仅添加少量任务特定参数，冻结或更新全部预训练参数，在 GLUE、SQuAD 等 11 个任务上刷新 SOTA，例如 GLUE 分数达 80.5%，SQuAD v1.1 F1 达 93.2。

2.5 模型分析与改进空间

2.5.1 性能与规模效应

BERT-LARGE 在小数据集（如 MRPC，3.6k 样本）上的性能显著优于 BASE，证明模型规模对泛化能力的提升作用。参数规模从 110M 增至 340M 时，GLUE 平均分数提升 7.0%，验证了深度双向架构与模型缩放的有效性。

2.5.2 预训练任务优化

现有 NSP 任务因简单二分类可能存在信息利用不足，后续研究可探索更复杂的句子关系（如因果、对比）；MLM 的固定掩码策略可改进为动态选择高频词或短语掩码，增强语义依赖建模。此外，跨语言预训练、多模态融合等方向可进一步拓展 BERT 的应用场景。

3 总结与思考

Transformer 通过自注意力机制革新序列建模，BERT 则证明深层双向预训练的巨大潜力。二者的成功推动 NLP 进入" 预训练 + 微调" 范式，而后续模型（如 GPT-3、T5）的涌现，印证了扩大模型规模、优化预训练任务、探索多模态融合的重要性。未来研究可聚焦于效率优化（如稀疏注意力）、小样本学习、可解释性增强等方向，推动模型在实际场景中的落地应用。

4 代码实现

4.1 Positional Encoding

```python
class PositionalEncoding(nn.Module):
    """
    compute sinusoid encoding.
    """
    def __init__(self, d_model, max_len, device):
        """
        constructor of sinusoid encoding class

        :param d_model: dimension of model
        :param max_len: max sequence length
        :param device: hardware device setting
        """
        super(PositionalEncoding, self).__init__()

        # same size with input matrix (for adding with input matrix)
        self.encoding = torch.zeros(max_len, d_model, device=device)
```

```
        self.encoding.requires_grad = False  # we don't need to compute gradient

        pos = torch.arange(0, max_len, device=device)
        pos = pos.float().unsqueeze(dim=1)
        # 1D => 2D unsqueeze to represent word's position

        _2i = torch.arange(0, d_model, step=2, device=device).float()
        # 'i' means index of d_model (e.g. embedding size = 50, 'i' = [0,50])
        # "step=2" means 'i' multiplied with two (same with 2 * i)

        self.encoding[:, 0::2] = torch.sin(pos / (10000 ** (_2i / d_model)))
        self.encoding[:, 1::2] = torch.cos(pos / (10000 ** (_2i / d_model)))
        # compute positional encoding to consider positional information of words

    def forward(self, x):
        # self.encoding
        # [max_len = 512, d_model = 512]

        batch_size, seq_len = x.size()
        # [batch_size = 128, seq_len = 30]

        return self.encoding[:seq_len, :]
        # [seq_len = 30, d_model = 512]
        # it will add with tok_emb : [128, 30, 512]
```

4.2 Multi-Head Attention

```
class MultiHeadAttention(nn.Module):

    def __init__(self, d_model, n_head):
        super(MultiHeadAttention, self).__init__()
        self.n_head = n_head
        self.attention = ScaleDotProductAttention()
        self.w_q = nn.Linear(d_model, d_model)
        self.w_k = nn.Linear(d_model, d_model)
        self.w_v = nn.Linear(d_model, d_model)
        self.w_concat = nn.Linear(d_model, d_model)

    def forward(self, q, k, v, mask=None):
        # 1. dot product with weight matrices
        q, k, v = self.w_q(q), self.w_k(k), self.w_v(v)

        # 2. split tensor by number of heads
        q, k, v = self.split(q), self.split(k), self.split(v)

        # 3. do scale dot product to compute similarity
        out, attention = self.attention(q, k, v, mask=mask)

        # 4. concat and pass to linear layer
        out = self.concat(out)
        out = self.w_concat(out)

        # 5. visualize attention map
        # TODO : we should implement visualization

        return out
```

```python

    def split(self, tensor):
        """
        split tensor by number of head

        :param tensor: [batch_size, length, d_model]
        :return: [batch_size, head, length, d_tensor]
        """
        batch_size, length, d_model = tensor.size()

        d_tensor = d_model // self.n_head
        tensor = tensor.view(batch_size, length, self.n_head, d_tensor).transpose(1, 2)
        # it is similar with group convolution (split by number of heads)

        return tensor

    def concat(self, tensor):
        """
        inverse function of self.split(tensor : torch.Tensor)

        :param tensor: [batch_size, head, length, d_tensor]
        :return: [batch_size, length, d_model]
        """
        batch_size, head, length, d_tensor = tensor.size()
        d_model = head * d_tensor

        tensor = tensor.transpose(1, 2).contiguous().view(batch_size, length, d_model)
        return tensor
```

4.3 Scale Dot Product Attention

```python
class ScaleDotProductAttention(nn.Module):
    """
    compute scale dot product attention

    Query : given sentence that we focused on (decoder)
    Key : every sentence to check relationship with Qeury(encoder)
    Value : every sentence same with Key (encoder)
    """

    def __init__(self):
        super(ScaleDotProductAttention, self).__init__()
        self.softmax = nn.Softmax(dim=-1)

    def forward(self, q, k, v, mask=None, e=1e-12):
        # input is 4 dimension tensor
        # [batch_size, head, length, d_tensor]
        batch_size, head, length, d_tensor = k.size()

        # 1. dot product Query with Key^T to compute similarity
        k_t = k.transpose(2, 3)  # transpose
        score = (q @ k_t) / math.sqrt(d_tensor)  # scaled dot product

        # 2. apply masking (opt)
        if mask is not None:
            score = score.masked_fill(mask == 0, -10000)
```

```python

        # 3. pass them softmax to make [0, 1] range
        score = self.softmax(score)

        # 4. multiply with Value
        v = score @ v

        return v, score
```

4.4 Layer Norm

```python
class LayerNorm(nn.Module):
    def __init__(self, d_model, eps=1e-12):
        super(LayerNorm, self).__init__()
        self.gamma = nn.Parameter(torch.ones(d_model))
        self.beta = nn.Parameter(torch.zeros(d_model))
        self.eps = eps

    def forward(self, x):
        mean = x.mean(-1, keepdim=True)
        var = x.var(-1, unbiased=False, keepdim=True)
        # '-1' means last dimension.

        out = (x - mean) / torch.sqrt(var + self.eps)
        out = self.gamma * out + self.beta
        return out
```

4.5 Position-wise Feed Forward

```python

class PositionwiseFeedForward(nn.Module):

    def __init__(self, d_model, hidden, drop_prob=0.1):
        super(PositionwiseFeedForward, self).__init__()
        self.linear1 = nn.Linear(d_model, hidden)
        self.linear2 = nn.Linear(hidden, d_model)
        self.relu = nn.ReLU()
        self.dropout = nn.Dropout(p=drop_prob)

    def forward(self, x):
        x = self.linear1(x)
        x = self.relu(x)
        x = self.dropout(x)
        x = self.linear2(x)
        return x
```

4.6 Encoder & Decoder Structure

```python
class EncoderLayer(nn.Module):

    def __init__(self, d_model, ffn_hidden, n_head, drop_prob):
        super(EncoderLayer, self).__init__()
```

```
        self.attention = MultiHeadAttention(d_model=d_model, n_head=n_head)
        self.norm1 = LayerNorm(d_model=d_model)
        self.dropout1 = nn.Dropout(p=drop_prob)

        self.ffn = PositionwiseFeedForward(d_model=d_model, hidden=ffn_hidden, drop_prob=drop_prob)
        self.norm2 = LayerNorm(d_model=d_model)
        self.dropout2 = nn.Dropout(p=drop_prob)

    def forward(self, x, src_mask):
        # 1. compute self attention
        _x = x
        x = self.attention(q=x, k=x, v=x, mask=src_mask)

        # 2. add and norm
        x = self.dropout1(x)
        x = self.norm1(x + _x)

        # 3. positionwise feed forward network
        _x = x
        x = self.ffn(x)

        # 4. add and norm
        x = self.dropout2(x)
        x = self.norm2(x + _x)
        return x

class DecoderLayer(nn.Module):

    def __init__(self, d_model, ffn_hidden, n_head, drop_prob):
        super(DecoderLayer, self).__init__()
        self.self_attention = MultiHeadAttention(d_model=d_model, n_head=n_head)
        self.norm1 = LayerNorm(d_model=d_model)
        self.dropout1 = nn.Dropout(p=drop_prob)

        self.enc_dec_attention = MultiHeadAttention(d_model=d_model, n_head=n_head)
        self.norm2 = LayerNorm(d_model=d_model)
        self.dropout2 = nn.Dropout(p=drop_prob)

        self.ffn = PositionwiseFeedForward(d_model=d_model, hidden=ffn_hidden, drop_prob=drop_prob)
        self.norm3 = LayerNorm(d_model=d_model)
        self.dropout3 = nn.Dropout(p=drop_prob)

    def forward(self, dec, enc, trg_mask, src_mask):
        # 1. compute self attention
        _x = dec
        x = self.self_attention(q=dec, k=dec, v=dec, mask=trg_mask)

        # 2. add and norm
        x = self.dropout1(x)
        x = self.norm1(x + _x)

        if enc is not None:
            # 3. compute encoder - decoder attention
            _x = x
            x = self.enc_dec_attention(q=x, k=enc, v=enc, mask=src_mask)

            # 4. add and norm
```

```
            x = self.dropout2(x)
            x = self.norm2(x + _x)

        # 5. positionwise feed forward network
        _x = x
        x = self.ffn(x)

        # 6. add and norm
        x = self.dropout3(x)
        x = self.norm3(x + _x)
        return x

class Decoder(nn.Module):
    def __init__(self, dec_voc_size, max_len, d_model, ffn_hidden, n_head, n_layers, drop_prob, device):
        super().__init__()
        self.emb = TransformerEmbedding(d_model=d_model,
                                        drop_prob=drop_prob,
                                        max_len=max_len,
                                        vocab_size=dec_voc_size,
                                        device=device)

        self.layers = nn.ModuleList([DecoderLayer(d_model=d_model,
                                                  ffn_hidden=ffn_hidden,
                                                  n_head=n_head,
                                                  drop_prob=drop_prob)
                                     for _ in range(n_layers)])

        self.linear = nn.Linear(d_model, dec_voc_size)

    def forward(self, trg, src, trg_mask, src_mask):
        trg = self.emb(trg)

        for layer in self.layers:
            trg = layer(trg, src, trg_mask, src_mask)

        # pass to LM head
        output = self.linear(trg)
        return output
```

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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.

并行化
训练快 ?

1 Introduction

Recurrent neural networks, long short-term memory [13] and gated recurrent [7] neural networks in particular, have been firmly established as state of the art approaches in sequence modeling and

*Equal contribution. Listing order is random. Jakob proposed replacing RNNs with self-attention and started the effort to evaluate this idea. Ashish, with Illia, designed and implemented the first Transformer models and has been crucially involved in every aspect of this work. Noam proposed scaled dot-product attention, multi-head attention and the parameter-free position representation and became the other person involved in nearly every detail. Niki designed, implemented, tuned and evaluated countless model variants in our original codebase and tensor2tensor. Llion also experimented with novel model variants, was responsible for our initial codebase, and efficient inference and visualizations. Lukasz and Aidan spent countless long days designing various parts of and implementing tensor2tensor, replacing our earlier codebase, greatly improving results and massively accelerating our research.

†Work performed while at Google Brain.

‡Work performed while at Google Research.

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transduction problems such as language modeling and machine translation [35, 2, 5]. Numerous efforts have since continued to push the boundaries of recurrent language models and encoder-decoder architectures [38, 24, 15].

Recurrent models typically factor computation along the symbol positions of the input and output sequences. Aligning the positions to steps in computation time, they generate a sequence of hidden states h_t, as a function of the previous hidden state h_{t-1} and the input for position t. This inherently sequential nature precludes parallelization within training examples, which becomes critical at longer sequence lengths, as memory constraints limit batching across examples. Recent work has achieved significant improvements in computational efficiency through factorization tricks [21] and conditional computation [32], while also improving model performance in case of the latter. The fundamental constraint of sequential computation, however, remains.

问题点1：
RNN的顺序时序
计算，难以并行
化

Attention mechanisms have become an integral part of compelling sequence modeling and transduction models in various tasks, allowing modeling of dependencies without regard to their distance in the input or output sequences [2, 19]. In all but a few cases [27], however, such attention mechanisms are used in conjunction with a recurrent network.

以前：需要结合RNN等。 ?

In this work we propose the Transformer, a model architecture eschewing recurrence and instead relying entirely on an attention mechanism to draw global dependencies between input and output. The Transformer allows for significantly more parallelization and can reach a new state of the art in translation quality after being trained for as little as twelve hours on eight P100 GPUs.

2 Background

The goal of reducing sequential computation also forms the foundation of the Extended Neural GPU [16], ByteNet [18] and ConvS2S [9], 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 [12]. 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 as described in section 3.2.

问题点2：CNN
长距离的编码差

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 [4, 27, 28, 22].

End-to-end memory networks are based on a recurrent attention mechanism instead of sequence-aligned recurrence and have been shown to perform well on simple-language question answering and language modeling tasks [34].

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. In the following sections, we will describe the Transformer, motivate self-attention and discuss its advantages over models such as [17, 18] and [9].

3 Model Architecture

Most competitive neural sequence transduction models have an encoder-decoder structure [5, 2, 35]. Here, the encoder maps an input sequence of symbol representations $(x_1, ..., x_n)$ to a sequence of continuous representations $\mathbf{z} = (z_1, ..., z_n)$. Given $\mathbf{z}$, the decoder then generates an output sequence $(y_1, ..., y_m)$ of symbols one element at a time. At each step the model is auto-regressive [10], consuming the previously generated symbols as additional input when generating the next.

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.

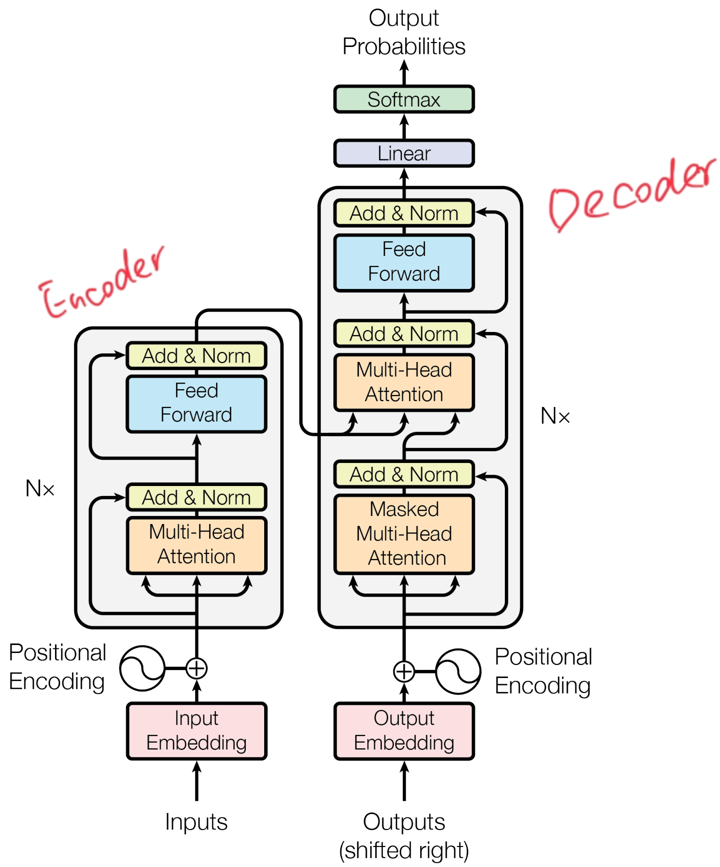


Figure 1: The Transformer - model architecture.

3.1 Encoder and Decoder Stacks

Encoder: The encoder is composed of a stack of $N = 6$ identical layers. 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. We employ a residual connection [11] around each of the two sub-layers, followed by layer normalization [1]. 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. To facilitate these residual connections, all sub-layers in the model, as well as the embedding layers, produce outputs of dimension $d_{\text{model}} = 512$.

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

3.2 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.

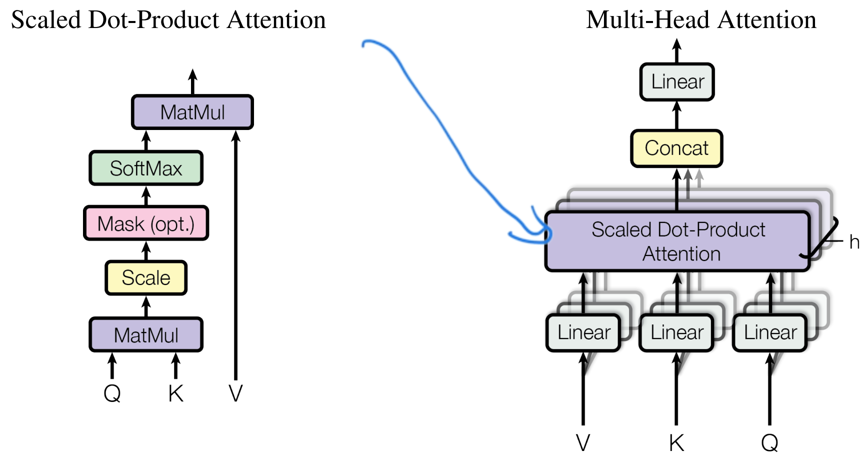


Figure 2: (left) Scaled Dot-Product Attention. (right) Multi-Head Attention consists of several attention layers running in parallel.

3.2.1 Scaled Dot-Product Attention

We call our particular attention "Scaled Dot-Product Attention" (Figure 2). 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.

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:

$$\mathrm{Attention}(Q, K, V) = \mathrm{softmax}(\frac{QK^T}{\sqrt{d_k}})V \tag{1}$$

The two most commonly used attention functions are additive attention [2], 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 [3]. 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 [4]. To counteract this effect, we scale the dot products by $\frac{1}{\sqrt{d_k}}$.

3.2.2 Multi-Head Attention

Instead of performing a single attention function with d_{model}-dimensional keys, values and queries, we found it beneficial to linearly project the queries, keys and values h times with different, learned linear projections to d_k, d_k and d_v dimensions, respectively. On each of these projected versions of queries, keys and values we then perform the attention function in parallel, yielding d_v-dimensional output values. These are concatenated and once again projected, resulting in the final values, as depicted in Figure 2.

[4]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.

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.

$$\mathrm{MultiHead}(Q,K,V) = \mathrm{Concat}(\mathrm{head_1},...,\mathrm{head_h})W^O$$
$$\text{where } \mathrm{head_i} = \mathrm{Attention}(QW_i^Q, KW_i^K, VW_i^V)$$

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.

3.2.3 Applications of Attention in our Model

The Transformer uses multi-head attention in three different ways:

- 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 [38, 2, 9].

(1) 编码-解码注意力层.

- 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.

(2) 编码器自注意力层.

- 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. See Figure 2.

(3) 解码器自注意力层.

3.3 Position-wise Feed-Forward Networks 位置前馈神经网络

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.

$$\mathrm{FFN}(x) = \max(0, xW_1 + b_1)W_2 + b_2 \tag{2}$$

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 $d_{ff} = 2048$.

3.4 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 [30]. In the embedding layers, we multiply those weights by $\sqrt{d_{\text{model}}}$.

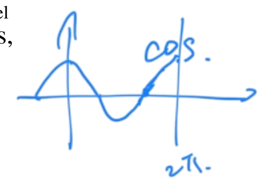
3.5 Positional Encoding 位置编码

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

Table 1: Maximum path lengths, per-layer complexity and minimum number of sequential operations for different layer types. n is the sequence length, d is the representation dimension, k is the kernel size of convolutions and r the size of the neighborhood in restricted self-attention.

Layer Type	Complexity per Layer	Sequential Operations	Maximum Path Length
Self-Attention	$O(n^2 \cdot d)$	$O(1)$	$O(1)$
Recurrent	$O(n \cdot d^2)$	$O(n)$	$O(n)$
Convolutional	$O(k \cdot n \cdot d^2)$	$O(1)$	$O(log_k(n))$
Self-Attention (restricted)	$O(r \cdot n \cdot d)$	$O(1)$	$O(n/r)$

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 [9].



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}.

We also experimented with using learned positional embeddings [9] instead, and found that the two versions produced nearly identical results (see Table 3 row (E)). We chose the sinusoidal version because it may allow the model to extrapolate to sequence lengths longer than the ones encountered during training.

正弦

允许推断比训练时长的序列

$PE_{(pos+k,2i)} = 2cos(\ ) P_{(pos,2i)}$

线性.

余弦非线性:

$PE_{(pos+k,2i+1)} =$

$PE^2_{(pos,2i+1)} -$

$sin^2(\ )$.

推断计算复杂度高.

4 Why Self-Attention

In this section we compare various aspects of self-attention layers to the recurrent and convolutional layers commonly used for mapping one variable-length sequence of symbol representations $(x_1, ..., x_n)$ to another sequence of equal length $(z_1, ..., z_n)$, with $x_i, z_i \in \mathbb{R}^d$, such as a hidden layer in a typical sequence transduction encoder or decoder. Motivating our use of self-attention we consider three desiderata.

One is the total computational complexity per layer. Another is the amount of computation that can be parallelized, as measured by the minimum number of sequential operations required.

The third is the path length between long-range dependencies in the network. Learning long-range dependencies is a key challenge in many sequence transduction tasks. One key factor affecting the ability to learn such dependencies is the length of the paths forward and backward signals have to traverse in the network. The shorter these paths between any combination of positions in the input and output sequences, the easier it is to learn long-range dependencies [12]. Hence we also compare the maximum path length between any two input and output positions in networks composed of the different layer types.

As noted in Table 1, a self-attention layer connects all positions with a constant number of sequentially executed operations, whereas a recurrent layer requires $O(n)$ sequential operations. In terms of computational complexity, self-attention layers are faster than recurrent layers when the sequence length n is smaller than the representation dimensionality d, which is most often the case with sentence representations used by state-of-the-art models in machine translations, such as word-piece [38] and byte-pair [31] representations. To improve computational performance for tasks involving very long sequences, self-attention could be restricted to considering only a neighborhood of size r in

总结：

1) 计算复杂度

2) 可并行化

3) 长距离依赖

4) 可解释性.

the input sequence centered around the respective output position. This would increase the maximum path length to $O(n/r)$. We plan to investigate this approach further in future work.

A single convolutional layer with kernel width $k < n$ does not connect all pairs of input and output positions. Doing so requires a stack of $O(n/k)$ convolutional layers in the case of contiguous kernels, or $O(log_k(n))$ in the case of dilated convolutions [18], increasing the length of the longest paths between any two positions in the network. Convolutional layers are generally more expensive than recurrent layers, by a factor of k. Separable convolutions [6], however, decrease the complexity considerably, to $O(k \cdot n \cdot d + n \cdot d^2)$. Even with $k = n$, however, the complexity of a separable convolution is equal to the combination of a self-attention layer and a point-wise feed-forward layer, the approach we take in our model.

比最快的卷积还快.(获得相同依赖).

As side benefit, self-attention could yield more interpretable models. We inspect attention distributions from our models and present and discuss examples in the appendix. Not only do individual attention heads clearly learn to perform different tasks, many appear to exhibit behavior related to the syntactic and semantic structure of the sentences.

5 Training

This section describes the training regime for our models.

5.1 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 [3], 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 [38]. 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.

5.2 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,(described on the bottom line of table 3), step time was 1.0 seconds. The big models were trained for 300,000 steps (3.5 days).

5.3 Optimizer

We used the Adam optimizer [20] 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:

$$lrate = d_{\text{model}}^{-0.5} \cdot \min(step\_num^{-0.5}, step\_num \cdot warmup\_steps^{-1.5}) \tag{3}$$

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 $warmup\_steps = 4000$.

5.4 Regularization

We employ three types of regularization during training:

Residual Dropout We apply dropout [33] to the output of each sub-layer, before it is added to the sub-layer input and normalized. 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 $P_{drop} = 0.1$.

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**	$2.3 \cdot 10^{19}$	

Label Smoothing During training, we employed label smoothing of value $\epsilon_{ls} = 0.1$ [36]. This hurts perplexity, as the model learns to be more unsure, but improves accuracy and BLEU score.

6 Results

6.1 Machine Translation

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 $P_{drop} = 0.1$, instead of 0.3.

For the base models, we used a single model obtained by averaging the last 5 checkpoints, which were written at 10-minute intervals. For the big models, we averaged the last 20 checkpoints. We used beam search with a beam size of 4 and length penalty $\alpha = 0.6$ [38]. These hyperparameters were chosen after experimentation on the development set. We set the maximum output length during inference to input length + 50, but terminate early when possible [38].

Table 2 summarizes our results and compares our translation quality and training costs to other model architectures from the literature. We estimate the number of floating point operations used to train a model by multiplying the training time, the number of GPUs used, and an estimate of the sustained single-precision floating-point capacity of each GPU [5].

6.2 Model Variations

To evaluate the importance of different components of the Transformer, we varied our base model in different ways, measuring the change in performance on English-to-German translation on the development set, newstest2013. We used beam search as described in the previous section, but no checkpoint averaging. We present these results in Table 3.

In Table 3 rows (A), we vary the number of attention heads and the attention key and value dimensions, keeping the amount of computation constant, as described in Section 3.2.2. While single-head attention is 0.9 BLEU worse than the best setting, quality also drops off with too many heads.

[5]We used values of 2.8, 3.7, 6.0 and 9.5 TFLOPS for K80, K40, M40 and P100, respectively.

Table 3: Variations on the Transformer architecture. Unlisted values are identical to those of the base model. All metrics are on the English-to-German translation development set, newstest2013. Listed perplexities are per-wordpiece, according to our byte-pair encoding, and should not be compared to per-word perplexities.

	N	d_{model}	d_{ff}	h	d_k	d_v	P_{drop}	ϵ_{ls}	train steps	PPL (dev)	BLEU (dev)	params $\times 10^6$
base	6	512	2048	8	64	64	0.1	0.1	100K	4.92	25.8	65
(A)				1	512	512				5.29	24.9	
				4	128	128				5.00	25.5	
				16	32	32				4.91	25.8	
				32	16	16				5.01	25.4	
(B)					16					5.16	25.1	58
					32					5.01	25.4	60
(C)	2									6.11	23.7	36
	4									5.19	25.3	50
	8									4.88	25.5	80
		256			32	32				5.75	24.5	28
		1024			128	128				4.66	26.0	168
			1024							5.12	25.4	53
			4096							4.75	26.2	90
(D)							0.0			5.77	24.6	
							0.2			4.95	25.5	
								0.0		4.67	25.3	
								0.2		5.47	25.7	
(E)	positional embedding instead of sinusoids									4.92	25.7	
big	6	1024	4096	16			0.3		300K	**4.33**	**26.4**	213

Table 4: The Transformer generalizes well to English constituency parsing (Results are on Section 23 of WSJ)

Parser	**Training**	**WSJ 23 F1**
Vinyals & Kaiser el al. (2014) [37]	WSJ only, discriminative	88.3
Petrov et al. (2006) [29]	WSJ only, discriminative	90.4
Zhu et al. (2013) [40]	WSJ only, discriminative	90.4
Dyer et al. (2016) [8]	WSJ only, discriminative	91.7
Transformer (4 layers)	WSJ only, discriminative	91.3
Zhu et al. (2013) [40]	semi-supervised	91.3
Huang & Harper (2009) [14]	semi-supervised	91.3
McClosky et al. (2006) [26]	semi-supervised	92.1
Vinyals & Kaiser el al. (2014) [37]	semi-supervised	92.1
Transformer (4 layers)	semi-supervised	92.7
Luong et al. (2015) [23]	multi-task	93.0
Dyer et al. (2016) [8]	generative	93.3

In Table 3 rows (B), we observe that reducing the attention key size d_k hurts model quality. This suggests that determining compatibility is not easy and that a more sophisticated compatibility function than dot product may be beneficial. We further observe in rows (C) and (D) that, as expected, bigger models are better, and dropout is very helpful in avoiding over-fitting. In row (E) we replace our sinusoidal positional encoding with learned positional embeddings [9], and observe nearly identical results to the base model.

6.3 English Constituency Parsing

To evaluate if the Transformer can generalize to other tasks we performed experiments on English constituency parsing. This task presents specific challenges: the output is subject to strong structural constraints and is significantly longer than the input. Furthermore, RNN sequence-to-sequence models have not been able to attain state-of-the-art results in small-data regimes [37].

We trained a 4-layer transformer with $d_{model} = 1024$ on the Wall Street Journal (WSJ) portion of the Penn Treebank [25], about 40K training sentences. We also trained it in a semi-supervised setting, using the larger high-confidence and BerkleyParser corpora from with approximately 17M sentences [37]. We used a vocabulary of 16K tokens for the WSJ only setting and a vocabulary of 32K tokens for the semi-supervised setting.

We performed only a small number of experiments to select the dropout, both attention and residual (section 5.4), learning rates and beam size on the Section 22 development set, all other parameters remained unchanged from the English-to-German base translation model. During inference, we increased the maximum output length to input length + 300. We used a beam size of 21 and $\alpha = 0.3$ for both WSJ only and the semi-supervised setting.

Our results in Table 4 show that despite the lack of task-specific tuning our model performs surprisingly well, yielding better results than all previously reported models with the exception of the Recurrent Neural Network Grammar [8].

In contrast to RNN sequence-to-sequence models [37], the Transformer outperforms the Berkeley-Parser [29] even when training only on the WSJ training set of 40K sentences.

7 Conclusion

In this work, we presented the Transformer, the first sequence transduction model based entirely on attention, replacing the recurrent layers most commonly used in encoder-decoder architectures with multi-headed self-attention.

For translation tasks, the Transformer can be trained significantly faster than architectures based on recurrent or convolutional layers. On both WMT 2014 English-to-German and WMT 2014 English-to-French translation tasks, we achieve a new state of the art. In the former task our best model outperforms even all previously reported ensembles.

We are excited about the future of attention-based models and plan to apply them to other tasks. We plan to extend the Transformer to problems involving input and output modalities other than text and to investigate local, restricted attention mechanisms to efficiently handle large inputs and outputs such as images, audio and video. Making generation less sequential is another research goals of ours.

The code we used to train and evaluate our models is available at `https://github.com/tensorflow/tensor2tensor`.

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Attention Visualizations

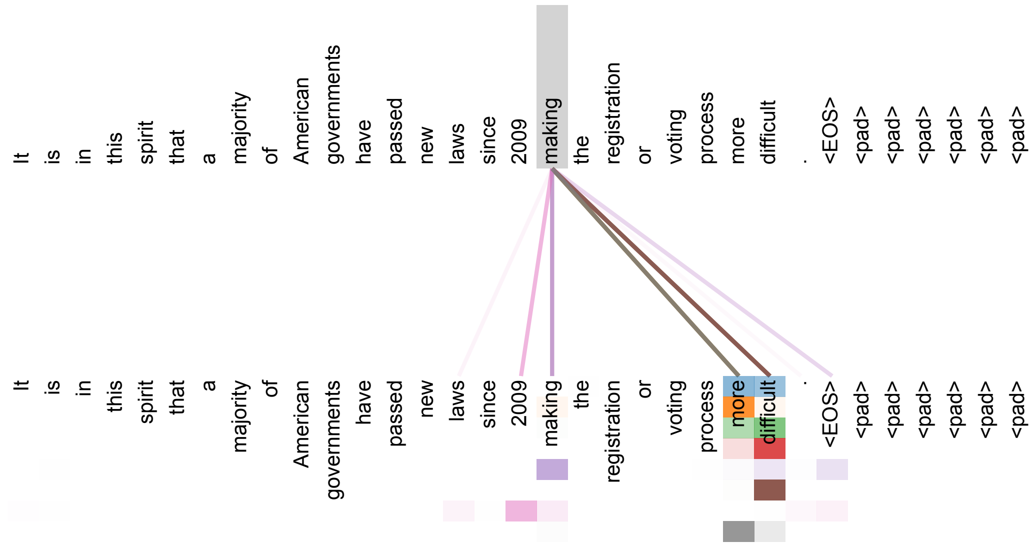

Figure 3: An example of the attention mechanism following long-distance dependencies in the encoder self-attention in layer 5 of 6. Many of the attention heads attend to a distant dependency of the verb 'making', completing the phrase 'making...more difficult'. Attentions here shown only for the word 'making'. Different colors represent different heads. Best viewed in color.

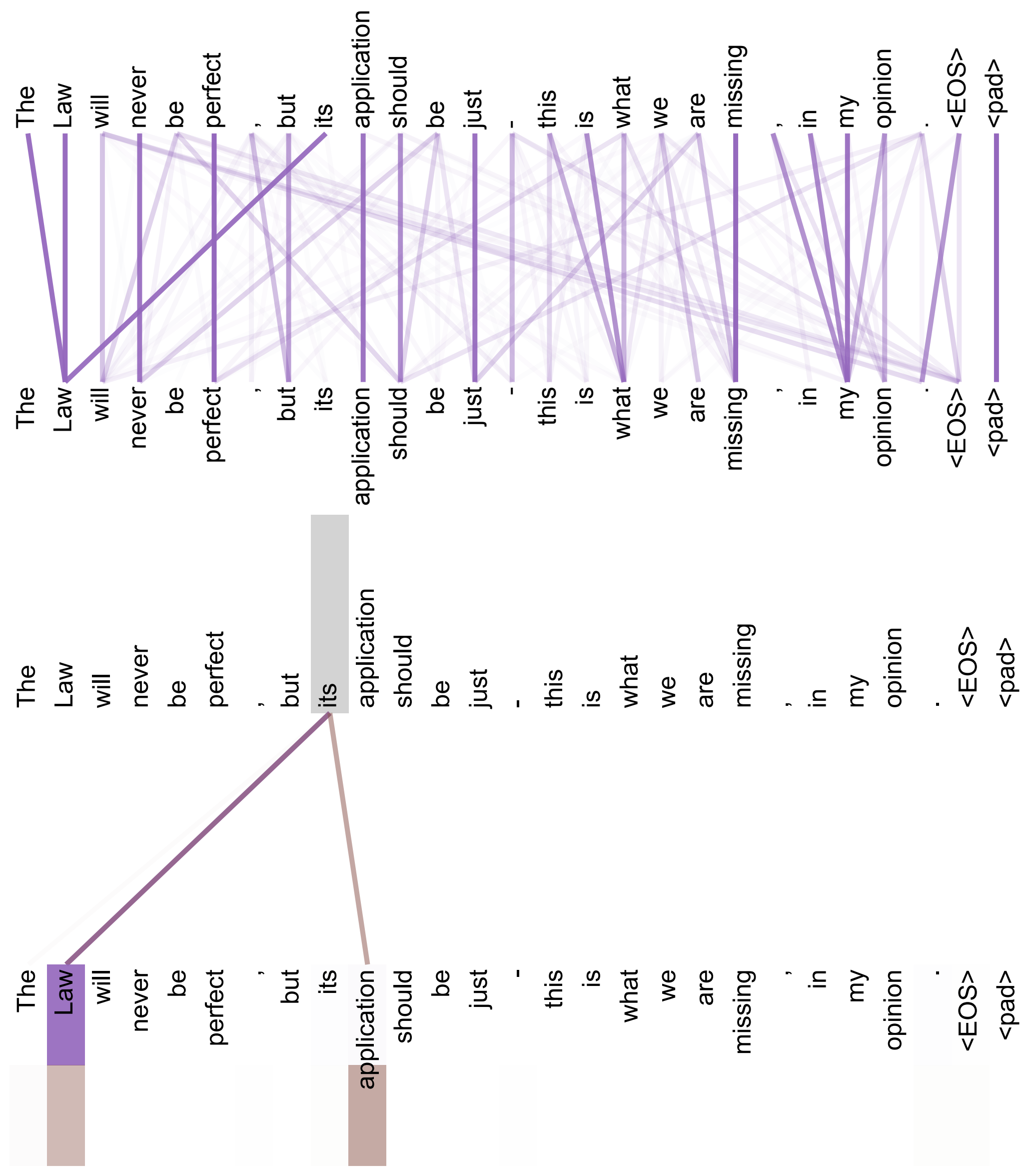

Figure 4: Two attention heads, also in layer 5 of 6, apparently involved in anaphora resolution. Top: Full attentions for head 5. Bottom: Isolated attentions from just the word 'its' for attention heads 5 and 6. Note that the attentions are very sharp for this word.

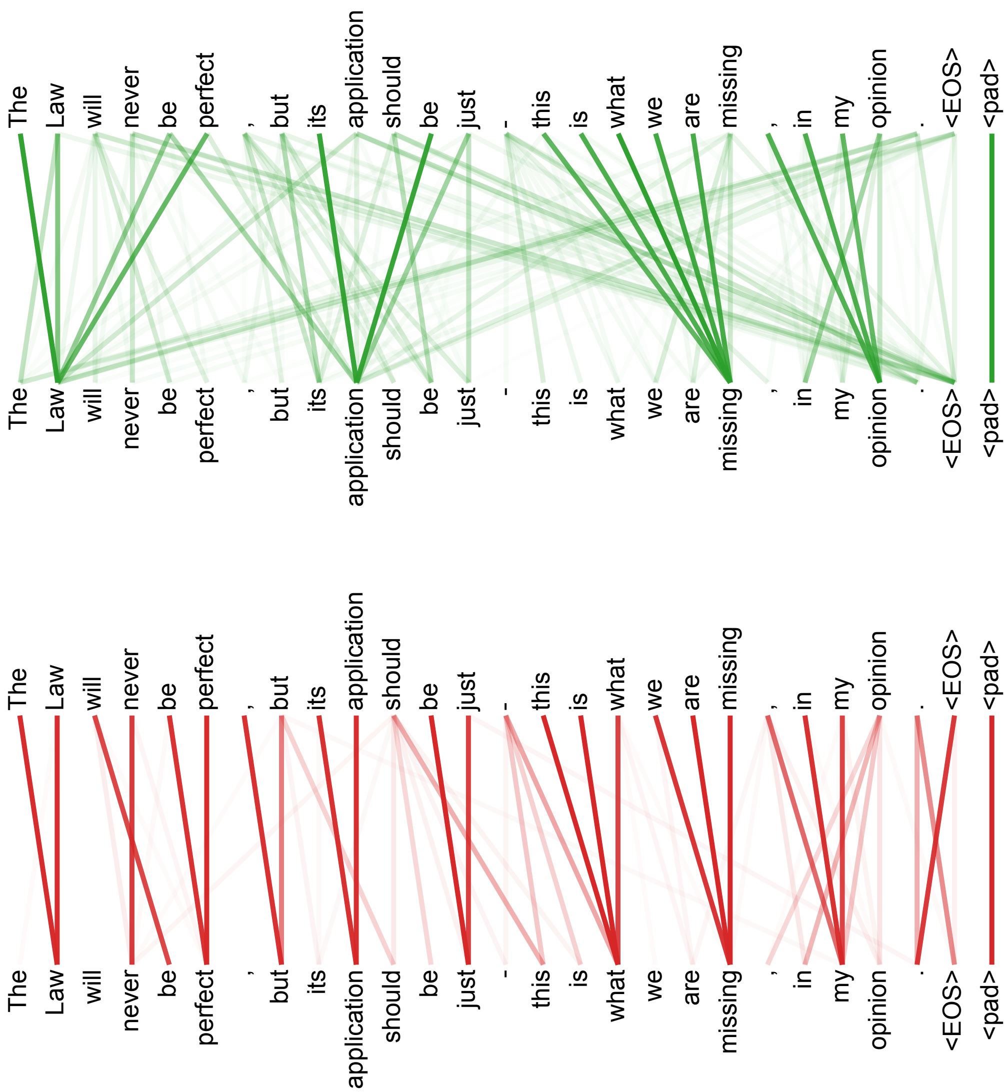

Figure 5: Many of the attention heads exhibit behaviour that seems related to the structure of the sentence. We give two such examples above, from two different heads from the encoder self-attention at layer 5 of 6. The heads clearly learned to perform different tasks.

BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding

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Abstract

We introduce a new language representation model called **BERT**, which stands for **B**idirectional **E**ncoder **R**epresentations from **T**ransformers. Unlike recent language representation models (Peters et al., 2018a; Radford et al., 2018), BERT is designed to pre-train deep bidirectional representations from unlabeled text by jointly conditioning on both left and right context in all layers. As a result, the pre-trained BERT model can be fine-tuned with just one additional output layer to create state-of-the-art models for a wide range of tasks, such as question answering and language inference, without substantial task-specific architecture modifications.

BERT is conceptually simple and empirically powerful. It obtains new state-of-the-art results on eleven natural language processing tasks, including pushing the GLUE score to 80.5% (7.7% point absolute improvement), MultiNLI accuracy to 86.7% (4.6% absolute improvement), SQuAD v1.1 question answering Test F1 to 93.2 (1.5 point absolute improvement) and SQuAD v2.0 Test F1 to 83.1 (5.1 point absolute improvement).

1 Introduction

Language model pre-training has been shown to be effective for improving many natural language processing tasks (Dai and Le, 2015; Peters et al., 2018a; Radford et al., 2018; Howard and Ruder, 2018). These include sentence-level tasks such as natural language inference (Bowman et al., 2015; Williams et al., 2018) and paraphrasing (Dolan and Brockett, 2005), which aim to predict the relationships between sentences by analyzing them holistically, as well as token-level tasks such as named entity recognition and question answering, where models are required to produce fine-grained output at the token level (Tjong Kim Sang and De Meulder, 2003; Rajpurkar et al., 2016).

There are two existing strategies for applying pre-trained language representations to downstream tasks: *feature-based* and *fine-tuning*. The feature-based approach, such as ELMo (Peters et al., 2018a), uses task-specific architectures that include the pre-trained representations as additional features. The fine-tuning approach, such as the Generative Pre-trained Transformer (OpenAI GPT) (Radford et al., 2018), introduces minimal task-specific parameters, and is trained on the downstream tasks by simply fine-tuning *all* pre-trained parameters. The two approaches share the same objective function during pre-training, where they use unidirectional language models to learn general language representations.

We argue that current techniques restrict the power of the pre-trained representations, especially for the fine-tuning approaches. The major limitation is that standard language models are unidirectional, and this limits the choice of architectures that can be used during pre-training. For example, in OpenAI GPT, the authors use a left-to-right architecture, where every token can only attend to previous tokens in the self-attention layers of the Transformer (Vaswani et al., 2017). Such restrictions are sub-optimal for sentence-level tasks, and could be very harmful when applying fine-tuning based approaches to token-level tasks such as question answering, where it is crucial to incorporate context from both directions.

In this paper, we improve the fine-tuning based approaches by proposing BERT: **B**idirectional **E**ncoder **R**epresentations from **T**ransformers. BERT alleviates the previously mentioned unidirectionality constraint by using a "masked language model" (MLM) pre-training objective, inspired by the Cloze task (Taylor, 1953). The masked language model randomly masks some of the tokens from the input, and the objective is to predict the original vocabulary id of the masked word based only on its context. Unlike left-to-right language model pre-training, the MLM objective enables the representation to fuse the left and the right context, which allows us to pre-train a deep bidirectional Transformer. In addition to the masked language model, we also use a "next sentence prediction" task that jointly pre-trains text-pair representations. The contributions of our paper are as follows:

- We demonstrate the importance of bidirectional pre-training for language representations. Unlike Radford et al. (2018), which uses unidirectional language models for pre-training, BERT uses masked language models to enable pre-trained deep bidirectional representations. This is also in contrast to Peters et al. (2018a), which uses a shallow concatenation of independently trained left-to-right and right-to-left LMs.

- We show that pre-trained representations reduce the need for many heavily-engineered task-specific architectures. BERT is the first fine-tuning based representation model that achieves state-of-the-art performance on a large suite of sentence-level *and* token-level tasks, outperforming many task-specific architectures.

- BERT advances the state of the art for eleven NLP tasks. The code and pre-trained models are available at `https://github.com/google-research/bert`.

2 Related Work

There is a long history of pre-training general language representations, and we briefly review the most widely-used approaches in this section.

2.1 Unsupervised Feature-based Approaches

Learning widely applicable representations of words has been an active area of research for decades, including non-neural (Brown et al., 1992; Ando and Zhang, 2005; Blitzer et al., 2006) and neural (Mikolov et al., 2013; Pennington et al., 2014) methods. Pre-trained word embeddings are an integral part of modern NLP systems, offering significant improvements over embeddings learned from scratch (Turian et al., 2010). To pre-train word embedding vectors, left-to-right language modeling objectives have been used (Mnih and Hinton, 2009), as well as objectives to discriminate correct from incorrect words in left and right context (Mikolov et al., 2013).

特征提取

These approaches have been generalized to coarser granularities, such as sentence embeddings (Kiros et al., 2015; Logeswaran and Lee, 2018) or paragraph embeddings (Le and Mikolov, 2014). To train sentence representations, prior work has used objectives to rank candidate next sentences (Jernite et al., 2017; Logeswaran and Lee, 2018), left-to-right generation of next sentence words given a representation of the previous sentence (Kiros et al., 2015), or denoising auto-encoder derived objectives (Hill et al., 2016).

ELMo and its predecessor (Peters et al., 2017, 2018a) generalize traditional word embedding research along a different dimension. They extract *context-sensitive* features from a left-to-right and a right-to-left language model. The contextual representation of each token is the concatenation of the left-to-right and right-to-left representations. When integrating contextual word embeddings with existing task-specific architectures, ELMo advances the state of the art for several major NLP benchmarks (Peters et al., 2018a) including question answering (Rajpurkar et al., 2016), sentiment analysis (Socher et al., 2013), and named entity recognition (Tjong Kim Sang and De Meulder, 2003). Melamud et al. (2016) proposed learning contextual representations through a task to predict a single word from both left and right context using LSTMs. Similar to ELMo, their model is feature-based and not deeply bidirectional. Fedus et al. (2018) shows that the cloze task can be used to improve the robustness of text generation models.

完形填空.

2.2 Unsupervised Fine-tuning Approaches

As with the feature-based approaches, the first works in this direction only pre-trained word embedding parameters from unlabeled text (Collobert and Weston, 2008).

微调

More recently, sentence or document encoders which produce contextual token representations have been pre-trained from unlabeled text and fine-tuned for a supervised downstream task (Dai and Le, 2015; Howard and Ruder, 2018; Radford et al., 2018). The advantage of these approaches is that few parameters need to be learned from scratch. At least partly due to this advantage, OpenAI GPT (Radford et al., 2018) achieved previously state-of-the-art results on many sentence-level tasks from the GLUE benchmark (Wang et al., 2018a). Left-to-right language model-

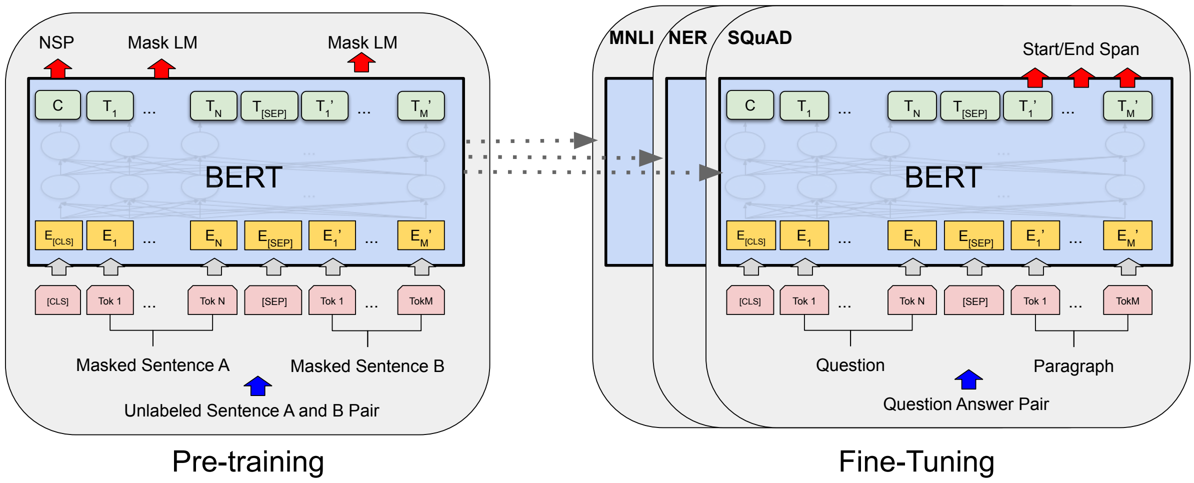

Figure 1: Overall pre-training and fine-tuning procedures for BERT. Apart from output layers, the same architectures are used in both pre-training and fine-tuning. The same pre-trained model parameters are used to initialize models for different down-stream tasks. During fine-tuning, all parameters are fine-tuned. `[CLS]` is a special symbol added in front of every input example, and `[SEP]` is a special separator token (e.g. separating questions/answers).

ing and auto-encoder objectives have been used for pre-training such models (Howard and Ruder, 2018; Radford et al., 2018; Dai and Le, 2015).

2.3 Transfer Learning from Supervised Data

There has also been work showing effective transfer from supervised tasks with large datasets, such as natural language inference (Conneau et al., 2017) and machine translation (McCann et al., 2017). Computer vision research has also demonstrated the importance of transfer learning from large pre-trained models, where an effective recipe is to fine-tune models pre-trained with ImageNet (Deng et al., 2009; Yosinski et al., 2014).

迁移学习

3 BERT

We introduce BERT and its detailed implementation in this section. There are two steps in our framework: *pre-training* and *fine-tuning*. During pre-training, the model is trained on unlabeled data over different pre-training tasks. For fine-tuning, the BERT model is first initialized with the pre-trained parameters, and all of the parameters are fine-tuned using labeled data from the downstream tasks. Each downstream task has separate fine-tuned models, even though they are initialized with the same pre-trained parameters. The question-answering example in Figure 1 will serve as a running example for this section.

A distinctive feature of BERT is its unified architecture across different tasks. There is minimal difference between the pre-trained architecture and the final downstream architecture.

Model Architecture BERT's model architecture is a multi-layer bidirectional Transformer encoder based on the original implementation described in Vaswani et al. (2017) and released in the `tensor2tensor` library.[1] Because the use of Transformers has become common and our implementation is almost identical to the original, we will omit an exhaustive background description of the model architecture and refer readers to Vaswani et al. (2017) as well as excellent guides such as "The Annotated Transformer."[2]

In this work, we denote the number of layers (i.e., Transformer blocks) as L, the hidden size as H, and the number of self-attention heads as A.[3] We primarily report results on two model sizes: $\textbf{BERT}_{\textbf{BASE}}$ (L=12, H=768, A=12, Total Parameters=110M) and $\textbf{BERT}_{\textbf{LARGE}}$ (L=24, H=1024, A=16, Total Parameters=340M).

$\text{BERT}_{\text{BASE}}$ was chosen to have the same model size as OpenAI GPT for comparison purposes. Critically, however, the BERT Transformer uses bidirectional self-attention, while the GPT Transformer uses constrained self-attention where every token can only attend to context to its left.[4]

[1] https://github.com/tensorflow/tensor2tensor

[2] http://nlp.seas.harvard.edu/2018/04/03/attention.html

[3] In all cases we set the feed-forward/filter size to be $4H$, i.e., 3072 for the $H = 768$ and 4096 for the $H = 1024$.

[4] We note that in the literature the bidirectional Trans-

Input/Output Representations To make BERT handle a variety of down-stream tasks, our input representation is able to unambiguously represent both a single sentence and a pair of sentences (e.g., ⟨ Question, Answer ⟩) in one token sequence. Throughout this work, a "sentence" can be an arbitrary span of contiguous text, rather than an actual linguistic sentence. A "sequence" refers to the input token sequence to BERT, which may be a single sentence or two sentences packed together.

We use WordPiece embeddings (Wu et al., 2016) with a 30,000 token vocabulary. The first token of every sequence is always a special classification token (`[CLS]`). The final hidden state corresponding to this token is used as the aggregate sequence representation for classification tasks. Sentence pairs are packed together into a single sequence. We differentiate the sentences in two ways. First, we separate them with a special token (`[SEP]`). Second, we add a learned embedding to every token indicating whether it belongs to sentence `A` or sentence `B`. As shown in Figure 1, we denote input embedding as E, the final hidden vector of the special `[CLS]` token as $C \in \mathbb{R}^H$, and the final hidden vector for the i^{th} input token as $T_i \in \mathbb{R}^H$.

For a given token, its input representation is constructed by summing the corresponding token, segment, and position embeddings. A visualization of this construction can be seen in Figure 2.

3.1 Pre-training BERT

Unlike Peters et al. (2018a) and Radford et al. (2018), we do not use traditional left-to-right or right-to-left language models to pre-train BERT. Instead, we pre-train BERT using two unsupervised tasks, described in this section. This step is presented in the left part of Figure 1.

①掩码语言模型

Task #1: Masked LM Intuitively, it is reasonable to believe that a deep bidirectional model is strictly more powerful than either a left-to-right model or the shallow concatenation of a left-to-right and a right-to-left model. Unfortunately, standard conditional language models can only be trained left-to-right *or* right-to-left, since bidirectional conditioning would allow each word to indirectly "see itself", and the model could trivially predict the target word in a multi-layered context.

In order to train a deep bidirectional representation, we simply mask some percentage of the input tokens at random, and then predict those masked tokens. We refer to this procedure as a "masked LM" (MLM), although it is often referred to as a *Cloze* task in the literature (Taylor, 1953). In this case, the final hidden vectors corresponding to the mask tokens are fed into an output softmax over the vocabulary, as in a standard LM. In all of our experiments, we mask 15% of all WordPiece tokens in each sequence at random. In contrast to denoising auto-encoders (Vincent et al., 2008), we only predict the masked words rather than reconstructing the entire input.

Although this allows us to obtain a bidirectional pre-trained model, a downside is that we are creating a mismatch between pre-training and fine-tuning, since the `[MASK]` token does not appear during fine-tuning. To mitigate this, we do not always replace "masked" words with the actual `[MASK]` token. The training data generator chooses 15% of the token positions at random for prediction. If the i-th token is chosen, we replace the i-th token with (1) the `[MASK]` token 80% of the time (2) a random token 10% of the time (3) the unchanged i-th token 10% of the time. Then, T_i will be used to predict the original token with cross entropy loss. We compare variations of this procedure in Appendix C.2.

Task #2: Next Sentence Prediction (NSP) Many important downstream tasks such as Question Answering (QA) and Natural Language Inference (NLI) are based on understanding the *relationship* between two sentences, which is not directly captured by language modeling. In order to train a model that understands sentence relationships, we pre-train for a binarized *next sentence prediction* task that can be trivially generated from any monolingual corpus. Specifically, when choosing the sentences `A` and `B` for each pre-training example, 50% of the time `B` is the actual next sentence that follows `A` (labeled as `IsNext`), and 50% of the time it is a random sentence from the corpus (labeled as `NotNext`). As we show in Figure 1, C is used for next sentence prediction (NSP).[5] Despite its simplicity, we demonstrate in Section 5.1 that pre-training towards this task is very beneficial to both QA and NLI. [6]

②下一句子预测

former is often referred to as a "Transformer encoder" while the left-context-only version is referred to as a "Transformer decoder" since it can be used for text generation.

[5] The final model achieves 97%-98% accuracy on NSP.

[6] The vector C is not a meaningful sentence representation without fine-tuning, since it was trained with NSP.

分类标记 整个序列的聚合表示 微调中使用 .
Classification Separator 问-答对 分隔标志

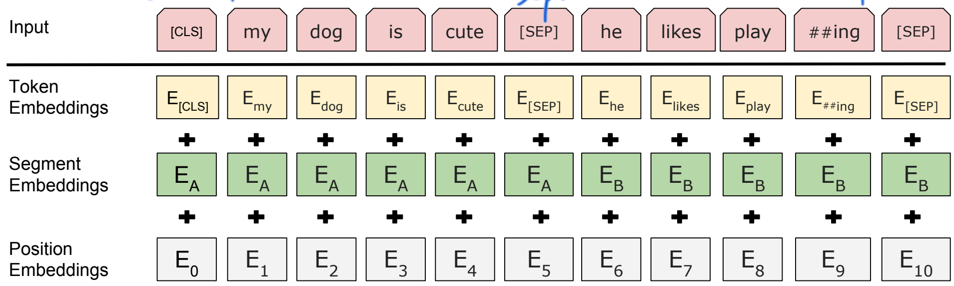

Figure 2: BERT input representation. The input embeddings are the sum of the token embeddings, the segmentation embeddings and the position embeddings.

The NSP task is closely related to representation-learning objectives used in Jernite et al. (2017) and Logeswaran and Lee (2018). However, in prior work, only sentence embeddings are transferred to down-stream tasks, where BERT transfers all parameters to initialize end-task model parameters.

Pre-training data The pre-training procedure largely follows the existing literature on language model pre-training. For the pre-training corpus we use the BooksCorpus (800M words) (Zhu et al., 2015) and English Wikipedia (2,500M words). For Wikipedia we extract only the text passages and ignore lists, tables, and headers. It is critical to use a document-level corpus rather than a shuffled sentence-level corpus such as the Billion Word Benchmark (Chelba et al., 2013) in order to extract long contiguous sequences.

2

3.2 Fine-tuning BERT

Fine-tuning is straightforward since the self-attention mechanism in the Transformer allows BERT to model many downstream tasks—whether they involve single text or text pairs—by swapping out the appropriate inputs and outputs. For applications involving text pairs, a common pattern is to independently encode text pairs before applying bidirectional cross attention, such as Parikh et al. (2016); Seo et al. (2017). BERT instead uses the self-attention mechanism to unify these two stages, as encoding a concatenated text pair with self-attention effectively includes *bidirectional* cross attention between two sentences.

For each task, we simply plug in the task-specific inputs and outputs into BERT and fine-tune all the parameters end-to-end. At the input, sentence `A` and sentence `B` from pre-training are analogous to (1) sentence pairs in paraphrasing, (2) hypothesis-premise pairs in entailment, (3) question-passage pairs in question answering, and (4) a degenerate text-∅ pair in text classification or sequence tagging. At the output, the token representations are fed into an output layer for token-level tasks, such as sequence tagging or question answering, and the `[CLS]` representation is fed into an output layer for classification, such as entailment or sentiment analysis.

(1) 释义 (2) 蕴含
(3) 问答 (4) 分类 序列标注

Compared to pre-training, fine-tuning is relatively inexpensive. All of the results in the paper can be replicated in at most 1 hour on a single Cloud TPU, or a few hours on a GPU, starting from the exact same pre-trained model.[7] We describe the task-specific details in the corresponding subsections of Section 4. More details can be found in Appendix A.5.

4 Experiments

In this section, we present BERT fine-tuning results on 11 NLP tasks.

4.1 GLUE

The General Language Understanding Evaluation (GLUE) benchmark (Wang et al., 2018a) is a collection of diverse natural language understanding tasks. Detailed descriptions of GLUE datasets are included in Appendix B.1.

To fine-tune on GLUE, we represent the input sequence (for single sentence or sentence pairs) as described in Section 3, and use the final hidden vector $C \in \mathbb{R}^H$ corresponding to the first input token (`[CLS]`) as the aggregate representation. The only new parameters introduced during fine-tuning are classification layer weights $W \in \mathbb{R}^{K \times H}$, where K is the number of labels. We compute a standard classification loss with C and W, i.e., $\log(\mathrm{softmax}(CW^T))$.

[7]For example, the BERT SQuAD model can be trained in around 30 minutes on a single Cloud TPU to achieve a Dev F1 score of 91.0%.

[8]See (10) in https://gluebenchmark.com/faq.

System	MNLI-(m/mm)	QQP	QNLI	SST-2	CoLA	STS-B	MRPC	RTE	**Average**
	392k	363k	108k	67k	8.5k	5.7k	3.5k	2.5k	-
Pre-OpenAI SOTA	80.6/80.1	66.1	82.3	93.2	35.0	81.0	86.0	61.7	74.0
BiLSTM+ELMo+Attn	76.4/76.1	64.8	79.8	90.4	36.0	73.3	84.9	56.8	71.0
OpenAI GPT	82.1/81.4	70.3	87.4	91.3	45.4	80.0	82.3	56.0	75.1
$\text{BERT}_{\text{BASE}}$	84.6/83.4	71.2	90.5	93.5	52.1	85.8	88.9	66.4	79.6
$\text{BERT}_{\text{LARGE}}$	**86.7/85.9**	**72.1**	**92.7**	**94.9**	**60.5**	**86.5**	**89.3**	**70.1**	**82.1**

Table 1: GLUE Test results, scored by the evaluation server (`https://gluebenchmark.com/leaderboard`). The number below each task denotes the number of training examples. The "Average" column is slightly different than the official GLUE score, since we exclude the problematic WNLI set.[8] BERT and OpenAI GPT are single-model, single task. F1 scores are reported for QQP and MRPC, Spearman correlations are reported for STS-B, and accuracy scores are reported for the other tasks. We exclude entries that use BERT as one of their components.

We use a batch size of 32 and fine-tune for 3 epochs over the data for all GLUE tasks. For each task, we selected the best fine-tuning learning rate (among 5e-5, 4e-5, 3e-5, and 2e-5) on the Dev set. Additionally, for $\text{BERT}_{\text{LARGE}}$ we found that fine-tuning was sometimes unstable on small datasets, so we ran several random restarts and selected the best model on the Dev set. With random restarts, we use the same pre-trained checkpoint but perform different fine-tuning data shuffling and classifier layer initialization.[9]

Results are presented in Table 1. Both $\text{BERT}_{\text{BASE}}$ and $\text{BERT}_{\text{LARGE}}$ outperform all systems on all tasks by a substantial margin, obtaining 4.5% and 7.0% respective average accuracy improvement over the prior state of the art. Note that $\text{BERT}_{\text{BASE}}$ and OpenAI GPT are nearly identical in terms of model architecture apart from the attention masking. For the largest and most widely reported GLUE task, MNLI, BERT obtains a 4.6% absolute accuracy improvement. On the official GLUE leaderboard[10], $\text{BERT}_{\text{LARGE}}$ obtains a score of 80.5, compared to OpenAI GPT, which obtains 72.8 as of the date of writing.

We find that $\text{BERT}_{\text{LARGE}}$ significantly outperforms $\text{BERT}_{\text{BASE}}$ across all tasks, especially those with very little training data. The effect of model size is explored more thoroughly in Section 5.2.

4.2 SQuAD v1.1

The Stanford Question Answering Dataset (SQuAD v1.1) is a collection of 100k crowd-sourced question/answer pairs (Rajpurkar et al., 2016). Given a question and a passage from Wikipedia containing the answer, the task is to predict the answer text span in the passage.

As shown in Figure 1, in the question answering task, we represent the input question and passage as a single packed sequence, with the question using the A embedding and the passage using the B embedding. We only introduce a start vector $S \in \mathbb{R}^H$ and an end vector $E \in \mathbb{R}^H$ during fine-tuning. The probability of word i being the start of the answer span is computed as a dot product between T_i and S followed by a softmax over all of the words in the paragraph: $P_i = \frac{e^{S \cdot T_i}}{\sum_j e^{S \cdot T_j}}$. The analogous formula is used for the end of the answer span. The score of a candidate span from position i to position j is defined as $S{\cdot}T_i + E{\cdot}T_j$, and the maximum scoring span where $j \geq i$ is used as a prediction. The training objective is the sum of the log-likelihoods of the correct start and end positions. We fine-tune for 3 epochs with a learning rate of 5e-5 and a batch size of 32.

Table 2 shows top leaderboard entries as well as results from top published systems (Seo et al., 2017; Clark and Gardner, 2018; Peters et al., 2018a; Hu et al., 2018). The top results from the SQuAD leaderboard do not have up-to-date public system descriptions available,[11] and are allowed to use any public data when training their systems. We therefore use modest data augmentation in our system by first fine-tuning on TriviaQA (Joshi et al., 2017) befor fine-tuning on SQuAD.

Our best performing system outperforms the top leaderboard system by +1.5 F1 in ensembling and +1.3 F1 as a single system. In fact, our single BERT model outperforms the top ensemble system in terms of F1 score. Without TriviaQA fine-

[9]The GLUE data set distribution does not include the Test labels, and we only made a single GLUE evaluation server submission for each of $\text{BERT}_{\text{BASE}}$ and $\text{BERT}_{\text{LARGE}}$.

[10]https://gluebenchmark.com/leaderboard

[11]QANet is described in Yu et al. (2018), but the system has improved substantially after publication.

System	Dev EM	Dev F1	Test EM	Test F1
Top Leaderboard Systems (Dec 10th, 2018)				
Human	-	-	82.3	91.2
#1 Ensemble - nlnet	-	-	86.0	91.7
#2 Ensemble - QANet	-	-	84.5	90.5
Published				
BiDAF+ELMo (Single)	-	85.6	-	85.8
R.M. Reader (Ensemble)	81.2	87.9	82.3	88.5
Ours				
$\text{BERT}_{\text{BASE}}$ (Single)	80.8	88.5	-	-
$\text{BERT}_{\text{LARGE}}$ (Single)	84.1	90.9	-	-
$\text{BERT}_{\text{LARGE}}$ (Ensemble)	85.8	91.8	-	-
$\text{BERT}_{\text{LARGE}}$ (Sgl.+TriviaQA)	**84.2**	**91.1**	**85.1**	**91.8**
$\text{BERT}_{\text{LARGE}}$ (Ens.+TriviaQA)	**86.2**	**92.2**	**87.4**	**93.2**

Table 2: SQuAD 1.1 results. The BERT ensemble is 7x systems which use different pre-training checkpoints and fine-tuning seeds.

System	Dev EM	Dev F1	Test EM	Test F1
Top Leaderboard Systems (Dec 10th, 2018)				
Human	86.3	89.0	86.9	89.5
#1 Single - MIR-MRC (F-Net)	-	-	74.8	78.0
#2 Single - nlnet	-	-	74.2	77.1
Published				
unet (Ensemble)	-	-	71.4	74.9
SLQA+ (Single)	-		71.4	74.4
Ours				
$\text{BERT}_{\text{LARGE}}$ (Single)	78.7	81.9	80.0	83.1

Table 3: SQuAD 2.0 results. We exclude entries that use BERT as one of their components.

tuning data, we only lose 0.1-0.4 F1, still outperforming all existing systems by a wide margin.[12]

4.3 SQuAD v2.0

The SQuAD 2.0 task extends the SQuAD 1.1 problem definition by allowing for the possibility that no short answer exists in the provided paragraph, making the problem more realistic.

We use a simple approach to extend the SQuAD v1.1 BERT model for this task. We treat questions that do not have an answer as having an answer span with start and end at the `[CLS]` token. The probability space for the start and end answer span positions is extended to include the position of the `[CLS]` token. For prediction, we compare the score of the no-answer span: $s_{\texttt{null}} = S{\cdot}C + E{\cdot}C$ to the score of the best non-null span $\hat{s_{i,j}} = \texttt{max}_{j \geq i} S{\cdot}T_i + E{\cdot}T_j$. We predict a non-null answer when $\hat{s_{i,j}} > s_{\texttt{null}} + \tau$, where the threshold τ is selected on the dev set to maximize F1. We did not use TriviaQA data for this model. We fine-tuned for 2 epochs with a learning rate of 5e-5 and a batch size of 48.

The results compared to prior leaderboard entries and top published work (Sun et al., 2018; Wang et al., 2018b) are shown in Table 3, excluding systems that use BERT as one of their components. We observe a +5.1 F1 improvement over the previous best system.

[12]The TriviaQA data we used consists of paragraphs from TriviaQA-Wiki formed of the first 400 tokens in documents, that contain at least one of the provided possible answers.

System	Dev	Test
ESIM+GloVe	51.9	52.7
ESIM+ELMo	59.1	59.2
OpenAI GPT	-	78.0
$\text{BERT}_{\text{BASE}}$	81.6	-
$\text{BERT}_{\text{LARGE}}$	**86.6**	**86.3**
Human (expert)†	-	85.0
Human (5 annotations)†	-	88.0

Table 4: SWAG Dev and Test accuracies. †Human performance is measured with 100 samples, as reported in the SWAG paper.

4.4 SWAG

The Situations With Adversarial Generations (SWAG) dataset contains 113k sentence-pair completion examples that evaluate grounded commonsense inference (Zellers et al., 2018). Given a sentence, the task is to choose the most plausible continuation among four choices.

When fine-tuning on the SWAG dataset, we construct four input sequences, each containing the concatenation of the given sentence (sentence `A`) and a possible continuation (sentence `B`). The only task-specific parameters introduced is a vector whose dot product with the `[CLS]` token representation C denotes a score for each choice which is normalized with a softmax layer.

We fine-tune the model for 3 epochs with a learning rate of 2e-5 and a batch size of 16. Results are presented in Table 4. $\text{BERT}_{\text{LARGE}}$ outperforms the authors' baseline ESIM+ELMo system by +27.1% and OpenAI GPT by 8.3%.

5 Ablation Studies

In this section, we perform ablation experiments over a number of facets of BERT in order to better understand their relative importance. Additional

Tasks	MNLI-m (Acc)	QNLI (Acc)	MRPC (Acc)	SST-2 (Acc)	SQuAD (F1)
	Dev Set				
$\text{BERT}_{\text{BASE}}$	84.4	88.4	86.7	92.7	88.5
No NSP	83.9	84.9	86.5	92.6	87.9
LTR & No NSP	82.1	84.3	77.5	92.1	77.8
+ BiLSTM	82.1	84.1	75.7	91.6	84.9

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增加随机初始化的双向. 效果下降.

Table 5: Ablation over the pre-training tasks using the $\text{BERT}_{\text{BASE}}$ architecture. "No NSP" is trained without the next sentence prediction task. "LTR & No NSP" is trained as a left-to-right LM without the next sentence prediction, like OpenAI GPT. "+ BiLSTM" adds a randomly initialized BiLSTM on top of the "LTR + No NSP" model during fine-tuning.

ablation studies can be found in Appendix C.

5.1 Effect of Pre-training Tasks

We demonstrate the importance of the deep bidirectionality of BERT by evaluating two pre-training objectives using exactly the same pre-training data, fine-tuning scheme, and hyperparameters as $\text{BERT}_{\text{BASE}}$:

No NSP: A bidirectional model which is trained using the "masked LM" (MLM) but without the "next sentence prediction" (NSP) task.

LTR & No NSP: A left-context-only model which is trained using a standard Left-to-Right (LTR) LM, rather than an MLM. The left-only constraint was also applied at fine-tuning, because removing it introduced a pre-train/fine-tune mismatch that degraded downstream performance. Additionally, this model was pre-trained without the NSP task. This is directly comparable to OpenAI GPT, but using our larger training dataset, our input representation, and our fine-tuning scheme.

We first examine the impact brought by the NSP task. In Table 5, we show that removing NSP hurts performance significantly on QNLI, MNLI, and SQuAD 1.1. Next, we evaluate the impact of training bidirectional representations by comparing "No NSP" to "LTR & No NSP". The LTR model performs worse than the MLM model on all tasks, with large drops on MRPC and SQuAD.

For SQuAD it is intuitively clear that a LTR model will perform poorly at token predictions, since the token-level hidden states have no right-side context. In order to make a good faith attempt at strengthening the LTR system, we added a randomly initialized BiLSTM on top. This does significantly improve results on SQuAD, but the results are still far worse than those of the pre-trained bidirectional models. The BiLSTM hurts performance on the GLUE tasks.

We recognize that it would also be possible to train separate LTR and RTL models and represent each token as the concatenation of the two models, as ELMo does. However: (a) this is twice as expensive as a single bidirectional model; (b) this is non-intuitive for tasks like QA, since the RTL model would not be able to condition the answer on the question; (c) this it is strictly less powerful than a deep bidirectional model, since it can use both left and right context at every layer.

5.2 Effect of Model Size

In this section, we explore the effect of model size on fine-tuning task accuracy. We trained a number of BERT models with a differing number of layers, hidden units, and attention heads, while otherwise using the same hyperparameters and training procedure as described previously.

Results on selected GLUE tasks are shown in Table 6. In this table, we report the average Dev Set accuracy from 5 random restarts of fine-tuning. We can see that larger models lead to a strict accuracy improvement across all four datasets, even for MRPC which only has 3,600 labeled training examples, and is substantially different from the pre-training tasks. It is also perhaps surprising that we are able to achieve such significant improvements on top of models which are already quite large relative to the existing literature. For example, the largest Transformer explored in Vaswani et al. (2017) is (L=6, H=1024, A=16) with 100M parameters for the encoder, and the largest Transformer we have found in the literature is (L=64, H=512, A=2) with 235M parameters (Al-Rfou et al., 2018). By contrast, $\text{BERT}_{\text{BASE}}$ contains 110M parameters and $\text{BERT}_{\text{LARGE}}$ contains 340M parameters.

It has long been known that increasing the model size will lead to continual improvements on large-scale tasks such as machine translation and language modeling, which is demonstrated by the LM perplexity of held-out training data shown in Table 6. However, we believe that this is the first work to demonstrate convincingly that scaling to extreme model sizes also leads to large improvements on very small scale tasks, provided that the model has been sufficiently pre-trained. Peters et al. (2018b) presented mixed results on the downstream task impact of increasing the pre-trained bi-LM size from two to four layers and Melamud et al. (2016) mentioned in passing that increasing hidden dimension size from 200 to 600 helped, but increasing further to 1,000 did not bring further improvements. Both of these prior works used a feature-based approach — we hypothesize that when the model is fine-tuned directly on the downstream tasks and uses only a very small number of randomly initialized additional parameters, the task-specific models can benefit from the larger, more expressive pre-trained representations even when downstream task data is very small.

5.3 Feature-based Approach with BERT

All of the BERT results presented so far have used the fine-tuning approach, where a simple classification layer is added to the pre-trained model, and all parameters are jointly fine-tuned on a downstream task. However, the feature-based approach, where fixed features are extracted from the pre-trained model, has certain advantages. First, not all tasks can be easily represented by a Transformer encoder architecture, and therefore require a task-specific model architecture to be added. Second, there are major computational benefits to pre-compute an expensive representation of the training data once and then run many experiments with cheaper models on top of this representation.

In this section, we compare the two approaches by applying BERT to the CoNLL-2003 Named Entity Recognition (NER) task (Tjong Kim Sang and De Meulder, 2003). In the input to BERT, we use a case-preserving WordPiece model, and we include the maximal document context provided by the data. Following standard practice, we formulate this as a tagging task but do not use a CRF

Hyperparams				Dev Set Accuracy		
#L	#H	#A	LM (ppl)	MNLI-m	MRPC	SST-2
3	768	12	5.84	77.9	79.8	88.4
6	768	3	5.24	80.6	82.2	90.7
6	768	12	4.68	81.9	84.8	91.3
12	768	12	3.99	84.4	86.7	92.9
12	1024	16	3.54	85.7	86.9	93.3
24	1024	16	3.23	86.6	87.8	93.7

Table 6: Ablation over BERT model size. #L = the number of layers; #H = hidden size; #A = number of attention heads. "LM (ppl)" is the masked LM perplexity of held-out training data.

类比验证集
Development Set

System	Dev F1	Test F1
ELMo (Peters et al., 2018a)	95.7	92.2
CVT (Clark et al., 2018)	-	92.6
CSE (Akbik et al., 2018)	-	**93.1**
Fine-tuning approach		
$\text{BERT}_{\text{LARGE}}$	96.6	92.8
$\text{BERT}_{\text{BASE}}$	96.4	92.4
Feature-based approach ($\text{BERT}_{\text{BASE}}$)		
Embeddings	91.0	-
Second-to-Last Hidden	95.6	-
Last Hidden	94.9	-
Weighted Sum Last Four Hidden	95.9	-
Concat Last Four Hidden	96.1	-
Weighted Sum All 12 Layers	95.5	-

Table 7: CoNLL-2003 Named Entity Recognition results. Hyperparameters were selected using the Dev set. The reported Dev and Test scores are averaged over 5 random restarts using those hyperparameters.

layer in the output. We use the representation of the first sub-token as the input to the token-level classifier over the NER label set.

To ablate the fine-tuning approach, we apply the feature-based approach by extracting the activations from one or more layers *without* fine-tuning any parameters of BERT. These contextual embeddings are used as input to a randomly initialized two-layer 768-dimensional BiLSTM before the classification layer.

Results are presented in Table 7. $\text{BERT}_{\text{LARGE}}$ performs competitively with state-of-the-art methods. The best performing method concatenates the token representations from the top four hidden layers of the pre-trained Transformer, which is only 0.3 F1 behind fine-tuning the entire model. This demonstrates that BERT is effective for both fine-tuning and feature-based approaches.

6 Conclusion

Recent empirical improvements due to transfer learning with language models have demonstrated that rich, unsupervised pre-training is an integral part of many language understanding systems. In particular, these results enable even low-resource tasks to benefit from deep unidirectional architectures. Our major contribution is further generalizing these findings to deep *bidirectional* architectures, allowing the same pre-trained model to successfully tackle a broad set of NLP tasks.

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Appendix for "BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding"

We organize the appendix into three sections:

- Additional implementation details for BERT are presented in Appendix A;
- Additional details for our experiments are presented in Appendix B; and
- Additional ablation studies are presented in Appendix C.

  We present additional ablation studies for BERT including:

  – Effect of Number of Training Steps; and
  – Ablation for Different Masking Procedures.

A Additional Details for BERT

A.1 Illustration of the Pre-training Tasks

We provide examples of the pre-training tasks in the following.

Masked LM and the Masking Procedure Assuming the unlabeled sentence is `my dog is hairy`, and during the random masking procedure we chose the 4-th token (which corresponding to `hairy`), our masking procedure can be further illustrated by

- 80% of the time: Replace the word with the `[MASK]` token, e.g., `my dog is hairy` → `my dog is [MASK]`
- 10% of the time: Replace the word with a random word, e.g., `my dog is hairy` → `my dog is apple`
- 10% of the time: Keep the word unchanged, e.g., `my dog is hairy` → `my dog is hairy`. The purpose of this is to bias the representation towards the actual observed word.

The advantage of this procedure is that the Transformer encoder does not know which words it will be asked to predict or which have been replaced by random words, so it is forced to keep a distributional contextual representation of *every* input token. Additionally, because random replacement only occurs for 1.5% of all tokens (i.e., 10% of 15%), this does not seem to harm the model's language understanding capability. In Section C.2, we evaluate the impact this procedure.

Compared to standard langauge model training, the masked LM only make predictions on 15% of tokens in each batch, which suggests that more pre-training steps may be required for the model

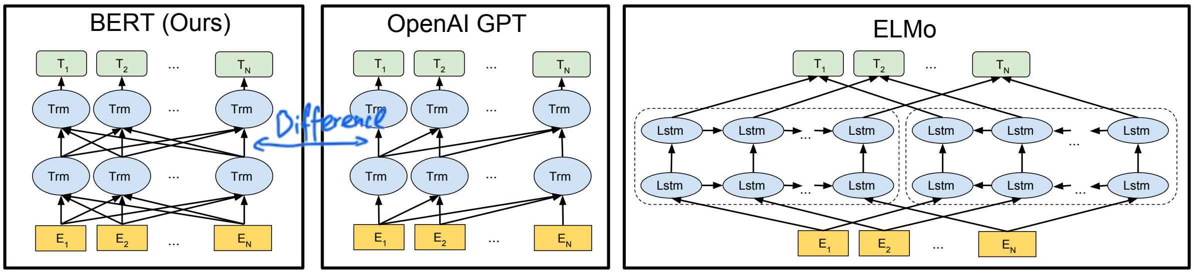

Figure 3: Differences in pre-training model architectures. BERT uses a bidirectional Transformer. OpenAI GPT uses a left-to-right Transformer. ELMo uses the concatenation of independently trained left-to-right and right-to-left LSTMs to generate features for downstream tasks. Among the three, only BERT representations are jointly conditioned on both left and right context in all layers. In addition to the architecture differences, BERT and OpenAI GPT are fine-tuning approaches, while ELMo is a feature-based approach.

to converge. In Section C.1 we demonstrate that MLM does converge marginally slower than a left-to-right model (which predicts every token), but the empirical improvements of the MLM model far outweigh the increased training cost.

Next Sentence Prediction The next sentence prediction task can be illustrated in the following examples.

Input = `[CLS] the man went to [MASK] store [SEP]`
`he bought a gallon [MASK] milk [SEP]`
Label = `IsNext`

Input = `[CLS] the man [MASK] to the store [SEP]`
`penguin [MASK] are flight ##less birds [SEP]`
Label = `NotNext`

A.2 Pre-training Procedure

To generate each training input sequence, we sample two spans of text from the corpus, which we refer to as "sentences" even though they are typically much longer than single sentences (but can be shorter also). The first sentence receives the A embedding and the second receives the B embedding. 50% of the time B is the actual next sentence that follows A and 50% of the time it is a random sentence, which is done for the "next sentence prediction" task. They are sampled such that the combined length is $\leq$ 512 tokens. The LM masking is applied after WordPiece tokenization with a uniform masking rate of 15%, and no special consideration given to partial word pieces.

We train with batch size of 256 sequences (256 sequences * 512 tokens = 128,000 tokens/batch) for 1,000,000 steps, which is approximately 40 epochs over the 3.3 billion word corpus. We use Adam with learning rate of 1e-4, $\beta_1 = 0.9$, $\beta_2 = 0.999$, L2 weight decay of 0.01, learning rate warmup over the first 10,000 steps, and linear decay of the learning rate. We use a dropout probability of 0.1 on all layers. We use a `gelu` activation (Hendrycks and Gimpel, 2016) rather than the standard `relu`, following OpenAI GPT. The training loss is the sum of the mean masked LM likelihood and the mean next sentence prediction likelihood.

Training of $\text{BERT}_{\text{BASE}}$ was performed on 4 Cloud TPUs in Pod configuration (16 TPU chips total).[13] Training of $\text{BERT}_{\text{LARGE}}$ was performed on 16 Cloud TPUs (64 TPU chips total). Each pre-training took 4 days to complete.

Longer sequences are disproportionately expensive because attention is quadratic to the sequence length. To speed up pretraing in our experiments, we pre-train the model with sequence length of 128 for 90% of the steps. Then, we train the rest 10% of the steps of sequence of 512 to learn the positional embeddings.

A.3 Fine-tuning Procedure

For fine-tuning, most model hyperparameters are the same as in pre-training, with the exception of the batch size, learning rate, and number of training epochs. The dropout probability was always kept at 0.1. The optimal hyperparameter values are task-specific, but we found the following range of possible values to work well across all tasks:

- **Batch size**: 16, 32

[13]https://cloudplatform.googleblog.com/2018/06/Cloud-TPU-now-offers-preemptible-pricing-and-global-availability.html

- **Learning rate (Adam)**: 5e-5, 3e-5, 2e-5
- **Number of epochs**: 2, 3, 4

We also observed that large data sets (e.g., 100k+ labeled training examples) were far less sensitive to hyperparameter choice than small data sets. Fine-tuning is typically very fast, so it is reasonable to simply run an exhaustive search over the above parameters and choose the model that performs best on the development set.

A.4 Comparison of BERT, ELMo ,and OpenAI GPT

Here we studies the differences in recent popular representation learning models including ELMo, OpenAI GPT and BERT. The comparisons between the model architectures are shown visually in Figure 3. Note that in addition to the architecture differences, BERT and OpenAI GPT are fine-tuning approaches, while ELMo is a feature-based approach.

The most comparable existing pre-training method to BERT is OpenAI GPT, which trains a left-to-right Transformer LM on a large text corpus. In fact, many of the design decisions in BERT were intentionally made to make it as close to GPT as possible so that the two methods could be minimally compared. The core argument of this work is that the bi-directionality and the two pre-training tasks presented in Section 3.1 account for the majority of the empirical improvements, but we do note that there are several other differences between how BERT and GPT were trained:

- GPT is trained on the BooksCorpus (800M words); BERT is trained on the BooksCorpus (800M words) and Wikipedia (2,500M words).

- GPT uses a sentence separator (`[SEP]`) and classifier token (`[CLS]`) which are only introduced at fine-tuning time; BERT learns `[SEP]`, `[CLS]` and sentence A/B embeddings during pre-training.

- GPT was trained for 1M steps with a batch size of 32,000 words; BERT was trained for 1M steps with a batch size of 128,000 words.

- GPT used the same learning rate of 5e-5 for all fine-tuning experiments; BERT chooses a task-specific fine-tuning learning rate which performs the best on the development set.

To isolate the effect of these differences, we perform ablation experiments in Section 5.1 which demonstrate that the majority of the improvements are in fact coming from the two pre-training tasks and the bidirectionality they enable.

A.5 Illustrations of Fine-tuning on Different Tasks

The illustration of fine-tuning BERT on different tasks can be seen in Figure 4. Our task-specific models are formed by incorporating BERT with one additional output layer, so a minimal number of parameters need to be learned from scratch. Among the tasks, (a) and (b) are sequence-level tasks while (c) and (d) are token-level tasks. In the figure, E represents the input embedding, T_i represents the contextual representation of token i, [CLS] is the special symbol for classification output, and [SEP] is the special symbol to separate non-consecutive token sequences.

B Detailed Experimental Setup

B.1 Detailed Descriptions for the GLUE Benchmark Experiments.

Our GLUE results in Table1 are obtained from `https://gluebenchmark.com/leaderboard` and `https://blog.openai.com/language-unsupervised`. The GLUE benchmark includes the following datasets, the descriptions of which were originally summarized in Wang et al. (2018a):

MNLI Multi-Genre Natural Language Inference is a large-scale, crowdsourced entailment classification task (Williams et al., 2018). Given a pair of sentences, the goal is to predict whether the second sentence is an *entailment*, *contradiction*, or *neutral* with respect to the first one.

QQP Quora Question Pairs is a binary classification task where the goal is to determine if two questions asked on Quora are semantically equivalent (Chen et al., 2018).

QNLI Question Natural Language Inference is a version of the Stanford Question Answering Dataset (Rajpurkar et al., 2016) which has been converted to a binary classification task (Wang et al., 2018a). The positive examples are (question, sentence) pairs which do contain the correct answer, and the negative examples are (question, sentence) from the same paragraph which do not contain the answer.

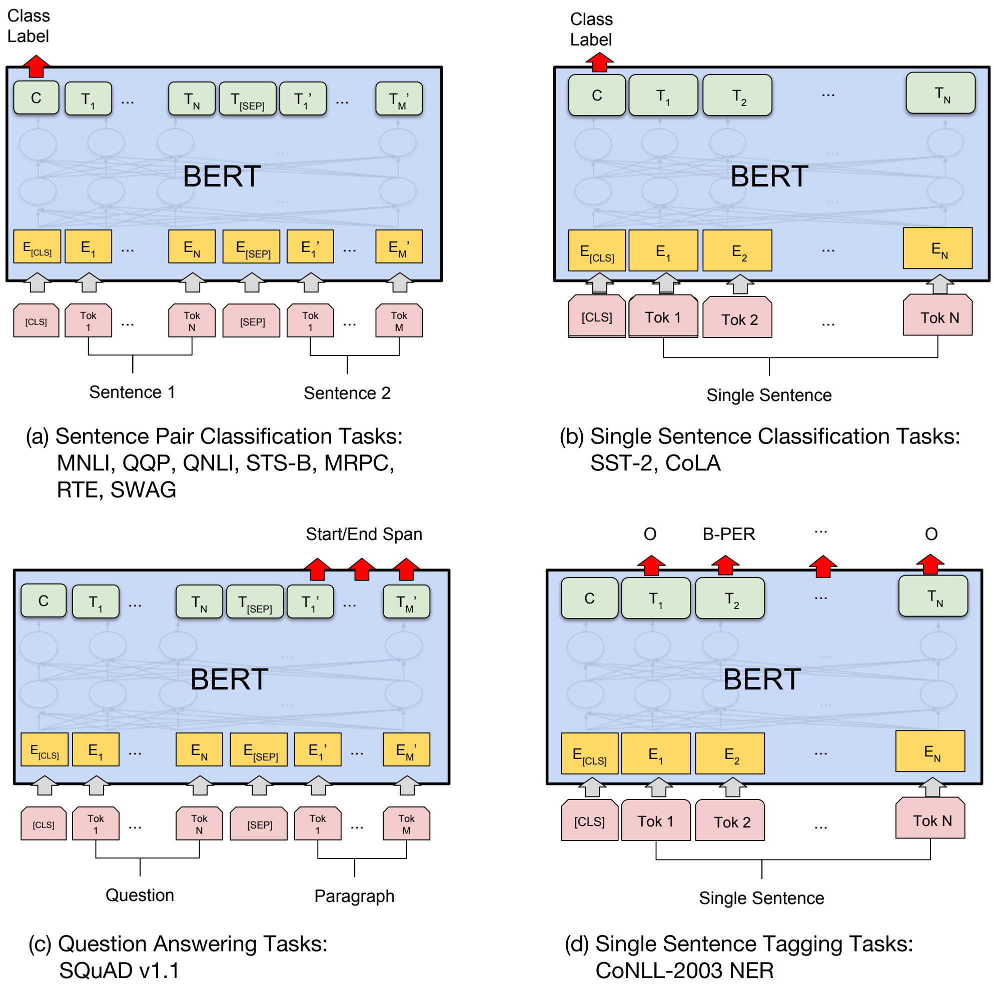

Figure 4: Illustrations of Fine-tuning BERT on Different Tasks.

SST-2 The Stanford Sentiment Treebank is a binary single-sentence classification task consisting of sentences extracted from movie reviews with human annotations of their sentiment (Socher et al., 2013).

CoLA The Corpus of Linguistic Acceptability is a binary single-sentence classification task, where the goal is to predict whether an English sentence is linguistically "acceptable" or not (Warstadt et al., 2018).

STS-B The Semantic Textual Similarity Benchmark is a collection of sentence pairs drawn from news headlines and other sources (Cer et al., 2017). They were annotated with a score from 1 to 5 denoting how similar the two sentences are in terms of semantic meaning.

MRPC Microsoft Research Paraphrase Corpus consists of sentence pairs automatically extracted from online news sources, with human annotations for whether the sentences in the pair are semantically equivalent (Dolan and Brockett, 2005).

RTE Recognizing Textual Entailment is a binary entailment task similar to MNLI, but with much less training data (Bentivogli et al., 2009).[14]

WNLI Winograd NLI is a small natural language inference dataset (Levesque et al., 2011). The GLUE webpage notes that there are issues with the construction of this dataset, [15] and every trained system that's been submitted to GLUE has performed worse than the 65.1 baseline accuracy of predicting the majority class. We therefore exclude this set to be fair to OpenAI GPT. For our GLUE submission, we always predicted the ma-

[14]Note that we only report single-task fine-tuning results in this paper. A multitask fine-tuning approach could potentially push the performance even further. For example, we did observe substantial improvements on RTE from multitask training with MNLI.

[15]https://gluebenchmark.com/faq

jority class.

C Additional Ablation Studies

C.1 Effect of Number of Training Steps

Figure 5 presents MNLI Dev accuracy after fine-tuning from a checkpoint that has been pre-trained for k steps. This allows us to answer the following questions:

1. Question: Does BERT really need such a large amount of pre-training (128,000 words/batch * 1,000,000 steps) to achieve high fine-tuning accuracy?
   Answer: Yes, $\text{BERT}_{\text{BASE}}$ achieves almost 1.0% additional accuracy on MNLI when trained on 1M steps compared to 500k steps.

2. Question: Does MLM pre-training converge slower than LTR pre-training, since only 15% of words are predicted in each batch rather than every word?
   Answer: The MLM model does converge slightly slower than the LTR model. However, in terms of absolute accuracy the MLM model begins to outperform the LTR model almost immediately.

C.2 Ablation for Different Masking Procedures

In Section 3.1, we mention that BERT uses a mixed strategy for masking the target tokens when pre-training with the masked language model (MLM) objective. The following is an ablation study to evaluate the effect of different masking strategies.

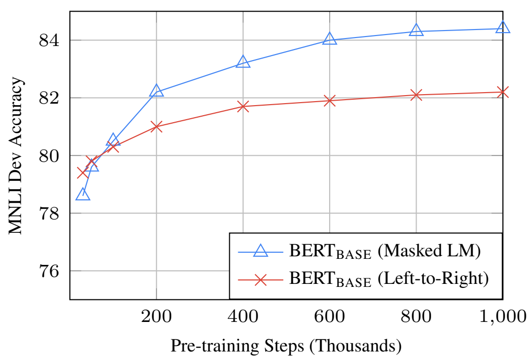

Figure 5: Ablation over number of training steps. This shows the MNLI accuracy after fine-tuning, starting from model parameters that have been pre-trained for k steps. The x-axis is the value of k.

Note that the purpose of the masking strategies is to reduce the mismatch between pre-training and fine-tuning, as the [MASK] symbol never appears during the fine-tuning stage. We report the Dev results for both MNLI and NER. For NER, we report both fine-tuning and feature-based approaches, as we expect the mismatch will be amplified for the feature-based approach as the model will not have the chance to adjust the representations.

Masking Rates			Dev Set Results		
MASK	SAME	RND	MNLI Fine-tune	NER Fine-tune	NER Feature-based
80%	10%	10%	84.2	95.4	94.9
100%	0%	0%	84.3	94.9	94.0
80%	0%	20%	84.1	95.2	94.6
80%	20%	0%	84.4	95.2	94.7
0%	20%	80%	83.7	94.8	94.6
0%	0%	100%	83.6	94.9	94.6

Table 8: Ablation over different masking strategies.

The results are presented in Table 8. In the table, MASK means that we replace the target token with the [MASK] symbol for MLM; SAME means that we keep the target token as is; RND means that we replace the target token with another random token.

The numbers in the left part of the table represent the probabilities of the specific strategies used during MLM pre-training (BERT uses 80%, 10%, 10%). The right part of the paper represents the Dev set results. For the feature-based approach, we concatenate the last 4 layers of BERT as the features, which was shown to be the best approach in Section 5.3.

From the table it can be seen that fine-tuning is surprisingly robust to different masking strategies. However, as expected, using only the MASK strategy was problematic when applying the feature-based approach to NER. Interestingly, using only the RND strategy performs much worse than our strategy as well.