Transformer review By Qiao

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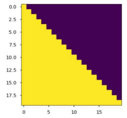
Credit:

- [The Annotated Transformer]
- [The Illustrated Transformer]
- [Attention Is All You Need]

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

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




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

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

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

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

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

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

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

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

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

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

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

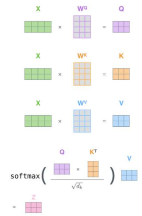
```python
class MyIterator(data.Iterator):
    def create_batches(self):
        if self.train:
            def pool(d, random_shuffler):
                for p in data.batch(d, self.batch_size * 100):
                    p_batch = data.batch(
                        sorted(p, key=self.sort_key),
   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

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

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

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

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

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

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

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

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

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

"We suspect that for large values of dk, 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 $\frac{1}{\sqrt{d_k}}$."

--- (Attention is all you need)

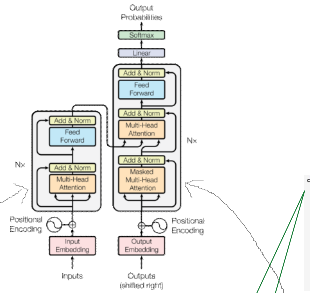
$$\mathrm{Attention}(Q,K,V) = \mathrm{softmax}(\frac{QK^T}{\sqrt{d_k}})V$$




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

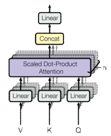
```python
def clones(module, N):
    "Produce N identical layers."
    return nn.ModuleList([copy.deepcopy(module) for _ in range(N)])
```

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

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




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

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

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

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

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

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

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




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

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

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

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

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

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

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

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

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

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

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

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

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

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

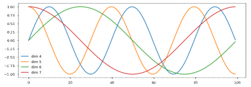
```python
class Embeddings(nn.Module):
    def __init__(self, d_model, vocab):
        super(Embeddings, self).__init__()
        self.lut = nn.Embedding(vocab, d_model)
        self.d_model = d_model

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

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

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

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

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

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

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

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

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




```python
        m = memory
        x = self.sublayer[0](x, lambda x: self.self_attn(x, x, x, tgt_mask))
        x = self.sublayer[1](x, lambda x: self.src_attn(x, m, m, src_mask))
        return self.sublayer[2](x, self.feed_forward)
```

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

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