

Fine-tuning Computational Info

LLMs for Drug-Drug Interaction Prediction

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1 GPT-4o Fine-tuning

Regarding the computational aspects, GPT-4o fine-tuning was performed via OpenAI API at a cost of approximately \$20.68 for 1,000 training examples over 3 epochs, totaling 827,007 trained tokens and lasting 1 hour and 2 minutes.

2 Fine-tuning of Open-weight LLMs

Table 1 details the computational resources required for each open-weight model. Phase 1 average time per trial represents the mean duration across all 1,000 trials including pruned trials. Phase 2 average time per trial represents the mean duration of full runs without pruning. Total time includes both phases plus intermediate processing.

During Phase 1, the SuccessiveHalvingPruner eliminated approximately 97–99% of trials before completion, yielding substantial compute savings. The pruner typically discarded unpromising configurations after 1–2 evaluations (iterations 5–10). On Phi-3.5 2.7B ($\approx 500\text{--}700$ tokens/s on our machine), each pruned trial took about 1 to 2 minutes of wall time, including validation. When we examined larger models like Gemma2 9B, which ran about 3 to 5 times slower, the time increased to roughly 4 to 8 minutes per pruned trial. Phase-2 throughput depended on model size. On models with 1.5–2.7 billion parameters, we observed about 1.5–3 trials/hour, while on models with 9 billion parameters, we observed about 0.4–0.8 trials/hour. The validation loss typically plateaued within the first 100–200 iterations; the remaining iterations confirmed stability and served as a guard against premature selection.

Table 1: Computational Resources per Model during the Optuna optimization process. Avg Time represents the average time per trial.

Model	Phase 1			Phase 2			Total	
	Trials	Avg Time	Dur.	Trials	Avg Time	Dur.	Time	Peak Mem.
DeepSeek R1 1.5B	1,000	1.2 min	20 hrs	12	15 min	3 hrs	23 hrs	35 GB
Phi-3.5 2.7B	1,000	1.8 min	30 hrs	10	95 min	16 hrs	46 hrs	42 GB
Qwen2.5 3B	1,000	1.9 min	32 hrs	11	85 min	15.5 hrs	47.5 hrs	44 GB
Gemma2 9B	1,000	4.2 min	70 hrs	9	110 min	16.5 hrs	86.5 hrs	78 GB