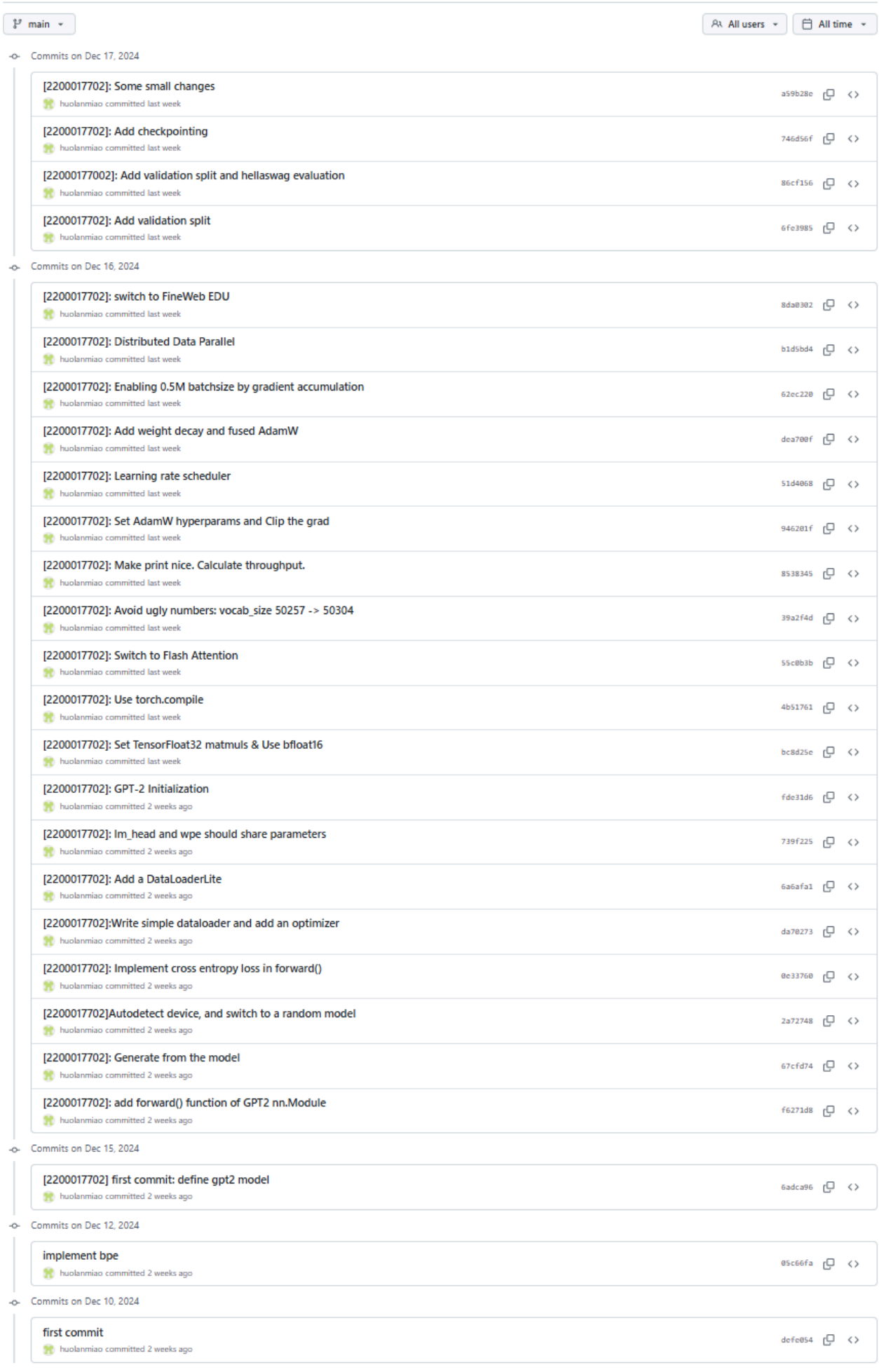
My commit history



Commit History

First commit

CausalSelfAttention: 将QKV和多头的运算，利用分块矩阵乘法的性质，只做一次矩阵乘法

1. 定义layer，3 * config.n_embd分别是QKV的weights

```
# n_embed = n_head * head_size
# key, query, value projections for all heads, but in a batch
self.c_attn = nn.Linear(config.n_embd, 3 * config.n_embd)
# output projection
self.c_proj = nn.Linear(config.n_embd, config.n_embd)
```

2. QKV一次算出来，然后分成Q、K、V，再分成多头

```
# 计算QKV然后分块
qkv = self.c_attn(x)
q, k, v = qkv.split(self.n_embd, dim=2)

# 分成多个头，每个头分别做self-attention
k = k.view(B, T, self.n_head, C // self.n_head).transpose(1, 2) # (B, nh, T, hs)
q = q.view(B, T, self.n_head, C // self.n_head).transpose(1, 2) # (B, nh, T, hs)
v = v.view(B, T, self.n_head, C // self.n_head).transpose(1, 2) # (B, nh, T, hs)
```

3. 对每个头分别做attention matrix的计算

```
# Batched attention mechanisms
att = (q @ k.transpose(-2, -1)) * (1.0 / math.sqrt(k.size(-1)))
```

4. Attention mask是通过将希望mask的位置赋为-inf，使得softmax之后概率为0。

```
# 实现注意力掩码，然后对Value做加权
att = att.masked_fill(self.bias[:,:,:T,:T] == 0, float('-inf'))
att = F.softmax(att, dim=-1)
y = att @ v # (B, nh, T, T) x (B, nh, T, hs) -> (B, nh, T, hs)
```

5. 合并每个head的结果，得到hidden_size与最初的embedding_dim相同

```
# .contiguous()确保返回一个连续的张量。
y = y.transpose(1, 2).contiguous().view(B, T, C)
# re-assemble all head outputs side by side
```

6. 最后做一次proj (n_embed * n_embed)，得到hidden_states

```
        # output projection
        y = self.c_proj(y)
```

MLP层：采用GELU激活函数，采用一种近似估计

https://pytorch.org/docs/stable/generated/torch.nn.GELU.html

GELU

CLASS torch.nn.GELU(*approximate='none'*) [SOURCE]

Applies the Gaussian Error Linear Units function.

$$\text{GELU}(x) = x * \Phi(x)$$

where $\Phi(x)$ is the Cumulative Distribution Function for Gaussian Distribution.

When the approximate argument is 'tanh', Gelu is estimated with:

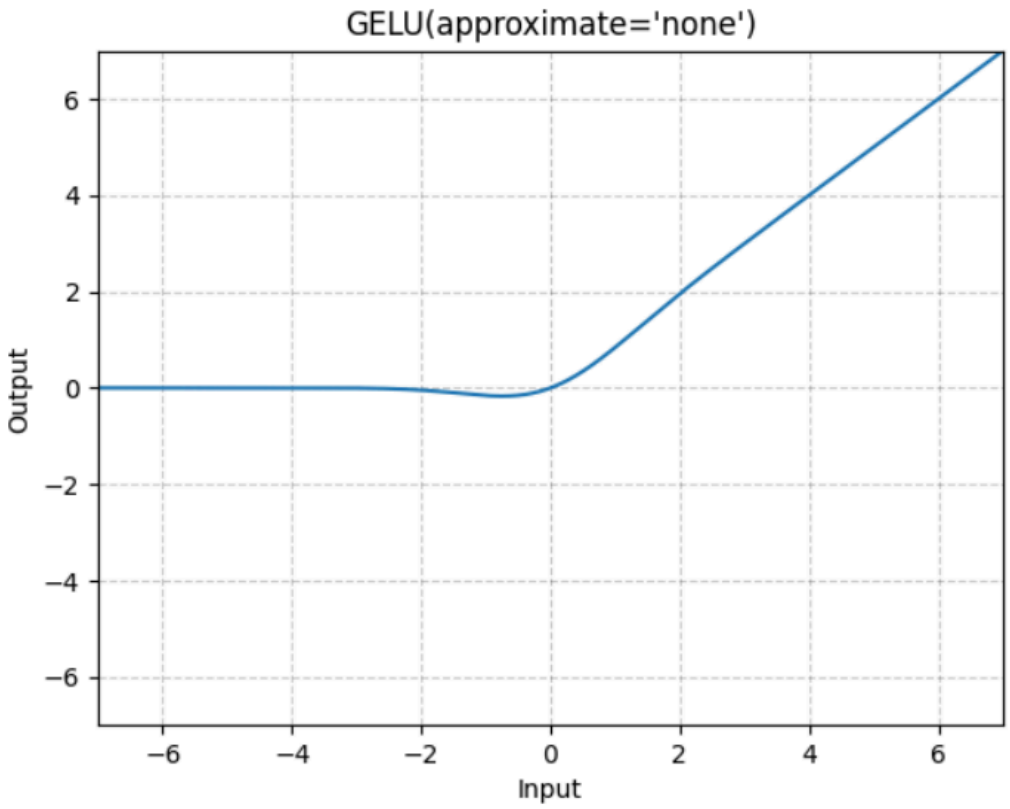
$$\text{GELU}(x) = 0.5 * x * (1 + \text{Tanh}(\sqrt{2/\pi} * (x + 0.044715 * x^3)))$$

Parameters

approximate (*str, optional*) – the gelu approximation algorithm to use: `'none'` | `'tanh'`. Default: `'none'`

Shape:

- Input: $(*)$, where $*$ means any number of dimensions.
- Output: $(*)$, same shape as the input.



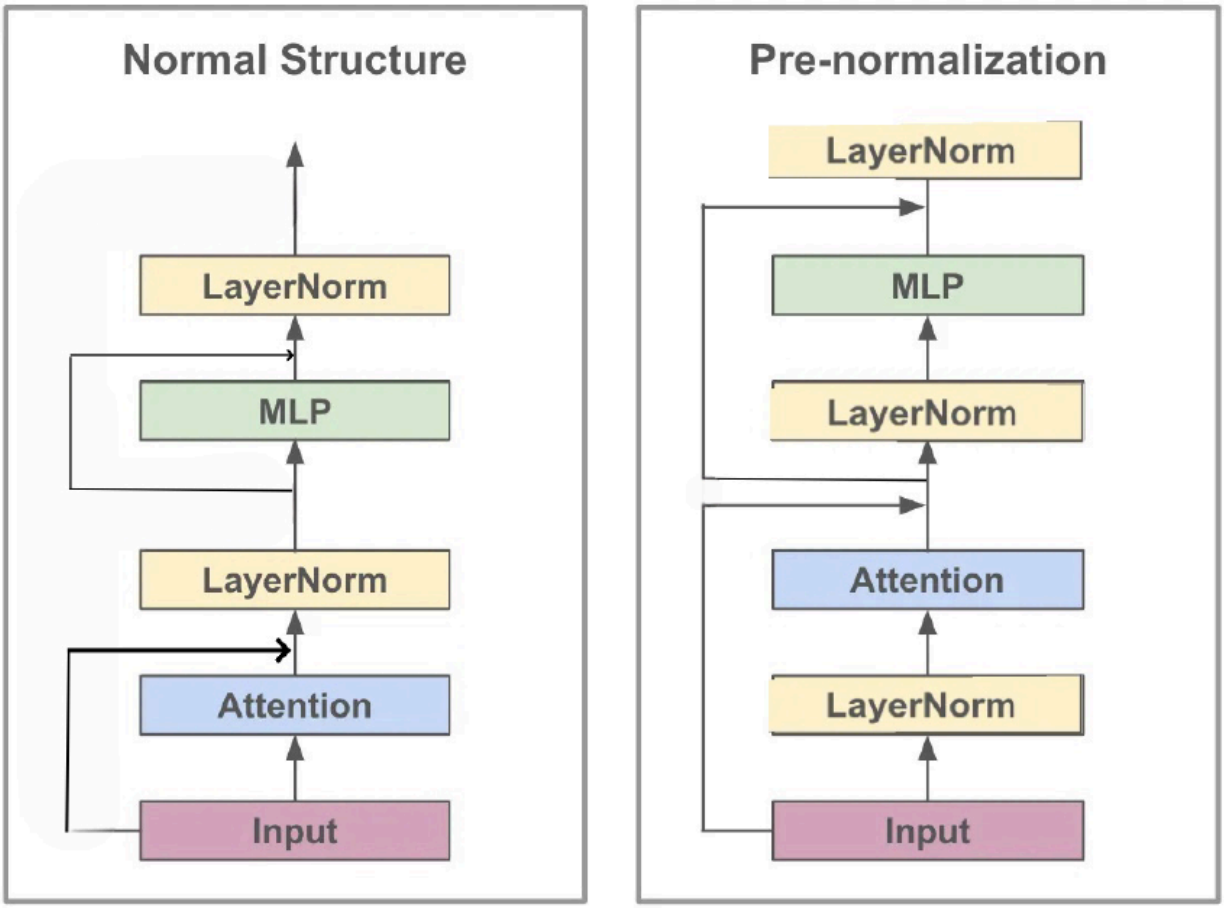
GeLU

Small Summerize

- **Attention**: map, get the relationship across tokens.
- **MLP**: reduce, think individually.

Block forward: layernorm前置，residual不做layernorm

1. We want clean residual pass way
2. 同一设置之下，Pre Norm结构往往更容易训练，但最终效果通常不如Post Norm。
   https://kexue.fm/archives/9009



数学表达：

$$\text{PRE} - \text{NORM} : x_{t+1} = x_t + F_t(Norm(x_t))$$

$$\text{POST} - \text{NORM} : x_{t+1} = Norm(x_t + F_t(x_t))$$

目前已知的实验结论是：同一设置之下，Pre Norm结构往往**更容易训练**，但**最终效果**通常不如Post Norm。

Pre & Post layernorm

GPTConfig() and GPT class

1. vocab_size的来源

```
block_size: int = 1024 # max sequence length
vocab_size: int = 50257 # number of tokens: 50,000 BPE merges + 256 bytes tokens + 1 <|endof
```

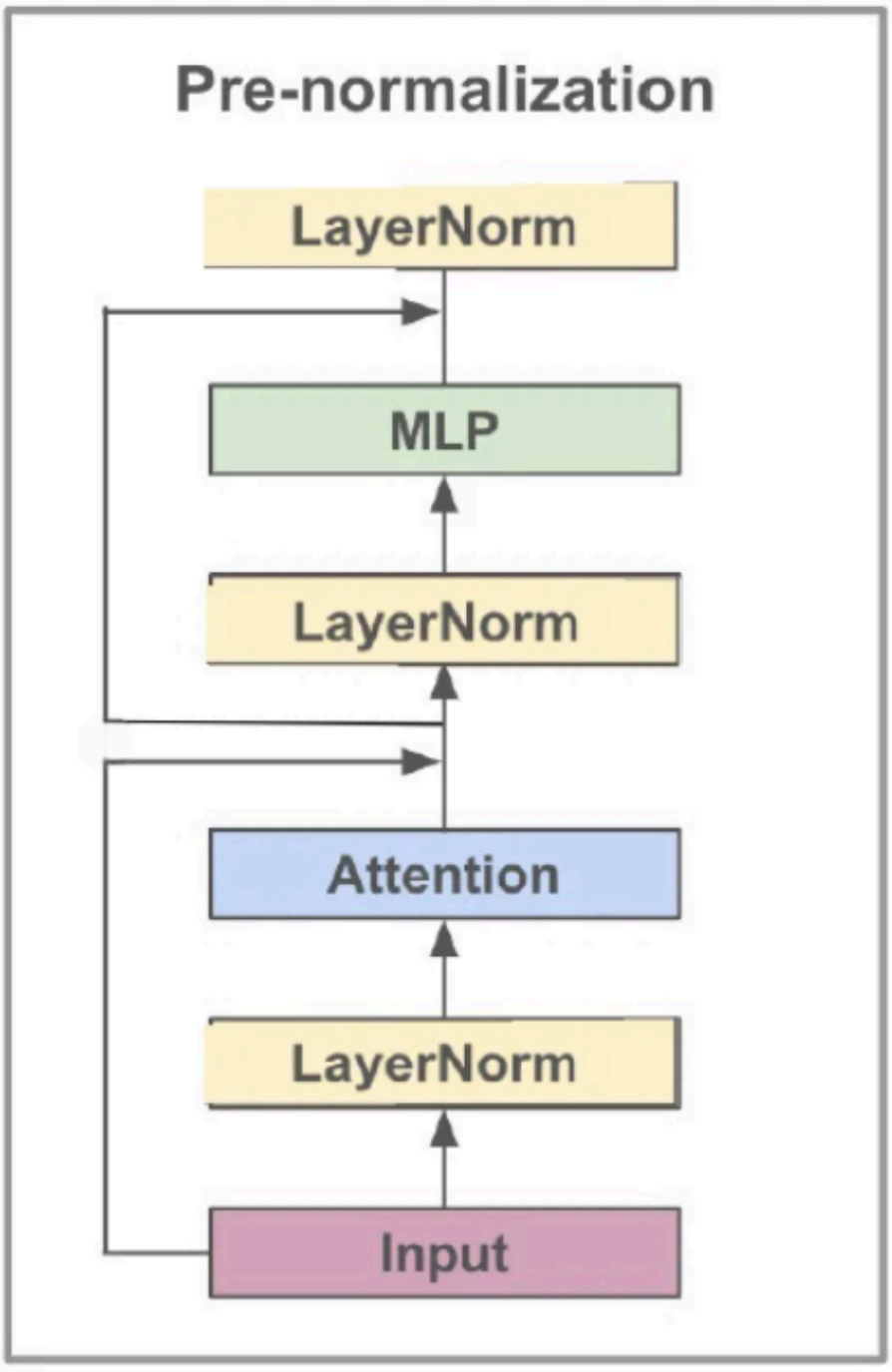
2. wte和wpe的维度

```
# Token Embedding [50257, 768]
wte = nn.Embedding(config.vocab_size, config.n_embd),
# Positional Embedding [1024, 768]
wpe = nn.Embedding(config.block_size, config.n_embd),
```

3. from_pretrained 负责从预训练模型加载权重

Add forward() function of GPT2 nn.Module

1. 输入的形状是(B, T)，即(batch, token_length)，这里的B是batched calculation计算一次的大小，并不等于用于更新梯度的batchsize，batchsize = B * T * num_accum_steps(需要串行的部分) * num_processes(可以放多张卡上并行)。token_length取决于设置的context_length，最多能根据多少个上文的token来预测下一个token。
2. 中间运算过程：先将token embedding和positional embedding加起来，其中pos embedding对于每一行相同，需要利用广播机制。然后，循环经过每个block，每个block中做attention和mlp，其中有前面提到的，clean residual和前置layernorm。最后做一次layernorm。相当于对下图，下面的部分迭代多次，再做最上面的layernorm。



Pre layernorm

3. 输出将hidden_states的维度 (B, T, n_embd) 经过 lm_head 映射到logits的维度(B, T, vocab_size)。每一行（总共B个句子）T个token，每个token都 tend to 前面的token，得到自己的hidden_state，以此预测自己的下一个token的概率。每一个位置预测的都是对应的下一个token的概率，(B, T)的输入得到的是(B, T)的预测输出，也就是将进行B*T次loss的计算。

Generate from the model

1. 预测下一个token。因为是在做inference，所以只需要拿到最后一个token预测出的下一个token的logits即可。

```
logits = model(x) # (B, T, vocab_size)
# take the logits at the last position
logits = logits[:, -1, :] # (B, vocab_size)
```

2. TopK选取概率最高的k个token，重新归一化，然后采样。这样可以避免sample到显然不合理的低概率值。topk_indices记录了选取的50个token到原词表中token的位置的映射。

```
topk_probs, topk_indices = torch.topk(probs, 50, dim=-1)
```

3. torch.gather根据给定索引从一个张量中提取元素。

```
# torch.gather(input, dim, index, out=None)
ix = torch.multinomial(topk_probs, 1) # (B, 1)
# gather the corresponding indices
xcol = torch.gather(topk_indices, -1, ix) # (B, 1)
```

Autodetect device, and switch to a random model

检测一下当前的设备是什么，然后to(device)。

Implement cross entropy loss in forward()

```
# 将logit展成(B*T, vocab_size)，与target(B*T, 1)计算CE loss。
loss = F.cross_entropy(logits.view(-1, logits.size(-1)), targets.view(-1))
```

Write simple dataloader and add an optimizer

尝试能否跑通训练过程。

```
using device: cuda
step 0, loss: 10.98649787902832
step 1, loss: 6.697659015655518
step 2, loss: 4.540412425994873
step 3, loss: 2.7975707054138184
step 4, loss: 1.6325037479400635
step 5, loss: 0.9096142053604126
step 6, loss: 0.508819580078125
step 7, loss: 0.2937222421169281
step 8, loss: 0.1840878278017044
step 9, loss: 0.12100420892238617
```

Add a DataLoaderLite

1. Load the text and encode into tokens.
2. 核心是next_batch()，取下一个data batch。

```
# 巧妙地错开一位，得到batched inputs和targets
buf = self.tokens[self.current_position : self.current_position+B*T+1]
x = (buf[:-1]).view(B, T) # inputs
y = (buf[1:]).view(B, T) # targets
# 顺序遍历整个语料，如果下一个batch将超过总长度，则重置读取位置
# advance the position in the tensor
self.current_position += B * T
# if loading the next batch would be out of bounds, reset
if self.current_position + (B * T + 1) > len(self.tokens):
    self.current_position = 0
```

3. Running output

```
using device: cuda
loaded 338024 tokens
1 epoch = 2640 batches
step 0, loss: 10.924686431884766
step 1, loss: 9.618416786193848
step 2, loss: 8.596650123596191
step 3, loss: 8.912147521972656
step 4, loss: 8.365449905395508
step 5, loss: 8.139814376831055
step 6, loss: 8.965357780456543
step 7, loss: 8.699417114257812
step 8, loss: 8.104934692382812
step 9, loss: 7.889430522918701
```

lm_head and word token embedding should share parameters

1. 为什么可以共用参数?
   因为wte是embedding matrix，lm_head是unembedding matrix。共享参数之后，相似语义的token，有相近的token embedding，进而在hidden_stated经过lm_head后，被预测到有相似的logit。
2. 好处：这两部分参数量很大，共享参数能够显著减少参数量，使得数据能被更充分的利用，训练更加高效。

```
# weight sharing scheme
self.transformer.wte.weight = self.lm_head.weight
```

3. It's a kind of **inductive bias**.

GPT-2 Initialization

1. Set the bias to 0.
2. Scale the std of the nn.linear layer.
3. Set the random seed.

```
"A modified initialization which accounts for the accumulation on the residual path with model de
```

Speedup the training process

Set TensorFloat32 matmuls

- Tensor Cores accelerate matrix multiplication by performing multiple multiply-accumulate operations simultaneously.
- Tensor Cores can perform mixed-precision matrix multiplications and accumulate results in higher precision.
- Run TensorCores in TF32 or BF16 is faster.

	A100 80GB PCIe	A100 80GB SXM
FP64	9.7 TFLOPS	
FP64 Tensor Core	19.5 TFLOPS	
FP32	19.5 TFLOPS	
Tensor Float 32 (TF32)	156 TFLOPS | 312 TFLOPS*	
BFLOAT16 Tensor Core	312 TFLOPS | 624 TFLOPS*	
FP16 Tensor Core	312 TFLOPS | 624 TFLOPS*	
INT8 Tensor Core	624 TOPS | 1248 TOPS*	

Flops of each precision

```
# 设置 float32 矩阵乘法的内部精度
# 可以显著提高训练速度
torch.set_float32_matmul_precision('high')
```

```
using device: cuda
loaded 338024 tokens
1 epoch = 20 batches
step 0, loss: 10.935506820678711, dt: 1261.48ms, tok/sec: 12987.94
step 1, loss: 9.398406028747559, dt: 1028.11ms, tok/sec: 15936.10
step 2, loss: 8.941734313964844, dt: 1034.39ms, tok/sec: 15839.25
step 3, loss: 8.818684577941895, dt: 1031.17ms, tok/sec: 15888.78
step 4, loss: 8.487004280090332, dt: 1031.76ms, tok/sec: 15879.67
```

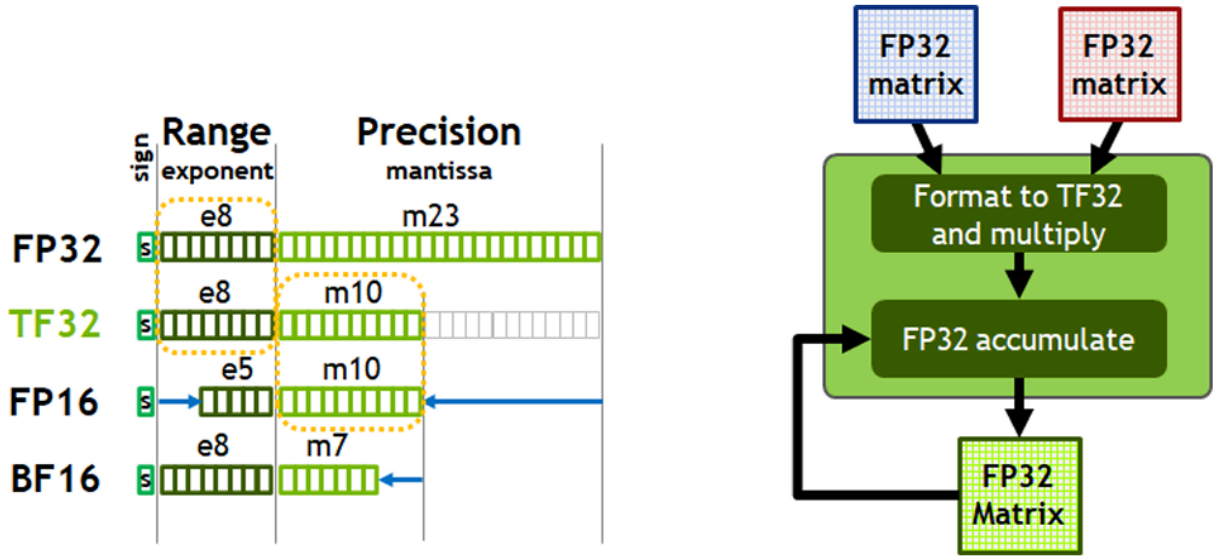
```
using device: cuda
loaded 338024 tokens
1 epoch = 20 batches
step 0, loss: 10.935468673706055, dt: 601.37ms, tok/sec: 27244.39
step 1, loss: 9.398317337036133, dt: 353.86ms, tok/sec: 46301.37
step 2, loss: 8.94157886505127, dt: 354.45ms, tok/sec: 46224.01
step 3, loss: 8.818318367004395, dt: 354.61ms, tok/sec: 46203.34
step 4, loss: 8.486916542053223, dt: 354.74ms, tok/sec: 46185.73
```

Use bfloat16

1. Same exponent bits(range), different mantissa bits(precision). No need for gradient scaler.
2. torch.autocast实现Automatic Mixed Precision，以提高性能同时保持准确性。一些对精度敏感的运算，例如activations、loss保持FP32，而matmul、conv将转变为BF16。

```
# 速度有一定提升
with torch.autocast(device_type=device, dtype=torch.bfloat16):
    logits, loss = model(x, y)
```

```
using device: cuda
loaded 338024 tokens
1 epoch = 20 batches
step 0, loss: 10.936103820800781, dt: 627.30ms, tok/sec: 26118.33
step 1, loss: 9.398155212402344, dt: 312.15ms, tok/sec: 52487.02
step 2, loss: 8.943115234375, dt: 311.01ms, tok/sec: 52680.04
step 3, loss: 8.822978019714355, dt: 310.76ms, tok/sec: 52721.59
step 4, loss: 8.487868309020996, dt: 311.29ms, tok/sec: 52632.83
```



TensorFloat-32 (TF32) provides the range of FP32 with the precision of FP16, 8x precision vs. BF16 (left). A100 accelerates tensor math with TF32 while supporting FP32 input and output data (right), enabling easy integration into DL and HPC programs and automatic acceleration of DL frameworks.

Figure 9. TensorFloat-32 (TF32)

TF32

Use torch.complie

Speedup mainly comes from reducing Python overhead and GPU read/writes.

1. No need for python interpreter: torch.compile sees the entire code and turn it into efficient code.
2. Kernel fusion: reduce GPU read/write.

```
# Take compilation time, but train faster.
model = torch.compile(model)
```

```
using device: cuda
loaded 338024 tokens
1 epoch = 20 batches
step 0, loss: 10.935880661010742, dt: 27732.57ms, tok/sec: 590.79
step 1, loss: 9.398301124572754, dt: 136.01ms, tok/sec: 120459.68
step 2, loss: 8.942550659179688, dt: 135.46ms, tok/sec: 120952.63
step 3, loss: 8.821760177612305, dt: 135.71ms, tok/sec: 120724.84
step 4, loss: 8.487848281860352, dt: 136.00ms, tok/sec: 120469.60
```

Use Flash Attention

```
# Flash Attention
y = F.scaled_dot_product_attention(q, k, v, is_causal=True)
# Attention
# (materializes the large (T,T) matrix for all the queries and keys)
# att = (q @ k.transpose(-2, -1)) * (1.0 / math.sqrt(k.size(-1)))
# att = att.masked_fill(self.bias[:,:,:T,:T] == 0, float('-inf'))
# att = F.softmax(att, dim=-1)
# y = att @ v # (B, nh, T, T) x (B, nh, T, hs) -> (B, nh, T, hs)
```

A kernel fusion algorithm, which torch.compile cannot find

- Rewrite the implementation of attention mechanism.
- More Flops, but less memory read/write
  - by making attention matrix never materialized
  - by online-softmax.....
    https://zhuanlan.zhihu.com/p/668888063

Insights behind Flash attention

1. Be aware of memory hierarchy
2. Flops doesn't matter, the whole memory access pattern matters.
3. There are some optimization that torch.compile can't find.

```
using device: cuda
loaded 338024 tokens
1 epoch = 20 batches
step 0, loss: 10.9359130859375, dt: 15738.08ms, tok/sec: 1041.04
step 1, loss: 9.398147583007812, dt: 96.13ms, tok/sec: 170428.02
step 2, loss: 8.94234848022461, dt: 97.89ms, tok/sec: 167379.46
step 3, loss: 8.820586204528809, dt: 97.14ms, tok/sec: 168665.73
step 4, loss: 8.487573623657227, dt: 97.39ms, tok/sec: 168226.82
```

Avoid ugly numbers: vocab_size 50257 -> 50304

- Single Instruction Multiple Thread: 实际上一个warp执行相同的指令，或者说执行同一个kernel function，一个warp包含32个thread，如果我们的参数不够好，可能会有remaining part导致耗费时间。
- 多出的vocab_size，对应的embedding将被置零，因为没有token对应到这些indices。

```
using device: cuda
loaded 338024 tokens
1 epoch = 20 batches
step 0, loss: 10.947336196899414, dt: 16484.30ms, tok/sec: 993.92
step 1, loss: 9.388265609741211, dt: 93.20ms, tok/sec: 175789.10
step 2, loss: 8.963359832763672, dt: 94.78ms, tok/sec: 172854.83
step 3, loss: 8.852533340454102, dt: 94.41ms, tok/sec: 173549.81
step 4, loss: 8.50554084777832, dt: 94.43ms, tok/sec: 173511.25
```

Details of model training----refer to GPT-3

```
To train all versions of GPT-3, we use Adam with 1 = 09, 2 = 095, and = 10 8, we clip the global

We also gradually increase the batch size linearly from a small value (32k tokens) to the full va

Data are sampled without replacement during training (until an epoch boundary is reached) to mini

All models use weight decay of 0.1 to provide a small amount of regularization.
```

AdamW hyperparameters

```
optimizer = torch.optim.AdamW(model.parameters(), lr=3e-4, betas=(0.9, 0.95), eps=1e-8)
```

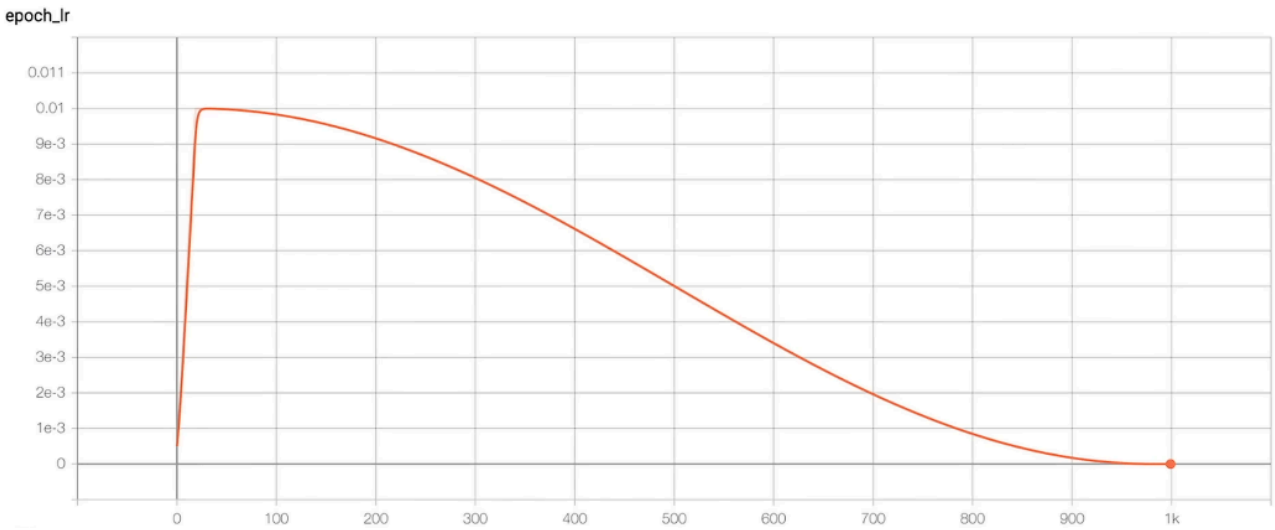
Clip the gradient

- Computes the total gradient norm (e.g., L2 norm across all parameters by default).
- If the norm exceeds the specified max_norm, the gradients are scaled down proportionally.
- Helps stabilize training, especially when using high learning rates or large models, by preventing gradient explosion.

```
# torch.nn.utils.clip_grad_norm_(parameters, max_norm, norm_type=2.0)
norm = torch.nn.utils.clip_grad_norm_(model.parameters(), 1.0)
```

```
using device: cuda
loaded 338024 tokens
1 epoch = 20 batches
step    0 | loss: 10.947336 | norm: 28.5686 | dt: 6138.27ms | tok/sec: 2669.16
step    1 | loss: 9.388454 | norm: 6.1851 | dt: 95.02ms | tok/sec: 172430.22
step    2 | loss: 8.949810 | norm: 2.4907 | dt: 96.79ms | tok/sec: 169278.56
step    3 | loss: 8.764482 | norm: 2.8624 | dt: 96.54ms | tok/sec: 169712.50
step    4 | loss: 8.771492 | norm: 10.1790 | dt: 96.01ms | tok/sec: 170650.22
step    5 | loss: 8.454670 | norm: 2.0210 | dt: 96.12ms | tok/sec: 170454.23
step    6 | loss: 8.338696 | norm: 2.4302 | dt: 96.32ms | tok/sec: 170096.03
step    7 | loss: 8.064600 | norm: 1.7912 | dt: 96.30ms | tok/sec: 170143.20
step    8 | loss: 7.772311 | norm: 2.0319 | dt: 95.98ms | tok/sec: 170696.84
step    9 | loss: 7.520995 | norm: 1.5736 | dt: 96.44ms | tok/sec: 169895.02
```

Learning rate scheduler



Learning rate scheduler

Add weight decay and fused AdamW

- The "W" in AdamW stands for "Weight Decay".
- Prevent overfitting by adding a penalty (**L2 regularization**) to the loss function.
- AdamW decouples weight decay from the optimization steps. The weight decay is applied directly to the parameters rather than being mixed with the gradient updates.

$$\theta_{t+1} = \theta_t - \eta \cdot \nabla_\theta J(\theta_t) + \lambda \cdot \theta_t$$

```
# 筛选所有需要梯度更新的参数
# start with all of the candidate parameters (that require grad)
param_dict = {pn: p for pn, p in self.named_parameters()}
param_dict = {pn: p for pn, p in param_dict.items() if p.requires_grad}
# 只对维度大于2D的参数做weight decay
# create optim groups. Any parameters that is 2D will be weight decayed, otherwise no.
# i.e. all weight tensors in matmuls + embeddings decay, all biases and layernorms don't.
decay_params = [p for n, p in param_dict.items() if p.dim() >= 2]
nodecay_params = [p for n, p in param_dict.items() if p.dim() < 2]
optim_groups = [
    {'params': decay_params, 'weight_decay': weight_decay},
    {'params': nodecay_params, 'weight_decay': 0.0}
]


# 如果有fused函数参数且在gpu上运行，则使用kernel fusion for AdamW optimization
# Create AdamW optimizer and use the fused version if it is available
fused_available = 'fused' in inspect.signature(torch.optim.AdamW).parameters
use_fused = fused_available and 'cuda' in device
print(f"using fused AdamW: {use_fused}")
optimizer = torch.optim.AdamW(optim_groups, lr=learning_rate, betas=(0.9, 0.95), eps=1e-8, fused=
```

Enabling 0.5M batchsize

Model Name	n_{params}	n_{layers}	d_{model}	n_{heads}	d_{head}	Batch Size	Learning Rate
GPT-3 Small	125M	12	768	12	64	0.5M	6.0×10^{-4}
GPT-3 Medium	350M	24	1024	16	64	0.5M	3.0×10^{-4}
GPT-3 Large	760M	24	1536	16	96	0.5M	2.5×10^{-4}
GPT-3 XL	1.3B	24	2048	24	128	1M	2.0×10^{-4}
GPT-3 2.7B	2.7B	32	2560	32	80	1M	1.6×10^{-4}
GPT-3 6.7B	6.7B	32	4096	32	128	2M	1.2×10^{-4}
GPT-3 13B	13.0B	40	5140	40	128	2M	1.0×10^{-4}
GPT-3 175B or “GPT-3”	175.0B	96	12288	96	128	3.2M	0.6×10^{-4}

Table 2.1: Sizes, architectures, and learning hyper-parameters (batch size in tokens and learning rate) of the models which we trained. All models were trained for a total of 300 billion tokens.

Determine the batchsize

```
# 因为显存无法放下整个batch，所以串行的运算grad_accum_steps次
# 以累积total_batch_size个loss和gradient
total_batch_size = 524288 # 2**19, ~0.5M, in number of tokens
grad_accum_steps = total_batch_size // (B * T)


# 梯度累积之后应求平均，因为每个mini_batch的大小都是B*T，所以只需要再除以grad_accum_steps
loss = loss / grad_accum_steps
```

```
using device: cuda
total desired batch size: 524288
=> calculated gradient accumulation steps: 32
loaded 338024 tokens
1 epoch = 20 batches
loaded 338024 tokens
1 epoch = 20 batches
num decayed parameter tensors: 50, with 124,354,560 parameters
num non-decayed parameter tensors: 98, with 121,344 parameters
using fused AdamW: True
step    0 | loss: 10.937969 | lr 6.0000e-05 | norm: 26.9896 | dt: 8847.89ms | tok/sec: 59255.72
step    1 | loss: 9.650049 | lr 1.2000e-04 | norm: 9.5442 | dt: 2890.59ms | tok/sec: 181377.28
step    2 | loss: 9.222029 | lr 1.8000e-04 | norm: 5.8025 | dt: 2891.99ms | tok/sec: 181289.75
step    3 | loss: 9.806954 | lr 2.4000e-04 | norm: 8.0335 | dt: 2895.77ms | tok/sec: 181053.32
step    4 | loss: 9.178097 | lr 3.0000e-04 | norm: 4.3161 | dt: 2895.10ms | tok/sec: 181095.20
```

Distributed Data Parallel

batchsize = B * T * grad_accum_steps(需要串行的部分) * num_processes(可以放多张卡上并行)

- Each process run the same source code, and has its only signiture RANK. 我们只让rank为0的master process打印输出。
- Wrap the model in DDP container, which **enables the overlap of the bachward pass and the synchronization between GPUs.**
- DDP会在loss.backward()的时候自动触发all-reduce，同时对num_processes求平均。
- Optimize the raw_model, not the DDP wrapped model. DDP只负责梯度的分布式同步，参数存储在raw_model中，优化器仍然需要更新原始模型的参数。

Use FinewebEDU dataset

1. Get the training datasets. Organize the file direction in a list.
2. Modify the dataloader. If the next position is out of range, then switch to the next shard and reset to the initial position.

Add validation split and hellaswag evaluation

1. Get val_dataloader using 'val' split of the datase.
2. Do evaluation every 100 training steps.

3. Hellaswag选取最合理的句子续写选项，比较模型对每个选项的average loss。

Add checkpointing

如果希望完全接续训练，除了保存当前权重之外，还需要保存optimizer状态。

Some small changes

1. `device_type` only refers to the type of the hardware where the tensor is stored "cpu" or "cuda", while `device` can includes the device identifier "cuda:0". Some function are restrict to the difference between them.
2. `model.require_backward_grad_sync` is actually used by both the forward and backward pass. During the forward pass, the `require_backward_grad_sync` flag doesn't directly influence the computation. However, the module may need to track whether the backward pass will require gradient synchronization based on this flag.