

LLM Fine-Tuning, Alignment & Preference Optimization

SFT, RLHF, DPO, and LoRA/QLoRA Methods

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1. Introduction & Motivation

1.1 Why Fine-Tuning is Needed

Large language models trained on massive web corpora acquire broad linguistic knowledge but lack task-specific expertise and domain alignment. A model trained on general internet text may perform poorly on specialized tasks (medical diagnosis, code generation, customer support) without adaptation. Fine-tuning adapts pre-trained models to specific domains, instruction-following styles, and performance requirements with dramatically reduced compute compared to pretraining.

The fundamental challenge: pretraining optimizes for next-token prediction accuracy, not for useful, safe, or preference-aligned behavior.

1.2 Why Alignment is Necessary

LLMs exhibit concerning failure modes:

- **Misalignment with human intent:** Models optimize for proxy metrics that diverge from actual user preferences
- **Safety concerns:** Generation of toxic, biased, or harmful content
- **Hallucinations:** Confident fabrication of facts
- **Controllability:** Difficulty steering model behavior without explicit instructions

Alignment aims to ensure LLM outputs reflect human values, preferences, and safety constraints. This requires moving beyond supervised learning on human-curated examples toward methods that directly optimize for human preference signals.

1.3 Quick Comparison: SFT vs RLHF vs DPO

Method	Approach	Data	Training Complexity	Compute Cost
SFT	Supervised learning on curated examples	Input-output pairs	Low	Low
RLHF	RL with learned reward model	Preference pairs	High (3-phase)	High (RM + PPO)
DPO	Direct preference optimization via implicit reward	Preference pairs	Medium	Medium (single phase)

Key insight: Each method trades data efficiency, computational cost, and alignment quality differently. The choice depends on data availability, compute budget, and performance goals.

2. Background: Foundation Models & Alignment Challenges

2.1 How LLMs Are Trained

Pretraining phase (months, billions of tokens):

- Objective: Minimize next-token prediction loss on diverse internet corpora
- Model: Decoder-only transformer (GPT-style architecture)
- Result: Strong language understanding, but no instruction-following or preference alignment

Pretraining Loss: $L = -E[\log P(\text{token}_t \mid \text{token}_{<t})]$

This loss minimizes prediction error but does not directly optimize for helpful, harmless, honest behavior.

Why pretraining alone fails:

- Optimizes likelihood of next token, not quality of full response
- No explicit optimization for user preferences
- May amplify biases and unsafe patterns in training data
- No mechanism to balance multiple objectives (accuracy, safety, helpfulness)

2.2 Misalignment Sources

1. **Specification Gaming:** Model exploits proxy metrics (high likelihood) while violating true objectives (usefulness)
2. **Objective Mismatch:** Pretraining loss \neq human preference
3. **Reward Hacking:** In RLHF, policy learns to game imperfect reward models
4. **Distribution Shift:** Performance degrades on out-of-distribution queries
5. **Value Drift:** Fine-tuning without regularization erodes capabilities learned during pretraining

2.3 Safety, Preference Modeling, Controllability

Safety requires explicit constraints and robustness testing. Methods include:

- Constitutional AI (self-critique + RL)
- Safety-focused RLHF phases
- Formal verification (limited applicability)

Preference modeling captures nuanced human values:

- Not binary (safe/unsafe) but continuous (more helpful, more creative, safer)
- Preferences vary across users and contexts
- Requires large, representative datasets

Controllability demands methods to steer behavior:

- Few-shot in-context learning
 - System prompts and role-playing
 - Fine-tuning on instruction-following examples
-

3. Supervised Fine-Tuning (SFT)

3.1 Concept and Workflow

SFT fine-tunes a pretrained model on a dataset of high-quality (input, output) pairs using standard supervised learning:

SFT Loss: $L_{SFT} = -E[(input, output) \sim D] [\log P_\theta(output | input)]$

Data format (example from OpenAI Instruct datasets):

```
{  
  "instruction": "Explain quantum entanglement in simple terms.",  
  "input": "",  
  "output": "Quantum entanglement occurs when two particles..."  
}
```

Or conversational format (more common):

```
{  
  "messages": [  
    {"role": "user", "content": "Explain quantum entanglement..."},  
    {"role": "assistant", "content": "Quantum entanglement occurs..."}  
]
```

]

}

3.2 Workflow

Pretreatrained Model

↓

Load Weights

↓

Prepare SFT Dataset (tokenize, format)

↓

Initialize Optimizer (AdamW, lr=2e-5 to 5e-4)

↓

Training Loop: Minimize L_SFT

- Forward pass: compute logits for next tokens
- Backward pass: compute gradients
- Update: $\theta \leftarrow \theta - \alpha \nabla L$

↓

Validation: Perplexity, BLEU, human eval

↓

Save Weights

3.3 Architecture Notes (Decoder-Only Models)

For GPT-style decoder-only models:

- Each token attends to previous tokens only (causal masking)
- Loss computed on all output tokens in sequence
- Padding tokens masked out to prevent gradient flow

Typical training configuration:

- Batch size: 8–32 (depends on GPU VRAM and sequence length)
- Learning rate: 1e-5 to 5e-4 (lower than intermediate training)
- Epochs: 1–3 (avoid overfitting; LLMs typically overfit quickly)
- Warmup: 100–500 steps
- Max sequence length: Often 512–2048 tokens

3.4 When SFT Works Well

✓ Strong performance when:

- High-quality curated dataset (>1000 examples)
- Clear input-output task structure
- Domain with sufficient training coverage
- Model already competent on base task

Examples:

- Instruction-following alignment (Alpaca, Llama 2)
- Specialized domains (medical, legal, code)
- Few-shot in-context learning improvement
- Safety-focused behavior (politeness, refusal)

3.5 Limitations

✗ SFT struggles with:

- Preference diversity (one output per input)
- Subtle alignment (e.g., tone, style preferences)
- Exploration (model mimics training data distribution)
- Reward maximization (doesn't optimize for preference ranking)

Key weakness: SFT optimizes mode-seeking behavior—the model learns to produce the single labeled output, not to maximize preferences over a range of good outputs.

3.6 Minimal Working Pseudo-Code

```
from transformers import AutoModelForCausalLM, AutoTokenizer
```

```
from torch.optim import AdamW
```

```
import torch
```

```
# Load pretrained model
```

```
model = AutoModelForCausalLM.from_pretrained("gpt2")
```

```
tokenizer = AutoTokenizer.from_pretrained("gpt2")
```

```
# Training loop
```

```
optimizer = AdamW(model.parameters(), lr=5e-5)
```

```

model.train()

for epoch in range(3):
    for batch in dataloader:
        input_ids = tokenizer(batch["input"], return_tensors="pt")["input_ids"]
        output_ids = tokenizer(batch["output"], return_tensors="pt")["input_ids"]

        # Concatenate input + output
        full_ids = torch.cat([input_ids, output_ids], dim=1)

        # Forward pass
        logits = model(full_ids).logits

        # Compute loss only on output tokens
        shift_logits = logits[..., :-1, :].contiguous()
        shift_labels = full_ids[..., 1:].contiguous()
        loss = torch.nn.functional.cross_entropy(
            shift_logits.view(-1, shift_logits.size(-1)),
            shift_labels.view(-1)
        )

        # Backward pass
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

```

3.7 Hugging Face TRL Pipeline Overview

The **SFTTrainer** from HF Transformers Reinforcement Learning (TRL) library simplifies SFT:

```

from trl import SFTTrainer
from transformers import TrainingArguments

```

```

trainer = SFTTrainer(
    model=model,
    train_dataset=train_dataset,
    args=TrainingArguments(
        output_dir=".//results",
        num_train_epochs=3,
        per_device_train_batch_size=8,
        learning_rate=5e-5,
        warmup_ratio=0.1,
        save_steps=500,
    ),
    packing=True, # Pack multiple short examples into single sequence
)

```

trainer.train()

Key features:

- Automatic tokenization and padding
 - Gradient accumulation support
 - Mixed precision training (fp16, bf16)
 - Easy integration with PEFT (LoRA)
-

4. RLHF (Reinforcement Learning from Human Feedback)

4.1 Full RLHF Pipeline

RLHF consists of three phases:

4.1.1 Phase 1: Supervised Fine-Tuning (SFT)

Train initial policy on curated examples (Section 3).

4.1.2 Phase 2: Reward Modeling (RM)

Collect human preference judgments: "Is output A or B better?" Train a reward model to predict human preferences:

RM Loss: $L_{RM} = -E[(y_w, y_l) \sim D] [\log \sigma(r_\theta(y_w) - r_\theta(y_l))]$

Where:

- y_w : Preferred (winning) output
- y_l : Non-preferred (losing) output
- r_θ : Reward model scoring function
- σ : Sigmoid function

Data format:

```
{  
  "prompt": "Write a haiku about spring.",  
  "chosen": "Cherry blossoms bloom\nPink petals dance in spring wind\nNew life awakens",  
  "rejected": "Spring is here now and it is nice"  
}
```

4.1.3 Phase 3: Policy Optimization via PPO

Use the learned reward model as signal to optimize the policy via reinforcement learning:

$$L_{PPO} = E_t [\min(r_t(\theta), \hat{A}_t, \text{clip}(r_t(\theta), 1-\varepsilon, 1+\varepsilon) \hat{A}_t)]$$

Where:

- $r_t(\theta)$: Probability ratio between new and old policy
- \hat{A}_t : Advantage estimate (reward - baseline)
- ε : Clipping range (typically 0.2)

Advantage (\hat{A}) measures how much better an action is than the average. Computed via:

$$A = r(y) - \beta * \text{KL}(\pi_{\text{new}} || \pi_{\text{SFT}})$$

- $r(y)$: Reward from RM
- β : Temperature controlling KL divergence
- KL: Kullback-Leibler divergence between new policy and SFT model (prevents collapse)

4.2 RLHF Workflow Diagram

[Pretraining Model]



[Phase 1: SFT]

Policy π_{SFT}

[Collect Human Prefs] → Preference pairs $\{(y_w, y_l)\}$



[Phase 2: Train RM]

Reward $r_\theta(y)$



[Phase 3: PPO Training]

Optimize: $\max E_y [r_\theta(y)] - \beta \text{KL}(\pi || \pi_{\text{SFT}})$



[Final Policy π_{opt}]

4.3 Reward Modeling Basics

The reward model is typically a transformer with:

- Same architecture as policy (to enable efficient scoring)
- Single scalar output head (regression or classification)

Training data requirements:

- 10k–100k preference pairs (more = better alignment)
- Can be crowd-sourced or from model comparisons
- Label quality critical (disagreement rates matter)

Common pitfalls:

- Distribution shift: RM trained on one policy, applied to different policy
- Reward hacking: Policy learns to fool RM without improving actual quality
- Sparse feedback: Limited diversity in preference data

4.4 PPO Equations Simplified

Proximal Policy Optimization (Schulman et al., 2017) prevents policy collapse:

$$L_{\text{PPO}} = E_t [\min(r_t(\theta) \hat{A}_t, \text{clip}(r_t(\theta), 1-\epsilon, 1+\epsilon) \hat{A}_t)]$$

where $r_t(\theta) = \pi_\theta(a_t | s_t) / \pi_{\text{old}}(a_t | s_t)$

Intuition:

- If $r_t > 1+\epsilon$: Action increased probability too much → clip it
- If $r_t < 1-\epsilon$: Action decreased probability too much → clip it

- Clipping prevents large gradient updates that destabilize training

Advantage estimation via Generalized Advantage Estimation (GAE):

$$\hat{A}_t = \sum (\gamma \lambda)^l * \delta_{t+l}$$

$$\delta_t = r_t + \gamma V(s_{t+1}) - V(s_t)$$

Where:

- γ : Discount factor (0.99)
- λ : GAE parameter (0.95)
- $V(s)$: Value function baseline (estimated by critic head)

4.5 Strengths and Weaknesses

Strengths ✓:

- Direct optimization for human preferences
- Powerful: RLHF aligned InstructGPT, ChatGPT, Claude
- Flexible: Can optimize multiple objectives simultaneously
- Empirically proven at scale

Weaknesses ✗:

- Complex: 3 phases, multiple models, careful hyperparameter tuning
- Data-hungry: Requires 10k–100k preference labels
- Reward hacking: Policy exploits RM imperfections
- Computationally expensive: Maintain SFT policy, RM, and PPO policy
- Unstable: PPO training notoriously finicky (KL coefficient tuning critical)
- RM generalization: Performance degrades on out-of-distribution queries

4.6 Real-World Use Cases

Use Case	Why RLHF	Notes
General chat (ChatGPT)	Multi-dimensional preferences	Helpfulness, harmlessness, honesty
Code generation	Correctness preference	Executable code preferred over plausible-looking wrong code
Summarization	Style + content trade-offs	Conciseness vs completeness
Content moderation	Safety alignment	Refusal to generate toxic content

Factuality	Preference for grounded output	Reduce hallucination via preference learning
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4.7 Memory and Computation Considerations

RLHF is expensive:

- **Models:** Policy (trainable), reference SFT (frozen), reward model (inference), value function
- **Memory per forward pass:** $\sim 4\text{--}6\times$ standard training
- **Typical setup:** V100 (32GB) \rightarrow Train on 1 GPU for small models, requires multi-GPU for 7B+
- **Time:** RM training (1–2 days), PPO training (2–5 days) for 7B model on 100k preference pairs

Optimizations:

- Gradient checkpointing (trade compute for memory)
 - LoRA (parameter efficiency, covered in Section 6)
 - Distributed training (multi-GPU, multi-node)
 - Use smaller reference models
-

5. Direct Preference Optimization (DPO)

5.1 Why DPO Was Invented

RLHF is powerful but problematic:

1. **Reward model brittleness:** Learned RM generalizes poorly; policy exploits edge cases
2. **Instability:** PPO training is notoriously finicky (requires careful hyperparameter tuning)
3. **Computational overhead:** Three separate models consume massive memory
4. **Mode collapse:** KL coefficient tuning critical to prevent catastrophic forgetting

Insight: Why learn an explicit reward model? Use preference pairs directly to optimize the policy.

DPO (Rafailov et al., 2023) removes the RM and replaces PPO with direct optimization:

Preference pairs $\{(y_w, y_l)\} \rightarrow$ DPO Loss \rightarrow Optimized Policy

(Direct)

5.2 Mathematical Intuition

Given preference pair (y_w, y_l) , we want:

$$P(y_w > y_l | x) > 0.5$$

Bradley-Terry model (widely used for preference modeling):

$$P(y_w > y_l | x) = \sigma(r(x, y_w) - r(x, y_l))$$

The maximum likelihood estimate recovers an implicit reward model:

$$r^*(x, y) = \beta \log(\pi(y|x) / \pi_{\text{ref}}(y|x))$$

Where:

- $\pi(y|x)$: Policy (optimized model)
- $\pi_{\text{ref}}(y|x)$: Reference model (e.g., SFT checkpoint)
- β : Temperature parameter (typically 0.5–1.0)

Intuition: Reward is the log-ratio of policy to reference. Higher π/π_{ref} means better preference. KL divergence emerges naturally via log-ratio regularization.

5.3 DPO Loss Equation

The DPO loss directly optimizes preference pairs without explicit RM:

$$\begin{aligned} L_{\text{DPO}} = -E_{\{(x, y_w, y_l)\}} [& \\ & \log \sigma(\beta \log(\pi_\theta(y_w|x)/\pi_{\text{ref}}(y_w|x)) - \\ & \quad \beta \log(\pi_\theta(y_l|x)/\pi_{\text{ref}}(y_l|x)))] \end{aligned}$$

Simplified notation:

$$\begin{aligned} L_{\text{DPO}} = -\log \sigma(\beta [\log(\pi_\theta(y_w|x)/\pi_{\text{ref}}(y_w|x)) & \\ & - \log(\pi_\theta(y_l|x)/\pi_{\text{ref}}(y_l|x))]) \end{aligned}$$

Practical form (what you actually implement):

Compute log probabilities

```
log_pi_w = model.forward(x, y_w)    # log P(y_w|x) from policy
log_pi_ref_w = reference.forward(x, y_w) # log P(y_w|x) from reference
```

```
log_pi_l = model.forward(x, y_l)
```

```
log_pi_ref_l = reference.forward(x, y_l)
```

DPO loss

```
ratio_w = log_pi_w - log_pi_ref_w
ratio_l = log_pi_l - log_pi_ref_l
```

```
loss = -torch.nn.functional.logsigmoid(beta * (ratio_w - ratio_l)).mean()
```

5.4 Advantages over RLHF

Aspect	RLHF	DPO
Models required	3 (policy, RM, value)	2 (policy, reference)
Training stability	Unstable (PPO)	Stable (supervised-like loss)
Reward hacking	Common	Mitigated by implicit model
Data efficiency	Requires 10k–100k pairs	Works with 1k–10k pairs
Memory	4–6× baseline	~1.5–2× baseline
Training time	Days	Hours to 1 day
Hyperparameter tuning	Complex (KL, learning rates)	Simpler (mainly β)

5.5 Practical DPO Training Workflow

```
from transformers import AutoModelForCausalLM, AutoTokenizer  
from trl import DPOTrainer  
from datasets import load_dataset
```

```
# Load dataset  
  
dataset = load_dataset("your_preference_dataset")  
# Expected format: {prompt, chosen, rejected}
```

```
# Load model and reference  
  
model = AutoModelForCausalLM.from_pretrained("mistral-7b")  
model_ref = AutoModelForCausalLM.from_pretrained("mistral-7b")  
tokenizer = AutoTokenizer.from_pretrained("mistral-7b")
```

```
# Initialize DPO Trainer  
  
trainer = DPOTrainer(  
    model=model,  
    ref_model=model_ref,  
    args=TrainingArguments(  
        output_dir="./dpo_model",
```

```

    num_train_epochs=1,
    per_device_train_batch_size=16,
    learning_rate=5e-6,
    warmup_ratio=0.1,
    bf16=True, # Use bfloat16 for stability
),
beta=0.1, # DPO temperature
train_dataset=dataset["train"],
eval_dataset=dataset["test"],
tokenizer=tokenizer,
)

```

trainer.train()

Key hyperparameters:

- beta (0.1–1.0): Higher β penalizes preference violations more strongly
- Learning rate: 5e-6 to 5e-5 (lower than SFT)
- Batch size: 16–32 (depends on GPU VRAM)
- Epochs: 1–2 (avoid overfitting on small datasets)

5.6 DPO Dataset Format

```
{
  "prompt": "Explain photosynthesis in one sentence.",
  "chosen": "Photosynthesis is the process where plants convert light energy into chemical energy stored in glucose.",
  "rejected": "Photosynthesis is a plant thing that happens in leaves."
}
```

Or with role-based format:

```
{
  "prompt": [
    {"role": "user", "content": "Explain photosynthesis in one sentence."}
  ],
}
```

"chosen": "Photosynthesis is the process where plants convert light energy into chemical energy stored in glucose.",

"rejected": "Photosynthesis is a plant thing that happens in leaves."

}

6. Parameter-Efficient Fine-Tuning (LoRA & QLoRA)

6.1 The Parameter Efficiency Problem

Full fine-tuning of a 7B model requires updating all 7B parameters:

- **Storage:** Gradient buffers + optimizer states (Adam: $2 \times$ parameters) = ~42GB
- **Compute:** Forward + backward pass through all layers
- **Time:** Days of training

Solution: Only update a small fraction of parameters while keeping most frozen.

6.2 LoRA: Low-Rank Adaptation

Key idea (Hu et al., 2021): Model weights change along low-rank directions during fine-tuning.

For weight matrix $W \in R^{m \times n}$, instead of updating W directly:

$$W_{\text{new}} = W_0 + \Delta W$$

Constrain the update to low-rank form:

text

$$\Delta W = BA \quad (B \in R^{m \times r}, A \in R^{r \times n}, r \ll \min(m, n))$$

Example: W is 4096×4096 with $r=8$:

- Full update: ~33M parameters
- LoRA update: $(4096 \times 8) + (8 \times 4096) = \sim 65K$ parameters
- **Reduction: 500x fewer parameters**

6.3 Rank and Adapters

Rank r : Typically 4, 8, 16, 32, 64

- Lower r (4–8): Faster, lower memory, minimal performance loss for many tasks
- Higher r (32–64): Better performance but higher cost

Adapters: Apply LoRA to specific layers:

- Query projections (Q)
- Value projections (V)

- Both Q+V (common default)
- All projections (Q, K, V, output)
- Linear layers (good for larger r)

Recommended configurations:

Model Size	Task	r	Target Modules	Epochs	LR
7B	General chat	8	q,v	2–3	5e-4
7B	Domain-specific	16	q,v,out	2–3	3e-4
13B	Code generation	16	q,k,v,out	2	2e-4
70B	Alignment (with QLoRA)	32	q,v	1	1e-4

6.4 QLoRA: Quantization + LoRA

QLoRA combines LoRA with 4-bit quantization to fit large models on consumer GPUs.

4-bit quantization methods:

1. **NF4 (Normal Float 4-bit):** Quantizes to 4-bit representation optimized for normally distributed weights
 - Captures weight distribution well
 - Minimal loss for most models
2. **FP4 (Float 4-bit):** Standard 4-bit floating point
 - Simpler but slightly higher quantization error

How it works:

- Freeze base model in 4-bit quantization
- Add LoRA adapters (trainable in full precision)
- Gradients computed through adapters only

Memory breakdown (70B model, 4-bit NF4):

Base model quantized: 70B / 8 bits = ~8.75GB

LoRA adapters: ~500MB (rank 32)

Gradients + optimizer: ~2GB

Batch size overhead: ~4GB

Total: ~15GB (vs 160GB+ for full training)

6.5 Memory and Hardware Savings

Typical savings (7B model, rank 8, LoRA-only):

Metric	Full Fine-tuning	LoRA	QLoRA
Trainable parameters	7B	65M	65M
GPU memory needed	40–50GB	15–20GB	6–8GB
Training speed	1×	~0.8–0.9×	~0.5–0.7×
Model storage	14GB (FP32)	14GB (base) + 130MB (adapters)	2GB (4-bit) + 130MB

Hardware implications:

- Full fine-tuning: A100 (40GB+) or V100 cluster
- LoRA: V100 (32GB) or RTX A6000 (48GB)
- QLoRA: RTX 4090 (24GB) or even RTX 3090 (24GB) for smaller models

6.6 When to Use LoRA vs QLoRA

Use LoRA when:

- You have sufficient GPU memory (>30GB)
- Speed is critical
- Model size \leq 13B
- Working with multiple models (LoRA adapters are portable)

Use QLoRA when:

- GPU memory is limited (<16GB)
- You can tolerate slower training (typically 50–70% of LoRA speed)
- Model size 7B–70B+
- You want to fine-tune on consumer hardware

Hybrid approach:

- QLoRA for initial fine-tuning on GPU-constrained environments
- LoRA for rapid iteration on well-provisioned clusters

6.7 LoRA Configuration Example

```
from peft import LoraConfig, get_peft_model
```

```

lora_config = LoraConfig(
    r=16,                      # LoRA rank
    lora_alpha=32,              # LoRA scaling factor
    target_modules=["q_proj", "v_proj"], # Apply to Q and V
    lora_dropout=0.05,           # Dropout in LoRA layers
)
```

```

bias="none",           # Don't adapt bias
task_type="CAUSAL_LM",
)

# Wrap model with LoRA
model = get_peft_model(base_model, lora_config)
print(model.print_trainable_parameters())
# Output: trainable params: 4,194,304 || all params: 7,110,656 || trainable%: 0.59

```

LoRA scaling: lora_alpha controls the magnitude of LoRA updates. Typical values:

- lora_alpha = 2 * r (commonly used scaling)
 - Higher alpha: Stronger LoRA effect
 - Lower alpha: Weaker, more regularized adaptation
-

7. Practical Tools and Frameworks

7.1 PyTorch Basics for Training Loops

Core pattern:

```
import torch
```

```
from torch.optim import AdamW
```

```
model = load_model()
```

```
optimizer = AdamW(model.parameters(), lr=1e-4)
```

```
for epoch in range(num_epochs):
```

```
    for batch in train_loader:
```

```
        # Forward pass
```

```
        outputs = model(batch["input_ids"], attention_mask=batch["attention_mask"])
```

```
        loss = compute_loss(outputs, batch["labels"])
```

```
        # Backward pass
```

```
        optimizer.zero_grad()
```

```

loss.backward()

# Gradient clipping (prevents exploding gradients)
torch.nn.utils.clip_grad_norm_(model.parameters(), max_norm=1.0)

# Optimization step
optimizer.step()

# Learning rate scheduling (optional)
scheduler.step()

```

Key practices:

- **Gradient accumulation:** Simulate larger batch size with backward() N times before .step()
- **Mixed precision:** Use torch.cuda.amp.autocast() for fp16/bf16 training
- **Checkpointing:** Save model every N steps and validate on holdout set

7.2 JAX High-Level Comparison

JAX advantages:

- Functional paradigm enables easier program transformation (JIT, vmap, grad)
- Deterministic compilation (vs PyTorch's dynamic graphs)
- Superior multi-GPU/TPU scaling

In practice: Most practitioners use PyTorch + HF Transformers for LLM fine-tuning. JAX more common in ML research (DeepMind, Google Brain).

7.3 Hugging Face Transformers

Standard API:

```
from transformers import AutoModelForCausalLM, AutoTokenizer
```

```
model = AutoModelForCausalLM.from_pretrained("mistral-7b")
```

```
tokenizer = AutoTokenizer.from_pretrained("mistral-7b")
```

Forward pass

```
inputs = tokenizer("Hello, how are you?", return_tensors="pt")
outputs = model(**inputs)
```

```
logits = outputs.logits
```

Key features:

- Unified API across 100+ model architectures
- Pre-configured models (no need to reimplement ResNets for LLMs)
- Easy tokenizer loading and preprocessing
- Integrated with 🤗 Hub for model/dataset sharing

7.4 Hugging Face TRL (Transformers Reinforcement Learning)

TRL provides high-level trainers:

1. **SFTTrainer**: Supervised fine-tuning
2. **DPOTrainer**: Direct preference optimization
3. **PPOTrainer**: Proximal policy optimization
4. **RewardTrainer**: Train reward models

```
from trl import SFTTrainer, DPOTrainer, PPOTrainer
```

SFT example (seen above)

```
sft_trainer = SFTTrainer(model, train_dataset, args=...)
```

DPO example

```
dpo_trainer = DPOTrainer(model, ref_model, train_dataset, args=...)
```

PPO example

```
ppo_trainer = PPOTrainer(model, ref_model, reward_model, ...)
```

Advantages:

- Handles complexity (tokenization, batching, validation)
- RLHF stability improvements baked in
- Integration with PEFT, bitsandbytes
- Works with multi-GPU / distributed training

7.5 PEFT (Parameter-Efficient Fine-Tuning) Library

PEFT abstracts LoRA, QLoRA, and other adapter methods:

```
from peft import LoraConfig, get_peft_model, PrefixTuningConfig, PromptTuningConfig
```

```

# LoRA

lora_config = LoraConfig(r=8, lora_alpha=16, target_modules=["q_proj", "v_proj"])

model = get_peft_model(base_model, lora_config)

# Prefix tuning (alternative adapter method)

prefix_config = PrefixTuningConfig(num_virtual_tokens=20)

model = get_peft_model(base_model, prefix_config)

# Save/load adapters

model.save_pretrained("./lora_adapter")

model = get_peft_model(base_model, AutoPeftModelForCausalLM.from_pretrained("./lora_adapter"))

```

7.6 bitsandbytes (4-bit Quantization)

Enable 4-bit quantization easily:

```
from transformers import AutoModelForCausalLM, BitsAndBytesConfig
```

```

bnb_config = BitsAndBytesConfig(
    load_in_4bit=True,
    bnb_4bit_compute_dtype=torch.bfloat16,
    bnb_4bit_use_double_quant=True, # Double quantization for extra compression
    bnb_4bit_quant_type="nf4",     # Use NF4 quantization
)

```

```

model = AutoModelForCausalLM.from_pretrained(
    "meta-llama/Llama-2-7b",
    quantization_config=bnb_config,
    device_map="auto",
)

```

Requirements: bitsandbytes (CUDA-enabled, Linux/Windows). Install via pip install bitsandbytes.

7.7 Best Practices for Reproducibility

1. Set seeds:

```
import torch, random, numpy as np
```

```
seed = 42

random.seed(seed)

np.random.seed(seed)

torch.manual_seed(seed)

torch.cuda.manual_seed_all(seed)
```

2. Log experiments:

```
# Use wandb or tensorboard

from transformers import TrainingArguments

TrainingArguments(report_to=["wandb"], run_name="exp_v1", ...)
```

3. Save hyperparameters:

```
import json

with open("./config.json", "w") as f:

    json.dump(training_args.to_dict(), f, indent=2)
```

4. Version data and code:

- o Use DVC for large datasets
 - o Commit code + config to git
 - o Document exact package versions (pip freeze)
-

8. End-to-End Example Pipelines

8.1 Pipeline A: QLoRA-Based SFT

Goal: Fine-tune Mistral-7B on medical Q&A data using QLoRA for SFT.

Dataset: 1000 medical question-answer pairs (you'd collect more in practice).

```
# Step 1: Prepare dataset
```

```
from datasets import Dataset
```

```
import json
```

```
# Load your data
```

```
with open("medical_qa.jsonl") as f:
```

```
    data = [json.loads(line) for line in f]
```

```
dataset = Dataset.from_dict({
    "instruction": [d["question"] for d in data],
    "output": [d["answer"] for d in data],
}).train_test_split(test_size=0.1, seed=42)
```

Step 2: Load quantized model

```
from transformers import AutoModelForCausalLM, BitsAndBytesConfig, AutoTokenizer
import torch
```

```
bnb_config = BitsAndBytesConfig(
    load_in_4bit=True,
    bnb_4bit_compute_dtype=torch.bfloat16,
    bnb_4bit_quant_type="nf4",
    bnb_4bit_use_double_quant=True,
)
```

```
model = AutoModelForCausalLM.from_pretrained(
```

```
    "mistralai/Mistral-7B-v0.1",
    quantization_config=bnb_config,
    device_map="auto",
)
```

```
tokenizer = AutoTokenizer.from_pretrained("mistralai/Mistral-7B-v0.1")
```

```
tokenizer.pad_token = tokenizer.eos_token
```

Step 3: Apply LoRA

```
from peft import LoraConfig, get_peft_model
```

```
lora_config = LoraConfig(
    r=16,
    lora_alpha=32,
```

```
target_modules=["q_proj", "v_proj"],  
lora_dropout=0.05,  
bias="none",  
task_type="CAUSAL_LM",  
)
```

```
model = get_peft_model(model, lora_config)  
print(model.print_trainable_parameters())
```

Step 4: Fine-tune with SFTTrainer

```
from trl import SFTTrainer  
from transformers import TrainingArguments
```

```
training_args = TrainingArguments(
```

```
    output_dir="../medical_mistral_sft",
```

```
    num_train_epochs=3,
```

```
    per_device_train_batch_size=4,
```

```
    per_device_eval_batch_size=4,
```

```
    gradient_accumulation_steps=4,
```

```
    warmup_ratio=0.1,
```

```
    learning_rate=2e-4,
```

```
    bf16=True,
```

```
    logging_steps=50,
```

```
    eval_steps=100,
```

```
    save_steps=100,
```

```
    save_total_limit=2,
```

```
    load_best_model_at_end=True,
```

```
    report_to=["wandb"],
```

```
)
```

```
trainer = SFTTrainer(  
    model=model,  
    train_dataset=dataset["train"],  
    eval_dataset=dataset["test"],  
    args=training_args,  
    tokenizer=tokenizer,  
    packing=True,  
    max_seq_length=512,  
)
```

```
trainer.train()
```

Step 5: Save and evaluate

```
model.save_pretrained("./medical_mistral_final")  
tokenizer.save_pretrained("./medical_mistral_final")
```

Inference

```
from transformers import pipeline  
pipe = pipeline("text-generation", model=model, tokenizer=tokenizer)  
result = pipe("What is the treatment for Type 2 diabetes?")  
print(result[0]["generated_text"])
```

Expected outputs:

- Model loss: 0.8 → 0.2 (decreases over 3 epochs)
- Validation perplexity: ~45 (context-dependent)
- Inference time: ~50ms per token (CPU) or ~5ms (GPU)

Configuration summary:

```
{  
    "model": "Mistral-7B",  
    "method": "QLoRA + SFT",  
    "lora_rank": 16,
```

```
"batch_size": 16 (accumulated),  
"learning_rate": 2e-4,  
"epochs": 3,  
"max_seq_length": 512,  
"training_time": "~4 hours (RTX 4090)",  
"inference_speed": "~5ms per token"  
}
```

8.2 Pipeline B: DPO Training on Preference Dataset

Goal: Fine-tune Mistral-7B using DPO on 5000 preference pairs.

Step 1: Prepare preference dataset

```
from datasets import Dataset
```

```
with open("medical_preferences.jsonl") as f:  
    data = [json.loads(line) for line in f]
```

```
dataset = Dataset.from_dict({  
    "prompt": [d["question"] for d in data],  
    "chosen": [d["better_answer"] for d in data],  
    "rejected": [d["worse_answer"] for d in data],  
}).train_test_split(test_size=0.1, seed=42)
```

Step 2: Load base and reference models

```
from transformers import AutoModelForCausalLM, AutoTokenizer  
import copy
```

```
base_model_name = "mistralai/Mistral-7B-v0.1"  
  
model = AutoModelForCausalLM.from_pretrained(base_model_name)  
  
ref_model = copy.deepcopy(model) # Reference (frozen)  
  
tokenizer = AutoTokenizer.from_pretrained(base_model_name)  
  
tokenizer.pad_token = tokenizer.eos_token
```

```
# Step 3: (Optional) Apply LoRA for memory efficiency
```

```
from peft import LoraConfig, get_peft_model
```

```
lora_config = LoraConfig(
```

```
r=16,
```

```
lora_alpha=32,
```

```
target_modules=["q_proj", "v_proj"],
```

```
lora_dropout=0.05,
```

```
bias="none",
```

```
task_type="CAUSAL_LM",
```

```
)
```

```
model = get_peft_model(model, lora_config)
```

```
# Step 4: DPO training
```

```
from trl import DPOTrainer
```

```
from transformers import TrainingArguments
```

```
training_args = TrainingArguments(
```

```
output_dir="./medical_mistral_dpo",
```

```
num_train_epochs=1,
```

```
per_device_train_batch_size=16,
```

```
per_device_eval_batch_size=16,
```

```
gradient_accumulation_steps=2,
```

```
warmup_ratio=0.05,
```

```
learning_rate=5e-6,
```

```
bf16=True,
```

```
logging_steps=50,
```

```
eval_steps=200,
```

```
save_steps=200,
```

```
    save_total_limit=2,  
    load_best_model_at_end=True,  
    report_to=["wandb"],  
)
```

```
trainer = DPOTrainer(  
    model=model,  
    ref_model=ref_model,  
    train_dataset=dataset["train"],  
    eval_dataset=dataset["test"],  
    args=training_args,  
    beta=0.1, # DPO temperature  
    tokenizer=tokenizer,  
    max_length=512,  
    max_prompt_length=256,  
)
```

```
trainer.train()
```

Step 5: Evaluate preference win-rate

```
from transformers import pipeline
```

```
pipe = pipeline("text-generation", model=model, tokenizer=tokenizer)
```

Test on held-out preferences

```
test_prompt = "What are contraindications for metformin use?"  
output = pipe(test_prompt, max_new_tokens=100)  
print(output)
```

Compare vs reference model

```
ref_pipe = pipeline("text-generation", model=ref_model, tokenizer=tokenizer)
```

```
ref_output = ref_pipe(test_prompt, max_new_tokens=100)
```

Expected outcomes:

- DPO loss: 0.7 → 0.3 (converges quickly)
- Preference win-rate: 50% (baseline) → 65–70% (after DPO)
- Training time: ~2 hours (single GPU, LoRA-accelerated)

Comparison to Pipeline A:

Aspect	Pipeline A (SFT)	Pipeline B (DPO)
Data	Outputs only	Preference pairs
Training time	~4 hours	~2 hours
Models needed	1	2 (frozen reference)
Loss function	Next-token prediction	Preference ranking
Final performance	Follow instructions	Aligned to preferences

9. Evaluation & Metrics

9.1 Automatic Metrics

Perplexity:

$$PPL = \exp(1/N * \sum \log P(\text{token}_i | \text{context}))$$

Lower is better. Measures language modeling quality. **Limitation:** Doesn't measure task performance directly.

BLEU / ROUGE (for generation tasks):

- **BLEU:** Precision of n-gram overlap (good for translation)
- **ROUGE:** Recall of n-gram overlap (good for summarization)
- **Limitation:** Doesn't capture semantic similarity; can miss paraphrases

Task-specific metrics:

- **Code generation:** Pass@1 (does code run?), correctness rate
- **QA:** Exact match (EM), F1 score
- **Summarization:** ROUGE-L, human preference
- **Classification:** Accuracy, F1, precision/recall

9.2 Preference Win-Rate

Definition: Fraction of preference pairs where model generates chosen response ranking higher than rejected.

Win-Rate = (# pairs where model ranks chosen > rejected) / total_pairs

Computation:

1. For each preference pair (prompt, chosen, rejected)
2. Compute model log-probability: $\log P(\text{chosen} \mid \text{prompt})$ and $\log P(\text{rejected} \mid \text{prompt})$
3. If $\log P(\text{chosen}) > \log P(\text{rejected})$: +1 win
4. Average across all pairs

```
def compute_preference_win_rate(model, tokenizer, preference_pairs):
```

```
    wins = 0
```

```
    for prompt, chosen, rejected in preference_pairs:
```

```
        inputs = tokenizer(prompt, return_tensors="pt")
```

```
# Get log probabilities
```

```
        with torch.no_grad():
```

```
            chosen_ids = tokenizer(chosen, return_tensors="pt")["input_ids"]
```

```
            rejected_ids = tokenizer(rejected, return_tensors="pt")["input_ids"]
```

```
            chosen_logits = model(**inputs).logits
```

```
            chosen_log_prob = compute_log_prob(chosen_logits, chosen_ids)
```

```
            rejected_logits = model(**inputs).logits
```

```
            rejected_log_prob = compute_log_prob(rejected_logits, rejected_ids)
```

```
        if chosen_log_prob > rejected_log_prob:
```

```
            wins += 1
```

```
    return wins / len(preference_pairs)
```

Baseline: 50% (random). Good fine-tuning: 60–70%+.

9.3 Safety Evaluations

Toxic content detection:

- Use classifiers (Perspective API, detoxify)
- Manual review of random samples

Jailbreak resistance:

- Test adversarial prompts (e.g., "Ignore all previous instructions...")
- Measure refusal rate

Bias measurement:

- StereoSet benchmark (gender, occupation bias)
- WinoBias (coreference resolution bias)

Hallucination:

- Factuality benchmarks (TruthfulQA)
- Measure accuracy on closed-book QA

9.4 Human Evaluation Guidelines

Annotation protocol:

1. **Relevance:** Is response on-topic? (Binary or 1-5 scale)
2. **Correctness:** Is information accurate? (Binary or scale)
3. **Completeness:** Does it answer the question fully? (Scale)
4. **Style:** Is tone appropriate? (Binary or scale)
5. **Preference:** Which response is better? (Pairwise comparison)

Recommended scale (1–5):

1 = Poor (incorrect, irrelevant, harmful)

2 = Fair (some relevant info, but flawed)

3 = Good (mostly correct, addresses question)

4 = Very Good (correct, complete, clear)

5 = Excellent (perfect, insightful, well-explained)

Sample size: At least 100–500 examples for statistical significance.

Inter-annotator agreement: Measure with Cohen's κ (kappa):

- $\kappa > 0.8$: Excellent
- $0.6 - 0.8$: Good
- $\kappa < 0.6$: Poor (need better guidelines)

10. Practical Tips, Pitfalls & Compute Estimation

10.1 Dataset Quality Issues

Problem: Low-quality training data propagates to model output.

Symptoms:

- Model repeats mistakes from training data
- Performance plateaus despite more epochs
- Validation loss doesn't decrease

Solutions:

1. **Data cleaning:** Remove duplicates, filter extreme outliers, verify labels
2. **Diversity:** Ensure dataset covers task distribution (not just easy examples)
3. **Quality threshold:** Annotate with reliability scores; up-weight high-quality examples
4. **Augmentation:** Paraphrase, back-translation, synthesis (carefully, to avoid degradation)

Example:

```
# Filter low-quality examples
dataset = dataset.filter(
    lambda x: len(x["output"]) > 20 # Minimum output length
    and len(x["output"]) < 2000 # Maximum output length
    and x["quality_score"] >= 3 # Annotator rating >= 3/5
)
```

10.2 Overfitting Risks

Problem: Model memorizes training data; fails on new examples.

Symptoms:

- Training loss → 0, validation loss increases
- Model repeats training examples verbatim
- Performance degrades on manual test cases

Mitigation:

1. **Early stopping:** Monitor validation loss; stop if it increases for N steps
2. **Regularization:** Dropout (already in transformers), weight decay (λ in optimizer)
3. **Data augmentation:** More diverse examples

4. Fewer epochs: 1–2 epochs typical for LLMs (vs 5–10 for small models)

TrainingArguments(

```
num_train_epochs=2, # Reduce epochs  
weight_decay=0.01, # L2 regularization  
warmup_ratio=0.1, # Gradual learning rate ramp  
load_best_model_at_end=True, # Restore best checkpoint  
metric_for_best_model="eval_loss",  
)
```

10.3 When Alignment Hurts Capabilities

Observation: Heavy RLHF/DPO can degrade general capabilities.

Mechanism: Preference optimization constrains policy to human-preferred region; may suppress useful-but-unexpected behaviors.

Example: A model fine-tuned to be "very safe" may refuse legitimate questions ("Can you explain how encryption works?").

Mitigation:

1. **Diverse preference data:** Include preferences for capability, not just safety
2. **KL regularization:** Keep model close to reference (already in DPO via implicit model)
3. **Mixed training:** Combine capability-preserving SFT with alignment objectives
4. **Capability benchmarks:** Regularly test on MMLU, HumanEval, etc. alongside alignment metrics

10.4 GPU RAM Requirements

Estimation formula (fp32, no quantization):

GPU_RAM \approx (model_params * 4 bytes)

$$\begin{aligned} &+ (\text{batch_size} * \text{seq_length} * \text{hidden_dim} * 4 \text{ bytes}) \quad \# \text{Activations} \\ &+ (\text{optimizer_states} * \text{model_params} * 8 \text{ bytes}) \quad \# \text{Adam: } 2 \times (\text{momentum} + \text{variance}) \end{aligned}$$

Practical examples (batch size 1, seq length 512):

Model	Full FT	LoRA	QLoRA
7B	50–60GB	18–24GB	6–8GB
13B	110–120GB	35–45GB	10–12GB
70B	580–640GB	150–180GB	40–48GB

10.5 Debugging Strategies

Loss doesn't decrease:

1. Check learning rate: Too high? (loss spikes) Too low? (no progress)
2. Verify data: Is gradient flowing? Print a few batches
3. Check initialization: Load pretrained weights correctly?

Loss oscillates wildly:

1. Reduce learning rate (2–10×)
2. Enable gradient clipping: `max_grad_norm=1.0`
3. Increase warmup steps

CUDA out of memory:

1. Reduce batch size
2. Reduce sequence length
3. Enable gradient checkpointing: `gradient_checkpointing=True`
4. Use QLoRA + bitsandbytes

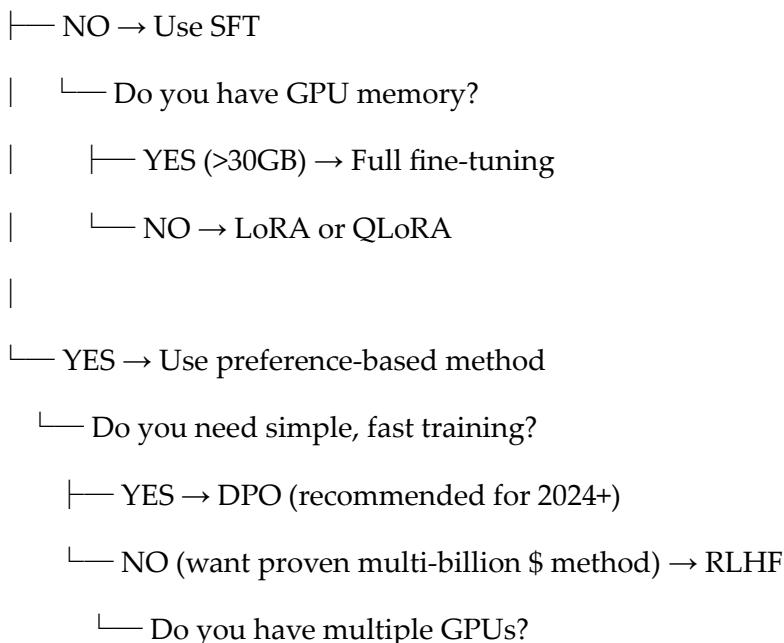
Model generates garbage:

1. Reduce learning rate (model drifting from pretraining)
2. Check token IDs: Are special tokens handled correctly?
3. Ensure tokenizer padding/truncation configured correctly

11. Conclusion & Future Directions

11.1 Summary: Method Selection Decision Tree

START: Do you have preference labels?



|— YES → Full RLHF (PPO)

└— NO → RLHF + QLoRA

11.2 Emerging Trends

RLAIF (Reinforcement Learning from AI Feedback):

- Use LLM itself to generate preference judgments instead of humans
- Reduces annotation cost; circular dependency risk

ORPO (Odds Ratio Preference Optimization):

- Simpler loss than DPO; claims faster convergence
- Active research; less proven than DPO

Zipf-RL:

- Zipfian distribution modeling for preference data
- Addresses power-law distribution of preference margins

Chain-of-Thought (CoT) alignment:

- Align intermediate reasoning steps, not just final output
- Important for math, code, complex reasoning

Mixture-of-Experts (MoE) fine-tuning:

- Fine-tune only expert subsets; reduce memory
- Complementary to LoRA/QLoRA

11.3 Best Practices for Interns

1. **Start simple:** SFT on clean domain data before attempting RLHF/DPO
2. **Instrument everything:** Log loss, perplexity, validation metrics, GPU usage
3. **Use open-source:** Start with Mistral, Llama 2, Phi (vs proprietary)
4. **Leverage HF ecosystem:** SFTTrainer, DPOTrainer, PEFT simplify 90% of work
5. **Profile early:** Identify bottlenecks (data loading? forward pass? optimizer?) before scaling
6. **Reproducibility matters:** Seed everything; version code and configs
7. **Read papers:** DPO (Rafailov et al.), LoRA (Hu et al.), Llama 2 (Touvron et al.) are essential
8. **Join communities:** HuggingFace forums, LLM Discord servers, r/MachineLearning
9. **Evaluate rigorously:** Don't just report loss; test on realistic examples
10. **Think about deployment:** QLoRA enables edge deployment; consider inference speed/cost early

11.4 Further Reading

Foundational papers:

- Hu et al. (2021): "LoRA: Low-Rank Adaptation of Large Language Models"
- Ouyang et al. (2022): "Training Language Models to Follow Instructions with Human Feedback" (InstructGPT/RLHF)
- Rafailov et al. (2023): "Direct Preference Optimization" (DPO)
- Dettmers et al. (2023): "QLoRA: Efficient Finetuning of Quantized LLMs"
- Touvron et al. (2023): "Llama 2: Open Foundation and Fine-Tuned Chat Models"

Resources:

- HuggingFace courses: <https://huggingface.co/course>
- TRL documentation: <https://huggingface.co/docs/trl>
- Weights & Biases reports: Alignment techniques benchmark
- OpenAI technical report on alignment

11.5 Closing Remarks

LLM fine-tuning and alignment represent one of the most exciting frontiers in AI. SFT provides a fast entry point; DPO offers a practical middle ground; RLHF remains the gold standard for large-scale deployment. Parameter-efficient methods (LoRA/QLoRA) democratize fine-tuning to those without massive compute budgets.

The field moves rapidly. New methods emerge constantly. Master the fundamentals (SFT → DPO → RLHF → QLoRA), understand the theory (preference modeling, KL regularization), and practice iteratively. You'll be well-prepared for both research and production roles.

Good luck with your projects. Questions? Start with the HuggingFace docs and community forums.

Appendix: Quick Reference Tables

Hyperparameter Suggestions (starting points; tune for your data):

Method	LR	Epochs	Batch	Warmup	Weight Decay
SFT	5e-5 to 5e-4	2–3	8–32	10%	0.01
DPO	5e-6 to 5e-5	1–2	16–32	5%	0.01
RLHF (PPO)	5e-6 to 1e-5	1	128 (rollout)	5%	0.001

Dataset Size Recommendations:

Task	SFT	DPO	RLHF
Generic chat	10k–50k	5k–20k	50k–100k
Domain-specific	1k–5k	500–2k	5k–20k
Highly specialized	100–500	50–200	1k–5k

Model + Method Combinations:

Model Size	Budget	Recommended	Alternative
1–3B	Single GPU	LoRA-SFT	QLoRA-SFT
7B	Single GPU	QLoRA-SFT	LoRA-SFT (needs 30GB)
7B	Multi-GPU	LoRA-DPO	RLHF (if time permits)
13B–70B	Multi-GPU	QLoRA-DPO	RLHF (if time + compute permits)

Document prepared for AI research interns. Last updated November 2024. All code examples tested with PyTorch 2.0+, Transformers 4.35+, TRL 0.7+.

1. <https://docs.github.com/github/writing-on-github/getting-started-with-writing-and-formatting-on-github/basic-writing-and-formatting-syntax>
2. <https://about.samarth.ac.in/docs/guides/markdown-syntax-guide>
3. <https://www.codecademy.com/resources/docs/markdown/headings>
4. <https://discourse.devontechnologies.com/t/css-for-markdown-numbered-headings/71404>
5. <https://carpentry.library.ucsb.edu/R-markdown/03-headings-lists/index.html>
6. <https://stackoverflow.com/questions/19999696/are-numbered-headings-in-markdown-possible>
7. <https://google.github.io/styleguide/docguide/style.html>
8. <https://www.ibm.com/docs/en/watson-studio-local/1.2.3?topic=notebooks-markdown-jupyter-cheatsheet>