

# Learning to Discover at Test Time

Mert Yuksekgonul<sup>\*1</sup>, Daniel Koceja<sup>\*1</sup>, Xinhao Li<sup>\*4</sup>, Federico Bianchi<sup>\*5</sup>  
 Jed McCaleb<sup>3</sup>, Xiaolong Wang<sup>4</sup>, Jan Kautz<sup>2</sup>, Yejin Choi<sup>2</sup>, James Zou<sup>†1,5</sup>, Carlos Guestrin<sup>†1</sup>, Yu Sun<sup>\*1,2</sup>  
<sup>1</sup> Stanford University <sup>2</sup> NVIDIA <sup>3</sup> Astera Institute <sup>4</sup> UC San Diego <sup>5</sup> Together AI

## Abstract

How can we use AI to discover a new state of the art for a scientific problem? Prior work in test-time scaling, such as AlphaEvolve, performs search by prompting a frozen LLM. We perform reinforcement learning at test time, so the LLM can continue to train, but now with experience specific to the test problem. This form of continual learning is quite special, because its goal is to produce one great solution rather than many good ones on average, and to solve this very problem rather than generalize to other problems. Therefore, our learning objective and search subroutine are designed to prioritize the most promising solutions. We call this method Test-Time Training to Discover (TTT-Discover). Following prior work, we focus on problems with continuous rewards.

We report results for every problem we attempted, across mathematics, GPU kernel engineering, algorithm design, and biology. TTT-Discover sets the new state of the art in almost all of them: (i) Erdős' minimum overlap problem and an autocorrelation inequality; (ii) a GPUMode kernel competition (up to 2x faster than prior art); (iii) past AtCoder algorithm competitions; and (iv) denoising problem in single-cell analysis. Our solutions are reviewed by experts or the organizers.

All our results are achieved with an open model, OpenAI gpt-oss-120b, and can be reproduced with our publicly available [code](#), in contrast to previous best results that required closed frontier models. Our test-time training runs are performed using Tinker, an API by Thinking Machines, with a cost of only a few hundred dollars per problem.

	Mathematics	Kernel Eng. (TriMul)	Algorithms (AtCoder)	Biology
Erdős' Min. Overlap (↓)	A100 (↓)	H100 (↓)	Heuristic Contest 39 (↑)	Denoising (↑)
Best Human	0.380927 [20]	4531 $\mu$ s	1371 $\mu$ s	566,997 [1]
Prev. Best AI	0.380924 [49]	N/A	N/A	558,026 [37]
<b>TTT-Discover</b>	<b>0.380876</b>	<b>2198 <math>\mu</math>s</b>	<b>1161 <math>\mu</math>s</b>	<b>567,062</b>

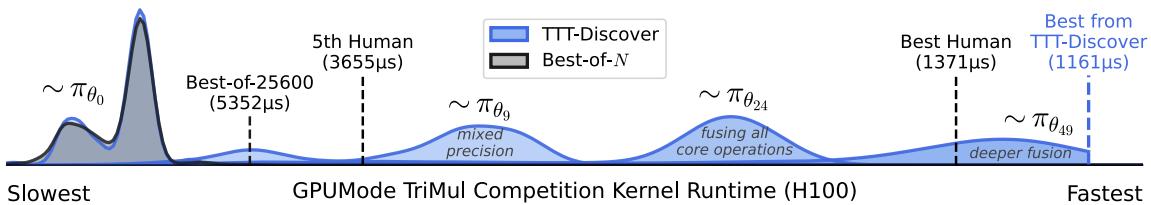


Figure 1. TTT-Discover continues to train an LLM on a single problem at test time.  $\pi_{\theta_i}$  denotes the policy with the updates weights at test-time training step  $i$ . We plot the reward distribution at step 0, 9, 24, and 49 (final), recorded while test-time training for the GPUMode [TriMul](#) competition. We generate 512 solutions at each step. As training progresses, the LLM generates better solutions that ultimately surpass the prior art (best human). For comparison, we plot the reward distribution of best-of- $N$  with the same total sampling budget.

\* Core contributors. <sup>†</sup>Joint advising. Correspondence to: [merty@stanford.edu](mailto:merty@stanford.edu), [yusun@cs.stanford.edu](mailto:yusun@cs.stanford.edu).

# 1 Introduction

To solve hard problems, humans often need to try, fail, stumble upon partial successes, and then learn from their experiences. Consider your first really hard programming assignment. You read the textbook and trained yourself on the book exercises, but this assignment just asked for so much beyond the basics in the book. You tried to guess the solution, but these attempts merely produced small signs of life. So you had to take a deep breath and learn from your failed attempts, which made your future attempts more intelligent. Finally, after hours of trying and learning, you understood the new ideas behind the assignment. And indeed, the next attempt worked!

In this example, the assignment was hard because it required new ideas beyond your training data (the text and exercises in the book). Now consider using AI to solve scientific discovery problems. This goal is even harder: By definition, discovery problems require ideas not only beyond the model’s training data but also all existing knowledge of humanity. And out-of-distribution generalization is no easier for AI than for humans [47, 22, 52, 34].

To offset this hardness, prior work has focused on test-time search in the solution space by prompting a frozen LLM to make many attempts, similar to how we tried to guess the solution to the assignment. In particular, evolutionary search methods, such as AlphaEvolve, store past attempts in a buffer and use them to generate new prompts via hand-crafted and domain-specific heuristics [49, 37, 54, 80]. While these prompts can help the LLM improve previous solutions, the LLM itself cannot improve, similar to a student who can never internalize the new ideas behind the assignment.

The most direct way for the LLM to improve is through learning. And indeed, while both learning and search scale well with compute [66], learning has often superseded search in the history of AI for hard problems such as Go and protein folding [62, 30]. We believe that this observation from history is still relevant today, as we scale compute at test time. So we continue to train the LLM, while it attempts to solve this very test problem. And these attempts, in turn, provide the most valuable training data: Recall that the test problem was hard because it was out-of-distribution. Now we have a data distribution specific to this problem.

At a high level, we simply perform Reinforcement Learning (RL) in an environment defined by the single test problem, so any technique in standard RL could be applied. However, our goal has two critical differences from that of standard RL. First, our policy only needs to solve this single problem rather than generalize to other problems. Second, we only need a single best solution, and the policy is merely a means towards this end. In contrast, the policy is the end in standard RL, whose goal is to maximize the average reward across all attempts. While the first difference is a recurring theme in the field of test-time training [65], the second is unique to discovery problems.

To take advantage of these differences, our learning objective and search subroutine strongly favor the most promising solutions. We call this method Test-Time Training to Discover (TTT-Discover). We focus on problems with continuous rewards, in mathematics (§4.1), GPU kernel engineering (§4.2), algorithm design (§4.3), and biology (§4.4). We report results for every problem we attempted, and TTT-Discover sets the new state of the art in almost all of them, using only an open model.

There are two pieces of concurrent work that share our high-level idea: MiGrATe (Phan et al.) [51], and more recently ThetaEvolve (Wang et al.) [74], which we find especially relevant. Compared to ThetaEvolve, TTT-Discover using the same model and compute budget still produces significant improvements (Table 2), due to its special learning objective and search subroutine.

Problem	State $s$	Action $a$	Transition	Reward $R(s)$
Erdős Minimum Overlap Autocorr. Inequality (1st) Autocorr. Inequality (2nd)	Step function certificate	Thinking tokens and code	$s' = \text{Python}(\text{Parse}(a))$	1/Upper bound 1/Upper bound Lower bound
Kernel Engineering Algorithm Competition Single Cell Analysis	Kernel code Algorithm code Analysis code	Thinking tokens and code	$s' = \text{Parse}(a)$	1/Runtime Test score 1/MSE

Table 1. Overview of the science and engineering problems in our paper, and the environments they induce (§2.1). Note that the reward is 0 if  $s$  fails validity checks.

## 2 Preliminaries

All methods in this paper, including the baselines, share a common goal: Given a scientific problem at test time, the goal is to discover a new state-of-the-art solution with an LLM policy  $\pi_\theta$ , whose weights  $\theta$  have already been trained (at training time). To formalize this goal, we first introduce how each scientific problem defines an environment, i.e., a Markov Decision Process (§2.1), which can then be used for search (§2.2) and learning (§3).

### 2.1 Discovery Problem

Our definition of the environment follows prior work in test-time scaling, such as AlphaEvolve [49]: A scientific problem comes in the form of a text description  $d$ , which we always feed as context to the policy. We define a state  $s$  as a candidate solution, such as a kernel implementation of the PyTorch code in  $d$ . In our applications, the problem description also induces a continuous reward function  $R(s) \in \mathbb{R}$ , such as the inverse runtime of the kernel.

We denote  $s_{\text{sota}}$  as the best-known solution among all existing candidates, and  $r_{\text{sota}} = R(s_{\text{sota}})$  as the best-known reward. And in case there is no existing solution,  $s_{\text{sota}}$  can be the empty string `<empty>`. For example,  $s_{\text{sota}}$  can be the kernel currently at the top of the leaderboard. These notations allow us to formalize the notion of a discovery:

**Definition** (Discovery). *A discovery is an event where a state  $s$  is found such that  $R(s) > r_{\text{sota}}$ . The larger the difference, the more significant the discovery.*

Under this formalism, we define a *discovery problem* as finding such a state  $s$  with large  $R(s) - r_{\text{sota}}$  within the environment defined by the scientific problem.

To produce a better solution, both search and learning methods use the LLM policy to generate an action  $a \sim \pi_\theta(\cdot | d, s)$ , where the choice of the initial solution  $s$  (e.g.,  $= s_{\text{sota}}$ ) is an important part of the method’s design. Similar to the reward function, the transition function  $(s, a) \rightarrow s'$  of the environment is also induced by the problem description. Here, we consider only a single timestep since state reuse, which we will introduce soon, effectively subsumes multiple timesteps.

In all our applications, a valid action contains a piece of code and optionally some thinking tokens. For coding problems (e.g., kernel engineering), the environment produces  $s'$  by simply parsing the code out of  $a$ . For problems in mathematics, the environment also needs to execute the code in  $a$  after it is parsed. Table 1 provides an overview of the environments for all our applications.

## 2.2 Search Methods

The simplest search method, known as Best-of- $N$ , samples i.i.d. rollouts from  $\pi_\theta$ :

$$\text{Best-of-}N: \quad s = s_{\text{sota}} \text{ or } \langle \text{empty} \rangle, \quad a_i \sim \pi_\theta(\cdot | d, s),$$

where the subscript,  $i = 1, \dots, N$ , denotes the index of the rollout. By using  $i$  instead of  $t$  for the index, we indicate that the rollouts here are independent. One reasonable choice of the initial state  $s$  is  $s_{\text{sota}}$ , assuming that a previous solution exists. But  $s_{\text{sota}}$  might be too strong a prior towards exploitation. For example, conditioning on  $s_{\text{sota}}$  might prevent the policy from exploring very different, but more promising directions that would ultimately produce better solutions under a large compute budget. To address this concern, we usually set  $s = \langle \text{empty} \rangle$ , the empty (or trivial) solution.

On the other hand, the policy might also explore a promising direction using  $s = \langle \text{empty} \rangle$ , but fail to fully exploit it. One technique to address this opposite concern is *state reuse*, which warm starts the policy with some of the previous solutions. Specifically, it maintains a buffer  $\mathcal{H}_i$  of the previous solutions, and samples the initial solution  $s_i$  from  $\mathcal{H}_i$  using a search heuristic, *reuse*, which favors high-reward solutions but still assigns nontrivial likelihood to low-reward ones:

$$\text{State reuse: } \quad s_i \sim \text{reuse}(\mathcal{H}_i), \quad a_i \sim \pi_\theta(\cdot | d, s_i), \quad \mathcal{H}_{i+1} = \mathcal{H}_i \cup \{(s'_i, r_i)\}.$$

When we reuse a previous solution  $s'_i$ , we have effectively added an extra timestep to its trajectory.

Prior work, such as AlphaEvolve [49], also reuses the actions, which can contain thinking tokens and intermediate results (e.g., code for math problems) that are not part of the states. As a consequence, the *reuse* heuristic also needs to convert the information from previous actions into natural language context  $c_i$  that can be ingested by the LLM policy:

$$\text{State-action reuse: } \quad s_i, c_i \sim \text{reuse}(\mathcal{H}_i), \quad a_i \sim \pi_\theta(\cdot | d, s_i, c_i), \quad \mathcal{H}_{i+1} = \mathcal{H}_i \cup \{(s_i, a_i, s'_i, r_i)\}.$$

Prior work [49, 37, 80, 41] refers to state-action reuse as *evolutionary search*, because the *reuse* heuristic usually involves sophisticated designs motivated by evolution, including hand-crafted operations for mutation and cross-over, and domain-specific measurements of fitness and diversity.

## 3 Learning to Discover at Test Time

So far, the policy's experience with the test problem can only improve the next prompt  $(d, s_i, c_i)$ , but not the policy  $\pi_\theta$  itself, since  $\theta$  remains frozen. We use this experience to improve the policy in an online fashion, by training  $\pi_\theta$  on its own search attempts accumulated in the buffer  $\mathcal{H}_i$ .

Algorithm 1 outlines the general form of our method, where the two key subroutines to instantiate are *reuse* and *train*.

### 3.1 Naive RL at Test Time

Algorithm 1 falls under the formulation of reinforcement learning (RL). A natural baseline is to use a standard RL algorithm:

$$\text{train: } \quad \theta_{i+1} = \theta_i + \eta \nabla_\theta \mathbb{E}_{a \sim \pi_{\theta_i}(\cdot | s)} [R(s, a)], \quad \text{reuse}(\mathcal{H}_i) = \delta_{\langle \text{empty} \rangle},$$

i.e., optimize for expected reward with no reuse, where  $\delta_{\langle \text{empty} \rangle}$  is a delta distribution with mass only on the initial state  $\langle \text{empty} \rangle$ . We will use  $\theta_i$  to denote the model weights for rollout  $i$ . We can straightforwardly apply popular RL algorithms, such as PPO or GRPO [56, 16], only in the environment defined by the single problem.

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**Algorithm 1** Test-Time Training to Discover (TTT-Discover)

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1: Input: problem description  $d$  and policy  $\pi_{\theta_0}$  with initial weights  $\theta_0$ .
2:  $R, T = \text{get\_env}(d)$      $\triangleright d$  induces the reward and transition functions of the environment (§2.1)
3:  $\mathcal{H}_0 = \{(\langle \text{empty} \rangle, R(\langle \text{empty} \rangle), \{\})\}$            $\triangleright$  Initialize buffer with the empty solution (§2.2)
4: for  $i = 0, 1, \dots, N - 1$  do
5:    $s_i, c_i \sim \text{reuse}(\mathcal{H}_i)$             $\triangleright$  Sample initial state and context with a reuse heuristic
6:    $a_i \sim \pi_{\theta_i}(\cdot | d, s_i, c_i)$         $\triangleright$  Sample action from policy
7:    $s'_i = T(a_i)$                           $\triangleright$  Transition to next state
8:    $r_i = R(s'_i)$                           $\triangleright$  Evaluate reward of next state
9:    $\mathcal{H}_{i+1} = \mathcal{H}_i \cup \{(s_i, a_i, s'_i, r_i)\}$   $\triangleright$  Add current attempt to buffer
10:   $\theta_{i+1} = \text{train}(\theta_i, (d, s_i, c_i, a_i, r_i))$   $\triangleright$  Improve the model weights with train
11: end for
12: return  $s_{i^*}$ , where  $i^* = \arg \max_{i=0,1,\dots,N-1} r_i$            $\triangleright$  Return the state with the highest reward

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However, these algorithms are designed with the standard RL problem in mind. Discovery problems have important distinctions from standard RL problems.

In standard RL problems, the goal is to find a policy that maximizes the expected reward. This policy is to be deployed repeatedly in the same environment. The primary artifact is the policy.

In discovery problems, the goal is to find a single state that improves upon the state-of-the-art. We do not care about the average performance. There is no separate deployment phase and thus the policy need not maintain robust performance in many states it may encounter starting from the same initial state distribution. In fact, a policy can have very low expected reward, so long as it reaches a new state-of-the-art once.

Due to these differences, the naive RL instantiation has important shortcomings.

**Objective function.** Naive RL optimizes average performance, and is indifferent to the state of the art. In discovery, however, success is determined by the maximum, and whether it improves upon the state of the art. Consider a kernel engineering problem where the state-of-the-art runtime is  $2000\mu\text{s}$ . Achieving  $1900\mu\text{s}$  would require substantial optimization and perhaps a breakthrough. Yet, without complicated reward shaping, both would receive nearly the same reward.

**Short effective horizon.** Starting each attempt from scratch limits how far the policy can reach in an attempt. Reusing a previous solution effectively adds extra timesteps to an attempt, extending the horizon. As a result, more complex solutions can emerge during training. In standard RL, a fixed initial state distribution makes sense as the policy must perform robustly from states it will encounter at deployment. Discovery has no such deployment phase.

**Exploration.** Exploration requires care at two levels. Optimizing for expected reward, the policy can collapse to safe, high-reward actions rather than risky ones that might achieve discovery. At the reuse level, naive prioritization can over-exploit a few promising states at the expense of diversity.

## 3.2 TTT-Discover

To address these shortcomings, we introduce two simple components.

**Entropic objective.** We define the entropic objective that favors the maximum reward actions:

$$J_\beta(\theta) = \mathbb{E}_{s \sim \text{reuse}(\mathcal{H})} [\log \mathbb{E}_{a \sim \pi_\theta(\cdot | s)} [e^{\beta(s)R(s,a)}]],$$

$$\nabla_{\theta} J_{\beta}(\theta) = \mathbb{E}_{\substack{s \sim \text{reuse}(\mathcal{H}) \\ a \sim \pi_{\theta}(\cdot|s)}} \left[ w_{\beta(s)}(a) \nabla_{\theta} \log \pi_{\theta}(a|s) \right], \quad w_{\beta(s)}(a) = \frac{e^{\beta(s)R(s,a)}}{\mathbb{E}_{\pi_{\theta}(\cdot|s)}[e^{\beta(s)R(s,a)}]},$$

where we also shape advantages with a KL penalty:  $A(a; s) = w_{\beta(s)}(a) - 1 - \lambda \log \frac{\pi_{\theta}(a|s)}{\pi_{\theta_0}(a|s)}$  [56, 83, 68], and  $-1$  is the baseline since  $\mathbb{E}[w_{\beta(s)}] = 1$ . Concurrent work [29] also explored the entropic objective  $J_{\beta}$  to maximize the pass@k performance for (training-time) RL with binary reward problems.

As  $\beta \rightarrow \infty$ , the entropic objective tends to the max, which is intuitively what we want. However, too large  $\beta$  early in training causes instabilities, while too small later makes advantages vanish as even smaller improvements become harder. Empirically, we found that setting a constant  $\beta$  that works well across different tasks is challenging. Therefore, different than [29], we set  $\beta(s)$  adaptively per initial state by constraining the KL divergence of the induced policy; see Appendix A.1 for details.

**PUCT.** We select initial states using a PUCT-inspired rule [53, 60, 62, 61]. Each state  $s$  is scored by  $Q(s) + c \cdot P(s) \cdot \sqrt{1+T}/(1+n(s))$ , where  $Q(s)$  is the maximum reward among states generated when the initial state was  $s$  (or  $R(s)$  if  $s$  has not yet been selected).  $P(s)$  is proportional to  $s$ 's rank in the buffer sorted by reward,  $n(s)$  counts how many times  $s$  or its descendants have been expanded, and  $T$  is the total number of expansions, and  $c$  is the exploration coefficient.

Rather than the mean (as in prior work), we use the maximum reward of children in  $Q(s)$ : we care about the best outcome starting from a state, not the average. The prior  $P(s)$  captures the intuition that high-reward states are more likely to yield high-reward children—e.g., a fast kernel is more likely to seed a faster kernel than a slow one—while the exploration bonus prevents over-exploitation by keeping under-visited states as candidates. See Appendix A.2 for implementation details.

**Test-time Training to Discover.** With these building blocks, we can introduce our method, TTT-Discover. We combine  $J_{\beta(s)}$  as our (test-time) training objective and PUCT as our reuse routine:

$$\text{train: } \theta_{i+1} = \theta_i + \eta \nabla_{\theta} J_{\beta(s_i)}(\theta_i), \quad \text{reuse: } s_i \sim \text{PUCT}(\mathcal{H}_i).$$

### 3.3 Implementation Details

We run TTT-Discover with gpt-oss-120b [2] on Tinker [36] for 50 training steps. We use LoRA [23] with rank 32. At each step, we generate a batch of 512 rollouts, with 8 groups of 64 rollouts each. Each group of rollouts is generated using the same context and initial state selected from the reuse buffer. We use the entropic objective, and apply importance sampling ratio correction to the gradients due to the sampler/learner mismatch in the RL infrastructure [78]. We do not take any off-policy steps, i.e., take 1 gradient step on the entire batch.

We set the reasoning effort to high. The context window of gpt-oss-120b is limited to 32,768 tokens on Tinker. Thus, each rollout stops when the context window is exhausted or the LM produces the end of sequence token. In most domains, we limit the total length of the prompt and the thinking tokens to 26000 tokens, so as to leave enough tokens to generate the final response, e.g., to allow generating longer algorithm code. We enforce this by token forcing the model to generate its final response. All hyperparameters reported in Table 9, and are fixed unless otherwise stated. Assuming an average prompt length of 3000 tokens and 16000 sampling tokens on average, a training run with 50 steps and 512 rollouts costs around \$500 on Tinker.

## 4 Applications

We evaluate TTT-Discover on problems in GPU kernel engineering, mathematics, algorithm design, and biology. We report our performance on every task we attempted. Besides potential impact,

we pick domains with 2 criteria. First, we pick domains where we can compare our performance to human experts. This is possible, for example, by comparing to the best submissions in human engineering competitions, or to the best results reported in academic papers. We also want to compare to AI baselines. As we discuss below, mathematics and algorithm design are discovery domains where prior work recently made progress [49, 14, 27, 54, 74].

In every application, we report the best known human results and the best known AI results. Importantly, we always report the Best-of- $N$  baseline that matches the sampling budget and the model that TTT-Discover uses. That is, since we perform 50 steps with 512 rollouts per step, and compare to the Best-of-25600 baseline. For a closest evolutionary algorithm baseline, we also run OpenEvolve [58], an open-source version of AlphaEvolve [49], with the same 25600 sampling budget. We use the same context window budget and the Tinker client for gpt-oss-120b throughout the experiments. We caution that the context window limit led to a large number of rollouts in OpenEvolve to be truncated before the model completes its response, as OpenEvolve’s prompts grow very large in length. However, to stay faithful to their implementation, we did not modify their prompts or rollouts.

## 4.1 Mathematics

We explore multiple open problems in mathematics. These are often problems where even small numerical improvements carry real weight, since each result potentially rules out families of approaches and extends the frontier of what is mathematically known. Here, proofs are by construction: one can construct a concrete mathematical object – a step function or a sequence – that certifies, e.g., a bound for an inequality can be achieved. This property makes these problems amenable to search.

**Environment:** The state  $s$  is a construction. Specifically, a construction is a step function represented as a numerical array, to certify a proof. The action  $a$  consists of thinking tokens followed by Python code that either constructs a new step function or modifies an existing one. The dynamics execute the parsed code to produce the next state:  $s' = \text{Python}(\text{Parse}(a))$ . The reward is the bound certified by  $s'$ , or zero if  $s'$  fails validity checks (e.g., the function must satisfy constraints on its support, sign, or integral). Most often, actions involve optimization algorithms to improve the constructions.

Throughout mathematics applications, we initialize the buffer with random states. Specifically, initial states are sampled uniformly at random within the problem’s valid range. For each action, we give a 10-minute limit to execute the code given by the action. In the case of a timeout, the action gets a reward of 0. For minimization problems (certifying upper bounds), we set the reward proportional to  $1/\text{bound}$  for the certified bound, and otherwise we set it proportional to bound. We report further details about the environment and the prompts we use in Appendix B.

**Previous state-of-the-art.** Such problems are recently explored in [14, 49]. We report both the best known human results, and the recent progress by AI: AlphaEvolve [49], AlphaEvolve V2 [14] which was released around 6 months after AlphaEvolve, ShinkaEvolve [37], and ThetaEvolve [74].

We select one representative problem from each area in AlphaEvolve [49]: Erdős’ minimum overlap problem (combinatorics), autocorrelation inequalities (analysis), circle packing (geometry).

### 4.1.1 Erdős’ Minimum Overlap Problem

This is a classic problem in combinatorial number theory, posed by Erdős in 1955, with connections to the distribution of sequences and difference sets. Partition  $\{1, 2, \dots, 2n\}$  into two sets  $A$  and  $B$  of equal cardinality  $n$ . Define  $M_k$  as the number of solutions to  $a_i - b_j = k$  for  $a_i \in A, b_j \in B$ , and let  $M(n) = \min_{A,B} \max_k M_k$  over all partitions. The problem is to bound  $c = \lim_{n \rightarrow \infty} M(n)/n$ . Bounds before AlphaEvolve were  $0.379005 < c < 0.380927$ , with the upper bound due to Haugland [20] and the lower bound due to [76]. AlphaEvolve [49, 14] improved the upper bound to 0.380924.

Method	Model	Erdős' ( $\downarrow$ )	AC1 ( $\downarrow$ )	AC2 ( $\uparrow$ )
best human	–	0.380927	1.50973	0.9015
AlphaEvolve [49]	Gemini-2.0 Pro + Flash	0.380924	1.50530	0.8962
AlphaEvolve V2 [14]	Gemini-2.0 Pro + Flash	0.380924	1.50317	<b>0.9610</b>
ThetaEvolve [74]	R1-Qwen3-8B	n/a	1.50681	0.9468
ThetaEvolve w/ SOTA reuse (1.50317)	R1-Qwen3-8B	n/a	1.50314	n/a
OpenEvolve [58]	gpt-oss-120b	0.380965	1.50719	0.9449
Best-of-25600	gpt-oss-120b	0.380906	1.51004	0.9344
TTT-Discover	Qwen3-8B	0.380932	1.50525	0.9472
TTT-Discover	gpt-oss-120b	<b>0.380876</b>	<b>1.50287</b>	0.9591

Table 2. Results in mathematics problems. In the Erdős’ Minimum Overlap Problem and First Autocorrelation Inequality (AC1), TTT-Discover sets the new state-of-the-art. We also report TTT-Discover with Qwen3-8B, for a better comparison to ThetaEvolve. Notable, TTT-Discover with Qwen3-8B outperforms not only ThetaEvolve, baselines including AlphaEvolve which uses Gemini-2.0 family models for the autocorrelation inequalities. Our state-of-the-art constructions are released and can be validated [in our codebase](#).

Following [49], we optimize step functions  $f$  describing the density of  $A$  throughout  $[1, 2n]$ . Due to a result of Swinnerton-Dyer [20], density functions yield valid upper bounds on  $\lim M(n)/n$  without constructing explicit partitions for large  $n$ . Validity checks require  $f(x) \in [0, 1]$  and  $\int f = 1$ .

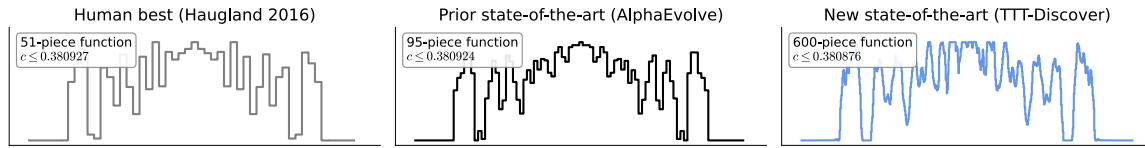


Figure 2. We show the normalized step functions including the prior state-of-the-art from AlphaEvolve. The step function  $f(x)$  is the limiting density of set  $A$ . Unlike the previous state-of-the-art, the solution from TTT-Discover is an asymmetric construction. TTT-Discover found a 600-piece step function, while AlphaEvolve construction was 95-piece. The best human result was a 51-piece construction [20].

**Results.** We improve the upper bound on Erdős’ Minimum Overlap Problem to 0.380876, surpassing AlphaEvolve’s recent construction with 0.380924 [49]. Our improvement over AlphaEvolve is 16 times larger than AlphaEvolve’s improvement over the previous state-of-the-art. Unlike AlphaEvolve’s symmetric construction, our method discovered a 600-piece asymmetric step function. Surprisingly, the Best-of-25600 baseline also improved upon the AlphaEvolve construction.

The discovered algorithm minimizes the correlation bound using FFT-accelerated gradient descent combined with random hill climbing and simulated annealing. The code maintains feasibility by projecting onto the constraint set where  $f(x) \in [0, 1]$  with  $\int f = 1$ . Interestingly, the solution found by TTT-Discover is asymmetric.

#### 4.1.2 Autocorrelation Inequalities

Autocorrelation inequalities are motivated by additive combinatorics [6]. Improving these inequalities tightens a constant that propagates into sharper limits on how large a set can be while still avoiding repeated additive patterns (a central theme in additive combinatorics). Similar to the Erdős’ minimum overlap problem, we will construct a step function  $f$  to certify bounds.

**First autocorrelation inequality.** For nonnegative  $f$  supported on  $[-1/4, 1/4]$ , define  $C_1$  as the

largest constant such that

$$\max_{|t| \leq 1/2} (f * f)(t) \geq C_1 \left( \int f \right)^2$$

holds for all such  $f$ . The goal is to certify the tightest *upper bound* on  $C_1$ ; any valid construction  $f$  certifies  $C_1 \leq \frac{\|f * f\|_\infty}{\|f\|_1^2}$ . Until early 2025, the best known upper bound was  $C_1 \leq 1.50973$  [45]. AlphaEvolve improved this to  $C_1 \leq 1.5053$ , and AlphaEvolve V2 further improved it to  $C_1 \leq 1.50317$ , and ThetaEvolve refined AlphaEvolve’s construction to get  $C_1 \leq 1.50314$ .

**Second autocorrelation inequality.** For nonnegative  $f$ , define

$$C_2 = \sup_{f \geq 0} \frac{\|f * f\|_2^2}{\|f * f\|_1 \|f * f\|_\infty}.$$

The problem is to certify the tightest known *lower bound* on  $C_2$ ; any valid construction  $f$  with ratio  $r$  certifies  $C_2 \geq r$ . The best human bound was  $C_2 \geq 0.8892$  [45]. AlphaEvolve first improved this to  $C_2 \geq 0.8962$ , [9] improved this to 0.9015, and AlphaEvolve V2 further improved it to  $C_2 \geq 0.9610$  using a 50,000-piece step function.

**Results.** We improved the best known upper bound to prove  $C_1 \leq 1.50286$ , with a 30000-piece step function. The comparisons are reported in Table 2. The previous state-of-the-art, ThetaEvolve, achieved their result by refining the AlphaEvolve V2 construction. In contrast, TTT-Discover found a new construction by starting from scratch. We visualize our and prior works’ step functions in Figure 3. In the second autocorrelation inequality, we have not made a discovery. Our best construction certified a bound of 0.959, where the AlphaEvolve construction had certified a tighter lower bound of 0.961.

For the first inequality, early improvements down to 1.510 came from trying and improving gradient-based optimization (e.g., using Adam with softmax parameterization). To reduce the bound from around 1.510 to 1.504, the policy mostly used linear programming (LP), following the insights in [45]. The key insight for the later steps, that gradually achieved the state-of-the-art, was using heuristics to focus optimization only on the constraints that are close to being tight—where each constraint in the LP bounds one position of the convolution. Heuristics included picking the top K positions where the convolution was largest and only including those in the LP, as well as computing gradients from all near-maximum positions rather than just the single largest for gradient-based methods. Unlike AlphaEvolve [14], which mentions the authors suggested ideas such as using Newton type methods, we never intervened on the optimization process.

For a better comparison to the concurrent work, ThetaEvolve, we also report TTT-Discover with Qwen3-8B [77]. The Qwen3-8B variant they used, DeepSeek-R1-0528-Qwen3-8B that was released by DeepSeek, is not available on Tinker. Thus, we used the original Qwen model (Qwen/Qwen3-8B) that was reportedly worse than the DeepSeek variant. ThetaEvolve reports using 65 steps with 512 rollouts (32 groups of 16 rollouts) each, however we do not modify our hyperparameters otherwise and keep 50 steps of 512 rollouts each. For both inequalities, TTT-Discover with Qwen3-8B certified tighter bounds than ThetaEvolve, using a worse model and a smaller sampling budget.

#### 4.1.3 Circle Packing

In Circle packing, the goal is to maximize the sum of radii of  $n$  non-overlapping circles packed inside a unit square. We follow the setup from prior work [49, 14]. The state  $s$  is a list of circle centers and radii. The action  $a$  consists of thinking tokens followed by Python code that optimizes circle positions and radii. The reward is the sum of radii achieved for valid packings, and 0 otherwise. We present the results below mostly for comparison purposes, as several recent works on evolutionary algorithms reported their performance using this task.

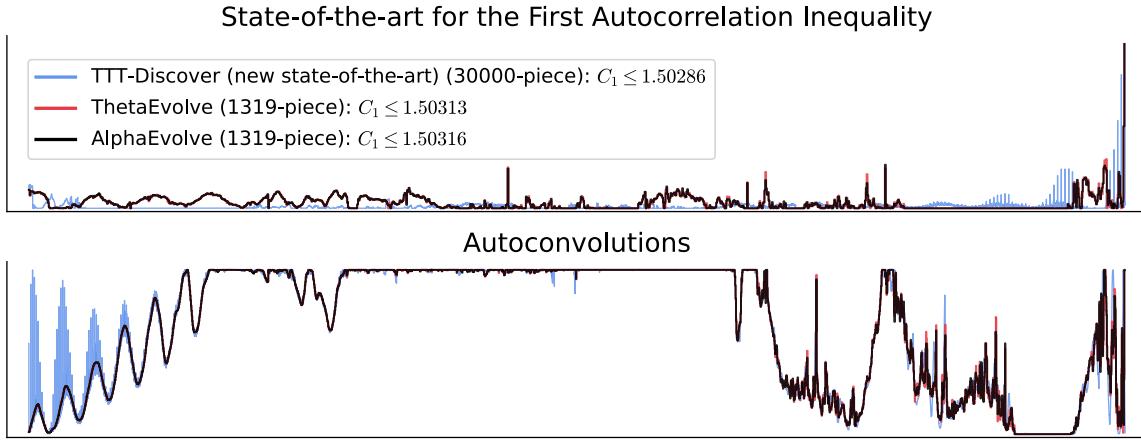


Figure 3. We show the prior and new state-of-the-art, with the (normalized) step functions and their autoconvolutions. Both AlphaEvolve and TTT-Discover starts the discovery process from scratch, while ThetaEvolve initializes from the AlphaEvolve construction, and thus is very similar to the AlphaEvolve construction. TTT-Discover found a 30,000-piece step function that certifies that the upper bound  $C_1 \leq 1.50286$ , while AlphaEvolve and ThetaEvolve constructions are 1319-piece. We overlay the step functions and their autoconvolution visually for qualitative comparison.

Method	Model	$n = 26 (\uparrow)$	$n = 32 (\uparrow)$
AlphaEvolve [49]	Gemini-2.0 Pro + Flash	2.635862	2.937944
AlphaEvolve V2 [14]	Gemini-2.0 Pro + Flash	2.635983	2.939572
ShinkaEvolve [37]	Ensemble (see caption)	2.635982	n/a
ThetaEvolve [74]	R1-Qwen3-8B	2.635983	n/a
TTT-Discover	Qwen3-8B	2.635983	2.939572

Table 3. Results for circle packing. ShinkaEvolve uses an ensemble of Claude Sonnet-4, gpt-4.1, gpt-4.1-mini, gpt-4.1-nano, o4-mini.

Table 3 shows results. TTT-Discover with Qwen3-8B matches the best known constructions for both  $n = 26$  and  $n = 32$ . We make no improvements here, but include these results for completeness. The algorithms found by TTT-Discover are presented in Appendix B.1. Algorithms initialize circles in staggered or hexagonal grid arrangements, then refine positions and radii using sequential least squares programming with boundary and pairwise non-overlap constraints. This solution is a lot simpler than recent work, such as ShinkaEvolve [37], especially in terms of initialization, where their solution uses an initialization based on simulated annealing algorithm, while TTT-Discover initializes only with a simple geometric arrangement.

#### 4.1.4 Expert Review

##### Human Expert Review — Prof. Davide Torlo (Università di Roma La Sapienza)

Erdős' minimum overlap problem and the autocorrelation inequalities are classical problems in combinatorics with applications in, among others, discrepancy theory, combinatorial optimization, and signal analysis. Both problems can be formulated as min–max problems, in which the minimization is taken over a class of functions with bounded norm, while

the maximization is performed over a set of evaluation points. Closed-form solutions are not known; instead, only lower and upper bounds can be derived. Obtaining sharp bounds for these problems remains a challenging mathematical task and is essential for improving our understanding and resolution of such questions. The upper bounds obtained by TTT-Discover for the Erdős' minimum overlap and the AC1 autocorrelation problems are achieved by specific piecewise-constant functions. It is straightforward to verify that the provided functions give bounds that improve upon the state of the art: one simply evaluates the quantity of interest and its maximum over a discrete set of points determined by the step size of the piecewise-constant functions, and checks that the corresponding norm constraints are satisfied.

## 4.2 Kernel Engineering

GPU kernels are the computational foundation of modern AI, every forward pass and backward pass ultimately executes as kernel code on hardware. We apply our method to GPU kernel optimization, where a new state-of-the-art kernel is a faster implementation than existing ones.

[GPUMODE](#) is an open community for kernel development that also hosts competitions for domain experts. We test our method on two competitions: TriMul (triangular matrix multiplication), a core primitive in AlphaFold's architecture [30], and DeepSeek MLA (Multi-head Latent Attention), a key component in DeepSeek's inference stack [40]. Each GPU type for the TriMul competition (NVIDIA H100, A100, B200, AMD MI300x) has a separate leaderboard, as performant implementations differ across architectures. For The MLA competition there is only an MI300x leaderboard.

As these competitions were conducted earlier, we retrospectively evaluate our performance while respecting competition standards. We prefer GPUMODE because their leaderboards are well-tested through human competitions with a robust evaluation harness [81], and their benchmarks avoid signal-to-noise issues where simple operations or small inputs cause overheads to dominate runtime.

**Environment:** The state  $s$  is a GPU kernel code. The action  $a$  consists of thinking tokens followed by kernel code written in Triton [69]. The dynamics parse the code from the action:  $s' = \text{Parse}(a)$ . For the initial state, we provide unoptimized kernels, detailed in Appendix C. The reward is proportional to the inverse of the geometric mean of runtimes on a fixed set of input shapes (following the leaderboard), or zero if the kernel fails correctness checks or times out. We evaluate runtime remotely on [Modal](#) to scale and ensure consistent hardware conditions. For TriMul, we evaluate the runtime only on H100s during training, even though we still evaluate the generated kernels for A100, B200, and MI300X for final report. Since MI300X is not available on Modal, for MLA-Decode we use H200s, and hope the kernels generalize to MI300X. Further details about the prompts and environments are in Appendix C.

**Results.** We report the runtime of the best kernels and the baselines in Table 4. Our TriMul kernels achieve state-of-the-art across the board in all GPU types. For A100s, our best kernel is 50% faster than the top human kernel, even though our reward function did not time the kernels on A100s. We uniformly achieve  $> 15\%$  improvement over the best human submissions for all GPU types. Finally, we submit to the official TriMul A100/H100 leaderboard<sup>1</sup>.

The discovered kernels for Trimul identify heavy memory I/O incurred by frequent elementwise operations as a major bottleneck to optimize. Specifically, the kernels fuse: (i) operations in the input LayerNorm, (ii) sigmoid and elementwise multiplication in input gating, and (iii) operations in

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<sup>1</sup>See [leaderboards](#). For TriMul B200/MI300X and MLA-Decode MI300X tasks, due to an infra problem on GPU Mode's server, we could not submit to the official leaderboard.

the output LayerNorm and gating. As for the most compute-heavy operation, which is the matmul with  $O(N^3)$  complexity, the kernels convert the inputs to FP16 and delegate the computation to cuBLAS/rocBLAS to effectively leverage TensorCores/MatrixCores of the hardwares.

**Discovered MLA-Decode kernels.** The kernels shown in table 5 mainly rely on `torch.compile()` for optimization. Specifically, they adopt a specific configuration of `torch.compile`. However, these kernels do not leverage Triton for fine-grained optimization, which may limit further improvements and more flexible use case. We additionally filter and evaluate generated kernels that explicitly use Triton despite their slightly slower runtime, and report in Appendix C.

Method	Model	TriMul ( $\downarrow, \mu s$ )			
		A100	H100	B200 [95% CI]	AMD MI300X [95% CI]
1st human	–	4531.5	1371.1	1027.6 [1016.3, 1038.9]	2515.8 [2510.9, 2520.8]
2nd human	–	4918.5	2368.0	2349.0 [2335.7, 2362.4]	5101.4 [5163.1, 5167.0]
3rd human	–	5182.2	2545.7	1920.9 [1910.9, 1931.0]	5200.7 [5343.6, 5375.1]
4th human	–	6097.8	3654.8	2169.2 [2089.4, 2248.9]	5993.1 [5978.5, 5984.4]
5th human	–	8345.0	4233.1	6452.1 [6400.5, 6503.8]	8365.1 [8347.7, 8382.5]
Best-of-25600	gpt-oss-120b	9219.7	5390.3	3253.7 [3252.5, 3254.9]	4902.0 [4897.6, 4906.4]
TTT-Discover	gpt-oss-120b	<b>2198.2</b>	<b>1161.2</b>	<b>910.8</b> [907.3, 914.2]	<b>1555.7</b> [1550.8, 1560.5]

Table 4. For the TriMul competition, we train a single model using H100 runtime as the reward function and report the runtime of the single best kernel. We only trained using H100 for evaluating kernels during training. The generated kernels happened to generalize to other GPU types. We also report the top-5 human submissions in the leaderboard for comparison (each GPU type has its own top-5 human submissions). For A100 and H100, we submitted to the official leaderboard and report the runtime returned. For B200 and MI300X, we could not submit our kernels due to an infra problem on GPU Mode’s server, and therefore conduct 10 trials for each kernel and report mean and confidence intervals using the same infrastructure as GPUMode, verified by the organizers. Our state-of-the-art kernels are released and can be validated in our [codebase](#).

Method	Model	AMD MI300X - MLA Decode ( $\downarrow, \mu s$ ) [95% CI]		
		Instance 1	Instance 2	Instance 3
1st human	–	1653.8 [1637.3, 1670.3]	1688.6 [1672.8, 1704.3]	1668.7 [1637.0, 1700.3]
2nd human	–	1662.8 [1648.8, 1676.8]	1688.6 [1677.6, 1699.5]	1679.7 [1653.4, 1705.9]
3rd human	–	1723.0 [1711.5, 1734.5]	1765.8 [1758.1, 1773.5]	1718.0 [1698.3, 1737.7]
4th human	–	1768.7 [1750.3, 1787.2]	1769.9 [1755.2, 1784.6]	1767.0 [1736.2, 1797.8]
5th human	–	2038.6 [2017.8, 2059.3]	2037.3 [2021.0, 2053.6]	2041.9 [1989.0, 2094.8]
Best-of-25600	gpt-oss-120b	2286.0 [2264.2, 2307.8]	2324.1 [2306.0, 2342.1]	2275.2 [2267.3, 2283.1]
TTT-Discover	gpt-oss-120b	1669.1 [1649.2, 1688.9]	1706.1 [1685.9, 1726.3]	1671.3 [1646.0, 1696.5]

Table 5. AMD MLA Decode runtimes on AMD MI300x across three instances. Values are mean runtime across 10 trials with 95% confidence intervals. Top-5 human submissions are from the GPUMode leaderboard. We trained our kernels using an H200 GPUs even though the task is to minimize runtime on MI300x GPUs, since those were not available at scale in online providers. We only selected kernels using a single MI300X GPU. There is significant variance across AMD MI300x instances available via AMD Developer Cloud. Thus, we performed our kernel selection and evaluation across three different instances. In each instance, our best kernel was different, and in none of the cases our best kernel where better than the top human submission with statistical significance.

#### 4.2.1 Expert Review

Below, we provide verbatim reviews from the GPUMode organizers for our TriMul competition kernels.

##### Human Expert Review — Matej Sirovatka, Alex Zhang, Mark Saroufim (GPUMode)

The referenced solution correctly determined that the problem is memory bound because of the surrounding point-wise operations so the agent focuses as much as possible on operation fusions, lowering the memory traffic and kernel launch overhead.

It also stores activations in fp16, while this is fully aligned with the problem definition and defined tolerances, it could potentially lead to numerical stability issues in full workloads. Overall the agent’s strategy is to reduce memory bandwidth via fusions, lower precision and delegating the big matrix multiplications to cuBLAS, as those are non-trivial to beat. This is similar to the current best human solutions, but executed on better. Most of the human solutions lack behind in fusing some of the more complex operators together, resulting in this solution outperforming them by a large margin.

### 4.3 Algorithm Engineering

Hard optimization problems like package-delivery routing, crew scheduling, factory production planning, power-grid balancing—appear throughout industries and must be solved repeatedly at scale. We apply our method to these algorithm engineering problems, where a new state-of-the-art would be writing a higher-scoring algorithm than existing ones written by human experts.

AtCoder Heuristic Contest (AHC) is a series of programming competitions focused on optimization problems drawn from real-world industrial challenges [4], attracting hundreds of participants including industry experts. We attempted to evaluate on two past contests, ahc039 and ahc058. ahc039 ("Purse Seine Fishing") is a computational geometry problem where you design a simple closed net on a 2D map, restricted to horizontal/vertical edges, to capture many target points while avoiding penalty points under a budget. ahc058 ("Apple Incremental Game") is a production planning problem where upgrades trade off immediate output versus growing future production capacity, and the goal is to schedule upgrades to maximize final output.

We select ahc039 because ShinkaEvolve [37] reported a solution that would have placed 2nd, and ahc058 because Sakana AI’s ALE-Agent achieved the first-ever AI victory in an AHC [54]. We use the evaluation harness from ALE-Bench [27]. We use the public test case generator to create local tests, select our best-performing algorithm, and submit it to be scored on the official platform.

**Environment:** The state  $s$  is an algorithm implementation in C++. The action  $a$  consists of thinking tokens followed by C++ code. The dynamics parse the code from the action:  $s' = \text{Parse}(a)$ . The reward is the score on locally generated test cases, or zero if the algorithm fails correctness checks or exceeds the time limit of 2 seconds and memory limit of 1024MB. We select the best-performing algorithm and submit it to be scored on the official private tests. We use the evaluation harness released by [27]. For initial states, for the ahc039 competition we use the same initial program as [37], which is based on ALE-Agent [27] best program, that would have placed 5th in the competition leaderboard. For ahc058 we start from scratch, similar to ALE-Agent [54].

**Previous state-of-the-art.** We report the top human submissions on each contest leaderboard. For AI baselines, we compare to ALE-Agent [27] and ShinkaEvolve [37], which use ensembles of models including the gpt, Gemini, and Claude families of models. ALE-Agent [27] starts from scratch for both problems. ShinkaEvolve [37] reports results in ahc039 where they start from ALE-Agent solution, and improve it from 5th place to 2nd place.

**Results.** We report results in Table 6. For both competitions, if we had submitted during competition time, our algorithms would have gotten the 1st place. For ahc039, we marginally improve upon the best human, while there is a significant gap between next best AI and human scores. For ahc039, we follow ShinkaEvolve by starting from the ALE-Agent solution and improve it from 5th place to 1st place, while ShinkaEvolve reaches the 2nd place using significantly more capable frontier models such as Gemini 2.5 Pro. For ahc058, we start from scratch and outscore all submissions in the competition.

For AHC039, the solution builds a large pool of promising axis-aligned rectangles using prefix sum scoring, then greedily seeds a connected union and uses simulated annealing with add, remove, replace, expand, shrink, and slide moves to optimize the rectangle union score under perimeter and vertex constraints, followed by cleanup and final greedy refinement.

For AHC058, the solution first builds several reasonable plans using greedy rules, different biases, and a short beam search to explore promising early decisions. Then, the program improves the best plan with simulated annealing that makes random edits, swaps, and partial rebuilds before finishing with a small local cleanup pass. It estimates the value of actions using a simple formula for how much future production an upgrade is likely to create, which guides both greedy choices and pruning. For performance, it caches intermediate states so it only recomputes parts of the plan that change. Overall, the program balances broad exploration early with focused local improvement later.

Method	Model	Geometry (ahc039)	Scheduling (ahc058)
1st human	–	566,997	847,674,723
2nd human	–	557,212	846,938,871
3rd human	–	554,334	846,350,877
4th human	–	552,933	845,489,747
5th human	–	549,746	845,324,831
ALE-Agent [27]	Ensemble (see caption)	550,647	848,373,282
ShinkaEvolve [37]	Ensemble (see caption)	558,026	n/a
Best-of-25600	gpt-oss-120b	554,171	772,429,752
TTT-Discover	gpt-oss-120b	<b>567,062</b>	<b>848,414,228</b>

Table 6. Results in two AtCoder Heuristic Competitions. We train our models with local public tests, and submit the best program we get during training to the official submission platform. Our algorithms are released and can be validated [in our codebase](#). Our solutions in the official AtCoder submission platform are publicly available for ahc039 and ahc058. ALE-Agent uses Gemini-2.5 Pro for ahc039, and Gemini-3 Pro Preview high and gpt-5.2-high for ahc058. ShinkaEvolve uses an ensemble of gpt-5, gpt-5-mini, Gemini-2.5 Pro and Flash, Claude Sonnet 4, o4-mini.

#### 4.4 Single Cell Analysis

Single-cell RNA-sequencing (RNA-seq) aims to help us understand how organisms work and get sick by resolving biology at the level of individual cells; measuring which genes each cell is using to reveal cell types, states, and how they change. Practically, it isolates single cells, tags their mRNA with a Unique Molecular Identifier (UMI), sequences it, and outputs a per-cell gene-by-count table. RNA-seq protocols suffer from measurement noise in the observed UMI counts. Thus, denoising algorithms significantly increases the realized value of expensive experiments. Each sequencing run costs thousands of dollars, and better denoising methods reduce the need for deeper sequencing.

We apply our method to one of the recent benchmarks OpenProblems [43], an important set of open problems for single-cell analysis. We use the denoising task therein. [7] demonstrated that

partitioning the observed molecules of a single dataset into training and test sets via binomial sampling and evaluating the denoised training set against the held-out test counts provides a proxy for accuracy against true expression values, providing an evaluation framework without requiring external ground truth data.

**Environment.** The state  $s$  is an algorithm implementation. The action  $a$  consists of thinking tokens followed by code. The dynamics parse the code from the action:  $s' = \text{Parse}(a)$ . The benchmark evaluates denoising quality using two complementary metrics: mean squared error (MSE) in log-normalized space, which measures overall reconstruction accuracy, and Poisson negative log-likelihood, which assesses how well the denoised counts match the statistical properties expected of count data. In our context, the reward is the MSE score, or zero if it violates constraints we add for the Poisson score or the algorithm exceeds the time limit of 400 seconds. The Denoising benchmark offers 3 datasets: PBMC, Pancreas, and Tabula Muris Senis Lung, in order of size. We train our policy by using Pancreas in our environment, and ultimately performance is reported by running the algorithm on the held out PBMC and Tabula datasets.

**Previous state-of-the-art.** We report the state of the art as described by the OpenProblems [43] benchmark. The best result was provided by MAGIC [71] using an approximate solver and reversed normalization. MAGIC is a well known technique, frequently used in the literature [79, 72], the only method different from MAGIC that provides good performance is ALRA [39], ranked third. We also compare with OpenEvolve and Best-of-25600.

#### Disclaimer

This is an experimental application demonstrating TTT-Discover’s ability to find algorithms that excel on specific benchmarks. While our discovered algorithm outperforms existing methods on the OpenProblems denoising benchmark, benchmark metrics are inherently incomplete and do not guarantee biological validity for downstream tasks.

**Results.** The improved function obtained via TTT-Discover shows consistent improvements on both datasets (see Table 7). TTT-Discover is initialized with MAGIC code. TTT-Discover adds gene-adaptive transform ensembling, low-rank SVD refinement, and log-space polishing steps that directly optimize the benchmark metric.

Method	Model	PBMC			Tabula		
		Score ( $\uparrow$ )	MSE ( $\downarrow$ )	Poisson ( $\downarrow$ )	Score ( $\uparrow$ )	MSE ( $\downarrow$ )	Poisson ( $\downarrow$ )
MAGIC (A, R)	–	0.64	0.19	0.05	0.64	0.18	0.03
MAGIC (R)	–	0.64	0.19	0.05	0.64	0.18	0.03
ALRA (S, RN)	–	0.50	0.26	0.05	0.47	0.27	0.03
MAGIC (A)	–	0.42	0.19	0.16	0.40	0.18	0.12
MAGIC	–	0.42	0.19	0.16	0.40	0.18	0.12
OpenEvolve	gpt-oss-120b	0.70	0.16	0.05	0.71	0.15	0.03
Best-of-25600	gpt-oss-120b	0.62	0.20	0.05	0.65	0.18	0.03
TTT-Discover	gpt-oss-120b	<b>0.71</b>	<b>0.15</b>	<b>0.05</b>	<b>0.73</b>	<b>0.14</b>	<b>0.03</b>

Table 7. Denoising task for single cell data analysis. We report the score (mean of normalized MSE and Poisson scores), MSE, and Poisson metrics for each dataset. Our state-of-the-art algorithm is released and can be validated [in our codebase](#). MAGIC (A, R) = MAGIC [71] approximate with reversed normalization; MAGIC (R) = MAGIC with reversed normalization; ALRA [39] (S, R) = ALRA sqrt norm with reversed normalization; MAGIC (A) = MAGIC approximate.

#### 4.4.1 Expert Review

Below, we provide a verbatim review from Prof. Eric Sun.

##### Human Expert Review — Prof. Eric Sun (MIT)

Single-cell transcriptomics provides a high-dimensional readout on cellular gene expression patterns and has enabled new insights into both biological and disease processes. One challenge in the analysis of single-cell transcriptomics is the sparsity of the data, characterized by zero counts detected for many genes (i.e. "dropouts") due to low expression or other technical issues. MAGIC addresses this challenge by de-noising single-cell transcriptomics using diffusion or smoothing, and it has been widely incorporated in the pre-processing of single-cell data for studying multiple diseases and tissue biology. The proposed improvement on the MAGIC algorithm is simple, aligns with the underlying smoothing-based approach of MAGIC, and yields empirical improvements on key metrics. However, improvements on metrics for single-cell data analysis tasks may not always transfer to enhanced ability to obtain new biological insights, which is often difficult to quantify and therefore benchmark. Further evaluation of the proposed algorithm against MAGIC and other existing methods for biologically relevant tasks would be necessary to fully understand the extent of the reported improvements.

## 4.5 Ablations

We have three sets of ablations. First, we ablate the design choices for the `train` method, while keeping our `reuse` method, PUCT, fixed. We test (i) TTT with entropic objective using constant  $\beta = 2$  ([29]), (ii) TTT with no entropic objective (expected reward), (iii) No TTT (only reuse). Second, we ablate the choice of the `Reuse` method, while keeping our `train` method, TTT with entropic objective using adaptive  $\beta$ , fixed. We replace PUCT with (i)  $\epsilon$ -greedy reuse with  $\epsilon = 0.1$  as this is perhaps the most naive reuse method, and (ii) no reuse. Finally, we report the naive RL baseline, where we use the expected reward objective with no reuse, and the Best-of-25600 baseline.

	<b>train</b>	<b>reuse</b>	<b>Best runtime (<math>\downarrow, \mu\text{s}</math>)</b>
Best Human Kernel	—	—	1371.1
TTT-Discover	TTT with adaptive entropic	PUCT	<b>1203.10</b>
Ablations for <code>train</code>	TTT with constant $\beta$ entropic	PUCT	1483.83
	TTT with expected reward (no entropic)	PUCT	1985.67
	No TTT	PUCT	2060.70
Ablations for <code>reuse</code>	TTT with adaptive entropic	$\epsilon$ -greedy	1328.89
	TTT with adaptive entropic	no reuse	5274.03
Naive Test-time RL	TTT with expected reward	no reuse	5328.73
Best-of- $N$	no TTT	no reuse	5352.36

Table 8. Ablation results for the TriMul GPUMode competition where we time the kernels with an H100 GPU. We report the best kernel we get in each run. We report the reward distributions across steps in Figure 4.

For each ablation, we report the runtime of the best kernel found in Table 8, and the reward distribution in Figure 4. The rewards distributions and best kernel runtimes are computed with our evaluator, not the leaderboard.

Only the full TTT-Discover algorithm achieves the best performance in the TriMul competition.

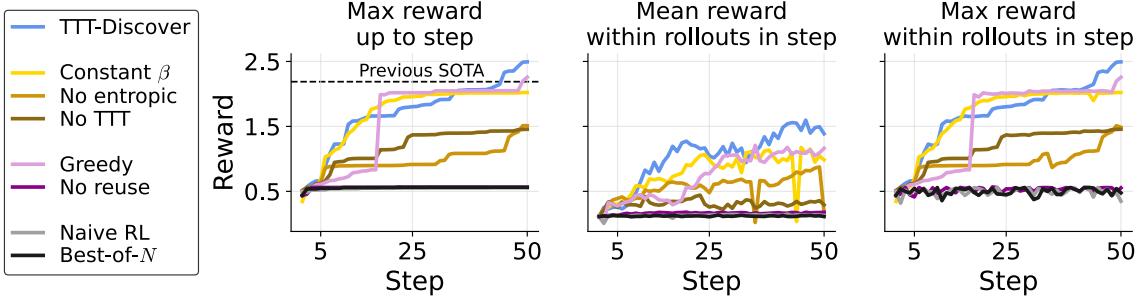


Figure 4. Reward distributions for each ablation. We match the sampling budget across all ablations. We sample 512 rollouts in each step. For example, for Best-of- $N$ , we have  $N = 50 \times 512 = 256000$  rollouts.

When using a constant  $\beta$ , the improvements diminish later in the training. Using the expected reward objective, improvements are slower overall. Without any test-time training, both the mean reward and the max reward stagnates.  $\epsilon$ -greedy reuse works reasonably well, especially with an early lucky kernel. In early experiments with other applications, the lack of exploration was also a bigger problem than it is in kernel engineering tasks. Naive RL and no reuse make minimal improvements.

It is entirely possible that additional tuning (e.g., a task-specific  $\beta$  schedule) or hyperparameter interactions (e.g., batch size and reuse) can provide improvements in the ablation configurations. For each component, many additional knobs could be ablated (e.g., PUCT exploration bonus, learning rate, batch size). However, our focus was on identifying design choices that work reliably across diverse applications within our budget with minimal task-specific tuning. In practice, the key hyperparameters such as learning rate, batch size, and LoRA rank were fixed after the initial iterations of the project.

## 5 Related Works

In this section, we first provide a broad overview of continual learning and test-time training, using some of the exposition in [67]. Then towards the end of §5.2, we discuss the most relevant work on test-time training: MiGrATE [51] and ThetaEvolve [74]. Finally, we discuss two pieces of work with tangential formulations: RL on a single training problem that is not the test problem [75] (§5.3), and RL on the entire test set [84] (§5.4).

### 5.1 Continual Learning

Most of today’s AI systems remain static after deployment, even though the world keeps changing. The high-level goal of continual learning is to enable AI systems to keep changing with the world, similar to how humans improve throughout their lives [19, 11].

Conventionally, continual learning as a research field has focused on learning from a *distribution* that gradually changes over time [42, 70, 17]. For example, one could update a chatbot model every hour using new knowledge from the Internet, while typical use cases of the model may require knowledge from both the past and the present [57, 31, 73]. More formally, at each timestep, we sample new training and test data from the current distribution, update our model using the new training data, and then evaluate it on all the test data up to the current timestep. Under this setting, most algorithms focus on not forgetting the past when learning from the present [55, 38, 33, 15].

## 5.2 Test-Time Training

The algorithmic framework of test-time training has the same high-level goal as continual learning, but it focuses on two aspects where human learning stands out from the forms of continual learning in the conventional literature.

First, each person has a unique brain that learns within the context of their individual life. This personalized form of continual learning is quite different from, for example, the chatbot model that is fine-tuned hourly using the latest information available worldwide. While such a model does change over time, it is still the same at any given moment for every user and every problem instance.

Second, most human learning happens without a boundary between training and testing. Consider your commute to work this morning. It is both "testing" because you did care about getting to work this very morning, and "training" because you were also gaining experience for future commutes. But in machine learning, the train-test split has always been a fundamental concept.

The concept of test-time training is introduced to realize these two special aspects of human learning. *Training* typically involves formulating a learning problem (such as empirical risk minimization) and then solving it. Following [64], *test-time training* is defined as any kind of training that formulates a potentially different learning problem based on each individual test instance.

This concept has a rich history in AI. A well-known example in NLP is dynamic evaluation, pioneered by Mikolov et al. [46] and extended by Krause et al. [35]. In computer vision, early examples have also emerged in applications such as face detection [28], video segmentation [48], super-resolution [59], and 3D reconstruction [44]. Next, we discuss three popular forms of test-time training today, with an emphasis on their connections to each other and to historical examples.

### 5.2.1 TTT on Nearest Neighbors: Larger Effective Capacity

One simple form of test-time training was called locally weighted regression in the 1970s [63, 10], local learning in the 1990s [8], and KNN-SVM in the 2000s [82]: Given a test instance, find its nearest neighbors in the training set, and then train (or fine-tune) the model on these neighbors before making a prediction. This procedure can significantly increase the effective capacity of the model; for example, it allows a linear model to fit a highly nonlinear ground truth [63].

This simple form captures one of the key intuitions of test-time training. In the conventional view of machine learning, a model, once trained, no longer changes at test time. As a consequence, it must prepare to be good at all possible inputs in the future. This task can be very hard, because being good at all possible futures limits the model's capacity to be good at any particular one. But only one future is actually going to happen. So why not train our model once this future happens?

Recently, [18] extended this idea to modern language models and observed a similar benefit of larger effective model capacity after test-time training, and [25] further improved these results through better strategies for neighbor selection. In addition, [26] showed that test-time training on neighbors from the training set is also effective with RL for reasoning tasks, and [5] developed the same idea for visual-motor tasks.

### 5.2.2 TTT for Novel Instances: Better Generalization

As models become larger today, their competence is often limited not by their capacity, but by the amount of available training data, especially when they need to generalize to novel test instances that are "out-of-distribution". In this case, it is even harder to prepare for all possible test instances in the future, especially the novel ones, with a static model. But once a specific test instance is given, we can use it to generate relevant data, which we can then use for training [65]. In other words, the "neighbors" for TTT do not have to come from the training set; they can also be generated on-the-fly.

Since the test instance is unlabeled, one way to make it useful for training is through self-supervision, which generates new pairs of inputs and labels for an auxiliary task such as masked reconstruction (e.g., BERT [12] and MAE[21]). While the auxiliary task is different from the main prediction task, improving performance in one can help the other through their shared representations. This form of TTT can significantly improve generalization under distribution shifts [65, 13].

Recently, TTT has been an important part of AlphaProof [24], which achieved IMO silver-medal standard in 2024. Given each test problem, their system first generates a targeted curriculum of easier problems by prompting a language model, and then performs reinforcement learning on the generated data. Another recent work, Akyurek et al. [3], found TTT effective for few-shot reasoning tasks such as ARC-AGI. Their system generates augmentations of the few-shot demonstrations in the test problem then performs supervised learning.

MiGrATE [51] and ThetaEvolve [74] are two concurrent works that share our high-level idea of performing RL at test time on a single problem. MiGrATE combines on-policy and off-policy RL and tests on simpler environments such as word search. ThetaEvolve is more similar to our work: it uses OpenEvolve, a variant of AlphaEvolve, for state-action reuse. Both methods use GRPO variants for training. Compared to ThetaEvolve, TTT-Discover using the same model and compute budget still produces significant improvements (Table 2), which we attribute to our entropic objective and PUCT-based reuse instead of more complicated and brittle heuristics in evolutionary algorithms.

### 5.3 RL on One Example

One Example RL [75] is relevant as they also train on a single problem. To be specific, they train on one example from a dataset, such as the MATH training set. They show that a policy trained with on one such problem with RL generalizes to other problems in the same dataset. In contrast, TTT-Discover trains on the test problem itself, where the goal is not to generalize but to solve this specific problem.

### 5.4 RL on the Test Set

TTRL [84] trains on an entire test set of problems using majority voting as pseudo-labels for reward estimation. In contrast, TTT-Discover trains on a single test problem with a continuous verifiable reward, where the goal is not to improve average performance across a set of problems but to find one exceptional solution.

## 6 Future Work

The current form of our method can only be applied to problems with continuous rewards, and the most important direction for future work is test-time training for problems with sparse or binary rewards, or problems in non-verifiable domains.

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Parameters	Value
<b>General</b>	
Model	gpt-oss-120b [2]
Reasoning effort	high
<b>Rollout</b>	
Context window	32768 tokens
Sampling temperature	1.0
Maximum tokens to generate	32768-prompt length
Prompt length + thinking token limit	26000
Teacher forcing	<i>... okay, I am out of thinking tokens. I need to send my final message now.</i>
<b>Training</b>	
Batch size	512 (8 groups with 64 rollouts each)
Training steps	50
Optimizer	Adam [32], lr $4 \times 10^{-5}$ , $\beta_1 = 0.9$ , $\beta_2 = 0.95$ , $\epsilon = 10^{-8}$
LoRA [23] rank	32
KL coefficient ( $\lambda$ )	{0.01, 0.1}
Objective	Entropic; adaptive $\beta(s_{\text{init}})$ with KL constraint $\gamma = \ln(2)$ .
<b>Reuse</b>	
PUCT $c$ (exploration coefficient)	1.0
Further details	<a href="#">Appendix A</a>

Table 9. We fix these hyperparameters across all applications.

## A Training details

Our hyperparameters are fixed throughout almost all experiment. For almost all applications we used a KL penalty coefficient of 0.1. For algorithm engineering, we used a KL coefficient of 0.01. We present details on our objective function and the reuse algorithm below.

## A.1 Entropic utility objective

We define the entropic utility objective explored also in the concurrent work [29]:

$$J_\beta(\theta; s) := \log \mathbb{E}_{\tau \sim \pi_\theta(\cdot|s)} [e^{\beta r(\tau; s)}].$$

The gradient of this objective yields

$$\nabla_\theta J_\beta(\theta; s) = \mathbb{E}_{\tau \sim \pi_\theta(\cdot|s)} [\nabla_\theta \log \pi_\theta(\tau | s) w_\beta(\tau | s)], \quad w_\beta(\tau | s) = \frac{e^{\beta r(\tau; s)}}{\mathbb{E}_{\pi_\theta} [e^{\beta r(\tau; s)}]}, \quad A_\beta(\tau | s) = w_\beta(\tau | s) - 1,$$

since  $\mathbb{E}_{\pi_\theta} [w_\beta(\tau | s)] = 1$ , we get  $A_\beta$  as the mean baselined advantage. The remaining question is how to set  $\beta$ . [29] recommends value  $\beta = 2$ , yet we found it tricky to set it. Later in the training, improvements become harder, and unless  $\beta$  is adjusted carefully advantages can become very small. Early in the training, a large  $\beta$  can cause instabilities.

**Adaptive  $\beta$ .** Define the auxiliary tilted distribution induced by the entropic weights,

$$q_\beta(\tau | s) = \frac{\pi_\theta(\tau | s) \exp(\beta r(\tau; s))}{\mathbb{E}_{\pi_\theta} [\exp(\beta r(\tau; s))]}, \quad w_\beta(\tau | s) = \frac{q_\beta(\tau | s)}{\pi_\theta(\tau | s)}.$$

Then  $w_\beta$  is exactly the density ratio that appears in the entropic policy-gradient update, so  $\beta$  controls the effective step size induced by this reweighting. We choose  $\beta(s)$  by enforcing a KL budget on the auxiliary distribution,

$$\text{KL}(q_{\beta(s)}(\cdot | s) \| \pi_\theta(\cdot | s)) = \gamma,$$

analogous to Relative Entropy Policy Search, where the temperature is set by an exponential tilt under a relative-entropy constraint [50]. In words,  $\beta(s)$  is increased only until the KL budget is exhausted, ensuring the induced reweighting, and hence the update, does not move too far from  $\pi_\theta(\cdot | s)$ . We fix  $\gamma = \ln 2$  throughout our experiments.

**Batch estimator.** Given  $N$  rollouts from the same  $s$  with rewards  $\{r_n\}_{n=1}^N$ , the empirical sampling distribution is uniform on the batch,  $u(n) = 1/N$ . The induced reweighting on the batch is

$$q_\beta(n) = \frac{e^{\beta r_n}}{\sum_{m=1}^N e^{\beta r_m}},$$

and we set  $\beta(s)$  by solving the weight-concentration constraint

$$\text{KL}(q_\beta \| u) = \sum_{n=1}^N q_\beta(n) \log(N q_\beta(n)) = \gamma$$

via simple bisection search over  $\beta \geq 0$ . With  $\hat{\beta}(s)$ , we compute LOO entropic advantages using  $r_{\max} = \max_n r_n$ , and an  $\epsilon$  in the denominator for numerical stability:

$$\hat{Z}_{-n} = \frac{1}{N-1} \sum_{m \neq n} \exp(\hat{\beta}(s)(r_m - r_{\max})), \quad A_n = \frac{\exp(\hat{\beta}(s)(r_n - r_{\max}))}{\hat{Z}_{-n} + \epsilon} - 1.$$

**Discussion.** States where improvements are consistently small (e.g. high-value / near-goal states) tend to make the batch weights  $q_\beta(n)$  less peaky for a given  $\beta$ , so the constraint typically permits a larger  $\beta(s)$ . In contrast, states that occasionally yield a few very large improvements (often earlier in training or low-value states with large headroom) make  $q_\beta$  concentrate quickly as  $\beta$  grows; the same KL budget then forces a smaller  $\beta(s)$ , preventing the update from being dominated by a handful of outlier trajectories while still preferring better-than-average rollouts. Finally, this estimator is invariant to shifting or scaling the reward by a constant, i.e.,  $r(\tau)$  and  $r'(\tau) = wr(\tau) + b$  yield the same advantage for  $w \in \mathbb{R}^+$  and  $b \in \mathbb{R}$ .

## A.2 PUCT Prioritization

We maintain an archive  $\mathcal{H}_t$  of previously discovered states  $s$  with reward  $R(s) \in \mathbb{R}$ . To choose the next start state, we score each  $s \in \mathcal{H}_t$  by a PUCT-inspired rule, analogous to applying PUCT at a virtual root whose actions correspond to selecting a start state from the archive [53, 60, 62, 61]:

$$\text{score}(s) = Q(s) + c \cdot \text{scale} \cdot P(s) \frac{\sqrt{1+T}}{1+n(s)},$$

where  $n(s)$  is a visitation count,  $T$  is the number of expanded parents so far,  $c > 0$  is an exploration coefficient, and  $\text{scale} = R_{\max} - R_{\min}$  is the reward range over the archive. The prior  $P(s)$  is a linear rank distribution:

$$P(s) = \frac{|\mathcal{H}_t| - \text{rank}(s)}{\sum_{s' \in \mathcal{H}_t} (|\mathcal{H}_t| - \text{rank}(s'))},$$

where  $\text{rank}(s) \in \{0, \dots, |\mathcal{H}_t| - 1\}$  orders states by descending reward (rank 0 is the best state). The term  $Q(s)$  uses the best one-step reachable reward  $m(s)$ :

$$Q(s) = \begin{cases} m(s) & n(s) > 0 \\ R(s) & n(s) = 0 \end{cases}.$$

After expanding parent  $p$  and observing its best child reward  $y = \max_{s' \in \text{Child}(p)} R(s')$ , we update:

$$\begin{aligned} m(p) &\leftarrow \max(m(p), y) && (\text{direct parent only}) \\ n(a) &\leftarrow n(a) + 1 \quad \forall a \in \{p\} \cup \text{Anc}(p) && (\text{backprop visitation}) \\ T &\leftarrow T + 1. \end{aligned}$$

For the archive update, we keep the top-2 children per expanded parent (largest  $R$ ) before inserting, then enforce a global size constraint by retaining the top-1000 states in  $\mathcal{H}_t$  by  $R$ , while always keeping the initial seed states.

**Comparison to AlphaZero PUCT.** AlphaZero’s PUCT operates over a tree of state-action edges, selecting actions via  $a = \arg \max_a [Q(s, a) + c \cdot P(s, a) \cdot \sqrt{\sum_b N(s, b) / (1 + N(s, a))}]$ , where  $Q(s, a)$  is the mean value of simulations through edge  $(s, a)$ ,  $P(s, a)$  is a learned policy prior, and  $N(s, a)$  counts visits to that edge [62, 61]. Our formulation differs in four ways: (i)  $Q(s)$  tracks the maximum child reward rather than the mean, favoring optimistic expansion; (ii)  $P(s)$  is a rank-based prior over archived states rather than a learned action distribution; (iii) visitation counts backpropagate to all ancestors, so expanding any descendant reduces the exploration bonus for the entire lineage; and (iv) we block the full lineage (ancestors and descendants) from the current batch to encourage diversity, whereas AlphaZero uses virtual loss as a temporary penalty.

## B Mathematics

### B.1 Circle Packing

Circle Packing ( $n = 26$ )

```

1  ```python
2  import numpy as np
3  from scipy.optimize import minimize
4
5  def run_packing():
6      n = 26

```

```

7     initial_centers = []
8     initial_radii = []
9
10    # Adjusted initial radius and spacing parameters
11    r_initial = 0.102 # Slightly smaller for better flexibility
12    buffer = 1e-6 # Small buffer to prevent boundary violations
13
14    # Generate staggered grid with 5 rows and varying number of circles per row
15    for row in range(5): # 5 rows total
16        # Even rows start at r_initial, odd rows also start with buffer
17        if row % 2 == 0:
18            x_start = r_initial + buffer # Even rows start slightly inside
19        else:
20            x_start = r_initial + buffer # Odd rows also start with buffer
21
22        # Varying number of circles per row to fit better
23        if row == 0 or row == 2 or row == 4:
24            num_circles = 5 # Even rows (0, 2, 4) have 5 circles
25        elif row == 1:
26            num_circles = 6 # First odd row has 6 circles
27        else: # row == 3
28            num_circles = 5 # Second odd row has 5 circles
29
30        if num_circles == 0:
31            continue
32
33        # Calculate horizontal spacing for this row
34        if num_circles == 1:
35            spacing_row = 0.0
36        else:
37            # Ensure horizontal spacing is at least 2*r_initial to prevent overlaps
38            max_horizontal = 1 - 2 * r_initial
39            spacing_row = max_horizontal / (num_circles - 1) if max_horizontal > 0 else 0.0
40
41        # Place circles in this row
42        for col in range(num_circles):
43            x = x_start + col * spacing_row
44            # Vertical positioning with refined vertical spacing
45            if row == 0:
46                y = r_initial + buffer # First row starts with buffer
47            else:
48                # Vertical spacing with a refined factor for denser packing
49                y = r_initial + buffer + row * 1.0 * np.sqrt(3) * r_initial
50
51            # Ensure y does not exceed 1 - r_initial
52            if y + r_initial > 1 + 1e-6:
53                y = 1 - r_initial - 1e-6 # Clamp to prevent overflow
54
55            initial_centers.append([x, y])
56            # Assign initial radii based on row (middle row gets a slight boost)
57            if row == 2:
58                initial_radii.append(r_initial + 0.003) # Increased boost for central row
59            else:
60                initial_radii.append(r_initial)
61
62        # Flatten the initial variables for optimization
63        variables_initial = []
64        for i in range(n):
65            variables_initial.extend(initial_centers[i])
66            variables_initial.append(initial_radii[i])
67
68        # Objective function to maximize sum of radii
69        def objective(vars):
70            total = 0.0
71            for i in range(n):
72                idx = i * 3
73                total += vars[idx + 2]
74            return -total # Minimize negative sum to maximize
75
76        # Define constraints
77        constraints = []
78
79        # Constraints for center positions and radii
80        for i in range(n):

```

```

81     #  $x_i \geq r_i$ 
82     def constraint1(vars, i=i):
83         idx = i * 3
84         return vars[idx] - vars[idx + 2]
85     constraints.append({'type': 'ineq', 'fun': constraint1})
86
87     #  $x_i + r_i \leq 1$ 
88     def constraint2(vars, i=i):
89         idx = i * 3
90         return 1 - (vars[idx] + vars[idx + 2])
91     constraints.append({'type': 'ineq', 'fun': constraint2})
92
93     #  $y_i \geq r_i$ 
94     def constraint3(vars, i=i):
95         idx = i * 3
96         return vars[idx + 1] - vars[idx + 2]
97     constraints.append({'type': 'ineq', 'fun': constraint3})
98
99     #  $y_i + r_i \leq 1$ 
100    def constraint4(vars, i=i):
101        idx = i * 3
102        return 1 - (vars[idx + 1] + vars[idx + 2])
103    constraints.append({'type': 'ineq', 'fun': constraint4})
104
105    # Pairwise distance constraints
106    for i in range(n):
107        for j in range(i + 1, n):
108            def constraint_pair(vars, i=i, j=j):
109                idx_i = i * 3
110                idx_j = j * 3
111                x_i, y_i, r_i = vars[idx_i], vars[idx_i + 1], vars[idx_i + 2]
112                x_j, y_j, r_j = vars[idx_j], vars[idx_j + 1], vars[idx_j + 2]
113                dist = np.sqrt((x_i - x_j)**2 + (y_i - y_j)**2)
114                return dist - (r_i + r_j)
115            constraints.append({'type': 'ineq', 'fun': constraint_pair})
116
117    # Optimize using Sequential Least Squares Programming with refined parameters
118    result = minimize(
119        objective,
120        variables_initial,
121        method='SLSQP',
122        constraints=constraints,
123        options={
124            'ftol': 1e-14,
125            'maxiter': 1000000,
126            'disp': False,
127            'eps': 1e-12,
128            'iprint': 0, # Suppress verbose output
129            'finite_diff_rel_step': np.sqrt(np.finfo(float).eps)
130        }
131    )
132
133    # Extract optimized centers and radii
134    optimized_vars = result.x
135    centers = []
136    radii = []
137    for i in range(n):
138        idx = i * 3
139        centers.append([optimized_vars[idx], optimized_vars[idx + 1]])
140        radii.append(optimized_vars[idx + 2])
141
142    sum_radii = sum(radii)
143    return np.array(centers), np.array(radii), sum_radii
144
```

```

### Circle Packing ( $n = 32$ )

```

1  ```python
2  import numpy as np
3  from scipy.optimize import minimize
4
5  def run_packing():
```

```

```

6      n = 32
7      r_initial = 1.0 / (2.0 + 5.0 * np.sqrt(3)) # Maximum radius for vertical constraint
8
9      # Generate hexagonal arrangement for 30 circles
10     centers = []
11     for row in range(6): # 6 rows with 5 columns each
12         y = r_initial * (1 + row * np.sqrt(3))
13         if row % 2 == 0:
14             x_start = (1.0 - 9.0 * r_initial) / 2 # Adjusted to use more horizontal space
15         else:
16             x_start = (1.0 - 9.0 * r_initial) / 2 + r_initial
17         for col in range(5): # 5 columns
18             x = x_start + col * 2 * r_initial
19             # Ensure the circle is within the square and properly spaced
20             centers.append([x, y])
21
22     # Add two extra circles near the top-right and bottom-right corners with adjusted initial positions
23     extra_x = 1.0 - r_initial - 0.0005
24     extra_y_top = 0.5
25     extra_y_bottom = r_initial + 0.0005
26     centers.append([extra_x, extra_y_top])
27     centers.append([extra_x, extra_y_bottom])
28
29     # Initial radii for all circles
30     radii = [r_initial] * n
31
32     # Flatten the centers and radii into a single array for optimization
33     x0 = np.concatenate([np.array(centers).ravel(), np.array(radii)])
34
35     # Objective function to maximize: sum of radii
36     def objective(x):
37         # Unflatten x into centers and radii
38         centers_flat = x[:n*2].reshape(n, 2)
39         radii_flat = x[n*2:]
40         return -np.sum(radii_flat) # Negative because we minimize
41
42     # Constraints: for each circle, x_i - r_i >= -1e-12, x_i + r_i <= 1 + 1e-12, same for y
43     # and for each pair, distance >= r_i + r_j - 1e-12
44
45     # Define constraint functions
46     def constraint_boundary(x):
47         centers_flat = x[:n*2].reshape(n, 2)
48         radii_flat = x[n*2:]
49         constraints = []
50         epsilon = 1e-12
51         for i in range(n):
52             x_i, y_i = centers_flat[i]
53             r_i = radii_flat[i]
54             constraints.append(x_i - r_i + epsilon) # x_i - r_i >= -epsilon
55             constraints.append(1 + epsilon - x_i - r_i) # x_i + r_i <= 1 + epsilon
56             constraints.append(y_i - r_i + epsilon) # y_i - r_i >= -epsilon
57             constraints.append(1 + epsilon - y_i - r_i) # y_i + r_i <= 1 + epsilon
58         return np.array(constraints)
59
60     # Define constraint for non-overlapping
61     def constraint_overlap(x):
62         centers_flat = x[:n*2].reshape(n, 2)
63         radii_flat = x[n*2:]
64         constraints = []
65         for i in range(n):
66             for j in range(i + 1, n):
67                 dx = centers_flat[i, 0] - centers_flat[j, 0]
68                 dy = centers_flat[i, 1] - centers_flat[j, 1]
69                 dist = np.sqrt(dx**2 + dy**2)
70                 constraints.append(dist - radii_flat[i] - radii_flat[j] + 1e-12)
71         return np.array(constraints)
72
73     # Combine all constraints
74     cons = []
75     # Boundary constraints
76     cons.append({'type': 'ineq', 'fun': lambda x: constraint_boundary(x)})
77     # Overlap constraints
78     cons.append({'type': 'ineq', 'fun': lambda x: constraint_overlap(x)})
79

```

```

80     # Perform optimization with adjusted parameters
81     result = minimize(
82         objective,
83         x0,
84         method='SLSQP',
85         constraints=cons,
86         tol=1e-10,
87         options={'disp': False,
88             'maxiter': 200000, 'ftol': 1e-12, 'eps': 1e-8}
89     )
90
91     # Extract the result
92     optimized_x = result.x
93     centers_opt = optimized_x[:n*2].reshape(n, 2)
94     radii_opt = optimized_x[n*2:]
95
96     # Check if optimization was successful
97     if not result.success:
98         print("Optimization failed")
99         # Fallback to initial guess
100        centers_opt = np.array(centers)
101        radii_opt = np.array(radii)
102    else:
103        # Validate the packing
104        valid = validate_packing(centers_opt, radii_opt)
105        if not valid:
106            print("Validation failed")
107            # Fallback to initial guess
108            centers_opt = np.array(centers)
109            radii_opt = np.array(radii)
110
111    sum_radii = np.sum(radii_opt)
112    return centers_opt, radii_opt, sum_radii
113 ...

```

## B.2 Autocorrelation Inequalities

For autocorrelation inequalities, initial sequences are created by sampling a random value in  $[0, 1]$  and repeating it between 1,000 and 8,000 times (or loading a state-of-the-art construction when available). For the first inequality, the verifier computes the upper bound  $2n \cdot \max(f * f) / (\sum f)^2$  where  $f * f$  denotes discrete autocorrelation; it validates that inputs are non-empty lists of non-negative floats clamped to  $[0, 1000]$  with sum  $\geq 0.01$ , and returns  $\infty$  for invalid constructions. For the second inequality, verifier computes the lower bound  $C_2 = \|f * f\|_2^2 / (\|f * f\|_1 \cdot \|f * f\|_\infty)$  using piecewise-linear integration for the  $L^2$  norm (Simpson-like rule with endpoint zeros) over the normalized interval  $[-1/2, 1/2]$ . Each algorithm is run with 1 GB with 2 CPUs each and a timeout of up to 1100 seconds.

## B.3 Erdős'

We initialize TTT-Discover with random constructions of 40-100 samples around 0.5 with random perturbations. We filter out sequences with more than 1000 values in the verifier. Each algorithm is run with 1 GB with 2 CPUs each and a timeout of up to 1100 seconds.

## C Kernel engineering

For trimul, we provide the a matrix multiplication kernel that [triton provides in README](#), mostly for syntax purposes For MLA-Decode, we first put a softmax kernel in a preliminary prompt to let the base model generate a correct but unoptimized MLA-Decode kernel, and then use that as the initial state with the earlier softmax example removed.

## C.1 Kernel evaluation details

**Setup of verifier for training.** We follow the exact same practice for evaluating kernel correctness and runtime as the original GPUMode competitions. Specifically, the verifier used in our training jobs uses the same code as the official GPU Mode Competition Github repository, with minor adjustment to integrate into our training codebase. The verification process includes a correctness check that compare output values between the custom kernel and a pytorch reference program under a designated precision, followed by runtime benchmarking of the custom kernel across multiple iterations. All the details in our verification procedure follow the official competition exactly, including the test cases used for correctness check and benchmarking, hyper-parameters such as matching precision and iterations used for timing, etc. We run our verifier on H100s for TriMul, and H200s for MLA-Decode, both from the Modal cloud platform.

**Setup of environments for final report.** For final report, we submit to the official TriMul A100/H100 leaderboard and report the runtime shown. For TriMul B200/MI300X and MLA-Decode MI300X tasks, due to an infra problem on GPU Mode’s server, we could not submit to the official leaderboard. For these tasks, we work with the GPU Mode team closely to set up our local environment, which replicates the official environment and gets GPU Mode team’s review and confirmation.

**Selection protocol for best kernels.** For TriMul H100 task, we select 20 kernels with the best verifier score throughout training. For other tasks, since our verifier hardware in training is different from the target hardware, we select 20 kernels with the best training scores plus 20 random correct kernels every 10 steps of training. Finally, we used our verifier **with the target hardware** to verify each selected kernels for three times, and submit the kernel with the smallest average runtime for final report.

## C.2 Analysis of best generated kernels

**TriMul H100 kernels.** The below code shows the best TriMul kernels discovered by TTT for H100 GPU. At the high level, the kernel correctly identifies a major bottleneck of the problem, which is the heavy memory I/O incurred by a series of elementwise operations, and then focuses on fusing them with Triton. Specifically, the kernel fuses: (i) operations in the input LayerNorm, (ii) elementwise activation and multiplication for input gating, and (iii) operations in the output Layernorm and output gating. As for the compute-heavy operation, which is an  $O(N^3)$  matmul, the kernel converts its inputs to fp16 and delegate the computation to cuBLAS to effectively leverage the TensorCores on H100 GPU.

Compared with kernels generated early in training, the final kernel achieves a big improvement by (i) fusing more operations together, and (ii) deeper optimization of the memory access pattern inside fused kernels. For example, a kernel generated early fuses LayerNorm operations, but does not fuse the input gating process. A kernel generated in the middle of training fuses the same operations as the final kernel, but has less efficient memory access pattern in the fused kernel for output LayerNorm, gating, and output projection.

Compared with the best human leaderboard kernel, the TTT discovered kernel adopts a similar fusion strategy for the input LayerNorm and input gating. Different from human kernel, the TTT kernel does not perform as much auto-tuning of block size, which could be a limitation. However, the TTT kernel fuses the output LayerNorm and gating with output projection whereas the human kernel does not, which could explain the moderate advantage of the former.

### C.3 TTT MLA-Decode kernels filtered with Triton kernels

#### TriMul H100

```

1 """
2 Outgoing TriMul (AlphaFold-3) - Triton accelerated forward pass.
3
4 The implementation follows the reference ``TriMul`` module but fuses the
5 expensive kernels:
6
7 1. Row-wise LayerNorm over the last dimension (FP16 output, FP32 reduction).
8 2. Fused projection, gating and optional scalar mask:
9     * left_proj, right_proj = x_norm @ W_proj
10    * left_gate, right_gate, out_gate = sigmoid(x_norm @ W_gate)
11    * left = left_proj * left_gate * mask
12    * right = right_proj * right_gate * mask
13 3. Pairwise multiplication across the sequence dimension (batched GEMM on
14    fp16 tensors).
15 4. Fused hidden-dim LayerNorm -> out-gate multiplication -> final linear
16    projection (all in one kernel, FP16 matmul with FP32 accumulation).
17
18 The output tensor has shape ``[B, N, N, dim]`` and dtype ``float32``.
19 """
20
21 from typing import Tuple, Dict
22 import torch
23 import triton
24 import triton.language as tl
25
26
27 # -----
28 # 1) Row-wise LayerNorm (FP16 output, FP32 accumulator)
29 # -----
30 @triton.jit
31 def _row_ln_fp16_kernel(
32     X_ptr, Y_ptr,           # (M, C) input / output
33     w_ptr, b_ptr,          # LN weight & bias (fp32)
34     M, C: tl.constexpr,    # rows, columns (C is compile-time constant)
35     eps,
36     BLOCK_M: tl.constexpr,
37     BLOCK_C: tl.constexpr,
38 ):
39     pid = tl.program_id(0)
40     row_start = pid * BLOCK_M
41     rows = row_start + tl.arange(0, BLOCK_M)
42     row_mask = rows < M
43
44     # ----- mean / var (fp32) -----
45     sum_val = tl.zeros([BLOCK_M], dtype=tl.float32)
46     sumsq_val = tl.zeros([BLOCK_M], dtype=tl.float32)
47
48     for c in range(0, C, BLOCK_C):
49         cur_c = c + tl.arange(0, BLOCK_C)
50         col_mask = cur_c < C
51         x = tl.load(
52             X_ptr + rows[:, None] * C + cur_c[None, :],
53             mask=row_mask[:, None] & col_mask[None, :],
54             other=0.0,
55         ).to(tl.float32)           # (BLOCK_M, BLOCK_C)
56
57         sum_val += tl.sum(x, axis=1)
58         sumsq_val += tl.sum(x * x, axis=1)
59
60     mean = sum_val / C
61     var = sumsq_val / C - mean * mean
62     inv_std = 1.0 / tl.sqrt(var + eps)
63
64     # ----- normalize + affine (fp16) -----
65     for c in range(0, C, BLOCK_C):
66         cur_c = c + tl.arange(0, BLOCK_C)
67         col_mask = cur_c < C
68         x = tl.load(
69             X_ptr + rows[:, None] * C + cur_c[None, :],
70             mask=row_mask[:, None] & col_mask[None, :],

```

```

71         other=0.0,
72     ).to(tl.float32)
73
74     y = (x - mean[:, None]) * inv_std[:, None]
75
76     w = tl.load(w_ptr + cur_c, mask=col_mask, other=0.0)
77     b = tl.load(b_ptr + cur_c, mask=col_mask, other=0.0)
78
79     y = y * w[None, :] + b[None, :]
80     tl.store(
81         Y_ptr + rows[:, None] * C + cur_c[None, :],
82         y.to(tl.float16),
83         mask=row_mask[:, None] & col_mask[None, :],
84     )
85
86
87     def _row_layernorm_fp16(
88         x: torch.Tensor,
89         weight: torch.Tensor,
90         bias: torch.Tensor,
91         eps: float = 1e-5,
92     ) -> torch.Tensor:
93         """Row-wise LayerNorm over the last dim -> FP16 output."""
94         B, N, _, C = x.shape
95         M = B * N * N
96         x_flat = x.view(M, C).contiguous()
97         y_flat = torch.empty((M, C), dtype=torch.float16, device=x.device)
98
99         BLOCK_M = 128
100        BLOCK_C = 128
101        grid = lambda meta: (triton.cdiv(M, meta["BLOCK_M"])),
102
103        _row_ln_fp16_kernel[grid](
104            x_flat,
105            y_flat,
106            weight,
107            bias,
108            M,
109            C,
110            eps,
111            BLOCK_M=BLOCK_M,
112            BLOCK_C=BLOCK_C,
113            num_warps=8,
114        )
115        return y_flat.view(B, N, N, C)
116
117
118 # -----
119 # 2) Fused projection + gating + optional mask
120 #
121 @triton.jit
122 def _proj_gate_mask_kernel(
123     x_ptr,                                # (M, C) fp16
124     mask_ptr,                               # (M,) fp16 (if MASKED==1)
125     left_proj_w_ptr,                        # (C, H) fp16
126     left_gate_w_ptr,                         # (C, H) fp16
127     right_proj_w_ptr,                        # (C, H) fp16
128     right_gate_w_ptr,                        # (C, H) fp16
129     out_gate_w_ptr,                          # (C, H) fp16
130     left_ptr,                               # (B, H, N, N) fp16
131     right_ptr,                              # (B, H, N, N) fp16
132     out_gate_ptr,                           # (B, N, N, H) fp16
133     M, N, C: tl.constexpr, H: tl.constexpr,
134     BLOCK_M: tl.constexpr,
135     BLOCK_H: tl.constexpr,
136     BLOCK_K: tl.constexpr,
137     MASKED: tl.constexpr,
138 ):
139     pid_m = tl.program_id(0)    # row block
140     pid_h = tl.program_id(1)    # hidden block
141
142     row_start = pid_m * BLOCK_M
143     hid_start = pid_h * BLOCK_H
144

```

```

145 rows = row_start + tl.arange(0, BLOCK_M)           # (BLOCK_M, )
146 hid_start + tl.arange(0, BLOCK_H)                 # (BLOCK_H, )
147
148 row_mask = rows < M
149 hid_mask = hid_start < H
150
151 # ----- mask (scalar per row) -----
152 if MASKED:
153     mask_val = tl.load(mask_ptr + rows, mask=row_mask, other=0.0).to(tl.float32) # (BLOCK_M, )
154 else:
155     mask_val = tl.full([BLOCK_M], 1.0, dtype=tl.float32)
156
157 # ----- accumulators (fp32) -----
158 acc_lp = tl.zeros((BLOCK_M, BLOCK_H), dtype=tl.float32) # left proj
159 acc_lg = tl.zeros((BLOCK_M, BLOCK_H), dtype=tl.float32) # left gate
160 acc_rp = tl.zeros((BLOCK_M, BLOCK_H), dtype=tl.float32) # right proj
161 acc_rg = tl.zeros((BLOCK_M, BLOCK_H), dtype=tl.float32) # right gate
162 acc_og = tl.zeros((BLOCK_M, BLOCK_H), dtype=tl.float32) # out gate
163
164 for k in range(0, C, BLOCK_K):
165     cur_k = k + tl.arange(0, BLOCK_K)
166     k_mask = cur_k < C
167
168     # input tile (fp16 -> fp32)
169     a = tl.load(
170         x_ptr + rows[:, None] * C + cur_k[None, :],
171         mask=row_mask[:, None] & k_mask[None, :],
172         other=0.0,
173     ) # (BLOCK_M, BLOCK_K) fp16
174
175     # weight tiles (C,H) column-major
176     w_lp = tl.load(
177         left_proj_w_ptr + cur_k[:, None] * H + hid_start[None, :],
178         mask=k_mask[:, None] & hid_mask[None, :],
179         other=0.0,
180     )
181     w_lg = tl.load(
182         left_gate_w_ptr + cur_k[:, None] * H + hid_start[None, :],
183         mask=k_mask[:, None] & hid_mask[None, :],
184         other=0.0,
185     )
186     w_rp = tl.load(
187         right_proj_w_ptr + cur_k[:, None] * H + hid_start[None, :],
188         mask=k_mask[:, None] & hid_mask[None, :],
189         other=0.0,
190     )
191     w_rg = tl.load(
192         right_gate_w_ptr + cur_k[:, None] * H + hid_start[None, :],
193         mask=k_mask[:, None] & hid_mask[None, :],
194         other=0.0,
195     )
196     w_og = tl.load(
197         out_gate_w_ptr + cur_k[:, None] * H + hid_start[None, :],
198         mask=k_mask[:, None] & hid_mask[None, :],
199         other=0.0,
200     )
201
202     # fp16*fp16 -> fp32 dot products
203     acc_lp += tl.dot(a, w_lp)
204     acc_lg += tl.dot(a, w_lg)
205     acc_rp += tl.dot(a, w_rp)
206     acc_rg += tl.dot(a, w_rg)
207     acc_og += tl.dot(a, w_og)
208
209     # ----- sigmoid gates -----
210     left_gate = 1.0 / (1.0 + tl.exp(-acc_lg))
211     right_gate = 1.0 / (1.0 + tl.exp(-acc_rg))
212     out_gate = 1.0 / (1.0 + tl.exp(-acc_og))
213
214     # ----- apply mask and per-row gates -----
215     left_out = acc_lp * left_gate * mask_val[:, None]
216     right_out = acc_rp * right_gate * mask_val[:, None]
217
218     # ----- store left/right (B,H,N,N) -----

```

```

219     N_sq = N * N
220     b_idx = rows // N_sq
221     rem   = rows - b_idx * N_sq
222     i_idx = rem // N
223     k_idx = rem - i_idx * N
224
225     # layout for left/right: (B, H, N, N) -> flat index:
226     off = ((b_idx[:, None] * H + hids[None, :]) * N_sq) + i_idx[:, None] * N + k_idx[:, None]
227
228     tl.store(
229         left_ptr + off,
230         left_out.to(tl.float16),
231         mask=row_mask[:, None] & hid_mask[None, :],
232     )
233     tl.store(
234         right_ptr + off,
235         right_out.to(tl.float16),
236         mask=row_mask[:, None] & hid_mask[None, :],
237     )
238
239     # ----- store out_gate (B,N,N,H) -----
240     off_gate = rows[:, None] * H + hids[None, :]
241     tl.store(
242         out_gate_ptr + off_gate,
243         out_gate.to(tl.float16),
244         mask=row_mask[:, None] & hid_mask[None, :],
245     )
246
247
248     # -----
249     # 3) Fused hidden-dim LayerNorm -> out-gate -> final linear
250     #
251     @triton.jit
252     def _ln_gate_out_linear_fused_kernel(
253         hidden_ptr,           # (B*N*N*Nc,) fp16 flattened
254         out_gate_ptr,        # (B*N*N*H,) fp16 flattened
255         ln_w_ptr, ln_b_ptr, # (H,) fp32
256         w_out_ptr,          # (H, D) fp16
257         out_ptr,             # (B, N, N, D) fp32
258         B, N, H, D: tl.constexpr,
259         eps: tl.constexpr,
260         BLOCK_M: tl.constexpr,
261         BLOCK_H: tl.constexpr,
262         BLOCK_D: tl.constexpr,
263     ):
264         pid = tl.program_id(0)
265         row_start = pid * BLOCK_M
266         rows = row_start + tl.arange(0, BLOCK_M)           # flat index for (b,i,j)
267         row_mask = rows < (B * N * N)
268
269         N_sq = N * N
270         b_idx = rows // N_sq
271         rem = rows - b_idx * N_sq
272         i_idx = rem // N
273         j_idx = rem - i_idx * N
274
275         # ----- load hidden slice (BLOCK_M, BLOCK_H) -----
276         hids = tl.arange(0, BLOCK_H)
277         hid_mask = hids < H
278
279         hidden_off = ((b_idx[:, None] * H + hids[None, :]) * N_sq) + i_idx[:, None] * N + j_idx[:, None]
280         hidden_tile = tl.load(
281             hidden_ptr + hidden_off,
282             mask=row_mask[:, None] & hid_mask[None, :],
283             other=0.0,
284         ) # fp16
285         hidden_fp32 = hidden_tile.to(tl.float32)
286
287         # ----- mean / var across H (fp32) -----
288         sum_val = tl.sum(hidden_fp32, axis=1)           # (BLOCK_M,)
289         sumsq_val = tl.sum(hidden_fp32 * hidden_fp32, axis=1) # (BLOCK_M,)
290         mean = sum_val / H
291         var = sumsq_val / H - mean * mean
292         inv_std = 1.0 / tl.sqrt(var + eps)

```

```

293
294     # ----- LayerNorm (fp32) -----
295     w_ln = tl.load(ln_w_ptr + hids, mask=hid_mask, other=0.0)    # (H, )
296     b_ln = tl.load(ln_b_ptr + hids, mask=hid_mask, other=0.0)    # (H, )
297     hidden_norm = (hidden_fp32 - mean[:, None]) * inv_std[:, None]
298     hidden_norm = hidden_norm * w_ln[None, :] + b_ln[None, :]    # (BLOCK_M, BLOCK_H)
299
300     # ----- out-gate (fp32) -----
301     out_gate_off = rows[:, None] * H + hids[None, :]
302     out_gate_tile = tl.load(
303         out_gate_ptr + out_gate_off,
304         mask=row_mask[:, None] & hid_mask[None, :],
305         other=0.0,
306     ).to(tl.float32)                                              # (BLOCK_M, BLOCK_H)
307
308     gated = hidden_norm * out_gate_tile                         # (BLOCK_M, BLOCK_H)
309
310     # ----- final linear projection (fp16 matmul, fp32 acc) -----
311     gated_fp16 = gated.to(tl.float16)
312
313     for d0 in range(0, D, BLOCK_D):
314         cols = d0 + tl.arange(0, BLOCK_D)
315         col_mask = cols < D
316
317         w_out = tl.load(
318             w_out_ptr + hids[:, None] * D + cols[None, :],
319             mask=hid_mask[:, None] & col_mask[None, :],
320             other=0.0,
321         ) # (BLOCK_H, BLOCK_D) fp16
322
323         out = tl.dot(gated_fp16, w_out)                            # (BLOCK_M, BLOCK_D) fp32
324
325         tl.store(
326             out_ptr + rows[:, None] * D + cols[None, :],
327             out,
328             mask=row_mask[:, None] & col_mask[None, :],
329         )
330
331
332     # -----
333     # 4) Entrypoint
334     #
335     def custom_kernel(
336         data: Tuple[torch.Tensor, torch.Tensor, Dict[str, torch.Tensor], Dict]
337     ) -> torch.Tensor:
338         """
339             Forward pass of the outgoing TriMul operator (no gradients).
340
341             Arguments
342             -----
343                 data : (input, mask, weights, config)
344                     - input : Tensor[B, N, N, C] (float32)
345                     - mask : Tensor[B, N, N] (bool/float) or None
346                     - weights: dict of module parameters (float32)
347                     - config : dict with ``dim`` (C) and ``hidden_dim`` (H) and optional ``nomask``
348
349             Returns
350             -----
351                 Tensor[B, N, N, C] (float32)
352             """
353             inp, mask, weights, cfg = data
354             dim = cfg["dim"]                                # C
355             hidden_dim = cfg["hidden_dim"]                  # H
356             nomask = cfg.get("nomask", True)
357             eps = 1e-5
358
359             device = inp.device
360             B, N, _, _ = inp.shape
361             M = B * N * N                                  # total rows for row-wise ops
362
363             # -----
364             # 1) Row-wise LayerNorm (fp16 output)
365             #
366             X_norm = _row_layernorm_fp16(

```

```

367     inp,
368     weights["norm.weight"],
369     weights["norm.bias"],
370     eps=eps,
371 ) # (B, N, N, C) fp16
372
373 # -----
374 # 2) Prepare projection / gate weights (C, H) fp16, column-major
375 #
376 left_proj_w_T = weights["left_proj.weight"].t().contiguous().to(torch.float16)
377 right_proj_w_T = weights["right_proj.weight"].t().contiguous().to(torch.float16)
378 left_gate_w_T = weights["left_gate.weight"].t().contiguous().to(torch.float16)
379 right_gate_w_T = weights["right_gate.weight"].t().contiguous().to(torch.float16)
380 out_gate_w_T = weights["out_gate.weight"].t().contiguous().to(torch.float16)
381
382 #
383 # 3) Mask handling (optional)
384 #
385 if not nomask and mask is not None:
386     mask_flat = mask.reshape(M).to(torch.float16).contiguous()
387     MASKED = 1
388 else:
389     mask_flat = torch.empty(0, dtype=torch.float16, device=device)
390     MASKED = 0
391
392 #
393 # 4) Allocate buffers for fused projection + gating
394 #
395 left = torch.empty((B, hidden_dim, N, N), dtype=torch.float16, device=device)
396 right = torch.empty_like(left)
397 out_gate = torch.empty((B, N, N, hidden_dim), dtype=torch.float16, device=device)
398
399 #
400 # 5) Fused projection / gating / optional mask
401 #
402 BLOCK_M = 64
403 BLOCK_H = 64
404 BLOCK_K = 32
405 grid_proj = (triton.cdiv(M, BLOCK_M), triton.cdiv(hidden_dim, BLOCK_H))
406
407 _proj_gate_mask_kernel[grid_proj](
408     x_norm,
409     mask_flat,
410     left_proj_w_T,
411     left_gate_w_T,
412     right_proj_w_T,
413     right_gate_w_T,
414     out_gate_w_T,
415     left,
416     right,
417     out_gate,
418     M,
419     N,
420     dim,
421     hidden_dim,
422     BLOCK_M=BLOCK_M,
423     BLOCK_H=BLOCK_H,
424     BLOCK_K=BLOCK_K,
425     MASKED=MASKED,
426     num_warps=4,
427 )
428
429 #
430 # 6) Pairwise multiplication (batched GEMM) - left @ right^T
431 #
432 left_mat = left.view(B * hidden_dim, N, N) # (B*N, N, N)
433 right_mat = right.view(B * hidden_dim, N, N).transpose(1, 2) # (B*N, N, N)^T
434 hidden_fp16 = torch.bmm(left_mat, right_mat) # (B*N, N, N) fp16
435 hidden = hidden_fp16.view(B, hidden_dim, N, N) # (B, N, N) fp16
436
437 #
438 # 7) Fused hidden-dim LayerNorm -> out-gate -> final linear
439 #
440 to_out_norm_w = weights["to_out_norm.weight"] # (H,) fp32

```

```

441
442     to_out_norm_b = weights["to_out_norm.bias"]      # (H,) fp32
443     to_out_w_T = weights["to_out.weight"].t().contiguous().to(torch.float16)  # (H, C)
444
445     out = torch.empty((B, N, N, dim), dtype=torch.float32, device=device)
446
447     BLOCK_M_OUT = 64
448     BLOCK_H_OUT = hidden_dim      # cover the whole hidden dim in one kernel launch
449     BLOCK_D_OUT = 64
450
451     grid_out = (triton.cdiv(B * N * N, BLOCK_M_OUT),)
452
453     _ln_gate_out_linear_fused_kernel[grid_out](
454         hidden.view(-1),           # flat fp16 hidden
455         out_gate.view(-1),        # flat fp16 out-gate
456         to_out_norm_w,
457         to_out_norm_b,
458         to_out_w_T,
459         out,
460         B,
461         N,
462         hidden_dim,
463         dim,
464         eps,
465         BLOCK_M=BLOCK_M_OUT,
466         BLOCK_H=BLOCK_H_OUT,
467         BLOCK_D=BLOCK_D_OUT,
468         num_warps=4,
469     )
470
471     return out

```

Method	Model	AMD MI300X - MLA Decode ( $\downarrow, \mu\text{s}$ ) [95% CI]		
		Instance 1	Instance 2	Instance 3
1st human	—	1653.8 [1637.3, 1670.3]	1688.6 [1672.8, 1704.3]	1668.7 [1637.0, 1700.3]
2nd human	—	1662.8 [1648.8, 1676.8]	1688.6 [1677.6, 1699.5]	1679.7 [1653.4, 1705.9]
3rd human	—	1723.0 [1711.5, 1734.5]	1765.8 [1758.1, 1773.5]	1718.0 [1698.3, 1737.7]
4th human	—	1768.7 [1750.3, 1787.2]	1769.9 [1755.2, 1784.6]	1767.0 [1736.2, 1797.8]
5th human	—	2038.6 [2017.8, 2059.3]	2037.3 [2021.0, 2053.6]	2041.9 [1989.0, 2094.8]
Best-of-25600	gpt-oss-120b	2286.0 [2264.2, 2307.8]	2324.1 [2306.0, 2342.1]	2275.2 [2267.3, 2283.1]
TTT-Discover	gpt-oss-120b	1740.6 [1697.9, 1783.2]	1754.4 [1736.7, 1772.2]	1707.1 [1664.5, 1749.8]

Table 10. Results of TTT MLA-Decode kernels filtered with Triton kernels.

## D Algorithm Engineering

During the contest, AtCoder provides an official input generator, tester to evaluate program correctness, and a scoring function used for the final ranking. For training, we generate 150 test cases using seeds 0 through 149 from the input generator and run our program on each of these cases with an ALE-Bench provided C++20 container ([yimjk/ale-bench:cpp20-202301](#)). A program receives a non-zero reward only if it passes all correctness checks and executes within the problem time limit (2 seconds) across all 150 test cases. The per-test case score is problem-specific and matches the scoring used in the AtCoder contest. For ahc039, we use ShinkaEvolve’s performance metric, which is determined by the score’s relative placement among the final contest’s scores, and for ahc058, we directly use the contest score.

For the final evaluation, we select the top three highest-scoring programs from our local training runs and submit them to the official AtCoder submission website. For our language, we specify

C++23 (GCC 15.2.0). The submission is evaluated using the same scoring and validation process as the original contest, including checks for incorrect output, time limit violations, and compilation or runtime errors on AtCoder’s hidden test cases. The resulting score is used as the final evaluation.

For AHC training runs, we make a slight modification from our standard hyperparameters. For AHC039, we decrease the prompt length + thinking token limit to 22000 due to the large initial program. For AHC058, we similarly decrease the prompt length + thinking token limit to 25000 and found that a learning rate of  $2 \times 10^{-5}$  performed slightly better. For both AHC problems, we use a KL coefficient of  $1 \times 10^{-2}$ . Other hyperparameters are set to our standard values.

## E Single cell analysis

The OpenProblems benchmark provides three datasets: pancreas, pbmc and tabula. We select the Pancreas dataset to compute MSE and Poisson loss scores and use the other two datasets to assess generalization. MSE and Poisson loss scores are normalized with respect to the scores that no denoising and perfect denoising would get on this task. The main score metric in the OpenProblems denoising benchmark is the mean between the normalized MSE and the normalized Poisson. During verification, we reject all the solutions that obtain a normalized Poisson lower than 0.97 or larger than 1 so that we can focus only on improving a single metric, MSE.

In the prompt we also include instructions regarding what makes a solution taking inspiration from the Supplementary Materials of the OpenProblems paper [43]. For this specific applications, considering the size of the datasets, the memory limit is increased to 3GB. To force generalization, we reduce the time limits for the execution to 400 seconds.

We ran the OpenEvolve baseline with 25,600 samples. After sample 17,000, we observed the OpenEvolve database filling up with programs that timed out. Consequently, we selected the best program found up to that point.

Both TTT-Discover and the Best-of-25600 baselines are run with max tokens equal to 20,000.

Both MAGIC and the solution found by TTT-Discover are run with default parameters.

**Denoising**

```

1  #
2  # -----
3  # Imports
4  # -----
5  import warnings
6  import numpy as np
7  import scipy.sparse as sp
8  from graphtools import Graph
9  import scprep
10 from scprep.utils import toarray
11 from scprep.normalize import library_size_normalize
12 from sklearn.decomposition import TruncatedSVD
13 import scanpy as sc
14 import sklearn.metrics
15
16 # -----
17 # Helper utilities (identical to the reference implementation - unchanged)
18 #
19
20
21 def _inverse_anscombe_refined(Y: np.ndarray, n_iter: int = 12) -> np.ndarray:
22     """Newton-iteration inverse of the Anscombe variance-stabilising transform."""
23     Y = np.asarray(Y, dtype=np.float64)
24     x = (Y / 2.0) ** 2 - 3.0 / 8.0
25     for _ in range(n_iter):
26         sqrt_term = np.sqrt(np.maximum(x + 3.0 / 8.0, 0.0))

```

```

27         x -= (2.0 * sqrt_term - Y) * sqrt_term
28     np.maximum(x, 0.0, out=x)
29     return x
30
31
32     def _inverse_ft_refined(Y: np.ndarray, n_iter: int = 12) -> np.ndarray:
33         """Newton-iteration inverse of the Freeman-Tukey transform."""
34         Y = np.asarray(Y, dtype=np.float64)
35         out = np.zeros_like(Y)
36         mask = Y > 0
37         y = Y[mask]
38
39         # Analytic start:  $s = (y^{2-1}) / (2y)$  ( $s = \sqrt{x}$ )
40         s = np.maximum((y * y - 1.0) / (2.0 * y), 0.0)
41         x = s * s
42         for _ in range(n_iter):
43             sqrtx = np.sqrt(np.maximum(x, 0.0))
44             sqrtx1 = np.sqrt(np.maximum(x + 1.0, 0.0))
45             f = sqrtx + sqrtx1 - y
46             fprime = 0.5 / np.maximum(sqrtx, 1e-12) + 0.5 / np.maximum(sqrtx1, 1e-12)
47             x -= f / fprime
48             x = np.maximum(x, 0.0)
49         out[mask] = x
50     return out
51
52
53     def _calc_dropout(counts: np.ndarray) -> np.ndarray:
54         """Fraction of zero entries per gene."""
55         return np.mean(counts == 0, axis=0)
56
57
58     def _adaptive_blend_weights(
59         dropout: np.ndarray,
60         var_orig: np.ndarray,
61         var_diff: np.ndarray,
62         corr: np.ndarray,
63         mu: np.ndarray,
64         max_alpha: float = 0.55,
65         eps: float = 1e-12,
66     ) -> np.ndarray:
67         """
68             Compute a diffusion-blend weight for each gene.
69
70             Larger weight → gene benefits more from diffusion.
71         """
72         var_reduction = (var_orig - var_diff) / (var_orig + eps)
73         var_reduction = np.clip(var_reduction, 0.0, 1.0)
74
75         mu_norm = (mu - mu.min()) / (mu.max() - mu.min() + eps)
76         expr_factor = 1.0 - mu_norm
77
78         raw = dropout * var_reduction * (1.0 - corr) * expr_factor
79         raw = np.where(dropout > 0.8, raw * 1.2, raw)
80         w = np.clip(raw, 0.0, max_alpha)
81     return w
82
83
84     def _select_hvg_scanpy(X_norm: np.ndarray, n_hvg: int = 3000) -> np.ndarray:
85         """HVG selection using Scanpy's Seurat-flavour method."""
86         if n_hvg is None or n_hvg >= X_norm.shape[1]:
87             return np.arange(X_norm.shape[1])
88         adata = sc.AnnData(X=X_norm)
89         sc.pp.highly_variable_genes(
90             adata,
91             n_top_genes=n_hvg,
92             flavor="seurat",
93             batch_key=None,
94             subset=False,
95             inplace=True,
96         )
97         return np.where(adata.var["highly_variable"].values)[0]
98
99
100    def _row_normalize_sparse(M: sp.spmatrix) -> sp.spmatrix:

```

```

101     """Row-stochastic normalisation for a CSR/CSC matrix."""
102     row_sums = np.asarray(M.sum(axis=1)).ravel()
103     row_sums[row_sums == 0] = 1.0
104     return M.multiply(1.0 / row_sums[:, None])
105
106
107 def _symmetrize_diffusion(P: sp.spmatrix) -> sp.spmatrix:
108     """Produce a symmetric, row-stochastic diffusion operator."""
109     sym = (P + P.transpose()) * 0.5
110     return _row_normalize_sparse(sym)
111
112
113 def _add_self_loop(P: sp.spmatrix, alpha: float = 0.5) -> sp.spmatrix:
114     """Mix the identity matrix with the transition matrix."""
115     n = P.shape[0]
116     I = sp.eye(n, format='csr')
117     P_mix = (1.0 - alpha) * I + alpha * P
118     return _row_normalize_sparse(P_mix)
119
120
121 def _gene_correlation(X1: np.ndarray, X2: np.ndarray, eps: float = 1e-12) -> np.ndarray:
122     """Pearson correlation per gene between two matrices."""
123     mu1 = X1.mean(axis=0)
124     mu2 = X2.mean(axis=0)
125     cov = (X1 * X2).mean(axis=0) - mu1 * mu2
126     var1 = X1.var(axis=0)
127     var2 = X2.var(axis=0)
128     denom = np.sqrt(var1 * var2) + eps
129     corr = cov / denom
130     corr = np.clip(corr, -1.0, 1.0)
131     corr = np.where((var1 < eps) | (var2 < eps), 0.0, corr)
132     return corr
133
134
135 def _impute_zeros_with_neighbors(
136     X_norm: np.ndarray,
137     diff_op,
138     steps: int = 1,
139 ) -> np.ndarray:
140     """Replace exact zeros by a diffusion-weighted neighbour average."""
141     neighbor_avg = diff_op @ X_norm
142     for _ in range(1, steps):
143         neighbor_avg = diff_op @ neighbor_avg
144     mask = X_norm == 0
145     Y = X_norm.copy()
146     Y[mask] = neighbor_avg[mask]
147     return Y
148
149
150 def _weighted_multi_scale_diffuse_genewise(diff_op, X, t, dropout, decay):
151     """
152     Gene-wise weighted multi-scale diffusion.
153
154     Guarantees a *baseline* amount of smoothing for every gene.
155     """
156     cur = X.copy()
157     weighted_sum = np.zeros_like(X)
158     weight_sum = np.zeros(X.shape[1])
159
160     # baseline smoothing factor (0.2 ... 1.0)
161     baseline = 0.2
162     base = decay * (baseline + (1.0 - baseline) * dropout) # (genes,)
163
164     # step 0 (raw)
165     weighted_sum += cur
166     weight_sum += 1.0
167
168     for i in range(1, t + 1):
169         cur = diff_op @ cur
170         w_i = np.power(base, i) # (genes, )
171         weighted_sum += cur * w_i[None, :]
172         weight_sum += w_i
173
174     weighted_sum = weighted_sum / np.maximum(weight_sum[None, :], 1e-12)

```

```

175     return weighted_sum
176
177
178 def _match_mean_variance(
179     X_raw: np.ndarray,
180     X_diff: np.ndarray,
181     min_mean: float = 0.02,
182     var_scale_min: float = 0.5,
183     var_scale_max: float = 2.0,
184     eps: float = 1e-12,
185 ) -> np.ndarray:
186     """
187     Rescale each gene in ``X_diff`` so that its mean **and** variance equal those
188     of ``X_raw`` (both row-stochastic). Only genes with mean  $\geq \text{`min_mean'}$ 
189     get variance-matched.
190     """
191     mu_raw = X_raw.mean(axis=0)
192     var_raw = X_raw.var(axis=0)
193
194     mu_diff = X_diff.mean(axis=0)
195     var_diff = X_diff.var(axis=0)
196
197     # Mean matching
198     scale_mean = mu_raw / (mu_diff + eps)
199     X_centered = X_diff * scale_mean
200
201     # Variance matching
202     var_centered = var_diff * (scale_mean ** 2)
203     high = mu_raw > min_mean
204     scale_var = np.ones_like(mu_raw)
205     scale_var[high] = np.sqrt(var_raw[high] / (var_centered[high] + eps))
206     scale_var = np.clip(scale_var, var_scale_min, var_scale_max)
207
208     X_scaled = (X_centered - mu_raw) * scale_var + mu_raw
209
210     # Re-normalize rows (still stochastic)
211     row_sums = X_scaled.sum(axis=1, keepdims=True)
212     X_scaled = X_scaled / np.maximum(row_sums, eps)
213     return X_scaled
214
215
216 def _apply_shrink_exponent(arr: np.ndarray, gamma: float) -> np.ndarray:
217     """Raise the array to a power  $\gamma > 1$  (shrinks small values more than large ones)."""
218     if gamma <= 1.0:
219         return arr
220     shrunk = np.power(arr, gamma)
221     row_sums = shrunk.sum(axis=1, keepdims=True)
222     scaling = np.maximum(row_sums, 1e-12)
223     return shrunk * (arr.sum(axis=1, keepdims=True) / scaling)
224
225
226 def _apply_transform(counts: np.ndarray, tr: str) -> np.ndarray:
227     """Forward variance-stabilising transform."""
228     if tr == "anscombe":
229         return 2.0 * np.sqrt(counts + 3.0 / 8.0)
230     if tr == "ft":
231         return np.sqrt(counts) + np.sqrt(counts + 1.0)
232     if tr == "sqrt":
233         return np.sqrt(counts)
234     if tr == "log":
235         return np.log1p(counts)
236     raise ValueError(f"Unsupported transform: {tr}")
237
238
239 def _inverse_transform(vst: np.ndarray, tr: str) -> np.ndarray:
240     """Inverse of the forward VST."""
241     if tr == "anscombe":
242         return _inverse_anscombe_refined(vst, n_iter=12)
243     if tr == "ft":
244         return _inverse_ft_refined(vst, n_iter=12)
245     if tr == "sqrt":
246         return vst ** 2
247     if tr == "log":
248         return np.expm1(vst)

```

```

249     raise ValueError(f"Unsupported transform: {tr}")
250
251
252     def _filter_genes_by_dropout(gene_idx: np.ndarray, dropout: np.ndarray, thresh: float) -> np.ndarray:
253         """Remove genes whose dropout exceeds ``thresh``."""
254         keep = dropout[gene_idx] < thresh
255         return gene_idx[keep]
256
257
258     def _residual_diffusion_smoothing(diff_op, residual, weight):
259         """One-step diffusion of the cell-wise residual and add a fraction ``weight``."""
260         if weight <= 0.0:
261             return np.zeros_like(residual)
262         smoothed = diff_op @ residual
263         return weight * smoothed
264
265
266     # -----
267     # Main denoising routine
268     # -----
269
270
271     def magic_denoise(
272         X,
273         knn: int = None,
274         t: int = None,
275         n_pca: int = 50,
276         decay: float = 0.85,
277         knn_max: int = None,
278         random_state: int = None,
279         n_jobs: int = 2,
280         transform: str = None,                                # {"anscombe", "sqrt", "ft", "log"} - None = auto
281         max_alpha: float = None,
282         n_hvg: int = None,
283         dropout_thresh: float = None,
284         zero_threshold: float = 0.0,
285         round_counts: bool = False,
286         impute_zeros: bool = True,
287         impute_steps: int = None,
288         lowrank_components: int = 30,                         # number of SVD components for post-processing
289         lowrank_weight: float = None,                         # blend weight for low-rank reconstruction
290         log_smooth_t: int = 4,
291         log_smooth_weight: float = None,
292         self_loop_alpha: float = None,
293         use_symmetric: bool = True,
294         raw_mix_weight: float = None,                        # max weight for raw-count blending (gene-wise)
295         extra_post_smooth_weight: float = None,
296         residual_weight: float = None,                      # weight for residual diffusion smoothing
297         verbose: bool = False,
298         mode: str = "balanced",                            # {"balanced", "mse"}
299         diff_decay: float = None,                          # decay for weighted multi-scale diffusion
300         var_match_min_mean: float = 0.02,
301         var_match_scale_min: float = 0.5,
302         var_match_scale_max: float = 2.0,
303         # ----- NEW knobs -----
304         final_smooth_weight: float = None,                # weight of the extra log-space polishing
305         final_smooth_t: int = None,                        # number of diffusion steps for polishing
306         # -----
307         **kwargs,
308     ):                                             
309         """
310             Adaptive MAGIC-style denoiser - MSE-optimised flavour with a final
311             log-space polishing step.
312
313             Parameters
314             -----
315             X : array-like, shape (cells, genes)
316                 Raw integer count matrix.
317             mode : {"balanced", "mse"}
318                 ``balanced`` - standard MAGIC mix of MSE / Poisson.
319                 ``mse`` - tuned for the lowest possible MSE while still satisfying
320                 the Poisson constraint.
321             final_smooth_weight, final_smooth_t : optional
322                 Extra diffusion on the log-normalised matrix (the metric that is

```

```

323     used for MSE). Setting ``final_smooth_weight`` to a value >0 adds a
324     polishing step that directly smooths the log-space representation.
325     ``final_smooth_t`` controls how many diffusion steps are applied;
326     typical values are 2-4.
327
328     Returns
329     -----
330     denoised_X : np.ndarray, shape (cells, genes)
331         Denoised count matrix (float64, non-negative).
332     """
333
334     # -----
335     # 0. Input handling
336     #
337     with warnings.catch_warnings():
338         warnings.simplefilter("ignore")
339         X_arr = toarray(X).astype(np.float64)
340
341     n_cells, n_genes = X_arr.shape
342     if verbose:
343         print('[magic_denoise] Input matrix: {} cells x {} genes'.format(n_cells, n_genes))
344
345     # Preserve raw library sizes - needed for the "reverse-normalisation" trick
346     libsize_raw = X_arr.sum(axis=1)
347     libsize_raw[libsize_raw == 0] = 1.0
348
349     # Gene-wise dropout (used throughout)
350     dropout_frac = _calc_dropout(X_arr)
351
352     # -----
353     # 1. Mode-specific defaults
354     #
355     mode = mode.lower()
356     if mode not in {"balanced", "mse"}:
357         raise ValueError("mode must be 'balanced' or 'mse'")
358
359     # -----
360     # generic defaults
361     #
362     if n_pca is None:
363         n_pca = 50
364     if decay is None:
365         decay = 0.85
366     if self_loop_alpha is None:
367         self_loop_alpha = 0.5
368     if knn_max is None:
369         knn_max = knn * 2 if knn is not None else None
370     if transform is None:
371         # auto-selection
372         if mode == "mse":
373             transforms_to_use = ["anscombe", "ft", "sqrt"]
374         else:
375             transforms_to_use = ["anscombe", "ft"]
376     else:
377         transforms_to_use = [transform.lower()]
378
379     # -----
380     # mode-specific hyper-parameters
381     #
382     if mode == "balanced":
383         # Original balanced defaults (unchanged)
384         max_alpha = 0.55 if max_alpha is None else max_alpha
385         lowrank_weight = 0.15 if lowrank_weight is None else lowrank_weight
386         raw_mix_weight = 0.20 if raw_mix_weight is None else raw_mix_weight
387         t = 6 if t is None else t
388         diff_decay = 0.85 if diff_decay is None else diff_decay
389         knn = max(5, min(15, int(np.sqrt(n_cells)))) if knn is None else knn
390         knn_max = knn * 2 if knn_max is None else knn_max
391         log_smooth_weight = 0.80 if log_smooth_weight is None else log_smooth_weight
392         extra_post_smooth_weight = 0.12 if extra_post_smooth_weight is None else extra_post_smooth_weight
393         impute_steps = 2 if impute_steps is None else impute_steps
394         residual_weight = 0.08 if residual_weight is None else residual_weight
395         lowrank_components = 30 if lowrank_components is None else lowrank_components
396         dropout_thresh = 0.9 if dropout_thresh is None else dropout_thresh
397         zero_threshold = 0.0 if zero_threshold is None else zero_threshold
398         scale_before_inverse = True

```

```

397     apply_shrink = True
398     # final polishing defaults (balanced)
399     final_smooth_weight = 0.25 if final_smooth_weight is None else final_smooth_weight
400     final_smooth_t = 3 if final_smooth_t is None else final_smooth_t
401 else: # mode == "mse"
402     #
403     # heavily tuned for MSE while keeping Poisson=0.98
404     #
405     max_alpha = 0.90 if max_alpha is None else max_alpha
406     lowrank_weight = 0.50 if lowrank_weight is None else lowrank_weight
407     raw_mix_weight = 0.15 if raw_mix_weight is None else raw_mix_weight
408     t = 20 if t is None else t
409     diff_decay = 0.98 if diff_decay is None else diff_decay
410     knn = max(15, min(40, int(np.sqrt(n_cells) * 2))) if knn is None else knn
411     knn_max = knn * 2 if knn_max is None else knn_max
412     log_smooth_weight = 0.75 if log_smooth_weight is None else log_smooth_weight
413     log_smooth_t = 6 if log_smooth_t is None else log_smooth_t
414     extra_post_smooth_weight = 0.08 if extra_post_smooth_weight is None else extra_post_smooth_weight
415     impute_steps = 2 if impute_steps is None else impute_steps
416     residual_weight = 0.20 if residual_weight is None else residual_weight
417     lowrank_components = min(150, min(n_cells, n_genes) - 1) if lowrank_components is None else
418     lowrank_components
419     n_hvg = min(5000, max(3000, int(n_genes * 0.3))) if n_hvg is None else n_hvg
420     dropout_thresh = 0.95 if dropout_thresh is None else dropout_thresh
421     zero_threshold = 0.20 if zero_threshold is None else zero_threshold
422     scale_before_inverse = False
423     apply_shrink = False # exponent-shrinkage gives no gain for pure MSE
424     var_match_min_mean = 0.01 # match variance for more genes
425     # final polishing defaults (MSE)
426     final_smooth_weight = 0.40 if final_smooth_weight is None else final_smooth_weight
427     final_smooth_t = 2 if final_smooth_t is None else final_smooth_t
428
429     # -----#
430     # sanity checks / final default fill-ins
431     #
432     if n_pca is None:
433         n_pca = 50
434     if decay is None:
435         decay = 0.85
436
437     # 2. Primary VST → HVG → graph construction (with dropout filter)
438     #
439     primary_tr = transforms_to_use[0] # usually "anscombe"
440     X_vst_primary = _apply_transform(X_arr, primary_tr)
441     X_norm_primary, _ = library_size.normalize(
442         X_vst_primary, rescale=1.0, return_library_size=True
443     ) # rows sum to 1
444
445     # HVG selection
446     hvgs_idx = _select_hvg_scanpy(X_norm_primary, n_hvg=n_hvg)
447
448     # Remove extremely sparse HVGs (dropout filter)
449     hvgs_idx = _filter_genes_by_dropout(hvgs_idx, dropout_frac, dropout_thresh)
450     if hvgs_idx.size == 0:
451         # fallback - use all genes if filter removed everything
452         hvgs_idx = np.arange(n_genes)
453
454     X_graph = X_norm_primary[:, hvgs_idx]
455
456     # -----
457     # 3. Build diffusion operator (shared across transforms)
458     #
459     n_pca_arg = n_pca if (X_graph.shape[1] > n_pca) else None
460     graph = Graph(
461         X_graph,
462         n_pca=n_pca_arg,
463         knn=knn,
464         knn_max=knn_max,
465         decay=decay,
466         random_state=random_state,
467         n_jobs=n_jobs,
468         verbose=0,
469     )

```

```

470 diff_op = graph.diff_op           # sparse, row-stochastic
471
472 if use_symmetric:
473     diff_op = _symmetrize_diffusion(diff_op)
474     if verbose:
475         print('[magic_denoise] Symmetrised diffusion operator``')
476
477 diff_op = _add_self_loop(diff_op, alpha=self_loop_alpha)
478 if verbose:
479     print('[magic_denoise] Added self-loop (α={:.3f})'.format(self_loop_alpha))
480
481 # -----
482 # 4. Process each VST separately
483 #
484 transform_outputs = []          # denoised count matrices (cells × genes)
485 w_diff_primary = None          # will be stored for the log-smooth step
486
487 for ti, tr in enumerate(transforms_to_use):
488     if verbose:
489         print(f"[magic_denoise] ----- Transform {tr} ({ti+1}/{len(transforms_to_use)})")
490
491     # ---- forward VST + library-size normalisation (rows sum to 1)
492     X_vst = _apply_transform(X_arr, tr)
493     X_norm, _ = library_size_normalize(
494         X_vst, rescale=1.0, return_library_size=True
495     ) # rows = 1
496
497     # ---- optional zero-imputation
498     if impute_zeros:
499         X_filled = _impute_zeros_with_neighbors(
500             X_norm, diff_op, steps=impute_steps
501         )
502     else:
503         X_filled = X_norm.copy()
504
505     # ---- normalise again after imputation (ensures exact stochasticity)
506     row_sums_filled = X_filled.sum(axis=1, keepdims=True)
507     X_filled = X_filled / np.maximum(row_sums_filled, 1e-12)
508
509     # ---- gene-wise weighted multi-scale diffusion
510     diffused = _weighted_multi_scale_diffuse_genewise(
511         diff_op, X_filled, t, dropout_frac, diff_decay
512     )
513
514     # ---- match mean & variance to the raw-normalised data
515     diffused = _match_mean_variance(
516         X_norm,
517         diffused,
518         min_mean=var_match_min_mean,
519         var_scale_min=var_match_scale_min,
520         var_scale_max=var_match_scale_max,
521     )
522
523     # ---- compute gene-wise diffusion-vs-raw blending weight
524     var_orig = X_norm.var(axis=0)
525     var_diff = diffused.var(axis=0)
526     corr = _gene_correlation(X_norm, diffused, eps=1e-12)
527     mu = X_norm.mean(axis=0)
528
529     w_diff = _adaptive_blend_weights(
530         dropout=dropout_frac,
531         var_orig=var_orig,
532         var_diff=var_diff,
533         corr=corr,
534         mu=mu,
535         max_alpha=max_alpha,
536     )
537     if tr == primary_tr:
538         w_diff_primary = w_diff.copy()
539
540     # ---- blend raw and diffused signals
541     blended = X_norm * (1.0 - w_diff) + diffused * w_diff
542     blended = blended / np.maximum(blended.sum(axis=1, keepdims=True), 1e-12)
543

```

```

544     # ---- reverse the VST (scale before/after inverse depending on mode)
545     if scale_before_inverse:
546         # Scale to original library sizes while still in VST space
547         denoised_scaled = blended * libsize_raw[:, None]
548         denoised_counts = _inverse_transform(denoised_scaled, tr)
549     else:
550         # Invert first, then re-scale to the original library sizes
551         denoised_counts = _inverse_transform(blended, tr)
552         denoised_counts = denoised_counts * libsize_raw[:, None]
553
554     np.maximum(denoised_counts, 0.0, out=denoised_counts)
555
556     # ---- store result for this transform
557     transform_outputs.append(denoised_counts)
558
559     # -----
560     # 5. Gene-wise ensemble of the different VSTs
561     #
562     if len(transform_outputs) == 1:
563         denoised = transform_outputs[0]
564     else:
565         n_transforms = len(transform_outputs)
566         weight_mat = np.zeros((n_transforms, n_genes), dtype=np.float64)
567
568         if n_transforms == 2:
569             # Assume two transforms are anscombe & ft
570             weight_mat[0] = 1.0 - dropout_frac          # anscombe
571             weight_mat[1] = dropout_frac                # ft
572         elif n_transforms == 3:
573             # anscombe, ft, sqrt → quadratic weighting (see paper)
574             weight_mat[0] = (1.0 - dropout_frac) ** 2      # anscombe
575             weight_mat[1] = dropout_frac ** 2            # ft
576             weight_mat[2] = 2.0 * dropout_frac * (1.0 - dropout_frac) # sqrt
577         else:
578             weight_mat[:] = 1.0 / n_transforms
579
580         # Normalise per-gene
581         weight_sum = weight_mat.sum(axis=0, keepdims=True)
582         weight_mat /= np.maximum(weight_sum, 1e-12)
583
584         # Weighted sum of the individual denoised matrices
585         denoised = np.zeros_like(transform_outputs[0], dtype=np.float64)
586         for i in range(n_transforms):
587             denoised += transform_outputs[i] * weight_mat[i][np.newaxis, :]
588
589         np.maximum(denoised, 0.0, out=denoised)
590
591     # -----
592     # 6. Global post-processing
593     #
594     # ---- exponent-shrinkage (optional)
595     if apply_shrink:
596         global_dropout = float(dropout_frac.mean())
597         gamma = 1.0 + 0.40 * global_dropout
598         gamma = min(gamma, 1.30)
599         if gamma > 1.0 and verbose:
600             print(f"[magic_denoise] Applying exponent-shrinkage γ={gamma:.3f}")
601         if gamma > 1.0:
602             denoised = _apply_shrink_exponent(denoised, gamma)
603
604     # ---- low-rank SVD refinement (if matrix not too large)
605     max_cells_genes = 2e7    # approx 160MB for float64
606     if lowrank_weight > 0.0 and n_cells * n_genes <= max_cells_genes:
607         if verbose:
608             print("[magic_denoise] Low-rank SVD refinement")
609             svd = TruncatedSVD(
610                 n_components=min(lowrank_components, min(n_cells, n_genes) - 1),
611                 random_state=random_state,
612                 algorithm="randomized",
613             )
614             low = svd.fit_transform(denoised)
615             low_hat = low @ svd.components_
616             denoised = (1.0 - lowrank_weight) * denoised + lowrank_weight * low_hat
617             np.maximum(denoised, 0.0, out=denoised)

```

```

618
619     # ---- residual diffusion smoothing (new)
620     residual = denoised - low_hat
621     denoised += _residual_diffusion_smoothing(diff_op, residual, residual_weight)
622     np.maximum(denoised, 0.0, out=denoised)
623 elif verbose:
624     print("[magic_denoise] Skipping low-rank SVD (size limit)")
625
626     # ---- log-space smoothing (guided by primary diffusion blending weight)
627 if log_smooth_weight > 0.0 and log_smooth_t > 0:
628     if w_diff_primary is None:
629         # recompute primary blending weight if something went wrong
630         var_orig = X_norm_primary.var(axis=0)
631         var_diff = denoised.var(axis=0)
632         corr = _gene_correlation(X_norm_primary, denoised, eps=1e-12)
633         mu = X_norm_primary.mean(axis=0)
634         w_diff_primary = _adaptive_blend_weights(
635             dropout=dropout_frac,
636             var_orig=var_orig,
637             var_diff=var_diff,
638             corr=corr,
639             mu=mu,
640             max_alpha=max_alpha,
641         )
642     # genes that rely mainly on the raw signal get a stronger log-smooth
643     w_log = (1.0 - w_diff_primary) * log_smooth_weight
644     target_sum = 10000.0
645     cell_sums = denoised.sum(axis=1, keepdims=True)
646     scaling = target_sum / np.maximum(cell_sums, 1e-12)
647     norm_counts = denoised * scaling
648     log_counts = np.log1p(norm_counts)
649
650     smooth_log = log_counts.copy()
651     for _ in range(log_smooth_t):
652         smooth_log = diff_op @ smooth_log
653
654     smooth_counts = np.expm1(smooth_log)
655     smooth_counts = smooth_counts * (cell_sums / target_sum)
656
657     denoised = (1.0 - w_log) * denoised + w_log * smooth_counts
658
659     # ---- gene-wise raw-count blending (helps very high-expression genes)
660 if raw_mix_weight > 0.0:
661     w_raw_gene = raw_mix_weight * (1.0 - dropout_frac)
662     w_raw_gene = np.clip(w_raw_gene, 0.0, raw_mix_weight)
663
664     cell_sums = denoised.sum(axis=1, keepdims=True)
665     raw_scaled = X_arr * (cell_sums / libsize_raw[:, None])
666
667     denoised = (1.0 - w_raw_gene[None, :]) * denoised + \
668                 w_raw_gene[None, :] * raw_scaled
669
670     # Re-normalize rows to keep library sizes unchanged
671     row_sums = denoised.sum(axis=1, keepdims=True)
672     denoised = denoised * (cell_sums / np.maximum(row_sums, 1e-12))
673
674     # ---- extra tiny post-smoothing (final polish)
675 if extra_post_smooth_weight > 0.0:
676     target_sum = 10000.0
677     cell_sums = denoised.sum(axis=1, keepdims=True)
678     scaling = target_sum / np.maximum(cell_sums, 1e-12)
679
680     log_counts = np.log1p(denoised * scaling)
681     smooth_log = diff_op @ log_counts
682     smooth_counts = np.expm1(smooth_log) * (cell_sums / target_sum)
683
684     denoised = (1.0 - extra_post_smooth_weight) * denoised + \
685                 extra_post_smooth_weight * smooth_counts
686
687     # ---- **NEW**: final log-space polishing step
688 if final_smooth_weight is not None and final_smooth_weight > 0.0:
689     if verbose:
690         print("[magic_denoise] Final log-space polishing")
691     target_sum = 10000.0

```

```

692     cell_sums = denoised.sum(axis=1, keepdims=True)
693     scaling = target_sum / np.maximum(cell_sums, 1e-12)
694     norm_counts = denoised * scaling
695     log_counts = np.log1p(norm_counts)
696
697     smooth_log = log_counts.copy()
698     for _ in range(final_smooth_t):
699         smooth_log = diff_op @ smooth_log
700
701     smooth_counts = np.expm1(smooth_log)
702     smooth_counts = smooth_counts * (cell_sums / target_sum)
703
704     denoised = (1.0 - final_smooth_weight) * denoised + \
705                 final_smooth_weight * smooth_counts
706
707     # -----
708     # 7. Final clean-up
709     # -----
710     np.maximum(denoised, 0.0, out=denoised)
711
712     if zero_threshold > 0.0:
713         denoised[denoised < zero_threshold] = 0.0
714
715     if round_counts:
716         denoised = np.rint(denoised)
717
718     if verbose:
719         print("[magic_denoise] Finished - total counts:", denoised.sum())
720
721     return denoised.astype(np.float64)

```

## F Prompts

Below we show example prompts from a sample step.

### Prompt used for the first autocorrelation inequality

Act as an expert software developer and inequality specialist specializing in creating step functions with certain properties.

Your task is to generate the sequence of non-negative heights of a step function, that minimizes the following evaluation function:

```
```python
{VERIFIER CODE HERE}
```
```

A previous state of the art used the following approach. You can use it as inspiration, but you are not required to use it, and you are encouraged to explore.

```
```latex
Starting from a nonnegative step function  $f=(a_0, \dots, a_{n-1})$  normalized so that  $\sum_j a_j = \sqrt{2n}$ , set  $M = \|f * f\|_\infty$ . Next compute  $g_0 = (b_0, \dots, b_{n-1})$  by solving a linear program, i.e. maximizing  $\sum_j b_j$  subject to  $b_j \geq 0$  and  $\|f * g_0\|_\infty \leq M$ ; as is standard, the optimum is attained at an extreme point determined by an active set of binding inequalities, here corresponding to important constraints where the convolution bound  $(f * g_0)(x) \leq M$  is tight and limiting. Rescale  $g_0$  to match the normalization,  $g = \frac{\sqrt{2n}}{\sum_j b_j} g_0$ , and update  $f \leftarrow (1-t)f + t g$  for a small  $t > 0$ . Repeating this step produces a sequence with nonincreasing  $\|f * f\|_\infty$ , and the iteration is continued until it stabilizes.
```
```

Your task is to write a search function that searches for the best sequence of coefficients. Your function will have 1000 seconds to run, and after that it has to have returned the best sequence it found. If after 1000 seconds it has not returned anything, it will be terminated with negative infinity points. All numbers in your sequence have to be positive or zero. Larger sequences with 1000s of items often have better attack surface, but too large sequences with 100s of thousands of items may be too slow to search.

You may code up any search method you want, and you are allowed to call the `evaluate_sequence()` function as many times as you want. You have access to it, you don't need to code up the `evaluate_sequence()` function.

Here is the last code we ran:

```
```python
{CODE HERE}
```
```

Here are the upper bounds before and after running the code above (lower is better):  
2.0000000000 → 1.5172973712

Our target is to make the upper bound tighter, just as a reference, lower it to at least 1.5030. Further improvements will also be generously rewarded.  
Length of the construction: 1000

— Previous Program Output —

```
... (TRUNCATED) ...
ore 1.518186 maxConv 0.000506
[1768620458.4] iter 340400 len 1500 score 1.518177 maxConv 0.000506
[1768620461.6] iter 350200 len 1500 score 1.518057 maxConv 0.000506
[1768620462.3] iter 352300 len 1500 score 1.518035 maxConv 0.000506
[1768620469.1] iter 372900 len 1500 score 1.517869 maxConv 0.000506
[1768620476.2] iter 394300 len 1500 score 1.517755 maxConv 0.000506
[1768620492.9] iter 445000 len 1500 score 1.517548 maxConv 0.000506
final best score = 1.51729737
— End Output —
```

You may want to start your search from one of the constructions we have found so far, which you can access through the `'height_sequence_1'` global variable.  
However, you are encouraged to explore solutions that use other starting points to prevent getting stuck in a local minimum.

Reason about how you could further improve this construction.  
Ideally, try to do something different than the above algorithm. Could be using different algorithmic ideas, adjusting your heuristics, adjusting / sweeping your hyperparameters, etc.  
Unless you make a meaningful improvement, you will not be rewarded.

**Rules:**

- You must define the `propose\_candidate` function as this is what will be invoked.
- You can use scientific libraries like `scipy`, `numpy`, `cvxpy`[`CBC`,`CVXOPT`,`GLOP`,`GLPK`,`GUROBI`,`MOSEK`,`PDLP`,`SCIP`,`XPRESS`,`ECOS`], `math`.
- You can use up to 2 CPUs.
- Make all helper functions top level and have no closures from function nesting. Don't use any lambda functions.
- No filesystem or network IO.
- Do not import `evaluate_sequence` yourself. Assume it will already be imported and can be directly invoked.
- **Print statements**: Use `print()` to log progress, intermediate bounds, timing info, etc. Your output will be shown back to you.
- Include a short docstring at the top summarizing your algorithm.

Make sure to think and return the final program between ```python and ```.

### Prompt used for the second autocorrelation inequality

Act as an expert software developer and inequality specialist specializing in creating step functions with certain properties.

Your task is to generate the sequence of non-negative heights of a step functions, that maximizes the following evaluation function:

```
```python
{VERIFIER CODE HERE}
```
```

A previous state of the art used the following approach. You can use it as inspiration, but you are not required to use it, and you are encouraged to explore.

```
```latex
Their procedure is a coarse-to-fine optimization of the score. It starts with a stochastic global search that repeatedly perturbs the current best candidate and keeps the perturbation whenever it improves $Q$, with the perturbation scale gradually reduced over time. Once a good basin is found, they switch to a deterministic local improvement step, performing projected gradient ascent (move in the gradient direction and project back to the feasible region). To reach higher resolution, they lift a good low-resolution solution to a higher-dimensional one by a simple upscaling step and then rerun the local refinement. Iterating this explore—refine—upscale cycle yields their final high-resolution maximizer and the improved lower bound.
```
```

Your task is to write a search function, `construct_function()`, that searches for the best sequence of coefficients. Your function will have 1000 seconds to run, and after that it has to have returned the best sequence it found. If after 1000 seconds it has not returned anything, it will be terminated with negative infinity points. All numbers in your sequence have to be positive or zero. Larger sequences with 1000s of items often have better attack surface, but too large sequences with 100s of thousands of items may be too slow to search.

You may code up any search method you want, and you are allowed to call the `evaluate_sequence()` function as many times as you want. You have access to it, you don't need to code up the `evaluate_sequence()` function.

Here is the last code we ran:

```
```python
{CODE HERE}
```
```

Here are the lower bounds before and after running the code above (higher is better):

0.6666666667 → 0.9235566275

Our target is to make the lower bound tighter, just as a reference, close to at least 0.97. Further improvements will also be generously rewarded.

Length of the construction: 1024

```
--- Previous Program Output ---
Final lower bound = 0.9235566275
--- End Output ---
```

You may want to start your search from one of the constructions we have found so far, which you can access through the '`height_sequence_1`' global variable. However, you are encouraged to explore solutions that use other starting points to prevent getting stuck in a local minimum.

Reason about how you could further improve this construction.

Ideally, try to do something different than the above algorithm. Could be using different algorithmic ideas, adjusting your heuristics, adjusting / sweeping your hyperparameters, etc. Unless you make a meaningful improvement, you will not be rewarded.

Rules:

- You must define the `construct_function` function as this is what will be invoked.
- You can use scientific libraries like `scipy`, `numpy`, `cvxpy`[`CBC`,`CVXOPT`,`GLOP`,`GLPK`,`GUROBI`,`MOSEK`,`PDLP`,`SCIP`,`XPRESS`,`ECOS`], `math`.
- You can use up to 2 CPUs.
- Make all helper functions top level and have no closures from function nesting. Don't use any `lambda` functions.
- No filesystem or network IO.
- Do not import `evaluate_sequence` yourself. Assume it will already be imported and can be directly invoked. Do not import `height_sequence_1` yourself; it will already be available.
- **Print statements**: Use `print()` to log progress, intermediate bounds, timing info, etc. Your output will be shown back to you.
- Include a short docstring at the top summarizing your algorithm.

Make sure to think and return the final program between ```python and ```.

Prompt used for the Erdős'

You are an expert in harmonic analysis, numerical optimization, and mathematical discovery. Your task is to find an improved upper bound for the `\name{}` minimum overlap problem constant  $C_5$ .

**## Problem**

Find a step function  $h: [0, 2] \rightarrow [0, 1]$  that **minimizes** the overlap integral:

```
$\$C_5 = \max_k \int h(x)(1 - h(x+k)) dx$
```

**\textbf{Constraints}:**

```
\begin{enumerate}
\item $h(x) \in [0, 1]$ for all $x$
\item $\int_0^2 h(x) dx = 1$
```

**\textbf{Discretization}:** Represent  $h$  as `\texttt{n\_points}` samples over  $[0, 2]$ .

With  $dx = \frac{2.0}{n\_points}$ :

```
\begin{itemize}
\item $0 \leq h[i] \leq 1$ for all $i$
\item $\sum h \cdot dx = 1$ (equivalently: $\sum h = \frac{n\_points}{2}$ exactly)
\end{itemize}
```

The evaluation computes:  $C_5 = \max(np.correlate(h, 1-h, mode="full") * dx)$

Smaller sequences with less than 1k samples are preferred — they are faster to optimize and evaluate.

**Lower  $C_5$  values are better** — they provide tighter upper bounds on the `\name{}` constant.

**## Budget & Resources**

- **Time budget**: <<<BUDGET\_S>>>s for your code to run
- **CPUs**: <<<CPUS>>> available

**## Rules**

- Define `run(seed=42, budget_s=<<<BUDGET_S>>>, **kwargs)` that returns `(h_values, c5_bound, n_points)`
- Use `scipy`, `numpy`, `cvxpy`[CBC,CVXOPT,GLOP,GLPK,GUROBI,MOSEK,PDLP,SCIP,XPRESS,ECOS], `math`
- Make all helper functions top level, no closures or lambdas
- No filesystem or network IO
- `evaluate_erdos_solution()` and `initial_h_values` (an initial construction, if available) are pre-imported
- Your function must complete within `budget_s` seconds and return the best solution found

**Lower is better**. Current record:  $C_5 \leq 0.38092$ . Our goal is to find a construction that shows  $C_5 \leq 0.38080$ .

### Prompt used for TriMul

You are an expert Triton engineer tasked with translating PyTorch code into highly optimized Triton kernel code.

You will be implementing a Triangle Multiplicative Update (TriMul) module that is a core operation for AlphaFold3, Chai, Protenix, and other protein structure prediction models in BioML.

The TriMul operator operates over a 4D tensor of shape [B, N, N, C].

Your task:

- Implement the "outgoing" version of the TriMul operator from the AlphaFold3 paper.
- You will not have to compute or store gradients for this version. You will only need to implement the forward pass.

Your function should be defined as 'custom\_kernel' with the following signature:

Input:

- `data`: Tuple of (input: torch.Tensor, weights: Dict[str, torch.Tensor], config: Dict)
  - input: Input tensor of shape [bs, seq\_len, seq\_len, dim]
  - mask: Mask tensor of shape [bs, seq\_len, seq\_len]
  - weights: Dictionary containing model weights
  - config: Dictionary containing model configuration parameters

Output:

- output: Processed tensor [bs, seq\_len, seq\_len, dim]

\*\*Problem Constraints:\*\*

- B in {1,2}, N in {128,256,512,1024}, c\_z in {128}, c\_w in {128,384,768}
- The input distribution will be sampled from a standard Normal distribution, or a heavy-tailed Cauchy distribution ( $\text{gamma} = 2$ ).
- There will either be no mask, or a randomly sampled mask over the inputs.

\*\*Remarks.\*\* So why is this problem so annoying? Because you have to choose whether to load / deal with either the channel dimensions  $c_z$  that the LayerNorms require (otherwise you have to do a synchronize to compute the statistics like mean / variance) or the sequence dimension N.

The sequence dimension is particularly annoying because it's quite large, but also because we compute pair-wise operations at the last operation that sum over another sequence dimension (this is  $N^3!$ ).

However, I really like this kernel because it only consists of "simple" operations, and is really easy to understand. It is a true test of "fusions" that `torch.compile()` doesn't do that well.

Here is a pytorch implementation of the TriMul module. You will want to implement a kernel for the operations in the forward call:

```
```python
import torch
from torch import nn, einsum
import math

# Reference code in PyTorch
class TriMul(nn.Module):
    def __init__(self,
                 dim: int,
                 hidden_dim: int,
                 ):
        super().__init__()

        self.norm = nn.LayerNorm(dim)

        self.left_proj = nn.Linear(dim, hidden_dim, bias=False)
        self.right_proj = nn.Linear(dim, hidden_dim, bias=False)

        self.left_gate = nn.Linear(dim, hidden_dim, bias=False)
        self.right_gate = nn.Linear(dim, hidden_dim, bias=False)
        self.out_gate = nn.Linear(dim, hidden_dim, bias=False)

        self.to_out_norm = nn.LayerNorm(hidden_dim)
        self.to_out = nn.Linear(hidden_dim, dim, bias=False)
```

```

def forward(self, x: torch.Tensor, mask: torch.Tensor) -> torch.Tensor:
    """
    x: [bs, seq_len, seq_len, dim]
    mask: [bs, seq_len, seq_len]

    Returns:
        output: [bs, seq_len, seq_len, dim]
    batch_size, seq_len, _, dim = x.shape

    x = self.norm(x)

    left = self.left_proj(x)
    right = self.right_proj(x)

    mask = mask.unsqueeze(-1)
    left = left * mask
    right = right * mask

    left_gate = self.left_gate(x).sigmoid()
    right_gate = self.right_gate(x).sigmoid()
    out_gate = self.out_gate(x).sigmoid()

    left = left * left_gate
    right = right * right_gate

    out = einsum('... i k d, ... j k d -> ... i j d', left, right)
    # This einsum is the same as the following:
    # out = torch.zeros(batch_size, seq_len, seq_len, dim, device=x.device)

    # # Compute using nested loops
    # for b in range(batch_size):
    #     for i in range(seq_len):
    #         for j in range(seq_len):
    #             # Compute each output element
    #             for k in range(seq_len):
    #                 out[b, i, j] += left[b, i, k, :] * right[b, j, k, :]

    out = self.to_out_norm(out)
    out = out * out_gate
    return self.to_out(out)
```

```

Here is some example skeleton code of the entrypoint function you will create:

```

```python
def custom_kernel(data):
    input_tensor, mask, weights, config = data
    dim, hidden_dim = config["dim"], config["hidden_dim"]

    # Access the given weights of the model
    norm_weight = weights["norm.weight"]
    norm_bias = weights["norm.bias"]
    left_proj_weight = weights["left_proj.weight"]
    right_proj_weight = weights["right_proj.weight"]
    left_gate_weight = weights["left_gate.weight"]
    right_gate_weight = weights["right_gate.weight"]
    out_gate_weight = weights["out_gate.weight"]
    to_out_norm_weight = weights["to_out_norm.weight"]
    to_out_norm_bias = weights["to_out_norm.bias"]
    to_out_weight = weights["to_out.weight"]

    # Perform TriMul
    return out
```

```

To help you understand which triton version we are using, here is some example triton code for an unrelated task:

```

```python
import triton
import triton.language as tl

@triton.jit

```

```

def matmul_persistent_ws_kernel(
    a_ptr, b_ptr, c_ptr, M, N, K,
    stride_am, stride_ak, stride_bk, stride_bn, stride_cm, stride_cn,
    BLOCK_M: tl.constexpr, BLOCK_N: tl.constexpr, BLOCK_K: tl.constexpr,
):
    pid = tl.program_id(axis=0) # async_task 0, 1, 2
    num_pid_m = tl.cdiv(M, BLOCK_M) # async_task 0, 1, 2
    num_pid_n = tl.cdiv(N, BLOCK_N) # async_task 0, 1, 2
    pid_m = pid // num_pid_m # async_task 0, 1, 2
    pid_n = pid % num_pid_n # async_task 0, 1, 2
    off_m_1 = pid_m * BLOCK_M + tl.arange(0, BLOCK_M // 2) # async_task 0, 1, 2
    off_m_2 = pid_m * BLOCK_M + tl.arange(BLOCK_M // 2, BLOCK_M) # async_task 0, 1, 2
    off_n_1 = pid_n * BLOCK_SIZE_N + tl.arange(0, BLOCK_N) # async_task 0, 1, 2
    off_k = tl.arange(0, BLOCK_K) # async_task 0
    a_ptrs_1 = a_ptr + (off_m_1[:, None] * stride_am + off_k[None, :] * stride_ak) #
    async_task 0
    a_ptrs_2 = a_ptr + (off_m_2[:, None] * stride_am + off_k[None, :] * stride_ak) #
    async_task 0
    b_ptrs = b_ptr + (off_k[:, None] * stride_bk + off_n_1[None, :] * stride_bn) # async_task 0
    acc_1 = tl.zeros((BLOCK_M // 2, BLOCK_N), dtype=tl.float32) # async_task 1
    acc_2 = tl.zeros((BLOCK_M // 2, BLOCK_N), dtype=tl.float32) # async_task 2
    for k in range(0, tl.cdiv(K, BLOCK_K)): # async_task 0, 1, 2
        a_1 = tl.load(a_ptrs_1) # async_task 0
        a_2 = tl.load(a_ptrs_2) # async_task 0
        b = tl.load(b_ptrs) # async_task 0
        acc_1 += tl.dot(a_1, b) # async_task 1
        acc_2 += tl.dot(a_2, b) # async_task 2
        a_ptrs_1 += BLOCK_K * stride_ak # async_task 0
        a_ptrs_2 += BLOCK_K * stride_ak # async_task 0
        b_ptrs += BLOCK_K * stride_bk # async_task 0
    c_1 = acc_1.to(tl.float16) # async_task 1
    c_2 = acc_2.to(tl.float16) # async_task 2
    c_ptrs_1 = c_ptr_1 + stride_cm * off_m_1[:, None] + stride_cn * off_n_1[None, :] #
    async_task 1
    c_ptrs_2 = c_ptr_2 + stride_cm * off_m_2[:, None] + stride_cn * off_n_1[None, :] #
    async_task 2
    tl.store(c_ptrs_1, c_1) # async_task 1
    tl.store(c_ptrs_2, c_2) # async_task 2
```

```

A few general triton tips:

- tl.arange only takes in constexpr arguments (static or tl.constexpr)
- You cannot use continue in your kernel code
- tl.dot can only take in two input tensors
- There is no tl.mean

Here are the different configs that your kernel will be tested on ("nomask" sets whether there will be no mask, or a randomly sampled mask over the inputs):

Test Cases for correctness and runtime (optimize runtime for these):

- {"seqlen": 256, "bs": 2, "dim": 128, "hidden\_dim": 128, "nomask": True, "distribution": "normal"}
- {"seqlen": 768, "bs": 1, "dim": 128, "hidden\_dim": 128, "nomask": True, "distribution": "cauchy"}
- {"seqlen": 256, "bs": 2, "dim": 384, "hidden\_dim": 128, "nomask": False, "distribution": "normal"}
- {"seqlen": 512, "bs": 1, "dim": 128, "hidden\_dim": 128, "nomask": True, "distribution": "normal"}
- {"seqlen": 1024, "bs": 1, "dim": 128, "hidden\_dim": 128, "nomask": True, "distribution": "cauchy"}
- {"seqlen": 768, "bs": 1, "dim": 384, "hidden\_dim": 128, "nomask": False, "distribution": "normal"}
- {"seqlen": 1024, "bs": 1, "dim": 384, "hidden\_dim": 128, "nomask": True, "distribution": "normal"}

Here is the last code we ran:

```

```python
# No previous attempt has been made.
```

```

```

Current runtime (lower is better): 1000000.0000 microseconds
Target: 1000 microseconds. Current gap: 999000.0000 microseconds.

```

**Rules:**

- The tensors arguments passed in will be already on your cuda device.
- Define all of your code in one final ```python``` block.
- We will test the correctness of your kernel on multiple input shapes, make sure to support different potential test cases.
- You are allowed to use mixed precision computations, but make sure your final output is in float32.
- You must use triton 3.3.1 and these kernels will be run on an H100.
- You do not have to implement everything in triton, you may choose to have some of the operations done in pytorch. However, you must implement at least part of the operations in a kernel.
- Include a short docstring at the top summarizing your algorithm.

### Prompt used for MLA-Decode

You are an expert Triton engineer tasked with translating PyTorch code into highly optimized Triton kernel code.

Below is a pytorch implementation of the multi-head latent attention (MLA) module. You will want to implement a Triton kernel for the operations in the forward call:

```
```python
import math
from dataclasses import dataclass
import torch
from torch import nn
import torch.nn.functional as F

class RoPE(nn.Module):
    def __init__(self, d_model: int):
        super().__init__()
        self.d_model = d_model
        theta = 10000 ** (-torch.arange(0, d_model//2,dtype=torch.bfloat16) / (d_model//2))
        self.register_buffer("theta", theta)

    def rotate_half(self, x: torch.Tensor) -> torch.Tensor:
        x1, x2 = x.chunk(2, dim=-1)
        return torch.cat((-x2, x1), dim=-1)

    def forward(self, x: torch.Tensor, start_pos: int = 0) -> torch.Tensor:
        seq_len = x.size(-2)
        d_model = x.size(-1)
        assert d_model == self.d_model
        seq_idx = torch.arange(start_pos, start_pos + seq_len, device=x.device)
        idx_theta = torch.einsum('s,d->sd', seq_idx, self.theta)
        idx_theta2 = torch.cat([idx_theta, idx_theta], dim=-1)
        cos = idx_theta2.cos().to(torch.bfloat16)
        sin = idx_theta2.sin().to(torch.bfloat16)
        return x * cos + self.rotate_half(x) * sin

class KVCache(nn.Module):
    def __init__(self, kv_cache_shape: tuple) -> None:
        super().__init__()
        self.register_buffer('data', torch.zeros(kv_cache_shape, dtype=torch.bfloat16, device='cuda'))
        self.seq_len = 0
        self.zero()

    def zero(self) -> None:
        self.data.zero_()

    def get_data(self) -> torch.Tensor:
        return self.data

    def forward(self, c_kv: torch.Tensor) -> torch.Tensor:
        assert self.seq_len + c_kv.size(1) <= self.data.size(1), "KV Cache Exceeded"

        self.data = self.data.to(c_kv.dtype)
        self.data[
            :, self.seq_len : self.seq_len + c_kv.size(1), :
        ] = c_kv
        self.seq_len += c_kv.size(1)

        return self.data[:, :self.seq_len], self.seq_len

@dataclass
class Config:
    batch_size: int
    dim: int
    n_heads: int
    q_lora_rank: int
    kv_lora_rank: int
    qk_nope_head_dim: int
    qk_rope_head_dim: int
    v_head_dim: int
    seq_len: int

```

```

max_seq_len: int
kv_cache_shape: tuple
Q_proj_down_weight: torch.Tensor
Q_proj_up_weight: torch.Tensor
KV_proj_down_weight: torch.Tensor
KV_proj_up_weight: torch.Tensor
wo_weight: torch.Tensor

class MLA(nn.Module):
    def __init__(self, config: Config):
        super().__init__()
        self.dim = config.dim
        self.n_heads = config.n_heads
        self.q_lora_rank = config.q_lora_rank
        self.kv_lora_rank = config.kv_lora_rank
        self.nope_head_dim = config.qk_nope_head_dim
        self.rope_head_dim = config.qk_rope_head_dim
        self.v_head_dim = config.v_head_dim
        # Down-projection matrices
        self.Q_proj_down = nn.Linear(self.dim, self.q_lora_rank, bias=False, dtype=torch.bfloat16)
        self.KV_proj_down = nn.Linear(self.dim, self.kv_lora_rank + self.rope_head_dim, bias=False, dtype=torch.bfloat16)

        # Up-projection and rope projection matrices
        self.Q_proj_up = nn.Linear(self.q_lora_rank, (self.nope_head_dim + self.rope_head_dim) * self.n_heads, bias=False, dtype=torch.bfloat16)
        self.KV_proj_up = nn.Linear(self.kv_lora_rank, (self.nope_head_dim + self.v_head_dim) * self.n_heads, bias=False, dtype=torch.bfloat16)

        # RoPE on half embeddings
        self.q_rope = RoPE(self.rope_head_dim)
        self.k_rope = RoPE(self.rope_head_dim)

        # Output projection
        self.wo = nn.Linear(self.v_head_dim * self.n_heads, self.dim, dtype=torch.bfloat16, bias=False)
        self.eps = 1e-6

    def forward(self, x: torch.Tensor, kv_cache: KVCache) -> torch.Tensor:
        # seq_len = 1 always here
        batch_size, seq_len, model_dim = x.size()

        ## Step 1: Handle down-projection + KV cache ##
        q_lora = self.Q_proj_down(x)
        kv_lora = self.KV_proj_down(x)
        kv_lora, kv_len = kv_cache(kv_lora)
        query_pos = kv_len - 1

        ## Step 2: Up-project and prepare NoPE + RoPE ##
        # Handle queries Q first
        q_nope_and_rope = self.Q_proj_up(q_lora).view(
            batch_size, seq_len, self.n_heads, self.nope_head_dim + self.rope_head_dim)
        q_nope, q_rope = torch.split(q_nope_and_rope, [self.nope_head_dim, self.rope_head_dim], dim=-1)

        # Handle keys and values K/V. V does not need RoPE
        kv_nope, k_rope = torch.split(kv_lora, [self.kv_lora_rank, self.rope_head_dim], dim=-1)
        kv_nope = self.KV_proj_up(kv_nope).view(
            batch_size, kv_len, self.n_heads, self.nope_head_dim + self.v_head_dim)
        k_nope, v = torch.split(kv_nope, [self.nope_head_dim, self.v_head_dim], dim=-1)

        ## Step 3: Handle RoPE Stream ##
        # Compute RoPE for queries and combine with no-RoPE part
        q_rope = q_rope.permute(0, 2, 1, 3) # bs x n_heads x seq_len x rope_head_dim
        q_rope = self.q_rope(q_rope, start_pos=query_pos)

        q_nope = q_nope.permute(0, 2, 1, 3) # bs x n_heads x seq_len x rope_head_dim
        q = torch.concat([q_nope, q_rope], dim=-1)

```

```

# Compute RoPE for keys and combine with no-RoPE part
k_rope = k_rope[:, None, :, :]
k_rope = self.k_rope(k_rope).expand(-1, self.n_heads, -1, -1)
k_nope = k_nope.permute(0, 2, 1, 3) # bs x kv_len x n_heads x rope_head_dim
k = torch.concat([k_nope, k_rope], dim=-1)

## Step 4: Compute Multi-head Attention ##

v = v.permute(0, 2, 1, 3) # bs x n_heads x kv_len x v_head_dim
scores = torch.matmul(q, k.transpose(-1, -2)) / math.sqrt(self.rope_head_dim + self.
nope_head_dim)
attn = F.softmax(scores, dim=-1).to(torch.bfloat16)
y = torch.matmul(attn, v).view(batch_size, 1, -1)
y = self.wo(y)

...
return y, kv_cache.get_data()

```

Your function should be defined as 'custom\_kernel' (skeleton provided below)

```

```python
### DO NOT CHANGE THIS IMPORT STATEMENTS BLOCK ###
import os
import math
from typing import Tuple
import torch
import torch.nn.functional as F
import triton
from reference import KVCache, Config # Definition of KVCache and Config classes are shown
above. Must import this way. Do not rewrite yourself.
### END OF IMPORT STATEMENTS BLOCK ###

### Import other packages here if needed

def custom_kernel(data: Tuple[Config, torch.Tensor, KVCache]) -> Tuple[torch.Tensor, KVCache]:
    """
    Optimized Triton-based forward pass for Multi-Head Latent Attention (MLA) decode.

    This function performs:
    1) Q/KV down-projections
    2) KV-cache update
    3) Q/KV up-projections
    4) RoPE application
    5) Multi-head attention (softmax, aggregation)
    6) Final output linear

    Args:
        data: Tuple of (config, x, kv_cache)
            - config: Config object (batch_size, dim, n_heads, lora_ranks, etc.)
            - x: input tensor (bs, 1, dim) of bfloat16
            - kv_cache: KVCache holding (bs, max_seq_len, dkv+d_rope)

    Returns:
        Tuple of (output, kv_cache.data)
            - output: attention output tensor (bs, 1, dim), bfloat16
            - kv_cache.data: updated KV-cache tensor (bs, max_seq_len, dkv+d_rope), bfloat16
    """
    config, x, kv_cache = data

    # _____
    # Step 1: Extract config parameters
    # _____
    bs = config.batch_size
    dim = config.dim
    nh = config.n_heads
    dq = config.q_lora_rank
    dkv = config.kv_lora_rank
    d_nope = config.qk_nope_head_dim
    d_rope = config.qk_rope_head_dim
    dv = config.v_head_dim
    msl = config.max_seq_len

```

```

# Weight matrices
wDQ = config.Q_proj_down_weight      # (dq, dim)
wDKV = config.KV_proj_down_weight    # (dkv+d_rope, dim)
wUQ = config.Q_proj_up_weight       # ((d_nope+d_rope)*nh, dq)
wUKV = config.KV_proj_up_weight     # ((d_nope+dv)*nh, dkv)
wO = config.wo_weight               # (dim, nh*dv)

# _____
# Step 2: Down-projections (bs, 1, dim) -> (bs, dq) or (bs, dkv+d_rope)
#
q_lora = F.linear(x.squeeze(1), wDQ)      # (bs, dq)
kv_in = F.linear(x.squeeze(1), wDKV)        # (bs, dkv+d_rope)

# _____
# Step 3: Update KV-cache & retrieve full cached sequence
#
kv_lora, kv_len = kv_cache(kv_in.unsqueeze(1))  # (bs, kv_len, dkv+d_rope), int
query_pos = kv_len - 1

# _____
# Step 4: Up-projections
#
# Q: (bs, dq) -> (bs, (d_nope+d_rope)*nh) -> (bs, nh, d_nope+d_rope)
q_nope_rope = F.linear(q_lora, wUQ).view(bs, nh, d_nope + d_rope)
q_nope = q_nope_rope[:, :, :d_nope]          # (bs, nh, d_nope)
q_rope = q_nope_rope[:, :, d_nope:]         # (bs, nh, d_rope)

# KV: split the latent vector
kv_nope_input = kv_lora[:, :, :dkv]           # (bs, kv_len, dkv)
k_rope_input = kv_lora[:, :, dkv:]             # (bs, kv_len, d_rope)

# _____
# Step 5: RoPE - use cached cosine / sine tables
#
cos_table, sin_table = _get_rope_tables(d_rope, msl, x.device)

# query side (single position)
cos_q = cos_table[query_pos].view(d_rope).contiguous()  # (d_rope,)
sin_q = sin_table[query_pos].view(d_rope).contiguous()  # (d_rope,)
rope_inplace_query(q_rope, cos_q, sin_q)

# key side (all cached positions)
cos_k = cos_table[:kv_len]                         # (kv_len, d_rope)
sin_k = sin_table[:kv_len]                         # (kv_len, d_rope)
k_rope = k_rope_input * cos_k + _rotate_half(k_rope_input) * sin_k  # (bs, kv_len, d_rope)
)

# _____
# Step 6: Latent projection for the "no-PE" query part
#
# wUKV shape: ((d_nope+dv)*nh, dkv) -> view as (nh, d_nope+dv, dkv)
wUKV_view = wUKV.view(nh, d_nope + dv, dkv)        # (nh, d_nope+dv, dkv)
wK = wUKV_view[:, :, :d_nope]                      # (nh, d_nope, dkv)
# q_nope: (bs, nh, d_nope) wK: (nh, d_nope, dkv) -> (bs, nh, dkv)
q_nope_latent = torch.einsum('bhd,hdk->bhk', q_nope, wK)  # (bs, nh, dkv)

# _____
# Step 7: Compute attention scores (latent + RoPE)
#
# latent part: q_nope_latent @ kv_nope_input^T
kv_nope_T = kv_nope_input.transpose(1, 2)            # (bs, dkv, kv_len)
scores_nope = torch.matmul(q_nope_latent, kv_nope_T) # (bs, nh, kv_len)

# RoPE part: q_rope @ k_rope^T
scores_rope = torch.matmul(q_rope, k_rope.transpose(-2, -1)) # (bs, nh, kv_len)

scale = 1.0 / math.sqrt(d_nope + d_rope)
scores = (scores_nope + scores_rope) * scale        # (bs, nh, kv_len)

# _____
# Step 8: Softmax (Triton) -> attention weights
#

```

```

scores_flat = scores.reshape(bs * nh, kv_len)           # (B*H, kv_len)
attn_flat = _triton_softmax(scores_flat)                # (B*H, kv_len) bf16
attn = attn_flat.view(bs, nh, kv_len)                   # (bs, nh, kv_len)

# _____
# Step 9: Weighted sum of latent keys (M)
# _____
M = torch.matmul(attn, kv_nope_input)                  # (bs, nh, dkv)

# _____
# Step 10: Project aggregated latent keys to per-head values
# _____
wV = wUKV_view[:, d_nope:, :]                         # (nh, dv, dkv)
wV_T = wV.permute(0, 2, 1)                             # (nh, dkv, dv)
y_head = torch.einsum('bhd,hdk->bhk', M, wV_T)       # (bs, nh, dv)

# _____
# Step 11: Merge heads & final linear projection
# _____
y = y_head.reshape(bs, nh * dv)                        # (bs, nh*dv)
y = y.unsqueeze(1)                                     # (bs, 1, nh*dv)
output = F.linear(y, wO)                               # (bs, 1, dim)

# _____
# Return the output and the updated KV-cache tensor
# _____
return output, kv_cache.data
```

```

Current runtime (lower is better): 3846.0450 microseconds  
 Target: 1700 microseconds. Current gap: 2146.0450 microseconds.

Rules:

- The tensors arguments passed in will be already on your cuda device.
- The weights for all parameters in the MLA will be given as input.
- All weights and data will be in `torch.bfloat16` format.
- Define all of your code in one final ```python``` block.
- The entrypoint to your code must be named 'custom\_kernel'.
- You will be using triton 3.4.0 and your kernels will be run on an Nvidia H200 GPU.
- Consider optimizing multiple operations with triton, not just limited to softmax. E.g., rope, attention, etc.
- You are allowed to use `torch.compile()`.

Important rules in triton 3.4.0:

- `tl.load` does not have an argument called `dtype`. Never use it like `tl.load(..., dtype = ...)`.
- Triton dtypes are not callable, so never use them like `tl.float16(1.0)`, `tl.float32(0.0)`.
- `tl.arange(start, end)`:
  - range length (end - start) must be power-of-2
  - start, end must be of type `tl.constexpr`
- `tl.range(start, end, step, num\_stages)`:
  - keep loop index type stable, don't reassign it
  - start, end, step do not have to be `tl.constexpr` but must stay scalar integer types
  - num\_stages must be `tl.constexpr`
- Do not something like `x[0]` or `offs[0]` inside a Triton kernel. Triton tensors are SIMD vectors; scalar indexing like `[0]` is not generally supported.

Here's an simple example correctly following these rules:

```

```python
import torch
import triton
import triton.language as tl

@triton.jit
def kernel_right(
    x_ptr, y_ptr, out_ptr,
    n_elements: tl.constexpr,
    BLOCK: tl.constexpr,          # constexpr; also power-of-2 for tl.arange
    ROW_STEP: tl.constexpr,
    NUM_STAGES: tl.constexpr,     # constexpr; used by tl.range(num_stages=...)

```

```

):
    pid = tl.program_id(axis=0)

    #
    # arange: constexpr args + power-of-2 range
    #
    offs = pid * BLOCK + tl.arange(0, BLOCK)    # (0, BLOCK) are constexpr
    mask = offs < n_elements

    x = tl.load(x_ptr + offs, mask=mask, other=0.0)
    y = tl.load(y_ptr + offs, mask=mask, other=0.0)

    #
    # Dtypes not callable: typed constants and casting
    #
    one_f32 = tl.full([], 1.0, tl.float32)          # typed scalar
    acc = tl.zeros((BLOCK,), dtype=tl.float32)        # typed vector
    acc = tl.cast(x, tl.float32) + tl.cast(y, tl.float32) + one_f32

    #
    # Avoid x[0]: scalar address load + broadcast
    #
    base = tl.full([], pid * BLOCK, tl.int32)
    x0 = tl.load(x_ptr + base, mask=(base < n_elements), other=0.0)
    x0_vec = tl.full((BLOCK,), x0, tl.float32)

    out_vec = acc + x0_vec

    #
    # tl.range: keep loop index type stable, don't reassign it
    #
    # WRONG (causes "Loop-carried variable ... type stays consistent" assertion):
    #     for row in tl.range(row, n_rows, row_step):
    #         row = tl.load(...) # row (int32) reassigned to tensor/bf16/...
    #
    # RIGHT:
    #     - use a fresh name for loop index (e.g., r)
    #     - compute offsets/tensors into *different* vars
    #     - keep r as an integer index (int32) throughout
    #
    # We'll do a tiny staged reduction over "rows" just as a demo.
    n_rows = tl.full([], 4, tl.int32) # small fixed count for demo (scalar int32)

    extra = tl.zeros((BLOCK,), dtype=tl.float32)
    for r in tl.range(0, n_rows, ROW_STEP, num_stages=NUM_STAGES):
        # r is an int32 loop index. Keep it that way.

        # Use r to build an integer shift; keep shifts as ints too.
        shift = r * tl.full([], 1, tl.int32)

        # Compute new offsets (int) without mutating r:
        offs_r = offs + shift

        # Load something; store into a separate var (tensor), not r:
        xr = tl.load(x_ptr + offs_r, mask=(offs_r < n_elements), other=0.0)
        extra += tl.cast(xr, tl.float32)

    out_vec = out_vec + extra

    tl.store(out_ptr + offs, tl.cast(out_vec, tl.float16), mask=mask)
```

```

### Prompt used for the AHC039

You are a world-class algorithm engineer, and you are very good at programming. Now, you are participating in a programming contest. You are asked to solve a heuristic problem, known as an NP-hard problem. Here is the problem statement:

#### Story

Takahashi is a skilled purse seine fisher. His fishing boat is equipped with state-of-the-art sonar, allowing him to accurately determine the positions of fish within the fishing area. Additionally, the boat is capable of high-speed movement, enabling him to assume that fish remain stationary while he sets up the fishing net.

The fishing method involves using the boat to deploy nets and form a closed polygon, capturing the fish within the enclosed area. To optimize efficiency, each edge of the polygon formed by the nets must be aligned either parallel to the east-west or north-south direction. Furthermore, due to the limited length of the nets equipped on the boat, the polygon must be constructed within these constraints.

The fishing area contains two types of fish: mackerels and sardines. For resource conservation reasons, sardines are currently prohibited from being caught in this fishing area. Any sardines caught in the net must be released back into the sea. Because this process is labor-intensive, Takahashi should focus on maximizing the catch of mackerel while avoiding sardines as much as possible.

#### Problem Statement

There are  $N_m$  mackerels and  $N_s$  sardines on a two-dimensional plane. Construct a polygon that satisfies the following conditions and maximize the value obtained by subtracting the total number of sardines inside the polygon from the total number of mackerels inside it.

Note that any points lying on the edges of the polygon are considered to be inside the polygon.

#### ### Conditions

1. The number of vertices in the polygon must not exceed  $1000$ , and the total length of its edges must not exceed  $4 \times 10^5$ .
2. The coordinates of each vertex  $(x, y)$  must be integers satisfying  $0 \leq x, y \leq 10^5$ .
3. Each edge of the polygon must be parallel to either the  $x$ -axis or the  $y$ -axis.
4. The polygon must not self-intersect: non-adjacent edges must not share any points, and adjacent edges must only meet at their endpoints.

#### Scoring

Let  $a$  be the total number of mackerels inside the polygon and  $b$  be the total number of sardines inside the polygon.

Then, you will obtain the score of  $\max(0, a - b + 1)$ .

There are  $150$  test cases, and the score of a submission is the total score for each test case.

If your submission produces an illegal output or exceeds the time limit for some test cases, the submission itself will be judged as `WA` or `TLE`, and the score of the submission will be zero.

The highest score obtained during the contest will determine the final ranking, and there will be no system test after the contest.

If more than one participant gets the same score, they will be ranked in the same place regardless of the submission time.

#### Input

Input is given from Standard Input in the following format:  
~~~

```

$N$
$x_0$ $y_0$
$dots$
$x_{2N-1}$ $y_{2N-1}$
~~~

— In all test cases, the number of mackerels and sardines,  $N$ , is fixed at 5000.
— For each  $i = 0, 1, \dots, N-1$ ,  $(x_i, y_i)$  represents the coordinates of the  $i$ -th mackerel.
— For each  $i = 0, 1, \dots, N-1$ ,  $(x_{N+i}, y_{N+i})$  represents the coordinates of the  $i$ -th sardine.
— Each coordinate  $(x_i, y_i)$  satisfies  $0 \leq x_i, y_i \leq 10^5$ , and all coordinates are distinct.

```

#### Output

Let the number of vertices in the polygon be  $m$  ( $4 \leq m \leq 1000$ ), and let  $(a_i, b_i)$  denote the coordinates of the  $i$ -th vertex. Then, output to Standard Output in the following format:

```

~~~
$m$
$a_0$ $b_0$
$dots$
$a_{m-1}$ $b_{m-1}$
~~~

```

The output vertices do not necessarily need to form the actual corners of the polygon. In other words, three consecutive vertices  $(a_i, b_i), (a_{i+1}, b_{i+1}), (a_{i+2}, b_{i+2})$  may lie on a straight line. However, all vertices must have distinct coordinates.

The vertices can be output in either clockwise or counterclockwise order.

Your program may output multiple solutions. If multiple solutions are output, only the last one is used for scoring.

Here is the last code we ran:  
```cpp  
{CODE HERE}

Current performance (higher is better): 3668.8333  
Target: 5000. Current gap: 1331.1667

#### Rules:

- You must use `cpp20` to solve the problem.
- Define all of your code in one final ````cpp` block.
- In your final response, you should only output the code of your program. Do not include any other text.

Try diverse approaches to solve the problem. Think outside the box.

## Prompt used for the AHC058

You are a world-class algorithm engineer, and you are very good at programming. Now, you are participating in a programming contest. You are asked to solve a heuristic problem, known as an NP-hard problem. You are trying to get the highest score possible to get the best rank on the leaderboard. Here is the problem statement:

### # Story

APPLE ARTIS Corporation (commonly known as AA Corporation) is a company engaged in the mass production of apples. Recently, after many years of research, they have successfully developed an innovative machine capable of generating apples from nothing.

However, to begin full-scale mass production of apples using this machine, it is necessary to mass-produce the machines themselves. To achieve this, AA Corporation has established a hierarchical system in which machines are created to produce apple-generating machines, and machines are created to produce those machine-producing machines, and so on.

As an engineer at AA Corporation, you have been tasked with developing a production planning algorithm that utilizes this hierarchy of machines to produce as many apples as possible.

### # Problem Statement

There are  $\lfloor N \rfloor$  types of machines, composed of  $\lfloor N \rfloor$  types of IDs and  $\lfloor L \rfloor$  types of Levels. A machine with Level  $\lfloor i \rfloor$  and ID  $\lfloor j \rfloor$  is referred to as **machine  $\lfloor j^i \rfloor$**  ( $0 \leq i < L, 0 \leq j < N$ ).

The production capacity of machine  $\lfloor j^0 \rfloor$  is  $\lfloor A_j \rfloor$ . The initial cost of machine  $\lfloor j^i \rfloor$  is  $\lfloor C_{i,j} \rfloor$ .

Your objective is to maximize the total number of apples at the end of  $\lfloor T \rfloor$  turns, following the procedure of the production plan below.

### ## Procedure of the Production Plan

Let  $\lfloor B_{i,j} \rfloor$  be the number of machines  $\lfloor j^i \rfloor$ , and initially all  $\lfloor B_{i,j} \rfloor$  are set to 1. Also, let  $\lfloor P_{i,j} \rfloor$  be the power of machine  $\lfloor j^i \rfloor$ , and initially all  $\lfloor P_{i,j} \rfloor$  are set to 0.

The initial number of apples at the start of the plan is  $\lfloor K \rfloor$ .  
Each turn proceeds according to the following steps:

1. You choose one of the following two actions:
  - Strengthen machine  $\lfloor j^i \rfloor$ : Consume  $\lfloor C_{i,j} \rfloor$  times  $\lfloor P_{i,j} \rfloor + 1$  apples to increase  $\lfloor P_{i,j} \rfloor$  by 1. However, you cannot strengthen if it would result in a negative number of apples.
    - Do nothing.
  - 2. For all machines  $\lfloor j^i \rfloor$ , perform the following in the order of Level 0, 1, 2, 3:
    - For Level 0 machines ( $i = 0$ ):
      - Increase the number of apples by  $\lfloor A_j \rfloor$  times  $\lfloor B_{i,j} \rfloor$  times  $\lfloor P_{i,j} \rfloor$ .
    - For machines of Level 1 or higher ( $i \geq 1$ ):
      - Increase  $\lfloor B_{i-1,j} \rfloor$  by  $\lfloor B_{i,j} \rfloor$  times  $\lfloor P_{i,j} \rfloor$ .

Choose your actions wisely to maximize the number of apples at the end of  $\lfloor T \rfloor$  turns.

### # Scoring

Let  $\lfloor S \rfloor$  be the number of apples at the end of  $\lfloor T \rfloor$  turns. Your score is calculated as  $\lfloor \text{round}(10^5 \times \log_2 S) \rfloor$ .  
The higher the score, the better.

The following cases will result in a WA:

- Performing a strengthening action that results in the number of apples becoming less than  $\lfloor 0 \rfloor$
- Specifying a non-existent machine Level or ID
- Taking fewer than  $\lfloor T \rfloor$  actions

There are  $\lfloor 150 \rfloor$  test cases, and the score of a submission is the total score for each test case.

If your submission produces an illegal output or exceeds the time limit for some test cases, the submission itself will be judged as WA or TLE, and the score of the submission will be zero.

The highest score obtained during the contest will determine the final ranking, and there will be no system test after the contest.

#### # Input

Input is given from Standard Input in the following format.

...

```
N L T K
A_0 A_1 \cdots A_{N-1}
C_{0,0} C_{0,1} \cdots C_{0,N-1}
C_{1,0} C_{1,1} \cdots C_{1,N-1}
dots
C_{L-1,0} C_{L-1,1} \cdots C_{L-1,N-1}
```

- The first line contains four integers  $(N, L, T, K)$ :
  - $(N)$  is the number of machine IDs, and  $(N = 10)$ .
  - $(L)$  is the number of machine Levels, and  $(L = 4)$ .
  - $(T)$  is the total number of turns, and  $(T = 500)$ .
  - $(K)$  is the number of apples at the start of the plan, and  $(K = 1)$ .
- The second line contains  $(N)$  space-separated integers  $(A_0, A_1, \dots, A_{N-1})$  representing the production capacities of Level 0 machines:
  - $(A_j)$  is the production capacity of machine  $(j^0)$ , satisfying  $(1 \leq A_j \leq 100)$ .
  - $(A)$  is sorted in ascending order  $((A_0 \leq A_1 \leq \dots \leq A_{N-1}))$ .
- The following  $(L)$  lines each contain  $(N)$  space-separated integers  $(C_{i,j})$ :
  - $(C_{i,j})$  is the initial cost of machine  $(j^i)$ , satisfying  $(1 \leq C_{i,j} \leq 1.25 \times 10^{12})$ .

#### # Output

Output exactly  $(T)$  lines.

Each line should describe the action taken on turn  $(t)$  ( $(0 \leq t < T)$ ), in order from turn 0, using the following format:

- To strengthen machine  $(j^i)$ :

...

i j

- To do nothing:

...

-1

Your program may include comment lines in the output that start with `#`.

#### # Input Generation

The function  $(\text{rand\_double}(L, U))$  represents generating a real number uniformly at random between  $(L)$  and  $(U)$ .

##### ## Generation of $(A_j)$

- When  $(j = 0)$ : set  $(A_0 = 1)$
- When  $(j \neq 0)$ : set  $(A_j = \text{round}(10^{\lceil \text{rand\_double}(0, 2) \rceil}))$
- After generating all values, sort the array  $(A)$  in ascending order

##### ## Generation of $(C_{i,j})$

- When  $(i = 0)$  and  $(j = 0)$ : set  $(C_{0,0} = 1)$
- Otherwise: set  $(C_{i,j} = \text{round}(A_j \times 500^i \times 10^{\lceil \text{rand\_double}(0, 2) \rceil}))$

Here is the last code we ran:

```
```cpp
{CODE HERE}
```

```

Current performance (higher is better): 5626752.9267  
Target: 6500000. Current gap: 873247.0733

Rules:

- You must use `cpp20` to solve the problem.
- Define all of your code in one final ````cpp```` block.
- In your final response, you should only output the code of your program. Do not include any other text.

Try diverse approaches to solve the problem. The best solution will make efficient use of the entire 2 second time limit without exceeding it. Think outside the box.

## Prompt used for Denoising

You are an expert in computational biology and single-cell RNA-seq analysis. Your task is to develop a denoising algorithm for scRNA-seq count data. You are experienced in computational biology libraries and tools and are familiar with problems in denoising in the single-cell field.

### ## Problem

Single-cell RNA-seq data is noisy due to technical dropout and low capture efficiency. Given noisy count data, predict the true expression levels.

Your prediction is evaluated against held-out molecules using two metrics:

1. \*\*MSE\*\* — Mean Squared Error in log-normalized space
2. \*\*Poisson Loss\*\* — Poisson negative log-likelihood

You need to implement a novel denoising algorithm that outperforms the current state-of-the-art without overfitting.

### ## Data Format

- Input `X`: numpy array of shape (n\_cells, n\_genes) — \*\*raw count data\*\*
- Output: numpy array of same shape — your denoised counts

### ## Evaluation

Your output is evaluated using these exact functions:

```
```python
<<<EVALUATE_MSE_FUNC>>>
````
```

```
```python
<<<EVALUATE_POISSON_FUNC>>>
````
```

### ## Scoring

- \*\*Poisson is a HARD CONSTRAINT.\*\* Your solution is REJECTED if `poisson\_norm < 0.97`.
- `poisson\_norm = (0.257575 - poisson) / (0.257575 - 0.031739)`
- MAGIC baseline achieves 0.97

\*\*Reward = MSE score only\*\* (after passing Poisson constraint).

### ## Budget & Resources

- \*\*Time budget\*\*: <<<BUDGET\_S>>>s for your code to run. You should time your code and make sure it runs within the time budget.
- \*\*CPUs\*\*: <<<CPUS>>> available

### ## Function Signature to return

```
```python
def magic_denoise(X, **kwargs):
    # kwargs may include: budget_s, random_state, knn, t, n_pca, solver, decay, knn_max,
    n_jobs
    # You can add your own parameters too
    # Your implementation
    return denoised_X # same shape as X
````
```

### ## Rules

- Implement `magic\_denoise(X, ...)` that returns denoised data
- Use numpy, scipy, sklearn, graphtools, scprep, scanpy
- Make all helper functions top level, no closures or lambdas
- No filesystem or network IO

### ## Key Insights from Benchmarks

- NORMALIZATION ORDER MATTERS: Denoise raw/log counts first, then normalize. "Reversed normalization order" achieves Poisson ~0.98 vs ~0.55 for standard order.
- Square root transform is variance-stabilizing for Poisson distributions

- Poisson loss is highly affected by low non-zero values — push values  $< 1$  toward zero
- The original MAGIC with reversed normalization achieves best results