Profiling & Optimization

Week 13 · CS 203: Software Tools and Techniques for AI

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The Performance Problem

Training is expensive:

- GPT-3 cost ~$4.6M to train
- LLaMA-65B: ~$2-3M in compute
- Even small models can burn through credits

Inference at scale is costly:

- ChatGPT serves millions of requests/day
- 100ms latency improvement = $1M+ savings/year

Developer time is expensive:

- Slow iteration cycles reduce productivity
- 10 min/epoch → 100 epochs = 16+ hours waiting

Goal: Make code faster and more efficient without sacrificing accuracy.

The Optimization Mindset

Donald Knuth's wisdom:

> "Premature optimization is the root of all evil. Yet we should not pass up our opportunities in that critical 3%."

The correct process:

1. **Make it work** (correctness first)
2. **Make it right** (clean code, tests)
3. **Profile to find bottlenecks** (measure, don't guess!)
4. **Make it fast** (optimize the 3% that matters)

Common mistake: Optimizing code that runs once during initialization while ignoring the training loop that runs millions of times.

Performance Metrics Overview

Training metrics:

- **Throughput**: Samples/second, batches/second
- **Epoch time**: Total time to process entire dataset
- **GPU utilization**: % of time GPU is actively computing
- **Memory usage**: Peak memory allocated

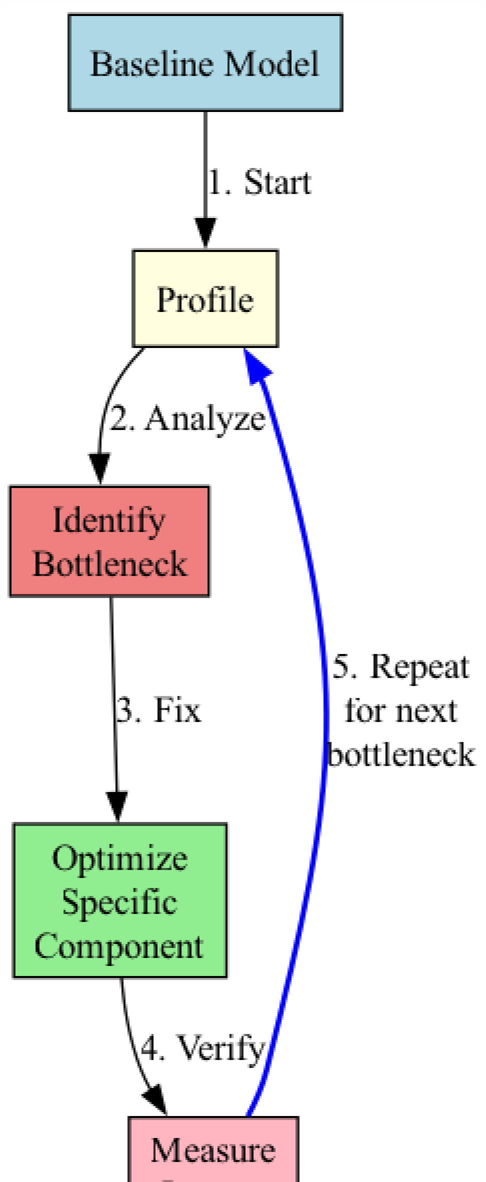
Inference metrics:

- **Latency**: Time per prediction (p50, p95, p99)
- **Throughput**: Predictions/second
- **First token latency**: Time to first output (for GenAI)

Cost metrics:

- **FLOPs**: Floating point operations (theoretical)
- **Energy**: kWh consumed

The Optimization Loop



Types of Bottlenecks

CPU-bound:

- Data loading and preprocessing
- Tokenization, data augmentation
- Host-to-device memory transfer

GPU compute-bound:

- Too many parameters
- Inefficient operations (small kernels, poor fusion)
- Suboptimal algorithms (e.g., naive attention)

GPU memory-bound:

- Out of memory (OOM) errors
- Batch size limited by VRAM
- Memory bandwidth saturation

Profiling Tool Hierarchy

Level 1: Quick checks (seconds)

- `nvidia-smi`: GPU utilization snapshot
- `time` command: Total execution time
- Manual timers: `time.time()`, `time.perf_counter()`

Level 2: Python profiling (minutes)

- `cProfile`: Function-level CPU profiling
- `line_profiler`: Line-by-line profiling
- `memory_profiler`: Memory usage per line

Level 3: Deep profiling (hours)

- PyTorch Profiler: Op-level GPU/CPU profiling
- Nsight Systems: System-wide CUDA profiling
- TensorBoard: Visual timeline analysis

Quick Check: nvidia-smi

Basic monitoring:

```
nvidia-smi
```

Watch mode (update every 1 second):

```
nvidia-smi -l 1
```

Key metrics:

- **GPU-Util**: % of time GPU was busy (aim for >85%)
- **Memory-Usage**: Current / Total VRAM
- **Power**: Current draw vs TDP
- **Temperature**: Thermal throttling at ~85°C

Red flags:

- GPU-Util < 50%: Likely CPU bottleneck

Python Profiling: cProfile

Built-in function-level profiler:

```python
import cProfile
import pstats

# Profile a function
profiler = cProfile.Profile()
profiler.enable()

train_model()  # Your code here

profiler.disable()
```

Output columns:

- `ncalls`: Number of calls
- `tottime`: Total time in function (excluding sub-calls)
- `cumtime`: Cumulative time (including sub-calls)
- `percall`: Time per call

cProfile Example Output

```
   ncalls  tottime  percall  cumtime  percall filename:lineno(function)
        1    0.002    0.002   45.231   45.231 train.py:23(train_epoch)
     1563   12.450    0.008   30.125    0.019 dataloader.py:45(__next__)
     1563    8.234    0.005   15.678    0.010 transforms.py:12(augment)
   156300    4.123    0.000    4.123    0.000 {method 'random' of '_random.Random'}
     1563    3.456    0.002   10.234    0.007 model.py:67(forward)
```

Analysis:

- Data loading (`__next__`) takes 30s out of 45s → CPU bottleneck!
- Random augmentation is expensive → consider caching or GPU augmentation
- Model forward pass is fast (10s) → GPU is underutilized

Line-Level Profiling: line_profiler

More granular than cProfile:

```python
from line_profiler import LineProfiler

lp = LineProfiler()
lp.add_function(preprocess_data)
lp.add_function(model.forward)

lp.enable()
train_one_epoch()
lp.disable()
```

Output:

```
Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
    15         1      12500.0  12500.0     45.2  img = cv2.imread(path)
    16         1       8500.0   8500.0     30.7  img = cv2.resize(img, (224, 224))
    17         1       6700.0   6700.0     24.1  img = normalize(img)
```


Insight: `cv2.imread` is the slowest → use faster libraries or cache.

Memory Profiling: memory_profiler

Track memory usage line by line:

```python
from memory_profiler import profile

@profile
def train_step(batch):
    images, labels = batch  # Line 1
    images = images.cuda()  # Line 2
    outputs = model(images)  # Line 3
    loss = criterion(outputs, labels)  # Line 4
```

Output:

```
Line #    Mem usage    Increment   Line Contents
================================================
     1     2145 MB        0 MB       images, labels = batch
     2     4290 MB     2145 MB       images = images.cuda()
     3     8580 MB     4290 MB       outputs = model(images)
     4     8585 MB        5 MB       loss = criterion(outputs, labels)
     5    12875 MB     4290 MB       loss.backward()
```

Insight: Gradients double memory (line 5) → use gradient checkpointing.

PyTorch Built-in Profiling

Torch profiler with CPU/GPU tracing:

```python
from torch.profiler import profile, record_function, ProfilerActivity

with profile(
    activities=[ProfilerActivity.CPU, ProfilerActivity.CUDA],
    record_shapes=True,
    profile_memory=True,
    with_stack=True
) as prof:
    with record_function("train_epoch"):
        for i, batch in enumerate(dataloader):
            if i >= 10:  # Profile first 10 batches
                break

            with record_function("forward"):
                output = model(batch)

            with record_function("backward"):
                loss.backward()

            prof.step()  # Signal step boundary
```

PyTorch Profiler Output

Table view:

```python
print(prof.key_averages().table(
    sort_by="cuda_time_total",
    row_limit=10
))
```

Output:

```
-------------------------------------------------------  ------------
Name                                         Self CPU time  Self CUDA time
-------------------------------------------------------  ------------
aten::conv2d                                        1.2ms       125.4ms
aten::batch_norm                                    0.8ms        45.2ms
aten::linear                                        0.5ms        78.3ms
```

Insights:

- Convolutions dominate GPU time (expected)
- HtoD memcpy is 23ms → data transfer bottleneck! Use `pin_memory`

TensorBoard Profiler Visualization

Export for TensorBoard:

```
with profile(
    activities=[ProfilerActivity.CPU, ProfilerActivity.CUDA],
    on_trace_ready=torch.profiler.tensorboard_trace_handler('./log/resnet18')
) as prof:
    train()
```

View in TensorBoard:

```
tensorboard --logdir=./log
```

Visualizations:

- **Timeline**: See GPU kernels, data loading, CPU ops on timeline
- **Operator view**: Breakdown by operation type
- **Kernel view**: GPU kernel efficiency
- **Trace view**: Detailed event trace

Interpreting GPU Timeline

Ideal timeline:

```
GPU: ██████████████████████ (100% busy)
CPU: █ █ █ █ █ █ █ █ █ █ █ (loading data)
```

CPU bottleneck:

```
GPU: █  █  █  █  █  █  █   (idle gaps)
CPU: ██████████████████████ (100% busy)
     ▲  ▲  ▲
     Gaps while waiting for data!
```

Memory transfer bottleneck:

```
GPU: █   █   █   █   █   █
MEM: ░███░███░███░███░███░ (memcpy)
     ▲ Large memory transfers stalling GPU
```

Data Loading Optimization

Problem: GPU idle while CPU loads data.

Solutions:

1. Multi-process data loading:

```
DataLoader(dataset,
    batch_size=32,
    num_workers=4,          # Spawn 4 worker processes
    pin_memory=True,        # Faster GPU transfer
    persistent_workers=True  # Reuse workers across epochs
)
```

2. Prefetching (automatic with `num_workers > 0`):

```
Worker 1: Load batch 1 → Load batch 3 → Load batch 5
Worker 2: Load batch 2 → Load batch 4 → Load batch 6
GPU:      Process batch 1 → Process batch 2 → Process batch 3
```

Data Loading Best Practices

Rule of thumb for `num_workers`:

- Start with `num_workers = min(4, num_cpus)`
- Profile and tune (diminishing returns after ~8)
- Too many workers → memory overhead

Optimization checklist:

```
DataLoader(
    dataset,
    batch_size=32,
    num_workers=4,              # Multi-process loading
```

Advanced: GPU preprocessing:

```
# Use NVIDIA DALI or Kornia for GPU-accelerated augmentation
import kornia.augmentation as K
augment = K.AugmentationSequential(
```

Mixed Precision Training Theory

Float32 (FP32):

- 1 sign bit, 8 exponent bits, 23 fraction bits
- Range: ~10^-38 to 10^38
- Standard for training

Float16 (FP16):

- 1 sign bit, 5 exponent bits, 10 fraction bits
- Range: ~10^-8 to 65504
- 2x memory savings, 2-3x speedup on Tensor Cores

Problem with pure FP16:

- Small gradients underflow to zero
- Large activations overflow to infinity
- Training diverges or converges poorly

Automatic Mixed Precision (AMP)

Solution: Mixed precision training

Strategy:

1. **Master weights** in FP32 (stored in optimizer)
2. **Forward pass** in FP16 (faster)
3. **Loss** in FP32 (precision for small values)
4. **Backward pass** in FP16 (faster)
5. **Gradient scaling** to prevent underflow
6. **Weight update** in FP32 (master weights)

Gradient scaling:

- Multiply loss by scale factor (e.g., 1024) before backward
- Prevents small gradients from becoming zero in FP16
- Unscale gradients before optimizer step

AMP Implementation in PyTorch

```python
from torch.cuda.amp import autocast, GradScaler

model = MyModel().cuda()
optimizer = torch.optim.Adam(model.parameters(), lr=1e-3)
scaler = GradScaler()  # Gradient scaler

for epoch in range(num_epochs):
    for batch in dataloader:
        images, labels = batch
        images, labels = images.cuda(), labels.cuda()

        optimizer.zero_grad()

        # Forward in FP16
        with autocast():
            outputs = model(images)
            loss = criterion(outputs, labels)

        # Backward with gradient scaling
        scaler.scale(loss).backward()
        scaler.step(optimizer)
```


Expected speedup: 1.5-3x on V100/A100/H100 GPUs with Tensor Cores.

AMP Best Practices

When to use AMP:

- ✅ Training CNNs, Transformers on modern GPUs (V100+)
- ✅ Large batch sizes (better Tensor Core utilization)
- ✅ Models with lots of matrix multiplications

When NOT to use AMP:

- ❌ Small models on old GPUs (no Tensor Cores)
- ❌ Models with numerical instability
- ❌ When accuracy drops significantly (rare)

Debugging AMP issues:

Memory Optimization: Gradient Checkpointing

Problem: Storing all activations for backprop uses O(N) memory.

Example (4-layer network):

```
Forward:  Input → Act1 → Act2 → Act3 → Act4 → Loss
Backward: ∇Loss ← ∇Act4 ← ∇Act3 ← ∇Act2 ← ∇Act1
          ▲       ▲       ▲       ▲       ▲
          Need to store all activations!
```

Memory usage: Batch_size × Num_layers × Hidden_dim

Solution: Gradient Checkpointing (Recomputation)

- Store only subset of activations (checkpoints)
- Recompute others during backward pass
- **Trade**: 20-30% slower for 50%+ memory savings

Gradient Checkpointing in PyTorch

```python
import torch.utils.checkpoint as checkpoint

class MyModel(nn.Module):
    def __init__(self):
        super().__init__()
        self.layer1 = nn.Linear(1024, 1024)
        self.layer2 = nn.Linear(1024, 1024)
        self.layer3 = nn.Linear(1024, 1024)

    def forward(self, x):
        # Checkpoint layer1 and layer2
        x = checkpoint.checkpoint(self._forward_layers, x)
        x = self.layer3(x)
        return x

    def _forward_layers(self, x):
        x = F.relu(self.layer1(x))
        x = F.relu(self.layer2(x))
        return x
```

Use case: Train larger models/batches that otherwise OOM.

Gradient Accumulation

Problem: Limited GPU memory → small batch size → poor convergence.

Solution: Accumulate gradients over multiple steps.

```
accumulation_steps = 4  # Effective batch size = 32 * 4 = 128

optimizer.zero_grad()
for i, batch in enumerate(dataloader):
    outputs = model(batch)
    loss = criterion(outputs, labels)

    # Normalize loss by accumulation steps
    loss = loss / accumulation_steps
    loss.backward()

    # Only step optimizer every N batches
    if (i + 1) % accumulation_steps == 0:
        optimizer.step()
        optimizer.zero_grad()
```

Effect: Simulates large batch training with limited memory.

Compute Optimization: torch.compile

PyTorch 2.0+ feature: JIT compilation for speedups.

```
import torch

model = MyModel()
model = torch.compile(model)  # Compile the model

# Training loop unchanged
for batch in dataloader:
    output = model(batch)  # First run: compile, subsequent: fast!
```

What it does:

- **Graph capture**: Traces model operations
- **Operator fusion**: Merges ops (e.g., Conv+BN+ReLU → 1 kernel)
- **Memory optimization**: Reuses buffers
- **CUDA graph**: Reduces kernel launch overhead

Expected speedup: 10-50% for free!

torch.compile Modes

```python
# Default mode (balanced)
model = torch.compile(model)

# Maximum performance (slower compile time)
model = torch.compile(model, mode="max-autotune")

# Reduce memory usage
model = torch.compile(model, mode="reduce-overhead")

# Debug mode (disable optimizations)
model = torch.compile(model, mode="default", dynamic=True)
```

Caveats:

- First run is slow (compilation overhead)
- Not all operations supported (fallback to eager)
- Dynamic shapes can trigger recompilation

Operator Fusion Example

Without fusion (3 kernel launches):

```
x = conv(input)     # Kernel 1: Convolution
x = bn(x)           # Kernel 2: Batch norm
x = relu(x)         # Kernel 3: ReLU
```

With fusion (1 kernel launch):

```
x = conv_bn_relu(input)  # Single fused kernel
```

Benefits:

- Fewer kernel launches (less overhead)
- Reduced memory bandwidth (no intermediate writes)
- Better cache locality

torch.compile does this automatically!

Flash Attention

Problem: Standard attention has $O(N^2)$ memory complexity.

Standard attention:

```
# Materialize full N×N attention matrix
scores = Q @ K.T  # (N, N) matrix
attn = softmax(scores)  # (N, N) matrix
```

Flash Attention (Dao et al., 2022):

- Tiled computation (never materialize full matrix)
- Fused kernel (attention + softmax in one pass)
- **Result**: 2-4x speedup, $O(N)$ memory instead of $O(N^2)$

Usage:

```
from torch.nn.functional import scaled_dot_product_attention

# PyTorch 2.0+ uses Flash Attention automatically!
```

System-Level Optimization

CPU affinity (bind processes to cores):

```
taskset -c 0-7 python train.py  # Use cores 0-7
```

NUMA awareness (multi-socket systems):

```
numactl --cpunodebind=0 --membind=0 python train.py
```

PCIe optimization (multi-GPU):

```
# Use GPUs on same PCIe switch
os.environ["CUDA_VISIBLE_DEVICES"] = "0,1"  # Same switch
```

Storage I/O:

- Use SSD over HDD for datasets
- Use RAM disk for small datasets (`tmpfs`)

Benchmarking Best Practices

1. Warmup runs (JIT compilation, cache warming):

```python
for _ in range(10):
    model(dummy_input)  # Warmup

# Now measure
start = time.time()
for _ in range(100):
    model(input_data)
```

2. Multiple runs (reduce variance):

```python
import numpy as np

times = []
for _ in range(100):
    start = time.perf_counter()
    model(input_data)
    times.append(time.perf_counter() - start)

print(f"Mean: {np.mean(times)*1000:.2f} ms")
```

Benchmarking Checklist

Environment control:

- [ ] Disable CPU frequency scaling (`performance` mode)
- [ ] Close background applications
- [ ] Fix random seeds (`torch.manual_seed(42)`)
- [ ] Use same device (GPU vs CPU)

Measurement:

- [ ] Warmup before timing (10+ iterations)
- [ ] Measure multiple runs (100+)
- [ ] Report mean, std, percentiles (p50, p95, p99)
- [ ] Synchronize CUDA ops (`torch.cuda.synchronize()`)

Comparison:

- [ ] Same hardware, same PyTorch version

Common Performance Anti-Patterns

1. Implicit CPU-GPU synchronization:

```python
# BAD: Forces sync every iteration
for i, batch in enumerate(dataloader):
    loss = train_step(batch)
    print(f"Loss: {loss.item()}")  # .item() syncs!

# GOOD: Batch logging
losses = []
for i, batch in enumerate(dataloader):
    loss = train_step(batch)
    losses.append(loss.detach())  # No sync
if i % 100 == 0:
    print(f"Avg loss: {torch.stack(losses).mean()}")
```

2. Small batch sizes (underutilize GPU):

- Batch size 1-8: Poor GPU utilization
- Batch size 32-128: Better (saturate GPU)

Common Performance Anti-Patterns (2)

3. Unnecessary data transfers:

```python
# BAD: Transfer to GPU every iteration
for batch in dataloader:
    batch = batch.cuda()  # Slow!

# GOOD: Use pin_memory + non_blocking
dataloader = DataLoader(..., pin_memory=True)
for batch in dataloader:
    batch = batch.cuda(non_blocking=True)  # Faster!
```

4. Inefficient tensor operations:

```python
# BAD: Python loop
result = []
for i in range(len(tensor)):
    result.append(tensor[i] * 2)

# GOOD: Vectorized operation
result = tensor * 2  # Much faster!
```

Case Study: Training Speedup

Baseline ResNet-50 on ImageNet:

- Batch size: 32
- Time per epoch: 120 minutes
- GPU utilization: 45%

Optimization steps:

Optimization	Speedup	Cumulative Time
Baseline	1.0x	120 min
+ num_workers=8	1.4x	86 min
+ Mixed precision (AMP)	1.9x	45 min
+ Larger batch (32→128)	2.3x	37 min
+ torch.compile	2.8x	31 min

Final result: 2.8x speedup, 74% faster!

Case Study: Memory Optimization

Problem: Training LLaMA-7B on single A100 (40GB VRAM) OOMs.

Optimization steps:

Technique	Memory Usage	Batch Size
Baseline FP32	52 GB	OOM
FP16	26 GB	1
+ Gradient checkpointing	18 GB	2
+ Gradient accumulation	18 GB	8 (effective)
+ Flash Attention	14 GB	4

Result: Fits on single GPU with effective batch size of 16!

Profiling Workflow Summary

Step 1: Establish baseline

- Measure throughput, latency, memory
- Profile with PyTorch Profiler
- Identify bottleneck category (CPU/GPU compute/GPU memory/I/O)

Step 2: Apply targeted optimization

- CPU bottleneck → `num_workers`, prefetching
- GPU compute → AMP, `torch.compile`, algorithmic improvements
- GPU memory → gradient checkpointing, smaller batch, model parallelism
- I/O → faster storage, caching, data format (HDF5, LMDB)

Step 3: Measure impact

- Re-run profiling
- Compare metrics

Optimization Priority

Quick wins (do first):

1. ✅ Enable AMP (5 min, 1.5-2x speedup)
2. ✅ Tune `num_workers` (10 min, 1.2-1.5x speedup)
3. ✅ Use `torch.compile` (1 line, 1.1-1.5x speedup)
4. ✅ Enable `pin_memory=True` (1 parameter, 1.1x speedup)

Medium effort (if needed):

5. ⚙️ Gradient accumulation (if memory-limited)
6. ⚙️ Larger batch size (if hardware allows)
7. ⚙️

Tools Ecosystem Summary

Profiling:

- `nvidia-smi`: GPU monitoring
- `cProfile`: Python function profiling
- `line_profiler`: Line-level profiling
- `memory_profiler`: Memory usage
- PyTorch Profiler: Deep PyTorch profiling
- TensorBoard: Visual profiling
- Nsight Systems/Compute: Expert CUDA profiling

Optimization:

- `torch.cuda.amp`: Mixed precision
- `torch.compile`: Graph optimization
- `torch.utils.checkpoint`: Gradient checkpointing
- `torch.nn.utils.prune`: Model pruning

Lab Preview

Today's mission:

1. **Part 1**: Profile ResNet-18 training and identify bottlenecks
2. **Part 2**: Optimize data loading (num_workers, pin_memory)
3. **Part 3**: Apply mixed precision training (AMP)
4. **Part 4**: Use gradient checkpointing to fit larger batch
5. **Part 5**: Apply torch.compile and measure speedup
6. **Part 6**: Create comprehensive performance comparison

Deliverable: Optimization report showing 2-3x speedup!

Key Takeaways

1. **Always profile before optimizing** - measure, don't guess
2. **Focus on the critical path** - optimize what matters (training loop)
3. **Quick wins first** - AMP, num_workers, torch.compile are easy
4. **Memory vs speed trade-offs** - gradient checkpointing, accumulation
5. **Benchmark properly** - warmup, multiple runs, synchronization
6. **Iterative process** - profile → optimize → measure → repeat

Remember: A 2x speedup means 2x more experiments, faster iteration, and cheaper costs!

Additional Resources

Documentation:

- PyTorch Profiler: https://pytorch.org/tutorials/recipes/recipes/profiler_recipe.html
- PyTorch Performance Tuning: https://pytorch.org/tutorials/recipes/recipes/tuning_guide.html
- torch.compile: https://pytorch.org/tutorials/intermediate/torch_compile_tutorial.html

Papers:

- Mixed Precision Training (Micikevicius et al., 2018)
- Flash Attention (Dao et al., 2022)
- Gradient Checkpointing (Chen et al., 2016)

Tools:

- TensorBoard: https://www.tensorflow.org/tensorboard
- Nsight Systems: https://developer.nvidia.com/nsight-systems
- py-spy: https://github.com/benfred/py-spy (sampling profiler)