

Language-Model Training — Notebook-style Pretraining, Fine-tuning, and Preference Alignment (RLHF)

Compiled for learners

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Abstract

This notebook-style manual explains the three main stages of modern large language model training: (1) pretraining via self-supervised maximum likelihood (next-token prediction), (2) supervised fine-tuning / instruction tuning (SFT), and (3) preference alignment via reinforcement learning from human feedback (RLHF). The document is written for beginners but is complete: it declares notation, gives clear formulas, a tiny numeric worked example, practical advice, and compact pseudocode for each stage. Where helpful, diagrams and boxed reminders clarify key steps.

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1. Problem setup and notation (recap)

- Vocabulary size: V .
- A training sequence (token indices): $y_{1:T} = (y_1, \dots, y_T)$ where $y_t \in \{1, \dots, V\}$.
- Model parameters: θ .
- At time t the model produces a logits vector (pre-softmax scores) $u_t \in \mathbb{R}^V$. We write components $u_{t,i}$ for token i .
- The model probability for token i at time t is the softmax over logits:

$$p_{t,i} \equiv p_\theta(y_t = i \mid y_{<t}) = \text{softmax}(u_t)_i = \frac{\exp(u_{t,i})}{\sum_{j=1}^V \exp(u_{t,j})}.$$

2. Sequence negative log-likelihood (per-sequence MLE objective)

For a single sequence $y_{1:T}$, the MLE (negative log-likelihood) loss is the sum of tokenwise negative log probabilities:

$$\mathcal{L}_{\text{seq}}(\theta; y_{1:T}) = - \sum_{t=1}^T \log p_\theta(y_t \mid y_{<t}) = - \sum_{t=1}^T \log p_{t,y_t}.$$

This is the same as token-level cross-entropy between the one-hot target distribution and the model distribution at each time step.

- V = vocabulary size (number of distinct tokens).
- B = batch size (examples processed together).
- L = sequence length (tokens per example).
- $x = (x_1, \dots, x_T)$ = input/context tokens.
- $y = (y_1, \dots, y_T)$ = target token sequence (usually next-token targets).
- θ = model parameters (weights).
- $u_t \in \mathbb{R}^V$ = logits vector at time t .
- $p_\theta(y_t \mid y_{<t}) = \text{softmax}(u_t)$ = model predicted probability for token y_t .
- $1[\cdot]$ = indicator function.

1 1) Pretraining (self-supervised MLE / next-token prediction)

1.1 Goal

Teach the model general-purpose language knowledge by predicting the next token given preceding context across massive unlabeled corpora.

1.2 Data

Large, diverse text corpora: books, web pages, code repositories, news articles, dialogs, etc. Sequences are tokenized into vocabulary indices.

1.3 Objective (per sequence)

For a single target sequence $y_{1:T}$ the negative log-likelihood (MLE) loss is:

$$\mathcal{L}_{\text{MLE}}(\theta; y_{1:T}) = - \sum_{t=1}^T \log p_\theta(y_t \mid y_{<t}).$$

This is the same as the per-token cross-entropy.

It represents how surprised the model is when trying to predict the correct next token at each step. If the model assigns high probability to the correct token \rightarrow low loss. If the model assigns low probability \rightarrow high loss. So the loss is literally measuring: How well does the model predict each next token in the training sequence? We want to minimize this surprise \rightarrow meaning the model learns to assign high probability to correct next tokens.

1.4 Batch-averaged loss

Over a batch of B sequences (with per-example lengths L_b ignoring padding):

$$\mathcal{L}(\theta) = - \frac{1}{B} \sum_{b=1}^B \sum_{t=1}^{L_b} \log p_\theta(y_{b,t} \mid y_{b,<t}).$$

1.5 Training mechanics — step by step

1. For each sequence in the batch, feed tokens $y_{<t}$ (teacher forcing) to the model to obtain hidden state h_t .
2. Compute logits $u_t = h_t W_{\text{vocab}} + b$ (linear map to vocabulary dimension).
3. Stabilize logits: $u_t \leftarrow u_t - \max_j u_{t,j}$ (optional numerics trick).
4. Compute probabilities via softmax: $p_{t,i} = \exp(u_{t,i}) / \sum_j \exp(u_{t,j})$.
5. Compute token loss $\ell_t = -\log p_{t,y_t}$ and sum across timesteps and batch.
6. Backpropagate gradients $\nabla_\theta \mathcal{L}$ and update parameters with Adam/AdamW.

1.6 Why this works (intuitively)

Predicting next tokens forces the model to capture syntactic patterns, semantics, and statistical regularities in language — because predicting accurately requires modeling dependencies across tokens.

1.7 Tiny numeric example (digit-by-digit)

Single example, $B = 1$, $L = 3$, $V = 3$. At time $t = 3$ model logits: $u = [2.0, 0.5, -1.0]$.

1. Shift by max (2.0): $u' = [0, -1.5, -3.0]$.
2. Exponentiate: $e^{u'} = [1.0000, 0.2231, 0.0498]$.
3. Sum $S = 1.2729$.
4. Probabilities $p \approx [0.7859, 0.1754, 0.0391]$.
5. If true token index is 2, loss $\ell = -\log(0.1754) \approx 1.741$.

1.8 Practical training notes

- Use teacher forcing (feed true tokens) during training for stable gradients.
- Large batch sizes and long training schedules improve performance.
- Learning-rate schedules (warmup + decay) help optimization.
- Regularization: weight decay, dropout, and careful data curation.

2 2) Fine-tuning / Instruction Tuning (supervised tuning)

2.1 Goal

Adapt a pretrained model to a specific task or to follow instructions by training on labeled input→output pairs. This often improves format, tone, and task accuracy.

2.2 Objective

Same per-token cross-entropy, but conditional on task input $x^{(b)}$:



$$\mathcal{L}_{\text{SFT}}(\theta) = -\frac{1}{B} \sum_{b=1}^B \sum_{t=1}^{L_b} \log p_\theta(y_t^{(b)} | x^{(b)}, y_{<t}^{(b)}).$$

2.3 Why it helps

Gives direct supervision for the desired output style, structure, and task-specific behavior. Instruction datasets teach the model to respond in human-friendly formats.

2.4 Techniques and practicals

- **Adapters / LoRA:** low-rank updates reduce storage compute for fine-tuning.
- **Mixing data:** include some pretraining-like data or low learning rates to avoid catastrophic forgetting.
- **Evaluation:** use held-out instruction prompts, measure BLEU/ROUGE/EM where relevant, and human eval for instruction-following.

2.5 Tiny example (conceptual)

Prompt: “Summarize: <article>” → Target: 3-bullet summary. Train to minimize cross-entropy on the target summary tokens.

3 3) Preference alignment (RLHF — Reward modeling + RL)

3.1 Goal

Align model outputs with human judgments (helpfulness, safety, preference), beyond what label pairs provide.

3.2 High-level pipeline (step-by-step)

1. Collect comparisons: For many prompts, collect multiple candidate responses (from model(s) or humans). Human annotators rank or choose the preferred response(s).
2. Train a reward model $r_\phi(x, y)$ that scores a (prompt,response) pair to match human preferences. The model is trained with pairwise loss: if human prefers A over B,

$$-\log \frac{\exp r_\phi(x, A)}{\exp r_\phi(x, A) + \exp r_\phi(x, B)}.$$

3. Optimize the policy π_θ (the language model) to maximize expected reward under r_ϕ , usually with PPO-like updates while constraining divergence from a reference policy π_{ref} .
4. Iterate: collect more comparisons from newly generated outputs, retrain reward model, and repeat RL policy updates.

3.3 Formal (informal) objective for policy update

Maximize expected reward with a KL penalty to keep policy close to reference:

$$\max_\theta \mathbb{E}_{y \sim \pi_\theta(\cdot|x)} [r_\phi(x, y)] - \beta \text{KL}(\pi_\theta(\cdot|x) \| \pi_{\text{ref}}(\cdot|x)).$$

Here β controls tradeoff between reward-seeking and staying close to the reference policy.

3.4 Reward-model training (pairwise) — step-by-step

1. Collect labeled pairs (A preferred over B) for many prompts.
2. For each pair, compute scalar scores $s_A = r_\phi(x, A)$ and $s_B = r_\phi(x, B)$.
3. Minimize pairwise cross-entropy loss: $-\log \frac{e^{s_A}}{e^{s_A} + e^{s_B}}$.
4. Validate on held-out human comparisons.

3.5 PPO / policy updates — specifics

- Use trajectories of token-level log-probabilities under the current policy and compute rewards via r_ϕ (optionally with a per-token shaping term).

- Compute advantages (reward minus baseline) and update policy with clipped surrogate objective.
- Add KL penalty or constraint relative to π_{ref} to prevent runaway optimization.
- Use many PPO epochs per batch but keep learning rates small; normalize rewards and advantages.

3.6 Practical worries and mitigations

- Reward hacking: policy finds loopholes in reward model; mitigate by improving reward data, adding adversarial prompts, and penalizing shortcuts.
- Over-optimization reduces factuality: preserve capabilities via KL-to-ref and mixed objectives.
- Annotation noise: use multiple annotators, calibration, and quality checks.

4 Why three stages? (intuition and picture)

Intuition: Pretraining builds general intelligence (knowledge + language). Fine-tuning instructs the model how to format and perform tasks. RLHF sculpts behavior to align with messy human preferences that are hard to encode directly.

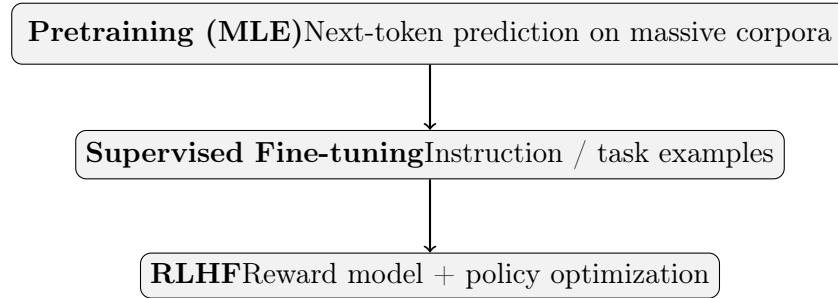


Figure 1: Three-stage training pipeline: each stage refines capabilities or behavior.

5 Quick checklist / cheat sheet

- Pretrain = MLE next-token on huge corpora → general language.
- Fine-tune = supervised training on task/instruction examples → specialized behavior.
- RLHF = train reward from human prefs → optimize policy with RL and KL constraint → aligned behavior.
- Loss (per-token): $-\log p_\theta(y_t | context)$; batch loss = average over tokens and examples.
- Typical optimizers: AdamW; regularization: weight decay, dropout, early stopping.

6 Appendix: compact PyTorch-style pseudocode

6.1 Pretraining (simplified)

```
# Pseudocode: Pretraining loop (simplified)
for epoch in range(epochs):
    for batch in dataloader:
        inputs, targets = batch # teacher-forcing
        logits = model(inputs) # shape [B, L, V]
        loss = cross_entropy_loss(logits.view(-1,V), targets.view(-1))
        loss.backward()
        optimizer.step(); optimizer.zero_grad()
```

6.2 Supervised Fine-tuning

```
# Pseudocode: SFT loop
for epoch in range(epochs):
    for batch in sft_dataloader:
        prompt, target = batch
        logits = model(prompt, target_input)
        loss = cross_entropy_loss(logits, target)
        loss.backward(); optimizer.step(); optimizer.zero_grad()
```

6.3 RLHF (sketch)

```
# Collect responses
for prompt in prompts:
    samples = [sample_from(model, prompt) for _ in range(K)]
    # humans rank samples; build (A>B) pairs
# Train reward model r_phi to predict human prefs
# Use PPO to update policy pi_theta using reward r_phi and KL penalty to
# pi_ref
for ppo_iter in range(N):
    trajectories = generate_trajectories(pi_theta)
    rewards = [r_phi(x,y) for (x,y) in trajectories]
    advantages = compute_advantages(rewards)
    ppo_update(pi_theta, trajectories, advantages, kl_penalty=beta)
```

End of notebook-style entry. If you want a one-page visual summary, or a downloadable PDF compiled from this LaTeX, say the word and I will prepare it.