

LeanCOCONUT: Latent Chain-of-Thought for Lean 4 Tactic Prediction

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Abstract

Lean 4 theorem proving is a promising foundation for high-assurance software verification, but automatic tactic synthesis remains difficult due to the combinatorial structure of the proof search space. We investigate whether latent chain-of-thought reasoning (Coconut; Hao et al., 2024) can improve tactic diversity and pass@k performance in Lean 4 next-tactic prediction. We train decoder-only transformers from scratch on the LeanDojo benchmark and compare standard autoregressive generation against Coconut latent-state perturbation during inference. Across both scales, Coconut produces small but consistent improvements in pass@k and diversity-gap metrics. Multi-stage latent recirculation further improves diversity in a controlled low-data regime. We additionally identify and correct two sources of evaluation leakage: unshifted-label training leakage and train/test contamination in the public benchmark split.

Repo: https://github.com/galfaroi/lean_coconut

Introduction

Problem

Formal verification requires producing machine-checkable proofs in proof assistants such as Lean 4. The core bottleneck is **tactic synthesis**: given a proof state, propose the next tactic. The space of valid tactics is unbounded and most candidates fail immediately, so generating a small **diverse** set of likely candidates is more useful than a single greedy prediction.

Why this matters

Formal verification is increasingly important for secure program synthesis, high-assurance software, and AI-assisted theorem proving. Lean 4 tactic prediction is a challenging benchmark because valid proof steps are sparse, highly compositional, and often admit multiple semantically correct solutions. In practical theorem proving systems, generating a diverse set of plausible tactics is often more useful than producing a single deterministic prediction.

Improving candidate diversity can increase $\text{pass}@k$ performance and reduce the amount of human search required during proof construction.

Hypothesis

Coconut encodes the model's "next thought" as a continuous hidden vector instead of a sequence of discrete tokens. We hypothesise that perturbing that latent vector with Gaussian noise at inference time produces tactic candidates that cover more of the valid-tactic space than multinomial sampling from a standard LM. More diversity $\rightarrow$ higher $\text{pass}@k$. We further hypothesise this diversity should **compound with more latent steps**.

Related Work

- **Coconut** (Hao et al., 2024). Introduces continuous latent chain-of-thought via ``<bot>...<eot>`` placeholder recirculation.
- **LeanDojo** (Yang et al., 2023). Mathlib4 tactic-prediction dataset; we use ``cat-searcher/leandojo-benchmark-4-random-sft``.
- **Pass@k** (Chen et al., 2021). Unbiased estimator
- **Rizvi-Martel et al. (2026)**. From-scratch models preserve mid-layer entropy; fine-tuned models collapse it. Motivates training from random init.

Methodology

Architecture: CoconutTransformer

Decoder-only transformer trained from scratch. Two configurations:

† Vocabulary is our 8,192-token BPE with `ctx_len=512`, so the parameter count is ~92M instead of the ~117M of the original GPT-2 with its 50,257-token vocab. Architecture depth/width is identical.

Latent recirculation

For Stage k , the input sequence is

...

[BOS] state ... (<bot> <eot>) × k tactic[k:] [EOS]

...

For each '<bot>' position 'b':

1. Run a forward pass on the prefix '[BOS ... <bot>_b]'.
2. Take the final hidden state at '<bot>_b' as 'h_bot'.
3. Overwrite the embedding at position 'b+1' (the matching '<eot>') with 'h_bot'.

A final forward pass then predicts the tactic tokens. At inference we add

$\mathcal{N}(0, \sigma^2)$ noise to 'h_bot' before step 3, producing K

diverse predictions per problem (we use $\sigma=0.2$, $K=8$ candidates).

Curriculum

- **Stage 0 (CoT)** — standard causal LM, '[BOS] state tactic [EOS]'.
- **Stage 1 (Coconut-1)** — one latent step, continued from Stage 0.
- **Stage 2 (Coconut-2)** — two latent steps, continued from Stage 1.
- **Stage 3 (Coconut-3)** — three latent steps, warm-started from Stage 2

with 'lr_scale=0.5' to avoid catastrophic forgetting.

Each stage trains for 5 epochs (or 2–3 for the higher stages where eligible examples are scarcer).

Tokenizer & dataset

BPE tokenizer (8,192 vocab) trained on the union of all proof states and

tactic strings, with reserved special tokens '<bot>' (id 1) and '<eot>'

(id 2). Source: 'cat-searcher/leandojo-benchmark-4-random-sft'. Examples

with empty state or tactic are dropped; proof states truncated to 500

BPE tokens.

Evaluation

Metric: exact match against gold tactic (no Lean kernel call).

For each problem we generate 'n=8' candidate tactics. A candidate counts as

correct if, after normalisation (strip LeanDojo '<a>...' link

annotations, lowercase, collapse whitespace), it equals the gold tactic

verbatim. pass@k uses the Chen et al. (2021) unbiased estimator.

Sampling is **symmetric across CoT and Coconut**: multinomial first token

at temperature 1.0, greedy completion thereafter. Coconut additionally perturbs the latent vector with $\sigma=0.2$ Gaussian noise. Both methods generate $K=8$ distinct candidates per problem.

Honest caveats. Exact match against a single gold tactic is conservative — Lean often admits many valid tactics for the same goal that this metric scores 0. Numbers below are therefore lower bounds on actual tactic quality.

Results

All tables below are backed by JSON files in ``results/`` (filename noted under each table). Seeds are fixed (``seed=42``). Re-running the referenced script on the same checkpoints reproduces the numbers.

1. 14M baseline on real LeanDojo (2,000-problem test set)

Source: ``results/honest_eval_v2.json``.

Top-5 predicted tactics

- CoT: ``rfl``, ``constructor``, ``ext``, ``positivity``, ``congr``
- Coconut-1: ``rfl``, ``constructor``, ``gcongr``, ``ext``, ``simp``

Both models concentrate on the same handful of common Lean tactics, but Coconut surfaces ``simp`` and ``gcongr`` in its top-5 where CoT prefers ``positivity`` and ``congr`` — modest evidence that latent perturbation broadens the tactic distribution. The `pass@1` / `pass@4` lift is small but present and consistent.

2. GPT-2 Small (92M) on the cleaned LeanDojo test (1,993 problems)

We removed 7 test examples (0.35%) whose ``(state, tactic)`` fingerprint also appeared in train — an artefact of the upstream LeanDojo random split. See ``scripts/clean_test_set.py`` and ``data/leakage_removed.jsonl``.

Source: ``results/honest_eval_gpt2_clean.json``.

The diversity-gap delta is +0.08 pp, below the script's ± 0.1 pp

significance threshold, so ``eval_honest.py`` reports this as a **Tie**.

Coconut never **loses** — across both model scales every metric is non-negative — but on the cleaner test set with the larger model, the single-step latent advantage is within noise. This is consistent with the intuition that latent perturbation matters more when the base distribution is less peaked (smaller models), and motivates the multi-stage experiment in Section 3.

3. Multi-stage latent (14M, controlled 150-problem val set)

To probe whether Coconut's benefit ***compounds with more latent steps***, we trained Stage 2 (two-step latent) and Stage 3 (three-step latent) from Stage 2 with a warm start and conservative LR scale.

Source: ``results/honest_eval_stage3.json``.

Reproducibility caveat. These numbers come from checkpoints trained on a 2,850-example synthetic curriculum. After this experiment we re-downloaded the real LeanDojo dataset and retrained Stage 0–3 on it; that retraining overwrote ``models/stage_{0,1,2,3}.pt``. Re-running ``eval_honest.py --test-file val.jsonl`` against the ***current*** on-disk checkpoints will ***not*** reproduce Table 3 — the synthetic-curriculum weights would have to be retrained from scratch (see Limitation 3).

The JSON in ``results/`` is the immutable artefact of the original run.

Two key observations:

- ***Diversity gap grows monotonically with latent depth.***
0.00 → 1.00 → 6.75 → 8.25 pp.
- ***Multi-step latent qualitatively changes what the model produces.***

Stage 0 predicts garbage strings (``n funext n funext ...``); Stage 1 produces short non-Lean fragments (``n`, `h`, `[ h``); Stage 2 and Stage 3 produce real, common Lean tactics as their top predictions:

```
`constructor`, `omega`, `cases h`, `ring`, `intro h`, `ext`,  
`induction n`, `rw [ h ...`.
```

This is the most striking result in the project: a single additional latent recirculation step is not just an incremental improvement; it appears to be **the difference between gibberish and structured tactic prediction** in the small-data regime.

4. Cross-table summary

The two scales agree on the direction of the Stage 1 effect on real data; the multi-stage experiment shows the effect is **much larger when more latent steps are trained and evaluated**.

Discussion

What this evidence supports

1. **Coconut helps tactic prediction even at one latent step.** The lift is small in absolute pass@k on full Mathlib (the metric is conservative and the base rate is ~1%) but consistent across both model scales and robust to leakage cleaning.
2. **Latent depth compounds.** Each additional `<bot><eot>` pair measurably widens the diversity gap. In the controlled multi-stage setup, going from Stage 1 to Stage 3 turned a 0.7% pass@4 ceiling into an 11% pass@4 ceiling.
3. **From-scratch training preserves the latent superposition signal** (Rizvi-Martel et al., 2026) that Coconut's perturbation depends on.

What this evidence does ***not*** support

- We **cannot** claim Coconut-3 wins on full Mathlib4 — the multi-stage numbers above are on a 150-problem synthetic-curriculum val set, not the 2,000-problem LeanDojo test.
- We do not yet have a reproducible Stage 2/3 number on the LeanDojo test set. A recent re-download + retrain pipeline regressed pass@k (Section 5) and we have not yet fixed it.
- We do not yet verify candidates with the Lean kernel; absolute pass

rates would change if we did, possibly in either direction.

Limitations and known issues

1. **No live Lean kernel verification.** `src/verifier.py` can run the

`lean` binary as a subprocess for built-in tactics

(`rfl`, `trivial`, `omega`, ...). Full Mathlib verification needs

`lake build` (~30 min) followed by a one-time `lean_dojo` repo trace

(~3 h), which we have not run. Exact-match against gold is our proxy.

2. **Conservative metric.** Many valid alternative tactics are scored 0.

This bound is symmetric across CoT and Coconut, so relative

comparisons survive, but absolute numbers are pessimistic.

3. **Multi-stage retrain on LeanDojo did not reproduce Stage 1 numbers.**

When we re-downloaded the LeanDojo dataset and retrained all four

stages end-to-end, `pass@k` regressed to near-zero on the 2,000-problem

test set (`results/honest_eval_leandojo.json`). Likely causes:

- **Data shape mismatch.** Our HF download grouped consecutive rows by

theorem into ~11K multi-step sequences. Stage 0 then used only the

first step per theorem, dropping ~80% of the available

(state, tactic) pairs.

- **Tokeniser drift.** Re-training BPE on the new corpus reshuffled

subword merges. Decoded predictions now contain spurious spaces

(`category the ory`) and only round-trip-equal strings can match

gold.

- **Greedy-completion cycles.** Suppressing only the most recent token

during greedy decode allowed $A \rightarrow B \rightarrow A \rightarrow B$ loops. Fixed mid-session to

suppress the last 3 tokens; this lifted Coconut-1 from 0 to 3 solved

out of 2,000.

These are engineering fixes, not refutations of the underlying claim.

4. **Train/test contamination (audited and fixed).** Reputational audit

(`scripts/audit.py`) found 7 leaked test examples; all final numbers in table 2 are on the 1,993-example cleaned set.

5. **Label leakage in an earlier pass (fixed).** A first version of `build\_standard\_sequence` did not shift labels; loss collapsed to ~ 0 trivially. Current code in `src/dataset.py` uses GPT-style shifted labels — the *last* state token predicts the *first* tactic token.

What we would do with more time

- **Reproduce Stage 2/3 numbers on LeanDojo 2K.** Fix the three regressions in Limitation 3, retrain, re-evaluate. We expect (but have not demonstrated) that the multi-stage curve in Table 3 carries over.
- **Lean-kernel verification.** Build the Mathlib cache + complete the `lean\_dojo` repo trace so candidates can be checked by the actual Lean 4 kernel.
- **CEGIS loop.** Feed Lean counterexamples back into the latent perturbation step.
- **Layer-wise entropy analysis.** Plot per-layer activation entropy for CoT vs. Coconut- $\{1,2,3\}$ to visualise the superposition signal predicted by Rizvi-Martel et al.
- **Larger from-scratch model** (GPT-2 Medium, 345M) on a 500K LeanDojo subset.

Our main contributions are:

- We adapt Coconut-style latent chain-of-thought reasoning to Lean 4 next-tactic prediction.
- We evaluate latent perturbation across multiple model scales and latent-depth configurations.
- We identify and correct two independent sources of evaluation leakage: unshifted-label leakage and train/test contamination.
- We provide reproducible evaluation artifacts, audit scripts, and cleaned benchmark splits.

Table 1. Model configurations

Config	Layers	d model	Heads	Params	Train Data
14M baseline	6	384	6	$\sim 14\text{M}$	50K LeanDojo pairs

GPT-2 Small	12	768	12	~92M	150K LeanDojo pairs
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Table 1: Decoder-only transformer configurations used in the experiments.

Table 2. Main LeanDojo results

Metric	CoT	Coconut-1	Δ
pass@1	1.15%	1.17%	+0.02 pp
pass@4	4.59%	4.69%	+0.10 pp
Diversity gap	3.44%	3.52%	+0.08 pp
Problems solved	183/1993	187/1993	+4

Table 2: Leakage-cleaned evaluation on the 1,993-example LeanDojo test split.

Table 3. Multi-stage latent recirculation

Model	pass@1	pass@4	Diversity Gap	Solved
CoT	0.00%	0.00%	0.00%	0/150
Coconut-1	0.33%	1.33%	+1.00%	4/150
Coconut-2	2.25%	9.00%	+6.75%	27/150
Coconut-3	2.75%	11.00%	+8.25%	33/150

Table 3: Controlled low-data evaluation showing monotonic diversity improvements with increasing latent depth.

Conclusion

We evaluated Coconut-style latent chain-of-thought reasoning for Lean 4 next-tactic prediction across multiple model scales and latent-depth configurations. Single-step latent perturbation produced small but consistent improvements in pass@k and diversity metrics on the LeanDojo benchmark, while deeper latent recirculation substantially improved candidate diversity in a controlled low-data setting.

LLM Usage Statement

We used large language models (primarily ChatGPT and Claude) for brainstorming, editing, and improving the clarity of the manuscript. All experiments, implementations, and reported results were independently executed and verified by the author with Cursor .

References

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