000 001 002 003 AVOIDING MODE COLLAPSE IN DIFFUSION MODELS FINE-TUNED WITH REINFORCEMENT LEARNING

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ABSTRACT

Fine-tuning foundation models via reinforcement learning (RL) has proven promising for aligning to downstream objectives. In the case of diffusion models (DMs), though RL training improves alignment from early timesteps, critical issues such as training instability and mode collapse arise. We address these drawbacks by exploiting the hierarchical nature of DMs: we train them dynamically at each epoch with a tailored RL method, allowing for continual evaluation and step-bystep refinement of the model performance (or alignment). Furthermore, we find that not every denoising step needs to be fine-tuned to align DMs to downstream tasks. Consequently, in addition to clipping, we regularise model parameters at distinct learning phases via a sliding-window approach. Our approach, termed Hierarchical Reward Fine-tuning (HRF), is validated on the Denoising Diffusion Policy Optimisation method, where we show that models trained with HRF achieve better preservation of diversity in downstream tasks, thus enhancing the fine-tuning robustness and at uncompromising mean rewards.

- 1 INTRODUCTION
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029 030 031 032 033 034 Diffusion models (DMs) are the *de facto* state of the art in prompt-based generative modelling across various tasks including text-to-image, text-to-video, molecular graph modelling and medical image reconstruction [\(Ramesh et al., 2021;](#page-11-0) [Rombach et al., 2022;](#page-11-1) [Ho et al., 2022;](#page-10-0) [Singer et al., 2023;](#page-11-2) [Jing](#page-10-1) [et al., 2022;](#page-10-1) [Song et al., 2022\)](#page-11-3). Most of these applications build on the original Denoising Diffusion Probabilistic Model (DDPM) by [Ho et al.](#page-10-2) [\(2020\)](#page-10-2), but the extension to other formulations and variants is fast growing. It includes Score-based and Flow matching generative models, among others [\(Song](#page-11-4) [and Ermon, 2019;](#page-11-4) [Song et al., 2020;](#page-11-5) [Lipman et al., 2022\)](#page-10-3).

036 037 038 039 040 041 042 043 044 045 Recent works use Reinforcement Learning (RL) to align DMs to downstream tasks that are otherwise difficult to address, e.g., via explicit class labelling, such as generating *aesthetic* images following a specific prompt, or producing images admitting significant JPEG compression rates. These methods, such as the Denoising Diffusion Policy Optimization (DDPO) [\(Black et al., 2024\)](#page-10-4) and others [\(Deng](#page-10-5) [et al., 2024;](#page-10-5) [Fan et al., 2023\)](#page-10-6), formulate the denoising steps as a Markov Decision Process (MDP) controlled through a reward function. Despite recent works [\(Ouyang et al., 2022;](#page-10-7) [Schulman et al.,](#page-11-6) [2017\)](#page-11-6) making RL fine-tuning more stable and accurate, the consequence for alignment in rewardbased DDPM extensions are skewed generated samples, which lead to *mode collapse*, i.e., when the model's inherent diversity vanishes. Fig. [1](#page-1-0) shows samples from DDPM and DDPO to illustrate that, although DDPO provides better samples than DDPM (in terms of the LAION aesthetic score in this case), it sacrifices sample diversity: the images look the same.

046 047 048 049 050 051 052 053 We build on the hierarchical interpretation of DDPMs [\(Sclocchi et al., 2024\)](#page-11-7) and propose a methodology called *Hierarchical Reward Fine-tuning* (HRF), which performs reward-based learning from different timesteps in the diffusion using a sliding window approach. In DDPM, the HRF window selection mechanism fixes high-level features and generates variations in low-level features, facilitating exploration while preserving the sample's semantics, as illustrated in Fig. [3.](#page-4-0) To achieve this, we identify distinct stages in the learning process, distinguishing between high- and low-level features, and apply online RL at each stage, thus effectively training intermediate steps in the diffusion. Our proposal thus enables a controlled learning scheme promoting sample diversity, mitigating mode collapse, and thus successfully aligning diffusion models (DMs) to downstream tasks.

 The proposed HRF is implemented and experimentally assessed in the generation of RL-optimised diversity-preserving samples within DDPM. To this end, we consider a DM pre-trained on CelebaHQ [\(Karras et al., 2018\)](#page-10-8), and fine-tuned over three downstream tasks originally considered in [\(Black](#page-10-4) [et al., 2024\)](#page-10-4): compressibility, incompressibility and LAION aesthetic score. Fig. [4](#page-7-0) shows a succinct illustration of the results of our method for each of these tasks.

- The key contributions of our work are:
	- Insights into the learning dynamics of DDPMs when fine-tuned via online RL.
	- A critical assessment of the state of the art, in terms of its inability to preserve sample diversity due to an overoptimisation in noisy (early) stages of the diffusion chain.
	- A novel framework for preserving sample diversity in DDPMs fine-tuned with RL, based on a hierarchical interpretation of diffusion models, called Hierarchical Reward Fine-tuning (HRF).
	- An experimental validation of HRF demonstrating: i) advantages in controlled learning, ii) reduced need for reward handcrafting, and iii) improved preservation of sample diversity compared to DDPO.

 Figure 1: Comparison of Image Synthesis Using CelebA-HQ-Based Models. 2D projection of CLIP embeddings for two sets of 1,000 samples: i) DDPM samples (black borders) and ii) DDPO samples fine-tuned with the LAION aesthetic reward (white borders). The DDPO samples were optimized to achieve a higher average aesthetic score (5.58 vs. 5.11), indicating better *aesthetic quality*. Notably, the DDPO samples cluster more tightly (red ellipse) around the highest-scoring DDPM sample, indicating a *mode collapse effect*. Both sets of samples were generated using the same seed.

108 109 2 RELATED WORK

110 111 2.1 HIERARCHICAL FEATURES OF DIFFUSION MODELS

112 113 114 115 116 117 118 119 120 121 Recent studies have highlighted the hierarchical nature of data generation in diffusion models, particularly in the case of images. For instance, [Sclocchi et al.](#page-11-7) [\(2024\)](#page-11-7) found that a phase transition occurs during the backward diffusion at a specific timestamp. Beyond this point, the probability of reconstructing high-level features drops rapidly, while low-level features (details) change slower. High-level features typically refer to global attributes, such as overall face structure or hair type, whereas low-level features involve finer details, like skin texture or small facial details. This implies that high-level features are more susceptible to temporal changes in the diffusion process, whereas low-level features remain relatively stable across the diffusion. This observation is pivotal in our work, as we will develop a methodological approach to learn favourable representations for downstream tasks at distinct steps in the diffusion process. The main rationale behind our diversity-preserving approach is to target the early steps of the diffusion process trajectory we are training on.

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2.2 DIFFUSION MODEL TRAINING AT DIFFERENT NOISE LEVELS

125 126 127 128 129 130 The learning dynamics and convergence properties of DDPM at different stages of the diffusion process have been studied by [Hang et al.](#page-10-9) [\(2023\)](#page-10-9), finding that convergence speed is related to the learning difficulty associated with each timestep. Additionally, [Xu et al.](#page-11-8) [\(2024\)](#page-11-8) adopted a perspective of curriculum learning and found that DDPMs learn the early steps easier than the later ones across the denoising procedure. This curriculum learning approach allows for the design of learning strategies tailored for each step of the diffusion, thus improving the convergence speed.

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2.3 TRAINING DIFFUSION MODELS WITH REINFORCEMENT LEARNING

133 134 135 136 137 138 139 140 Approaches to train DDPMs by modelling the diffusion chain as an MDP leverage different loss formulations and regularization techniques [\(Black et al., 2024;](#page-10-4) [Fan et al., 2023;](#page-10-6) [Deng et al., 2024\)](#page-10-5). However, they all build upon the same RL setup: they refine loss definitions and mitigate the degeneration of sample diversity through regularization and hyperparameter tuning, but they do not exploit the hierarchical nature of data generation inherent in diffusion models. This means that although these approaches successfully fine-tune the models for downstream tasks in terms of their achieved rewards, they do so struggling to propagate learning across all diffusion steps in a controlled manner, ultimately compromising diversity. Our contribution aims to address this limitation.

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3 BACKGROUND

144 3.1 DIFFUSION MODELS

146 147 148 149 150 Let us consider denoising diffusion probabilistic models (DDPMs) [\(Ho et al., 2020;](#page-10-2) [Sohl-Dickstein](#page-11-9) [et al., 2015\)](#page-11-9), which represent a distribution $p(x_0|c)$ over data samples $x_0 \in \mathcal{X}$ conditioned on contexts $c \in \mathcal{C}$. This distribution is defined by reversing the forward Markovian process $q(x_t|x_{t-1}, c)$, where the chain $\{x_t\}_{t=0}^T$ is a sequence of samples with increasing levels of noise such that x_0 represents a clean data sample and x_T a completely noisy one, where all the data structure has been broken.

151 152 The transition probability of the backward process is typically modelled as a Gaussian with a learnable mean $\mu_{\theta}(x_t, c, t)$ and a fixed variance σ_t^2 [\(Ho et al., 2020;](#page-10-2) [Song et al., 2021\)](#page-11-10), that is,

$$
p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t, c) = \mathcal{N}(\mathbf{x}_{t-1}|\mu_{\theta}(\mathbf{x}_t, c, t), \sigma_t^2 I). \tag{1}
$$

155 The mean $\mu_{\theta}(x_t, c, t)$ is usually parameterised by a neural network trained with the objective:

$$
L_{\text{DDPM}}(\theta) = \mathbb{E}_{(\mathbf{x}_0, c) \sim p(\mathbf{x}_0, c), t \sim U\{0, T\}, \mathbf{x}_t \sim q(\mathbf{x}_t | \mathbf{x}_0)} \left[\| \mu(\mathbf{x}_0, t) - \mu_\theta(\mathbf{x}_t, c, t) \|^2 \right],\tag{2}
$$

157 158 159 160 where $\mu(x_0, t) = \mathbb{E}(x_t|x_0)$ is the expectation of x_t under the forward process defined by the transition kernel $q(x_t|x_{t-1})$. This objective maximizes a variational lower bound on the log-likelihood of the data [\(Ho et al., 2020;](#page-10-2) [Luo, 2022\)](#page-10-10).

161 Once the DDPM is trained, i.e., the neural net $\mu_{\theta}(x_t, c, t)$ is learned, data generation occurs via sampling. This starts by first drawing a pure-noise sample $x_T \sim \mathcal{N}(0, I)$ and then realising the

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162 163 164 reverse process in equation [1](#page-2-0) to produce the sequence (or trajectory) $\{x_T, x_{T-1}, \ldots, x_0\}$, where x_0 is the desired sample.

3.2 DIFFUSION MODEL AS A SEQUENTIAL DECISION-MAKING PROCESS

182 183 184 185 186 187 188 189 Figure 2: Equivalence of the backward process of a diffusion model as a sequential decisionmaking process. The initial state distribution of this MDP corresponds to an isotropic Gaussian, $\rho_0(s_0) \sim \mathcal{N}(0, I)$, where we assign the noise instance to the initial state $s_0 = x_T$. The agent follows a sequence of decisions a_t determined by the policy $\pi_\theta(a_t | s_t) := p_\theta(x_{T-t-1} | x_{T-t})$, moving from a noisy state x_{T-t} to a less noisy one x_{T-t-1} until it reaches to the sample x_0 , illustrated as the terminal state s_T in the diagram. This process generates the whole denoising trajectory $\tau = \{x_T, x_{T-1}, x_{T-2}, \ldots, x_0\}$, which is associated with a reward. In the case of DDPO, the reward model R only depends on the final, i.e., sample $r(x_0)$.

190 191 192 193 194 195 196 As a starting point, let us consider the denoising diffusion policy optimization (DDPO) formulation [\(Black et al., 2024\)](#page-10-4). In this setting, the DDPM backward process can be interpreted as an MDP, where the policy describes how an agent moves from a state s_t with a noisy sample x_{T-t} to a state s_{t-1} with a cleaner sample x_{T-t-1} , through its *denoising actions* $a_t : x_{T-t} \to x_{T-t-1}$. This occurs from the initial state s₀, where a noise sample is drawn from an isotropic Gaussian distribution $\rho_0 \sim \mathcal{N}(0, I)$ and assigned to x_T , until arriving at a terminal state s_T , where the sample x_0 is generated. Fig. [2](#page-3-0) illustrates this RL formulation of DDPM.

197 198 199 200 201 202 In DDPO, a *denoising* neural network p_θ is used to directly estimate s_t at timestep $t - 1$ (or, indirectly, estimate the corresponding noise), defining the policy $\pi_{\theta}(a_t, s_t)$. In this post-training framework, the diffusion model parameters θ can be directly optimized via policy gradient estimation to maximize any arbitrary scalar-reward signal over the sample. x_0 In other words, the agent learns to denoise trajectories in order to maximize the expected reward, leveraging the denoising diffusion reinforcement learning (DDRL) objective [\(Black et al., 2024\)](#page-10-4):

$$
\mathcal{J}_{\text{DDRL}}(\theta) = \mathbb{E}_{c \sim p(c), \mathbf{x}_0 \sim p_{\theta}(\mathbf{x}_0|c)}[r(\mathbf{x}_0, c)].
$$
\n(3)

204 205 A critical aspect of this formulation is that the reward $R(s_t, a_t)$ only considers the final sample x_0 , neglecting every non-terminal state s_T , or equivalently samples $x_{t\neq0}$, as depicted in Figure [2.](#page-3-0)

206 207 208 209 Furthermore, DDPOs compute gradients either via a score function method, also known as RE-INFORCE [\(Schulman et al., 2015\)](#page-11-11), or optimising a surrogate objective via importance sampling [\(Schulman et al., 2017\)](#page-11-6). The latter, denoted $DDPO_{IS}$ with gradient given by

(DDPO_{IS})
$$
\nabla_{\theta} \mathcal{J} = \mathbb{E}_{\mathbf{x}_{T:0} \sim p_{\theta_{old}}} \bigg[\sum_{t=0}^{T} \frac{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)}{p_{\theta_{old}}(\mathbf{x}_{t-1}|\mathbf{x}_t)} \nabla_{\theta} \log p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) r(\mathbf{x}_0) \bigg], \tag{4}
$$

213 214 215 is used as a baseline in our paper to compare the proposed method.^{[1](#page-3-1)} Note that computing p_θ and log p_θ in equation [4](#page-3-2) is straightforward when p_θ is a conditional Gaussian distribution.

¹ From now on, when we refer to DDPO, we mean $DDPO_{IS}$ unless specified otherwise.

3.3 DIVERSITY LOSS DUE TO OVERPARAMETERIZATION IN THE EARLY PHASES OF DENOISING

As discussed in Secs. [2.1](#page-2-1) and [2.2,](#page-2-2) learning in DDPM models is more effective during the noisy stages of diffusion and becomes increasingly difficult as noise is reduced. We confirm that this trend also applies to RL-based diffusion via a succinct experimental example. By employing injection sampling, a process where sampling is started with the fine-tuned model and then switched to the base model at step t to continue the sampling, we observed that interventions made in the noisier stages of the denoising process have the most significant impact on the resulting samples. A detailed description of the experiment can be found in Appendix [A.1.](#page-12-0)

4 HIERARCHICAL REWARD FINE-TUNING FOR DIFFUSION MODELS

 Figure 3: Hierarchical Reward Fine-tuning (HRF). In DDPO (purple), the entire denoising trajectory is influenced, affecting both high- and low-level features. In contrast, HRF intervenes at later timesteps of the trajectory, selecting an specific timestep t based on a *window selection schema*. At this point, an intermediate state $s_t \sim \rho_t$ is drawn from a new prior distribution, primarily adjusting low-level features while preserving high-level features and diversity, yet still achieving high rewards (s_T^1) yellow star). During policy rollouts, HRF generates divergent trajectories from s_t by introducing noise at intermediate timesteps. This serves as a *low-level feature exploration mechanism* to discover regions with higher reward potential (s_T^2 yellow star) given the high-level information set by the new prior ρ_t . In both cases, the dataset of trajectories and rewards \mathcal{D}^{π_θ} is used to estimate the gradients via Monte Carlo sampling, which are then applied to update the diffusion model parameters. HRF-D dynamically adjusts the vertical window selection line during fine-tuning.

> This section describes our main contribution by defining the problem statement and the methodology employed to solve it.

4.1 HIERARCHICAL REPRESENTATION OF TRAINING

 Our approach, HRF, is underpinned by the hierarchical nature of sample generation in diffusion models as identified by [Sclocchi et al.](#page-11-7) [\(2024\)](#page-11-7). With this in mind, we propose the training diagram illustrated in Figure [3.](#page-4-0) Each training step starts at a noisy step t using an image prior, guiding the model to learn from favorable policies at that stage. This is achieved by computing the trajectories and their corresponding rewards for every chosen initial step and then propagating the learning to those starting points. This approach leverages the fact that structural changes in generated samples occur at different stages of the diffusion chain, where the rate of change varies depending on the learning difficulty [\(Xu et al., 2024;](#page-11-8) [Hang et al., 2023\)](#page-10-9). The methodology remains flexible enough to **270 271 272** allow evaluation on fully denoised samples for each step t , while also facilitating the assessment of reward functions at intermediate steps. This capability helps in selecting better policies throughout the diffusion chain.

273 274 275 276 277 We propose two variants of the aforementioned methodology based on the window selection mechanism: HRF, which uses manually defined windows for selecting initial steps, and HRF-D, which employs a *dynamic window sampling* strategy. Refer to Section [4.3](#page-5-0) for more details about the window selection schemes.

278 279 280 281 282 283 284 A major benefit of our proposed methodology is the control over when and where to optimize the DMs distinct phases, particularly for training using RL on downstream rewards that are hard to describe explicitly. Furthermore, HRF is independent of the chosen loss definitions since it still uses the final sample to represent the information conveyed in the segment of the denoising trajectory under evaluation. Another significant benefit of HRF comes from splitting the learning task into multiple training steps (abiding by the hierarchical nature of training), which allows us to optimize hyper-parameters or skip phases in a controlled manner.

4.2 TRAJECTORY OF INTEREST SAMPLING

287 288 289 We define each denoising step in the diffusion chain as $p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t, c)$. For a given time step t, we use importance sampling so that the objective function defined in DDPO with our modified trajectory window is:

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$$
\text{(DDPO}_{\text{IS}_{\text{window}}}) \ \nabla_{\theta} \mathcal{J} = \mathbb{E}_{\mathbf{x}_{0:t} \sim p_{\theta_{\text{old}}}} \bigg[\sum_{t=0}^{t} \frac{p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_{t}, c)}{p_{\theta_{\text{old}}}(\mathbf{x}_{t-1} | \mathbf{x}_{t}, c)} \nabla_{\theta} \log p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_{t}, c) r(\mathbf{x}_{0}) \bigg], \qquad (5)
$$

where the likelihood is computed over the modified diffusion trajectory. This is from $t \to 0$, as its computed over the intermediate step selected by the window selection mechanism to the final state. We also employ trust regions to address inaccurate estimations of p_{θ} .

298 299 300 301 302 303 To maintain the consistency of our MDP definition, and as importance sampling operates over the batch where the likelihood is computed, it is important to ensure that the initial sampling step originates from the same distribution. In the original formulation of DDPO, this is achieved by defining the initial state as a sample from random noise. To replicate these conditions for each batch, we start with a clean image, add random noise up to step t a total of n times, based on a scheduler, and generate trajectories for n samples per batch.

304 Our MDP definition could be written as:

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$$
s_t = (c, t, \mathbf{x}_t) \quad \pi(a_t \mid s_t) = p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t, c) \qquad P(s_{t+1} \mid s_t, a_t) = (\delta_c, \delta_{t-1}, \delta_{\mathbf{x}_{t-1}})
$$

$$
a_t = \mathbf{x}_{t-1} \qquad \rho_0(s_0) = (p(c), \delta_t, \rho(x_{\text{noised}})) \qquad R(s_t, a_t) = \begin{cases} r(\mathbf{x}_0, c) & \text{if } t = 0\\ 0 & \text{otherwise} \end{cases}
$$

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where $\rho(x_{\text{noise}})$ is the distribution of the initial state at step t, which is obtained by adding noise sampled from $\mathcal{N}(0, I)$ to a clean image x_0 up to step t.

314 315 316 For $t = T$, the distribution of the initial state is equal to $\mathcal{N}(0, I)$, which is the original definition provided by DDPO. Generally, this framework is flexible enough to be adapted to any method that uses the original MDP formulation for diffusion models.

318 319 4.3 WINDOW SELECTION

320 321 322 323 We evaluate two window selection schemes: (1) predefined windows that determine initial sampling steps and (2) dynamic window selection, where windows are dynamically chosen by evaluating policies at each noise step. In the dynamic approach, we identify the step t that optimizes the sampling trajectory by finding the policy $\pi(a_t | s_t)$ that *maximizes reward variation while minimizing divergence from the image prior* $\rho(x_{\text{noised}})$. This reward is given by:

 $R_{\theta,t} = \text{Reward from } \tilde{x}_{t\to0} \mid \pi(a_t \mid s_t), \quad \pi_{\text{best}}(a_t \mid s_t) = \max_t (R_{\theta,t} - R_{\theta,t+1}) \ \forall t \in [T-1,0].$

where $\tilde{x}_{t\to 0}$ is the noise-free version of x_t . We incorporate a diversity-promoting term by considering the mean distance between samples (at each step) and the prior. The optimal policy is defined as:

$$
\pi_{\text{best}}(a_t \mid s_t) = \max_t ((R_{\theta,t} - R_{\theta,t+1}) - \beta \cdot D(\rho_0(s_0), \tilde{x}_{t \to 0})) \quad \forall t \in [T-1,0],
$$

where β is a hyperparameter and D is a distance metric such as cosine distance:

 $D(\rho_0(s_0), \tilde{x}_{t\to 0})$ = mean $(D_{\cos}(\rho_0(s_0), \tilde{x}_{t\to 0}))$ \forall samples at step t.

339 With this, our training process is as follows:

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340 341 342 343 344 *Algorithm [1:](#page-6-0) Initial Step*. For a predefined window, a sampling cluster C is generated for each epoch. For each sample within the batch, a starting step t_i is sampled from a uniform distribution over the cluster C, and the final state s_0 for the current batch is generated. If we are dynamically selecting the initial step, we sample all possible intermediate states and select the ones that maximizes the objective detailed above in section [4.3.](#page-5-0)

345 346 347 348 349 *Algorithm [2:](#page-6-1) Hierarchical Training*. It extends this sampling strategy to the full batch training process. Initially, several reference images are sampled from the selected initial steps (Initial Step). For each batch, noise is added to the final state of the reference image per batch s_0 to create new initial states $\{s_i\}_{i=t}^{\text{num}_\text{batches}}$. The algorithm then generates trajectories for a specified number of samples from the corresponding starting steps and applies DDPO to each clipped trajectory.

5 EXPERIMENTS

5.1 TASKS AND REWARD FUNCTIONS

371 372 373 374 375 We employed three downstream tasks as outlined in [Black et al.](#page-10-4) [\(2024\)](#page-10-4): compressibility, incompressibility, and aesthetic quality. The first two tasks are defined by the size of images after applying a JPEG compression algorithm, serving as the reward function. For aesthetic quality, we utilized the LAION aesthetic model [\(Schuhmann, 2022\)](#page-11-12), a multilayer perceptron that assigns a scalar value from 1 to 10 to indicate the aesthetic quality of an image.

376 377 These tasks show RL's ability to optimize objectives like compressibility, which are hard to encode in a loss function. The LAION aesthetic model further demonstrates how RL leverages human feedback to align diffusion models [\(Ouyang et al., 2022\)](#page-10-7).

Figure 4: Alignment of diffusion model to downstream tasks. This figure shows the visual performance of a diffusion model on three tasks: aesthetic quality, incompressibility, and compressibility. DDPO and HRF achieve similar semantic changes, but HRF better preserves visual diversity, especially for aesthetic quality. While DDPO risks mode collapse by generating similar high-reward images, **HRF** maintains diversity while improving rewards. **HRF-D** shows a significant visual shift, with samples differing greatly from the originals but maintaining high diversity. Compressibility skews towards darker samples, yet retains diverse representations.

5.2 EXPERIMENTAL SETUP

 We train our base model using DDPO and our proposed DDPO-based methods with three random seeds each, applying early stopping at a common stable point. First, we train DDPO to a target reward, then fine-tune our hierarchical models to achieve similar scores, resulting in 16 models: one baseline, one DDPO per task, three HRF per task, and one HRF-D per task. We evaluated these models via the following performance indices:

- 1. Inception Score (IS) [Salimans et al.](#page-11-13) [\(2016\)](#page-11-13): Measures both sample quality and diversity by evaluating the probability of generated samples belonging to distinct classes. A higher score indicates better visual quality and diversity, while a score closer to baseline score reflects preserved sample diversity and distribution.
- 2. Vendi Score [\(Dan Friedman and Dieng, 2023\)](#page-10-11), which measures diversity as the exponential of the Shannon entropy of a similarity matrix. It approximates the effective number of distinct classes in a sample based on a distance metric. For our evaluation, scores closer to baseline indicate better sample diversity preservation.
- 3. Reward Score: Evaluates a model's adaptability to a given downstream task by assigning a numerical value to task-specific performance. Higher scores indicate better alignment with the task, providing an intuitive measure for comparing model behavior under similar conditions.
- Hyperparameter settings and resources can be found in Appendix [A.2.](#page-12-1)
- 5.3 ABLATIONS ON WINDOW SELECTION IN HIERARCHICAL REWARD FINE-TUNING

 We performed a sensitivity analysis on window selection based on three regimes: baseline, early, and later stages, each trained with three seeds. With 40 sampling steps (*0 = noisiest, 40 = final image*), the windows used are:

- 1. Baseline: [(8,12), (18,22), (28,32)]—three equidistant windows.
- 2. Early: [(3,7), (18,22), (28,32)]—first window shifted to noisier states.
- 3. Later: [(8,12), (28,32)]—middle window removed, iterating more on the last window.

 Figure [5](#page-8-0) shows that different rewards favor different strategies: *Aesthetic Quality* prefers less noisy windows, while *Compressibility* and *Incompressibility* favor noisier ones.

Figure 5: **Rewards (y-axis) vs Diversity (x-axis, Vendi Score)**. Ablations on window selections for three hierarchical regimes: baseline (blue), early (orange) and latter stages (green) over the three downstream tasks considered. Each result is reported as the average of three-run seeds.

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5.4 RESULTS

Table 1: Reward Mean and standard error for each downstream task across using **google/ddpm-celebahq-256** as pretrained model. All samples were generated using the same initial noise to ensure a fair comparison. **Baseline** refers to the generative capabilities of the pretrained model. DDPO displays results from the fine-tuned models using DDPO with importance sampling (see Section [3.2\)](#page-3-3). **HRF** represents our proposed method based on the average results reported on different window selection schemas (see Section [5.3\)](#page-7-1). On the other side, **HRF-D** results are obtained using a *dynamic window selection* method.

Downstream Tasks	Baseline	DDPO	HRF	HRF-D
Aesthetic Quality (\uparrow better)	5.11 ± 0.01	5.55 ± 0.01	5.18 ± 0.01	5.41 ± 0.01
Compressibility $(\downarrow$ better)	17.26 ± 0.05	5.30 ± 0.06	8.40 ± 0.08	5.20 ± 0.07
Incompressibility (\uparrow) better)	17.26 ± 0.05	21.59 ± 0.08	23.81 ± 0.10	38.77 ± 0.15

Table 2: Sample Diversity Assessment Using Inception Score. The Inception Score (IS) represents the mean value calculated across 2, 142 images, with values closer to baseline indicating better diversity preservation.

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472 474 We evaluated the baseline DDPM model's generation capacity, measuring the mean reward over 2,142 samples for the three downstream tasks considered. Reproducing the DDPO method from [Black et al.](#page-10-4) [\(2024\)](#page-10-4), our approach outperformed the baseline across all tasks considered (see Table [1\)](#page-8-1).

475 476 477 478 479 480 The HRF and HRF-D methods performed on par with –or better than– standard DDPO. While achieving similar mean rewards, our approach successfully optimized the reward without collapsing samples into a single mode, thus preserving diversity. This claim was validated via the Inception Score (IS) [\(Salimans et al., 2016;](#page-11-13) [Heusel et al., 2017\)](#page-10-12) as described in Section [5.2.](#page-7-2) Table [2](#page-8-2) shows that HRF and HRF-D achieved IS values closer to the baseline, indicating improved sample diversity over DDPO while successfully fine-tuning the model for the tasks of interest.

481 482 483 484 485 Table [3](#page-9-0) further validates our claims. Vendi Scores closer to the baseline indicate better diversity preservation, and both HRF and HRF-D outperformed DDPO in that regard. While higher Vendi scores typically mean more diversity, our goal is to maintain diversity within the support of the original distribution, making excessive diversity undesirable for this study. These metrics were computed using 2, 142 samples. For more details on how the scores change as the number of samples increases, refer to Appendix [A.4.](#page-12-2)

486 487 488 489 490 Table 3: Sample Diversity Assessment Using Vendi Score computed using cosine similarity metric on raw pixels and CLIP embeddings. Vendi score measures the number of distinct classes: scores closer to the baseline preserve the same number of unique samples, indicating better sample diversity preservation. Higher values show greater diversity but do not guarantee preservation within the original distribution support.

The evidence shows a trade-off between optimizing for a downstream objective and maintaining sample diversity, as reinforcement learning inherently skews samples toward policy preferences. Our approach appears to balance this trade-off by focusing on learning dynamics and training in a more controlled step-wise manner, rather than manipulating the reward.

In summary, our findings suggest that our RL-based training approach achieved comparable performance to DDPO in reward optimization, while better preserving model diversity. This highlights the robustness and efficacy of HRF and HRF-D as a method, showcasing its potential for enhancing model performance across various tasks while avoiding mode collapse.

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6 CONCLUSIONS

512 513 514 515 516 517 518 519 We have presented HRF, a novel methodological framework that leverages the hierarchical nature of data generation in diffusion models and improves the multi-step decision-making interpretation. In this line, we have also introduced a phase training scheme that enhances specific parts of the diffusion model during fine-tuning. The method provides new insights into learning via reinforcement learning and the effects on each diffusion step. Our hierarchical formulation has proven to be an effective method for fine-tuning diffusion models on downstream tasks while successfully preserving the inherent models' diversity. Our evaluation utilized known and validated metrics such as the Inception Score (IS) and Vendi Score to measure the performance of the generative models considered, thus providing a trustworthy assessment of the

521 522 523 524 525 526 527 528 529 Future work. Some future work directions include optimizing cluster selection and hyperparameters to balance learning and sample diversity. Also, exploring alternative RL formulations within this framework could yield interesting results. While we showed that manual step selection improves performance, finding optimal training scenarios remains an open question that we initially explored with HRF-D, which employs an algorithm to identify optimal training steps, but it is not yet fully optimized and requires further research. Finally, we find it extremely necessary to define benchmarks with specific pre-trained models and tasks to measure and compare different post-training strategies, as this is an area rather unexplored. Methodologies like the one proposed in this paper would benefit from better and more concise evaluation.

530 531 532 Limitations. Our method aims to control diffusion models to align with downstream tasks via reward functions, offering benefits like avoiding mode collapse. However, risks include generating explicit content, and more research is needed to understand its broader impact.

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540 541 REFERENCES

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584

542 543 544 Kevin Black, Michael Janner, Yilun Du, Ilya Kostrikov, and Sergey Levine. Training diffusion models with reinforcement learning. In *International Conference on Learning Representations*, 2024. URL <https://openreview.net/forum?id=YCWjhGrJFD>.

545 546 547 Dan Dan Friedman and Adji Bousso Dieng. The vendi score: A diversity evaluation metric for machine learning. *Transactions on machine learning research*, 2023.

548 549 550 Fei Deng, Qifei Wang, Wei Wei, Matthias Grundmann, and Tingbo Hou. PRDP: Proximal reward difference prediction for large-scale reward finetuning of diffusion models. *Preprint arXiv:2402.08714*, 2024.

- **551 552 553 554 555 556** Ying Fan, Olivia Watkins, Yuqing Du, Hao Liu, Moonkyung Ryu, Craig Boutilier, Pieter Abbeel, Mohammad Ghavamzadeh, Kangwook Lee, and Kimin Lee. DPOK: Reinforcement learning for fine-tuning text-to-image diffusion models. In A. Oh, T. Naumann, A. Globerson, K. Saenko, M. Hardt, and S. Levine, editors, *Advances in Neural Information Processing Systems*, volume 36, pages 79858–79885. Curran Associates, Inc., 2023.
- **557 558 559** Tiankai Hang, Shuyang Gu, Chen Li, Jianmin Bao, Dong Chen, Han Hu, Xin Geng, and Baining Guo. Efficient diffusion training via Min-SNR weighting strategy. In *IEEE/CVF International Conference on Computer Vision*, pages 7407–7417, 2023.
- **560 561 562 563 564 565** Martin Heusel, Hubert Ramsauer, Thomas Unterthiner, Bernhard Nessler, and Sepp Hochreiter. GANs trained by a two time-scale update rule converge to a local Nash equilibrium. In I. Guyon, U. Von Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc., 2017. URL [https://proceedings.neurips.cc/paper_files/paper/](https://proceedings.neurips.cc/paper_files/paper/2017/file/8a1d694707eb0fefe65871369074926d-Paper.pdf) [2017/file/8a1d694707eb0fefe65871369074926d-Paper.pdf](https://proceedings.neurips.cc/paper_files/paper/2017/file/8a1d694707eb0fefe65871369074926d-Paper.pdf).
- **567 569** Jonathan Ho, Ajay Jain, and Pieter Abbeel. Denoising diffusion probabilistic models. In H. Larochelle, M. Ranzato, R. Hadsell, M.F. Balcan, and H. Lin, editors, *Advances in Neural Information Processing Systems*, volume 33, pages 6840–6851. Curran Associates, Inc., 2020.
	- Jonathan Ho, William Chan, Chitwan Saharia, Jay Whang, Ruiqi Gao, Alexey Gritsenko, Diederik P. Kingma, Ben Poole, Mohammad Norouzi, David J. Fleet, and Tim Salimans. Imagen video: High definition video generation with diffusion models. *Preprint arXiv: 2210.02303*, 2022.
- **574 575 576 577** Bowen Jing, Gabriele Corso, Jeffrey Chang, Regina Barzilay, and Tommi Jaakkola. Torsional diffusion for molecular conformer generation. In S. Koyejo, S. Mohamed, A. Agarwal, D. Belgrave, K. Cho, and A. Oh, editors, *Advances in Neural Information Processing Systems*, volume 35, pages 24240–24253. Curran Associates, Inc., 2022.
	- Tero Karras, Timo Aila, Samuli Laine, and Jaakko Lehtinen. Progressive growing of GANs for improved quality, stability, and variation. In *International Conference on Learning Representations*, 2018.
- **582 583** Yaron Lipman, Ricky TQ Chen, Heli Ben-Hamu, Maximilian Nickel, and Matt Le. Flow matching for generative modeling. *arXiv preprint arXiv:2210.02747*, 2022.
- **585 586** Calvin Luo. Understanding diffusion models: A unified perspective. *Preprint arXiv:2208.11970*, 2022.
- **587 588 589 590 591 592 593** Long Ouyang, Jeffrey Wu, Xu Jiang, Diogo Almeida, Carroll Wainwright, Pamela Mishkin, Chong Zhang, Sandhini Agarwal, Katarina Slama, Alex Ray, John Schulman, Jacob Hilton, Fraser Kelton, Luke Miller, Maddie Simens, Amanda Askell, Peter Welinder, Paul F Christiano, Jan Leike, and Ryan Lowe. Training language models to follow instructions with human feedback. In S. Koyejo, S. Mohamed, A. Agarwal, D. Belgrave, K. Cho, and A. Oh, editors, *Advances in Neural Information Processing Systems*, volume 35, pages 27730–27744. Curran Associates, Inc., 2022. URL [https://proceedings.neurips.cc/paper_files/paper/](https://proceedings.neurips.cc/paper_files/paper/2022/file/b1efde53be364a73914f58805a001731-Paper-Conference.pdf) [2022/file/b1efde53be364a73914f58805a001731-Paper-Conference.pdf](https://proceedings.neurips.cc/paper_files/paper/2022/file/b1efde53be364a73914f58805a001731-Paper-Conference.pdf).

A APPENDIX

 A.1 INJECTION SAMPLING

 When investigating the impact of learning with the MDP formulation we propose that most of the learning prowess is being done at the early steps of the diffusion model (the noisier states). To verify this experimentally we propose the following method:

- 1. Sample 15 trajectories with all fine-tuned models using DDPO on three tasks.
	- 2. Select initial injection steps: [38, 35, 30, 25, 20, 10], where 40 is the noisiest and 0 is the final sample.
- 3. Resample 15 trajectories, switching to the base model at selected injection steps, and compute all trajectory variations.
- 4. Compute cosine distances between denoised images of the original and fine-tuned models for all starting timesteps for the same starting seed. This is between the estimated noiseless image for each timestep.
- 5. Plot the distances for all three models.

 Following these steps we get the differences that each model makes for the denoising trajectory at different timesteps. We confirm that most of the differences in the final image come from the early stages of the diffusion model [6.](#page-13-0) This insight further solidifies the fact that almost all of the learning tends to happen at the early stages of the diffusion model due to the training inherent dynamics.

 A.2 IMPLEMENTATION DETAILS

 We provide the implementation details we used, such as computational resources and relevant hyperparameters settings. All this hyperparameters may be subject to changes and exploration, especially in the HRF implementations. Where the hyperparameters where found experimentally.

 A.2.1 RESOURCE DETAILS

 For HRF: GPU experiments were conducted on the default NVIDIA system within the cloud computing provider Hyperstack, with one A100 Tensor Core GPU and 150GB of GPU memory. The training time for each iteration took approximately 4 hours. Inference for the reward model was performed on a single NVIDIA L4 GPU and takes about 2 minutes per 40 images.

A.3 FULL HYPERPARAMETERS

A.4 VENDI SCORE

 We conducted an empirical analysis of the incrementally computed Vendi Score using the cosine distance metric on CLIP embeddings. The results are shown in Figure [7](#page-15-0) . The analysis begins with an initial sample size of 500, increasing by 5 samples at each step until reaching 2000. Afterwards, the sample size is increased by 500 samples per step until reaching a total of 11, 000 samples. We ended up using 2, 142 samples to compute the Vendi Score, capturing the major increase in diversity.

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Table 4: Full Hyperparameters for Aesthetic Quality

Table 5: Full Hyperparameters for Compressibility and Incompressibility

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number of DDPM samples (x-axis).. The analysis starts with 500 images, increasing by 5 samples per step until reaching 2, 000, after which steps increase by 500 samples up to a total of 11, 000. The vertical line marks the Vendi Score at 2, 142 samples, the same number used for diversity evaluation in ablation studies and Table [3](#page-9-0) This consistent sample size ensures a fair comparison of diversity

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