

000 MAD: MANIFOLD ATTRACTED DIFFUSION

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002
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005 006 007 ABSTRACT

009
010 Score-based diffusion models are a highly effective method for generating sam-
011 ples from a distribution of images. We consider scenarios where the training data
012 comes from a noisy version of the target distribution, and present an efficiently
013 implementable modification of the inference procedure to generate noiseless sam-
014 ples. Our approach is motivated by the manifold hypothesis, according to which
015 meaningful data is concentrated around some low-dimensional manifold of a high-
016 dimensional ambient space. The central idea is that noise manifests as low magni-
017 tude variation in off-manifold directions in contrast to the relevant variation of the
018 desired distribution which is mostly confined to on-manifold directions. We intro-
019 duce the notion of an extended score and show that, in a simplified setting, it can
020 be used to reduce small variations to zero, while leaving large variations mostly
021 unchanged. We describe how its approximation can be computed efficiently from
022 an approximation to the standard score and demonstrate its efficacy on toy prob-
023 lems, synthetic data, and real data.

024 1 INTRODUCTION

025 Score-based diffusion models are a state-of-the-art approach for image synthesis, often outperform-
026 ing alternatives like generative adversarial networks (GANs) and variational autoencoders (VAEs)
027 in sample quality and diversity (Ho et al., 2020; Song & Ermon, 2020). These models learn a neural
028 network by adding noise to data samples during training, according to some forward process. The
029 network can then be used to reverse this process during inference. Essentially, they denoise an image
030 with independent Gaussian pixel values into samples from the data distribution.

031 However, real-world datasets are often corrupted by noise arising from measurement er-
032 rors, compression artifacts, or data collection processes (Gupta & Gupta, 2019; Brummer &
033 De Vleeschouwer, 2019). In this case, standard diffusion models trained directly on noisy data
034 will learn to reproduce this corruption in their generated samples. We aim to address this by de-
035 veloping a method that can generate samples that approximately come from the clean distribution,
036 despite being trained on noisy data.

037 A well-established paradigm for understanding data with a high-dimensional representation is the
038 *manifold hypothesis*: meaningful data distributions are concentrated near a low-dimensional man-
039 ifold embedded in the ambient space (Bengio et al., 2013; Fefferman et al., 2016). For instance,
040 natural images, despite being represented as a d -dimensional array, where d can be in the millions,
041 exhibit intrinsic dimensions that are far lower (Pope et al., 2021). This viewpoint will be the basis
042 of our approach as we interpret noise as low-magnitude variations in directions orthogonal to the
043 manifold, whereas meaningful variations of the underlying data correspond to movements along the
044 manifold itself. The central idea is to exploit this geometric structure during the inference process
045 to suppress the former while preserving the latter.

046 The manifold hypothesis has previously been considered in the context of diffusion models to study
047 their convergence behavior, e.g. in Bortoli (2022), Tang & Yang (2024), and Potaptchik et al. (2024).
048 It has also been argued in Stanczuk et al. (2024) that diffusion models can be leveraged to estimate
049 the intrinsic dimension of data manifolds. Some existing works tackle the problem of noisy training
050 (Daras et al., 2023; Lu et al., 2025), but require adapting the training process. Outside the gen-
051 erative setting, there are also traditional manifold denoising techniques predating diffusion models
052 (Hein & Maier, 2006; Gong et al., 2010; Wang & Carreira-Perpiñán, 2010; Fefferman et al., 2018;
053 Faigenbaum-Golovin & Levin, 2023).

This work introduces *Manifold Attracted Diffusion (MAD)*, an efficiently implementable modification to the inference procedure of score-based models. We define the concept of an “extended score”, which coincides with the standard score when that exists, but is also well-defined for Dirac delta distributions. In fact, it treats them essentially as Gaussians with a certain non-zero variance. This property can be leveraged in the inference procedure to reduce small off-manifold variations to almost zero while leaving larger on-manifold variations mostly unchanged, resulting in a soft thresholding effect. Thereby our method implicitly “attracts” the generated samples towards a low-dimensional structure, effectively filtering out noise. Importantly, a suitable approximation to the extended score can be computed easily from an approximation to the standard score, which enables the use of established training methods as well as pretrained networks under some conditions that are, e.g., satisfied by the framework of Karras et al. (2022). Our key contributions include:

- The formal definition and analysis of the extended score;
- An inference algorithm that reduces noise in generated samples without needing a special training procedure, making it compatible with established frameworks and pretrained models;
- Empirical validation on toy problems and real-world image data, such as FFHQ, AFHQ, ImageNet, and EMPIAR-11618 (cryo electron microscopy data).

We also distinguish our work from other diffusion-based approaches. Methods for posterior sampling, such as DPS (Chung et al., 2023; 2022), are designed to solve inverse problems (Daras et al., 2024), such as denoising a single given image. Our goal is different: we learn from a dataset of noisy images to produce new, clean samples from the underlying distribution.

This paper is structured as follows. In Section 2, we review the necessary background on score-based diffusion models. In Section 3, we formally introduce the extended score and analyze its properties. Section 4 details our proposed inference algorithm and, in Section 5, we present numerical experiments that validate our approach.

2 BACKGROUND

We will be working with the probability flow ODE formulation of diffusion models, largely following the framework of Karras et al. (2022). For more background and the connection to other diffusion model formulations we refer to Karras et al. (2022) and the references therein. Given a data distribution p_0 on \mathbb{R}^d we consider the stochastic process $(X_\sigma)_{\sigma \in [0, \sigma_{\max}]}$ with $X_0 \sim p_0$ and

$$X_\sigma = X_0 + \mathcal{N}(0, \sigma^2 \mathbb{I}), \quad \sigma > 0.$$

The corresponding densities are given by

$$p_\sigma = p_0 * g_{\sigma^2}, \tag{1}$$

where $g_{\sigma^2}(x) = (2\pi\sigma^2)^{-d/2} \exp(-\frac{\|x\|^2}{2\sigma^2})$ is the density of $\mathcal{N}(0, \sigma^2 \mathbb{I})$. The central idea behind score-based diffusion models is to generate a sample $x_0 \sim X_0$ from a sample $x_{\sigma_{\max}} \sim X_{\sigma_{\max}}$, where $x_{\sigma_{\max}}$ is, in practice, approximated by simply sampling from $\mathcal{N}(0, \sigma_{\max}^2 \mathbb{I})$, as for a sufficiently large σ_{\max} this should only introduce a negligible error. One way to achieve this is by evolving the ODE

$$dx_t = -\dot{\sigma}(t)\sigma(t)Sp_{\sigma(t)}(x_t)dt, \tag{2}$$

where $\sigma: [0, T] \rightarrow [0, \sigma_{\max}]$ is some noise schedule and the score operator is given by

$$S: P(\mathbb{R}^d) \rightarrow C(\mathbb{R}^d, \mathbb{R}^d), \quad p \mapsto \nabla_x \log p,$$

where $P(\mathbb{R}^d) := \{p \in C^1(\mathbb{R}^d, \mathbb{R}): \int_{\mathbb{R}^d} p(x) dx = 1, p(x) > 0 \forall x \in \mathbb{R}^d\}$ is the set of densities that are positive everywhere in \mathbb{R}^d . Note that, for $\sigma > 0$, $p_0 * g_{\sigma^2}$ is a density even if p_0 is not. The fact that the score may not be well-defined for p_0 , e.g. because the data distribution is supported on some lower-dimensional subset in \mathbb{R}^d , is avoided in practice by generating a sample x_δ with δ close to 0. It can be shown (Song et al., 2021; Karras et al., 2022) that evolving a sample $x_{t_1} \sim X_{t_1}$ from t_1 to t_2 according to (2) yields a sample $x_{t_2} \sim X_{t_2}$.

Of course, this is only useful provided that we have access to the score, which depends on the data distribution, and from which we usually have only a finite number of samples. Remarkably, it turns

108 out that a useful approximation of the score can be learned by training a neural network on these
 109 samples. A common practice, motivated by numerical stability, is to learn the so-called denoiser
 110 function D , which is simply a shifted and scaled version of the score, i.e. $D(x, \sigma) = \sigma^2 Sp_\sigma(x) + x$.
 111 This denoiser function is then approximated by a neural network D_θ using a loss based on

$$\mathbb{E}_{y \sim X_0} \mathbb{E}_{\eta \sim \mathcal{N}(0, \sigma^2 \mathbb{I})} \|D_\theta(y + \eta) - y\|_2^2$$

114 which is minimized by the denoiser function. However, as the expectation over the data distribution
 115 must be replaced by the empirical expectation based on the available data samples, this loss
 116 has, in general, many global minima. Nonetheless, employing neural networks utilizing an adapted
 117 U-Net architecture (Ronneberger et al., 2015; Ho et al., 2020; Dhariwal & Nichol, 2021) appears to
 118 introduce sufficient bias towards a good approximation of the score. This approximation capability
 119 is primarily founded on the empirical observation that using it to generate images by evolving
 120 equation 2 (or related differential equations) produces realistic samples. An analytical description
 121 of how D_θ approximates D is still an open problem. As the purpose of the work is to introduce a
 122 novel inference procedure, we will simply assume that we can obtain a suitable approximation to
 123 the score by some established training method.

124 3 CONCEPT: THE EXTENDED SCORE

126 Let $M(\mathbb{R}^d)$ denote the set of probability measures on \mathbb{R}^d .

128 **Definition 3.1** (Extended score). *For $d \in \mathbb{R}^d$, $p \in M(\mathbb{R}^d)$, $\gamma \in (0, \infty)$, let*

$$129 \quad H_\gamma: M(\mathbb{R}^d) \rightarrow C(\mathbb{R}^d, \mathbb{R}^d), \quad p \mapsto (1 + \gamma)S(p * g_\gamma) + \gamma \frac{d}{d\gamma} S(p * g_\gamma)$$

131 and

$$132 \quad H_0: \widetilde{M}(\mathbb{R}^d) \rightarrow \{f: \mathbb{R}^d \rightarrow \mathbb{R}^d\}, \quad p \mapsto \lim_{\gamma \rightarrow 0} H_\gamma p,$$

134 where $\widetilde{M}(\mathbb{R}^d) := \{p \in M(\mathbb{R}^d): \lim_{\gamma \rightarrow 0} (H_\gamma p)(x) \in \mathbb{R}^d \forall x \in \mathbb{R}^d\}$.

136 We first note that H_0 coincides with the score for probability distributions with density in $P(\mathbb{R}^d)$,
 137 which we can view as a subset of $M(\mathbb{R}^d)$ by identifying a density function $p \in P(\mathbb{R}^d)$ with the
 138 measure given by $p(A) = \int_A p(x)dx$ for $A \subseteq \mathbb{R}^d$ (see Section A.2 for a proof).

139 **Lemma 3.2.** *Let $p \in P(\mathbb{R}^d)$. Then $H_0 p = Sp$.*

140 It is, however, also well-defined for, e.g., Dirac delta measures. Specifically, let δ denote the Dirac
 141 delta at 0, then

$$143 \quad H_\gamma \delta(x) = (1 + \gamma)S(g_\gamma)(x) + \gamma \frac{d}{d\gamma} S(g_\gamma)(x) = -\frac{(1 + \gamma)x}{\gamma} + \gamma \frac{d}{d\gamma} \left(-\frac{x}{\gamma}\right) = -x.$$

145 In particular it holds that $H_0 \delta(x) = -x$, i.e. we obtain¹ a function which, similar to the score for
 146 Gaussians, yields at each point a vector pointing towards the mode of the probability distribution.
 147 This generalizes to mixtures of Dirac delta distributions, where $H_0 p$ will point towards the location
 148 of the nearest Dirac delta in the mixture (see Section A.2 for a proof).

149 **Lemma 3.3.** *Let $n \in \mathbb{N}$, $\mu_1, \dots, \mu_n \in \mathbb{R}^d$, $c_1, \dots, c_n \in \mathbb{R}_+$ such that $\sum_i c_i = 1$ and $p =$
 150 $\sum_{i \in [n]} c_i \delta_{\mu_i}$. Then*

$$153 \quad H_0 p(x) = - \sum_{i \in [n]} z_i(x)(x - \mu_i),$$

155 where $W_i = \{x \in \mathbb{R}^d: \|x - \mu_i\| \leq \|x - \mu_j\| \forall j \in [n]\}$ is a Voronoi region and

$$157 \quad z_i(x) = \begin{cases} 0 & x \notin W_i, \\ 1 & x \in \text{int } W_i, \\ c_i \left(\sum_{j: x \in W_j} c_j\right)^{-1} & x \in \partial W_i. \end{cases}$$

161 ¹Note that in this simple case, $H_\gamma \delta$ is already the same as $H_0 \delta$, which is not the case in more complicated
 scenarios, e.g. for mixtures of Dirac deltas.

162 Note that the first two cases in the expression for $z_i(x)$ cover almost every (w.r.t the Lebesgue
 163 measure) $x \in \mathbb{R}^d$ and the third case is only needed if x is equally distant to multiple μ_i .

164 By combining the expressions of the extended score for a Dirac delta and for a non-degenerate
 165 Gaussian distribution, it is possible to derive an explicit expression of the extended score for any
 166 (possibly degenerate) Gaussian distribution. This is achieved by exploiting how the extended score
 167 behaves with respect to products of measures, see Appendix A.1 for the details.

168 We have the rather peculiar property that $H_0\delta = Sg_1$, i.e. the extended score of the Dirac delta
 169 matches the score of a variance 1 Gaussian. At this point, it should be noted that it is impossible to
 170 find a nice extension of the score operator that includes Dirac delta distributions, as

$$172 \quad Sg_\gamma(x) = -\frac{x}{\gamma},$$

173 which diverges for $x \neq 0$ as $\gamma \rightarrow 0$. As such any extension is necessarily discontinuous with respect
 174 to any topology in which $\lim_{\gamma \rightarrow 0} g_\gamma = \delta$.

175 However, the ability of the extended score to treat distributions with positive variance like they
 176 were Dirac delta distributions will, in fact, be the cornerstone of our proposed inference technique.
 177 Under the manifold hypothesis, the clean data distribution has significant variation only along a
 178 small number of directions. Given noise in the ambient pixel space, which has a much higher
 179 dimension than the image manifold, the variance in off-manifold directions due to noise should
 180 be much smaller (e.g. for isotropic Gaussian noise η the variance in each direction is of order $\sim d^{-\frac{1}{2}}\mathbb{E}[\|\eta\|]$). Thus, noise can be suppressed by using the extended score. **This principle is formally
 181 justified in Appendix A.1, where we derive the extended score for a distribution supported on a low-
 182 dimensional subspace and show that it strongly attracts samples in the off-manifold directions while
 183 preserving the standard score in the on-manifold directions.**

184 4 IMPLEMENTATION

185 In view of the property of the extended score just discussed, we would like to design an inference
 186 procedure that is able to generate samples with less noise, if compared to the samples obtained via
 187 the usual score. To this end we first note that, due to (1), we have

$$188 \quad S(p_{\sigma(t)} * g_\gamma) = S(p_0 * g_{\sigma(t)^2} * g_\gamma) = S(p_0 * g_{\sigma(t)^2 + \gamma}) = S(p_{\sqrt{\sigma(t)^2 + \gamma}}).$$

189 So, given a network trained to approximate the score for any $\sigma \in [0, \sigma_{\max}]$, as is the case in the
 190 framework of Karras et al. (2022), we also have an approximation to the extended score with a given
 191 small $\gamma > 0$, where the γ -derivative can be obtained, e.g., by a finite difference² approximation. As
 192 the desirable properties of the extended score hold in the $\gamma \rightarrow 0$ limit, which we cannot compute
 193 directly, we instead need to choose a suitable dependence $\gamma(t)$ with $\lim_{t \rightarrow 0} \gamma(t) = 0$.

194 A basic way to conduct inference with the standard score is evolving (2) simply via Euler method,
 195 i.e. initializing with $x_0 \sim \mathcal{N}(0, \sigma(t_0)^2 \mathbb{I})$ and iterating

$$196 \quad x_{i+1} = x_i - (t_{i+1} - t_i) \dot{\sigma}(t_i) \sigma(t_i) S_\theta(\sigma(t_i), x_i), \quad (3)$$

197 where $S_\theta(\sigma, x) \approx Sp_\sigma(x)$ is the learned approximation of the score. We will instead, based on
 198 Definition 3.1, consider the iteration

$$199 \quad x_{i+1} = x_i - m(t_i)(t_{i+1} - t_i) \dot{\sigma}_\gamma(t_i) \sigma_\gamma(t_i) \left((1 + \gamma(t_i)) S_\theta(\sigma_\gamma(t_i), x_i) + \gamma(t_i) \frac{d}{d\gamma} S_\theta(\sigma_\gamma(t_i), x_i) \right), \quad (4)$$

200 where $\sigma_\gamma(t) = \sqrt{a\sigma(t)^2 + b\gamma(t)}$, $a, b > 0$ are manually chosen parameters, and $m(t_i)$ is a cor-
 201 rection factor determined as explained below. Note that this reduces to (3) for $a = 1$, $b = 0$, and
 202 $m(t) = (1 + \gamma(t))^{-1}$, so essentially the choices of a , b , and m determine to what extent we would
 203 like the inference to push points onto a manifold at a given time step. **More precisely, increasing
 204 a or reducing b corresponds to lessening the effect of the extended score and thereby limiting the
 205 denoising effect. Conversely, reducing a or increasing b yield a stronger denoising effect. As such,
 206 a and b can be seen as regularization parameters, and their choice is problem dependent. While in**

207 ²Note that one could also compute the exact derivative of the score network using automatic differentiation
 208 (AD). However, since PyTorch is not optimized for forward mode AD this is significantly more expensive than
 209 a second evaluation of the network and did not yield any clear improvements in the numerical experiments.

the idealized case of the $\gamma \rightarrow 0$ limit, analyzed in Section 3, Diracs and variance 1 Gaussians are treated in the same way, the choice of a and b adjusts this equivalence in practice, causing variations below this (soft) threshold to be compressed significantly. Note that we currently do not determine the explicit dependence of this threshold on the parameters. However, since we cannot expect to know the optimal threshold for a data distribution in practice, a parameter optimization seems unavoidable anyway. We further enforce $\sigma_\gamma(t) = t$ to match the scheduling of Karras et al. (2022), as it allows us to take advantage of their optimized choice of time steps and leads to better comparability. Lastly, we introduce a parameter $p > 0$ to regulate the relative speed of convergence of σ and γ via $\gamma(t) = \sigma(t)^p$.

With these choices, (4) simplifies to

$$x_{i+1} = x_i - m(t_i)(t_{i+1} - t_i)t_i((1 + \gamma(t_i))S_\theta(t_i, x_i) + \frac{b\gamma(t_i)}{2t_i} \frac{d}{d\sigma} S_\theta(t_i, x_i)), \quad (5)$$

where $\frac{d}{d\sigma} S_\theta$ denotes the derivative of $S_\theta: [0, \sigma_{\max}] \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ w.r.t its first argument, and $\gamma(t_i)$ is a solution of

$$\sqrt{a\gamma(t_i)^{\frac{2}{p}} + b\gamma(t_i)} = t_i.$$

We observe that in the case of $S_\theta(\sigma, x) = -\frac{x-\mu}{\sigma^2}$, which corresponds to an initial distribution consisting of a Dirac delta at μ , the standard score inference rule (3) with $\sigma(t) = t$ evaluates to

$$x_{i+1} = x_i - \frac{t_i - t_{i+1}}{t_i}(x_i - \mu) = (1 - \frac{t_i - t_{i+1}}{t_i})x_i + \frac{t_i - t_{i+1}}{t_i}\mu. \quad (6)$$

This means that, if $\frac{t_i - t_{i+1}}{t_i} \geq \Delta > 0$ for every i , we have

$$\|x_{i+k} - \mu\| \leq (1 - \Delta)^k \|x_i - \mu\|,$$

i.e. convergence to μ at a geometric rate. We would like our inference rule to mimic this behavior for simple Dirac deltas, which is accomplished by choosing the correction factor as

$$m(t_i) = \left(1 + \gamma(t_i) - \frac{b\gamma(t_i)}{t_i^2}\right)^{-1}, \quad (7)$$

see Section A.2 in the appendix for a detailed derivation. Note that, as long as $\gamma(t_i) \in o(t_i^{-2})$ we have $\lim_{t \rightarrow 0} m(t) = 1$. Putting it all together, we arrive at the following algorithm.

Algorithm 1 Inference with extended score

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1: function INFERENCE( $S_\theta, a, b, p, \delta, (t_i)_{i \in \{0, \dots, N\}}$ )
2:   sample  $x_0 \sim \mathcal{N}(0, t_0^2 \mathbb{I})$  ▷ Generate Gaussian sample
3:   for  $i \in \{0, \dots, N - 1\}$  do
4:      $\gamma_i = \mathbf{solve}(a\gamma_i^{2/p} + b\gamma_i - t_i^2 = 0)$  ▷ Determine  $\gamma_i$  using a root finding algorithm
5:      $s_i = S_\theta(t_i, x_i)$  ▷ Evaluate the score network
6:      $\tilde{s}_i = S_\theta((1 + \delta)t_i, x_i)$ 
7:      $s'_i = \frac{\tilde{s}_i - s_i}{\delta t_i}$  ▷ Compute an approximation to the derivative
8:      $m_i = (1 + \gamma_i - \frac{b\gamma_i}{t_i^2})^{-1}$  ▷ Compute correction factor
9:      $x_{i+1} = x_i - m_i(t_{i+1} - t_i)t_i((1 + \gamma_i)s_i + \frac{b\gamma_i}{2t_i}s'_i)$  ▷ Update sample
10:   return  $x_N$ 

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5 NUMERICAL EXPERIMENTS

In section 5.1 (toy examples in \mathbb{R}^2) and in section 5.2 (FFHQ, AFHQv2, and ImageNet) we present some illustrative numerical simulations to build intuition of the “manifold attraction” property of the extended score on clean datasets. Further, in sections 5.3 (synthetic dataset) and 5.4 (CIFAR-10) we provide controlled experiments showing qualitatively and quantitatively (FID scores) the denoising effect of the extended score. Finally, in section 5.5 we test MAD with real Cryo-EM data.

We emphasize that MAD addresses a specific blind generative denoising task where only noisy data is available, and the specific degradation model may be unknown. In this context, there are no established benchmarks, and a comparison with other (non-generative) manifold denoising approaches would not be meaningful, because they tackle a different problem.

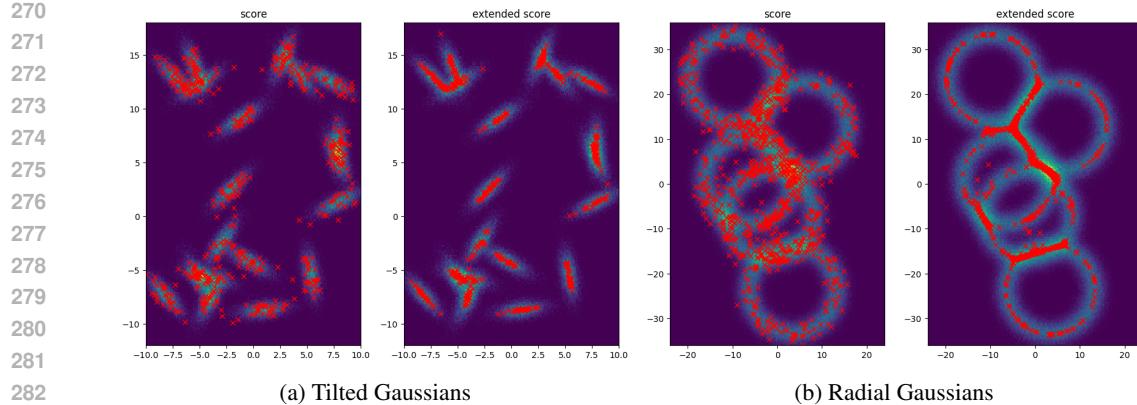


Figure 2: Target distribution is displayed as a histogram colormap. Red crosses indicate samples generated either via standard score inference (left) or extended score inference (right). Extended score parameters are $p = 1.3$, $a = 1$, $b = 1.1$ for (a) and $p = 2$, $a = 2$, $b = 30$ for (b).

5.1 ILLUSTRATIVE EXAMPLES IN \mathbb{R}^2

We visualize the evolution according to the extended score in \mathbb{R}^2 for relatively simple distributions, where the (extended) score can be computed explicitly (see Appendix A.1). Figure 1 displays the inference trajectories for a degenerate Gaussian mixture, which behaves like a Dirac delta at 0 in the x_2 -direction and a Gaussian in the x_1 -direction as the means are chosen such that the different mixture components affect each other very little. We can see that for the Gaussians with variances 0.2 and 0.5 respectively, using the extended score causes all trajectories to end up at the respective means, i.e. it behaves as if we had Dirac deltas (in the x_1 -direction) at these locations. For the higher variance Gaussians the extended score trajectories still end up closer to the mean than they would for standard score, but this variance reduction effect decreases significantly as the variance of the Gaussians increases. All together, we essentially have a soft thresholding effect, where variances below a certain value are shrunk to 0, while large enough variances are left almost unchanged.

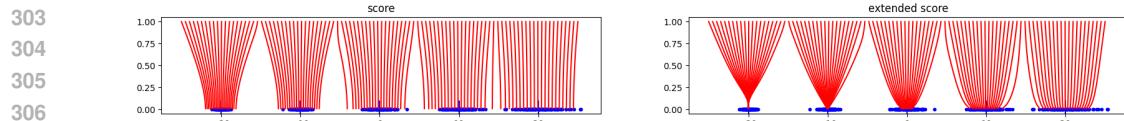
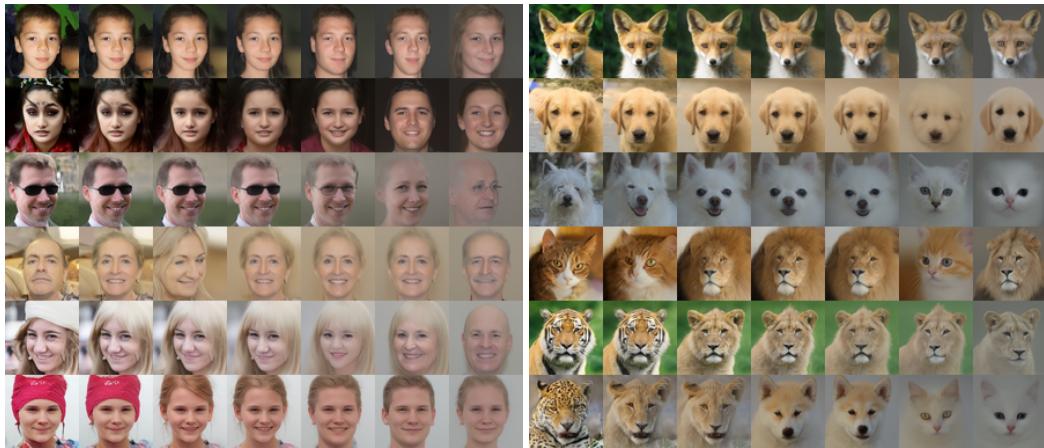


Figure 1: Comparison of inference trajectories (red) and samples (blue) for Gaussian mixture $p(x_1, x_2) = \delta(x_2) \sum_{i=1}^5 \frac{1}{5} (2\pi v_i)^{-\frac{1}{2}} \exp\left(-\frac{(x_1 - \mu_i)^2}{2v_i}\right)$ with equal weights, variances $v = (0.2, 0.5, 1, 2, 4)$, and means $\mu = (-20, -10, 0, 10, 20)$. Extended score is applied with parameters $a = b = n = 1$.

In Figure 2a we consider a mixture of Gaussians with covariance matrices $\Sigma_i = R_i \text{diag}(1.7, 0.2)$, where the R_i , $i \in \{1, \dots, 21\}$, are randomly chosen rotation matrices, i.e. around each mean of the mixture we have large variance in one direction and small variance in the direction orthogonal to the first one. Locally this can be viewed as a 1.5-variance Gaussian along some 1-dimensional affine linear subspace to which Gaussian noise with covariance matrix $0.2\mathbb{I}$ is added, resulting in a 1.7 variance in one direction and a 0.2 variance in the other. The denoising effect is clear: the extended score inference moves the points onto the affine linear subspace corresponding to the first principal direction of each Gaussian, while leaving the spread along the affine linear subspace almost unchanged. In Figure 2b we demonstrate that this effect is not limited to affine linear manifolds, by considering a mixture of radial Gaussians of the form $p(x) = C \sum_{i=1}^5 \exp\left(-\frac{\|x - \mu_i\| - r}{2v}\right)$ with variance $v = 2.5$, radius $r = 10$, randomly chosen means μ_i , and C a normalizing constant.

324 5.2 EFFECTS ON FFHQ, AFHQv2, AND IMAGENET
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326
327 While the last section provides some basic intuition for the effects of our inference method, it is,
328 of course, not so clear how this translates to much more complicated distributions in much higher
329 dimensions. We will explore this question using our inference method with the pretrained score
330 networks from Karras et al. (2022) for³ FFHQ (Karras et al. (2019)), AFHQv2 (Choi et al. (2020)),
331 and ImageNet (Deng et al. (2009)), where we also use the time schedule suggested in Karras et al.
332 (2022), and only vary the hyperparameters specific to our method, i.e. a , b , p , and δ in Algorithm 1.
333 Since these datasets are arguably essentially noiseless, the effect of the extended score will be visible
334 on the different features of the images. The following two sections consider noisy datasets.
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336



352 Figure 3: In both subfigures, all images in each row start from the same latent noise sample, and
353 the leftmost column uses standard score whereas second to last columns use Algorithm 1 with $\delta =$
354 0.0001 , $p = 8$, $a = 2.5$, and, left to right, $b \in \{2, 5, 10, 20, 40, 80\}$. Further examples in Figure 10.
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358 In Figure 3, we showcase the impact of our inference methods on the generation of human or animal
359 faces using the pretrained score networks for FFHQ and AFHQv2, respectively. Note that increasing
360 the parameter b in Algorithm 1 results in a greater impact of the extended score, i.e. we expect
361 stronger attraction to the manifold of primary variation. We observe that for all values of b , we
362 generate samples with qualitatively the same facial features, but for larger values of b , we always get
363 a plain single-colored background. In case of faces, it seems quite clear that the direction of primary
364 relevance should correspond to essential facial features that are present in all the data, whereas the
365 background variation, as well as features like glasses and head wear, are split across a much larger
366 number of directions and are thresholded out first. We also observe similar effects on ImageNet,
367 e.g. in the examples in Figure 4, where the extended score inference seems to focus on generating
368 one primary object, while progressively thresholding out everything else as we increase b . However,
369 since ImageNet contains a large variety of objects, the primary directions differ between classes,
370 and thus the effect of extended score inference with a given choice of hyperparameters is much
371 more varied across different starting noise images (see Figure 11 in the Appendix).

372 Although Algorithm 1 is deterministic when started with the same random seed, i.e. such that it starts
373 from the same latent noise image, it relies on a score network trained through a highly stochastic
374 process. Consequently, even small changes of the iterates x_i can build up and lead to the genera-
375 tion of a significantly different image. As can be seen in Figure 3, in general the algorithm is not
376 particularly suited for orthogonal projection on the manifold of, in this case, faces, i.e. it does not
377 simply generate the same face as standard inference would but without background. However, as
378 showcased in Figure 9 in the Appendix, there are often certain ranges of parameters that lead to
379 rather similar images and may be used for manual adjustment of a generated image.



Figure 4: Each row starts from the same latent noise sample, and the leftmost column uses standard score whereas second to last columns use Algorithm 1 with $\delta = 0.001$, $p = 12$, and $a = 8$, $b \in \{5, 20, 50, 80, 250\}$ for the top row, $a = 4$, $b \in \{2, 10, 30, 60, 100\}$ for the bottom row.

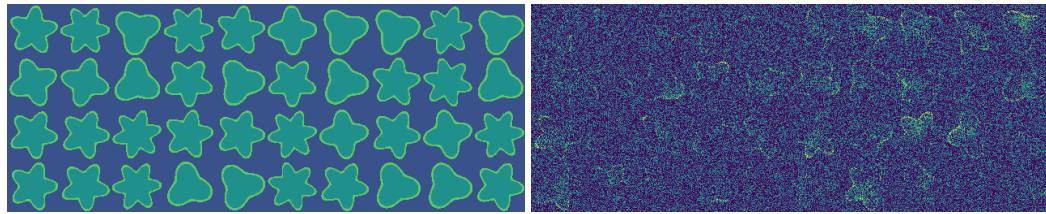


Figure 5: Grid of clean samples from the synthetic data set (left); grid of corresponding noisy samples (right). Each sample is an 8-bit grayscale 64×64 image, displayed via viridis colormap.

5.3 DENOISING SYNTHETIC DATA

We created a synthetic dataset of clean samples, added noise, and trained a diffusion model only on the noisy data. Our clean distribution consists of 8-bit grayscale 64×64 images depicting 4 different shapes, each appearing with equal probability and rotated by an angle chosen uniformly at random (see Figure 5, left). As such, this probability distribution is essentially supported on 4 disjoint 1-dimensional manifolds in pixel space. We then add two types of corruption to obtain noisy samples. Firstly, we blot out large parts of the shape, by uniformly randomly picking 50 locations on the boundary of the shape and subtracting Gaussian bump functions centered at those locations from the clean image. Secondly, we add i.i.d. Gaussian noise to each pixel, resulting in images where the original shapes can hardly be discerned from a single image (see Figure 5, right). We then trained a DDPM++ model⁴ on a set of 100 000 of such noisy samples for a duration of 3 mimg, i.e. 30 repeats per image. When using the trained network for standard score inference we obtain a reproduction of the corrupted samples (see Figure 6, right). In contrast, running our extended score inference, we obtain samples showing the original shapes (see Figure 6, left). Figure 12 in the Appendix illustrates the dependence on the extended score parameters δ , a , b , and p . In order to test whether our method works on corrupted training data beyond the case of Gaussian noise, we also trained a DDPM++ model, using the same training settings, on a set of 100 000 synthetic samples, where each pixel was set to 0 with probability 0.5 (see Figure 14 in Appendix A.3). As can be seen in Table 1, for both cases extended score inference leads to a significant improvement in FID compared to the standard score, which generates samples with essentially the same distance to the clean data as the noisy data.

5.4 DENOISING CIFAR-10

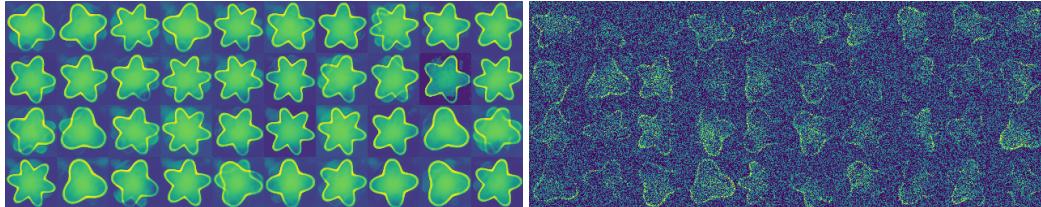
Next, we test whether the denoising capabilities of our method extend to real data. Specifically we train a DDPM++ model on CIFAR-10 with additive Gaussian noise. While standard score inference

³Note that these networks have been trained on images from these datasets which have been downsampled to a 64×64 resolution.

⁴Using the method from the accompanying github to Karras et al. (2022) with default settings except for cond = 0 and augment = 0, which took roughly 14 hours on a single A100 GPU.

Noisy dataset	training data	standard generation	extended generation
CIFAR-10, Gaussian noise	136.87	147.47	77.15
synthetic data, Gaussian noise	320.56	319.42	189.51
synthetic data, pixel removal	233.86	234.40	163.14

436

437 Table 1: FIDs with respect to the corresponding clean dataset, computed from 10 000 images.
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449 Figure 6: Grid of samples generated from consecutive random seeds by Algorithm 1 with parameters
delta = 0.02, p = 8, a = 0.002, and b = 15 (left); grid of samples generated by inference with standard
score (right). Each sample is an 8-bit grayscale 64×64 image, displayed via viridis colormap.450
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458 Figure 7: Trained on CIFAR-10 with additive Gaussian noise and generated by standard score infer-
ence (right) or by extended score inference (left).462
463 produces image with roughly the amount of noise of the images it was trained on, extended score
464 inference produces significantly cleaner images, both visually (Figure 7) as well as in the FID scores
465 (Table 1). The intermediate images generated during inference (see Figure 15 in Appendix A.3)
466 strongly indicate that this effect cannot simply be achieved by truncated sampling.

467

468 5.5 DENOISING REAL DATA

469
470 In this section we test our method on real data from single-particle Cryo-Electron Microscopy (see
471 Cheng et al. (2015) for an introduction), where many particles of the same type are suspended in liq-
472 uid, frozen, and put under an electron microscope. This produces extremely noisy 2D-images which
473 need to be refined before further steps like 3D reconstruction can be attempted. This presents an op-
474 portunity to investigate the performance of our method on practically relevant real world data with
475 non-Gaussian noise. We use the EMPIAR-11618 (Bacic et al., 2021) dataset of 68 401 grayscale
476 images with 256×256 resolution. They were extracted from raw data and undergone some prepro-
477 cessing, but are still very noisy (see Figure 8, top left). We trained a DDPM++ model⁵ on this data
478 and used our method to generate samples (see Figure 8, right) whose shapes correspond strongly to
479 what has been obtained by Bacic et al. (2021), see Figure 8, bottom. We emphasize that the net-
480 work has only ever seen noisy data and has in no way been specifically adjusted based on a priori
481 knowledge of these shapes. This can be seen by the fact that standard score inference generates
482 noisy samples, very similar to those in the training set (see Figure 16 in the Appendix). The pa-
483 rameters used for Figure 8 of the extended score inference have been determined by hand with such
484 knowledge, of course, but similar results are generated for a wide range of parameter choices (see485
486 ⁵In order to compensate for the higher resolution we reduced the number of feature channels in the ddpmpp
487 architecture from 128 to 32, but otherwise used the same settings as for the synthetic data. Training took
488 roughly 60 hours on two A100 GPUs.

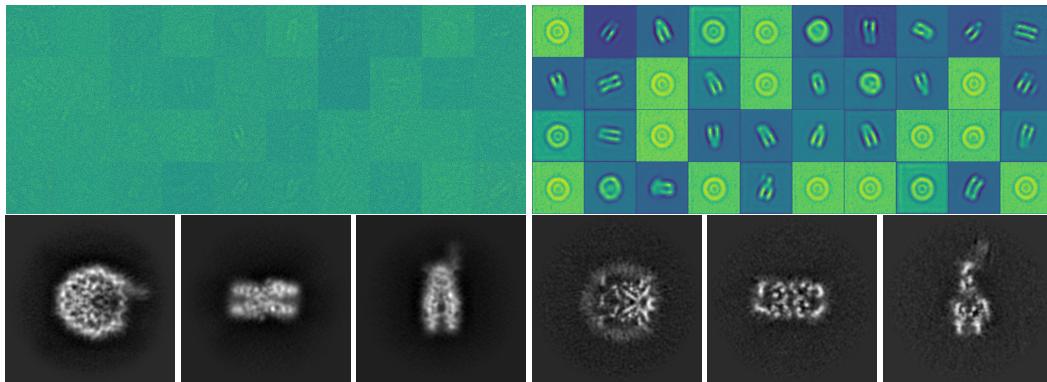


Figure 8: Images from the EMPIAR-11618 dataset (left). Samples generated by Algorithm 1 with parameters $\delta = 0.001$, $p = 8$, $a = 0.01$, and $b = 2$ (right). Shapes obtained by Bacic et al. (2021) (bottom), taken from (wwPDB Consortium, 2023, EMD-17944). The colormap is applied with normalization per image to enhance contrast.

Figure 13 in the Appendix). In particular, this demonstrates a significant capability of the extended score to guide generation towards samples from the underlying image manifold, also in the case of real data with extreme noise corruption caused by physical measurement modalities. This example serves as proof of concept for the validation of our approach: reaching state-of-the-art performance is outside the scope of this work, and would require incorporating more prior domain knowledge.

6 CONCLUSION

We introduced Manifold Attracted Diffusion (MAD), a novel inference approach for score-based diffusion models to generate clean samples from a distribution despite training on noisy datasets. Based on the manifold hypothesis, our method utilizes the underlying geometry to suppress off-manifold variations while preserving on-manifold variations, which results in attracting samples toward a low-dimensional structure. It can leverage established training algorithms and pretrained models. The required computation cost is **at most** twice that of standard inference, due to requiring a second evaluation of the score network. **However, we observed empirically that it is enough to use the extended score only in the last half of the inference steps, yielding an additional computational cost of 50%, but additional investigation on this aspect is required.** Numerical experiments on both synthetic and real data demonstrate that MAD successfully suppresses noise.

Future directions include extending MAD to solve inverse problems, as in Cryo-EM for denoising individual images, or for other denoising or image restoration tasks. This would benefit from integration with conditional diffusion models, as explored in diffusion posterior sampling frameworks (Chung et al., 2023; 2022). Developing automatic and adaptive parameter selection for $\gamma(t)$ would enhance the methods robustness and applicability. Further theoretical analysis of the extended score may lead to an improved incorporation into the inference procedure, in particular one could combine it with inference techniques using noise injection or higher order ODE discretization schemes. Future work should also involve a rigorous quantitative study comparing the performance and computational trade-offs of MAD against training-time methods, finetuning on limited clean data, and other relevant inference-time baselines such as truncated sampling (Daras et al., 2025). Furthermore, it would be valuable to investigate whether the MAD framework could be adapted to time-unconditioned generative models (Sun et al., 2025), or if our method fundamentally relies on a time-dependent score. Finally, a promising future direction, motivated by the conceptual similarities to classifier-free guidance (Ho & Salimans, 2021), is to explore whether our extended score can serve as a more interpretable, geometrically-grounded method for improving general generation quality, even for models trained on clean data.

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663 A APPENDIX

664 A.1 THE EXTENDED SCORE FOR PRODUCTS OF MEASURES

665 In the following lemma, we derive the expression of the extended score of the product of two mea-
 666 sures. In this section, the superscripts denote the dimension of the domain.

667 **Lemma A.1.** *Let $d_1 + d_2 = d$. Take $p_1 \in \widetilde{M}(\mathbb{R}^{d_1})$ and $p_2 \in \widetilde{M}(\mathbb{R}^{d_2})$. Then the product measure
 668 $p = p_1 \otimes p_2$ belongs to $\widetilde{M}(\mathbb{R}^d)$ and*

$$669 H_0^d p(x) = (H_0^{d_1} p_1(x_1), H_0^{d_2} p_2(x_2)),$$

670 where $x = (x_1, x_2) \in \mathbb{R}^{d_1+d_2}$.

671 *Proof.* We have that $g_\gamma^d(x) = g_\gamma^{d_1}(x_1)g_\gamma^{d_2}(x_2)$. Thus, by Fubini’s theorem, we have

$$672 (p * g_\gamma^d)(x) = (p_1 * g_\gamma^{d_1})(x_1) \cdot (p_2 * g_\gamma^{d_2})(x_2).$$

673 Thus

$$674 \log(p * g_\gamma^d)(x) = \log(p_1 * g_\gamma^{d_1})(x_1) + \log(p_2 * g_\gamma^{d_2})(x_2).$$

675 Taking a gradient with respect to x we obtain

$$676 S^d(p * g_\gamma^d)(x) = (S^{d_1}(p_1 * g_\gamma^{d_1})(x_1), 0_{d_2}) + (0_{d_1}, S^{d_2}(p_2 * g_\gamma^{d_2})(x_2)).$$

677 Therefore, since the expression of $H_\gamma^d(p)$ is linear in $S^d(p * g_\gamma^d)$, we obtain

$$678 H_\gamma^d(p)(x) = (H_\gamma^{d_1}(p_1)(x_1), 0_{d_2}) + (0_{d_1}, H_\gamma^{d_2}(p_2)(x_2)) = (H_\gamma^{d_1}(p_1)(x_1), H_\gamma^{d_2}(p_2)(x_2)).$$

679 Taking the limit as $\gamma \rightarrow 0$, the result follows. \square

680 This result can be used to calculate the extended score of a degenerate distribution p , namely, a
 681 distribution supported on a lower-dimensional affine subspace of \mathbb{R}^d . Since the score, and thus the
 682 extended score, is equivariant with respect to rotations and translations, without loss of generality,
 683 we can assume that p is supported on $\{(x_1, 0_{d_2}) \in \mathbb{R}^d : x_1 \in \mathbb{R}^{d_1}\}$ with density $p_1 \in P(\mathbb{R}^{d_1})$,
 684 namely,

$$685 p = p_1 \otimes \delta_{d_2},$$

686 where $\delta_{d_2} \in \widetilde{M}(\mathbb{R}^{d_2})$ is the Dirac delta centered at 0 in \mathbb{R}^{d_2} . By Lemmata 3.2 and A.1, we obtain
 687 that the extended score of p is given by

$$688 H_0^d p(x) = (H_0^{d_1} p_1(x_1), H_0^{d_2} p_2(x_2)) = (S^{d_1} p_1(x_1), -x_2),$$

702 where we have also used that $H_0\delta(x) = -x$.
 703

704 In the particular case when p_1 is a non-degenerate Gaussian distribution on \mathbb{R}^{d_1} with mean $\mu_1 \in \mathbb{R}^{d_1}$
 705 and covariance $\Sigma_1 \in \mathbb{R}^{d_1 \times d_1}$, namely $p_1 = \mathcal{N}(\mu_1, \Sigma_1)$, we have

$$706 H_0^d p(x) = (-\Sigma_1^{-1}(x_1 - \mu_1), -x_2).$$

707 As expected, this coincides with the standard score of the (non-degenerate) Gaussian distribution
 708 $\mathcal{N}(\mu_1, 0_{d_2}), \Sigma)$ on \mathbb{R}^d , where Σ is the block matrix given by
 709

$$710 \Sigma = \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \mathbb{I}^{d_2} \end{bmatrix}.$$

713 A.2 PROOFS AND DERIVATIONS

715 *Proof of Lemma 3.2.* By standard properties of approximate identities (Grafakos, 2014, Exam-
 716 ple 1.2.17 and Theorem 1.2.19(2)), for $f \in C(\mathbb{R}^d)$ bounded we have that

$$717 \lim_{\gamma \rightarrow 0} (f * g_\gamma)(x) = f(x), \quad x \in \mathbb{R}^d,$$

719 Analogously, with $h_\gamma(x) := \frac{1}{\gamma} \|x\|^2 g_\gamma(x)$ by (Grafakos, 2014, Theorem 1.2.21(b)) we get that
 720

$$721 \lim_{\gamma \rightarrow 0} (f * h_\gamma)(x) = Cf(x), \quad x \in \mathbb{R}^d,$$

723 where $C = \int_{\mathbb{R}^d} (2\pi)^{-\frac{d}{2}} \|z\|^2 e^{-\frac{\|z\|^2}{2}} dz < \infty$. In addition, we observe that
 724

$$725 \frac{\partial}{\partial x_i} g_\gamma(x) = -\frac{x_i}{\gamma} g_\gamma(x)$$

726 and

$$728 \frac{d}{d\gamma} g_\gamma(x) = \left(\frac{-d}{2\gamma} + \frac{\|x\|^2}{2\gamma^2}\right) g_\gamma(x) = \frac{1}{2\gamma} (h_\gamma(x) - dg_\gamma(x)).$$

730 Consequently, as $p(x) > 0$ for all $x \in \mathbb{R}^d$, by assumption

$$\begin{aligned} 732 \lim_{\gamma \rightarrow 0} \gamma \frac{d}{d\gamma} S(p * g_\gamma) &= \lim_{\gamma \rightarrow 0} \gamma \frac{d}{d\gamma} \frac{\nabla_x(p * g_\gamma)}{p * g_\gamma} = \lim_{\gamma \rightarrow 0} \gamma \frac{d}{d\gamma} \frac{\nabla_x p * g_\gamma}{p * g_\gamma} \\ 733 &= \lim_{\gamma \rightarrow 0} \gamma \frac{(p * g_\gamma)(\nabla_x p * \frac{d}{d\gamma} g_\gamma) - (\nabla_x p * g_\gamma)(p * \frac{d}{d\gamma} g_\gamma)}{(p * g_\gamma)^2} \\ 734 &= \lim_{\gamma \rightarrow 0} \frac{(p * g_\gamma)((\nabla_x p * h_\gamma) - d(\nabla_x p * g_\gamma)) - (\nabla_x p * g_\gamma)((p * h_\gamma) - d(p * g_\gamma))}{2(p * g_\gamma)^2} \\ 735 &= \frac{p(C\nabla_x p - d\nabla_x p) - \nabla_x p(Cp - dp)}{2p^2} \\ 736 &= 0. \end{aligned}$$

742 Moreover, it holds that

$$744 \lim_{\gamma \rightarrow 0} S(p * g_\gamma) = \lim_{\gamma \rightarrow 0} \frac{\nabla_x(p * g_\gamma)}{p * g_\gamma} = \frac{\lim_{\gamma \rightarrow 0} \nabla_x p * g_\gamma}{\lim_{\gamma \rightarrow 0} p * g_\gamma} = \frac{\nabla_x p}{p} = Sp,$$

746 which completes the proof. \square
 747

748 *Proof of Lemma 3.3.* We write $h_i(x) := c_i e^{-\frac{\|x - \mu_i\|^2}{2\gamma}}$, i.e. $p * g_\gamma = \sum_{i \in [n]} (2\pi\gamma)^{-\frac{d}{2}} h_i$, and observe
 749 that
 750

$$751 S(p * g_\gamma)(x) = - \sum_{i \in [n]} \frac{x - \mu_i}{\gamma} w_i(x),$$

753 where

$$755 w_i := \frac{h_i}{\sum_{j \in [n]} h_j}.$$

756 We observe that

$$758 \frac{d}{d\gamma} w_i(x) = \frac{(\sum_{j \in [n]} h_j(x))^{\frac{\|x - \mu_i\|^2}{2\gamma^2}} h_i(x) - h_i(x) \sum_{j \in [n]} \frac{\|x - \mu_j\|^2}{2\gamma^2} h_j(x)}{(\sum_{j \in [n]} h_j(x))^2}$$

760 and

$$762 H_\gamma p(x) = (1 + \gamma)S(p * g_\gamma)(x) + \gamma \frac{d}{d\gamma} S(p * g_\gamma)(x) = \gamma S(p * g_\gamma)(x) + \frac{d}{d\gamma} \gamma S(p * g_\gamma)(x).$$

764 We will first show that the second term vanishes for $\gamma \rightarrow 0$. To this end, we note

$$766 \frac{d}{d\gamma} \gamma S(p * g_\gamma)(x) = - \sum_{i \in [n]} (x - \mu_i) \frac{(\sum_{j \in [n]} h_j(x))^{\frac{\|x - \mu_i\|^2}{2\gamma^2}} h_i(x) - h_i(x) \sum_{j \in [n]} \frac{\|x - \mu_j\|^2}{2\gamma^2} h_j(x)}{(\sum_{j \in [n]} h_j(x))^2}$$

$$769 = - \frac{\sum_{i, j \in [n]} h_i(x) h_j(x) (x - \mu_i) (\|x - \mu_i\|^2 - \|x - \mu_j\|^2)}{2\gamma^2 (\sum_{j \in [n]} h_j(x))^2}.$$

772 Let $x \in W_k$ and $i, j \in [n]$ such that $x \notin W_i \vee x \notin W_j$, then

$$774 \lim_{\gamma \rightarrow 0} \frac{h_i(x) h_j(x)}{\gamma^2 (\sum_{j \in [n]} h_j(x))^2} \leq \lim_{\gamma \rightarrow 0} \frac{h_i(x) h_j(x)}{\gamma^2 h_k(x)^2} = \lim_{\gamma \rightarrow 0} \frac{c_i c_j}{\gamma^2 c_k^2} e^{\frac{2\|x - \mu_k\|^2 - \|x - \mu_i\|^2 - \|x - \mu_j\|^2}{2\gamma}} = 0$$

777 as $2\|x - \mu_k\|^2 - \|x - \mu_i\|^2 - \|x - \mu_j\|^2 < 0$ by definition of W_i . Since $\|x - \mu_i\|^2 - \|x - \mu_j\|^2 = 0$
778 if⁶ $x \in W_i \cap W_j$, and $h_i(x) \geq 0$ for every $x \in \mathbb{R}^d$, $i \in [n]$, we have

$$779 \lim_{\gamma \rightarrow 0} \frac{d}{d\gamma} \gamma S(p * g_\gamma)(x) = 0.$$

782 We proceed by noting that

$$784 \lim_{\gamma \rightarrow 0} \frac{h_j(x)}{h_i(x)} = \lim_{\gamma \rightarrow 0} \frac{c_j}{c_i} e^{-\frac{\|x - \mu_j\|^2 - \|x - \mu_i\|^2}{2\gamma}} = \begin{cases} 0, & \|x - \mu_i\| < \|x - \mu_j\| \\ \frac{c_j}{c_i}, & \|x - \mu_i\| = \|x - \mu_j\| \\ \infty, & \|x - \mu_i\| > \|x - \mu_j\| \end{cases}$$

788 and, consequently, using the conventions that $\frac{1}{0} = \infty$ and $\frac{1}{\infty} = 0$,

$$790 \lim_{\gamma \rightarrow 0} w_i(x) = \lim_{\gamma \rightarrow 0} \frac{h_i(x)}{\sum_{j \in [n]} h_j(x)}$$

$$791 = \lim_{\gamma \rightarrow 0} \left(1 + \sum_{j \in [n], j \neq i} \frac{h_j(x)}{h_i(x)} \right)^{-1}$$

$$792 = \begin{cases} 0, & x \notin W_i \\ 1, & (x \in W_i) \wedge (x \notin W_j \forall j \in [n] \setminus \{i\}) \\ (\sum_{j \in J} \frac{c_j}{c_i})^{-1}, & i \in J \subseteq [n] : x \in \bigcap_{j \in J} W_j(x) \end{cases}$$

800 Thus

$$801 H_0 p(x) = \lim_{\gamma \rightarrow 0} H_\gamma p(x) = \lim_{\gamma \rightarrow 0} \gamma S(p * g_\gamma)(x) = - \sum_{i \in [n]} (x - \mu_i) z_i(x).$$

804 This concludes the proof. □

806 *Derivation of equation (7).* For $S_\theta(\sigma, x) = -\frac{x - \mu}{\sigma^2}$, we have

$$808 \frac{d}{d\sigma} S_\theta(\sigma, x) = \frac{2(x - \mu)}{\sigma^3}$$

809 ⁶In particular, if $i = j$.



Figure 9: Generated with Algorithm 1 from the same latent noise sample with $\delta = 0.0001$, $p = 8$, and, from left to right, $b \in \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10\}$ as well as, from top to bottom, $a \in \{1, 3, 5, 7\}$.

and thus (5) evaluates to

$$\begin{aligned} x_{i+1} &= x_i - m(t_i)(t_{i+1} - t_i)t_i((1 + \gamma(t_i))(-\frac{x_i - \mu}{t_i^2}) + \frac{b\gamma(t_i)}{2t_i} \frac{2(x_i - \mu)}{t_i^3}) \\ &= x_i - m(t_i) \frac{t_i - t_{i+1}}{t_i} (x_i - \mu) \left(1 + \gamma(t_i) - \frac{b\gamma(t_i)}{t_i^2}\right). \end{aligned}$$

We would like to force this to match the standard score inference step in (6), for this special case of $S_\theta(\sigma, x)$, which is achieved by choosing

$$m(t_i) = \left(1 + \gamma(t_i) - \frac{b\gamma(t_i)}{t_i^2}\right)^{-1}.$$

□

A.3 ADDITIONAL NUMERICAL EXAMPLES

Additional examples related to the datasets FFHQ and AFHQv2 are shown in Figure 10. Additional examples related to ImageNet are shown in Figure 11.

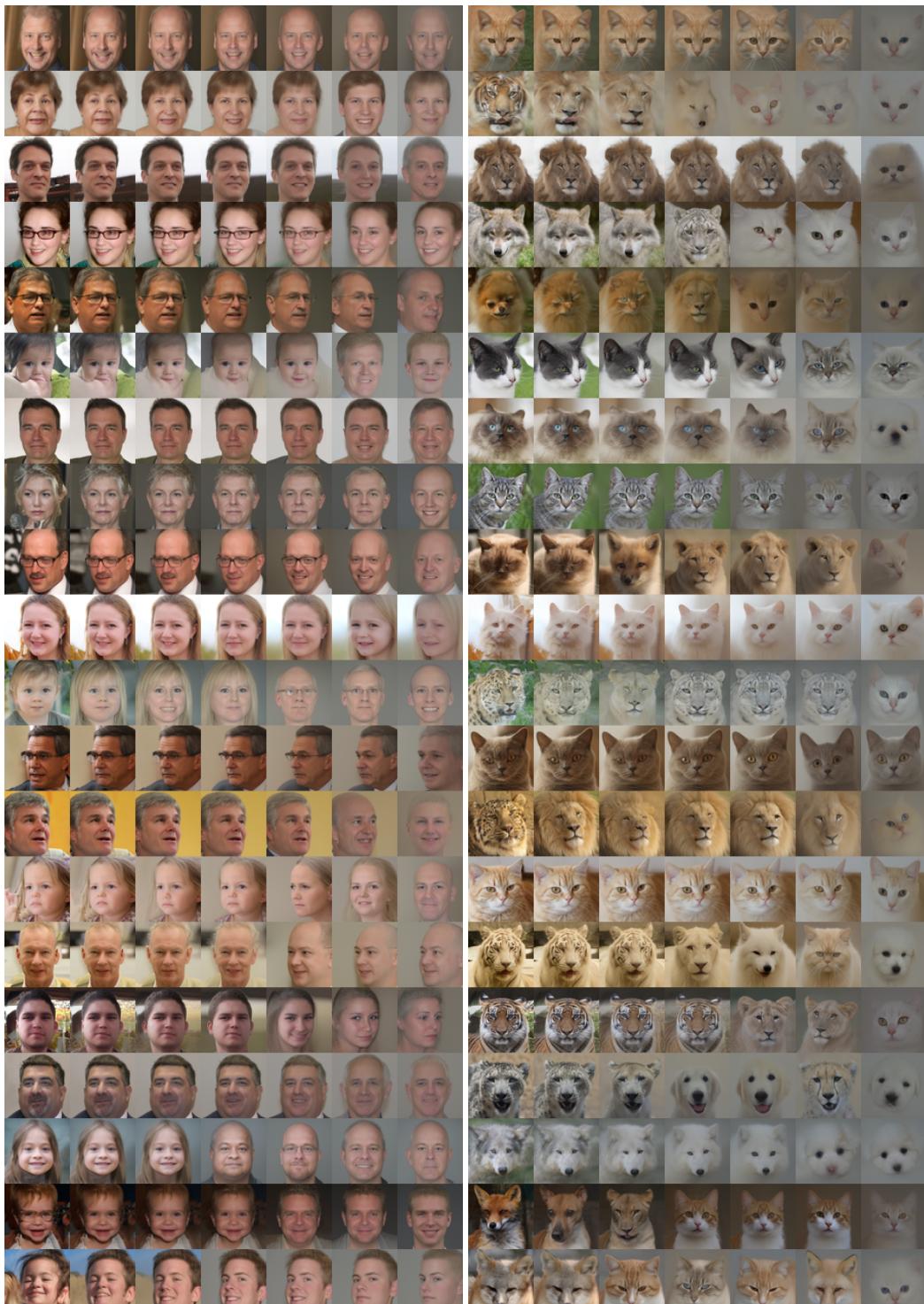
Figure 12 and Figure 13 show that the samples generated by extended score inference have a strong dependence on the chosen hyperparameters, but a significant emergence of structure can be observed for many different choices. Despite being a simpler problem, the generation seems to be less stable w.r.t. hyperparameter choices for the synthetic data. One reason for this might be that we have a 1-dimensional manifold of images that is harder to find than the one underlying the EMPIAR-11618 data, which is, of course, not explicitly known but can be assumed to be higher-dimensional. It may also be due to a shorter training duration (3mimg compared to 10mimg), which would be consistent with the generation being much more stable w.r.t. the hyperparameters for FFHQ, AFHQv2, and ImageNet as the networks for those problems have been trained significantly longer.

In Figure 14, we show the results with the synthetic dataset with 50% pixel removal. We see that images generated by standard score inference replicate the corruption present in the training set, while the images generated by extended score inference exhibit all key features of the clean data, while eliminating the corruption due to pixel removal.

In Figure 15, we compare the inference paths for standard and extended score generations: applying truncated sampling to the standard score generation would not be enough to obtain the denoising effect.

Additional images from the EMPIAR-11618 dataset, as well as images generated by standard score inference, are shown in Figure 16.

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914 Figure 10: In both subfigures, all images in each row starts from the same latent noise sample
915 and the leftmost column uses standard score whereas second to last columns use Algorithm 1 with
916 $\delta = 0.0001$, $p = 8$, $a = 2.5$, and, from left to right, $b \in \{2, 5, 10, 20, 40, 80\}$. The rows are
917 generated from consecutive random seeds.

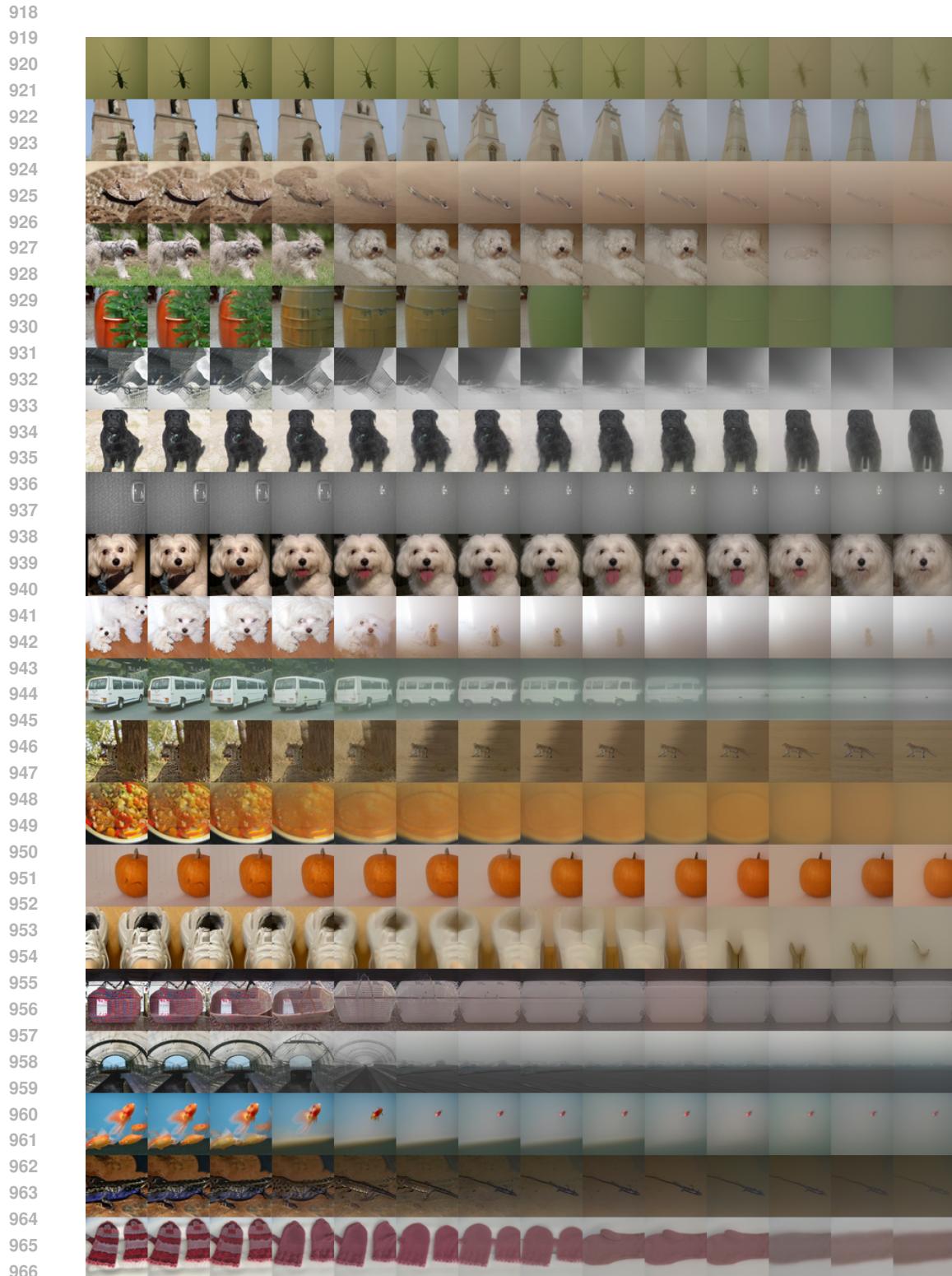
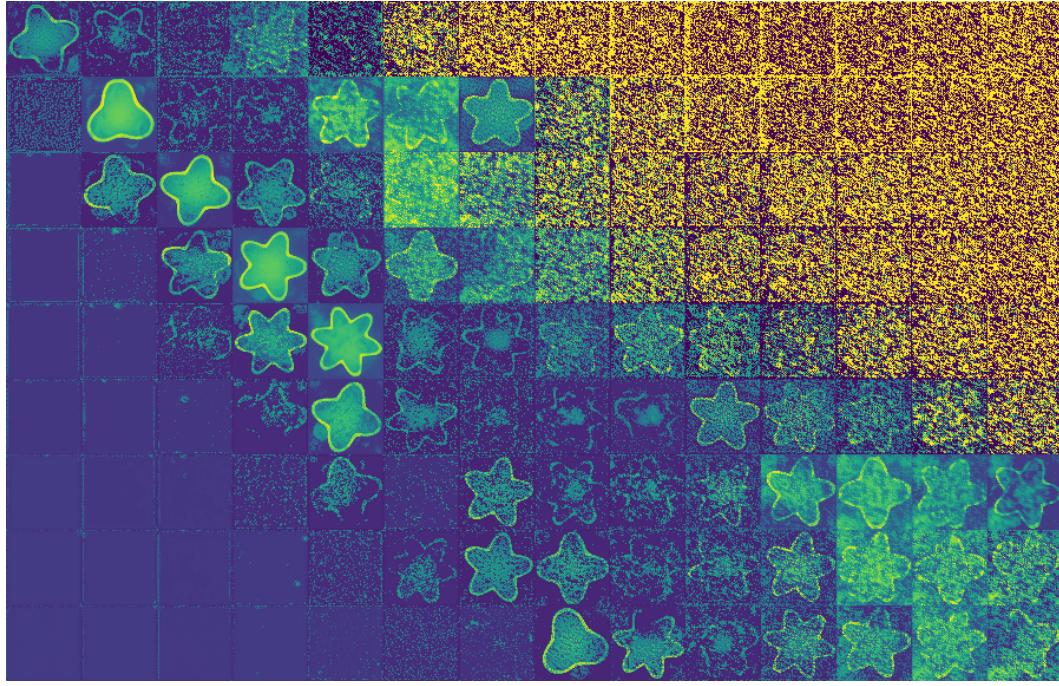


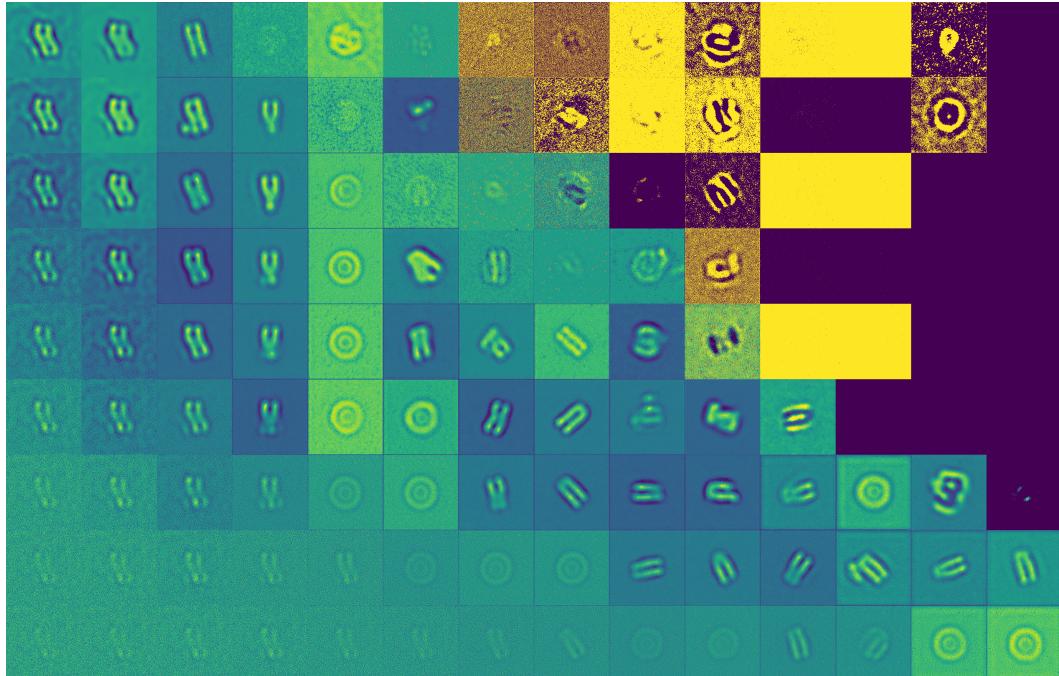
Figure 11: All images in each row starts from the same latent noise sample and the leftmost column uses standard score whereas second to last columns use Algorithm 1 with $\delta = 0.001$, $p = 12$, $a = 4$, and, from left to right, $b \in \{1, 2, 5, 10, 15, 20, 25, 30, 35, 40, 50, 60, 70\}$. The rows are generated from consecutive random seeds.

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995 Figure 12: Generated with Algorithm 1 from the same latent noise sample with $\delta = 0.02$, $p = 8$,
 996 and, from left to right, $b \in \{10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 75\}$ as well as, from top to bottom,
 997 $a \in \{0.0015, 0.002, 0.0025, 0.003, 0.0035, 0.004, 0.0045, 0.005, 0.0055\}$.
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1022 Figure 13: Generated with Algorithm 1 from the same latent noise sample with $\delta = 0.001$, $p = 8$,
 1023 and, from left to right, $b \in \{0.25, 0.5, 1, 2, 4, 8, 16, 32, 64, 128, 256, 512, 1024, 2048\}$ as well as, from top to bottom,
 1024 $a \in \{0.0005, 0.001, 0.002, 0.005, 0.01, 0.02, 0.05, 0.1, 0.2\}$.
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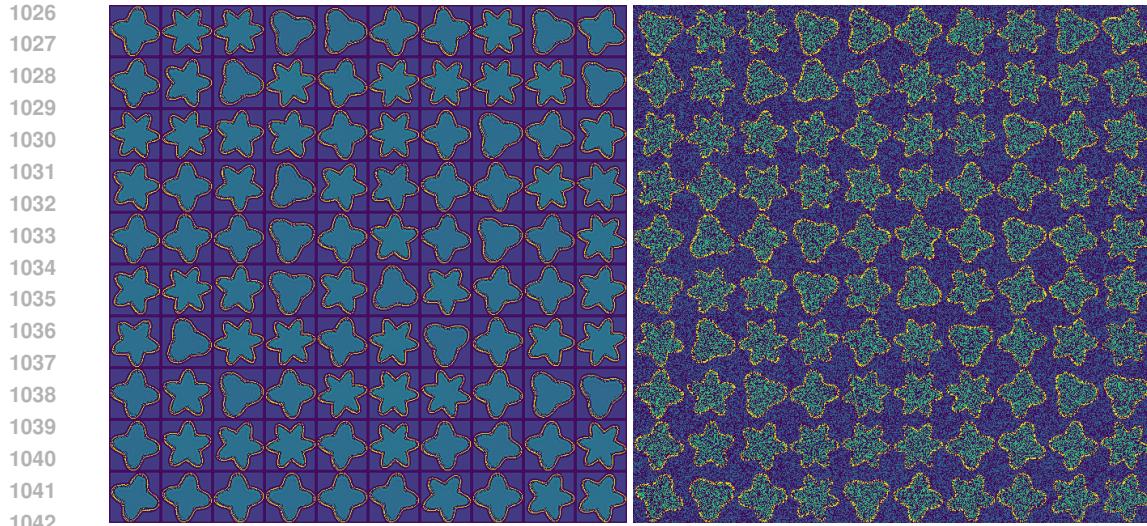


Figure 14: Comparison of generated images using a network trained on our synthetic dataset with pixel removal noise, specifically in a given image every pixel is set to 0 with probability 0.5. Images generated by standard score inference (right). Images generated by extended score inference (left).

A.4 LLM USE

LLMs were used to polish the writing for parts of the text, to suggest related work, and as a coding aid. All those suggestions have only been implemented after thorough manual review. No LLMs were involved in any way in the mathematical derivations.

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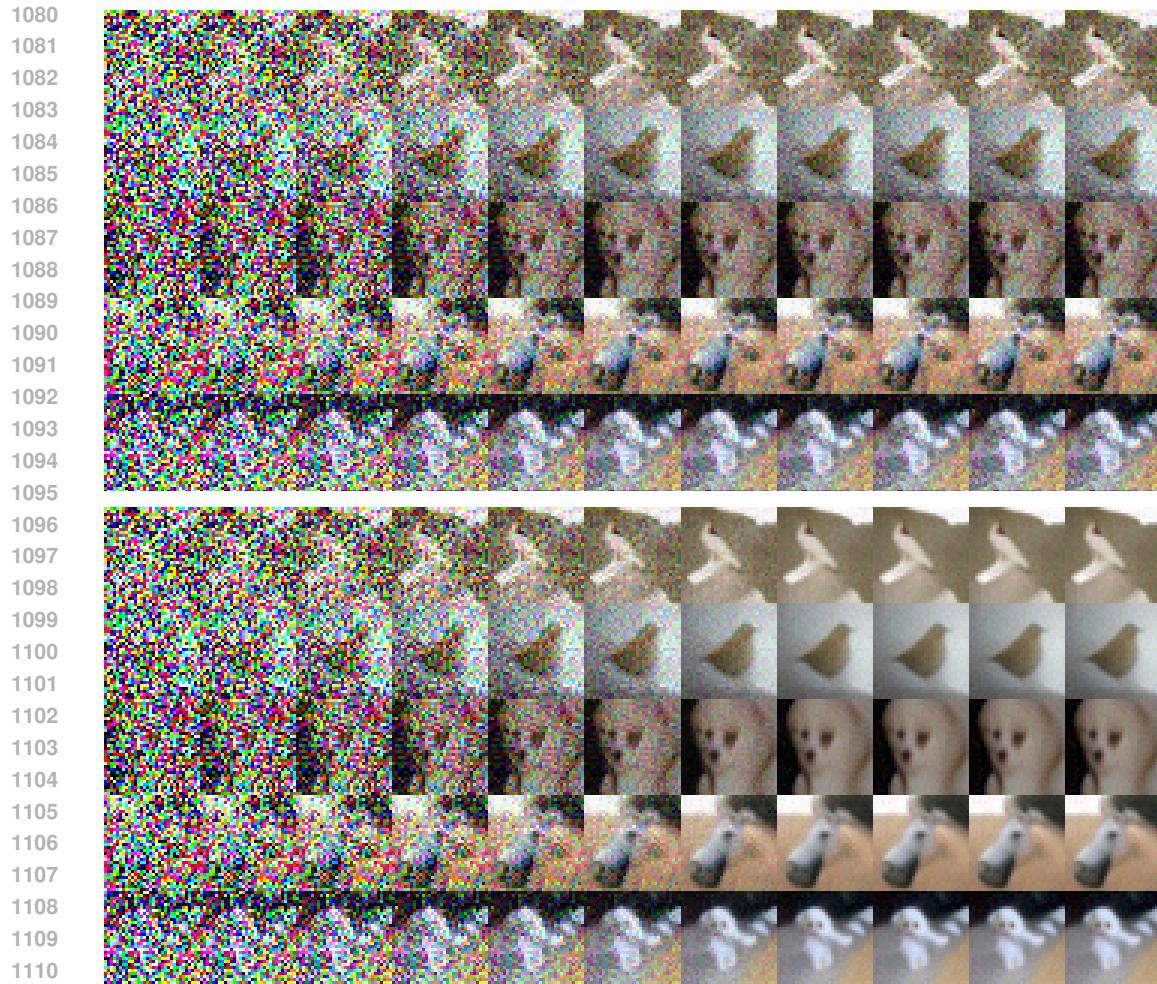


Figure 15: Illustrating the inference path for standard score generation (top) compared to extended score generation (bottom), displaying every second image generated during the inference procedure starting at step 20.

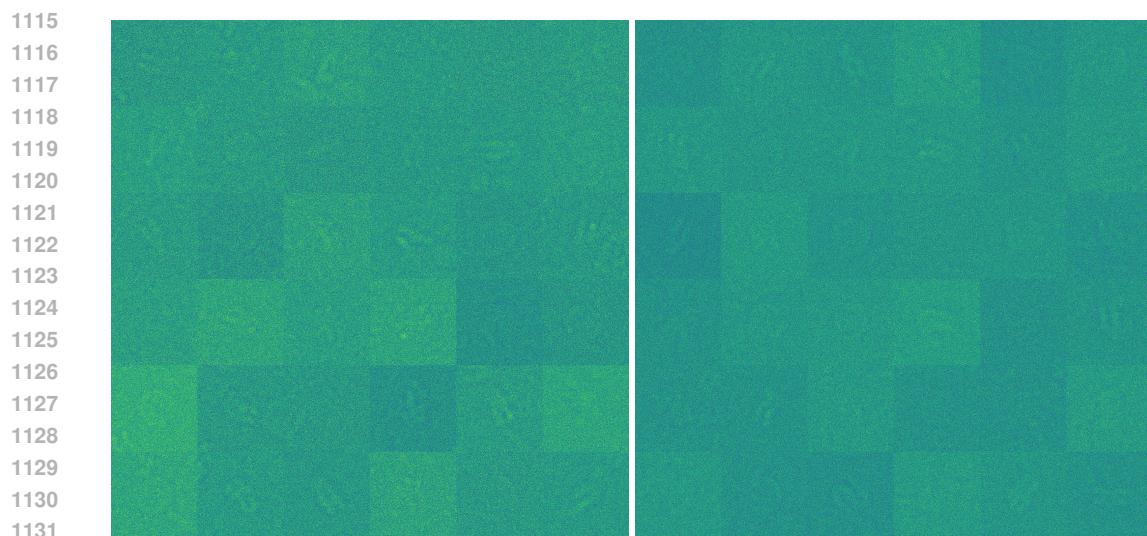


Figure 16: Images from the EMPIAR-11618 dataset (left). Images generated by standard score inference (right).