Note

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Transformer as a Graph Neural Network

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Warning

The tutorial aims at gaining insights into the paper, with code as a mean of explanation. The implementation thus is NOT optimized for running efficiency. For recommended implementation, please refer to the official examples.

In this tutorial, you learn about a simplified implementation of the Transformer model. You can see highlights of the most important design points. For instance, there is only single-head attention. The complete code can be found here.

The overall structure is similar to the one from the research papaer Annotated Transformer.

The Transformer model, as a replacement of CNN/RNN architecture for sequence modeling, was introduced in the research paper: Attention is All You Need. It improved the state of the art for machine translation as well as natural language inference task (GPT). Recent work on pre-training Transformer with large scale corpus (BERT) supports that it is capable of learning high-quality semantic representation.

The interesting part of Transformer is its extensive employment of attention. The classic use of attention comes from machine translation model, where the output token attends to all input tokens.

Transformer additionally applies *self-attention* in both decoder and encoder. This process forces words relate to each other to combine together, irrespective of their positions in the sequence. This is different from RNN-based model, where words (in the source sentence) are combined along the chain, which is thought to be too constrained.

Attention layer of Transformer

In the attention layer of Transformer, for each node the module learns to assign weights on its in-coming edges. For node pair (i, j) (from i to j) with node $x_i, x_j \in \mathbb{R}^n$, the score of their connection is defined as follows:

$$\begin{aligned} q_j &= W_q \cdot x_j \\ k_i &= W_k \cdot x_i \\ v_i &= W_v \cdot x_i \\ \text{score} &= q_j^T k_i \end{aligned}$$

where $W_q, W_k, W_v \in \mathbb{R}^{n \times d_k}$ map the representations x to "query", "key", and "value" space respectively.

There are other possibilities to implement the score function. The dot product measures the similarity of a given query q_j and a key k_i: if j needs the information stored in i, the query vector at position j (q_j) is supposed to be close to key vector at position i (k_i).

The score is then used to compute the sum of the incoming values, normalized over the weights of edges, stored in wv. Then apply an affine layer to wv to get the output o:

$$\begin{aligned} w_{ji} &= \frac{\exp\{\text{score}_{ji}\}}{\sum\limits_{(k,i)\in E} \exp\{\text{score}_{ki}\}} \\ \mathrm{wv}_i &= \sum_{(k,i)\in E} w_{ki} v_k \\ o &= W_o \cdot \mathrm{wv} \end{aligned}$$

Multi-head attention layer

In Transformer, attention is *multi-headed*. A head is very much like a channel in a convolutional network. The multi-head attention consists of multiple attention heads, in which each head refers to a single attention module. $\mathrm{wv}^{(i)}$ for all the heads are concatenated and mapped to output o with an affine layer:

$$o = W_o \cdot \text{concat}\left(\left[\mathrm{wv}^{(0)}, \mathrm{wv}^{(1)}, \cdots, \mathrm{wv}^{(h)}\right]\right)$$

The code below wraps necessary components for multi-head attention, and provides two interfaces.

- `get` maps state 'x', to query, key and value, which is required by following steps(`propagate_attention`).
- `get_o` maps the updated value after attention to the output o for post-processing.

```python
class MultiHeadAttention(nn.Module):
    "Multi-Head Attention"
    def __init__(self, h, dim_model):
        "h: number of heads; dim_model: hidden dimension"
        super(MultiHeadAttention, self).__init__()
        self.d_k = dim_model // h
        self.h = h
        # W_q, W_k, W_v, W_o
        self.linears = clones(nn.Linear(dim_model, dim_model), 4)

    def get(self, x, fields='qkv'):
        "Return a dict of queries / keys / values."
        batch_size = x.shape[0]
        ret = {}
        if 'q' in fields:
            ret['q'] = self.linears[0](x).view(batch_size, self.h, self.d_k)
        if 'k' in fields:
            ret['k'] = self.linears[1](x).view(batch_size, self.h, self.d_k)
        if 'v' in fields:
            ret['v'] = self.linears[2](x).view(batch_size, self.h, self.d_k)
        return ret

    def get_o(self, x):
        "get output of the multi-head attention"
        batch_size = x.shape[0]
        return self.linears[3](x.view(batch_size, -1))
```

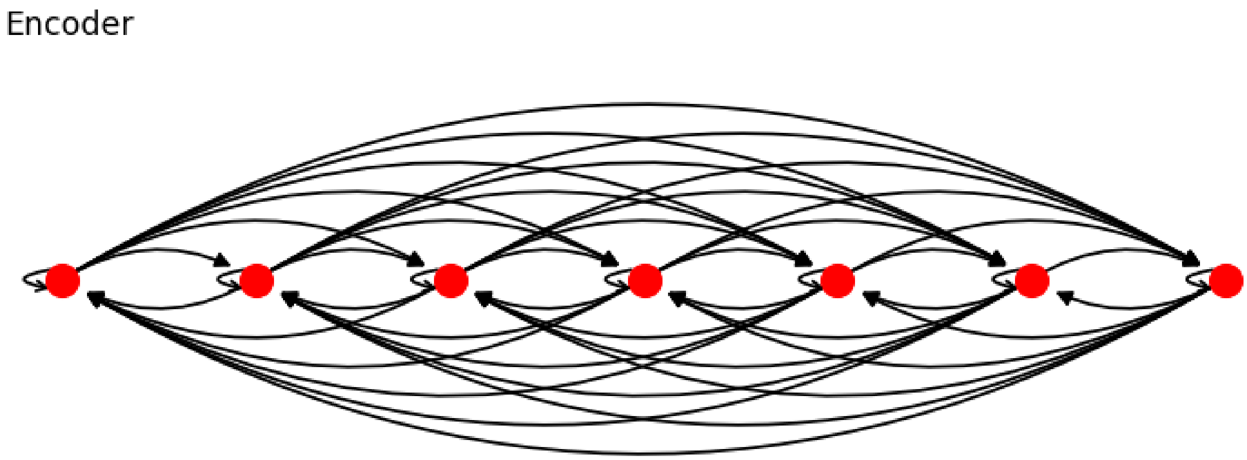
How DGL implements Transformer with a graph neural network

You get a different perspective of Transformer by treating the attention as edges in a graph and adopt message passing on the edges to induce the appropriate processing.

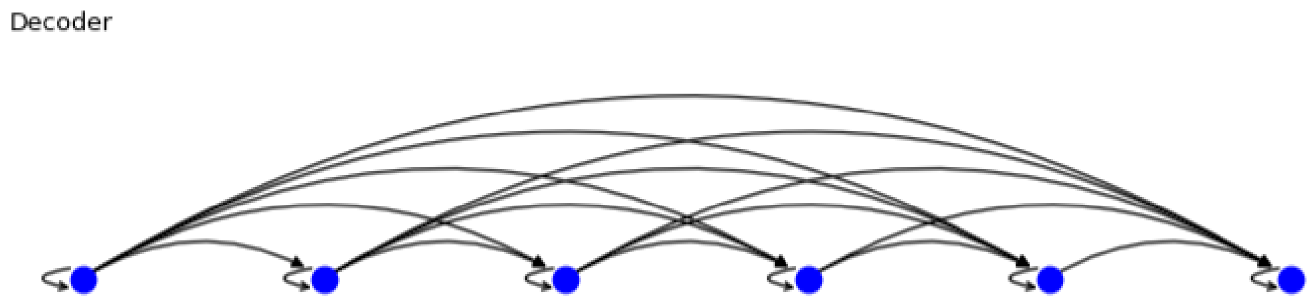
Graph structure

Construct the graph by mapping tokens of the source and target sentence to nodes. The complete Transformer graph is made up of three subgraphs:

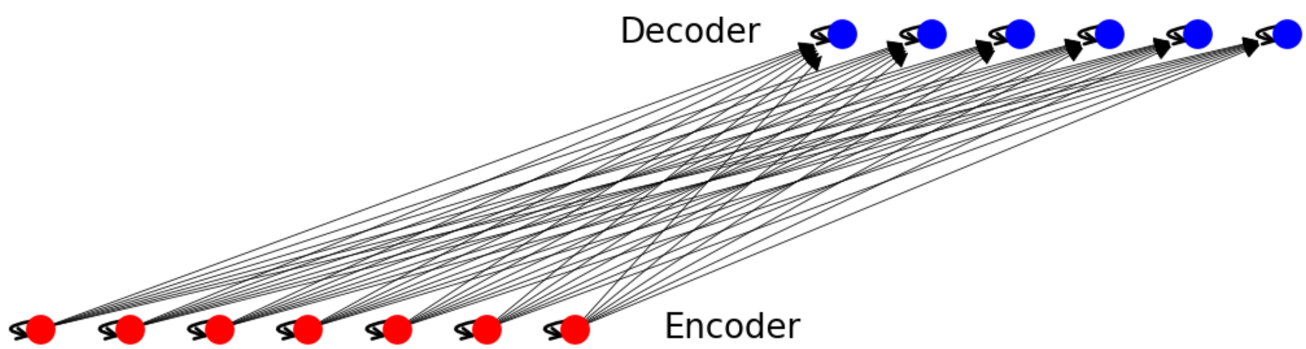
Source language graph. This is a complete graph, each token s_i can attend to any other token s_j (including self-loops).



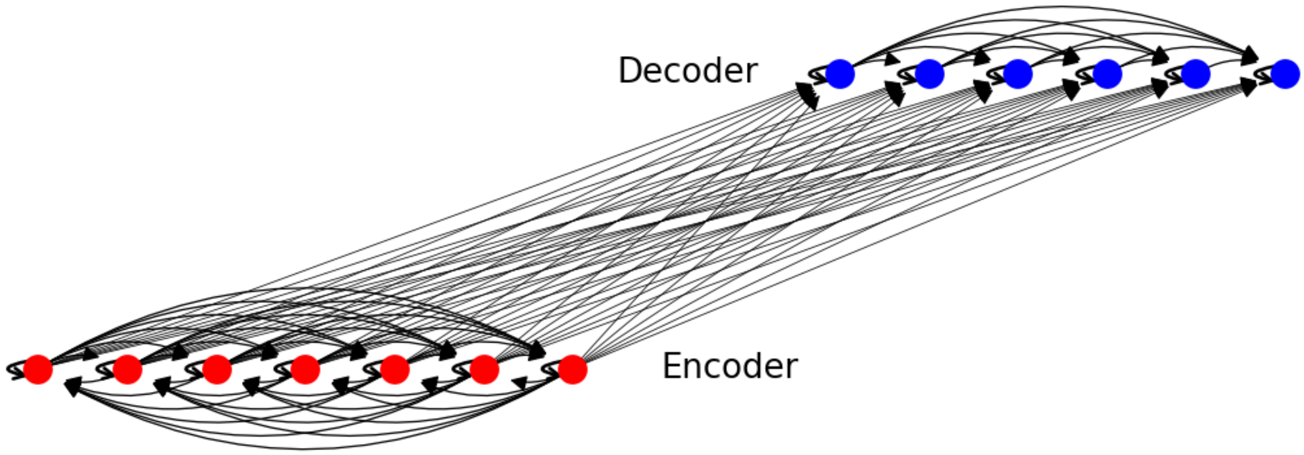
Target language graph. The graph is half-complete, in that t_i attends only to t_j if $i > j$ (an output token can not depend on future words).



Cross-language graph. This is a bi-partitie graph, where there is an edge from every source token s_i to every target token t_j, meaning every target token can attend on source tokens.



The full picture looks like this:



Pre-build the graphs in dataset preparation stage.

Message passing

Once you define the graph structure, move on to defining the computation for message passing.

Assuming that you have already computed all the queries q_i, keys k_i and values v_i. For each node i (no matter whether it is a source token or target token), you can decompose the attention computation into two steps:

1. **Message computation:** Compute attention score score_{ij} between i and all nodes j to be attended over, by taking the scaled-dot product between q_i and k_j. The message sent from j to i will consist of the score score_{ij} and the value v_j.
2. **Message aggregation:** Aggregate the values v_j from all j according to the scores score_{ij}.

Simple implementation

Message computation

Compute `score` and send source node's `v` to destination's mailbox

```
def message_func(edges):
    return {'score': ((edges.src['k'] * edges.dst['q'])
                      .sum(-1, keepdim=True)),
            'v': edges.src['v']}
```

Message aggregation

Normalize over all in-edges and weighted sum to get output

```
import torch as th
import torch.nn.functional as F

def reduce_func(nodes, d_k=64):
    v = nodes.mailbox['v']
    att = F.softmax(nodes.mailbox['score'] / th.sqrt(d_k), 1)
    return {'dx': (att * v).sum(1)}
```

Execute on specific edges

```
import functools.partial as partial
def naive_propagate_attention(self, g, eids):
    g.send_and_recv(eids, message_func, partial(reduce_func, d_k=self.d_k))
```

Speeding up with built-in functions

To speed up the message passing process, use DGL's built-in functions, including:

- `fn.src_mul_egdes(src_field, edges_field, out_field)` multiplies source's attribute and edges attribute, and send the result to the destination node's mailbox keyed by `out_field`.
- `fn.copy_edge(edges_field, out_field)` copies edge's attribute to destination node's mailbox.
- `fn.sum(edges_field, out_field)` sums up edge's attribute and sends aggregation to destination node's mailbox.

Here, you assemble those built-in functions into `propagate_attention`, which is also the main graph operation function in the final implementation. To accelerate it, break the `softmax` operation into the following steps. Recall that for each head there are two phases.

1. Compute attention score by multiply src node's `k` and dst node's `q`
   - `g.apply_edges(src_dot_dst('k', 'q', 'score'), eids)`
2. Scaled Softmax over all dst nodes' in-coming edges
   - Step 1: Exponentialize score with scale normalize constant
     - `g.apply_edges(scaled_exp('score', np.sqrt(self.d_k)))`

$$\text{score}_{ij} \leftarrow \exp\left(\frac{\text{score}_{ij}}{\sqrt{d_k}}\right)$$

- Step 2: Get the "values" on associated nodes weighted by "scores" on in-coming edges of each node; get the sum of "scores" on in-coming edges of each node for normalization. Note that here wv is not normalized.

  - `msg: fn.src_mul_edge('v', 'score', 'v'), reduce: fn.sum('v', 'wv')`

$$\mathrm{wv}_j = \sum_{i=1}^{N} \mathrm{score}_{ij} \cdot v_i$$

  - `msg: fn.copy_edge('score', 'score'), reduce: fn.sum('score', 'z')`

$$\mathrm{z}_j = \sum_{i=1}^{N} \mathrm{score}_{ij}$$

The normalization of wv is left to post processing.

```
def src_dot_dst(src_field, dst_field, out_field):
    def func(edges):
        return {out_field: (edges.src[src_field] * edges.dst[dst_field]).sum(-1,
keepdim=True)}

    return func

def scaled_exp(field, scale_constant):
    def func(edges):
        # clamp for softmax numerical stability
        return {field: th.exp((edges.data[field] / scale_constant).clamp(-5, 5))}

    return func


def propagate_attention(self, g, eids):
    # Compute attention score
    g.apply_edges(src_dot_dst('k', 'q', 'score'), eids)
    g.apply_edges(scaled_exp('score', np.sqrt(self.d_k)))
    # Update node state
    g.send_and_recv(eids,
                    [fn.src_mul_edge('v', 'score', 'v'), fn.copy_edge('score', 'score')],
                    [fn.sum('v', 'wv'), fn.sum('score', 'z')])
```

Preprocessing and postprocessing

In Transformer, data needs to be pre- and post-processed before and after the `propagate_attention` function.

Preprocessing The preprocessing function `pre_func` first normalizes the node representations and then map them to a set of queries, keys and values, using self-attention as an example:

$$x \leftarrow \mathrm{LayerNorm}(x)$$
$$[q, k, v] \leftarrow [W_q, W_k, W_v] \cdot x$$

Postprocessing The postprocessing function `post_funcs` completes the whole computation correspond to one layer of the transformer: 1. Normalize wv and get the output of Multi-Head Attention Layer o.

$$\mathrm{wv} \leftarrow \frac{\mathrm{wv}}{z}$$
$$o \leftarrow W_o \cdot \mathrm{wv} + b_o$$

add residual connection:

$$x \leftarrow x + o$$

2. Applying a two layer position-wise feed forward layer on x then add residual connection:

$$x \leftarrow x + \mathrm{LayerNorm}(\mathrm{FFN}(x))$$

where FFN refers to the feed forward function.

```python
class Encoder(nn.Module):
    def __init__(self, layer, N):
        super(Encoder, self).__init__()
        self.N = N
        self.layers = clones(layer, N)
        self.norm = LayerNorm(layer.size)

    def pre_func(self, i, fields='qkv'):
        layer = self.layers[i]
        def func(nodes):
            x = nodes.data['x']
            norm_x = layer.sublayer[0].norm(x)
            return layer.self_attn.get(norm_x, fields=fields)
        return func

    def post_func(self, i):
        layer = self.layers[i]
        def func(nodes):
            x, wv, z = nodes.data['x'], nodes.data['wv'], nodes.data['z']
            o = layer.self_attn.get_o(wv / z)
            x = x + layer.sublayer[0].dropout(o)
            x = layer.sublayer[1](x, layer.feed_forward)
            return {'x': x if i < self.N - 1 else self.norm(x)}
        return func

class Decoder(nn.Module):
    def __init__(self, layer, N):
        super(Decoder, self).__init__()
        self.N = N
        self.layers = clones(layer, N)
        self.norm = LayerNorm(layer.size)

    def pre_func(self, i, fields='qkv', l=0):
        layer = self.layers[i]
        def func(nodes):
            x = nodes.data['x']
            if fields == 'kv':
                norm_x = x # In enc-dec attention, x has already been normalized.
            else:
                norm_x = layer.sublayer[l].norm(x)
            return layer.self_attn.get(norm_x, fields)
        return func

    def post_func(self, i, l=0):
        layer = self.layers[i]
        def func(nodes):
            x, wv, z = nodes.data['x'], nodes.data['wv'], nodes.data['z']
            o = layer.self_attn.get_o(wv / z)
            x = x + layer.sublayer[l].dropout(o)
            if l == 1:
                x = layer.sublayer[2](x, layer.feed_forward)
            return {'x': x if i < self.N - 1 else self.norm(x)}
        return func
```

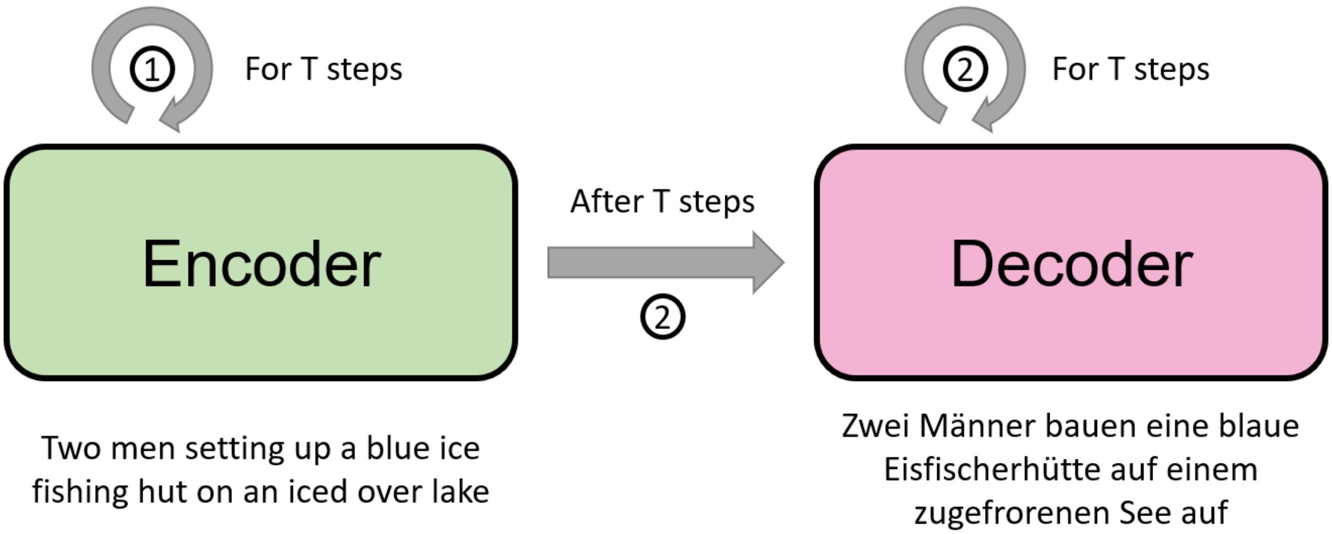
This completes all procedures of one layer of encoder and decoder in Transformer.

Note

The sublayer connection part is little bit different from the original paper. However, this implementation is the same as The Annotated Transformer and OpenNMT.

Main class of Transformer graph

The processing flow of Transformer can be seen as a 2-stage message-passing within the complete graph (adding pre- and post- processing appropriately): 1) self-attention in encoder, 2) self-attention in decoder followed by cross-attention between encoder and decoder, as shown below.



```python
class Transformer(nn.Module):
    def __init__(self, encoder, decoder, src_embed, tgt_embed, pos_enc, generator, h,
d_k):
        super(Transformer, self).__init__()
        self.encoder, self.decoder = encoder, decoder
        self.src_embed, self.tgt_embed = src_embed, tgt_embed
        self.pos_enc = pos_enc
        self.generator = generator
        self.h, self.d_k = h, d_k

    def propagate_attention(self, g, eids):
        # Compute attention score
        g.apply_edges(src_dot_dst('k', 'q', 'score'), eids)
        g.apply_edges(scaled_exp('score', np.sqrt(self.d_k)))
        # Send weighted values to target nodes
        g.send_and_recv(eids,
                        [fn.src_mul_edge('v', 'score', 'v'), fn.copy_edge('score',
'score')],
                        [fn.sum('v', 'wv'), fn.sum('score', 'z')])

    def update_graph(self, g, eids, pre_pairs, post_pairs):
        "Update the node states and edge states of the graph."

        # Pre-compute queries and key-value pairs.
        for pre_func, nids in pre_pairs:
            g.apply_nodes(pre_func, nids)
        self.propagate_attention(g, eids)
        # Further calculation after attention mechanism
        for post_func, nids in post_pairs:
            g.apply_nodes(post_func, nids)

    def forward(self, graph):
        g = graph.g
        nids, eids = graph.nids, graph.eids

        # Word Embedding and Position Embedding
        src_embed, src_pos = self.src_embed(graph.src[0]), self.pos_enc(graph.src[1])
        tgt_embed, tgt_pos = self.tgt_embed(graph.tgt[0]), self.pos_enc(graph.tgt[1])
        g.nodes[nids['enc']].data['x'] = self.pos_enc.dropout(src_embed + src_pos)
        g.nodes[nids['dec']].data['x'] = self.pos_enc.dropout(tgt_embed + tgt_pos)

        for i in range(self.encoder.N):
            # Step 1: Encoder Self-attention
            pre_func = self.encoder.pre_func(i, 'qkv')
            post_func = self.encoder.post_func(i)
            nodes, edges = nids['enc'], eids['ee']
            self.update_graph(g, edges, [(pre_func, nodes)], [(post_func, nodes)])

        for i in range(self.decoder.N):
            # Step 2: Dncoder Self-attention
            pre_func = self.decoder.pre_func(i, 'qkv')
            post_func = self.decoder.post_func(i)
            nodes, edges = nids['dec'], eids['dd']
            self.update_graph(g, edges, [(pre_func, nodes)], [(post_func, nodes)])
            # Step 3: Encoder-Decoder attention
            pre_q = self.decoder.pre_func(i, 'q', 1)
            pre_kv = self.decoder.pre_func(i, 'kv', 1)
            post_func = self.decoder.post_func(i, 1)
            nodes_e, nodes_d, edges = nids['enc'], nids['dec'], eids['ed']
            self.update_graph(g, edges, [(pre_q, nodes_d), (pre_kv, nodes_e)],
[(post_func, nodes_d)])

        return self.generator(g.ndata['x'][nids['dec']])
```

> **Note**
>
> By calling `update_graph` function, you can create your own Transformer on any subgraphs with nearly the same code. This flexibility enables us to discover new, sparse structures (c.f. local attention mentioned here). Note in this implementation you don't use mask or padding, which makes the logic more clear and saves memory. The trade-off is that the implementation is slower.

Training

This tutorial does not cover several other techniques such as Label Smoothing and Noam Optimizations mentioned in the original paper. For detailed description about these modules, read The Annotated Transformer written by Harvard NLP team.

Task and the dataset

The Transformer is a general framework for a variety of NLP tasks. This tutorial focuses on the sequence to sequence learning: it's a typical case to illustrate how it works.

As for the dataset, there are two example tasks: copy and sort, together with two real-world translation tasks: multi30k en-de task and wmt14 en-de task.

- **copy dataset**: copy input sequences to output. (train/valid/test: 9000, 1000, 1000)
- **sort dataset**: sort input sequences as output. (train/valid/test: 9000, 1000, 1000)
- **Multi30k en-de**, translate sentences from En to De. (train/valid/test: 29000, 1000, 1000)
- **WMT14 en-de**, translate sentences from En to De. (Train/Valid/Test: 4500966/3000/3003)

> **Note**
>
> Training with wmt14 requires multi-GPU support and is not available. Contributions are welcome!

Graph building

Batching This is similar to the way you handle Tree-LSTM. Build a graph pool in advance, including all possible combination of input lengths and output lengths. Then for each sample in a batch, call `dgl.batch` to batch graphs of their sizes together in to a single large graph.

You can wrap the process of creating graph pool and building BatchedGraph in `dataset.GraphPool` and `dataset.TranslationDataset`.

```
graph_pool = GraphPool()

data_iter = dataset(graph_pool, mode='train', batch_size=1, devices=devices)
for graph in data_iter:
    print(graph.nids['enc']) # encoder node ids
    print(graph.nids['dec']) # decoder node ids
    print(graph.eids['ee']) # encoder-encoder edge ids
    print(graph.eids['ed']) # encoder-decoder edge ids
    print(graph.eids['dd']) # decoder-decoder edge ids
    print(graph.src[0]) # Input word index list
    print(graph.src[1]) # Input positions
    print(graph.tgt[0]) # Output word index list
    print(graph.tgt[1]) # Ouptut positions
    break
```

Output:

```
tensor([0, 1, 2, 3, 4, 5, 6, 7, 8], device='cuda:0')
tensor([ 9, 10, 11, 12, 13, 14, 15, 16, 17, 18], device='cuda:0')
tensor([ 0,  1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11, 12, 13, 14, 15, 16, 17,
        18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35,
        36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53,
        54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71,
        72, 73, 74, 75, 76, 77, 78, 79, 80], device='cuda:0')
tensor([ 81,  82,  83,  84,  85,  86,  87,  88,  89,  90,  91,  92,  93,  94,
         95,  96,  97,  98,  99, 100, 101, 102, 103, 104, 105, 106, 107, 108,
        109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122,
        123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136,
        137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150,
        151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 161, 162, 163, 164,
        165, 166, 167, 168, 169, 170], device='cuda:0')
tensor([171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184,
        185, 186, 187, 188, 189, 190, 191, 192, 193, 194, 195, 196, 197, 198,
        199, 200, 201, 202, 203, 204, 205, 206, 207, 208, 209, 210, 211, 212,
        213, 214, 215, 216, 217, 218, 219, 220, 221, 222, 223, 224, 225],
       device='cuda:0')
tensor([28, 25,  7, 26,  6,  4,  5,  9, 18], device='cuda:0')
tensor([0, 1, 2, 3, 4, 5, 6, 7, 8], device='cuda:0')
tensor([ 0, 28, 25,  7, 26,  6,  4,  5,  9, 18], device='cuda:0')
tensor([0, 1, 2, 3, 4, 5, 6, 7, 8, 9], device='cuda:0')
```

Put it all together

Train a one-head transformer with one layer, 128 dimension on copy task. Set other parameters to the default.

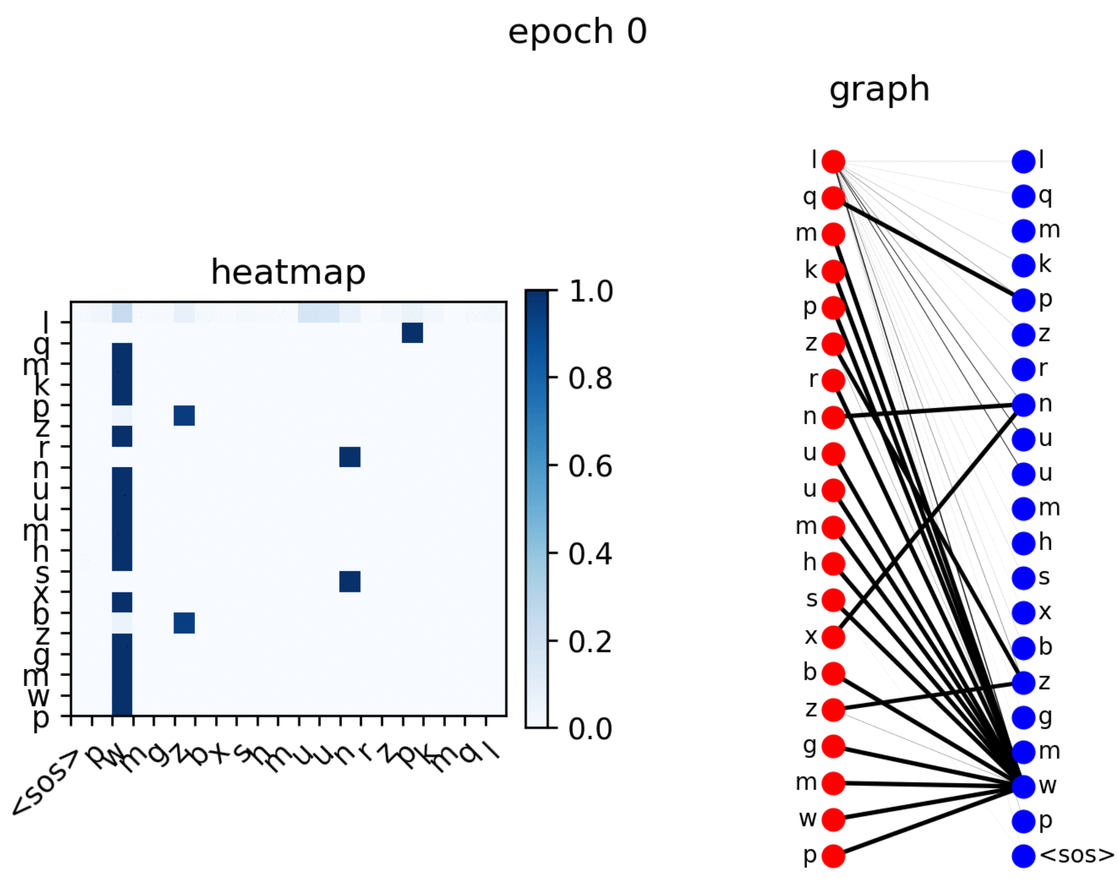
Inference module is not included in this tutorial. It requires beam search. For a full implementation, see the GitHub repo.

```
from tqdm import tqdm
import torch as th
import numpy as np

from loss import LabelSmoothing, SimpleLossCompute
from modules import make_model
from optims import NoamOpt
from dgl.contrib.transformer import get_dataset, GraphPool

def run_epoch(data_iter, model, loss_compute, is_train=True):
    for i, g in tqdm(enumerate(data_iter)):
        with th.set_grad_enabled(is_train):
            output = model(g)
            loss = loss_compute(output, g.tgt_y, g.n_tokens)
    print('average loss: {}'.format(loss_compute.avg_loss))
    print('accuracy: {}'.format(loss_compute.accuracy))

N = 1
batch_size = 128
devices = ['cuda' if th.cuda.is_available() else 'cpu']

dataset = get_dataset("copy")
V = dataset.vocab_size
criterion = LabelSmoothing(V, padding_idx=dataset.pad_id, smoothing=0.1)
dim_model = 128

# Create model
model = make_model(V, V, N=N, dim_model=128, dim_ff=128, h=1)

# Sharing weights between Encoder & Decoder
model.src_embed.lut.weight = model.tgt_embed.lut.weight
model.generator.proj.weight = model.tgt_embed.lut.weight

model, criterion = model.to(devices[0]), criterion.to(devices[0])
model_opt = NoamOpt(dim_model, 1, 400,
                    th.optim.Adam(model.parameters(), lr=1e-3, betas=(0.9, 0.98), eps=1e-
9))
loss_compute = SimpleLossCompute

att_maps = []
for epoch in range(4):
    train_iter = dataset(graph_pool, mode='train', batch_size=batch_size, devices=devices)
    valid_iter = dataset(graph_pool, mode='valid', batch_size=batch_size, devices=devices)
    print('Epoch: {} Training...'.format(epoch))
    model.train(True)
    run_epoch(train_iter, model,
              loss_compute(criterion, model_opt), is_train=True)
    print('Epoch: {} Evaluating...'.format(epoch))
    model.att_weight_map = None
    model.eval()
    run_epoch(valid_iter, model,
              loss_compute(criterion, None), is_train=False)
    att_maps.append(model.att_weight_map)
```

Visualization

After training, you can visualize the attention that the Transformer generates on copy task.

```
src_seq = dataset.get_seq_by_id(VIZ_IDX, mode='valid', field='src')
tgt_seq = dataset.get_seq_by_id(VIZ_IDX, mode='valid', field='tgt')[:-1]
# visualize head 0 of encoder-decoder attention
att_animation(att_maps, 'e2d', src_seq, tgt_seq, 0)
```



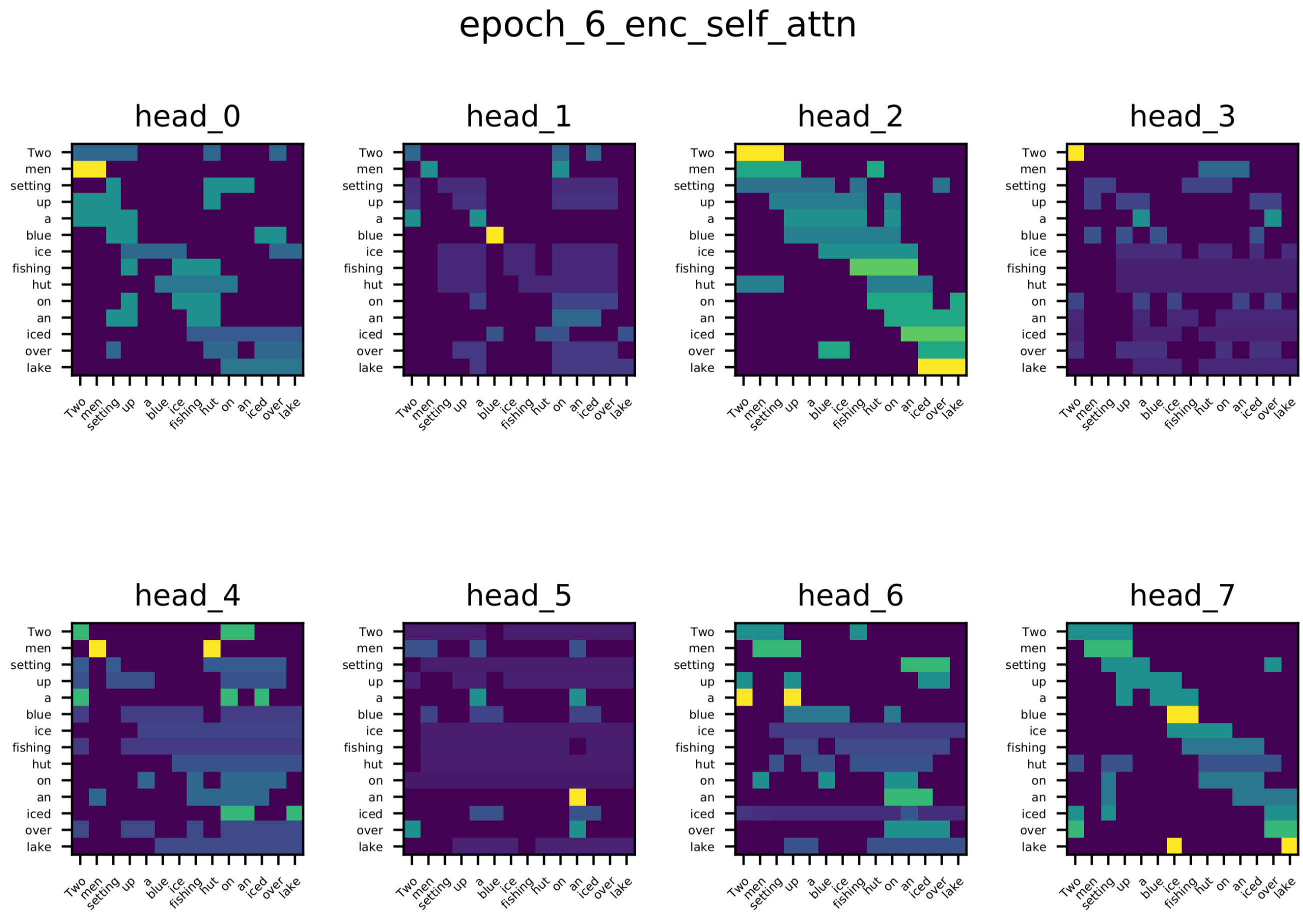
from the figure you see the decoder nodes gradually learns to attend to corresponding nodes in input sequence, which is the expected behavior.

Multi-head attention

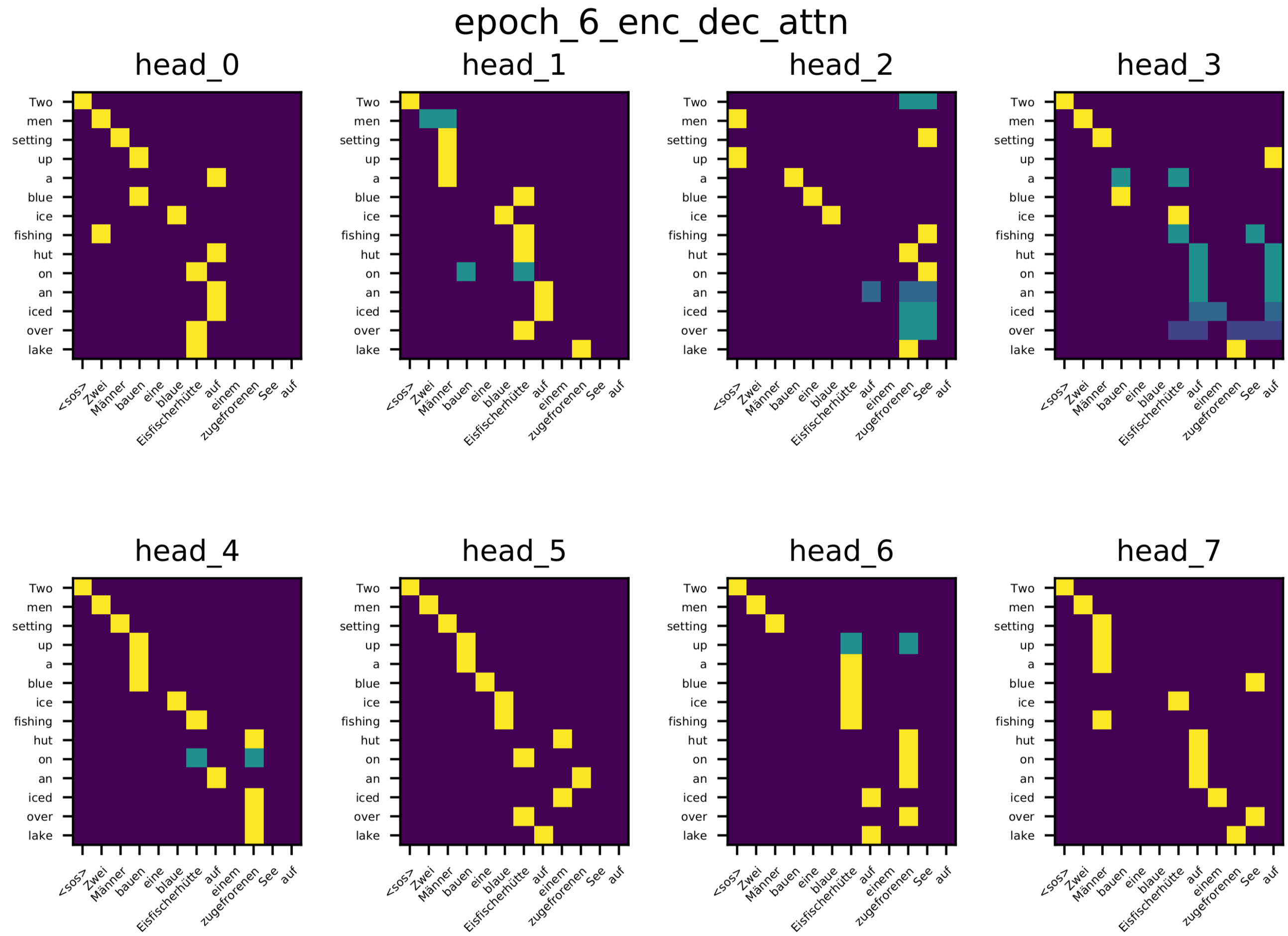
Besides the attention of a one-head attention trained on toy task. We also visualize the attention scores of Encoder's Self Attention, Decoder's Self Attention and the Encoder-Decoder attention of an one-Layer Transformer network trained on multi-30k dataset.

From the visualization you see the diversity of different heads, which is what you would expect. Different heads learn different relations between word pairs.

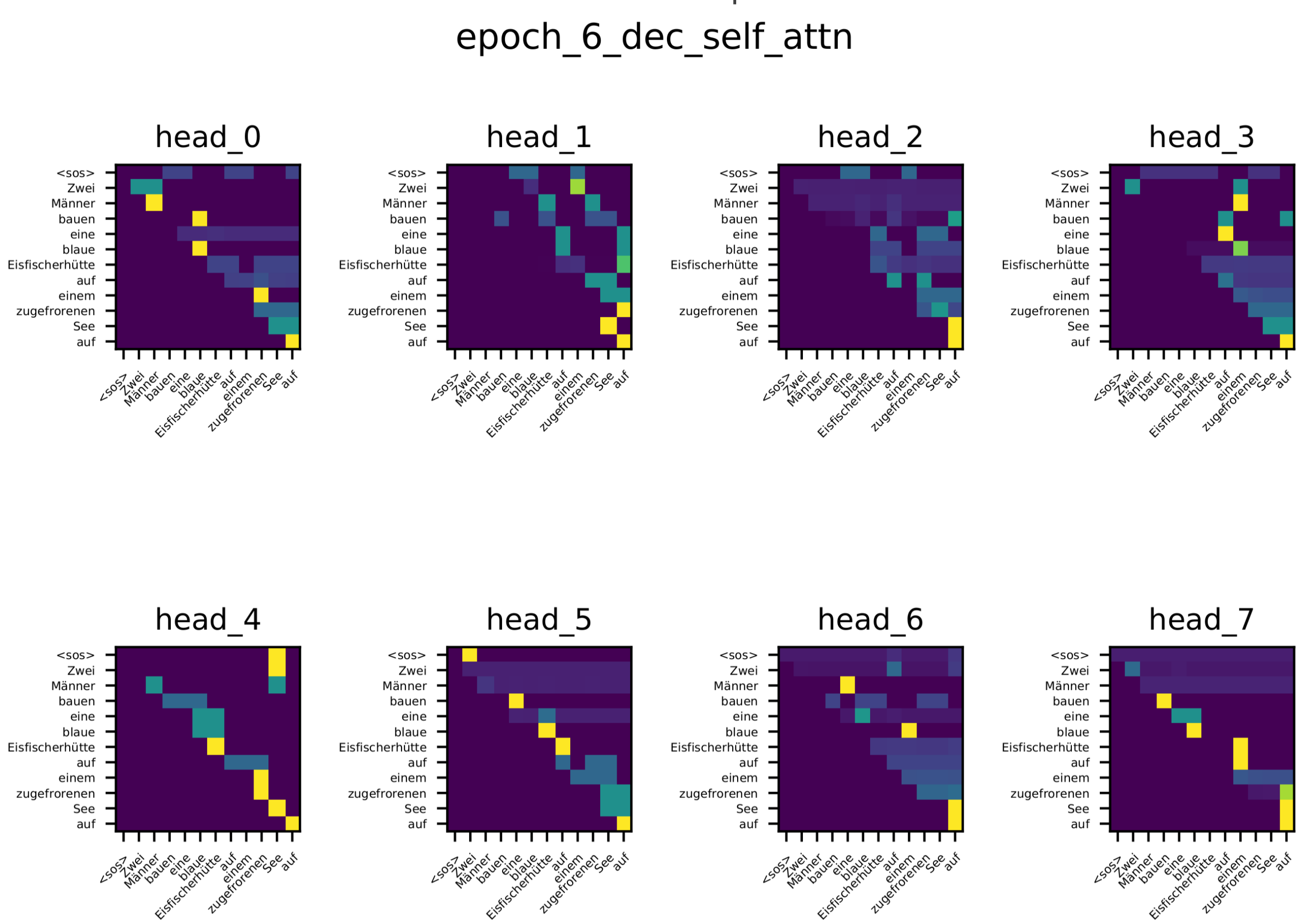
- **Encoder Self-Attention**



- **Encoder-Decoder Attention** Most words in target sequence attend on their related words in source sequence, for example: when generating “See” (in De), several heads attend on “lake”; when generating “Eisfischerhütte”, several heads attend on “ice”.



- **Decoder Self-Attention** Most words attend on their previous few words.



Adaptive Universal Transformer

A recent research paper by Google, Universal Transformer, is an example to show how `update_graph` adapts to more complex updating rules.

The Universal Transformer was proposed to address the problem that vanilla Transformer is not computationally universal by introducing recurrence in Transformer:

- The basic idea of Universal Transformer is to repeatedly revise its representations of all symbols in the sequence with each recurrent step by applying a Transformer layer on the representations.
- Compared to vanilla Transformer, Universal Transformer shares weights among its layers, and it does not fix the recurrence time (which means the number of layers in Transformer).

A further optimization employs an adaptive computation time (ACT) mechanism to allow the model to dynamically adjust the number of times the representation of each position in a sequence is revised (refereed to as **step** hereafter). This model is also known as the Adaptive Universal Transformer (AUT).

In AUT, you maintain an active nodes list. In each step t, we compute a halting probability: $h (0 < h < 1)$ for all nodes in this list by:

$$h_i^t = \sigma(W_h x_i^t + b_h)$$

then dynamically decide which nodes are still active. A node is halted at time T if and only if $\sum_{t=1}^{T-1} h_t < 1 - \varepsilon \leq \sum_{t=1}^{T} h_t$. Halted nodes are removed from the list. The procedure proceeds until the list is empty or a pre-defined maximum step is reached. From DGL's perspective, this means that the "active" graph becomes sparser over time.

The final state of a node s_i is a weighted average of x_i^t by h_i^t:

$$s_i = \sum_{t=1}^{T} h_i^t \cdot x_i^t$$

In DGL, implement an algorithm by calling `update_graph` on nodes that are still active and edges associated with this nodes. The following code shows the Universal Transformer class in DGL:

```python
class UTransformer(nn.Module):
    "Universal Transformer(https://arxiv.org/pdf/1807.03819.pdf) with
ACT(https://arxiv.org/pdf/1603.08983.pdf)."
    MAX_DEPTH = 8
    thres = 0.99
    act_loss_weight = 0.01
    def __init__(self, encoder, decoder, src_embed, tgt_embed, pos_enc, time_enc,
generator, h, d_k):
        super(UTransformer, self).__init__()
        self.encoder,  self.decoder = encoder, decoder
        self.src_embed, self.tgt_embed = src_embed, tgt_embed
        self.pos_enc, self.time_enc = pos_enc, time_enc
        self.halt_enc = HaltingUnit(h * d_k)
        self.halt_dec = HaltingUnit(h * d_k)
        self.generator = generator
        self.h, self.d_k = h, d_k

    def step_forward(self, nodes):
        # add positional encoding and time encoding, increment step by one
        x = nodes.data['x']
        step = nodes.data['step']
        pos = nodes.data['pos']
        return {'x': self.pos_enc.dropout(x + self.pos_enc(pos.view(-1)) +
self.time_enc(step.view(-1))),
                'step': step + 1}

    def halt_and_accum(self, name, end=False):
        "field: 'enc' or 'dec'"
        halt = self.halt_enc if name == 'enc' else self.halt_dec
        thres = self.thres
        def func(nodes):
            p = halt(nodes.data['x'])
            sum_p = nodes.data['sum_p'] + p
            active = (sum_p < thres) & (1 - end)
            _continue = active.float()
            r = nodes.data['r'] * (1 - _continue) + (1 - sum_p) * _continue
            s = nodes.data['s'] + ((1 - _continue) * r + _continue * p) * nodes.data['x']
            return {'p': p, 'sum_p': sum_p, 'r': r, 's': s, 'active': active}
        return func

    def propagate_attention(self, g, eids):
        # Compute attention score
        g.apply_edges(src_dot_dst('k', 'q', 'score'), eids)
        g.apply_edges(scaled_exp('score', np.sqrt(self.d_k)), eids)
        # Send weighted values to target nodes
        g.send_and_recv(eids,
                        [fn.src_mul_edge('v', 'score', 'v'), fn.copy_edge('score',
'score')],
                        [fn.sum('v', 'wv'), fn.sum('score', 'z')])

    def update_graph(self, g, eids, pre_pairs, post_pairs):
        "Update the node states and edge states of the graph."
        # Pre-compute queries and key-value pairs.
        for pre_func, nids in pre_pairs:
            g.apply_nodes(pre_func, nids)
        self.propagate_attention(g, eids)
        # Further calculation after attention mechanism
        for post_func, nids in post_pairs:
            g.apply_nodes(post_func, nids)

    def forward(self, graph):
        g = graph.g
        N, E = graph.n_nodes, graph.n_edges
```

```
        nids, eids = graph.nids, graph.eids

        # embed & pos
        g.nodes[nids['enc']].data['x'] = self.src_embed(graph.src[0])
        g.nodes[nids['dec']].data['x'] = self.tgt_embed(graph.tgt[0])
        g.nodes[nids['enc']].data['pos'] = graph.src[1]
        g.nodes[nids['dec']].data['pos'] = graph.tgt[1]

        # init step
        device = next(self.parameters()).device
        g.ndata['s'] = th.zeros(N, self.h * self.d_k, dtype=th.float, device=device)    #
accumulated state
        g.ndata['p'] = th.zeros(N, 1, dtype=th.float, device=device)                    #
halting prob
        g.ndata['r'] = th.ones(N, 1, dtype=th.float, device=device)                     #
remainder
        g.ndata['sum_p'] = th.zeros(N, 1, dtype=th.float, device=device)                #
sum of pondering values
        g.ndata['step'] = th.zeros(N, 1, dtype=th.long, device=device)                  #
step
        g.ndata['active'] = th.ones(N, 1, dtype=th.uint8, device=device)                #
active

        for step in range(self.MAX_DEPTH):
            pre_func = self.encoder.pre_func('qkv')
            post_func = self.encoder.post_func()
            nodes = g.filter_nodes(lambda v: v.data['active'].view(-1), nids['enc'])
            if len(nodes) == 0: break
            edges = g.filter_edges(lambda e: e.dst['active'].view(-1), eids['ee'])
            end = step == self.MAX_DEPTH - 1
            self.update_graph(g, edges,
                              [(self.step_forward, nodes), (pre_func, nodes)],
                              [(post_func, nodes), (self.halt_and_accum('enc', end),
nodes)])

        g.nodes[nids['enc']].data['x'] =
self.encoder.norm(g.nodes[nids['enc']].data['s'])

        for step in range(self.MAX_DEPTH):
            pre_func = self.decoder.pre_func('qkv')
            post_func = self.decoder.post_func()
            nodes = g.filter_nodes(lambda v: v.data['active'].view(-1), nids['dec'])
            if len(nodes) == 0: break
            edges = g.filter_edges(lambda e: e.dst['active'].view(-1), eids['dd'])
            self.update_graph(g, edges,
                              [(self.step_forward, nodes), (pre_func, nodes)],
                              [(post_func, nodes)])

            pre_q = self.decoder.pre_func('q', 1)
            pre_kv = self.decoder.pre_func('kv', 1)
            post_func = self.decoder.post_func(1)
            nodes_e = nids['enc']
            edges = g.filter_edges(lambda e: e.dst['active'].view(-1), eids['ed'])
            end = step == self.MAX_DEPTH - 1
            self.update_graph(g, edges,
                              [(pre_q, nodes), (pre_kv, nodes_e)],
                              [(post_func, nodes), (self.halt_and_accum('dec', end),
nodes)])

        g.nodes[nids['dec']].data['x'] =
self.decoder.norm(g.nodes[nids['dec']].data['s'])
        act_loss = th.mean(g.ndata['r']) # ACT loss
```

```
        return self.generator(g.ndata['x'][nids['dec']]), act_loss * self.act_loss_weight
```

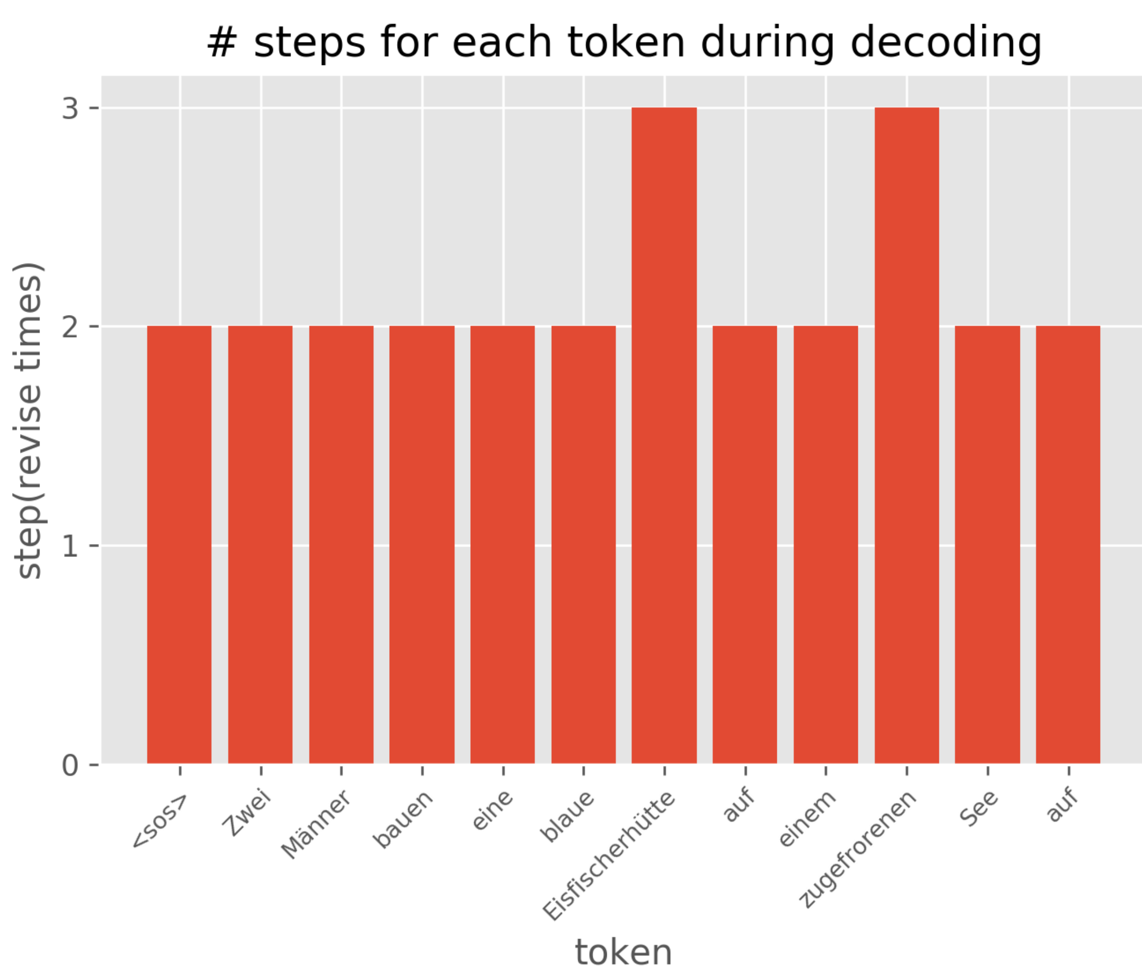
Call `filter_nodes` and `filter_edge` to find nodes/edges that are still active:

Note

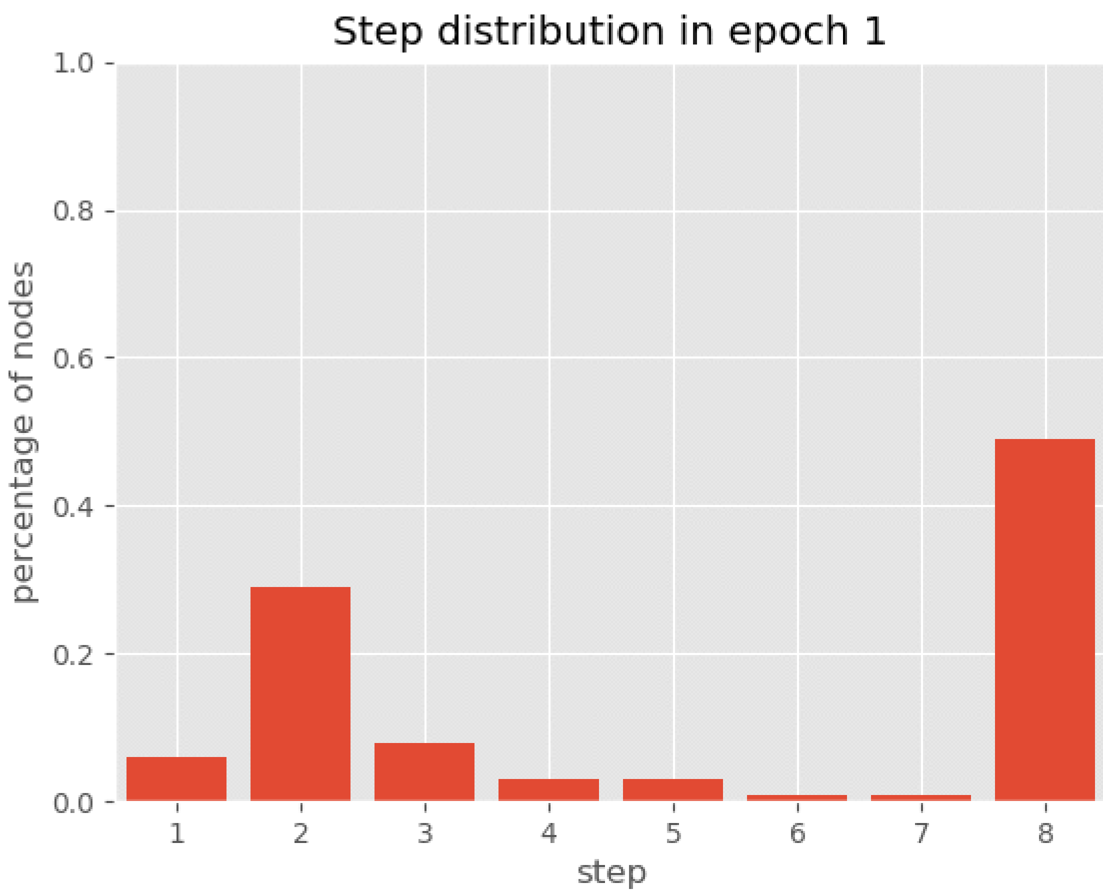
- `filter_nodes()` takes a predicate and a node ID list/tensor as input, then returns a tensor of node IDs that satisfy the given predicate.
- `filter_edges()` takes a predicate and an edge ID list/tensor as input, then returns a tensor of edge IDs that satisfy the given predicate.

For the full implementation, see the GitHub repo.

The figure below shows the effect of Adaptive Computational Time. Different positions of a sentence were revised different times.



You can also visualize the dynamics of step distribution on nodes during the training of AUT on sort task(reach 99.7% accuracy), which demonstrates how AUT learns to reduce recurrence steps during training.



Note

The notebook itself is not executable due to many dependencies. Download 7_transformer.py, and copy the python script to directory `examples/pytorch/transformer` then run `python 7_transformer.py` to see how it works.

Total running time of the script: (0 minutes 0.000 seconds)

Download Python source code: 7_transformer.py

Download Jupyter notebook: 7_transformer.ipynb