

Deep Learning System Design



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The logo depicts a cube puzzle gradually coming together, reflecting the journey of learning. Each piece represents a fragment of knowledge, and as they fall into place, they reveal the larger structure of understanding. It conveys the idea that growth is a process — knowledge is completed bit by bit.

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Part I

Introduction

Chapter 1

Introduction

1.1 Operations challenges with LLMs

- **Long download times** (*e.g.*, Bloom LLM is 330GB).
- **Longer deploy times** (*e.g.*, Bloom takes 30 ~ 45 mins to load the model into GPU).
- Along with increases in model size often come increases in **inference latency**.
- **Managing GPUs**
- **Peculiarities of text data**: unlike other fields, texts have ambiguities.
- **Token limits for a model** create bottlenecks
- **Hallucinations cause confusion**
- **Bias and ethical considerations**
- **Security concerns**
- **Controlling costs**: *e.g.*, GPUs, infra, storage, operational costs like energy consumption during both training and inference.

1.2 LLMOps Essentials

- **Compression** is the practice of making models smaller.
 - **Quantizing** is the process of reducing precision in preference of lowering the memory requirements.
 - **Pruning** is the process of weeding out and removing any parts of the model we deem unworthy.
 - **Knowledge distillation** takes the large LLM and train a smaller language model to copy it.
 - **Low-rank approximation** is a trick to simplify large matrices or tensors to find a lower dimensional representation.

- **Mixture of Experts** (MoE) is a technique where we replace the feed-forward (FF) layers in a transformer with MoE layers instead. FF layers are notorious for being parameter-dense and computationally intensive, so replacing them with something better can often have a large effect. MoEs are a group of sparsely activated models. They differ from ensemble techniques in that typically only one or a few expert models will be run, rather than combining results from all models. The sparsity is often induced by a *gate mechanism* that learns which experts to use and/or a router mechanism that determines which experts should even be consulted.
- **Distributed computing** is a technique used in DL to parallelize and speed up large, complex neural networks by dividing the workload across multiple devices or nodes in a cluster. This approach significantly reduces training and inference times by enabling concurrent computation, data parallelism, and model parallelism.
 - **Data parallelism**: splitting up the data and running them through multiple copies of the model or pipeline.
 - **Tensor parallelism**: This approach takes advantage of matrix multiplication properties of split up the activations across multiple processors, running the data through and then combining them on the other side of the processors.
 - **Pipeline parallelism**: This creates a pipeline, as input data will go to the first GPU, process, then transfer to the next GPU, and so on until it's run through the entire model.
 - **3D parallelism**: We want to take advantages of all three parallelism practices as they can all be run together. This is known as 3D parallelism, which combines data, tensor and pipeline parallelism (DP+TP+PP) together. Since each technique and thus dimension will require at least two GPUs to run 3D parallelism, we will need at least eight GPUs to get started.

1.3 LLM Operations Infrastructures

- Data infrastructure is the foundation of DataOps. (*e.g.*, Airflow, Prefect, and Mage)
- Experiment trackers (*e.g.*, MLFlow and Weights & Biases)
- Model registry
- Feature stores (*e.g.*, Feast) is a centralized system for managing, storing, and serving features (the inputs to machine learning models) in a consistent and reliable way. It sits between your raw data sources and your ML models, making it easier to build, deploy, and maintain production ML systems. Why do we need it? In ML, the same features are used in two places:
 - Training – when building the model.
 - Serving/Inference – when the model is deployed to make predictions.
- Vector databases (*e.g.*, Qdrant, Pinecone, and Milvus) are specialized databases that store vectors along with some metadata around the vector, which makes them great for storing embeddings. The power of vector databases isn't in their storage but in the way that they search through the data.

- Monitoring systems (*e.g.*, whylogs and [1](#)): ML models are often fail silently (*e.g.*, data drift [1](#)).
- GPU-enabled workstations (*e.g.*, H100 provides 80GB and NVL [2](#))
 - If you aren't sure which GPU you need to run which model, multiply the number of billions of parameters by two, since most models at inference will default to run at half precision, FP16 or BF16, which means we need at least 2 bytes for every parameter. You will need a little extra as well for embedding model, which will be about another gigabyte, and more for the actual tokens. One token is about 1MB. For 16 batches of this size, you will need an extra 8GB of space.
 - For training you will need a lot more space (*e.g.*, full precision, optimizer tensors and gradients). Roughly you need 16 bytes for every parameter, so to train a 7B parameter model, you will need 112GB of memory.
- Deployment service (*e.g.*, NVIDIA Triton Inference Service, MLServer, Seldon, BentoML)

¹Data drift in Machine Learning (ML) systems refers to changes in the statistical properties of input data (or the relationship between inputs and outputs) over time, which can degrade model performance if not monitored and addressed.

²NVIDIA Link is NVIDIA's high-speed interconnect technology. It allows GPUs (and sometimes CPUs) to communicate with each other much faster than PCIe. In multi-GPU systems (like deep learning servers, HPC, or AI supercomputers), GPUs need to share data frequently (*e.g.*, gradients and parameters). If they only use PCIe, communication is slower, creating a bottleneck.

Chapter 2

Preliminaries

2.1 Complexity of Matrix Multiplication

Matrix multiplication is a fundamental operation in many computational tasks, including neural networks. The complexity of multiplying two matrices depends on their dimensions. Let's dive into the specifics.

- Let A be a matrix of size $m \times k$.
- Let B be a matrix of size $k \times n$.
- The result C will be a matrix of size $m \times n$.

Standard Matrix Multiplication: For each element c_{ij} in the resulting matrix C :

$$c_{ij} = \sum_{l=1}^k a_{il} \cdot b_{lj}$$

This involves:

- Multiplications: k multiplications for each element c_{ij} .
- Additions: $k - 1$ additions for each element c_{ij} .

Complexity

- The total number of elements in C is $m \times n$.
- Therefore, the total number of multiplications is $m \times n \times k$.
- The total number of additions is $m \times n \times (k - 1)$.

Thus, the total complexity is $O(m \times n \times k)$.

Even though there are several advanced methods, the standard $O(m \times n \times k)$ complexity is often used in practice, due to the simplicity and efficiency of implementation on modern hardware. Optimized libraries (like BLAS, cuBLAS for GPUs) leverage hardware-specific optimizations to improve practical performance.

Part II

Data Engineering

Chapter 3

Data Engineering for LLMs

Data engineering is the development, implementation, and maintenance of systems and processes that take in raw data and produce high-quality, consistent information that supports downstream use cases, such as analysis and machine learning.

There isn't more valuable asset than your data. All successful AI and ML initiatives are built on a good data engineering foundation. It's important then that we acquire, clean, and curate our data.

3.1 Models and the Foundation

The most important dataset you will need to collect when training is the model weights of a pretrained model.

3.1.1 Evaluating LLMs

When evaluating a model, you will need two things: *(i)* a *metric* and *(ii)* a *dataset*.

Metrics

- ROUGE (Recall-Oriented Understudy for Gisting Evaluation)
- BLEU (BiLingual Evaluation Understudy)
- BPC (*e.g.*, Perplexity): The bits per character (BPC) evaluation is an example of an entropy-based evaluation for language models.

Industry benchmarks

- GLUE (General Language Understanding Evaluation) is essentially a standardized test for language models to measure performance versus humans and each other on language tasks meant to test understanding.

- SuperGLUE
- MMLU (Massive Multitask Language Understanding).

Responsible AI benchmarks

- HONEST evaluation metric compares how hurtful prompt completions are for different genders.
- Some datasets:
 - WinoBias dataset focuses on gender bias.
 - CALM
 - WinoQueer

Developing your own benchmark

- [OpenAI's Evals library](#)
- [Huggingface's Evaluate](#)

Evaluating code generators The basic setup looks like this:

1. Have your model generate code based on docstrings.
2. Run the generated code in a safe environment on prebuilt tests to ensure they work and that no errors are thrown
3. Run the generated code through a profiler and record the time it takes to complete.
4. Run the generated code through a security scanner and count the number of vulnerabilities.
5. Run the generated code against architectural fitness functions to determine artifacts like how much coupling, integrations, and internal dependencies there are.
6. Run steps 1 to 5 on another LLM.
7. Compare results.

Evaluating model parameters There's a lot you can learn by simply looking at the parameters of an ML model. For instance, an untrained model will have a completely random distribution.

```

1 import weightwatcher as ww
2 from transformers import GPT2Model
3
4 gpt2_model = GPT2Model.from_pretrained("gpt2")
5 gpt2_model.eval()
6
7 watcher = ww.WeightWatcher(model=gpt2_model)
8 details = watcher.analyze(plot=False)
9 print(details.head())
10 #   layer_id   name      D   ...   warning   xmax   xmin

```

11	# 0	2	Embedding	0.076190	... over-trained	3837.188332	0.003564
12	# 1	8	Conv1D	0.060738	...	2002.124419	108.881419
13	# 2	9	Conv1D	0.037382	...	712.127195	46.092445
14	# 3	14	Conv1D	0.042383	...	1772.850274	95.358278
15	# 4	15	Conv1D	0.062197	...	626.655218	23.727908

The spectral analysis plots evaluate the frequencies of eigenvalues for each layer of a model. These plots tell you whether a model (or layer) looks well-trained and generalizes well or is unstable/poorly conditioned. Shape of the Spectrum (How eigenvalues are distributed)

- Power-law exponent (α):
 - Good if between 2 and 6: the layer is well-trained.
 - Bad if $\alpha > 6$: layer might be undertrained or over-regularized.
- Fit quality (Dks):
 - Low Dks: spectrum matches the expected “heavy-tailed” shape, reliable.
 - High Dks: poor fit, unstable or unstructured layer.

3.2 Data for LLMs

It has been shown that data is the most important part of training an LLM.

Table 3.1: Summary of datasets

Dataset	Contents	Size	LastUpdate
WikiText	English Wikipedia	<1GB	2016
Wiki-40B	Multi-lingual Wikipedia	10GB	2020
Europarl	European Parliament proceedings	1.5GB	2011
Common Crawl	The internet	~ 300GB	Ongoing
OpenWebText	Curated internet using Reddit	55GB	2019
The Pile	Everything above plus specialty datasets (books, law, med)	825GB	2020
RedPajama	GitHub, arXiv, Books, Wikipedia, StackExchange , and multiple version of Common Crawl	5TB	2023
OSCAR	Highly curated multilingual dataset with 166 languages	9.4TB	Ongoing

3.2.1 Data cleaning and preparation

If you pulled any of the previously mentioned datasets, you might be surprised to realize most of them are just giant text dumps. There are no labels or annotations, and feature engineering hasn’t been done at all.

LLMs are trained via self-supervised manner to predict the next word or a masked word, so a lot of traditional data cleaning and preparation processes are unneeded. This fact leads many to believe that data cleaning as a whole is unnecessary.

Data cleaning and curation are difficult, time-consuming, and ultimately subjective tasks that are difficult to tie to key performance indicators (KPIs). Still, taking the time and resources to clean your data will create a more consistent and unparalleled user experience.

The right frame of mind when preparing your dataset:

1. Take your pie of data and determine a schema for the features
2. Make sure all the features conform to a distribution that makes sense for the outcome you're trying to get through normalization or scaling.
3. Check the data for bias/anomalies (most businesses skip this step by using automated checking instead of informed verification).
4. Convert the data into a format for the model to ingest (for LLMs, it's through tokenization and embedding).
5. Train, check, and retrain.

Note

For more information, check out Fundamentals of Data Engineering, WizardLM, and LIMA: Less Is More for Alignment.

Instruct Schema is one of the most effective and widely used data formats for fine-tuning models. Instruction tuning works on the principle that providing a model with explicit instructions for a task leads to better performance than simply giving it raw prompts and answers. In this approach, the data explicitly demonstrates what the model should do, making it clearer and more aligned with human intent. However, preparing such datasets is more demanding than assembling general web data, since each entry must be carefully constructed to match a structured format, typically including an instruction, optional input, and the expected output. You need to prepare your data to match a format that will look something like this:

```

1 ###Instruction
2
3 {user input}
4
5 ###Input
6
7 {meta info about the instruction}
8
9 ###Response
10
11 {model output}
```

It is a structured way of formatting data so that each example clearly contains:

- An instruction (what the model should do).
- An input (optional context or data the model works on).
- An output (the desired response).

For instance,

```

1 {
2   "instruction": "Translate the following English text into Korean.",
3   "input": "The stock market saw significant volatility today due to global
4     economic concerns.",
5   "output": "<Translations>"
6 }
```

Note

- EvolInstruct: WizardLM
- Self-instruct format, Alpaca

Ensuring proficiency with speech acts When preparing a dataset for training a model, the most important factor is ensuring the data truly reflects the task you want the model to perform. Misaligned or overly generic data reduces performance and can cause unpredictable behavior.

Dataset alignment:

- Training data must match the intended task (e.g., don't train on Titanic survivors if you want to predict Boston housing prices).
- In real-world use cases (like fast-food ordering), interactions are more diverse and unpredictable than generic datasets suggest.

Robustness and Risks:

- Instruction datasets require intentional design: if a model is only trained on “helpful” responses, it might follow harmful instructions (e.g., “help me take over the world”).
- With tool access (Google, HR docs), this becomes even riskier.

Understanding speech acts (directives, representatives, commissives, expressives, declarations, verdictives) helps design datasets that match realistic user interactions.

- In language learning, this means learners should not only know grammar/vocabulary but also how to perform speech acts appropriately:
 - How to make polite requests
 - How to refuse without sounding rude
 - How to apologize or thank in culturally acceptable ways
- In AI / LLM context, it means training the model to:
 - Generate outputs that correctly perform the intended communicative function (e.g., distinguish between an instruction, a suggestion, or a formal declaration).
 - Handle pragmatic nuances, politeness, indirectness, etc.

Speech acts refer to the various functions language can perform in communication beyond conveying information. They are a way of categorizing utterances based on their intended effect or purpose in a conversation. In short, it is an action performed through speaking. For example:

- Assertives → stating something true/false.
- Directives → requesting, commanding (e.g., “Get it done in the next three days”).
- Commissives → promising, committing (e.g., “I swear”).

- Expressives → greetings, apologizing (*e.g.*, “You are the best”).
- Declarations → enacting something by saying it (*e.g.*, “I now pronounce you married”).
- Questions (*e.g.*, “What is this?”)

Annotating the data Annotation is labeling your data, usually in a positionally aware way. For speech recognition tasks, annotations would identify the different words as noun, verb, adjective, or adverb. Annotations essentially give us metadata that makes it easier to reason about and analyze our datasets.

There are tools to help with the task:

- [Prodigy](#): multimodal annotation tool.
- [doccano](#): Open-source web-based platform for data annotation.
- [Praat](#): The audio annotation tool.
- [Galileo](#): Galileo’s LLM studio helps create prompt, evaluate and speed up annotation.

3.3 Text Processors

We need to transform our dataset into something that can be consumed by the LLM. Simply, we need to turn the text into numbers.

3.3.1 Tokenization

The tokenization is often ignored when working with an LLM through an API, but it is actually vitally important for every subsequent step, and it affects the LLM’s performance significantly.

Word-based Word-based tokenizers most commonly split on whitespace, but there are other methods like using regex, dictionaries, or punctuation.

Character-based Character-based encoding methods are the most straightforward and easiest to implement since we split on the UTF-8 character encodings. However, it comes with a major loss of information and fails to keep relevant syntax, semantics, or morphology (morpheme like prefix and suffixes) of the text.

Subword-based Subword-based tokenizers have proven to be the best option so far.

- BPE
- WordPiece
- SentencePiece

3.3.2 Embeddings

Embeddings provide meaning to the vectors generated during tokenization.

Part III

Training LLMs

Chapter 4

Training LLMs: How to generate the generator

4.1 Multi-GPU environments

Training is a resource-intensive endeavor. A model that only takes a single GPU to run inference on may take 10 times that many to train if, for nothing else, to parallelize your work and speed things up so you aren't waiting for a thousand years for it to finish training.

4.1.1 Setting up

It should be pointed out up front that while multi-GPU environments are powerful, they are also expensive. For the rest of us, setting up a virtual machine (VM) in Google's Compute Engine is one of the easiest methods.

Google Virtual Machine One of the easiest ways to create a multi-GPU environment is to set up a VM on Google's cloud.

1. Create a Google Cloud Project (GCP).
 - Set up billing
 - Download the gcloud CLI.
2. After setting up your account, GCP sets your GPU quotas to 0. Quotas are used to manage your costs. You need to increase to 2 or more, since we plan to use multiple GPUs.
3. Init by "gcloud init"
- 4.

4.1.2 Libraries

DeepSpeed: DeepSpeed is an optimization library for distributed deep learning. DeepSpeed is powered by Microsoft and implements various enhancements for speed in training and inference,

like handling extremely long or multiple inputs in different modalities, quantization, caching weights and inputs, and, probably the hottest topic right now, scaling up to thousands of GPUs.

To install,

1. Install PyTorch
2. `pip install deepspeed`

Accelerate: From HuggingFace, Accelerate is made to help abstract the code for parallelizing and scaling to multiple GPUs away from you so that you can focus on the training and inference side.

To install,

1. `pip install accelerate`

PyTorch FSDP Install PyTorch with distributed support (CUDA version must match drivers):

```
1 pip install torch torchvision torchaudio
2
3 # (Optional) For speedups
4 pip install torchmetrics accelerate
```

Ensure passwordless SSH between nodes if you're on a bare-metal or HPC cluster.

Create `train_fsdp.py`:

```
1 import torch
2 import torch.nn as nn
3 import torch.optim as optim
4 import torch.distributed as dist
5 from torch.distributed.fsdp import FullyShardedDataParallel as FSDP
6 from torch.distributed.fsdp.wrap import transformer_auto_wrap_policy
7
8 # --- Simple Transformer block ---
9 class ToyBlock(nn.Module):
10     def __init__(self):
11         super().__init__()
12         self.fc1 = nn.Linear(1024, 4096)
13         self.act = nn.ReLU()
14         self.fc2 = nn.Linear(4096, 1024)
15
16     def forward(self, x):
17         return self.fc2(self.act(self.fc1(x)))
18
19 class ToyModel(nn.Module):
20     def __init__(self, depth=6):
21         super().__init__()
22         self.layers = nn.Sequential(*[ToyBlock() for _ in range(depth)])
23
24     def forward(self, x):
25         return self.layers(x)
26
27 def main():
28     dist.init_process_group("nccl")
29     torch.cuda.set_device(dist.get_rank() % torch.cuda.device_count())
```

```

30
31     model = ToyModel().cuda()
32
33     # Auto-wrap large layers with FSDP
34     auto_wrap_policy = transformer_auto_wrap_policy
35     model = FSDP(model, auto_wrap_policy=auto_wrap_policy)
36
37     optimizer = optim.AdamW(model.parameters(), lr=1e-4)
38
39     for step in range(20):
40         x = torch.randn(8, 1024).cuda()
41         y = model(x).mean()
42         y.backward()
43         optimizer.step()
44         optimizer.zero_grad()
45         if dist.get_rank() == 0:
46             print(f"Step {step} done.")
47
48     dist.destroy_process_group()
49
50 if __name__ == "__main__":
51     main()

```

If your node has 4 GPUs:

```
torchrun -nproc_per_node=4 train_fsd.py
```

- 4 processes (one per GPU).
- NCCL backend handles GPU communication.

Let's try running multiple nodes

- Node 0: 10.0.0.1
- Node 1: 10.0.0.2
- 4 GPUs per node
- Total world size = 8 (2 nodes × 4 GPUs)

```

1 **On Node 0 (rank 0):**
2
3 torchrun --nnodes=2 --nproc_per_node=4 \
4     --node_rank=0 \
5     --master_addr=10.0.0.1 \
6     --master_port=29500 \
7     train_fsd.py
8
9 **On Node 1 (rank 1):**
10
11 torchrun --nnodes=2 --nproc_per_node=4 \
12     --node_rank=1 \
13     --master_addr=10.0.0.1 \
14     --master_port=29500 \
15     train_fsd.py

```

- `--nnodes=2`: total number of nodes.

- `-nproc_per_node=4`: GPUs per node.
- `-node_rank`: each node's unique index.
- `-master_addr`: IP/hostname of rank 0 node.
- `-master_port`: open port for coordination.
- Activation checkpointing: Saves memory by discarding intermediate activations during forward pass and recomputing them during backward pass.
- Mixed precision: Uses FP16 or BF16 for computations (faster, less memory) while keeping FP32 for stability in some ops.

Full Example with FSDP + Checkpointing + AMP:

```

1 import torch
2 import torch.nn as nn
3 import torch.optim as optim
4 import torch.distributed as dist
5 from torch.distributed.fsdp import FullyShardedDataParallel as FSDP
6 from torch.distributed.fsdp.wrap import transformer_auto_wrap_policy
7 from torch.utils.checkpoint import checkpoint
8
9 # --- A block with activation checkpointing ---
10 class CheckpointedBlock(nn.Module):
11     def __init__(self):
12         super().__init__()
13         self.fc1 = nn.Linear(1024, 4096)
14         self.act = nn.ReLU()
15         self.fc2 = nn.Linear(4096, 1024)
16
17     def forward(self, x):
18         def forward_fn(x):
19             return self.fc2(self.act(self.fc1(x)))
20         # checkpoint will discard activations & recompute in backward
21         return checkpoint(forward_fn, x)
22
23 # --- Toy Model ---
24 class ToyModel(nn.Module):
25     def __init__(self, depth=6):
26         super().__init__()
27         self.layers = nn.Sequential(*[CheckpointedBlock() for _ in range(depth)]
28     ]
29
30     def forward(self, x):
31         return self.layers(x)
32
33 def main():
34     dist.init_process_group("nccl")
35     torch.cuda.set_device(dist.get_rank() % torch.cuda.device_count())
36
37     # Build model
38     model = ToyModel().cuda()
39     auto_wrap_policy = transformer_auto_wrap_policy
40     model = FSDP(model, auto_wrap_policy=auto_wrap_policy)
41
42     optimizer = optim.AdamW(model.parameters(), lr=1e-4)
43
44     # Use mixed precision autocast (bf16 preferred if hardware supports it)
45     scaler = torch.cuda.amp.GradScaler(enabled=True) # works for fp16

```

```

45
46     for step in range(20):
47         x = torch.randn(8, 1024).cuda()
48
49         with torch.cuda.amp.autocast(dtype=torch.bfloat16): # or torch.float16
50             y = model(x).mean()
51
52         # backward with gradient scaler
53         scaler.scale(y).backward()
54         scaler.step(optimizer)
55         scaler.update()
56         optimizer.zero_grad()
57
58         if dist.get_rank() == 0:
59             print(f"Step {step} done.")
60
61     dist.destroy_process_group()
62
63 if __name__ == "__main__":
64     main()

```

- Checkpointing: Wrap the forward function with `torch.utils.checkpoint.checkpoint`.
- AMP (Automatic Mixed Precision):
 - Use `torch.cuda.amp.autocast` for forward pass.
 - Use `torch.cuda.amp.GradScaler` for loss scaling (needed for FP16, not BF16).
- BF16 vs FP16:
 - Use BF16 if your GPUs are A100/H100 (more stable).
 - Use FP16 + GradScaler for V100 or older cards.
- Full State Dict: Gather the full parameters on rank 0 and save them. (simpler, larger files).
- Sharded State Dict: Each rank saves only its shard. (efficient, but needs all shards to reload).
- Rank 0 only writing: Typically only rank 0 writes to disk to avoid file conflicts.

```

1 import os
2 import torch
3 from torch.distributed.fsdp import FullyShardedDataParallel as FSDP
4 from torch.distributed.fsdp import StateDictType, FullStateDictConfig
5
6 CHECKPOINT_DIR = "./checkpoints"
7
8 def save_checkpoint(model, optimizer, step):
9     # Ensure only rank 0 writes the file
10    rank = torch.distributed.get_rank()
11    os.makedirs(CHECKPOINT_DIR, exist_ok=True)
12
13    # Switch to FULL state dict (gathered on rank 0)
14    # offload_to_cpu=True: keeps memory usage down when gathering full state.
15    full_sd_config = FullStateDictConfig(offload_to_cpu=True, rank0_only=True)
16    with FSDP.state_dict_type(model, StateDictType.FULL_STATE_DICT,
17                             full_sd_config):
18        model_state = model.state_dict()

```

```

18     optim_state = optimizer.state_dict()
19
20     if rank == 0: # only rank 0 writes to disk.
21         save_path = os.path.join(CHECKPOINT_DIR, f"step_{step}.pt")
22         torch.save({"model": model_state, "optimizer": optim_state, "step":
23                     step}, save_path)
24         print(f"[Rank 0] Saved checkpoint to {save_path}")
25
26 def load_checkpoint(model, optimizer, load_path):
27     # Load only on rank 0
28     rank = torch.distributed.get_rank()
29     map_location = "cpu" if rank == 0 else "meta" # meta avoids OOM on other
30     ranks
31     checkpoint = torch.load(load_path, map_location=map_location)
32
33     # Use FULL state dict context
34     full_sd_config = FullStateDictConfig(offload_to_cpu=True, rank0_only=True)
35     with FSDP.state_dict_type(model, StateDictType.FULL_STATE_DICT,
36                               full_sd_config):
37         model.load_state_dict(checkpoint["model"])
38
39     # Broadcast model weights to all ranks
40     torch.distributed.barrier()
41     optimizer.load_state_dict(checkpoint["optimizer"])
42     print(f"[Rank {rank}] Loaded checkpoint from {load_path}")

```

Library	Core Idea	Strengths / Use Cases
DeepSpeed	Distributed training engine with ZeRO (Zero Redundancy Optimizer) sharding	<ul style="list-style-type: none"> - ZeRO-1/2/3: memory savings via parameter/gradient/optimizer sharding - Offloading to CPU/NVMe - Mixture of Experts (MoE) support - Great for very large dense or MoE models
FSDP (Fully Sharded Data Parallel)	Native PyTorch module for full parameter, gradient, optimizer sharding	<ul style="list-style-type: none"> - First-party, stable, integrated in PyTorch - ZeRO-3-like memory scaling - Easy to use with Hugging Face Accelerate/Lightning
Megatron-LM	Parallelism library from NVIDIA (TP, PP, SP, EP)	<ul style="list-style-type: none"> - Tensor Parallelism (TP) for matmuls - Pipeline Parallelism (PP) for layer distribution - Sequence/Expert Parallelism for long-context and MoE - Standard for 30B–100B+ scale

Table 4.1: Comparison of Core Libraries for Multi-GPU LLM Training

- Up to 13B on few GPUs → FSDP (simpler, first-party).
- >30B or MoE, multi-node → Megatron-LM + (FSDP or DeepSpeed ZeRO).
- When GPU memory is tight → DeepSpeed ZeRO-3 (with offload).

4.2 Basic Training Techniques

Unlike traditional ML models, LLMs are often trained in stages:

- [Optuna](#): Open source hyperparameter optimization (HPO) framework for machine learning, including Large Language Models (LLMs).

Chapter 5

Parameter Efficient Fine-Tuning

5.1 LoRA

When fine-tuning a neural network for a new task, we adjust its weights W by learning an update ΔW , yielding

$$W' = W + \Delta W.$$

LoRA (Low-Rank Adaptation) avoids updating W directly. Motivated by the ****intrinsic rank hypothesis****—the idea that task-critical changes lie in a low-dimensional subspace—LoRA parameterizes the update as a low-rank product:

$$\Delta W = BA, \quad W' = W + BA,$$

while keeping W frozen. Here $B \in \mathbb{R}^{d \times r}$ and $A \in \mathbb{R}^{r \times d}$ with $r \ll d$, so BA is a low-rank approximation to the full update.

This factorization dramatically reduces trainable parameters. Instead of learning all d^2 entries of ΔW (for a $d \times d$ weight), LoRA learns only the factors B and A , totaling $2dr$ parameters—much smaller when $r \ll d$. (The same idea applies to non-square $W \in \mathbb{R}^{d \times k}$, using $B \in \mathbb{R}^{d \times r}$ and $A \in \mathbb{R}^{r \times k}$, for a cost of $r(d + k)$ instead of dk .)

5.2 QLoRA

While LoRA reduces the number of *trainable* parameters, it still requires storing and using the full-precision base model W during fine-tuning. For very large LLMs (tens or hundreds of billions of parameters), this memory demand can exceed the capacity of a single GPU.

QLoRA (Quantized Low-Rank Adaptation) addresses this by combining LoRA with parameter *quantization*. Instead of keeping W in 16- or 32-bit precision, QLoRA stores it in a lower-bit format (typically 4-bit). During training:

- The frozen base weights W are kept in 4-bit quantized form, greatly reducing memory usage.

- On-the-fly, W is *dequantized* into higher precision (e.g., 16-bit) for computations.
- As in LoRA, trainable low-rank adapters A, B are introduced to capture task-specific updates.

The update rule remains

$$W' = W + BA,$$

but now W is quantized, while A, B are small full-precision matrices.

Part IV

LLM Services

Chapter 6

LLM Services: A Practical Guide

Production refers to the phase where the model is integrated into live or operational environment to perform its intended tasks or provide services to end users. It's a crucial phase in making the model available for real-world applications and services. In this chapter, we will explore how to package up an LLM into a service or API so that it can take on-demand requests. Then, we will study how to set up a cluster in the cloud where you can deploy this service.

6.1 Creating an LLM service

6.1.1 Model Compilation

The success of any model in production is dependent on the hardware it runs on. Unfortunately, when programming in a high-level language like Python-based frameworks like PyTorch or TensorFlow, the model won't be optimized to take full advantage of the hardware. This is where compiling comes into play. Compiling is the process of taking code written in a high-level language and converting or lowering it to machine-level code that the computer can process quickly. Compiling your LLM can easily lead to major inference and cost improvements.

Kernel Tuning In DL, and high-performance computing, a kernel is a small program or function designed to run on a GPU or other similar processors. These routines are developed by the hardware vendor to maximize chip efficiency.

During kernel tuning, the most suitable kernels are chosen from a large collection of highly optimized kernels.

Kernel Fusion A GPU kernel is the tiny function that runs on each element. **Fusion** = do several elementwise ops in one kernel so each element is read from VRAM ¹ once, processed in registers, then written back once.

¹VRAM is technically a type of DRAM, but it is optimized for storing images and video data that the GPU (Graphics Processing Unit) requires for processing various graphics. It is primarily responsible for storing textures, frame buffers, image data, video data, and other graphics-related data [1].

The $y = \text{ReLU}(x + b)$ example

Assume x and b are the same length (or b is broadcast on the last dim).
Without fusion (two kernels: add, then ReLU):

1. For every element i :
2. Read $x[i]$ from VRAM
3. Read $b[i]$ from VRAM
4. Compute $t = x[i] + b[i]$
5. Write t to VRAM \leftarrow intermediate array
6. Read t from VRAM
7. Compute $y = \max(t, 0)$
8. Write y to VRAM

Global-memory ops per element: 5 (read x , read b , write t , read t , write y) Two kernel launches (one for add, one for ReLU).

With fusion (one kernel: add+ReLU together)

1. For every element i :
2. Read $x[i]$ from VRAM
3. Read $b[i]$ from VRAM
4. Compute $t = x[i] + b[i]$ (kept in a register, not VRAM)
5. Compute $y = \max(t, 0)$
6. Write y to VRAM

Global-memory ops per element: 3 (read x , read b , write y) One kernel launch.

ReLU Example:

```

1 import torch, time
2
3 B, C = 4096, 4096
4 x = torch.randn(B, C, device="cuda", dtype=torch.float32)
5 b = torch.randn(C, device="cuda", dtype=torch.float32)
6
7 def add_relu_unfused(x, b):
8     # Eager mode typically launches two kernels (add, then relu)
9     return torch.relu(x + b)
10
11 # PyTorch 2.x compiler (Inductor) generates fused kernels automatically
12 # This fuses common elementwise chains (like add ReLU) into single kernels.
13 add_relu_fused = torch.compile(add_relu_unfused, backend="inductor")
14
15 # Correctness check
16 with torch.no_grad():
17     y1 = add_relu_unfused(x, b)
18     y2 = add_relu_fused(x, b)
19     print("max |diff| =", (y1 - y2).abs().max().item())
20

```

```

21 # Simple timing
22 def bench(fn, iters=50, warmup=10):
23     for _ in range(warmup):
24         fn(x, b); torch.cuda.synchronize()
25     t0 = time.perf_counter()
26     for _ in range(iters):
27         fn(x, b)
28     torch.cuda.synchronize()
29     return (time.perf_counter() - t0) * 1000 / iters
30
31 print("Unfused   :", bench(add_relu_unfused), "ms/iter")
32 print("Fused     :", bench(add_relu_fused),   "ms/iter")

```

Graph Optimization Graph optimization = semantics-preserving rewrites of the op graph (fold, fuse, simplify, relayout, retype, reschedule) so the lowered kernels do less work with less memory traffic

TensorRT NVIDIA TensorRT is an SDK that converts a trained model into an optimized “engine” and then runs that engine with very low latency/high throughput on NVIDIA GPUs. It includes an optimizer (compiler) and a lightweight runtime.

How it works (typical workflow):

1. Import your model (usually ONNX; there are parsers and framework bridges).
2. Build an optimized engine: TensorRT selects fast kernels ("tactics"), fuses layers, lowers precision (FP16/INT8) if allowed, and specializes to your shapes/hardware.
3. Serialize the engine to a .plan file (so you can load it instantly in production).
4. Run it via the TensorRT runtime (C++/Python).

```

1 import tensorrt as trt
2
3 logger = trt.Logger(trt.Logger.WARNING)
4 builder = trt.Builder(logger)
5 network = builder.create_network(1 << int(trt.NetworkDefinitionCreationFlag.
6     EXPLICIT_BATCH))
7 parser = trt.OnnxParser(network, logger)
8
9 with open("model.onnx", "rb") as f:
10     assert parser.parse(f.read()), parser.get_error(0)
11
12 config = builder.create_builder_config()
13 config.set_memory_pool_limit(trt.MemoryPoolType.WORKSPACE, 4 << 30) #
14     workspace budget
15 config.set_flag(trt.BuilderFlag.FP16) # enable mixed precision if supported
16
17 # Dynamic-shape profile for input "input" (name must match your ONNX)
18 profile = builder.create_optimization_profile()
19 profile.set_shape("input", min=(1,3,224,224), opt=(8,3,224,224), max
20     =(32,3,224,224))
21 config.add_optimization_profile(profile)
22
23 engine = builder.build_engine(network, config)
24 with open("model.plan", "wb") as f:
25     f.write(engine.serialize())

```

ONNX Runtime **ONNX**, which stands for Open Neural Network Exchange, is an open source format and ecosystem designed for representing and interoperating between different deep learning frameworks. It was created to address the challenge of model portability and compatibility. ONNX is an IR (intermediate representation) and it allows you to represent models trained in some deep learning framework (*e.g.*, TensorFlow, PyTorch) in a standardized format easily consumed by other frameworks and it facilitates the exchange of models between different tools and environments. Unlike TensorRT, ONNX Runtime is intended to be hardware-agnostic, meaning it can be used with a variety of hardware accelerators, including CPUs, GPUs, and specialized hardware like TPUs.

6.1.2 LLM storage strategies

Now we have a compiled model, we need to think about how our service will access it. This step is critical, because boot times can be a nightmare when working with LLMs since it can take a long time to load such large assets into memory.

Object storage systems break up assets into small fractional bits called objects. They allow us to federate the entire asset across multiple machines and physical memory locations, a powerful tool that powers the cloud, and to cheaply store large objects on hardware.

Fusing is the process of mounting a bucket to your machine as if it were an external hard drive.

Baking the Model Baking is the process of putting your model into the Docker image. It is considered an *anti-pattern*.

- Gigantic images: every update means pushing/pulling multi-GB layers → slow CI/CD, slow Kubernetes rollouts, higher storage costs.
- Tight coupling: a new model version requires a full image rebuild and redeploy (harder A/B tests, slower rollbacks, no "one image, many models").
- Poor caching: one byte change in weights invalidates a huge layer; your build cache won't help much.
- Security issue

Hybrid: download once, reuse many Download the model at boot time but store it in a volume that is mounted at boot time. While this doesn't help at all with the first deployment in a region, it does substantially help any new instances, as they can simply mount this same volume and have the model available to load without having to download.

- At boot (when the service starts up), your service (or an init step) pulls the model from S3/MinIO/HF/etc.
- It stores the files on a persistent volume that's mounted into the container.
- Subsequent pods/containers on the same node (or across nodes if using a shared RWX volume) just mount the volume—no re-download.
- You keep your app image small and decouple model updates from image builds.

6.1.3 Adaptive request batching

A typical API will accept and process requests in the order they are received, processing them immediately and as quickly as possible. However, anyone who's trained a ML model has come to realize that there are mathematical and computational advantages to running inference in batches of powers of 2 (16, 32, 64, etc), particularly when GPUs are involved, where we can take advantage of better memory alignment or vectorized instructions parallelizing computations across the GPU cores.

Why power of 2 is better Reference: [CUDA C++ Best Practices Guide](#)

<https://datascience.stackexchange.com/questions/20179/what-is-the-advantage-of-keeping-batch-size-a-power-of-2>

What adaptive batching does is essentially pool requests together over a certain period of time. Once the pool receives the configured maximum batch size or the timer runs out, it will run inference on the entire batch through the model, sending the results back to the individual clients that requested them. Essentially, it's a queue. Setting one up yourself can and will be a huge pain; thankfully, most ML inference services offer this out of the box, and almost all are easy to implement. For example, in **BentoML**, add `@bentoml Runnable.method(batchable=True)` as a decorator to your predict function, and in **Triton Inference Server**, add `dynamic_batching{}` at the end of your model definition file.

If that sounds easy, it is. Typically, you don't need to do any further finessing, as the defaults tend to be very practical. That said, if you are looking to maximize every bit of efficiency possible in the system, you can often set a maximum batch size, which will tell the batcher to run once this limit is reached, or a batch delay, which does the same thing but for the timer. Increasing either will result in longer latency but likely better throughput, so typically these are only adjusted when your system has plenty of latency budget.

Overall, the benefits of adaptive batching include better use of resources and higher throughput at the cost of a bit of latency. This is a valuable trade-off, and we recommend giving your product the latency bandwidth to include this feature. In our experience, optimizing for throughput leads to better reliability and scalability and thus greater customer satisfaction. Of course, when latency times are extremely important or traffic is few and far between, you may rightly forgo this feature.

6.1.4 Flow Control

Rate limiters and access keys are critical protections for an API, especially one sitting in front of an expensive LLM. Rate limiters control the number of requests a client can make to an API within a specified time, which helps protect the API server from abuse, such as distributed denial of service (DDoS) attacks, where an attacker makes numerous requests simultaneously to overwhelm the system and hinder its function.

Rate limiters can also protect the server from bots that make numerous automated requests in a short span of time. This helps manage the server resources optimally so the server is not exhausted due to unnecessary or harmful traffic. They are also useful for managing quotas, thus ensuring all users have fair and equal access to the API's resources. By preventing any single user from using excessive resources, the rate limiter ensures the system functions smoothly for

all users.

All in all, rate limiters are an important mechanism for controlling the flow of your LLM's system processes. They can play a critical role in dampening bursty workloads and preventing your system from getting overwhelmed during autoscaling and rolling updates, especially when you have a rather large LLM with longer deployment times. Rate limiters can take several forms, and the one you choose will be dependent on your use case.

Types of rate limiters

- Fixed window
- Sliding window log
- Token bucket
- Leaky bucket

A rate limiter can be applied at multiple levels, from the entire API to individual client requests to specific function calls.

```

1 from typing import Optional
2
3 from fastapi import FastAPI, Depends, HTTPException, status, Request
4 from fastapi.security import APIKeyHeader
5 from slowapi import Limiter, _rate_limit_exceeded_handler
6 from slowapi.errors import RateLimitExceeded
7 from slowapi.util import get_remote_address
8
9 # ----- Config -----
10 # In real apps, load from a DB or env/secret manager.
11 VALID_KEYS = {"1234567890abcdefg"}
12
13 # Displayed in Swagger UI as the auth "scheme" name
14 api_key_header = APIKeyHeader(name="X-API-Key", scheme_name="APIKey",
15                               auto_error=False)
16
17 # Prefer per-key limiting; fall back to client IP (useful when no key provided)
18 def rate_key(request: Request) -> str:
19     key = request.headers.get("X-API-Key")
20     return f"key:{key}" if key else f"ip:{request.client.host}"
21
22 # Use in-memory storage for single-process dev.
23 # For multi-workers/replicas, switch to: storage_uri="redis://redis:6379/0"
24 limiter = Limiter(key_func=rate_key, storage_uri="memory://")
25
26 # ----- App setup -----
27 app = FastAPI(title="API-Key + Rate Limit Example")
28 app.state.limiter = limiter
29 app.add_exception_handler(RateLimitExceeded, _rate_limit_exceeded_handler)
30
31 # If running behind a reverse proxy/load balancer, trust X-Forwarded-*.
32 # In production, replace ["*"] with your proxy host/IP(s).
33
34 # ----- Auth dependency -----
35 async def require_api_key(api_key: Optional[str] = Depends(api_key_header)) ->
36     str:
37     """
38     Validates the X-API-Key header against our allow-list.
39     Returns the key (or user id associated with it) for downstream use.
40     """
41     if not api_key or api_key not in VALID_KEYS:

```

```

40         # RFC-friendly header (helps some clients know how to auth)
41         raise HTTPException(
42             status_code=status.HTTP_401_UNAUTHORIZED,
43             detail="Invalid or missing API key",
44             headers={"WWW-Authenticate": "APIKey"},
45         )
46     return api_key
47
48 # ----- Routes -----
49 @app.get("/health", include_in_schema=False)
50 async def health() -> dict:
51     return {"ok": True}
52
53 @app.get("/hello")
54 @limiter.limit("5/minute")           # per-key if present; else per-IP
55 async def hello(request: Request, api_key: str = Depends(require_api_key)):
56     # SlowAPI needs 'request'; dependency injects validated 'api_key'.
57     return {"message": "Hello World"}
58
59 # Optional: run directly with 'python main.py'
60 if __name__ == "__main__":
61     import uvicorn
62     uvicorn.run("main:app", host="127.0.0.1", port=8000, reload=True)

```

- You (the API owner) issue a unique key (*i.e.*, `VALID_KEYS`) to each user/app.
- The client keeps that key and sends it with every request.
- Because the client passes the key in an HTTP header. Your example uses an `X-API-Key` header via `APIKeyHeader`.
- The dependency `require_api_key(...)` reads the header, checks it against `VALID_KEYS`, and returns 401 if it's missing/invalid.
- The rate limiter's `key_func` (`rate_key`) also reads the same header to bucket requests per key.

To test in SwaggerUI:

- Click Authorize.
- You'll see a field for APIKey (because `APIKeyHeader` is used).
- Paste "12345678abcdefg" and authorize

LiteLLM LLM proxy server

6.1.5 Streaming responses

6.1.6 Feature store

When it comes to running ML models in production, feature stores really simplify the inference process. We first introduced these in chapter 3, but as a recap, feature stores establish a centralized source of truth. They answer crucial questions about your data:

Who is responsible for the feature? What is its definition? Who can access it? Let's take a look at setting one up and querying the data to get a feel for how they work. We'll be using Feast, which is open source and supports a variety of backends. To get started, let us pip install feast and then run the init command in your terminal to set up a project, like so:

The app we are building is a question-and-answer service. Q&A services can greatly benefit from a feature store's data governance tooling. For example, point-in-time joins help us answer questions like "Who is the president of x?" where the answer is expected to change over time. Instead of querying just the question, we *query the question with a timestamp*, and the point-in-time join will return whatever the answer to the question was in our database at that point in time. In the next listing, we pull a Q&A dataset and store it in a parquet format in the data directory of our Feast project.

```

1 import pandas as pd
2 from datasets import load_dataset
3 import datetime
4
5 from sentence_transformers import SentenceTransformer
6 model = SentenceTransformer("all-MiniLM-L6-v2")
7
8 def save_qa_to_parquet(path):
9     squad = load_dataset("squad", split="train[:5000]")
10    ids = squad["id"]
11    questions = squad["question"]
12    answers = [answer["text"][0] for answer in squad["answers"]]
13    qa = pd.DataFrame(
14        zip(ids, questions, answers),
15        columns=["question_id", "questions", "answers"],
16    )
17    qa["embeddings"] = model.encode(questions) # feature
18    qa["created"] = utcnow() # ingest time
19    qa["datetime"] = qa["created"].dt.floor("h") # Event time (when the new
    fact becomes true)
20    qa.to_parquet(path) # offline store file
21
22 if __name__ == "__main__":
23     path = "./data/qa.parquet"
24     save_qa_to_parquet(path)

```

- `DataFrame.to_parquet` in pandas is a method used to write a pandas DataFrame to the binary Parquet file format.
 - Parquet is a columnar storage format optimized for efficient data storage and retrieval, especially in big data environments.
- Creating a tiny feature table with:
 - Entity key: `question_id`
 - Features: embeddings (and you could treat answers, questions as features for the demo)
 - Time columns: `datetime` (event time), `created` (ingest time)

```

1 from feast import Entity, FeatureView, Field, FileSource, ValueType
2 from feast.types import Array, Float32, String
3 from datetime import timedelta
4
5 path = "./data/qa.parquet"

```

```

6
7 question = Entity(name="question_id", value_type=ValueTypes.STRING)
8
9 question_feature = Field(name="questions", dtype=String)
10
11 answer_feature = Field(name="answers", dtype=String)
12
13 embedding_feature = Field(name="embeddings", dtype=Array(Float32))
14
15 questions_view = FeatureView(
16     name="qa",
17     entities=[question],
18     ttl=timedelta(days=1),
19     schema=[question_feature, answer_feature, embedding_feature],
20     source=FileSource(
21         path=path,
22         event_timestamp_column="datetime",
23         created_timestamp_column="created",
24         timestamp_field="datetime",
25     ),
26     tags={},
27     online=True,
28 )

```

6.1.7 Retrieval-augmented generation

6.1.8 LLM service libraries

If you are starting to feel a bit overwhelmed about all the tooling and features you need to implement to create an LLM service, there are several libraries aim to do all of this for you! Some open source libraries of note are **vLLM** and **OpenLLM** (by BentoML).

Most of these toolings are still relatively new and under active development, and they are far from feature parity with each other, so pay attention to what they offer.

6.2 Setting up infrastructure

Setting up infrastructure is a critical aspect of modern software development, and we shouldn't expect machine learning to be any different. To ensure scalability, reliability, and efficient deployment of our applications, we need to plan a robust infrastructure that can handle the demands of a growing user base. This is where **Kubernetes** comes into play.

Kubernetes, often referred to as k8s, is an open source container orchestration platform that helps automate and manage the deployment, scaling, and management of containerized applications. It is designed to simplify the process of running and coordinating multiple containers across a cluster of servers, making it easier to scale applications and ensure high availability. We are going to talk a lot about k8s in this chapter, and while you don't need to be an expert, it will be useful to cover some basics to ensure we are all on the same page.

At its core, k8s works by grouping containers into logical units called *Pods*, which are the smallest deployable units in the k8s ecosystem. These pods are then scheduled and managed by the k8s control plane (*i.e.*, the brain of Kubernetes), which oversees their deployment, scaling,

and updates. This control plane consists of several components that collectively handle the orchestration and management of containers.

- Control Plane
 - API server: this is the gate to talk to k8s.
 - Scheduler: Decides which worker node will run your pod.
 - Controller manager: Watches everything and fixes it if it drifts from your request.
- Worker Nodes: each node is a computer (physical or virtual). It runs:
 - Kubelet: The assistant on each node. This talks to the control plane and makes sure the right containers (*i.e.*, pod) are running.

How it works?

- You tell Kubernetes: “Run 3 pods of my web app.”
- API Server receives the request.
- Scheduler decides where to place pods.
- Controller Manager keeps checking until 3 pods are alive.
- Kubelet on each worker starts the containers.
- Kube-Proxy sets up networking so users can reach your app.

6.2.1 Provisioning clusters

The first thing to do when starting any project is to set up a *cluster*. A cluster is a collective of worker machines or nodes where we will host our applications.

- On GCP:

```
1 gcloud container clusters create <NAME>
```

- On AWS

```
1 eksctl create cluster
```

- Provisioning a cluster is like building an “empty factory”: control room (control plane), power, network, and a small set of machines (nodes) to start with. In short, it creates and prepares the cluster.
- Node Auto-Provisioning (NAP) is an auto-hire manager that watches your job queue (unschedulable Pods) and, when there aren’t enough machines, buys and installs the right new machines automatically—and removes them later when work slows down. In short, it dynamically adds new nodes/pools to an existing cluster (not create the cluster itself).

6.2.2 Autoscaling

One of the big selling points to setting up a k8s cluster is *autoscaling*. Autoscaling is an important ingredient in creating robust production-grade services. The main reason is that **we never expect any service to receive static request volume**.

Autoscaling and NAP

Autoscaling can be considered as a family of mechanisms at different layers, and NAP is one specific (infrastructure) member of that family.

The HPA (horizontal pod autoscaler) watches CPU and memory resources and will tell the deployment service to increase or decrease the number of replicas.

The first service we'll need is one that can **collect the GPU metrics**. From this, we have *NVIDIA's Data Center GPU Manager (DCGM)*, which provides a metrics exporter that can export GPU metrics. DCGM exposes a host of GPU metrics, including temperature and power usage, which can create some fun dashboards, but the most useful metrics for autoscaling are utilization and memory utilization.

From here, the data will go to a service like *Prometheus*. Prometheus is an open source monitoring system used to monitor Kubernetes clusters and the applications running on them. Prometheus collects metrics from various sources and stores them in a time-series database, where they can be analyzed and queried. Prometheus can collect metrics directly from Kubernetes APIs and from applications running on the cluster using a variety of collection mechanisms such as exporters, agents, and sidecar containers. It's essentially an aggregator of services like DCGM, including features like alerting and notification. It also exposes an HTTP API for service for external tooling like Grafana to query and create graphs and dashboards with.

While Prometheus provides a way to store metrics and monitor our service, the metrics aren't exposed to the internals of Kubernetes. For an HPA to gain access, we will need to register yet another service to either the custom metrics API or external metrics API. By default, Kubernetes comes with the *metrics.k8s.io* endpoint that exposes resource metrics, CPU, and memory utilization. To accommodate the need to scale deployments and pods on custom metrics, two additional APIs were introduced: *custom.metrics.k8s.io* and *external.metrics.k8s.io*. There are some limitations to this setup, as currently, only one "adapter" API service can be registered at a time for either one. This limitation mostly becomes a problem if you ever decide to change this endpoint from one provider to another.

For this service, Prometheus provides the *Prometheus Adapter*, which works well, but from our experience, it wasn't designed for production workloads. Alternatively, we would recommend *KEDA*. KEDA (Kubernetes Event-Driven Autoscaling) is an open source project that provides event-driven autoscaling for Kubernetes. It offers more flexibility in terms of the types of custom metrics that can be used for autoscaling.

While Prometheus Adapter requires configuring metrics inside a ConfigMap, any metric already exposed through the Prometheus API can be used in KEDA, providing a more streamlined and friendly user experience. It also offers scaling to and from 0, which isn't available through HPAs, allowing you to turn off a service completely if there is no traffic. That said, you can't scale from 0 on resource metrics like CPU and memory and, by extension, GPU metrics, but it is useful when you are using traffic metrics or a queue to scale.

Putting this all together, you'll end up with the architecture shown in figure 6.7. Compared to

figure 6.6, you'll notice at the bottom that DCGM is managing our GPU metrics and feeding them into Prometheus Operator. From Prometheus, we can set up external dashboards with tools like Grafana. Internal to k8s, we'll use KEDA to set up a custom.metrics.k8s.io API to return these metrics so we can autoscale based on the GPU metrics. KEDA has several CRDs, one of which is a ScaledObject, which creates the HPA and provides the additional features.

While autoscaling provides many benefits, it's important to be aware of its limitations and potential problems, which are only exacerbated by LLM inference services. Proper configuration of the HPA is often an afterthought for many applications, but it becomes mission-critical when dealing with LLMs. LLMs take longer to become fully operational, as the GPUs need to be initialized and model weights loaded into memory; these aren't services that can turn on a dime, which often can cause problems when scaling up if not properly prepared for. Additionally, if the system scales down too aggressively, it may result in instances being terminated before completing their assigned tasks, leading to data loss or other problems. Lastly, flapping is just such a concern that can arise from incorrect autoscaling configurations. Flapping happens when the number of replicas keeps oscillating, booting up a new service only to terminate it before it can serve any inferences.

Summary You want Kubernetes to **add or remove Pods (and maybe nodes) based on GPU load** (e.g., how busy the GPU is, how much GPU memory is used).

- DCGM (NVIDIA): the thermometer for your GPUs. It reads GPU stats (utilization, memory used, temperature, power) and exposes them as metrics.
- Prometheus: the notebook + calculator. It scrapes (collects) those DCGM metrics and stores them so you can query/graph/alert.
- Adapter (KEDA or Prometheus Adapter): the translator for Kubernetes. It takes Prometheus metrics and exposes them to Kubernetes' autoscaling APIs so HPAs can use them.
 - By default, Kubernetes only knows basic resource metrics (CPU & memory) via metrics.k8s.io.
 - To scale on custom metrics (like GPU utilization), you must expose them via: custom.metrics.k8s.io (object-scoped) or external.metrics.k8s.io (external/global), through one adapter per API (limitation of the design).
- HPA (Horizontal Pod Autoscaler): the replica dial. It looks at a metric (e.g., GPU utilization) and scales Pods up/down.
- Cluster-level scaling (CA/NAP/Karpenter): the machine buyer. If more Pods need room, these can add nodes (and later remove them). NAP can even create new node *types* if needed.

The flow with GPUs:

- DCGM exports GPU metrics.
- Prometheus scrapes and stores them.
- KEDA (or Prometheus Adapter) publishes those metrics to Kubernetes as autoscaling metrics.

- HPA reads that metric and scales Pod replicas.
- If Pods don't fit on current nodes, Cluster Autoscaler / NAP may add nodes (and later remove them).

6.2.3 Rolling Updates

Rolling updates or rolling upgrades is a strategy that gradually implements the new version of an application to reduce downtime and maximize agility. It works by gradually creating new instances and turning off the old ones, replacing them in a methodical manner. This update approach allows the system to remain functional and accessible to users even during the update process, otherwise known as zero downtime. Rolling updates also make it easier to catch bugs before they have too much effect and rollback faulty deployments.

Rolling updates is a feature built into k8s and another major reason for its wide-spread use and popularity. Kubernetes provides an automated and simplified way to carry out rolling updates.

6.2.4 Inference Graphs

Inference graphs are the crème filling of a donut, the muffin top of a muffin, and the toppings on a pizza: they are just phenomenal. Inference graphs allow us to create sophisticated flow diagrams at inference in a resource-saving way. Consider figure 6.8, which shows us the building blocks for any inference graph.

Generally, any time you have more than one model, it's useful to consider an inference graph architecture. Your standard LLM setup is usually already at least two models: an encoder and the language model itself.

Usually, when we see LLMs deployed in the wild, these two models are deployed together. You send text data to your system, and it returns generated text. It's often no big deal, but when deployed as a sequential inference graph instead of a packaged service, we get some added bonuses. First, the encoder is usually much faster than the LLM, so we can split them up since you may only need one encoder instance for every two to three LLM instances. Encoders are so small that this doesn't necessarily help us out that much, but it saves the hassle of redeploying the entire LLM if we decide to deploy a new encoder model version. In addition, an inference graph will set up an individual API for each model, which allows us to hit the LLM and encoder separately.

This is really useful if we have a bunch of data we'd like to preprocess and save in a VectorDB; we can use the same encoder we already have deployed. We can then pull this data and send it directly into the LLM.

The biggest benefit of an inference graph is that it allows us to separate the API and the LLM. The API sitting in front of the LLM is likely to change much more often as you tweak prompts, add features, and fix bugs. The ability to update the API without having to deploy the LLM will save your team a lot of effort.

Let's now consider figure 6.9, which provides an example inference graph deployment using Seldon. In this example, we have an encoder model, an LLM, a classifier model, and a simple API that combines the results. Whereas we would have to build a container and the interface

for each of these models, Seldon creates an orchestrator that handles communication between a user’s request and each node in the graph.

Summary Don’t ship your entire AI pipeline as one big black-box service. Instead, split it into small model services and wire them together as a graph at inference time.

6.2.5 Monitoring

6.3 Production Challenges

6.3.1 Model updates and retraining

6.3.2 Load testing

6.3.3 Troubleshooting poor latency

One of the biggest bottlenecks when it comes to your model’s performance in terms of latency and throughput has nothing to do with the model itself but comes from **data transmission of the network**. One of the simplest methods to improve this I/O constraint is to **serialize the data before sending it across the wire**, which can have a large effect on ML workloads where the payloads tend to be larger, including LLMs where prompts tend to be long.

To serialize the data, we utilize a framework known as *Google Remote Procedure Call (gRPC)*. gRPC is an API protocol similar to REST, but instead of sending JSON objects, we **compress the payloads into a binary serialized format using Protocol Buffers**, also known as *protobufs*. By doing this, we can send more information in fewer bytes, which can easily give us orders of magnitude improvements in latency. Luckily, most inference services will implement gRPC along with their REST counterparts right out of the box, which is extremely convenient since the major hurdle to using gRPC is setting it up.

A major reason for this convenience is the Seldon V2 Inference Protocol, which is widely implemented. The only hurdle, then, is ensuring our client can serialize and deserialize messages to take advantage of the protocol. In listing 6.13, we show an example client using MLServer to do this. It’s a little bit more in depth than your typical curl request, but a closer inspection shows the majority of the complexity is simply converting the data from different types as we serialize and deserialize it.

6.3.4 Resource management

6.3.5 Cost engineering

Part V

Prompt Engineering

Chapter 7

Prompt Engineering

7.1 Prompting your model

7.1.1 Few-shot prompting

7.1.2 One-shot prompting

7.1.3 Zero-shot prompting

7.2 Prompt engineering basics

Part VI

A Systems View for LLMs

Chapter 8

Understanding GPUs

Chapter 9

Model Efficiency

You can understand efficiency of your deep learning regime as consisting of 3 different components.

- **Computation:** Time spent on your GPU computing actual *floating point operations per second (FLOPS)*
- **Bandwidth:** Time spent transferring tensors within a GPU
- **Overhead:** Everything else

9.1 Computation

You can't really shrink the number of operations like multiplies/adds without changing the model/algorithm (*e.g.*, smaller layers, pruning, low-rank tricks).

But you can often shrink time by reducing fewer memory trips, better packing, fusing steps, batching requests, and so on.

Hardware keeps getting faster than it speeds up IO operations. FLOPs (chef speed) roughly double quicker than memory bandwidth.

Suppose your GPU peaks at 300 TFLOPs and 1 TB/s memory bandwidth.

- To fully use 300 TFLOPs, your *kernels*¹ need 300 FLOPs per byte (roofline rule: performance $\min(\text{peak FLOPs}, \text{bandwidth} \times \text{FLOPs/byte})$).
- If your workload only does 50 FLOPs/byte, memory limits you to 50 TFLOPs no matter how beefy the chefs are—the pantry can't feed them fast enough.

What this means for LLMs (simple takeaways):

- **Prefill** (big matmuls): often compute-bound \rightarrow use mixed precision (FP8/16), fuse ops, and batch to keep math units hot.

¹A kernel is a single function the GPU runs in parallel (*e.g.*, "do this matmul," "add two tensors," "apply GELU"). Your model is a chain of many kernels.

- **Decode** (one token at a time): often memory-bound due to KV-cache reads → shrink bytes (KV quantization, MQA/GQA), fuse tiny ops, batch tokens across requests, speculative decoding to raise work per memory fetch.
- Across the board: arrange data contiguously, prefetch, use CUDA graphs/compiler, and avoid tons of micro-kernels.

9.2 Bandwidth

Bandwidth cost is the time and energy spent moving data. In deep-learning kernels, that can mean:

- CPU ↔ GPU transfers,
- Node ↔ node transfers (network),
- GPU DRAM ↔ on-chip compute (global memory ↔ registers/shared memory (SRAM)).

Our focus is on the last one. It dominates many GPU operations: moving tensors in and out of GPU DRAM ² can be far more expensive than the math itself. That’s why memory-bound kernels (little math per byte moved) often run much slower than you’d expect.

Memory bandwidth cost

Each time you launch a GPU kernel, intermediate results are typically written back to global memory and read again by the next kernel and it is called memory bandwidth cost. If each step does only a tiny bit of math, you’re mostly paying for reads/writes and these operations are called *memory-bound operations*.

9.2.1 Kernel Fusion (Operator Fusion)

Kernel fusion (or Operator fusion) combines multiple ops so intermediates stay on-chip instead of bouncing to DRAM. That cuts global reads/writes and lifts you out of the memory-bound regime.

²`nvidia-smi` shows up GPU’s DRAM, and DRAM is the primary resource of causing CUDA Out of Memory errors.

Point-wise operation example

Point-wise operation refers to an operation that each output element depends only on the corresponding input element, with no interaction across elements.

There are 4 global accesses.

```
1 x1 = x.cos()    # read x,   write x1
2 x2 = x1.cos()  # read x1,  write x2
```

With fusion (2 global accesses total):

```
1 x2 = x.cos().cos() # read x once, write x2 once
```

Cutting global traffic like this is often close to a $2\times$ speedup for simple pointwise chains. In `x.cos()`, for every index `i`, the kernel computes `y[i] = cos(x[i])`. There's no neighborhood, no reduction, no matrix multiply - each element is handled in isolation. Let's consider a simple example:

In short, kernel fusion do several steps in one pass. Instead of: “do op A \rightarrow write result to memory \rightarrow read it back \rightarrow do op B”, we combine them so data stays on-chip while we keep computing. That avoids slow trips to (global) memory.

Most kernels are limited by memory bandwidth, not raw FLOPs. If we don't have to write/read intermediates, we save bandwidth and time. That's why two separate PyTorch ops are a chance to fuse and speed things up.

One of counterintuitive observation is that the computational costs of `x.cos().cos()` and `x.cos()` are similar once fused. This is because, the expensive part is often moving `x` through memory. If you keep the value in registers and apply `cos` twice before writing, the extra math is tiny compared to the avoided memory traffic. This is also why GELU vs ReLU are closer in runtime than you'd expect: after fusion, both mostly cost the same memory movement.

There are a couple of caveats that make this a bit tricky.

1. The GPU needs to know what's going to happen next when performing the current operation. So, you can't do this optimization in eager-mode, where PyTorch runs operators one operation at a time.
2. We actually need to generate CUDA code for this, which opens up a whole new can of worms.

Example

Think of two "speed limits" on a GPU:

1. Memory bandwidth — how fast you can move data to/from global memory.
2. Compute throughput — how fast you can do math.

On an A100:

- Bandwidth $\approx 1.5 \text{ TB/s} = 1.5 \times 10^{12} \text{ bytes/s}$.
- Compute $\approx 19.5 \text{ TFLOP/s} = 19.5 \times 10^{12} \text{ float ops/s}$.
- A float32 is 4 bytes.

We can only read: $1.5 \times 10^{12} \text{ bytes/s} / 4 \text{ bytes} \approx 375 \text{B numbers/s}$.

For something like $y = 2 \times x$, each element:

- read 4 bytes (x),
- write 4 bytes (y).
- Total 8 bytes per element.

So max elements/s $\approx 1.5 \times 10^{12} / 8 = 187.5 \text{B elems/s}$.

This operations is memory-bound. Each element does $\approx 1 \text{ flop}$ (a multiply). If you can process at most 187.5B elems/s, that's $\approx 187.5 \text{GFLOP/s}$. This is tiny compared to 19.5 TFLOP/s. The math units are mostly waiting on memory.

To use the GPU's compute fully, you need high *arithmetic intensity* ^a (many flops per byte), *e.g.*, matrix multiplications.

^ahow much math you do per byte of data moved from main memory.

9.3 Overhead

Overhead is everything that isn't real math or moving tensors. For example, time spent in the Python interpreter? Overhead. Time spent in the PyTorch framework? Overhead. Time spent launching CUDA kernels.

This is a problem since, GPUs are insanely fast. If the GPU can do hundreds of trillions of FLOPs per second but Python can only do tens of millions, then any time you spend in Python (or framework layers) is like idling a rocket engine at a red light. For tiny ops, the setup time dominates; the math itself is over in a blink.

If you do lots of small ops (*e.g.*, add a few numbers many times), you pay the overhead each time. The GPU's compute is barely used, so your speed is capped by Python/framework/kernal-launch overhead, not by hardware.

Practical fixes (what to do):

- Batch work / make tensors bigger. Fewer, larger ops amortize overhead.
- Fuse ops. Do more math per read/write (*e.g.*, fuse activation, bias, scale).

- Vectorize in Python. Replace Python loops with tensor ops; avoid per-element Python.
- Use `torch.compile` (PyTorch 2+). Lets the compiler capture graphs, fuse, and lower overhead.
- Prefetch/async where possible. Overlap transfers and compute.
- If CPU-bound and tiny arrays: consider NumPy or even C++ for critical loops.
- Custom kernels (*e.g.*, Triton/CUDA) when patterns are regular and hot.

Part VII

LLM Inference

Chapter 10

Understanding LLM Inference

Most widely used decoder-only LLMs (*e.g.*, GPT) are trained with a causal language modeling objective—effectively, next-token prediction. Given an input token sequence, they generate the continuation autoregressively until a stopping criterion is reached (*e.g.*, a maximum length) or a special `<END>` token is produced. The inference process naturally splits into two stages: (i) the *prefill* phase, which reads users inputs and (ii) the *decode* phase, which generates responses.

Tokens. Tokens are the smallest units the model consumes. A common rule of thumb is that one token corresponds to roughly four English characters (the exact ratio depends on the tokenizer). Text is always tokenized before entering the model.

10.1 Prefill Phase

During prefill, the model ingests the entire input sequence (*e.g.*, user/system prompt) and constructs the attention memory—namely the keys and values, often called the *KV cache*—to be reused during generation. Because the full input is available from the start, this stage parallelizes well: it resembles a matrix–matrix workload and typically drives the GPU close to peak utilization.

10.2 Decoding Phase

Decoding then emits output one token at a time. Each new token must attend to all tokens seen so far (the original prompt plus previously generated outputs), which makes this step inherently sequential. At each step, the computation behaves more like matrix–vector multiplication and generally uses the GPU less efficiently than prefill.

For every token produced, the model must *fetch* a substantial portion of the KV cache from GPU memory. As the context grows, the data transferred per step increases, so latency is governed more by memory bandwidth than by raw compute—decoding is thus *memory-bound*.

Intuition. Imagine typing an answer character by character, but before each keystroke you skim all prior notes to remain consistent. The typing (compute) is quick; the skimming (memory

access) is what slows you down.

For instance, with a 1,000-token prompt, generating 200 tokens means token #1 attends over roughly 1,000 tokens, while token #200 attends over roughly 1,200 tokens.

Because decoding is the usual bottleneck, many inference optimizations focus here: more efficient attention mechanisms, improved KV-cache handling (*e.g.*, paging, quantization, head sharing), and strategies such as speculative or look-ahead decoding that reduce sequential work.

10.3 Batching

The simplest way to improve GPU utilization, and effectively throughput, is through batching. Since multiple requests use the same model, the memory cost of the weights is spread out. Larger batches getting transferred to the GPU to be processed all at once will leverage more of the compute available.

Batch sizes, however, can only be increased up to a certain limit, at which point they may lead to a memory overflow. To better understand why this happens requires looking at key-value (KV) caching and LLM memory requirements.

Traditional batching (also called static batching) is suboptimal. This is because for each request in a batch, the LLM may generate a different number of completion tokens, and subsequently they have different execution times. As a result, all requests in the batch must wait until the longest request is finished, which can be exacerbated by a large variance in the generation lengths. There are methods to mitigate this, such as in-flight batching, which will be discussed later.

10.4 KV-Caching

One common optimization for the decode phase is *KV caching*. The decode phase generates a single token at each time step, but each token depends on the key and value tensors of all previous tokens (including the input tokens' KV tensors computed at prefill, and any new KV tensors computed until the current time step).

To avoid recomputing all these tensors for all tokens at each time step, it's possible to cache them in GPU memory. Every iteration, when new elements are computed, they are simply added to the running cache to be used in the next iteration. In some implementations, there is one KV cache for each layer of the model.

10.5 LLM memory requirement

In effect, the two main contributors to the GPU LLM memory requirement are model weights and the KV cache:

- **Model weights:** Memory is occupied by the model parameters. As an example, a model with 7 billion parameters (such as Llama 2 7B), loaded in 16-bit precision (FP16 or BF16) would take roughly $7\text{B} \times \text{sizeof}(\text{FP16}) \approx 14\text{ GB}$ in memory.

- **KV caching:** Memory is occupied by the caching of self-attention tensors to avoid redundant computation.

With batching, the KV cache of each of the requests in the batch must still be allocated separately, and can have a large memory footprint. The formula below delineates the size of the KV cache, applicable to most common LLM architectures today.

$$\begin{aligned} \text{Size of KV cache per token in bytes} = \\ 2 \times (\text{n_layers}) \times (\text{n_heads} \times \text{dim_head}) \times (\text{precision_in_bytes}) \end{aligned}$$

- The first factor of 2 accounts for the K and V matrices.
- Commonly, the value of $(\text{num_heads} \times \text{dim_head})$ is equal the `hidden_size` (or dimension of the model, `d_model`) of the transformer. These model attributes are commonly found in model cards or associated config files.

This memory size is required for each token in the input sequence, across the batch of inputs.

For example, with a Llama2 7B model in 16-bit precision and a batch size of 1, the size of the KV cache will be $1 \times 4096 \times 2 \times 32 \times 4096 \times 2$ bytes, where 4096 is the sequence length. In sum, it takes around 2 GB.

Managing this KV cache efficiently is a challenging endeavor. Growing linearly with batch size and sequence length, the memory requirement can quickly scale. Consequently, it limits the throughput that can be served, and poses challenges for long-context inputs. This is the motivation behind several optimizations featured.

10.6 Scaling up LLMs with model parallelization

One way to reduce the per-device memory footprint of the model weights is to distribute the model over several GPUs. Spreading the memory and compute footprint enables running larger models, or larger batches of inputs. Model parallelization is a necessity to train or infer on a model requiring more memory than available on a single device, and to make training times and inference measures (latency or throughput) suitable for certain use cases. There are several ways of parallelizing the model based on how the model weights are split.

- Pipeline parallelism
- Tensor parallelism
- Sequence parallelism

10.6.1 Pipeline parallelism

Pipeline parallelism involves sharding the model (vertically) into chunks, where each chunk comprises **a subset of layers that is executed on a separate device**.

The main limitation of this method is that, due to the sequential nature of the processing, some devices or layers may remain idle while waiting for the output (activations, gradients) of previous layers. This results in inefficiencies or *pipeline bubbles* in both the forward and backward passes.

10.6.2 Tensor Parallelism

Tensor parallelism involves sharding (horizontally) individual layers of the model into smaller, independent blocks of computation that can be executed on different devices. Attention blocks and multi-layer perceptron (MLP) layers are major components of transformers that can take advantage of tensor parallelism. In multi-head attention blocks, each head or group of heads can be assigned to a different device so they can be computed independently and in parallel.

10.6.3 Sequence Parallelism

Tensor parallelism has limitations, as it requires layers to be divided into independent, manageable blocks. It's not applicable to operations like LayerNorm and Dropout, which are instead replicated across the tensor-parallel group. While LayerNorm and Dropout are computationally inexpensive, they do require a considerable amount of memory to store (redundant) activations.

Sequence parallelism (SP) splits work along the sequence length dimension across multiple GPUs. Instead of every GPU holding all tokens of each sequence, each GPU holds a slice of tokens (*e.g.*, tokens 0–255 on GPU0, 256–511 on GPU1). It's usually used together with tensor/model parallelism to cut activation memory and enable longer context or larger batches.

10.7 Optimizing the attention mechanism

- Multi-head attention
- Multi-query attention
- Grouped-query attention
- Flash attention

10.8 Model optimization techniques

10.8.1 Quantization

Quantization is the process of reducing the precision of a model's weights and activations. Most models are trained with 32 or 16 bits of precision, where each parameter and activation element takes up 32 or 16 bits of memory—a single-precision floating point. However, most deep learning models can be effectively represented with eight or even fewer bits per value.

Reducing the precision of a model can yield several benefits. If the model takes up less space in memory, you can fit larger models on the same amount of hardware. Quantization also means you can transfer more parameters over the same amount of bandwidth, which can help to accelerate models that are bandwidth-limited.

There are many different quantization techniques for LLMs involving reduced precision on either the activations, the weights, or both. It's much more straightforward to quantize the weights because they are fixed after training. However, this can leave some performance on the table because the activations remain at higher precisions. GPUs don't have dedicated hardware for

multiplying INT8 and FP16 numbers, so the weights must be converted back into a higher precision for the actual operations.

It's also possible to quantize the activations, the inputs of transformer blocks and network layers, but this comes with its own challenges. Activation vectors often contain outliers, effectively increasing their dynamic range and making it more challenging to represent these values at a lower precision than with the weights.

One option is to find out where those outliers are likely to show up by passing a representative dataset through the model, and choosing to represent certain activations at a higher precision than others (LLM.int8()). Another option is to borrow the dynamic range of the weights, which are easy to quantize, and reuse that range in the activations.

10.8.2 Sparsity

Similar to quantization, it's been shown that many deep learning models are robust to pruning, or replacing certain values that are close to 0 with 0 itself. Sparse matrices are matrices where many of the elements are 0. These can be expressed in a condensed form that takes up less space than a full, dense matrix.

GPUs in particular have hardware acceleration for a certain kind of structured sparsity, where two out of every four values are represented by zeros. Sparse representations can also be combined with quantization to achieve even greater speedups in execution. Finding the best way to represent large language models in a sparse format is still an active area of research, and offers a promising direction for future improvements to inference speeds.

10.8.3 Distillation

10.9 Model Serving Techniques

10.9.1 In-Flight Batching

10.9.2 Speculative inference

Chapter 11

Flash Attention

- Fast — excerpt from the paper: "We train BERT-large (seq. length 512) 15
- Memory-efficient — compared to vanilla attention, which is quadratic in sequence length, $O(N^2)$, this method is sub-quadratic/linear in N ($O(N)$). We'll see later why how.
- Exact — meaning it's not an approximation of the attention mechanism (like *e.g.*, sparse, or low-rank matrix approximation methods) — its outputs are the same as in the "vanilla" attention mechanism.
- IO aware — compared to vanilla attention, flash attention is sentient.

Over the years GPUs have been adding compute capacity (FLOPS) at a faster pace than increasing the memory throughput (TB/s).

It doesn't matter if you can compute at exaFLOPS speeds if there is no data to be processed. These 2 need to be closely aligned, and since the hardware lost that balance we have to make our software compensate for it.

We argue that a missing principle is making attention algorithms IO-aware – accounting for reads and writes between levels of GPU memory.

That is, modern GPUs have several types of memory:

- SRAM – fast, on-chip, small
- HBM – slower than SRAM, large size. That's what we usually address as GPU memory.

To conduct computation, data must be transferred from HBM to SRAM, and this transfer is not overhead-free!

The Flash Attention algorithm proposes a method of computing attention in tiles, without explicitly materializing the attention scores tensor. Here, materializing a matrix means that at any given time, the matrix exist in its full shape in memory.

It's easy to see that this matrix requires $O(n^2)$ of memory to store. For large sequence lengths, that's a lot of data. So, if we manage to avoid explicitly materializing this matrix, we can save lots of memory.

However, this matrix is necessary for transformer training as it is a part of backpropagation and gradient calculation. The authors propose that it's better to recalculate this matrix during the backward pass (again without explicit materialization). Not only does this save lots of memory, but it also provides huge speedups as we don't need to transfer this enormous matrix between different GPU memory types.

Overall, such an approach did not only speed up calculations by taking GPU I/O specifics into account, but also allowed processing huge sequence lengths as memory complexity drops to $O(n)$.

In sum,

- Load a small block of Q and K into SRAM.
- Compute just that block of scores ($Q \cdot K$).
- Do a streaming softmax: keep a running max and sum so softmax stays numerically stable without needing all tokens at once.
- Immediately apply that softmax block to the matching V block and accumulate partial outputs.
- Move to the next tile. When all tiles are processed, you already have the final output—no big attention matrix ever stored.

This is called an IO-aware algorithm: it minimizes slow memory traffic and maximizes use of the GPU's fast memory.

What attention normally does (and why it's slow)

Given per-head matrices:

- $Q \in \mathbb{R}^{N \times d}, K \in \mathbb{R}^{N \times d}, V \in \mathbb{R}^{N \times d_v}$
- Scores: $S = \frac{QK^\top}{\sqrt{d}}$ (size $N \times N$)
- Output: $O = \text{softmax}(S)V$

Naive kernels materialize S (size (N^2)), apply softmax row-wise, then multiply by V . Problem: writing/reading (N^2) scores to HBM (GPU DRAM) is *memory-bound* and explodes memory as N grows (e.g., $4k$ tokens $\rightarrow 16M(4k^2)$ scores per head).

The core idea of FlashAttention is to compute over tile with stream and never form S in HBM. In other words, do attention in tiles that fit in on-chip SRAM to minimize HBC traffic, and keep only tiny per-row summaries in HBM. For each tile:

1. Load a block of Q and a block of K, V into SRAM.
2. Compute partial scores $S_{\text{blk}} = Q_{\text{blk}}K_{\text{blk}}^\top/\sqrt{d}$.
3. Apply a streaming softmax update so you don't need the whole row at once.
4. Immediately multiply by V_{blk} and accumulate partial outputs for that row block.
5. Move to the next block of K/V and repeat.

11.1 The streaming (online) softmax trick

For one output row i (one query token), the softmax over all keys $j = 1 \dots N$ is:

$$o_i = \sum_{j=1}^N \frac{e^{s_{ij}}}{\sum_{k=1}^N e^{s_{ik}}} v_j, \quad s_{ij} = \frac{q_i \cdot k_j}{\sqrt{d}} + \text{mask/bias}.$$

We process keys in chunks (*i.e.*, tiles). Maintain per-row running stats:

- m_i : running max score seen so far (for numerical stability)
- ℓ_i : running sum of exp-shifted scores, *i.e.*, $\ell_i = \sum e^{s_{ij}-m_i}$
- z_i : running weighted sum of values, $z_i = \sum e^{s_{ij}-m_i} v_j$

When you see a new block with per-row block max $m_i^{\text{blk}} = \max_j s_{ij}^{\text{blk}}$ and sums

- $\ell_i^{\text{blk}} = \sum_j e^{s_{ij}^{\text{blk}}-m_i^{\text{blk}}}$,
- $z_i^{\text{blk}} = \sum_j e^{s_{ij}^{\text{blk}}-m_i^{\text{blk}}} v_j$,

update with running stats:

$$\begin{aligned} m_i^{\text{new}} &= \max(m_i, m_i^{\text{blk}}), \\ \ell_i^{\text{new}} &= \ell_i e^{m_i - m_i^{\text{new}}} + \ell_i^{\text{blk}} e^{m_i^{\text{blk}} - m_i^{\text{new}}}, \\ z_i^{\text{new}} &= z_i e^{m_i - m_i^{\text{new}}} + z_i^{\text{blk}} e^{m_i^{\text{blk}} - m_i^{\text{new}}}. \end{aligned}$$

At the end of all blocks:

$$o_i = \frac{z_i}{\ell_i}.$$

classic log-sum-exp fusion with dynamic max shifting keeps numbers well-scaled without needing all s_{ij} at once.

Example

- scores (two tiles): $s = [1, 3|0, 2]$
- 2-D values:
 - $(v_1 = [1, 0])$
 - $(v_2 = [0, 2])$
 - $(v_3 = [-1, 1])$
 - $(v_4 = [3, 1])$

Define $a = e^{-2} \approx 0.135335$, $b = e^{-1} \approx 0.367879$.

- **Tile 1:** $[1, 3]$ with $[v_1, v_2]$

- block max: $m^{\text{blk}} = 3$
- block sums (shift by m^{blk}):

$$\ell^{\text{blk}} = e^{1-3} + e^{3-3} = a + 1$$

$$z^{\text{blk}} = av_1 + 1 \cdot v_2 = a[1, 0] + [0, 2] = [a, , 2]$$

- merge into running stats (start from $m = -\infty, \ell = 0, z = 0$):

$$m \leftarrow 3, \quad \ell \leftarrow a + 1, \quad z \leftarrow [a, 2].$$

- **Tile 2:** $[0, 2]$ with $[v_3, v_4]$

- block max: $m^{\text{blk}} = 2$
- block sums:

$$\ell^{\text{blk}} = a + 1, \quad z^{\text{blk}} = av_3 + 1 \cdot v_4 = a[-1, 1] + [3, 1] = [3 - a, 1 + a].$$

- merge (global max stays $m^{\text{new}} = \max(3, 2) = 3$):

$$\ell \leftarrow \ell \cdot e^{3-3} + \ell^{\text{blk}} \cdot e^{2-3} = (a + 1) + (a + 1), b \approx \boxed{1.55300179}$$

$$z \leftarrow z \cdot e^{3-3} + z^{\text{blk}} \cdot e^{2-3} = [a, 2] + b[3 - a, 1 + a] \approx \boxed{[1.18918654, 2.41766651]}.$$

- **Finalize** (elementwise divide by scalar ℓ)

$$o = \frac{z}{\ell} \approx \left[\frac{1.18918654}{1.55300179}, \frac{2.41766651}{1.55300179} \right] = \boxed{[0.76573417, 1.55676994]}.$$

- **Sanity check** (plain softmax on all 4 keys) Weights from $s = [1, 3, 0, 2]$ are $\approx [0.08714, , 0.64391, , 0.03206, , 0.23688]$.

$$\begin{aligned} \sum_j w_j v_j &= 0.08714[1, 0] + 0.64391[0, 2] + 0.03206[-1, 1] + 0.23688[3, 1] \\ &= [0.76573417, 1.55676994], \end{aligned}$$

which matches the streaming result exactly.

Part VIII

Parallelism

Chapter 12

Data Parallelism

12.1 Data Parallel

The first step of the typical training loop for deep learning models is to split a dataset into batches so that we can feed them into the model and compute gradients corresponding to them. As the model size grows up, we couldn't fit the model into a single GPU. The *data parallelism* tries to tackle the issue by clone the model across multiple GPUs so that each GPU can take a small portion of the batches for each iteration. Data Parallel (sometimes referred to as “single-node data parallel”) is typically used when you have **multiple GPUs on a single machine**.

Let's say the batch size is 10 and we have 5 GPUs. Then, each GPU takes 2 batches and calculate gradients by on its own. The calculated gradients are then synchronized across the GPUs pretending they are computed on a single GPU. Finally, the synchronized gradient information is going to be distributed to them.

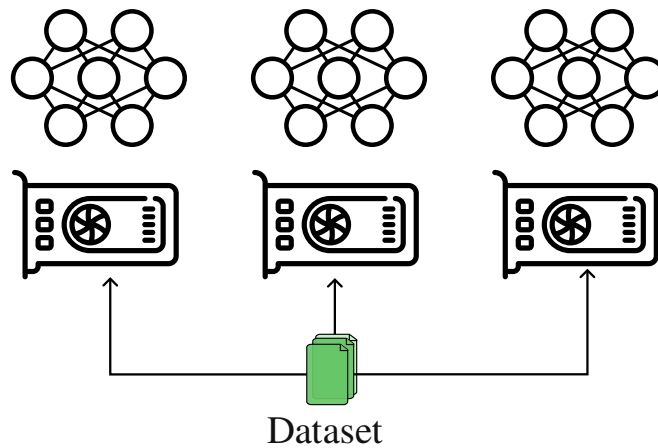
There are some important things to mention:

1. One process (or master thread) becomes a bottleneck for gradient aggregation and parameter updates.
2. As you increase the number of GPUs, or try to involve multiple machines, communication overhead grows significantly and can slow down training.
3. Each GPU holds a copy of the entire model, which can be large.

12.2 Distributed Data Parallel

To alleviate such issues, we can adopt an approach called *Distributed Data Parallel* (DDP), which is designed to scale training across many GPUs, potentially across multiple machines (nodes). Modern deep learning frameworks (like PyTorch `torch.nn.parallel.DistributedDataParallel`) typically recommend DDP as the best practice for multi-GPU/multi-node training due to better performance and scalability. During backpropagation, gradients are shared among GPUs through efficient communication primitives, resulting in synchronized model parameters across all GPUs.

Key benefits:



- Scalability: You can increase the number of GPUs (and even add more machines) to handle large datasets and bigger models.
- Performance: DDP typically provides better performance than older methods like `NN.DATAPARALLEL` (in PyTorch) because it uses *all-reduce* and eliminates the single “master” bottleneck.
- Flexibility: You can combine DDP with other parallelization strategies (*e.g.*, model parallel, sharded data parallel, pipeline parallel) if needed.

12.2.1 Concepts and Terminology

All-Reduce is a collective communication operation commonly used in distributed computing (especially in high-performance computing and deep learning). In simple terms:

- Each process (or GPU) starts with its own data (*e.g.*, local gradients).
- These data are combined (usually via a reduction operation like sum, mean, min, or max) across all processes.
- The result of that reduction (*e.g.*, the summed gradients) is then shared back so that every process receives the same reduced value.
- Hence the name: “all” (everyone gets the result) + “reduce” (combine data).

Basic Terms:

- World Size: The total number of processes engaged in the distributed job. Often, we run one process per GPU, so world size is the number of GPUs.
- Rank: A unique integer ID assigned to each process. Ranks typically range from 0 to `world_size - 1`. Rank 0 is often referred to as the “leader” or “master” process, but in DDP, every process does roughly the same work.
- Local Rank: When multiple GPUs reside on a single node, local rank identifies which GPU a specific process is mapped to on that local machine (*e.g.*, 0 for the first GPU, 1 for the second, etc.).

- Backend: The communication backend used for synchronization (*e.g.*, nccl). For GPU training, NCCL is typically recommended because it's optimized for high-performance GPU-to-GPU communication.
- Initialization Method: Describes how processes connect with each other (*e.g.*, a TCP store, a file-based store). This allows all processes to know who's who in the cluster.

12.2.2 How DDP Works Under the Hood

1. Process Per GPU: Each GPU runs the same script in its own process.
2. Data Subset: A DistributedSampler ensures that each process sees a unique subset of data. This prevents overlap in data usage among GPUs.
3. Full Model Copy: Each GPU has a full replica of the model in memory.
 - For massive models, consider *Sharded DDP* (*e.g.*, PyTorch's FSDP or DeepSpeed ZeRO) to split parameters across GPUs.
4. All-Reduce Gradient Sync: After backprop, gradients are summed (or averaged) across processes with an all-reduce operation. This keeps all models in sync.

Chapter 13

Pipeline Parallelism

13.1 Introduction

The basic idea of the data parallel is to distribute the model across GPUs. However, if the model size is bigger than the VRAM of GPU, the model wouldn't fit in a single GPU. To resolve the issue, we have to split the model across GPUs. For instance, we can put the half of the model into the first GPU and the remaining half into the second GPU. This approach is often called *model parallelism*. Let's closely look at one of the model parallelism approaches, called *pipeline parallelism*.

Pipeline Parallelism is a strategy for distributing large deep learning models across multiple devices (GPUs) by splitting the model layers into sequential stages. Rather than replicating the entire model on each GPU or sharding the parameters themselves, pipeline parallelism assigns a subset of layers to each device in a pipeline-like fashion. This technique is especially helpful when:

- The model is too large to fit on a single GPU, but it can be split into chunks (layers/stages).
- You want to keep multiple GPUs actively working on different portions (stages) of the forward and backward pass concurrently.

13.1.1 Illustration of the Pipeline

In pipeline parallelism, the model is divided into N sub-networks, and each sub-network is placed on a different GPU (or sometimes on multiple GPUs if you have many layers). Think of it like an assembly line:

- Sub-Network 1: Layers $1 \sim k$
- Sub-Network 2: Layers $(k + 1) \sim m$
- Sub-Network 3: Layers $(m + 1) \sim \dots$
- and so on.

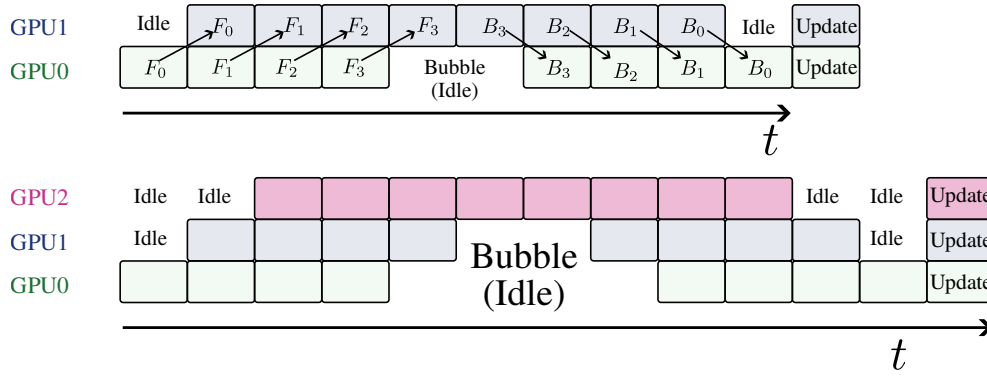


Figure 13.1: The Illustration of the pipeline parallel on two GPUs. As you can see the *bubble* (*i.e.*, underutilization) tends to grow as we increase the number of GPUs. It updates once at the end.

The input minibatch is then split into smaller micro-batches (smaller pieces of data), which flow sequentially through these sub-networks. In other words, the micro-batch is the basic unit of the input to the pipeline parallelism.

- While Stage 1 is processing the next micro-batch, Stage 2 can concurrently work on the intermediate outputs from Stage 1's previous micro-batch.

On each stage, for each microbatch that backpropagates through that stage's layers, the stage adds the microbatch gradients into its local grad buffers:

$$\text{grads_stage} += \text{dLoss/dParam (microbatch k)}$$

Mixed precision usually applies loss scaling before accumulation.

Example: Imagine a 2-stage pipeline parallel setup (for simplicity):

- GPU 0: Holds Layers 1–3
- GPU 1: Holds Layers 4–6

If you have a batch of data with 32 samples, you might split it into 4 micro-batches of size 8 each. Then, forward Pass can be processed as follows:

1. Micro-Batch 1
 - (a) Step A: GPU 0 processes layers 1–3 for micro-batch 1.
 - (b) Step B: Once GPU 0 is done with those layers, it sends the activations for micro-batch 1 over to GPU 1.
 - (c) Step C: GPU 1 then processes layers 4–6 for micro-batch 1.
2. Micro-Batch 2

- (a) As soon as GPU 0 finishes Step A for micro-batch 1 and passes the data to GPU 1, GPU 0 is free to start micro-batch 2 (layers 1–3).
 - (b) Meanwhile, GPU 1 is busy processing micro-batch 1 (layers 4–6).
 - (c) Once GPU 0 finishes its part for micro-batch 2, it sends those activations to GPU 1—which will be ready to handle them as soon as it’s done with micro-batch 1.
3. Micro-Batch 3 and 4
- (a) This pattern continues in an overlapping fashion: while GPU 1 is busy with micro-batch 2, GPU 0 can start on micro-batch 3, and so on.

The key benefit is concurrency:

- While GPU 0 is processing micro-batch 2, GPU 1 can process micro-batch 1.
- This overlap leads to higher GPU utilization.

Backward pass is a bit more complex because:

- You need gradient signals to flow in the reverse order of the forward pipeline.
- Each stage waits until it receives the gradient from the next stage before it can compute its own local gradients and pass them back to the previous stage.

However, the overall concept is similar—multiple stages can run backprop (on different micro-batches) in parallel, thereby keeping all GPUs busy.

13.1.2 Pipeline Bubbles

When using pipeline parallelism, you often hear about *pipeline bubbles* (or underutilization). This refers to idle times on some GPUs before the assembly line is fully loaded or after it starts to wind down.

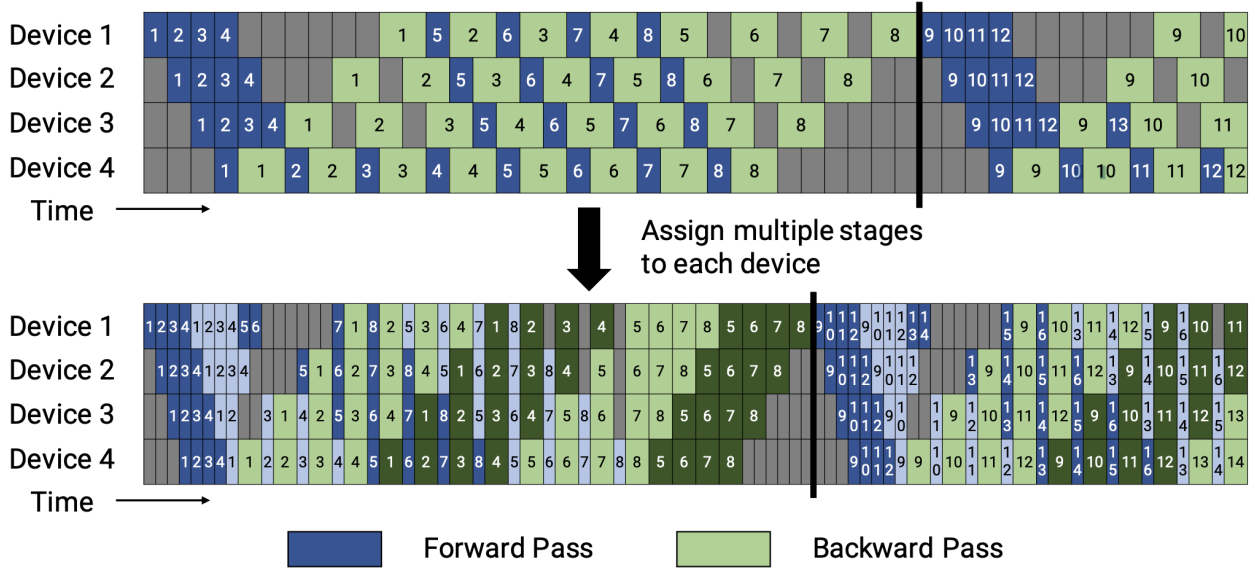
- Start-up Bubble: In the very beginning, GPU 1 must wait until GPU 0 finishes the first forward pass for micro-batch 1. GPU 1 sits idle during that initial delay.
- Wind-down Bubble: After the last micro-batch enters GPU 0, GPU 1 continues to process the pipeline while GPU 0 is idle.

The percentage of idle can be computed as follows:

$$\frac{1 - m}{m + n - 1},$$

where m is the number of microbatches and n is the number of GPUs.

These bubbles can lead to less-than-ideal speedups, but you can mitigate them by using enough micro-batches to keep the pipeline busy most of the time.



13.2.2 Interleaved Schedule

This schedule requires the number of microbatches to be an integer multiple of the stage of pipeline. In this schedule, each device can perform computation for multiple subsets of layers(called a model chunk) instead of a single contiguous set of layers. *i.e.*, Before device 1 had layer 1-4; device 2 had layer 5-8; and so on. But now device 1 has layer 1,2,9,10; device 2 has layer 3,4,11,12; and so on. With this scheme, each device in the pipeline is assigned multiple pipeline stages and each pipeline stage has less computation. This mode is both memory-efficient and time-efficient.

13.3 Zero Bubble

Chapter 14

Tensor Parallelism

14.1 Introduction

Let's go over an example:

- x is a row vector of shape $[1, d_{\text{in}}]$ (the input).
- W is a weight matrix of shape $[d_{\text{in}}, d_{\text{out}}]$.
- output is $[1, d_{\text{out}}]$.

We have two GPUs, GPU 0 and GPU 1. We want to split (shard) the weight matrix W across two GPUs. One common approach is column parallelism:

- GPU 0 holds columns $[0, 1]$
- GPU 1 holds columns $[2, 3]$

This means each GPU stores some columns of W . Let's denote:

$$W = [W_{\text{left}} \mid W_{\text{right}}]$$

where

- W_{left} is a 4×2 matrix on GPU 0,
- W_{right} is a 4×2 matrix on GPU 1.

In numeric form, suppose

$$W = \begin{bmatrix} 1 & 2 & 5 & 6 \\ 3 & 4 & 7 & 8 \\ 2 & 0 & 3 & 1 \\ -1 & 4 & 8 & 2 \end{bmatrix}.$$

Then, for column parallel:

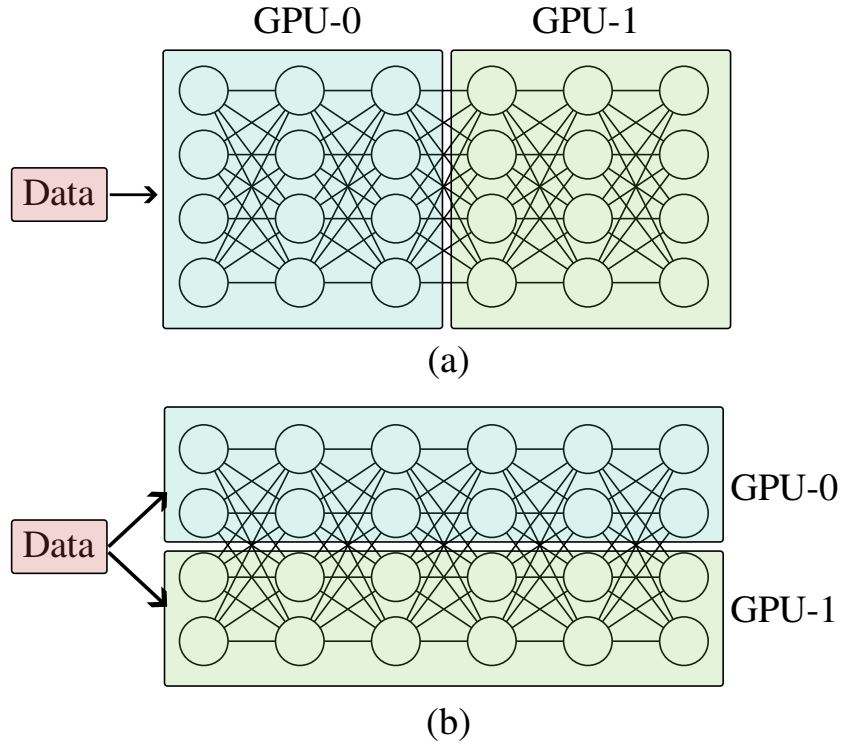


Figure 14.1: (a): Pipeline parallelism. (b) Tensor parallelism.

- GPU 0:

$$W_{\text{left}} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 2 & 0 \\ -1 & 4 \end{bmatrix}.$$

- GPU 1:

$$W_{\text{right}} = \begin{bmatrix} 5 & 6 \\ 7 & 8 \\ 3 & 1 \\ 8 & 2 \end{bmatrix}.$$

Given the input

$$x = [1, 2, 0, 1].$$

We can treat x as a row vector $[1, 4]$. For column parallelism, each GPU needs the entire input x so it can multiply by its subset of columns:

- We copy the x to both GPU 0 and GPU 1.
 - This is typically a small overhead compared to storing large weight matrices.
- Then, compute the matrix multiplications for each matrix.
- Finally, concatenate the outputs.

$$\text{output} = [\text{partial}_0 \mid \text{partial}_1] = [6, 14, 27, 24].$$

- Some frameworks do a ring-all-gather, or they might place this final output on one GPU if needed, etc.

When we do backprop, we can update the model's parameters in the opposite direction.

In Megatron-LM, all Transformer layers, except normalization layer, are using row or column parallelism.

Tensor parallelism can be costly primarily due to the significant communication overhead involved when distributing large model layers across multiple GPUs, requiring frequent data exchange between devices which can become a bottleneck, especially when dealing with very large models and limited network bandwidth; this communication cost often outweighs the benefits of parallel computation, making it a major drawback of tensor parallelism.

Chapter 15

N-Dim Parallelism

Chapter 16

DualPipe

16.1 Introduction

16.1.1 All-to-All vs Point-to-Point

When orchestrating multiple GPUs, we need them to communicate with each other to share information like gradients and model parameters. There are two main types of communication patterns:

1. All-to-all communication.
2. Point-to-point communication.

All-to-all communication involves every GPU in the system simultaneously exchanging data with all other GPUs. The canonical analogy is a group chat where everyone needs to share their updates with everyone else. All-to-all communication is expensive and involves a ton of communication overhead. There are several clever algorithms like ring-AllReduce that can reduce this overhead, but it's still often a bottleneck.

Point-to-point communication, on the other hand, is a communication between just two GPUs (the analogy here is a private conversation). One GPU sends data directly to another specific GPU without involving the rest of the system. This is much more efficient in terms of network bandwidth and latency. In practice, point-to-point communication is strongly preferred when possible because it's significantly cheaper in terms of computational resources.

16.2 DualPipe

Finer-Grained stages: divide each chunk into 4 components:

- Attention,
- All-to-all dispatch(Handles communication between devices),
- MLP(Multi-Layer Perceptron),



Figure 16.1: An illustration of dualpipe.

- All-to-all combine(merge output across devices).

For a backward chunk, the attention and MLP split further into two parts: backward for input(B) and backward for weights(W) like Zero Bubble.

Bidirectional pipeline scheduling which feeds micro-batches from both ends of the pipeline simultaneously and a significant portion of communications can be fully overlapped (See the 2 black arrows in following diagram). In order to support bidirectional pipeline scheduling, DualPipe requires keeping two copies of the model parameters. If we have 8 devices with a 8 layers model, in the Zero Bubble Schedule, each device has a corresponding layer. But in the DualPipe Schedule, in order to handle bidirectional pipeline, the device 0 should have model's layer0 and layer7, and the device 7 should have model's layer7 and layer0.

Part IX

Compression

Chapter 17

Model Compression

17.1 Introduction

haha

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