HW3

November 17, 2025

1 Libraries & Hyperparameters

[350]:
```
import torch
import torch.nn as nn
# import torch.nn.functional as F
import math
from transformers import AutoTokenizer
from torch.utils.data import TensorDataset, DataLoader
import numpy as np
import copy
import matplotlib.pyplot as plt
import seaborn as sns
# from tokenizers import Tokenizer
# from tokenizers.models import BPE
# from tokenizers.trainers import BpeTrainer
# from tokenizers.pre_tokenizers import Whitespace

from collections import defaultdict

plt.rcParams["font.family"] = "serif"
plt.rcParams["font.serif"] = ["Times New Roman"]

np.random.seed(42)
```

[299]:
```
# Tokenization
VOCAB_SIZE = 500
# Data Preparation
SEQ_LEN = 50
# Model
EMBED_DIM = 128
HIDDEN_DIM = 128
NUM_LAYERS = 2

BATCH_SIZE = 64
grad_clip = 1
lr = 3e-5
betas = (0.9, 0.98)
```

```
wd = 0.05
```

2 Data Preparation

2.1 Load the Tiny Shakespeare text

[280]:
```
corpus = []
skip_referrence = True
with open("input.txt", "r") as f:
    for line in f:
        line = line.strip('\n')
        if line == "":
            skip_referrence = True
            continue
        if skip_referrence:
            skip_referrence = False
            continue
        corpus.append(line)
```

2.2 Tokenization

We tried BPE tokenizer directly as following code block, however the behavior of the model on this vocabulary was not good enough. Thus we turned to GPT2 Pre-tokenizer + Byte Pair Encoding.

[281]:
```
# tokenizer = Tokenizer(BPE())
# tokenizer.pre_tokenizer = Whitespace()
# trainer = BpeTrainer(vocab_size = VOCAB_SIZE)
# tokenizer.train_from_iterator([corpus], trainer)
# stoi = dict(sorted(list(tokenizer.get_vocab().items()), key = lambda x:␣
↪(len(x[0]), x[0])))
# itos = {i: s for s, i in sorted(list(stoi.items()), key = lambda x: x[1])}
# tokenized_corpus = []
# for line in corpus:
#     pieces = tokenizer.encode(line).ids
#     tokenized_corpus += pieces
```

Most of this part is borrowed from HuggingFace, with slight modification to fit better in this small corpus.

[282]:
```
word_freqs = defaultdict(int)
tokenizer = AutoTokenizer.from_pretrained("gpt2")
corpus_ = []
for text in corpus:
    words_with_offsets = tokenizer.backend_tokenizer.pre_tokenizer.
↪pre_tokenize_str(text)
    new_words = [word for word, offset in words_with_offsets]
    for word in new_words:
```

```
        if word.isupper():
            word = word.capitalize()
        word_freqs[word] += 1
    corpus_ += new_words
```

[ ]:
```
alphabet = []
for word in word_freqs.keys():
    for letter in word:
        if letter not in alphabet:
            alphabet.append(letter)
alphabet.sort()
vocab = ["<|endoftext|>"] + alphabet.copy()
vocab = alphabet.copy()
splits = {word: [c for c in word] for word in word_freqs.keys()}
```

[284]:
```
def compute_pair_freqs(splits):
    pair_freqs = defaultdict(int)
    for word, freq in word_freqs.items():
        split = splits[word]
        if len(split) == 1:
            continue
        for i in range(len(split) - 1):
            pair = (split[i], split[i + 1])
            pair_freqs[pair] += freq
    return pair_freqs
def merge_pair(a, b, splits):
    for word in word_freqs:
        split = splits[word]
        if len(split) == 1:
            continue
        i = 0
        while i < len(split) - 1:
            if split[i] == a and split[i + 1] == b:
                split = split[:i] + [a + b] + split[i + 2 :]
            else:
                i += 1
        splits[word] = split
    return splits
```

[285]:
```
merges = {}
while len(vocab) < VOCAB_SIZE:
    pair_freqs = compute_pair_freqs(splits)
    best_pair = ""
    max_freq = None
    for pair, freq in pair_freqs.items():
        if max_freq is None or max_freq < freq:
            best_pair = pair
```

```
            max_freq = freq
    splits = merge_pair(*best_pair, splits)
    merges[best_pair] = best_pair[0] + best_pair[1]
    vocab.append(best_pair[0] + best_pair[1])
vocab = sorted(set(vocab), key = lambda x: (len(x), x))
```

We greedily tokenize the corpus.

[286]:
```
stoi = {tok: i for i, tok in enumerate(vocab)}
itos = {i: tok for tok, i in stoi.items()}
MAX_WORD_LEN = len(vocab[-1])
def tokenize_word(word, vocab):
    tokens = []
    i = 0
    l = len(word)
    while i < l:
        for j in range(min(i + MAX_WORD_LEN, l), i, -1):
            piece = word[i:j]
            if piece in vocab:
                i = j
                tokens.append(stoi[piece])
                break
    return tokens
```

[287]:
```
tokenized_corpus = []
for word in corpus_:
    pieces = tokenize_word(word, vocab)
    # print(pieces)
    # for p in pieces:
    #     print(itos[p], end = " ")
    # print()
    tokenized_corpus += pieces
```

[288]:
```
for i in range(5):
    print(corpus_[i])
    tokens = tokenize_word(corpus_[i], vocab)
    print(tokens)
    for token in tokens:
        print(itos[token], end = " ")
    print()
```

```
Before
[70, 363]
Be fore
Ġwe
[354]
Ġwe
Ġproceed
```

```
[416, 92, 99]
Ġpro ce ed
Ġany
[295, 61]
Ġan y
Ġfurther
[187, 164, 376]
Ġf ur ther
```

2.3 Sequence formatting

[289]:
```
inputs = []
targets = []
for i in range(len(tokenized_corpus) - SEQ_LEN):
    inputs.append(tokenized_corpus[i : i + SEQ_LEN])
    targets.append(tokenized_corpus[i + 1: i + 1 + SEQ_LEN])
inputs = torch.tensor(inputs, dtype=torch.long)
targets = torch.tensor(targets, dtype=torch.long)

print("inputs shape:", inputs.shape)
print("targets shape:", targets.shape)
```

```
inputs shape: torch.Size([423593, 50])
targets shape: torch.Size([423593, 50])
```

2.4 Data split

To make sure there's no data leakage, we should split the dataset directly by the order of token sequences, i.e. the first 80% as train and the last 20% as validation.

[290]:
```
SEQ_COUNT = int(len(inputs) * .8)
train_X = inputs[:SEQ_COUNT]
train_y = targets[:SEQ_COUNT]
val_X = inputs[SEQ_COUNT:]
val_y = targets[SEQ_COUNT:]
print(train_X.shape, train_y.shape)
print(val_X.shape, val_y.shape)
```

```
torch.Size([338874, 50]) torch.Size([338874, 50])
torch.Size([84719, 50]) torch.Size([84719, 50])
```

2.5 Token embedding

RoPE is better for very long context windows. Now that we've chosen SEQ_LEN = 50, we'll use simple sinusoidal positional embeddings.

[291]:
```
class PositionalEmbedding(nn.Module):
    def __init__(self, embed_dim, max_seq_len, base: float = 10000.0):
        super().__init__()
```

```
        pos_emd = torch.zeros(max_seq_len, embed_dim)
        position = torch.arange(0, max_seq_len).unsqueeze(1)
        div_term = torch.exp(torch.arange(0, embed_dim, 2) * (-math.log(base) /
 ↪embed_dim))
        pos_emd[:, 0::2] = torch.sin(position * div_term)
        pos_emd[:, 1::2] = torch.cos(position * div_term)
        # self.pos_emd = pos_emd
        self.register_buffer("pos_emd", pos_emd)

    def forward(self, x):
        # x in shape of [Batch, Tokens, Dims]
        # use broadcast
        B, T, D = x.size()
        return x + self.pos_emd[:T, :].unsqueeze(0)
```

3 Implement a Tiny Transformer

[292]:
```
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
class RMSNorm(nn.Module):
    def __init__(self, embed_dim = EMBED_DIM, eps = 1e-8):
        super().__init__()
        self.eps = eps
        self.scale = nn.Parameter(torch.ones(embed_dim))

    def forward(self, x):
        # x is of shape [Batch, Tokens, Dims]
        # normalize the embedding dimensions
        rms = x.pow(2).mean(dim = -1, keepdim = True).add(self.eps).sqrt()
        return x / rms * self.scale

class SelfAttention(nn.Module):
    def __init__(self, embed_dim = EMBED_DIM, mask = True):
        super().__init__()
        self.embed_dim = embed_dim
        self.scale = 1.0 / math.sqrt(embed_dim)
        self.q = nn.Linear(embed_dim, embed_dim)
        self.k = nn.Linear(embed_dim, embed_dim)
        self.v = nn.Linear(embed_dim, embed_dim)
        self.proj = nn.Linear(embed_dim, embed_dim)
        self.mask = mask

    def forward(self, x):
        B, T, D = x.shape
        q = self.q(x) # each in [B, T, Q] here Q = D
        k = self.k(x)
        v = self.v(x) # [B, T, V]
```

```
        # k.transpose(1, 2) in [B, K, T] where K = Q
        attn_scores = torch.bmm(q, k.transpose(1, 2)) * self.scale
        # out [B, T, T]

        # mask (i, j) if j > i for dimension T
        # out = sum att[i, j] v[j] over j in dimension T
        # hence only keeping lower triangle
        if self.mask:
            causal_mask = torch.tril(torch.ones(T, T, device=x.device)).bool()
            attn_scores = attn_scores.masked_fill(~causal_mask, float('-inf'))

        # softmax on dimension V
        attn_probs = torch.softmax(attn_scores, dim=-1)
        out = torch.bmm(attn_probs, v)  # [B, T, V]
        out = self.proj(out) # [B, T, D]
        return out, attn_probs

class TransformerBlock(nn.Module):
    def __init__(self, embed_dim = EMBED_DIM, ffnn_hidden = HIDDEN_DIM):
        super().__init__()
        self.attn = SelfAttention(embed_dim)
        self.ffnn = nn.Sequential(
            nn.Linear(embed_dim, ffnn_hidden),
            nn.GELU(),
            nn.Linear(ffnn_hidden, embed_dim)
        )
        self.rms1 = RMSNorm(embed_dim)
        self.rms2 = RMSNorm(embed_dim)

    def forward(self, x):
        attn_out, attn_map = self.attn(self.rms1(x))
        x = x + attn_out
        ffnn_out = self.ffnn(self.rms2(x))
        x = x + ffnn_out
        return x, attn_map

class TinyTransformer(nn.Module):
    def __init__(self, vocab_size = VOCAB_SIZE, embed_dim = EMBED_DIM,
                 num_layers = NUM_LAYERS, ffnn_hidden = HIDDEN_DIM,
                 max_seq_len = SEQ_LEN):
        super().__init__()
        self.token_emb = nn.Embedding(vocab_size, embed_dim)
        self.pos_enc = PositionalEmbedding(embed_dim, max_seq_len)
        self.layers = nn.ModuleList(
            [TransformerBlock(embed_dim, ffnn_hidden) for _ in␣
 ↪range(num_layers)])
        self.rms_final = RMSNorm(embed_dim)
```

```
        self.lm_head = nn.Linear(embed_dim, vocab_size, bias=False)

    def forward(self, idx, need_attn=False):
        # idx in shape [B, T]
        x = self.token_emb(idx)
        x = self.pos_enc(x)
        attn_maps = []
        for layer in self.layers:
            x, attn_map = layer(x)
            if need_attn:
                attn_maps.append(attn_map)
        x = self.rms_final(x)
        logits = self.lm_head(x)
        return (logits, attn_maps) if need_attn else (logits, None)
```

4 Model Training

[293]:
```
def evaluate(model, dataloader):
    model.eval()
    total_loss = 0.0
    total_tokens = 0
    loss_fn = nn.CrossEntropyLoss(reduction = "sum") # for Perplexity

    with torch.no_grad():
        for xb, yb in dataloader:
            xb = xb.to(device)
            yb = yb.to(device)
            logits, _ = model(xb)
            B, T, D = logits.shape
            loss = loss_fn(logits.view(B*T, D), yb.view(B*T))
            total_loss += loss.item()
            total_tokens += B * T
    avg_loss = total_loss / total_tokens
    ppl = math.exp(avg_loss)
    return avg_loss, ppl
```

[300]:
```
train_dataset = TensorDataset(train_X, train_y)
val_dataset = TensorDataset(val_X, val_y)

train_loader = DataLoader(train_dataset, batch_size=BATCH_SIZE, shuffle=True)
val_loader = DataLoader(val_dataset, batch_size=BATCH_SIZE, shuffle=False)

model = TinyTransformer().to(device)
optimizer = torch.optim.AdamW(model.parameters(), lr = lr,
                              betas = betas, weight_decay = wd)
```

[301]:

```
num_epochs = 20
loss_fn = nn.CrossEntropyLoss()
train_loss_ = []
val_loss_ = []
val_ppl_ = []
slices = []

NUM_BATCH = train_X.shape[0] // BATCH_SIZE + (
    1 if train_X.shape[0] % BATCH_SIZE == 0 else 0)
for epoch in range(num_epochs):
    model.train()
    running_loss = 0.0
    for i, (xb, yb) in enumerate(train_loader):
        xb = xb.to(device)
        yb = yb.to(device)

        logits, _ = model(xb)  # [B, T, D]
        B, T, D = logits.shape
        loss = loss_fn(logits.view(B*T, D), yb.view(B*T))

        optimizer.zero_grad()
        loss.backward()
        torch.nn.utils.clip_grad_norm_(model.parameters(), grad_clip)
        optimizer.step()
        if i % 500 == 0:
            print(f"{i:4}" + "/" + str(NUM_BATCH), "batch loss =", loss.item())
        running_loss += loss.item()

    # evaluate
    val_loss, val_ppl = evaluate(model, val_loader)
    train_loss = running_loss / len(train_loader)
    train_loss_.append(train_loss)
    val_loss_.append(val_loss)
    val_ppl_.append(val_ppl_)
    slices.append(copy.deepcopy(model))
    print(f"Epoch {epoch+1}/{num_epochs} | train_loss {train_loss:.4f} |␣
↪val_loss {val_loss:.4f} | val_ppl {val_ppl:.3f}")
```

```
   0/5294 batch loss = 6.3902130126953125
 500/5294 batch loss = 5.603116512298584
1000/5294 batch loss = 5.462903022766113
1500/5294 batch loss = 5.308985710144043
2000/5294 batch loss = 5.062462329864502
2500/5294 batch loss = 4.881281852722168
3000/5294 batch loss = 4.781650543212891
3500/5294 batch loss = 4.644182205200195
4000/5294 batch loss = 4.570744037628174
4500/5294 batch loss = 4.424808979034424
```

```
5000/5294 batch loss = 4.411384105682373
Epoch 1/20 | train_loss 4.9576 | val_loss 4.4839 | val_ppl 88.578
   0/5294 batch loss = 4.367015838623047
 500/5294 batch loss = 4.289495468139648
1000/5294 batch loss = 4.345645904541016
1500/5294 batch loss = 4.278390884399414
2000/5294 batch loss = 4.210529327392578
2500/5294 batch loss = 4.117604732513428
3000/5294 batch loss = 4.096757411956787
3500/5294 batch loss = 4.110508441925049
4000/5294 batch loss = 4.044566631317139
4500/5294 batch loss = 4.034152984619141
5000/5294 batch loss = 4.0079522132873535
Epoch 2/20 | train_loss 4.1616 | val_loss 4.2110 | val_ppl 67.423
   0/5294 batch loss = 3.9908642768859863
 500/5294 batch loss = 3.99162220954895
1000/5294 batch loss = 3.9859116077423096
1500/5294 batch loss = 3.9033703804016113
2000/5294 batch loss = 3.962441921234131
2500/5294 batch loss = 3.8631808757781982
3000/5294 batch loss = 3.9603981971740723
3500/5294 batch loss = 3.863771438598633
4000/5294 batch loss = 3.843601703643799
4500/5294 batch loss = 3.8578710556030273
5000/5294 batch loss = 3.9044573307037354
Epoch 3/20 | train_loss 3.9219 | val_loss 4.0885 | val_ppl 59.651
   0/5294 batch loss = 3.903183698654175
 500/5294 batch loss = 3.788572311401367
1000/5294 batch loss = 3.9221911430358887
1500/5294 batch loss = 3.7333099842071533
2000/5294 batch loss = 3.808300733566284
2500/5294 batch loss = 3.825962781906128
3000/5294 batch loss = 3.779961585998535
3500/5294 batch loss = 3.689647912979126
4000/5294 batch loss = 3.758289098739624
4500/5294 batch loss = 3.733891487121582
5000/5294 batch loss = 3.7929563522338867
Epoch 4/20 | train_loss 3.7829 | val_loss 4.0124 | val_ppl 55.281
   0/5294 batch loss = 3.723968505859375
 500/5294 batch loss = 3.7517528533935547
1000/5294 batch loss = 3.732694149017334
1500/5294 batch loss = 3.7171454429626465
2000/5294 batch loss = 3.7043628692626953
2500/5294 batch loss = 3.707407236099243
3000/5294 batch loss = 3.630192279815674
3500/5294 batch loss = 3.6709144115448
4000/5294 batch loss = 3.659444570541382
4500/5294 batch loss = 3.7107934951782227
```

```
5000/5294 batch loss = 3.7371323108673096
Epoch 5/20 | train_loss 3.6856 | val_loss 3.9609 | val_ppl 52.507
   0/5294 batch loss = 3.671360492706299
 500/5294 batch loss = 3.62782621383667
1000/5294 batch loss = 3.617067813873291
1500/5294 batch loss = 3.5487585067749023
2000/5294 batch loss = 3.663928747177124
2500/5294 batch loss = 3.5612688064575195
3000/5294 batch loss = 3.6489319801330566
3500/5294 batch loss = 3.593162775039673
4000/5294 batch loss = 3.5601465702056885
4500/5294 batch loss = 3.630521297454834
5000/5294 batch loss = 3.5761122703552246
Epoch 6/20 | train_loss 3.6111 | val_loss 3.9221 | val_ppl 50.508
   0/5294 batch loss = 3.6614110469818115
 500/5294 batch loss = 3.577645778656006
1000/5294 batch loss = 3.5225865840911865
1500/5294 batch loss = 3.5440173149108887
2000/5294 batch loss = 3.498671770095825
2500/5294 batch loss = 3.584014654159546
3000/5294 batch loss = 3.600620746612549
3500/5294 batch loss = 3.5596299171447754
4000/5294 batch loss = 3.4759154319763184
4500/5294 batch loss = 3.6235973834991455
5000/5294 batch loss = 3.5270309448242188
Epoch 7/20 | train_loss 3.5516 | val_loss 3.8952 | val_ppl 49.165
   0/5294 batch loss = 3.5978851318359375
 500/5294 batch loss = 3.5966145992279053
1000/5294 batch loss = 3.566756010055542
1500/5294 batch loss = 3.5705535411834717
2000/5294 batch loss = 3.571927547454834
2500/5294 batch loss = 3.480666399002075
3000/5294 batch loss = 3.481130599975586
3500/5294 batch loss = 3.5287537574768066
4000/5294 batch loss = 3.5110387802124023
4500/5294 batch loss = 3.449521541595459
5000/5294 batch loss = 3.4010913372039795
Epoch 8/20 | train_loss 3.5022 | val_loss 3.8736 | val_ppl 48.114
   0/5294 batch loss = 3.486612558364868
 500/5294 batch loss = 3.5179638862609863
1000/5294 batch loss = 3.4721386432647705
1500/5294 batch loss = 3.4650135040283203
2000/5294 batch loss = 3.5153136253356934
2500/5294 batch loss = 3.588919162750244
3000/5294 batch loss = 3.481585741043091
3500/5294 batch loss = 3.4176855087280273
4000/5294 batch loss = 3.410244941711426
4500/5294 batch loss = 3.510824203491211
```

```
5000/5294 batch loss = 3.406198501586914
Epoch 9/20 | train_loss 3.4602 | val_loss 3.8534 | val_ppl 47.154
   0/5294 batch loss = 3.4047844409942627
 500/5294 batch loss = 3.4145071506500244
1000/5294 batch loss = 3.3896517753601074
1500/5294 batch loss = 3.4201254844665527
2000/5294 batch loss = 3.4027271270751953
2500/5294 batch loss = 3.5129785537719727
3000/5294 batch loss = 3.4008688926696777
3500/5294 batch loss = 3.444234609603882
4000/5294 batch loss = 3.4549455642700195
4500/5294 batch loss = 3.3516595363616943
5000/5294 batch loss = 3.4665777683258057
Epoch 10/20 | train_loss 3.4239 | val_loss 3.8400 | val_ppl 46.527
   0/5294 batch loss = 3.3927605152130127
 500/5294 batch loss = 3.332500696182251
1000/5294 batch loss = 3.4279091358184814
1500/5294 batch loss = 3.2912240028381348
2000/5294 batch loss = 3.3777735233306885
2500/5294 batch loss = 3.4166383743286133
3000/5294 batch loss = 3.413107395172119
3500/5294 batch loss = 3.444436550140381
4000/5294 batch loss = 3.438514471054077
4500/5294 batch loss = 3.3485419750213623
5000/5294 batch loss = 3.358513832092285
Epoch 11/20 | train_loss 3.3920 | val_loss 3.8306 | val_ppl 46.091
   0/5294 batch loss = 3.414003849029541
 500/5294 batch loss = 3.34806752204895
1000/5294 batch loss = 3.3963820934295654
1500/5294 batch loss = 3.322866439819336
2000/5294 batch loss = 3.309598922729492
2500/5294 batch loss = 3.3278615474700928
3000/5294 batch loss = 3.4055674076080322
3500/5294 batch loss = 3.385599374771118
4000/5294 batch loss = 3.368709087371826
4500/5294 batch loss = 3.3082761764526367
5000/5294 batch loss = 3.440295457839966
Epoch 12/20 | train_loss 3.3636 | val_loss 3.8214 | val_ppl 45.666
   0/5294 batch loss = 3.3613345623016357
 500/5294 batch loss = 3.3738222122192383
1000/5294 batch loss = 3.3684756755828857
1500/5294 batch loss = 3.2893712520599365
2000/5294 batch loss = 3.364840030670166
2500/5294 batch loss = 3.3129584789276123
3000/5294 batch loss = 3.3817615509033203
3500/5294 batch loss = 3.386246919631958
4000/5294 batch loss = 3.4030301570892334
4500/5294 batch loss = 3.356894016265869
```

```
5000/5294 batch loss = 3.3039660453796387
Epoch 13/20 | train_loss 3.3376 | val_loss 3.8130 | val_ppl 45.285
   0/5294 batch loss = 3.280695915222168
 500/5294 batch loss = 3.2736480236053467
1000/5294 batch loss = 3.4114773273468018
1500/5294 batch loss = 3.3242621421813965
2000/5294 batch loss = 3.295977830886841
2500/5294 batch loss = 3.4093387126922607
3000/5294 batch loss = 3.2655811309814453
3500/5294 batch loss = 3.342923641204834
4000/5294 batch loss = 3.294598340988159
4500/5294 batch loss = 3.352964401245117
5000/5294 batch loss = 3.3088223934173584
Epoch 14/20 | train_loss 3.3139 | val_loss 3.8087 | val_ppl 45.090
   0/5294 batch loss = 3.292949914932251
 500/5294 batch loss = 3.396984577178955
1000/5294 batch loss = 3.288557529449463
1500/5294 batch loss = 3.2766427993774414
2000/5294 batch loss = 3.3123302459716797
2500/5294 batch loss = 3.3089911937713623
3000/5294 batch loss = 3.3714425563812256
3500/5294 batch loss = 3.2674150466918945
4000/5294 batch loss = 3.288177728652954
4500/5294 batch loss = 3.287961483001709
5000/5294 batch loss = 3.266645908355713
Epoch 15/20 | train_loss 3.2924 | val_loss 3.8040 | val_ppl 44.879
   0/5294 batch loss = 3.2542178630828857
 500/5294 batch loss = 3.2752585411071777
1000/5294 batch loss = 3.269796848297119
1500/5294 batch loss = 3.236529588699341
2000/5294 batch loss = 3.2818856239318848
2500/5294 batch loss = 3.2779784202575684
3000/5294 batch loss = 3.2288739681243896
3500/5294 batch loss = 3.2361578941345215
4000/5294 batch loss = 3.264878511428833
4500/5294 batch loss = 3.2899558544158936
5000/5294 batch loss = 3.24092173576355
Epoch 16/20 | train_loss 3.2726 | val_loss 3.8025 | val_ppl 44.811
   0/5294 batch loss = 3.2611782550811768
 500/5294 batch loss = 3.2552905082702637
1000/5294 batch loss = 3.231029748916626
1500/5294 batch loss = 3.262840986251831
2000/5294 batch loss = 3.238638401031494
2500/5294 batch loss = 3.2664666175842285
3000/5294 batch loss = 3.2890784740448
3500/5294 batch loss = 3.3341753482818604
4000/5294 batch loss = 3.3355841636657715
4500/5294 batch loss = 3.147444248199463
```

```
5000/5294 batch loss = 3.290396213531494
Epoch 17/20 | train_loss 3.2542 | val_loss 3.8014 | val_ppl 44.763
   0/5294 batch loss = 3.2390472888946533
 500/5294 batch loss = 3.256007432937622
1000/5294 batch loss = 3.247067928314209
1500/5294 batch loss = 3.2651355266571045
2000/5294 batch loss = 3.3150177001953125
2500/5294 batch loss = 3.2326903343200684
3000/5294 batch loss = 3.222816228866577
3500/5294 batch loss = 3.1895110607147217
4000/5294 batch loss = 3.1498517990112305
4500/5294 batch loss = 3.223426580429077
5000/5294 batch loss = 3.16745662689209
Epoch 18/20 | train_loss 3.2371 | val_loss 3.8011 | val_ppl 44.749
   0/5294 batch loss = 3.231670618057251
 500/5294 batch loss = 3.2736830711364746
1000/5294 batch loss = 3.3001251220703125
1500/5294 batch loss = 3.3421576023101807
2000/5294 batch loss = 3.2151246070861816
2500/5294 batch loss = 3.2029433250427246
3000/5294 batch loss = 3.167503595352173
3500/5294 batch loss = 3.204571485519409
4000/5294 batch loss = 3.2866687774658203
4500/5294 batch loss = 3.189556360244751
5000/5294 batch loss = 3.2073349952697754
Epoch 19/20 | train_loss 3.2211 | val_loss 3.8001 | val_ppl 44.704
   0/5294 batch loss = 3.2288198471069336
 500/5294 batch loss = 3.1839210987091064
1000/5294 batch loss = 3.193129539489746
1500/5294 batch loss = 3.2571301460266113
2000/5294 batch loss = 3.2382919788360596
2500/5294 batch loss = 3.161642551422119
3000/5294 batch loss = 3.1884799003601074
3500/5294 batch loss = 3.1512513160705566
4000/5294 batch loss = 3.198305130004883
4500/5294 batch loss = 3.2008771896362305
5000/5294 batch loss = 3.255891799926758
Epoch 20/20 | train_loss 3.2061 | val_loss 3.8028 | val_ppl 44.828
```

[ ]:
```
# total parameters
i = 0
for p in model.parameters():
    i += math.exp(sum(math.log(s) for s in p.shape))
print(int(round(i)))
```

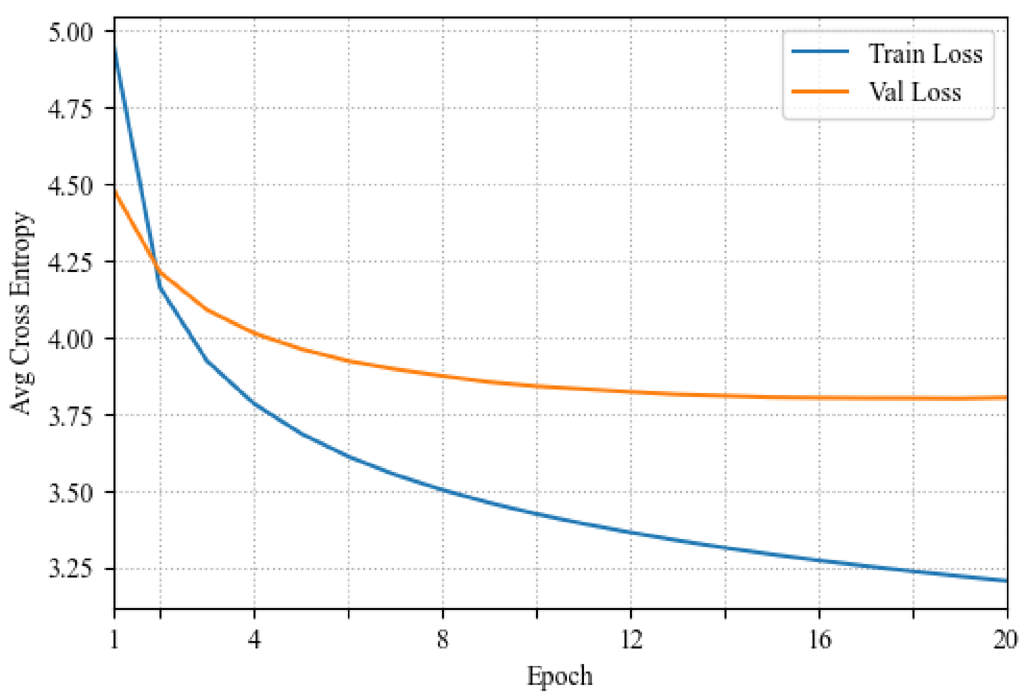
```
326784
```

5 Visualization & Interpretation

The best PPL on the validation set is 44.704 (epoch=19) and as training stops the PPL is 44.828.

5.1 Training and Validation Loss Curves over Epochs

[334]:
```
X = np.linspace(1, num_epochs, num_epochs)
plt.figure(figsize = (6, 4))
plt.plot(X, train_loss_, label = "Train Loss")
plt.plot(X, val_loss_, label = "Val Loss")
plt.xlabel("Epoch")
plt.ylabel("Avg Cross Entropy")
plt.xticks([1] + [2 * i for i in range(1, 11)],
           labels = [1] + [" " if i % 4 != 0 else i for i in range(2, 21, 2)])
plt.xlim(1, 20)
plt.legend()
plt.grid(True, 'major', linestyle = ':')
plt.show()
```



5.2 Attention Heatmaps

[459]:
```
def tokenize(text, vocab):
    tokens = []
    tokenizer = AutoTokenizer.from_pretrained("gpt2")
```

```
    words_with_offsets = tokenizer.backend_tokenizer.pre_tokenizer.
↪pre_tokenize_str(text)
    new_words = [word for word, offset in words_with_offsets]
    for word in new_words:
        if word.isupper():
            word = word.capitalize()
        tokens += tokenize_word(word, vocab)
    return tokens
def encode(tokens, transformed_space = False, replaced = ' '):
    if transformed_space:
        return [stoi[t] if t[0] != replaced else stoi['Ġ' + t[1:]] for t in␣
↪tokens]
    return [stoi[t] for t in tokens]
def decode(token_ids, show_space = False, replace = ' '):
    tokens = [itos[int(t)] for t in token_ids]
    if show_space:
        for i in range(len(tokens)):
            if tokens[i][0] == 'Ġ':
                tokens[i] = replace + tokens[i][1:]
    return tokens
```

[414]:
```
tokenize('Hello world!', vocab)
```

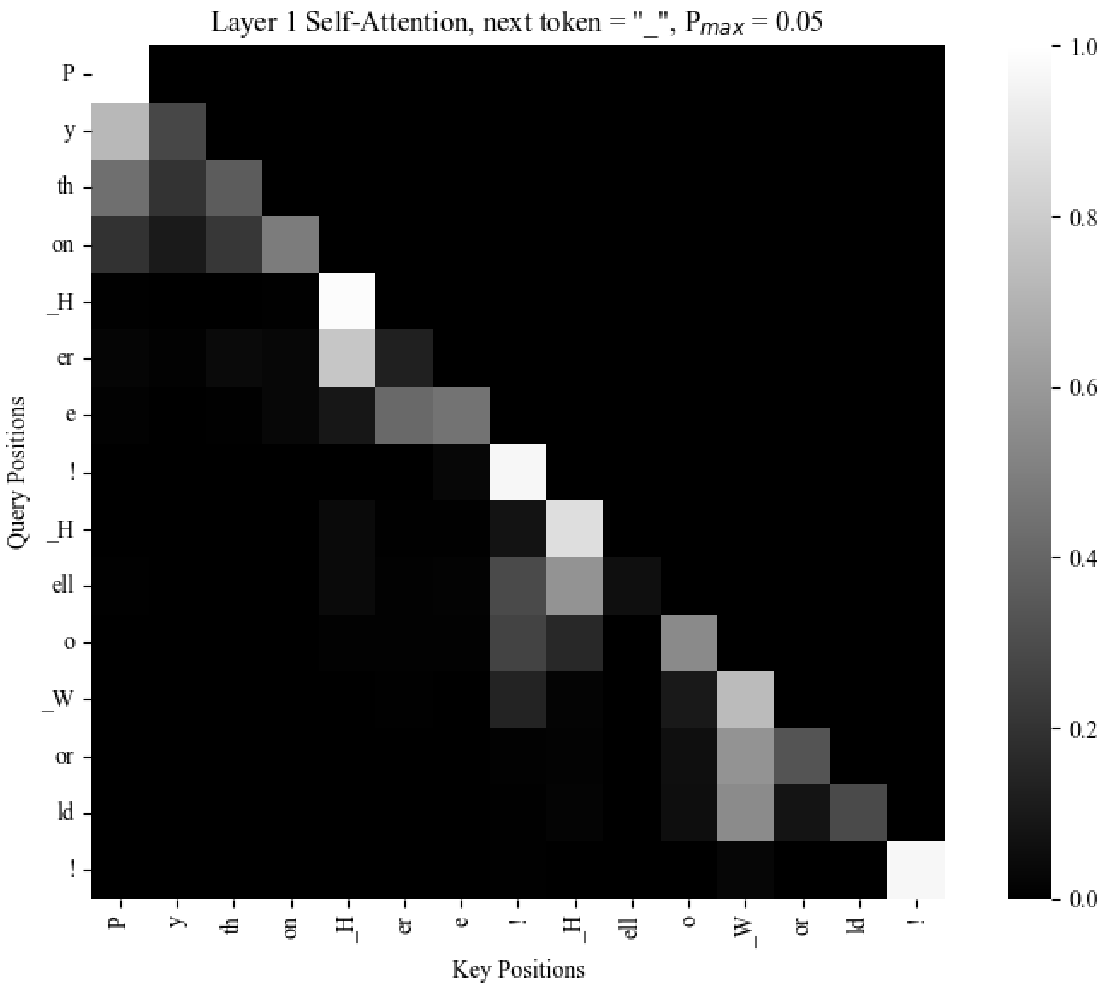
[414]:
```
[71, 131, 51, 430, 128, 0]
```

Here the space is replaced with a underscore.

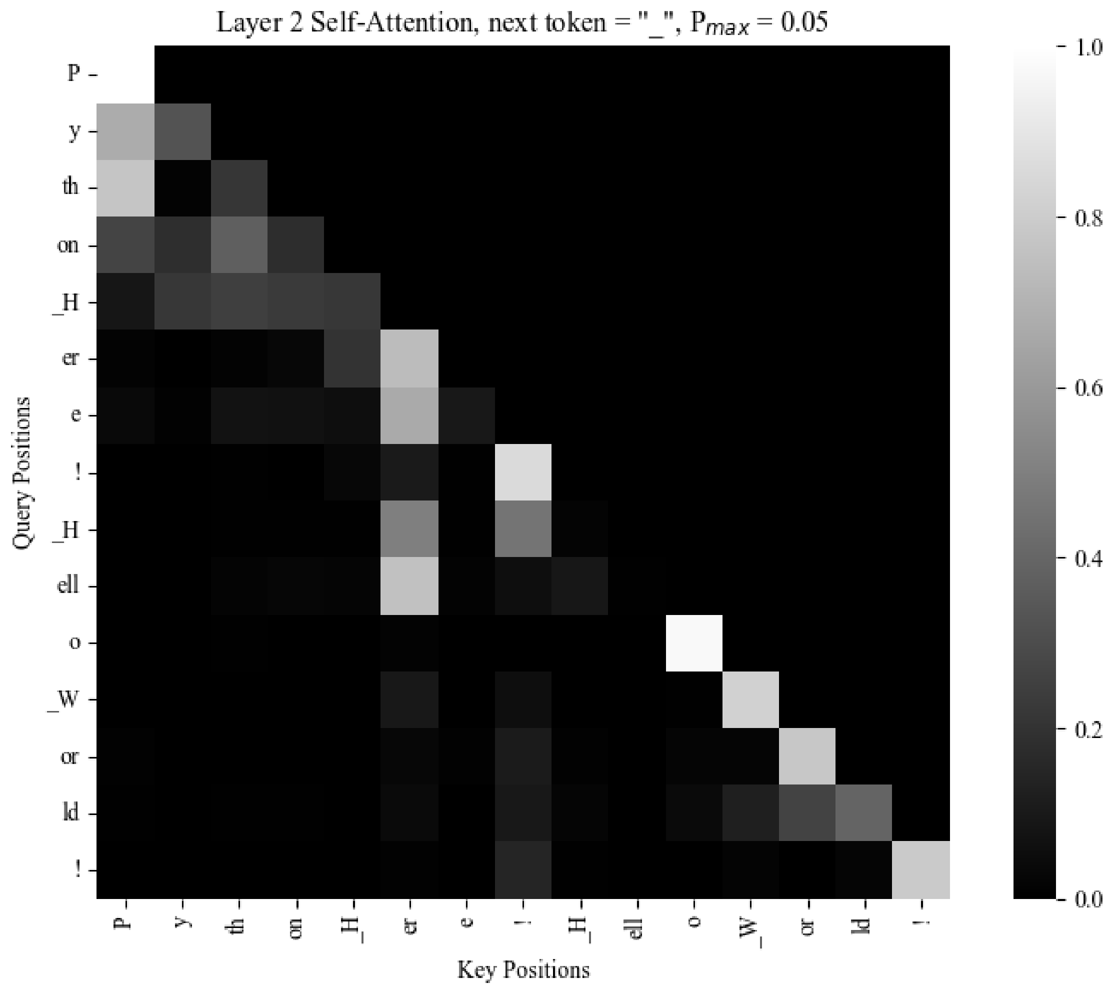
[525]:
```
def plot_attention(model, vocab, text, idx = 0, max_seq_len=SEQ_LEN,␣
↪figsize=(8, 6),
                   layers = None):
    model.eval()
    tokens = tokenize(text, vocab)
    tokens = tokens[:max_seq_len]
    x = torch.tensor(tokens, dtype=torch.long).unsqueeze(0).to(device)

    with torch.no_grad():
        logits, attn_maps = model(x, need_attn=True)

    i = torch.argmax(logits[0, idx, :]).item()
    prob = torch.softmax(logits[0, idx, :], dim = 0)[i].item()
    next_token = itos[i]
    if next_token[0] == 'Ġ':
        next_token = '_' + next_token[1:]

    token_strings = decode(tokens, show_space = True, replace = '_')
    T = len(tokens)
```

```
    for layer_i, attn in enumerate(attn_maps):
        assert idx <= T
        if layers and layer_i not in layers:
            break
        attn = attn[idx].cpu()  # take batch index 0

        if attn.dim() == 3:
            attn = attn.squeeze(0)

        plt.figure(figsize=figsize)
        sns.heatmap(attn[:T, :T],
                    xticklabels=token_strings,
                    yticklabels=token_strings,
                    cmap="grey",
                    square=True)
        plt.title(f"Layer {layer_i+1} Self-Attention, next token =␣
↪\"{next_token}\", " +
                  r"P$_{max}$" + f" = {prob:.2f}")
        plt.xlabel("Key Positions")
        plt.ylabel("Query Positions")
        plt.xticks(rotation=90)
        plt.yticks(rotation=0)
        plt.tight_layout()
        plt.show()
```

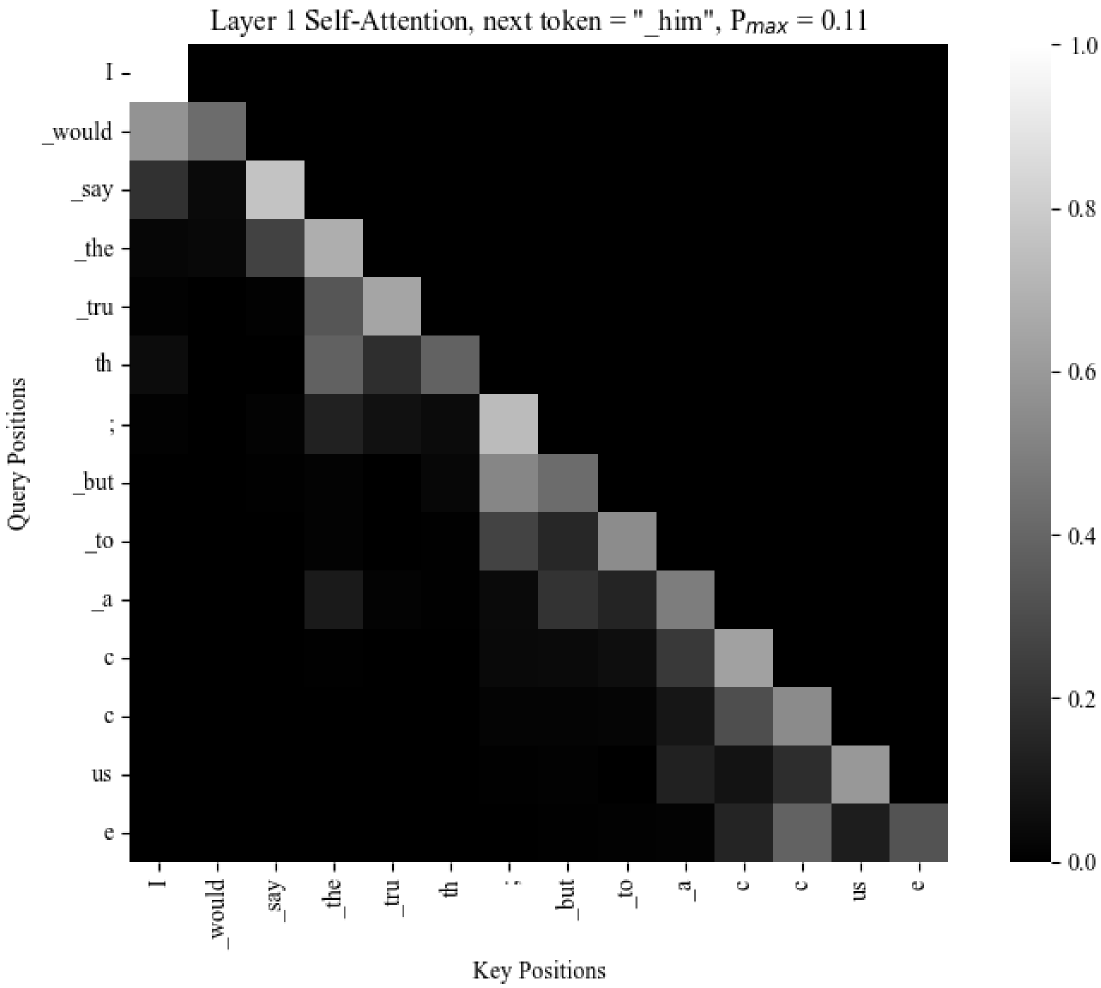
[526]:
```
plot_attention(slices[-2], vocab, "Python Here! Hello World!", idx = -1)
```



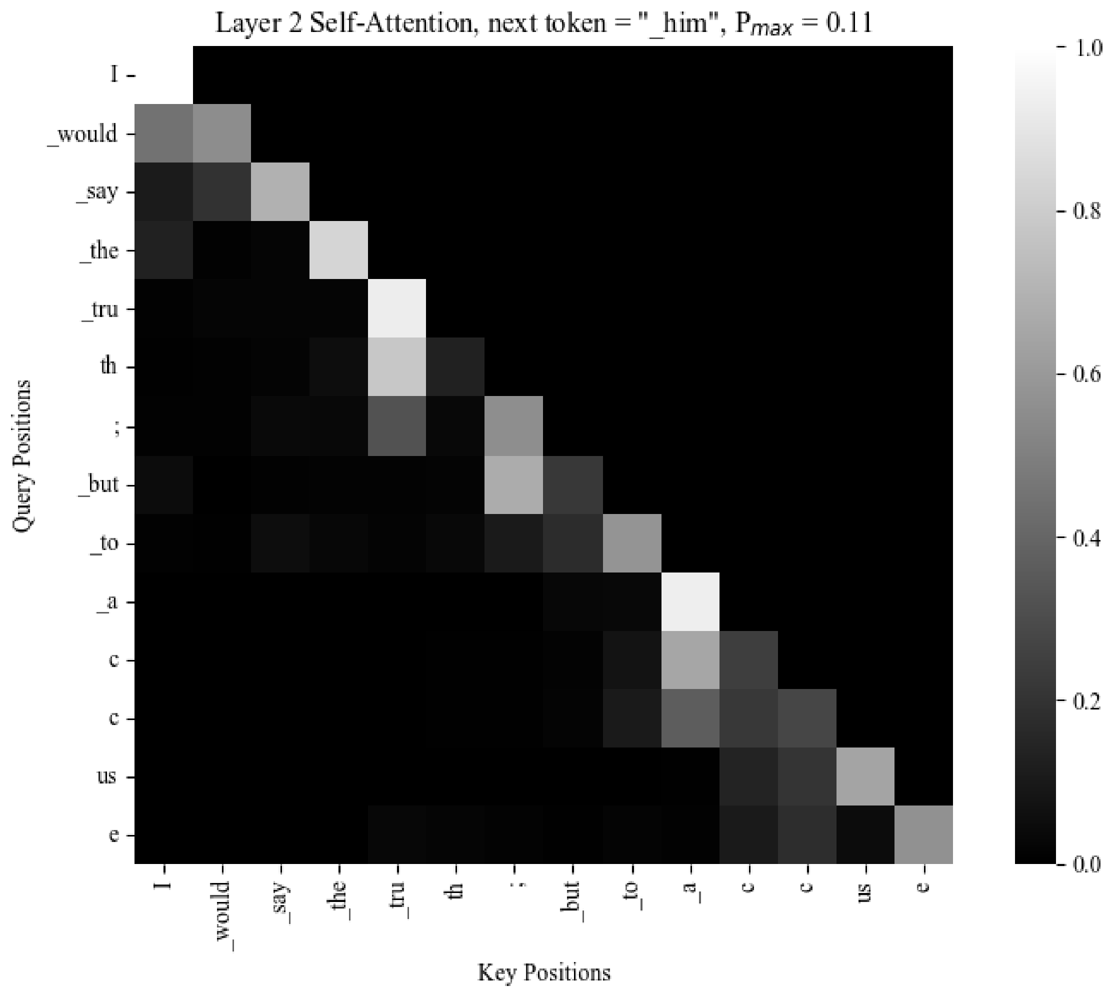
Layer 1 Self-Attention, next token = "_", P_{max} = 0.05
Query Positions
Key Positions
P
y
th
on
_H
er
e
!
_H
ell
o
_W
or
ld
!
1.0
0.8
0.6
0.4
0.2
0.0




```
[527]: plot_attention(slices[-2], vocab, "I would say the truth; but to accuse", idx =
       -1)
```

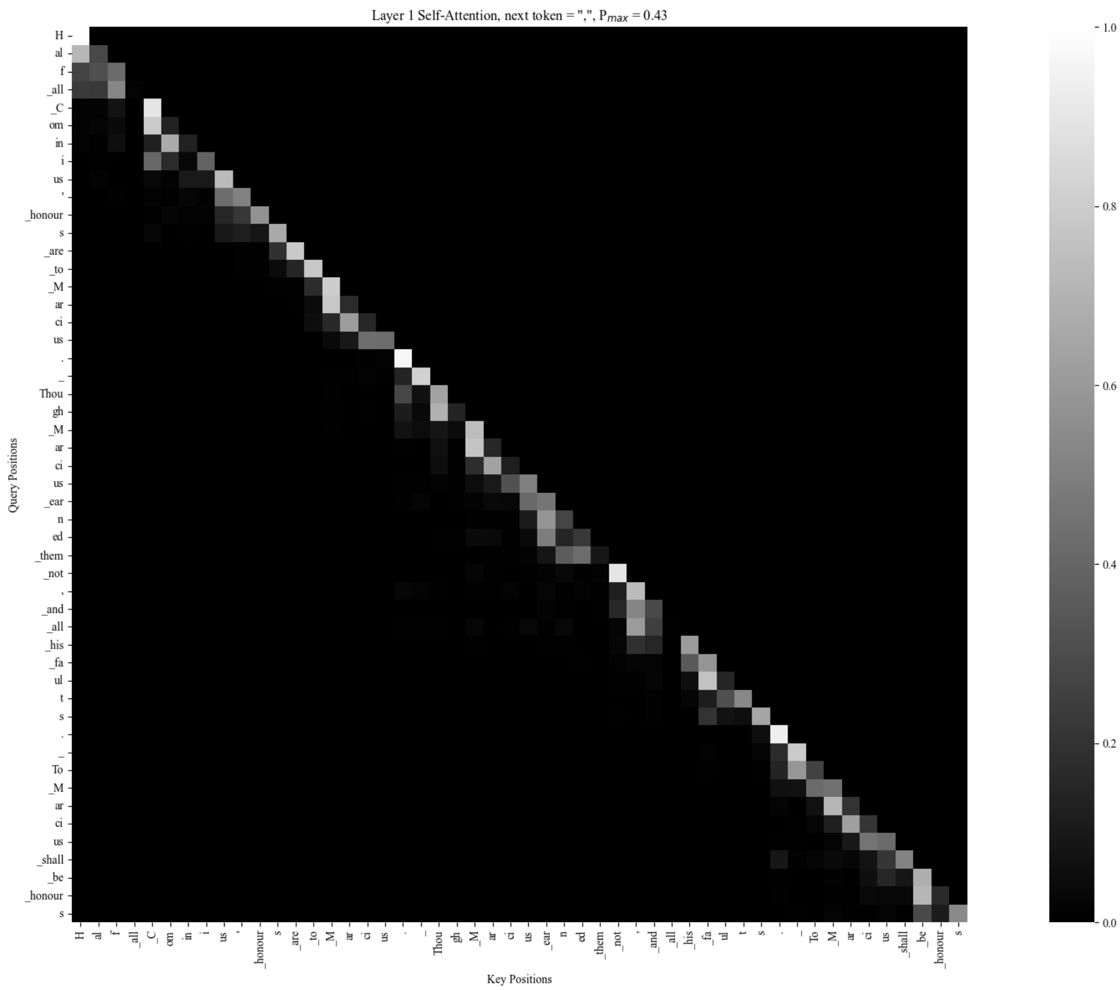


Layer 1 Self-Attention, next token = "_him", P_{max} = 0.11
Query Positions
I
_would
_say
_the
_tru
th
;
_but
_to
_a
c
c
us
e
Key Positions
1.0
0.8
0.6
0.4
0.2
0.0

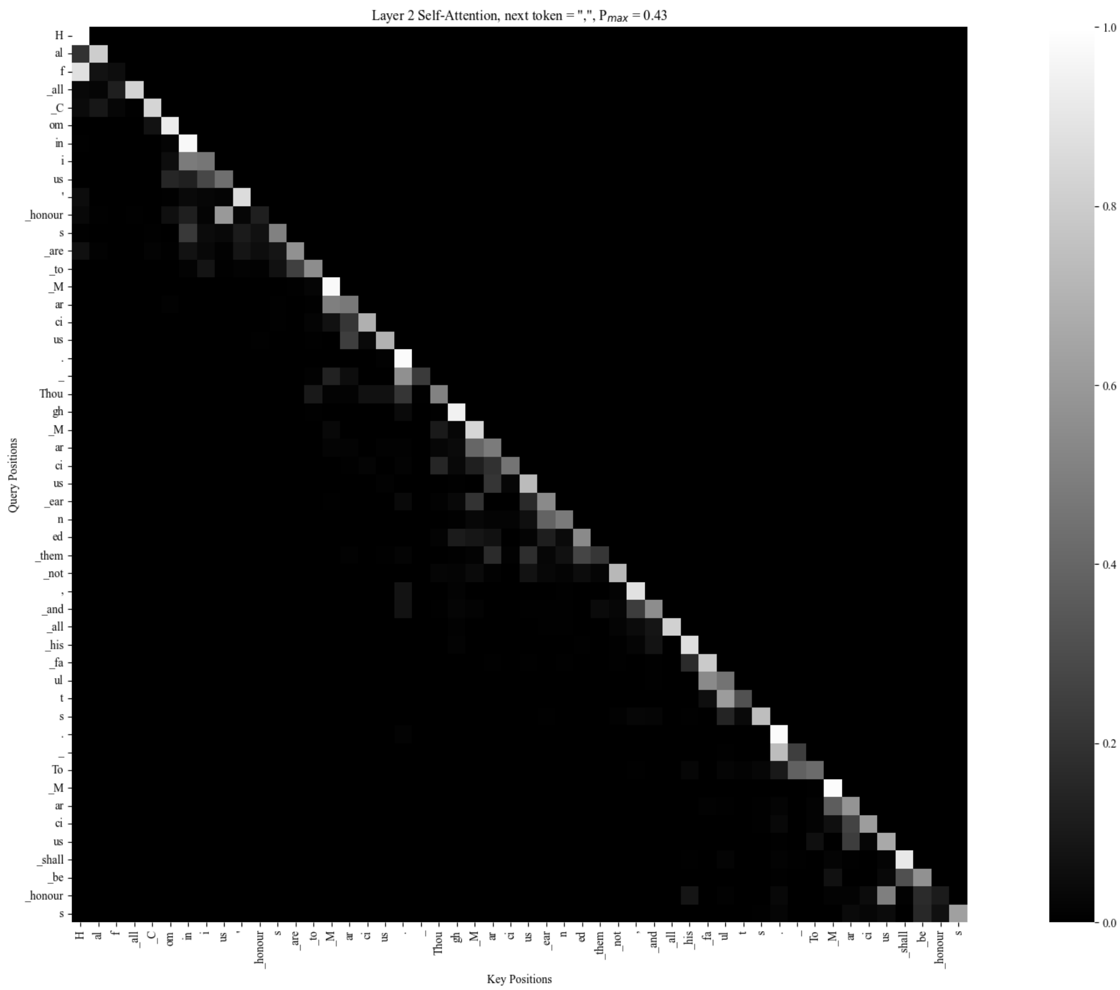


[528]:

```
plot_attention(slices[-2], vocab,
               "Half all Cominius' honours are to Marcius. Though Marcius␣
↪earned them not, and all his faults. To Marcius shall be honours",
               -1, figsize = (20, 12))
```



Layer 1 Self-Attention, next token = ",", P_{max} = 0.43
Query Positions
Key Positions



5.3 Sample Generation

[486]:
```
def generate(model, vocab, text, epoch = 1, max_seq_len = SEQ_LEN, loop_inf =
 ↪False):
    model.eval()
    tokens = tokenize(text, vocab)
    tokens = tokens[:max_seq_len]
    if len(tokens) >= max_seq_len and not loop_inf:
        return
    probs = []
    while epoch > 0:
        if len(tokens) > max_seq_len and not loop_inf:
            break
        if len(tokens) > max_seq_len and loop_inf:
            x = x = torch.tensor(tokens[-SEQ_LEN:], dtype=torch.long).
 ↪unsqueeze(0).to(device)
```

```python
        else:
            x = torch.tensor(tokens, dtype=torch.long).unsqueeze(0).to(device)
        with torch.no_grad():
            logits, attn_maps = model(x, need_attn=True)

            i = torch.argmax(logits[0, -1, :]).item()
            prob = torch.softmax(logits[0, -1, :], dim = 0)[i].item()
            next_token = itos[i]
        probs.append((next_token, prob))
        tokens.append(i)
        epoch -= 1

    token_strings = decode(tokens, show_space = True, replace = ' ')
    return token_strings, probs
```

[513]:
```python
token_strings, probs = generate(slices[-2], vocab,
                                "Hello world! This is Python! ", epoch = 18)
print(*token_strings, sep = "", end = "")
```

```
Hello world! This is Python! I am appear to the crown,And I am advance
```

[514]:
```python
token_strings, probs = generate(slices[-2], vocab,
    "Against him first: he's a very dog to the commonalty. ", epoch = 18)
print(*token_strings, sep = "", end = "")
```

```
Against him first: he's a very dog to the commonalty. I have a king, I'll not
beggar,And, as
```

6 Discussion & Reflection

What patterns do you observe in the attention maps?

The attention maps typically show that most semantically holistic combinations of tokens makes the model concentrate more on, generally reflecting the local dependency of natural language.

In early stages, the model remains underfitting and attention maps could be noisy and more uniform (shown below), but later the diagonal bands show up and structured spikes, triangles appear.

Interestingly, the vertical spikes and mutual attention show frequently on pairs or single punctuation, which shows the model gradually grasp the structure of the language through the punctuations.

Which hyperparameters (learning rate, context length, model size) had the greatest impact on stability?

I think the answer is Learning rate.

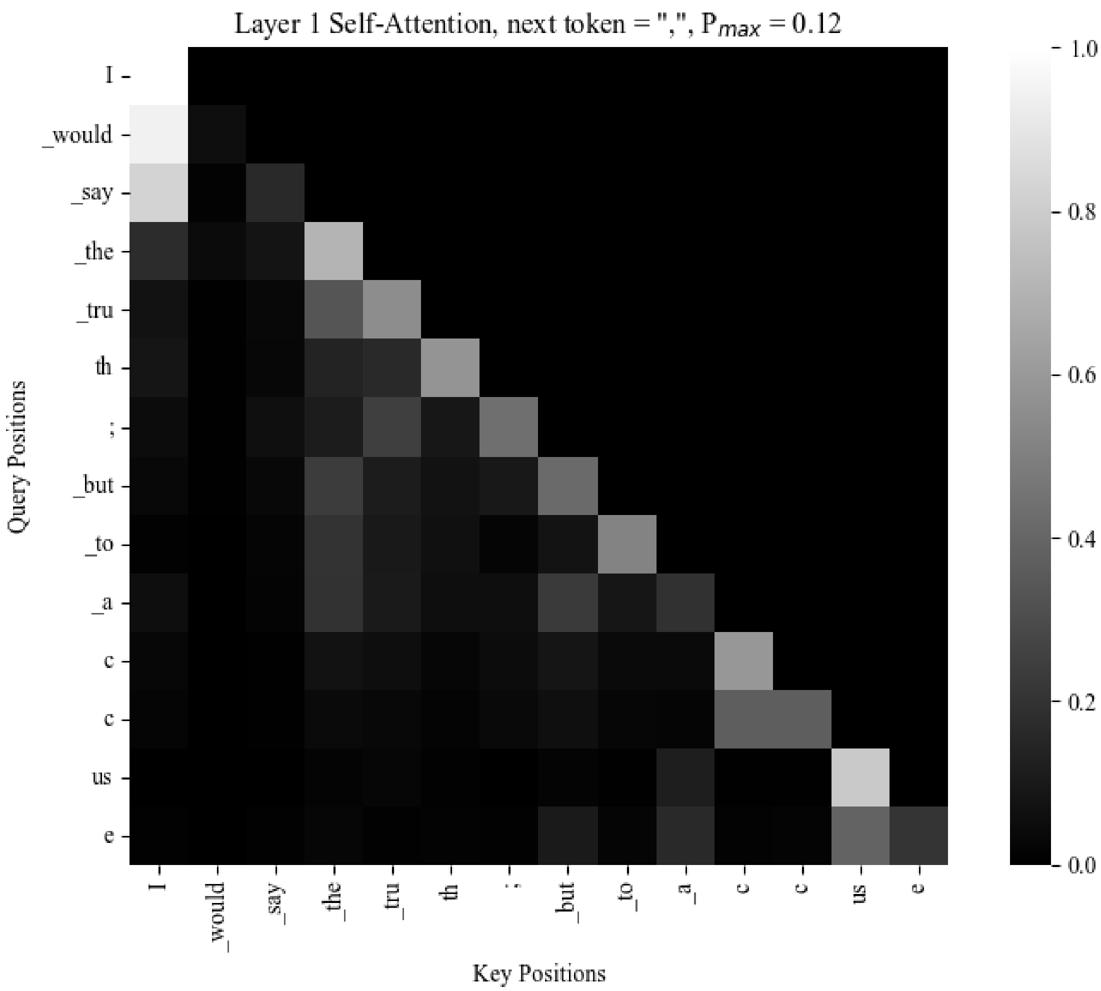
I trained this model under many learning rates and when it's too high, e.g. $>$ 3e-3, the model learns nothing and the validation loss increases steadily. If it's too low or with a higher weight decay coefficient in AdamW, the model learns nothing (probably extremely slow) and got stuck. You have to maintain it or reduce it carefully in a feasible interval.

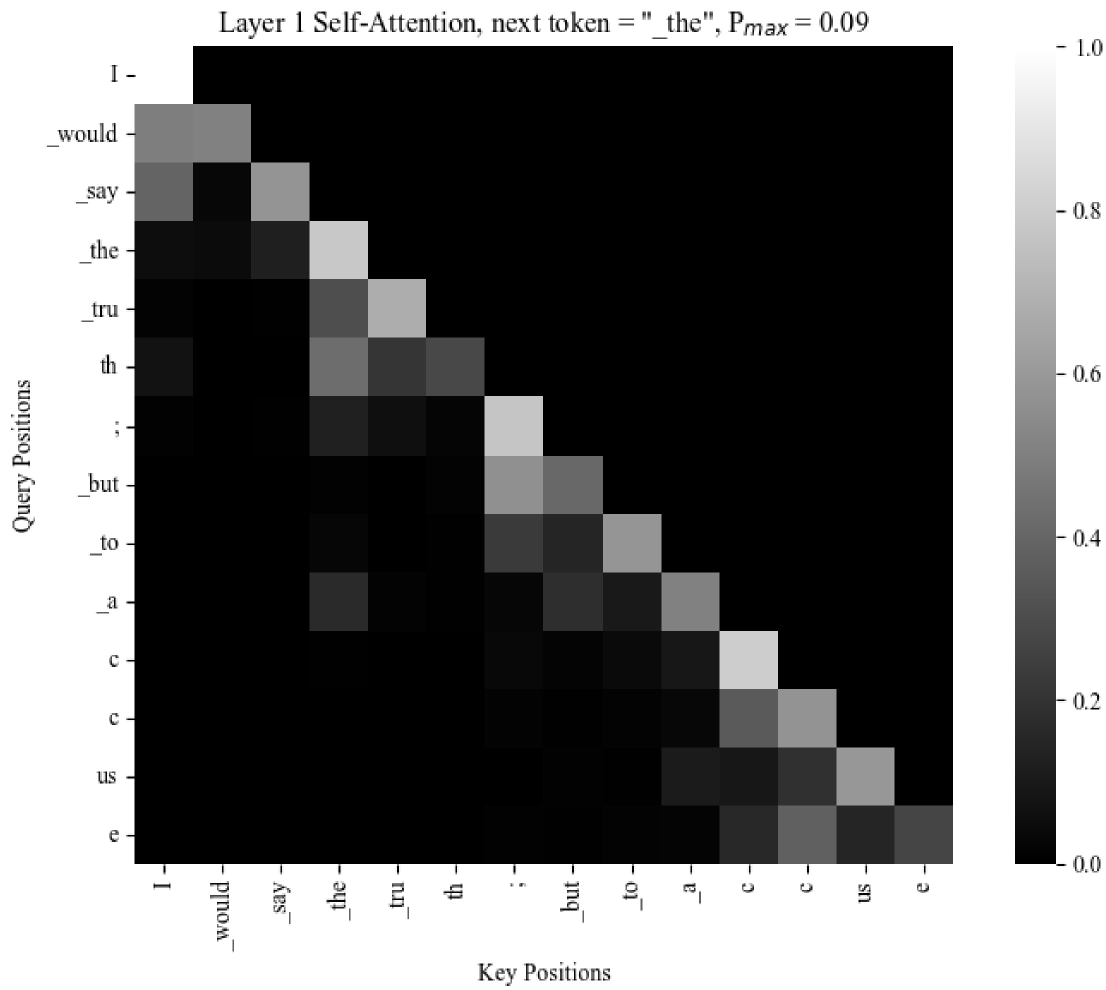
Context length has lighter influence on the stability if it is in the reasonable range. If context length is too short, which is unreasonable, the data leakage could easily take place and the model will exhibit very good performance on validation set, though meaningless. Longer context makes the model understands better, but not always greatly helpful.

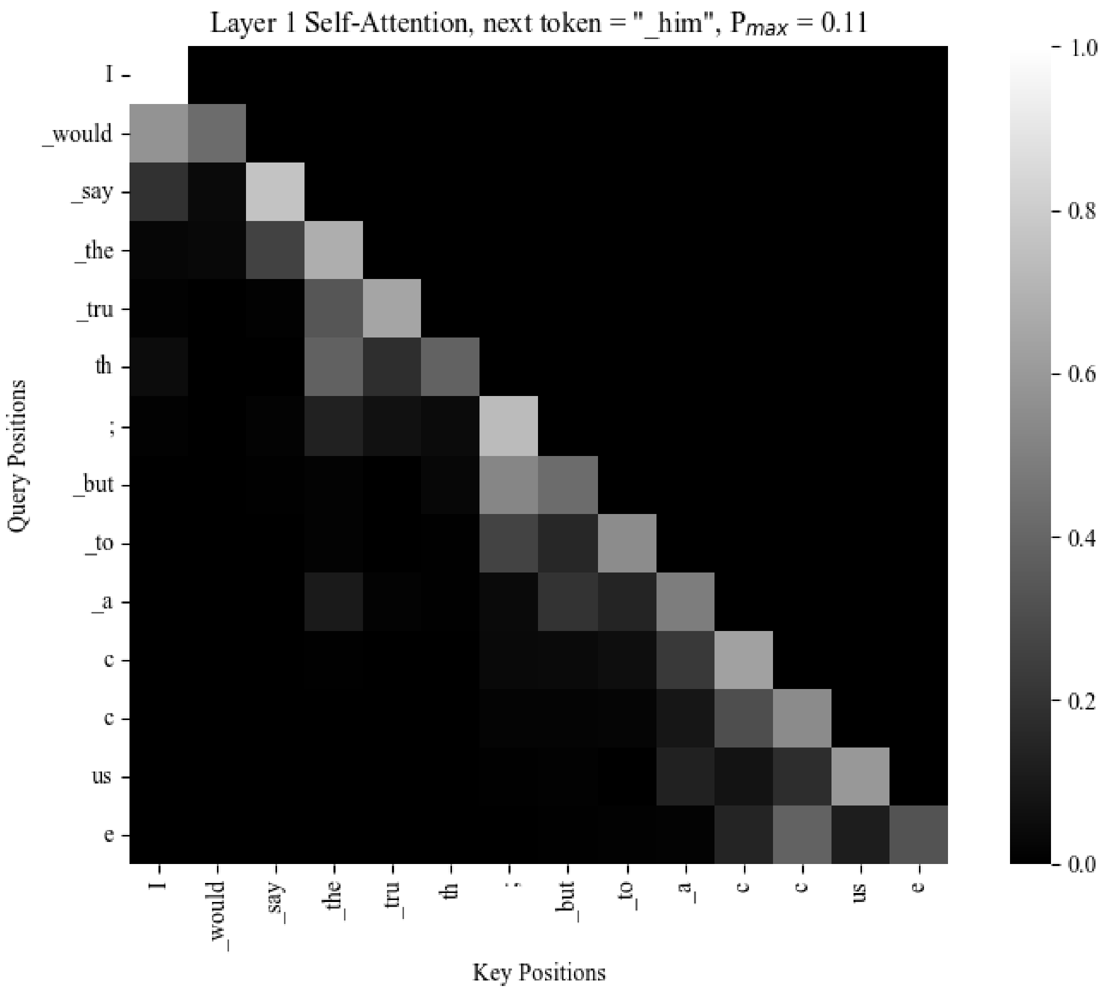
Model size: since we are only asked to implement 2 Transformer blocks, the parameters related to the model size which we can fiddle with are hidden state dimension (in FFN) and the embedding dimension. These had little impact on stability, again, in the reasonable range. For example, I tried hidden_dim = 16, 32, 512 and all results (val loss) are almost the same.

How does attention evolve as the model trains over epochs?

[533]:
```
for t in [0, 9, 18]:
    plot_attention(slices[t], vocab, "I would say the truth; but to accuse",
                   idx = -1, layers = [0])
```




Layer 1 Self-Attention, next token = "_the", P_{max} = 0.09
Query Positions
Key Positions
I
_would
_say
_the
_tru
th
;
_but
_to
_a
c
c
us
e
1.0
0.8
0.6
0.4
0.2
0.0



We can see from these graphs that, the attention at first was chaotic (epoch = 1), no specific patterns were shown. However, as we trained it for longer time (epoch = 10), patterns show up, such as attention focuses on semantically holistic token combinations (e.g. the attention for the whole word "accuse" were high amongst pairs of its sublevel tokens, or "the" is with high attention on the following "truth" = "tru" + "th"). As we train it further (epoch = 19), some pairs of attention are enhanced and some are diminished, for example, "I" has lower attention on "the".

What role do positional encodings play - could the model function without them?

No. Although we have causal masks, the positional encodings plays an important role in guaranteeing the model is not positional or permutation invariant: "You can jump like rabbits" is totally different from "Can rabbits jump like you" semantically. Causal masks are not sufficient to enable the model to catch structural information encoded in positions.

Reflect on runtime and memory footprint - where are the bottlenecks?

1. The attention map seems to be activated mainly along the diagonal line – could be reduced. As embed_dim (vocab_size) goes up, the computation could be of cost O(d_embed^2).

2. Matrix multiplication in Q, K, V also costs computationally O(d_model^2).
3. Attention recomputes a lot when the model is performing autoregressive generation. Each time only 1 token is selected and generated.

7 AI Tool Usage Disclosure

AI Tools Used ChatGPT (OpenAI, GPT-4 Configuration)

AI Contribution The author asked ChatGPT to check whether the implementation is correct and how to improve it. ChatGPT also helped in writing only abstract and problem definition.

Personal Contribution The author has written almost all of this code and the report (from Dataset description to the end). No AI assistant like Copilot was used in code writing. Some parts are inspired by the online documentation and forum posts about PyTorch and other package libraries. Some parameters are discussed with friends of the author.