Training-free Aligning Diffusion Models with Probability-Regularized Noise Optimization

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Abstract

1 Introduction

- Introduction on Diffuison Models.
- Drawback of Diffusion Models -> not align with the goal -> Align with reward
- Related work: LLM Alignment, RL-based, Guidance-based, noise/latent optimization-based.
- Contribution in this work:
  - We focus noise optimization-based method. Rigorously study the limit distribution and per-step improvement.
  - A key issue in noise optimization is reward-hacking. We reveal that when the noise drives away from standard Gaussian, reward-hacking happens. Thus we propose a probability-regularized noise optimization method to force the noise stay within the high probability region of the standard Gaussian.
  - We also extend to optimizing non-differentiable reward functions by revealing the best way of gradient approximation.
  - We conduct experiment on several popular reward function, and show that noise optimization can achieve sota scores without reward hacking and any training, albeit can with the cost of more time at generation.
  - We remark that the optimized images can serve as dataset for finetuning in the future.

1.1 Diffusion Models

In recent years, diffusion models have been recognized as state-of-the-art for generating high-quality images, demonstrating exceptional resolution, fidelity, and diversity [Ho et al., 2020, Dhariwal and Nichol, 2021, Song et al., 2020b]. These models are also notably easy to train and can be effectively extended to conditional generation [Ho and Salimans, 2022]. Broadly speaking, diffusion models work by learning to reverse the diffusion of data into noise, a process that can be described by a stochastic differential equation (SDE) [Song et al., 2020b, Karras et al., 2022]:

$$dx_t = f(t)x_t dt + g(t)dw_t, \tag{1}$$

where dw_t is the standard Wiener process, and $f(t)$ and $g(t)$ are the drift and diffusion coefficients, respectively. The reverse process relies on the score function $\epsilon(x_t, t) \overset{\text{def.}}{=} \nabla_x \log p(x_t)$, and its closed form can be expressed either as an ordinary differential equation (ODE) [Song et al., 2020b]:

$$dx_t = \left(f(t)x_t - \frac{1}{2}g^2(t)\epsilon(x_t, t) \right) dt, \tag{2}$$

or as an SDE:

$$dx_t = \left(f(t)x_t - g^2(t)\epsilon(x_t, t)\right) dt + g(t)dw_t. \tag{3}$$

With the ability to evaluate $\epsilon(x_t, t)$, it becomes possible to generate samples from noise by numerically solving the ODE (2) or the SDE (3). The training process, therefore, involves learning a parameterized surrogate $\epsilon_\theta(x_t, t)$ for $\epsilon(x_t, t)$ following a denoising score matching framework described in [Song et al., 2020b, Karras et al., 2022].

1.1.1 Aligning Generative Models

Generative models, e.g., Large Language Models (LLM) and Diffusion models, are trained on large-scale unlabeled and mixed-quality data, with an aim to capture the distribution of the data. However, when deploying these generative models for specific tasks, it is not good to sample from the orginally learned distribution directly, as this distribution is not aligned with the task-specific goal. For example, in image generation, people wishes to generated images that is aesthetically pleasing, not just a random image. Therefore, before putting the generative models into use, it is necessary to align the generative models with the task-specific goal.

Aligning Generative models has become a heated topic since the sucesss of alignming LLMs with Reinforcement Learning from Human Feeback (RLHF) [Ouyang et al., 2022, Liu et al., 2023a, OpenAI, 2022, Bai et al., 2022], where human evaluators are asked to rank the outputs of large AI models according to their personal preferences, with an aim to improve the generation quality of these models.

For diffusion models, RLHF has also gained sufficient attention recently, as the very recent series of works like [Deng et al., 2024, Uehara et al., 2024, Yuan et al., 2024, Song et al., 2023a, Dong et al., 2023, Sun et al., 2023, Zhang et al., 2023, Prabhudesai et al., 2023, Black et al., 2023, Fan et al., 2023].

Broadly speaking, given a generative models θ and its corresponding distribution $p_\theta(x)$. The most common setting in the alignment problem is that there exists a reward model $r(x)$, which can evaluate the generated samples with a real-valued score. Such reward models can either be obtained by training a neural network with human feedback, or using some pre-defined metrics. The goal of alignment is to improve the distribution $p_\theta(x)$, namely, the generated sample should have as high reward as possible. A common mathematical formulation in RLHF is to maximize the expected reward, while the obtained distribution should not deviate too much from the original distribution. This can be formulated as the following KL-regularized optimization problem:

$$\max_p \mathbb{E}_{x\sim p(x)} r(x) - \lambda KL(p||p_\theta). \tag{4}$$

existing models require training for every new reward model

1.1.2 Aligning Diffusion Models with Noise Optimization

In this work, we specifically focus on aligning diffusion models, and propose to align Diffusion Models by directly optimizing the latent noise.

Spefically, as we have introduced above, sampling from diffusion boils down to solving the ODE (2) or SDE (3). When solving for the ODE (2), the solving process can be viewed a mapping that maps the initial noise x_T into the generated sample x_0. Similarly, when solving for the SDE (3), the solving process can be viewed as a mapping that maps both the noise x_T and the Wiener process w_t into the generated sample x_0. With this observation, we can regard the solving process as a mapping $M(z)$ that maps the noise vectors z drawn from the standard Gaussian distribution to the generated samples.

As one can see, since the generated samples are determined by the noise vectors, it is to treat the noise vectors as the optimization variable, and optimize the noise vectors directly to maximize the reward. Mathematically, the optimization problem can be formulated as:

$$\max_z r((M(z))). \tag{5}$$

By solving this optimization problem, we can obtain the optimized noise vectors, and then use the optimized noise vectors to generate the optimized samples. Consider that $r(\cdot)$ is differentiable, we can use gradient-based optimization methods to solve this optimization problem.

Algorithm 1 Direct Noise Optimization with Differentiable Reward

Require: Initial noise z_0, stepsize η, number of iterations T.
for $t = 1$ to T **do**
  $z_t = z_{t-1} + \eta \nabla r(M(z_{t-1}))$.
end for
return Optimized sample $M(z_T)$.

1.1.3 Aligning Generative Models via prompt optimization

There are also some works that align the generative models by optimizing the prompt. For example, in the work of , the authors propose to optimize the prompt of LLMs to achieve the goal of the task. The prompt optimization can be viewed as a special case of the noise optimization, where the noise is the prompt. As we will show some example in Appendix.

2 Understanding Noise Optimization

- Use toy example to show the evolving of distribution.
- Show that the noise-to-image mapping is continuous and smooth, using DDIM and DDPM as example.
- Theoretical results, limit distribution, per-step improvement.

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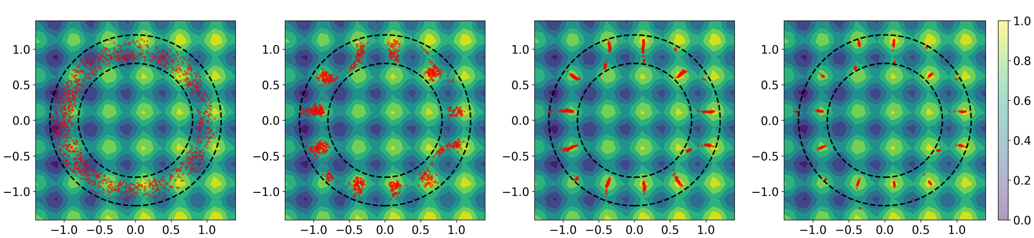
We remark that directly optimizing the noise vectors can be viewed as sampling from an improved distribution. Spefically, let us denote that $g_t(z)$ as an mapping that define the procedure of optimizing z with t gradient steps. For example, with the z_0 and z_T in Algorithm 1, we have $g_T(z_0) = z_T$. We denote $p_t(x)$ as the distribution of the generated samples after t steps of optimization, namely, $x \sim p_t(x)$ if $x = M(g_t(z))$ and $z \sim \mathcal{N}(0, I)$.

Figure: Toy example of the evolving of distribution. Showing that the point are moving towards the closest local minimum.

Let us first present a simple example while the distribution is the uniform distribution on the ring whose radius is between 0.8 and 1.2. We run the optimization with the reward function $r(x) = \sin(4\pi x[1]) + \sin(4\pi x[2]) - \left((x[1]-1)^2 - x[2]^2\right)/5$, which is a highly nonconvex function with many local minima, maxima and saddle points. We can see that the distribution of the samples are moving towards the local maxima of the reward function.



(a) Initial (b) 10 steps (c) 50 steps (d) 100 steps

Figure 1: evolving of distribution

Now let us states some assumptions before analyzing the noise optimization.

Assumption 1. *Throughout this paper, we have these assumptions:*

1. *For some constant B, $r(x) \geq B$ for all x.*

2. *$r \circ M$ is L-smooth, meaning that $\|\nabla^2 r \circ M(z)\| \leq L$.*

shows that the noise-to-image mapping is continuous and smooth, especially for continuous distribution. DDIM and DDPM, can just cite [Tang et al., 2024a]

Suppose that we choose the stepsize η in Algorithm 1 such that $\eta \leq 1/L$. We can analytically quantified the improvement of the distribution after each step of optimization. Spefically, we can use the expected reward as the metric to measure the improvement.

$$\mathbb{E}_{x \sim p_{t+1}(x)} r(x) \geq \mathbb{E}_{x \sim p_t(x)} r(x) + \frac{1}{2L} \mathbb{E}_{z_0 \sim N(0,I)} \left\| \nabla_z r \circ M(z)_{|z=g^i(z_0)} \right\|_2^2 > \mathbb{E}_{x \sim p_t(x)} r(x).$$

When does the distribution stop improving? As we can see, the distribution will stop improving when the expected gradient norm is zero. some discussion here

Different initialization leads to different samples. As we can see that the optimization process is sensitive to the initialization. For example, in the toy example, we can see that different initialization will leads to different images. This is also true for image diffusion models.

3 Understaning Reward-Hacking in Noise Optimization

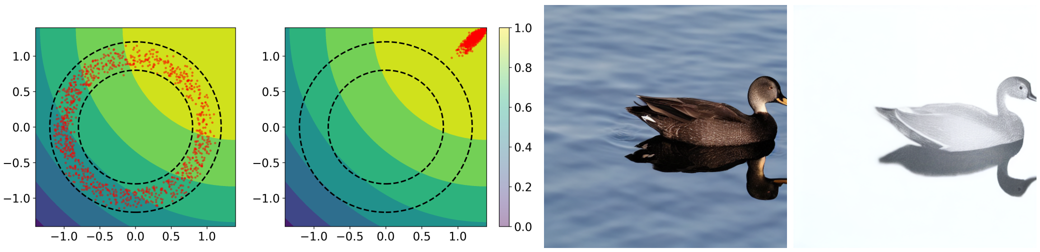
- Definition of reward-hacking: The reward is high but the generated images are out-of-distribution.
- Show examples of reward-hacking: Toy example, SD v1.5 with white reward and black prompt.
- Understand the reason of reward-hacking - Claim: Diffuison models generated out-of-manifold samples if and if only the initial noise is rare sample. The noise drives away from standard Gaussian during optimization.
- Use two concentration inequalities to measure the probability of sampled noise. Claim: The probability can be used to measure the degree of out-of-distribution.
- Four empricial evidence to support the claim.
  - Toy example: Show the noise-to-sample mapping. Use color to indicate the probability of sampled noise.
  - Set the noise to rare sample, e.g., all zero, all equal, etc. Bad images happen
  - Show some empirical investigation: Toy example, SD v1.5 with white reward. Compute the probability of sampled noise. When the probability of sampled noise is low, the reward-hacking happens.
  - For manifold-preserved reward, reward-hacking is less likely to happen. This is reflected in the probability of sampled noise.
- A plausible explination of why rare sample lead to out-of-distribution: The NN have high approximation error on rare samples.
- Formulate the probability-regularized noise optimization problem.

While noise optimization is an effective way to align diffusion models with the reward, sometimes it may have the issue of reward-hacking. Spefically, reward-hacking means that the optimized samples are no longer in the support of pretrained distribution $p_\theta(x)$. In the example of image diffusion models, reward-hacking may lead to the generation of unnatrual images.

Definition 1 (Reward-Hacking)**.** *We say that the noise optimization has the issue of reward-hacking if the expected reward is high, but the generated samples are out-of-distribution.*

Figure: Toy example of reward-hacking. SD v1.5 with white reward and black duck prompt. Before optimization and after optimization.

In this example, we present two examples using both the simple diffusion models in the toy example and the open-sourced image diffusion model SD v1.5. For the toy example, we optimize the reward fucntion $r(x) = -(x[1] - 1.4)^2 - (x[2] - 1.4)^2$ with 1000 gradient steps. For the SD v1.5, we optimize the whiteness reward, i.e., for an image $M \in [0, 255]^{3\times H\times W}$, we define the reward as $r(M) = -\sum_{i=1}^{3}\sum_{j=1}^{H}\sum_{k=1}^{W} M[i, j, k]$, and do the optimization with 30 steps. For both example, we use Adam optimizer with learning rate $1e-2$.



(a) Initial (b) 1000 steps (c) Black Duck (d) 50 steps

Figure 2: examples of reward-hacking

We identify that the main reason of reward-hacking is that optimized noise vectors becomes rare samples of standard Gaussian distribution. By saying rare samples, we mean that it is of extremely low probability to sample such noise vectors from the standard Gaussian distribution.

Since the diffusion models are trained on the standard Gaussian noise, when the noise vectors are rare samples, the neural network of diffusion models could have large approximation error on these rare samples. This leads to the generation of out-of-manifold samples.

3.1 Quantifying OOD via Concentration Inequalities

Therefore, to prevent reward-hacking, we propose to regularize the noise vectors to stay within the high probability region of the standard Gaussian distribution. We can achieve this by adding a regularization term to the optimization problem.

The regularization terms are designed with the inspiration from the classical concentration inequality for Gaussian Distribution. Specifically, for a sample $z \sim \mathcal{N}(0, I_n)$, we group it into m subvectors: $z = [z_1^1, ..., z_m^k], n = m \cdot k,\ z_i = [z_i^1, ..., z_i^k] \sim \mathcal{N}(0, I_k)$. $z = [z_1^1, ..., z_m^k], n = m \cdot k,\ z_i = [z_i^1, ..., z_i^k] \sim \mathcal{N}(0, I_k)$. We use the following two concentration inequalities for the mean and covariance matrix:

$$\Pr\left[\left\|\frac{1}{m}\sum_{i=1}^{m} z_i\right\| > M\right] < p_1(M) \overset{\text{def.}}{=} \max\left\{2e^{-\frac{mM^2}{2k}}, 1\right\} \tag{6}$$

$$\Pr\left[\left\|\frac{1}{m}\sum_{i=1}^{m} z_i z_i^\top - I_k\right\| > M\right] < p_2(M) \overset{\text{def.}}{=} \max\left\{2e^{-\frac{m\left(\max\left\{\sqrt{1+M}-1-\sqrt{\frac{k}{m}}, 0\right\}\right)^2}{2}}, 1\right\} \tag{7}$$

Remark 1. *According to [Wainwright, 2019], the two inequalities are tight when m/k is large. On the other hand, using a large k allows use to examine the covariance of different subvectors in the noise vector. For example, using $k = 1$ is a bad choice, as it only examines the mean and variance the noise vector, but not the covariance of different subvectors. In practice, we found that choosing k to be around $m/100$ to be an empirical good choice. In Appendix, we also provide a grid search for guiding the choice of k.*

A important thing to note is that the two inequalities are invariant to the permutation of the subvectors, i.e., for any permutation matrix Π, if z follows standard Gaussian probability, the permuted vector Πz will have the same probability behavior. This is due to the permutation-invariant property of the standard Gaussian distribution. With this observation, a natural idea is to examine the probability of many permuted vectors, i.e., given b permutation matrices $\Pi_1, ..., \Pi_b$, we wish to examine whether the all the vectors $\Pi_1 z, ..., \Pi_b z$ lies in the high probability region of the standard Gaussian distribution.

With this two concentration inequalities, we can measure the plausiblity of the sampled noise vectors. Specifically, given b permutation matrices $\Pi_1, ..., \Pi_b$, we can define the probability of the sampled noise vectors as: We denote $M_1(z) = \left\|\frac{1}{m}\sum_{i=1}^{m} z_i\right\|$ and $M_2(z) = \left\|\frac{1}{m}\sum_{i=1}^{m} z_i z_i^\top - I_k\right\|$

$$P(z) \stackrel{\text{def.}}{=} \min\left\{\min_{i\in\{1,\ldots,b\}} p_1\left(M_1(\Pi_i z)\right), \min_{i\in\{1,\ldots,b\}} p_2\left(M_2(\Pi_i z)\right)\right\}. \tag{8}$$

If the probability $P(z)$ is low, it means that there is a permutation matrix Π_i such that the noise vector $\Pi_i z$ lies in the low probability region of the standard Gaussian distribution, therefore, the noise vector z is less likely to be sampled from the standard Gaussian distribution.

Remark 2. *For the numbers of permutation matrices b, we can set it to be $b = 100$ throughout this work, and the used permutation matrices are randomly generated. Using a small b may make it less capable in locating the out-of-distribution case. But we will show that the probability $P(z)$ is robust to the choice of b as long as it is sufficiently large. More details can be found in Appendix.*

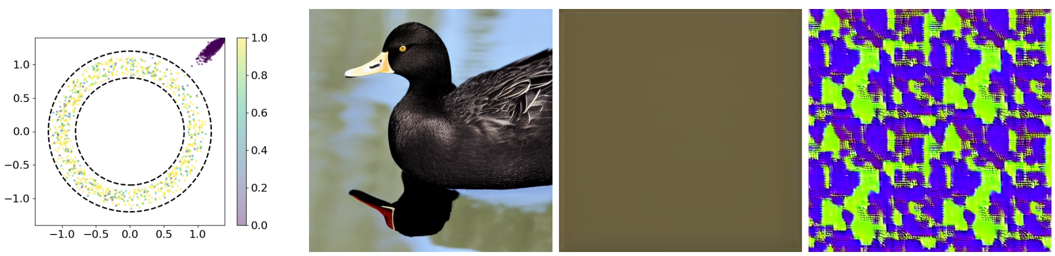
Figure: Four empricial evidence to support the claim.

Figure 1: One image, with color indicating the probability of sampled noise.

Figure 2: SD v1.5, set the noise to all zero. set part of the noise to be repetitive

Figure 3: Show the optimization trajectory of optimizing white reward, y-axis is the prob. prob is decreasiing

Figure 4: Show the optimization trajectory of optimizing aesthetic reward, y-axis is the prob. prob is not decreasiing



(a) Toy example (b) $P(z) = 0.36$ (c) Zero: $P(z) = 0.00$ (d) Repeat: $P(z) = 0.02$

Figure 3: examples of reward-hacking

Remark 3. *A possible reason that rare samples lead to out-of-distribution is that the neural network have high approximation error on rare samples.*

3.2 Probability-Regularized Noise Optimization

With these two inequalities, we propose the following probability-regularized noise optimization problem:

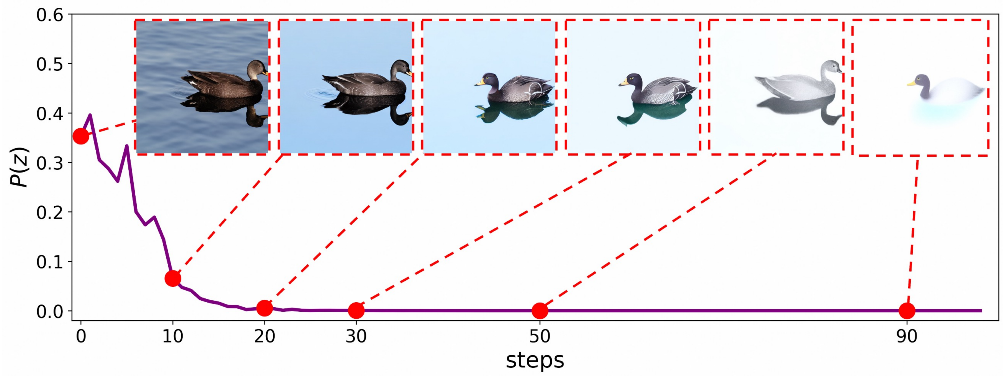
$$\max_z r((M(z))) + \mu \mathbb{E}_\Pi \left[\log p_1\left(M_1(\Pi z)\right) + \log p_2\left(M_2(\Pi z)\right)\right]. \tag{9}$$

In particular, for the regularization term, we use the expectation of the probability over the permutation matrices, rather than the minimum probability $P(z)$, this is because the expectation is more smooth for optimization.

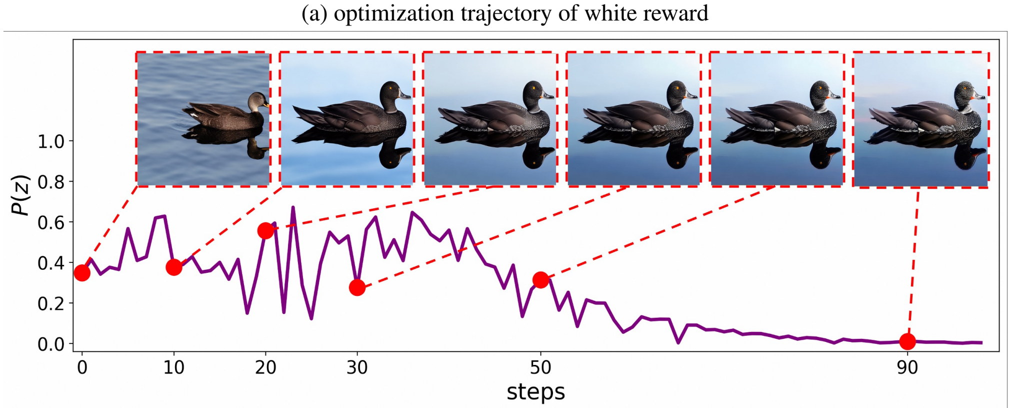
This can be similarly tackled by the gradient-based optimization algorithm.

4 Tackling Non-Differentiable Reward Functions

- In many case, we may face non-differential reward: 1. The metric, by design, is non-differentiable. 2. The reward is a third-party black-box. 3. The reward is represented by a huge neural network, thus the gradient is hard to compute.
- We study three way to extend noise optimization to non-differentiable reward functions, and identified the optimal one.



(a) optimization trajectory of white reward



(b) optimization trajectory of aesthetic reward

Figure 4: optimization trajectory

We remark that the noise optimization can also be extended to non-differentiable reward. Specifically, for the problem $\max_z r(M(x))$ with r is non-differentiable, we can see that the problem is partially differentiable as we can compute the gradient of M. In this case, we can estimate the gradient $\nabla_z r(M(z))$ via

$$\hat{g}(z) = \hat{h}(y) \cdot \nabla_z M(z),$$

where $\hat{h}(y) = (r(y_1) - r(y))(y_1 - y)$ and $y_1 = M(z + \xi), y = M(z)$, ξ is a small and random perturbation vector.

Theorem: provably efficient for the gradient estimation.

5 Experiments

- Major experiment 1: Black animal with whiteness reward, white animal with blackness reward. The main purpose is to prove the effectiveness of probability regularization.
- Major experiment 2: Benchmarking three NN-based reward functions with SD 1.5: aesthetic, pick score, hps. For these reward, it is less likely to hack them. But the regularization can also be helpful. When optimize one of them, use the other two as test metrics. Show that the score is superior to the one obtained by directly optimizing the image.
- Comparing three ways of non-differentiable optimization. Use Jpeg and aesthetic score. The purpose is to show that the optimal way is the one we proposed.
- Demonstrative experiments: 1. Use multi-modal LLM as reward function. show that it is less likely to hack it 2. use SDXL as base model for optimization. describe the computing cost. using complex prompt
- Experiments in Appendix:

- Tuning the regularization parameter.
- Visualization of optimization with images.
- finetuning on optimized images.
- Demonstrate the faliure of some common metrics. CLIP score, mlm-filter and some other metrics on the black and white example.
- more demonstartive examples

5.1 Examine the Effectiveness of Probability Regularization

Discuss the metrics used, the top-k mean of pixels value, because the classical metrics fails. detiails in appendix.

Figure: y-axis: value of the metric, probability, over-optimize metric. two legends: with and without regularization.

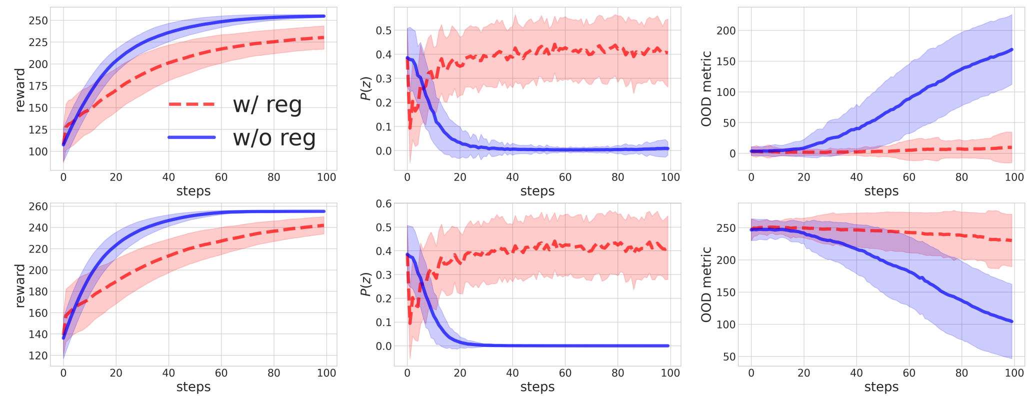


Figure 5: The effectiveness of probability regularization.

example images: white and black, with and without regularization.

(a) White w/o reg (b) White w/ reg (c) Black w/o reg (d) Black w/ reg

Figure 6: examples of optimized image with and without regularization

main conclusion: similar to the four empirical evidence mentioned above. the probability can reflect the level of out-of-distribution. penalizing the probability can prevent reward-hacking.

for the algorithm without regularization, we use the leanring rate 0.001, while for with regularization. we use the learning rate 0.01.

Remark 4. *We provide hyperparameters analysis for the regularization coefficients in Appendix.*

we run the experiment with 1000 samples, with the randomly generated animial prompt.

5.2 Benchmarking Three NN-based Reward Functions

Figure: y-axis: three metrics, probability. six legends: optimize three metrics * with/without regularization.

Table: comparing the score of the three metrics to existing works. for our methods, report the scores under time/steps.

we run the experiment with 1000 samples, with the randomly generated animial prompt.

main conclusion: optimizing these reward functions trained on human feedback is less likely to lead to reward-hacking, but not impossible. The regularization can also be helpful. This can be shown by using the other two as test metrics. Noise optimization can easily beat sota RL methods without any training on the reward function. Albeit the cost of more time at generation.

Remark 5. *we provide the Visualization of optimization in appendix.*

Remark 6. *To explore a possible way to alleviate the sampling cost, we also show that it works well by finetuning the model on optimized images in appendix.*

5.3 Comparing Three Ways of Non-Differentiable Optimization

main conclusion: the optimal way is the one we proposed. note that existing RL like DDPO consider only non-differentiable reward functions, we show that this case can also be handled by our method. Using estimated gradient is slower than using the true gradient, but it is still faster than RL methods.

Figure: Jpeg and aesthetic score. comparing the three ways.

5.4 Demonstrative Experiments

Figure: 1. Optimizing SDXL w.r.t aesthetic score, trajectory. 2. Optimizing SD v1.5 w.r.t multi-modal LLM, trajectory.

We believe our method have the potential in many real-world applications, such as the ID-preserving tasks in [Chen et al., 2024, Guo et al., 2024].

6 Conclusions

- Noise optimization is an effective way to align diffusion models, but be cautious about reward-hacking. By preventing the noise from being rare, we can alleviate the reward-hacking.
- It is training-free, but requires more time to generate images.
- A possible way to alleviate the time cost is to use the generated images as dataset for finetuning.

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Appendix

A Proofs

B hyperparameters

B.1 The η in DDIM

Comparing optimizing full noise and only initial noise. optimizing full noise tends to be faster.

B.2 Effect of learning rate on reward-hacking

B.3 m and k

B.4 Numbers of permutation matrices

B.5 Regularization coefficients

hyperparameters of regularization coefficients on white, aesthetic, hps, pick score

C Faliure of in existing metrics in capturing the reward-hacking phenomenon

D Visualization of optimization with images

E More Demonstrative Examples

F Comparing to Prompt tuning

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