

# OpenBioML PyTorch Lightning workshop (2/2)

Adrian Wälchli, Research Engineer Luca Antiga, CTO

#### OpenBioML PyTorch Lightning workshop

Session 1: Thu 23 Feb, 3pm ET

Session 2: Thu 2 Mar, 3pm ET

https://harvard.zoom.us/j/97375262666



#### OpenBioML PyTorch Lightning workshop

#### **Session 1**

- Intro to PyTorch Lightning + Fabric
- Hands-on: raw PyTorch -> Fabric -> PyTorch Lightning Trainer
- A look into OpenFold

By the end of Session 1 we saw how to build a model with PyTorch Lightning and Fabric and train it. Distributed. On a SLURM cluster.



#### OpenBioML PyTorch Lightning workshop

#### **Session 2**

- Intro to core distributed concepts and what's new in PyTorch 2.0
- Hands-on: how to debug and optimize performance, single node and distributed,
   running benchmarks
- More on OpenFold

By the end of Session 2 you will know how to make sure you are setting up your training correctly and verify you are leveraging your hardware the best.



#### Join us here

discord

discord.gg/MWAEvnC5fU

forums

lightning.ai/forums

twitter

@LightningAl



https://linktr.ee/lightningai



#### PyTorch Lightning

#### You do the science, we do the engineering

33 million+

780+
CONTRIBUTORS



13,000+ PROJECTS USING LIGHTNING 6,000+ SLACK MEMBERS ♣

10,000+ ORGANIZATIONS BUILD WITH LIGHTNING













https://lightning.ai





## Scale your models, without the boilerplate

Lightning's open-source ecosystem is designed for researchers and developers who require flexibility and performance at scale.

O pip install lightning



#### **Build AI without the boilerplate**

Lightning simplifies your deep learning code by taking care of engineering boilerplate, so you can focus on the problems that matter to you.



#### Unlock deep learning at scale

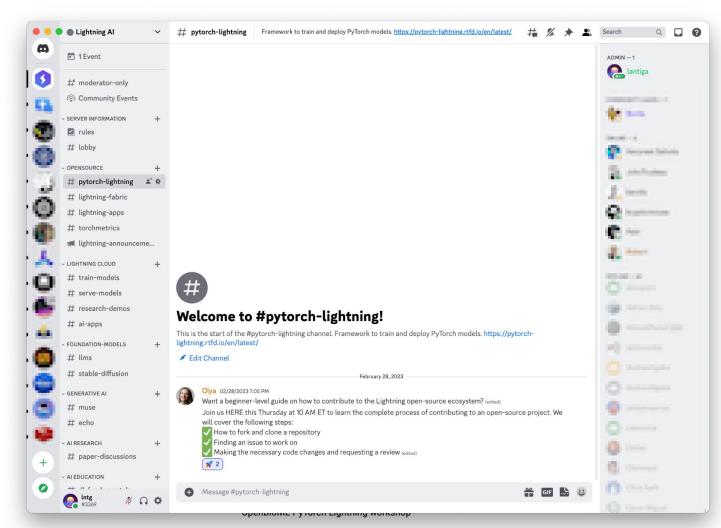
Work seamlessly with distributed computing environments like multi-GPU and TPU clusters and scale projects to large models and data.

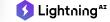


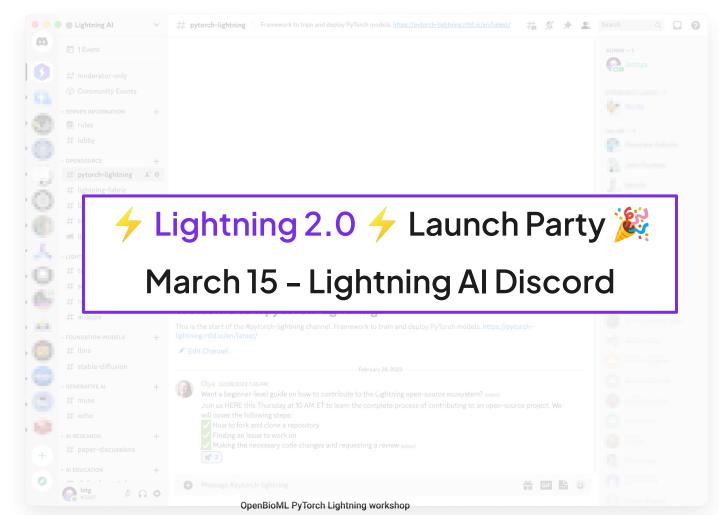
#### Create with the community

Join over 100,000 users and companies using Lightning to create their Al future. Tap into cuttingedge research and take it to production.





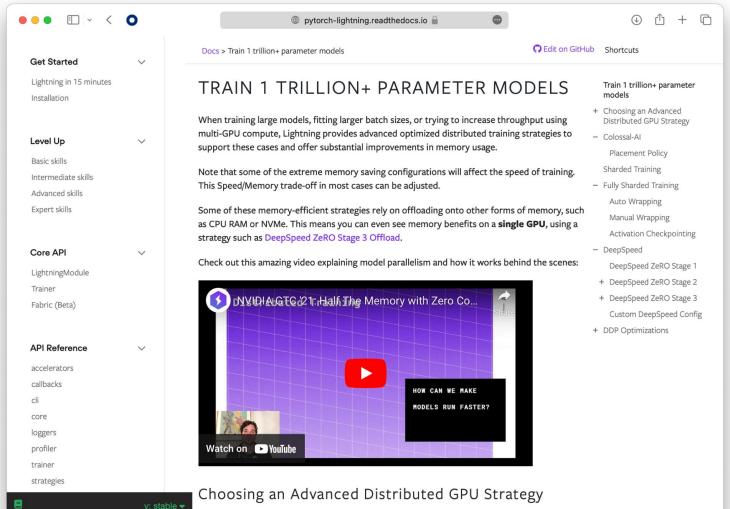






#### Intro: Scaling out and going fast







## PyTorch Lightning

#### Organized PyTorch

LightningModule

```
import lightning as L
from torch import n, optim
encoder = nn.Sequential(nn.Linear(28 * 28, 64), nn.ReLU(), nn.Linear(64, 3))
decoder = nn.Sequential(nn.Linear(3, 64), n.ReLU(), nn. Linear (64, 28 * 28))
class LitAutoEncoder(L.LightningModule):
    def _init__(self, encoder, decoder):
        super()._init__()
        self.encoder = encoder
        self.decoder = decoder
    def training_step(self, batch, batch_idx):
        X, y = batch
        X = x. view(x.size(0), -1)
        z = self.encoder(x)
        x_{hat} = self.decoder(z)
        loss = nn. functional.mse_loss(x_hat, x)
        self.log("train_loss", loss) return loss
    def configure_optimizers( self):
        optimizer = optim.Adam(self.parameters(), lr=le-3)
        return optimizer
autoencoder = LitAutoEncoder(encoder, decoder)
dataset = MIST(os.getcwd(), download=True, transform=ToTensor())
train_loader = utils.data.DataLoader (dataset)
trainer = L.Trainer(limit_train_batches=100, max_epochs=1)
trainer.fit(model=autoencoder, train_dataloaders=train_loader)
```

#### PyTorch Lightning

Accelerators

GPU, TPU, HPU, IPU, MPS

**Strategies** 

DDP, FSDP, DeepSpeed, Colossal AI

Precision

Callbacks

```
# train on 4 GPUs
trainer = Trainer(
     devices=4,
     accelerator="qpu"
# train 1B+ parameter models with Deepspeed/fsdp
trainer = Trainer(
    devices=4.
    accelerator="qpu",
    strategy="deepspeed_stage_2",
    precision=16
# 20+ helpful flags for rapid idea iteration
trainer = Trainer(
    max_epochs=10,
    min_epochs=5,
    overfit batches=1
# access the latest state of the art techniques
trainer = Trainer(callbacks=[StochasticWeightAveraging(...)])
```



#### **Fabric**

3 Your code

1 Fabric object

dataloader

2 Setup model, optimizer,

```
import lightning as L
def train(fabric, model, optimizer, dataloader):
    # Training loop
   model.train()
   for epoch in range(num_epochs):
        for i, batch in enumerate(dataloader):
            . . .
def main():
    # (Optional) Parse command line options
   args = parse_args()
    # Configure Fabric
    fabric = L.Fabric(..., strategy="deepspeed")
    # Instantiate objects
   model = \dots
   optimizer = ...
   train dataloader = ...
    # Set up objects
   model, optimizer = fabric.setup(model, optimizer)
   train_dataloader = fabric.setup_dataloaders(train_dataloader)
   # Run training loop
   train(fabric, model, optimizer, train_dataloader)
if __name__ == "__main__":
   main()
```



```
fabric = Fabric(accelerator="gpu", strategy="ddp", devices=8, num_nodes=4)
```

```
trainer = Trainer(accelerator="gpu", strategy="ddp", devices=8, num_nodes=4)
```

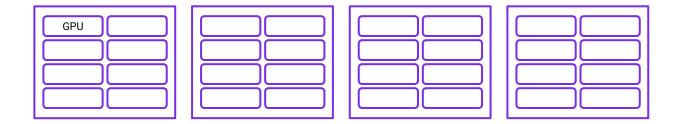
```
fabric = Fabric(accelerator="gpu", strategy="ddp", devices=8, num_nodes=4)
```

```
trainer = Trainer(accelerator="gpu", strategy="ddp", devices=8, num_nodes=4)
```



```
fabric = Fabric(accelerator="gpu", strategy="ddp", devices=8, num_nodes=4)

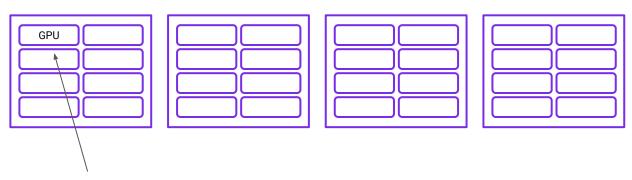
trainer = Trainer(accelerator="gpu", strategy="ddp", devices=8, num_nodes=4)
```





```
fabric = Fabric(accelerator="gpu", strategy="ddp", devices=8, num_nodes=4)

trainer = Trainer(accelerator="gpu", strategy="ddp", devices=8, num_nodes=4)
```



Think one process per accelerator



#### Under the hood

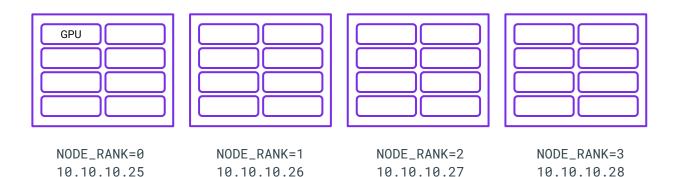
MASTER\_PORT: free port on machine with NODE\_RANK 0

MASTER\_ADDR: address of NODE\_RANK 0 node

WORLD\_SIZE: the total number of GPUs/processes

NODE\_RANK: id of the node in the cluster

MASTER\_PORT=23456
MASTER\_ADDR="10.10.10.25"
WORLD\_SIZE=32



#### Under the hood

WORLD\_SIZE: the total number of GPUs/processes

NODE\_RANK: id of the node

LOCAL\_RANK: id of the process in each node

GLOBAL\_RANK: unique id of the process



#### Under the hood

WORLD\_SIZE: the total number of GPUs/processes

NODE\_RANK: id of the node

LOCAL\_RANK: id of the process in each node

GLOBAL\_RANK: unique id of the process

MASTER PORT=23456 MASTER\_ADDR="10.10.10.25" WORLD SIZE=32 GLOBAL\_RANK 16 24 25 10 18 19 26 27 11 12 13 20 21 28 29 14 15 22 23 30 31 NODE\_RANK=0 NODE\_RANK=1 NODE\_RANK=2 NODE\_RANK=3 10.10.10.25 10.10.10.26 10.10.10.27 10.10.10.28



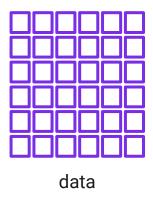
#### In Lightning / Fabric

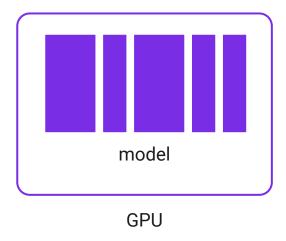
```
from lightning.fabric import Fabric

# Devices and num nodes determine how many processes there are fabric = Fabric(devices=8, num_nodes=4) fabric.launch()
```

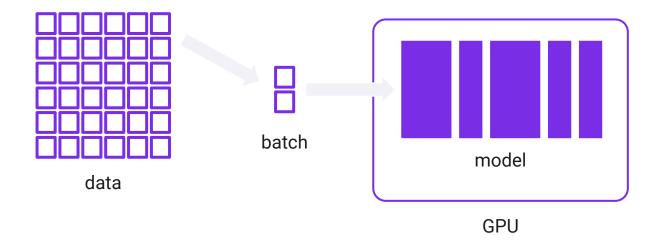
```
# The total number of processes running across all devices and nodes
fabric.world_ size # 4 * 8 = 32
# The global index of the current process across all devices and nodes
fabric.global_rank # -> {0, 1, 2, 3, 4, ..., 31}
# The index of the current process among the processes running on the
local node
fabric.local_rank # -> {0, 1, 2, 3, 4, 5, 6, 7}
# The index of the current node
fabric.node_rank \# -> \{0, 1, 2, 3\}
# Do something only on rank 0
if fabric.global_rank == 0:
```



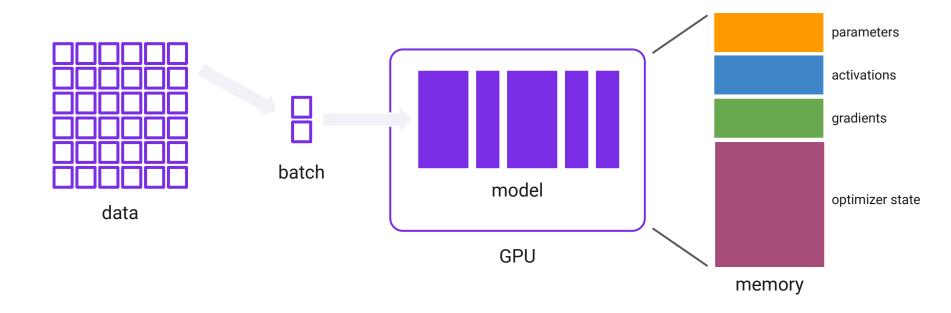






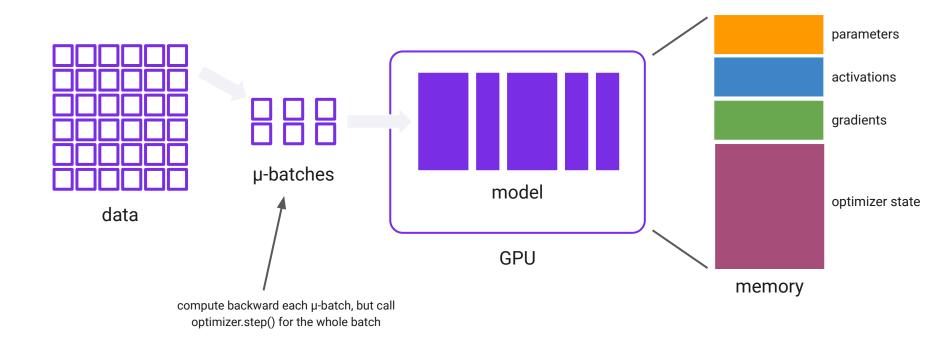






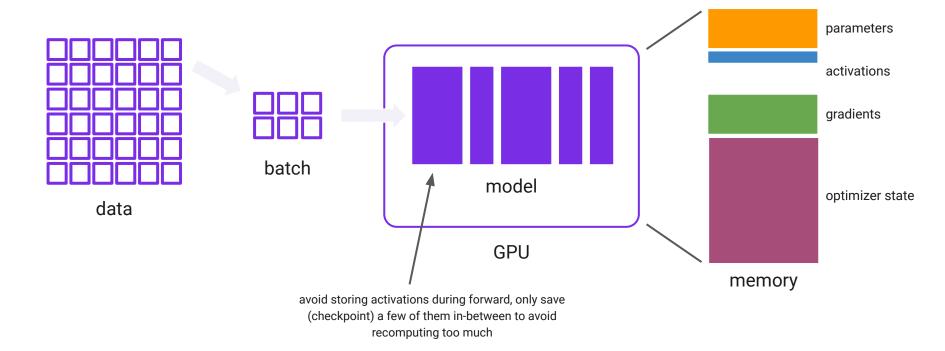


#### **Gradient accumulation**

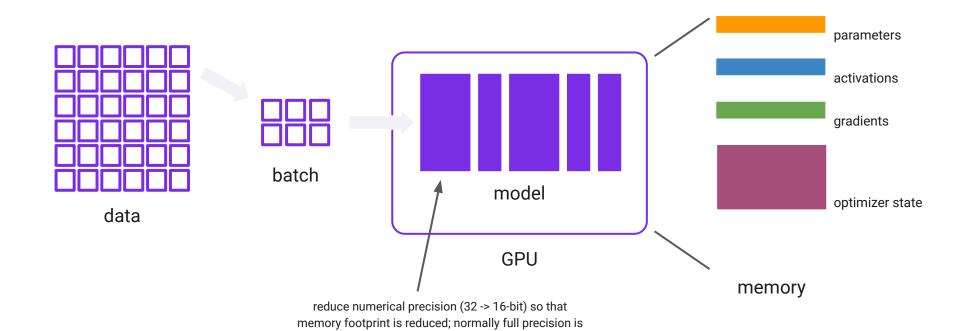




#### Activation/Gradient checkpointing

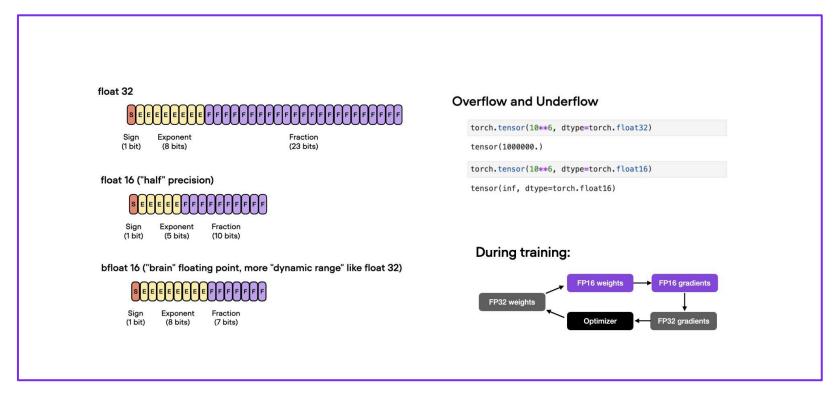


#### Mixed precision



automatically restored at computation time

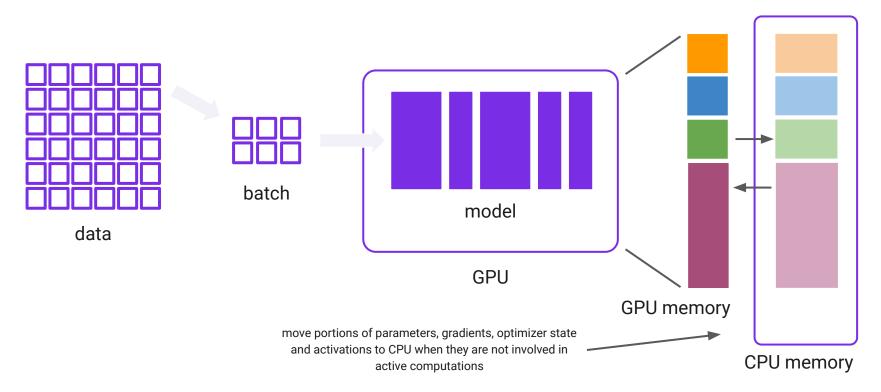
#### Mixed precision



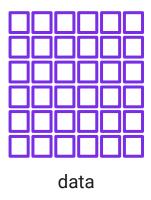
Sebastian Rashka, https://lightning.ai/pages/courses/deep-learning-fundamentals/

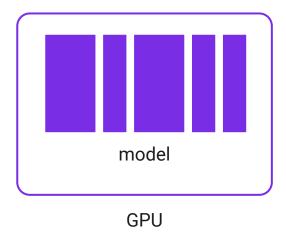


#### Offloading

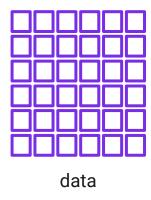








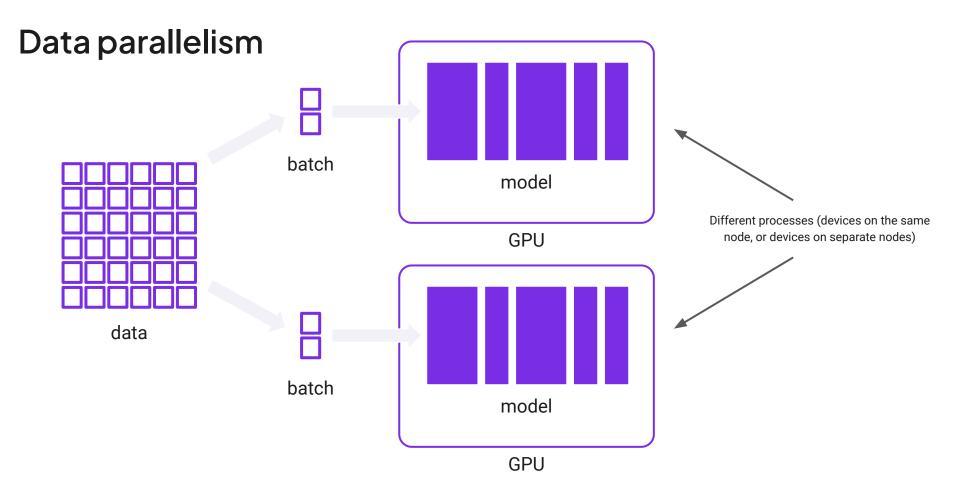


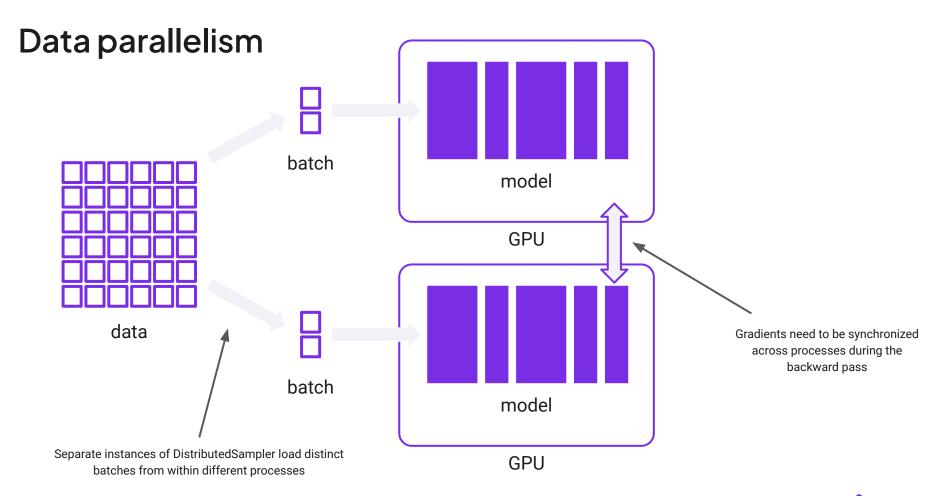


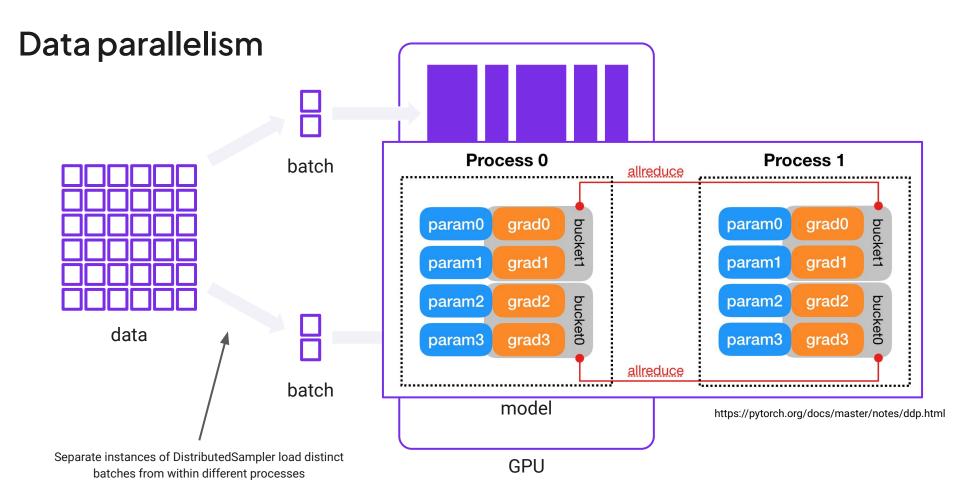


GPU

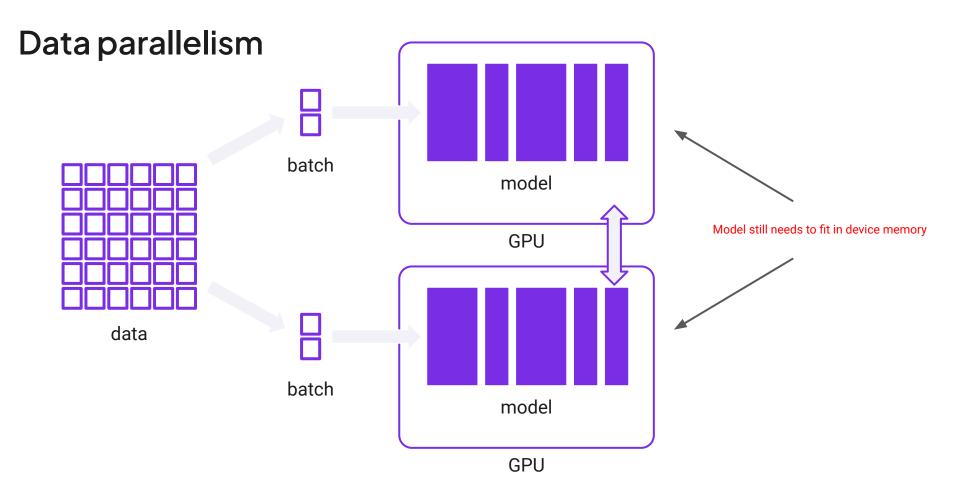


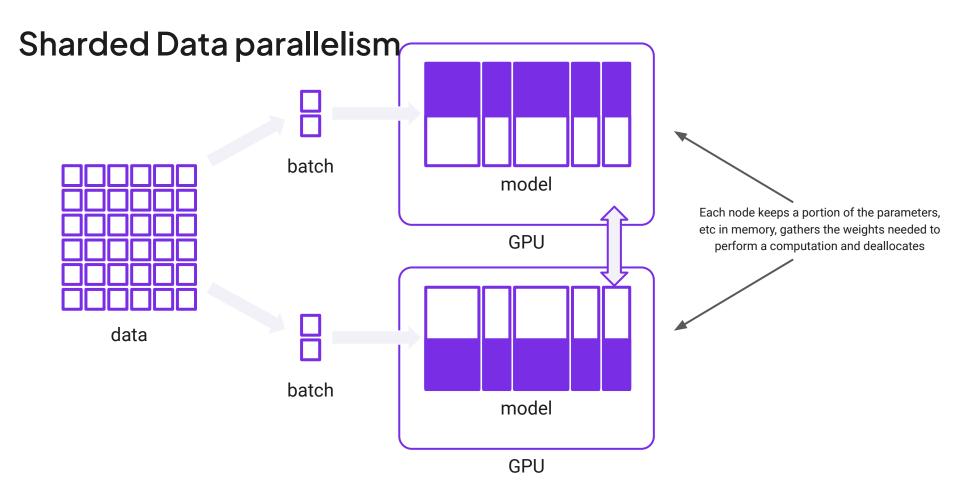




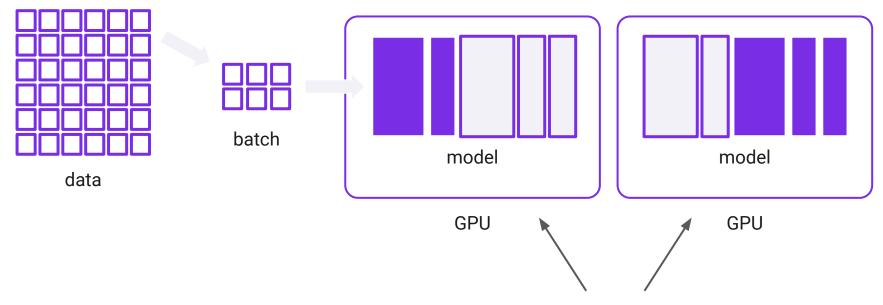




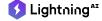


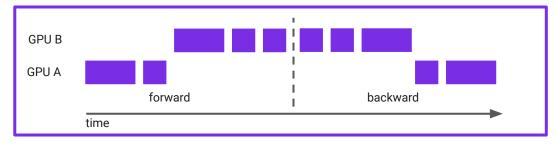


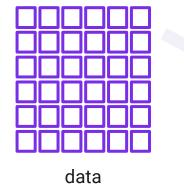




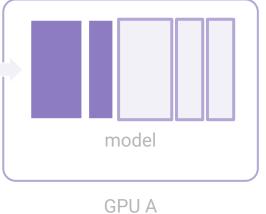
Distribute model parameters across machines in contiguous blocks

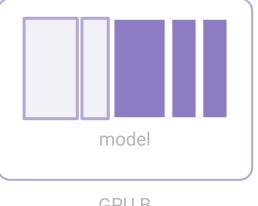


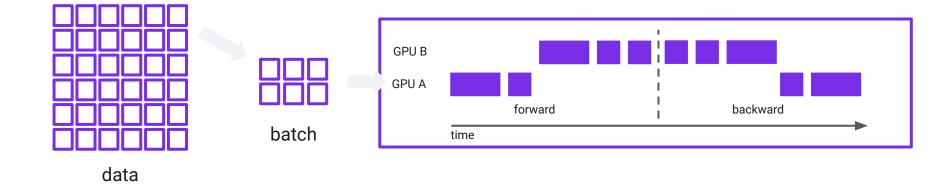






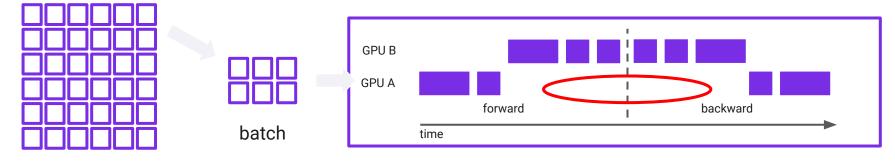








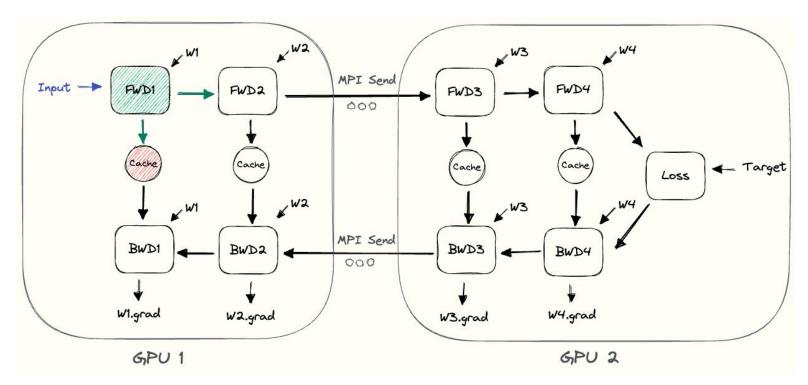
data







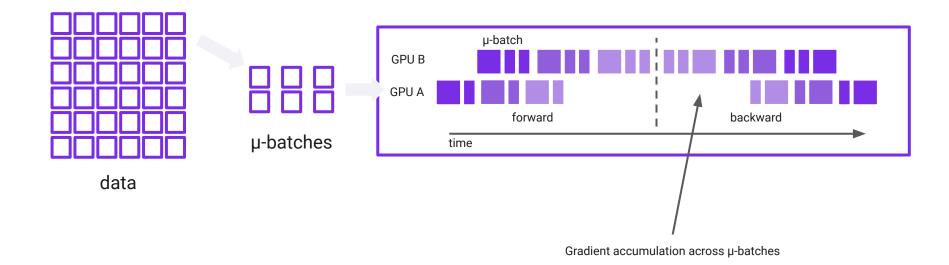
### Naive model parallelism



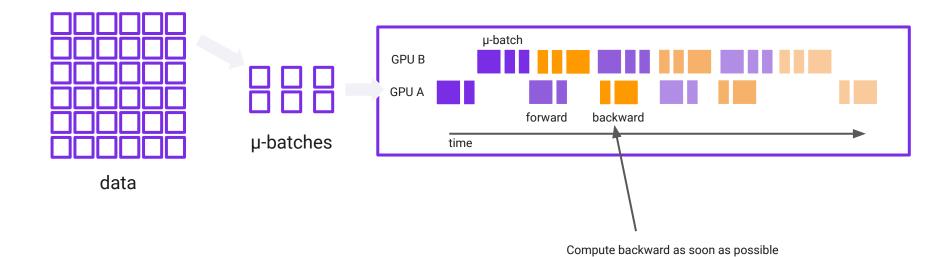
https://siboehm.com/articles/22/pipeline-parallel-training



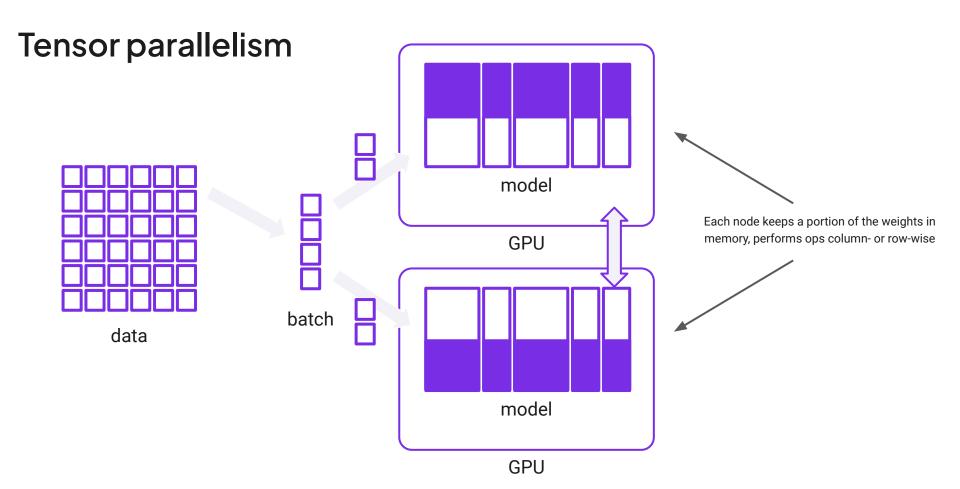
# Pipeline parallelism



# Interleaved pipeline parallelism



Bubble gets better as more nodes participate

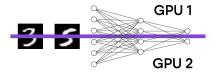




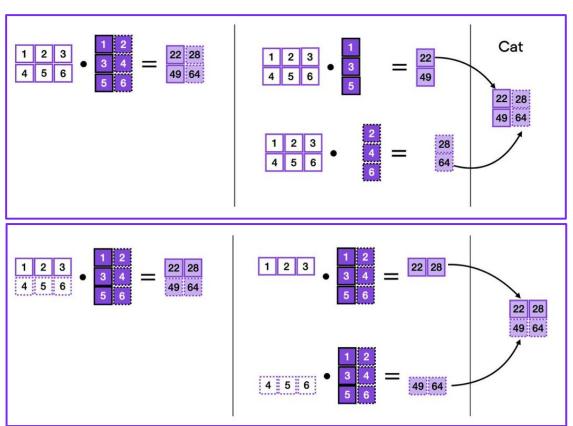
### Tensor parallelism

https://sebastianraschka.com/blog/2023/pytorch-faster.html

Column-wise



**Row-wise** 

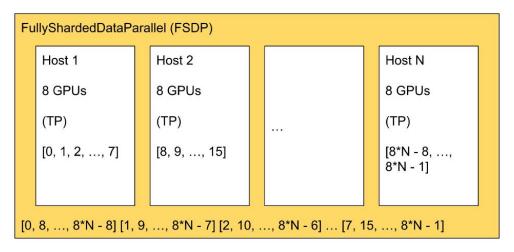


#### Combining parallelism: 2D, 3D, 4D

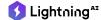
E.g. Sharded Data Parallel + Tensor Parallel in separate parallel dimensions:

- Data Parallel across hosts
- Tensor Parallel within each host

Other example: Megatron-LM



Wanchao Liang, Two Dimensional Parallelism Using Distributed Tensors



#### **DDP**

DDP - sharded DDP that shards **model parameters**, optimizer state and gradients across DDP ranks. It can optionally offload to CPU.

trainer = Trainer(accelerator="gpu", strategy="ddp", devices=8, num\_nodes=4)



#### DeepSpeed

- DeepSpeed ZeRO Stage 1 Shard optimizer states, remains at speed parity with DDP whilst providing memory improvement
- DeepSpeed ZeRO Stage 2 Shard optimizer states and gradients, remains at speed parity with DDP whilst providing even more memory improvement
- DeepSpeed ZeRO Stage 2 Offload Offload optimizer states and gradients to CPU. Increases distributed communication volume and GPU-CPU device transfer, but provides significant memory improvement
- DeepSpeed ZeRO Stage 3 Shard optimizer states, gradients, parameters and optionally activations.
   Increases distributed communication volume, but provides even more memory improvement
- DeepSpeed ZeRO Stage 3 Offload Offload optimizer states, gradients, parameters and optionally activations to CPU. Increases distributed communication volume and GPU-CPU device transfer, but even more significant memory improvement.
- DeepSpeed Activation Checkpointing Free activations after forward pass. Increases computation, but provides memory improvement for all stages.



#### DeepSpeed

```
trainer = Trainer(accelerator="gpu", devices=8, num_nodes=4, strategy="deepspeed_stage_1")
trainer = Trainer(accelerator="gpu", devices=8, num_nodes=4, strategy="deepspeed_stage_2")
trainer = Trainer(accelerator="gpu", devices=8, num_nodes=4, strategy="deepspeed_stage_2_offload")
trainer = Trainer(accelerator="gpu", devices=8, num_nodes=4, strategy="deepspeed_stage_3")
trainer = Trainer(accelerator="gpu", devices=8, num_nodes=4, strategy="deepspeed_stage_3")
```



#### DeepSpeed

```
import lightning as L
from lightning.pytorch.strategies import DeepSpeedStrategy
import deepspeed
class MyModel(L.LightningModule):
    def configure_sharded_model(self):
        self.block_1 = nn.Sequential(nn.Linear(32, 32),
nn.ReLU())
        self.block_2 = torch.nn.Linear(32, 2)
    def forward(self, x):
        # Use the DeepSpeed checkpointing function instead of
calling the module directly
        x = deepspeed.checkpointing.checkpoint(self.block_1, x)
        return self.block_2(x)
```

```
model = MyModel()
trainer = L.Trainer(accelerator="gpu", devices=4,
strategy="deepspeed_stage_3_offload", precision=16)
# Enable CPU Activation Checkpointing
trainer = Trainer(
    accelerator="gpu",
    devices=4.
    strategy=DeepSpeedStrategy(
        stage=3.
        offload_optimizer=True, # Enable CPU Offloading
        cpu_checkpointing=True, # Offload activations to CPU
    precision=16,
trainer.fit(model)
```



# FSDP (Fully Sharded Data Parallel)

FSDP - sharded DDP that **shards model parameters**, **optimizer state** and **gradients** across DDP ranks.

It optionally **offloads activations** and **optimizer state** to CPU.

```
trainer = Trainer(accelerator="gpu", strategy="fsdp", devices=8, num_nodes=4)
```



#### ColossalAl

ColossalAI - Zero-DP with dynamic chunk-based memory management and other configurable parallelization strategies.

```
class MyModel(LightningModule):
    def __init__(self):
        super().__init__()
        # don't instantiate layers here
        # move the creation of layers to
`configure_sharded_model`

def configure_sharded_model(self):
    # create all your layers here
    self.layers = nn.Sequential(...)
```

```
from lightning_colossalai import ColossalAIStrategy

model = MyModel()
my_strategy = ColossalAIStrategy(placement_policy="auto")

trainer = Trainer(accelerator="gpu", devices=4, precision=16, strategy=my_strategy)

trainer.fit(model)
```

Monitors the consumption of CUDA memory during the warmup phase and collects CUDA memory usage of all auto-grad operations

Automatically manages the data transmission between GPU and CPU according to collected CUDA memory usage information



### Going fast

#### Eager mode

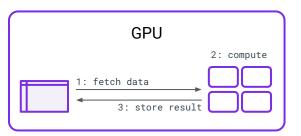
execute

execute

execute

execute

```
def forward(self, x):
   B, T, C = x.size()
   q, k ,v = self.c_attn(x).split(self.n_embd, dim=2) ——————
   k = k.view(B, T, self.n_head, C // self.n_head).transpose(1, 2)
   q = q.view(B, T, self.n_head, C // self.n_head).transpose(1, 2)
   v = v.view(B, T, self.n_head, C // self.n_head).transpose(1, 2)
   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)
   att = self.attn_dropout(att)
   y = att @ v
   y = y.transpose(1, 2).contiguous().view(B, T, C)
   y = self.resid_dropout(self.c_proj(y))
```



#### Going fast: bottleneck

#### Eager mode

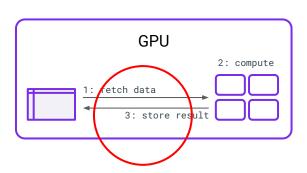
execute

execute

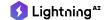
execute

execute

```
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   att = att.masked_fill(self.bias[:,:,:T,:T] == 0, float('-inf'))
   att = F.softmax(att, dim=-1)
   att = self.attn_dropout(att)
   y = att @ v
   y = y.transpose(1, 2).contiguous().view(B, T, C)
   y = self.resid_dropout(self.c_proj(y))
```



Bottleneck on modern hardware



# Going fast: bottleneck

#### Eager mode

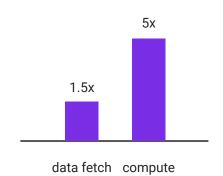
execute

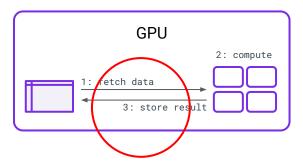
execute

execute

execute

```
def forward(self, x):
   B, T, C = x.size()
   q, k ,v = self.c_attn(x).split(self.n_embd, dim=2)
   k = k.view(B, T, self.n_head, C // self.n_head).transpose(1, 2)
   q = q.view(B, T, self.n_head, C // self.n_head).transpose(1, 2)
   v = v.view(B, T, self.n_head, C // self.n_head).transpose(1, 2)
   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)
   att = self.attn_dropout(att)
   y = att @ v
   y = y.transpose(1, 2).contiguous().view(B, T, C)
   y = self.resid_dropout(self.c_proj(y))
```





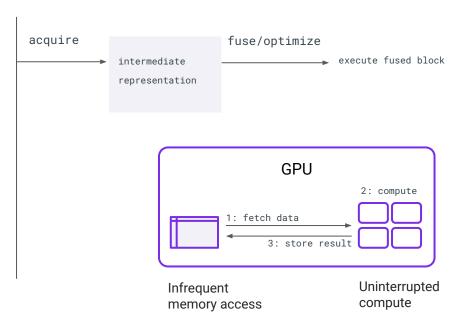
Bottleneck on modern hardware



#### Going fast: compiled mode

```
def forward(self, x):
   B, T, C = x.size()
   q, k ,v = self.c_attn(x).split(self.n_embd, dim=2)
    k = k.view(B, T, self.n_head, C // self.n_head).transpose(1, 2)
   q = q.view(B, T, self.n_head, C // self.n_head).transpose(1, 2)
   v = v.view(B, T, self.n_head, C // self.n_head).transpose(1, 2)
   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)
   att = self.attn_dropout(att)
   y = att @ v
   y = y.transpose(1, 2).contiguous().view(B, T, C)
   y = self.resid_dropout(self.c_proj(y))
```

#### Compiled mode





### Going fast: PyTorch 2.0

```
model = NanoGPT(config)
model = torch.compile(model)
model(x)

# Works with PyTorch Lightning (+ Fabric)
model = MyLitModule()
model = torch.compile(model)
trainer.fit(model)

Program acquisition
through tracing
bytecode, optimization
Optimized execution,
based on OpenAl Triton
```



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```

Status: DDP supported, FSDP support in the works



#### **Demo: Model Parallel**

github.com/Lightning-Al/open-bio-ml-workshop



# Performance Optimization



#### Minimize framework overhead

Compile: Use torch.compile whenever possible

Logging: Log often for development, log less for long training runs

Checkpointing: Minimize frequency, checkpoint often only if training is unstable

Validation: Tune frequency based on dataset sizes



## Maximize throughput

Compile: Use torch.compile whenever possible

Mixed precision: Speed + memory, prefer bfloat16 if available

Batch Size: Increase until OOM, avoid Malloc retries

Num Workers: Increase if GPU is waiting on data, consumes more CPU memory

# Best practices

Avoid unnecessary GPU synchronization

Create tensors directly on the device

```
# Avoid these:
output.item()
output.numpy()
output.cpu()

torch.cuda.empty_cache()
```

```
# bad
t = torch.rand(4, 4).cuda()

# LightningModule:
torch.rand(4, 4, device=self.device)

# Fabric:
torch.rand(4, 4, device=fabric.device)
```



## Performance flags

#### **Speed (default)**

```
# PyTorch / Fabric
torch.use_deterministic_algorithms(False)
torch.backends.cudnn.benchmark = True

# Trainer
trainer = Trainer(benchmark=True, deterministic=False)
```

#### **Determinism**

```
# PyTorch / Fabric
torch.use_deterministic_algorithms(True)
torch.backends.cudnn.benchmark = False
# Trainer
trainer = Trainer(benchmark=False, deterministic=True)
```

# Comparing Trainer vs. PyTorch

#### Run "barebones"

```
# Disable logging, checkpointing, etc.
trainer = Trainer(..., barebones=True)
```

Recommended for comparing implementations and unit testing!



#### Tensor cores

Perform costly matrix multiplications in lower precision (internal)

**Lightning** informs you if you have tensor cores

```
# Default
torch.set_float32_matmul_precision("high")

# Lower precision matrix multiplication
torch.set_float32_matmul_precision("highest")
torch.set_float32_matmul_precision("medium")
```

WARNING: You are using a CUDA device ('NVIDIA GeForce RTX 3090') that has Tensor Cores. To properly utilize them, you should set `torch.set\_float32\_matmul\_precision('medium' | 'high')` which will trade-off precision for performance.



#### Find bottlenecks (framework)

#### **Configure profiler**

```
# Trainer
trainer = Trainer(profiler="simple", ...)
trainer.fit(...)
```

#### **Output after fit**

Action		-1	Mean duration (s)		Total time (	s)
[LightningModule]BoringMode	l.prepare_data	1	10.0001		20.00	
run_training_epoch	· · -	1	6.1558	ı	6.1558	
run_training_batch		-	0.0022506	ı	0.015754	
[LightningModule]BoringMode	l.optimizer_step	- 1	0.0017477	- 1	0.012234	
[LightningModule]BoringMode	l.val_dataloader	- 1	0.00024388	- 1	0.00024388	
on_train_batch_start		- 1	0.00014637	- 1	0.0010246	
[LightningModule]BoringMode	l.teardown	- 1	2.15e-06	- 1	2.15e-06	
[LightningModule]BoringMode	l.on_train_start	- 1	1.644e-06	- 1	1.644e-06	
[LightningModule]BoringMode	l.on_train_end	- 1	1.516e-06	- 1	1.516e-06	
[LightningModule]BoringMode	l.on_fit_end	-1	1.426e-06	- 1	1.426e-06	
[LightningModule]BoringMode.	l.setup	-	1.403e-06		1.403e-06	
[LightningModule]BoringMode	l.on_fit_start	- 1	1.226e-06	- 1	1.226e-06	



# Find bottlenecks (PyTorch)

#### **Configure profiler**

```
# Trainer
trainer = Trainer(profiler="pytorch", ...)
trainer.fit(...)
```

#### **Output after fit**

Name	Self CPU %	Self CPU	CPU total %	CPU total	CPU time avg	Self CUDA	Self CUDA %	CUDA total	CU
D	3.48%	47.673ms	39.44%	540.549ms	180.183ms	0.000us	0.00%	113.315ms	
ProfilerStep*									
ol][profile][Strategy]SingleDeviceStrategy.backward	32.14%	440.445ms	32.18%	441.004ms	147.001ms	0.000us	0.00%	3.000us	
utograd::engine::evaluate_function: EmbeddingBackwa	0.00%	57.000us	27.61%	378.372ms	63.062ms	0.000us	0.00%	4.470ms	
EmbeddingBackward0	0.00%	21.000us	27.60%	378.277ms	63.046ms	0.000us	0.00%	2.834ms	
aten::embedding_backward	0.00%	15.000us	27.60%	378.256ms	63.043ms	0.000us	0.00%	2.834ms	
aten::embedding_dense_backward	0.03%	360.000us	27.60%	378.241ms	63.040ms	659.000us	0.11%	2.834ms	
cudaStreamSynchronize	27.51%	377.063ms	27.51%	377.063ms	41.896ms	0.000us	0.00%	0.000us	
[pl][profile]run_training_batch	0.05%	710.000us	26.02%	356.661ms	178.331ms	0.000us	0.00%	117.272ms	
<pre>[pl][profile][LightningModule]LitGPT.optimizer_step</pre>	0.00%	51.000us	25.97%	355.951ms	177.976ms	0.000us	0.00%	117.272ms	
Optimizer.step#AdamW.step	23.54%	322.614ms	25.97%	355.900ms	177.950ms	0.000us	0.00%	117.272ms	
l][profile][Strategy]SingleDeviceStrategy.training	0.02%	224.000us	3.64%	49.858ms	16.619ms	0.000us	0.00%	175.918ms	
[pl][module]gpt.GPT: gpt	0.06%	773.000us	3.62%	49.634ms	16.545ms	0.000us	0.00%	175.918ms	
cudaDeviceSynchronize	3.26%	44.698ms	3.26%	44.698ms	44.698ms	0.000us	0.00%	0.000us	
cudaLaunchKernel	2.01%	27.556ms	2.01%	27.556ms	5.968us	14.669ms	2.55%	14.669ms	
aten::linear	0.11%	1.443ms	1.65%	22.615ms	76.922us	0.000us	0.00%	150.840ms	
aten::to	0.12%	1.584ms	1.33%	18.255ms	14.318us	0.000us	0.00%	56.977ms	
aten::_to_copy	0.27%	3.708ms	1.26%	17.297ms	17.850us	0.000us	0.00%	58.926ms	
aten::mm	0.58%	7.996ms	0.85%	11.625ms	26.361us	209.986ms	36.56%	211.492ms	
autograd::engine::evaluate_function: MmBackward0	0.10%	1.334ms	0.82%	11.205ms	76.224us	0.000us	0.00%	138.901ms	
MmBackward0	0.10%	1.370ms	0.72%	9.871ms	67.150us	0.000us	0.00%	138.901ms	

Self CPU time total: 1.371s Self CUDA time total: 574.402ms





OpenFold Update: Lightning 2.0!

#### Reach out!

discord

discord.gg/MWAEvnC5fU

forums

lightning.ai/forums

twitter

@LightningAl



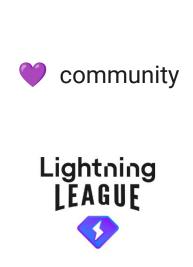
https://linktr.ee/lightningai



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William Falcon







https://linktr.ee/lightningai



#### **Thanks**

