Classifier-Free Diffusion Guidance

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Abstract

Classifier guidance is a recently introduced method to trade off mode coverage and sample fidelity in conditional diffusion models post training, in the same spirit as low temperature sampling or truncation in other types of generative models. This method combines the score estimate of a diffusion model with the gradient of an image classifier and thereby requires training an image classifier separate from the diffusion model. We show that guidance can be performed by a pure generative model without such a classifier: we jointly train a conditional and an unconditional diffusion model, and find that it is possible to combine the resulting conditional and unconditional scores to attain a trade-off between sample quality and diversity similar to that obtained using classifier guidance.

1 Introduction

Diffusion models have recently emerged as an expressive and flexible family of generative models, delivering competitive sample quality and likelihood scores on image and audio synthesis tasks [15, 16, 5, 17, 8]. These models have delivered audio synthesis performance rivaling the quality of autoregressive models with substantially fewer inference steps [2, 9], and they have delivered ImageNet generation results outperforming BigGAN-deep [1] and VQ-VAE-2 [11] in terms of FID score and classification accuracy score [6, 3].

Dhariwal and Nichol [3] proposed *classifier guidance*, a technique to boost the sample quality of a diffusion model using an extra trained classifier. Using classifier guidance, they generate high fidelity, non-diverse ImageNet samples that match or exceed the Inception scores of truncated BigGAN, and by varying the strength of the classifier gradient, they can trade off Inception score [14] and FID score [4] (or precision and recall) in a manner similar to varying the truncation parameter of BigGAN.

Prior to classifier guidance, it was not known how to generate "low temperature" samples from a diffusion model similar to those produced by truncated BigGAN: naive ways of doing so, such as scaling the model score vectors or decreasing the amount of Gaussian noise added during sampling, are ineffective. Classifier guidance resolves this issue but raises more questions. Because classifier guidance mixes a score estimate with a classifier gradient during sampling, classifier-guided diffusion sampling can be interpreted as attempting to confuse an image classifier with a gradient-based adversarial attack. This raises the question of whether classifier guidance is successful at boosting classifier-based metrics such as FID and Inception score (IS) simply because it is adversarial against such classifiers. Stepping in direction of classifier gradients also bears some resemblance to GAN training, particularly with nonparameteric generators; this also raises the question of whether classifier-guided diffusion models perform well on classifier-based metrics because they are beginning to resemble GANs, which are already known to perform well on such metrics.

To resolve these questions, we present *classifier-free guidance*, our guidance method which avoids any classifier entirely. Rather than sampling in the direction of the gradient of an image classifier, our method instead mixes the score estimates of a conditional diffusion model and a jointly trained unconditional diffusion model. By sweeping over the mixing weight, we attain a FID/IS tradeoff

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similar to that attained by classifier guidance. Our results demonstrate that pure generative diffusion models are capable of synthesizing extremely high fidelity samples possible with other types of generative models.

2 Background

Let $\mathbf{x}$ be data drawn from a data distribution $p(\mathbf{x})$. We train a diffusion model in continuous time [17, 2, 8]: letting $\mathbf{z} = \{\mathbf{z}_\lambda \,|\, \lambda \in [\lambda_{\min}, \lambda_{\max}]\}$ for hyperparameters $\lambda_{\min} < \lambda_{\max} \in \mathbb{R}$, the forward process $q(\mathbf{z}|\mathbf{x})$ is the variance-preserving Markov process [15] specified as

$$q(\mathbf{z}_\lambda|\mathbf{x}) = \mathcal{N}(\alpha_\lambda \mathbf{x}, \sigma_\lambda^2 \mathbf{I}), \text{ where } \alpha_\lambda^2 = 1/(1+e^{-\lambda}),\ \sigma_\lambda^2 = 1-\alpha_\lambda^2 \tag{1}$$

$$q(\mathbf{z}_\lambda|\mathbf{z}_{\lambda'}) = \mathcal{N}((\alpha_\lambda/\alpha_{\lambda'})\mathbf{z}_{\lambda'}, \sigma_{\lambda|\lambda'}^2 \mathbf{I}), \text{ where } \lambda < \lambda',\ \sigma_{\lambda|\lambda'}^2 = (1-e^{\lambda-\lambda'})\sigma_\lambda^2 \tag{2}$$

We will use the notation $p(\mathbf{z})$ (or $p(\mathbf{z}_\lambda)$) to denote the marginal of $\mathbf{z}$ (or $\mathbf{z}_\lambda$) when $\mathbf{x} \sim p(\mathbf{x})$. Note that $\lambda = \log \alpha_\lambda^2/\sigma_\lambda^2$, so λ can be interpreted as the log signal-to-noise ratio of $\mathbf{z}_\lambda$, and the forward process runs in the direction of decreasing λ. Conditioned on $\mathbf{x}$, the forward process can be described in reverse by the transitions $q(\mathbf{z}_{\lambda'}|\mathbf{z}_\lambda, \mathbf{x}) = \mathcal{N}(\tilde{\boldsymbol{\mu}}_{\lambda'|\lambda}(\mathbf{z}_\lambda, \mathbf{x}), \tilde{\sigma}_{\lambda'|\lambda}^2 \mathbf{I})$, where

$$\tilde{\boldsymbol{\mu}}_{\lambda'|\lambda}(\mathbf{z}_\lambda, \mathbf{x}) = e^{\lambda-\lambda'}(\alpha_{\lambda'}/\alpha_\lambda)\mathbf{z}_\lambda + (1-e^{\lambda-\lambda'})\alpha_{\lambda'}\mathbf{x}, \quad \tilde{\sigma}_{\lambda'|\lambda}^2 = (1-e^{\lambda-\lambda'})\sigma_{\lambda'}^2 \tag{3}$$

The reverse process generative model $p_\theta(\mathbf{z})$ starts from $p_\theta(\mathbf{z}_{\lambda_{\min}}) = \mathcal{N}(\mathbf{0}, \mathbf{I})$. We specify the transitions:

$$p_\theta(\mathbf{z}_{\lambda'}|\mathbf{z}_\lambda) = \mathcal{N}(\tilde{\boldsymbol{\mu}}_{\lambda'|\lambda}(\mathbf{z}_\lambda, \mathbf{x}_\theta(\mathbf{z}_\lambda)), (\tilde{\sigma}_{\lambda'|\lambda}^2)^{1-v}(\sigma_{\lambda|\lambda'}^2)^v) \tag{4}$$

During sampling, we apply this transition along an increasing sequence $\lambda_{\min} = \lambda_1 < \cdots < \lambda_T = \lambda_{\max}$ for T timesteps. If the model $\mathbf{x}_\theta$ is correct, then as $T \to \infty$, we obtain samples from an SDE whose sample paths are distributed as $p(\mathbf{z})$ [17]. The variance is a log-space interpolation of $\tilde{\sigma}_{\lambda'|\lambda}^2$ and $\sigma_{\lambda|\lambda'}^2$ as suggested by [10]; for simplicity we use a constant hyperparameter v rather than learned $\mathbf{z}_\lambda$-dependent v. Note that variances simplify to $\tilde{\sigma}_{\lambda'|\lambda}^2$ as $\lambda' \to \lambda$, so v has an effect only when sampling with non-infinitesimal timesteps as done in practice.

The reverse process mean comes from an estimate $\mathbf{x}_\theta(\mathbf{z}_\lambda) \approx \mathbf{x}$ plugged into $q(\mathbf{z}_{\lambda'}|\mathbf{z}_\lambda, \mathbf{x})$ [5, 8] ($\mathbf{x}_\theta$ also receives λ as input, but we suppress this to keep our notation clean). We parameterize $\mathbf{x}_\theta$ in terms of $\boldsymbol{\epsilon}$-prediction [5]: $\mathbf{x}_\theta(\mathbf{z}_\lambda) = (\mathbf{z}_\lambda - \sigma_\lambda \boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda))/\alpha_\lambda$, and we train on the objective

$$\mathbb{E}_{\boldsymbol{\epsilon},\lambda}\left[\|\boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda) - \boldsymbol{\epsilon}\|_2^2\right] \tag{5}$$

where $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$, $\mathbf{z}_\lambda = \alpha_\lambda \mathbf{x} + \sigma_\lambda \boldsymbol{\epsilon}$, and λ is drawn from a distribution $p(\lambda)$ over $[\lambda_{\min}, \lambda_{\max}]$. This objective is denoising score matching [18] over multiple noise scales [16], and when $p(\lambda)$ is uniform, the objective is proportional to the variational lower bound on the marginal log likelihood of the latent variable model $\int p_\theta(\mathbf{x}|\mathbf{z})p_\theta(\mathbf{z})d\mathbf{z}$, ignoring the term for the unspecified $p_\theta(\mathbf{x}|\mathbf{z})$ and for the prior at $\mathbf{z}_{\lambda_{\min}}$ [8]. For a different distribution $p(\lambda)$, the objective can be interpreted as weighted variational lower bound whose weighting can be tuned for sample quality [5]. We use a $p(\lambda)$ inspired by the cosine noise schedule of [10]: sampling λ is given by $\lambda = -2 \log \tan(au + b)$ for uniformly distributed $u \in [0, 1]$, where $b = \arctan(e^{-\lambda_{\max}/2})$ and $a = \arctan(e^{-\lambda_{\min}/2}) - b$. This represents a hyperbolic secant distribution modified to be supported on a bounded interval. For finite timestep sampling, we use λ values corresponding to uniformly spaced $u \in [0, 1]$.

Because the loss for $\boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda)$ is denoising score matching for all λ, the score $\boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda)$ learned by our model estimates the gradient of the log-density of the distribution of our noisy data $\mathbf{z}_\lambda$, that is $\boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda) \approx -\sigma_\lambda \nabla_{\mathbf{z}_\lambda} \log p(\mathbf{z}_\lambda)$; note, however, that because we use unconstrained neural networks to define $\boldsymbol{\epsilon}_\theta$, there need not exist any scalar potential whose gradient is $\boldsymbol{\epsilon}_\theta$. Sampling from the learned diffusion model resembles using Langevin diffusion to sample from a sequence of distributions $p(\mathbf{z}_\lambda)$ that converges to the conditional distribution $p(\mathbf{x})$ of the original data $\mathbf{x}$.

In the case of conditional generative modeling, the data $\mathbf{x}$ is drawn jointly with conditioning information $\mathbf{c}$, i.e. a class label for class-conditional image generation. The only modification to the model is that the reverse process function approximator receives $\mathbf{c}$ as input, as in $\boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda, \mathbf{c})$.

3 Guidance

An interesting property of certain generative models, such as GANs and flow-based models, is the ability to perform truncated or low temperature sampling by decreasing the variance or range of noise inputs to the generative model at sampling time. The intended effect is to decrease the diversity of the samples while increasing the quality of each individual sample. Truncation in BigGAN [1], for example, yields a tradeoff curve between FID score and Inception score for low and high amounts of truncation, respectively. Low temperature sampling in Glow [7] has a similar effect.

Unfortunately, straightforward attempts of implementing truncation or low temperature sampling in diffusion models are ineffective. For example, scaling model scores or decreasing the variance of Gaussian noise in the reverse process cause the diffusion model to generate blurry, low quality samples [3].

3.1 Classifier guidance

To obtain a truncation-like effect in diffusion models, Dhariwal and Nichol [3] introduce *classifier guidance*, where the diffusion score $\boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda, \mathbf{c}) \approx -\sigma_\lambda \nabla_{\mathbf{z}_\lambda} \log p(\mathbf{z}_\lambda|\mathbf{c})$ is modified to include the gradient of the log likelihood of an auxiliary classifier model $p_\theta(\mathbf{c}|\mathbf{z}_\lambda)$ as follows:

$$\tilde{\boldsymbol{\epsilon}}_\theta(\mathbf{z}_\lambda, \mathbf{c}) = \boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda, \mathbf{c}) - w\sigma_\lambda \nabla_{\mathbf{z}_\lambda} \log p_\theta(\mathbf{c}|\mathbf{z}_\lambda) \approx -\sigma_\lambda \nabla_{\mathbf{z}_\lambda}[\log p(\mathbf{z}_\lambda|\mathbf{c}) + w \log p_\theta(\mathbf{c}|\mathbf{z}_\lambda)],$$

where w is a parameter that controls the strength of the classifier guidance. This modified score $\tilde{\boldsymbol{\epsilon}}_\theta(\mathbf{z}_\lambda, \mathbf{c})$ is then used in place of $\boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda, \mathbf{c})$ when sampling from the diffusion model, which has the effect of up-weighting the probability of data for which the classifier $p_\theta(\mathbf{c}|\mathbf{z}_\lambda)$ assigns high likelihood to the correct label: data that can be classified well scores high on the Inception score of perceptual quality [14], which rewards generative models for this by design. Dhariwal and Nichol [3] therefore find that by setting $w > 0$ they can improve the Inception score of their diffusion model, at the expense of decreased diversity in their samples. Interestingly, they obtain their best results when applying classifier guidance to an already class-conditional model as described above, and they find that applying guidance to an unconditional model performs less well: the effects of class-conditioning and guidance thus seem complimentary.

3.2 Classifier-free guidance

A downside of classifier guidance is that it requires an additional classifier model and thus complicates the training pipeline. This model has to be trained on noisy data $\mathbf{z}_\lambda$, so it is not possible to plug in a standard pre-trained classifier. We explore an alternative method of modifying $\boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda, \mathbf{c})$ to achieve the same effect of boosting the perceptual quality as measured by the Inception score without requiring an auxiliary classifier. We call this new method *classifier-free guidance*.

Instead of training a separate classifier model, we choose to train an unconditional denoising diffusion model $p_\theta(\mathbf{z})$ parameterized through a score estimator $\boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda)$ together with the conditional model $p_\theta(\mathbf{z}|\mathbf{c})$ parameterized through $\boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda, \mathbf{c})$. We use a single neural network to parameterize both models, where for the unconditional model we can simply input zeros for the class identifier $\mathbf{c}$ when predicting the score, i.e. $\boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda) = \boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda, \mathbf{c} = \mathbf{0})$. We jointly train the unconditional and conditional models simply by randomly setting $\mathbf{c}$ to the unconditional class identifier.

We then perform sampling using the following linear combination of the conditional and unconditional score estimates:

$$\tilde{\boldsymbol{\epsilon}}_\theta(\mathbf{z}_\lambda, \mathbf{c}) = (1 + w)\boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda, \mathbf{c}) - w\boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda) \tag{6}$$

Eq. (6) has no classifier gradient present, so taking a step in the $\tilde{\boldsymbol{\epsilon}}_\theta$ direction cannot be interpreted as a gradient-based adversarial attack on an image classifier. Furthermore, $\tilde{\boldsymbol{\epsilon}}_\theta$ is constructed from score estimates that are non-conservative vector fields due to the use of unconstrained neural networks, so there in general cannot exist a scalar potential such as a classifier log likelihood for which $\tilde{\boldsymbol{\epsilon}}_\theta$ is the classifier-guided score.

Despite the fact that there in general cannot exist a classifier for which Eq. (6) is the classifier-guided score, it is in fact inspired by the gradient of an implicit classifier $p^i(\mathbf{c}|\mathbf{z}_\lambda) \propto p(\mathbf{z}_\lambda|\mathbf{c})/p(\mathbf{z}_\lambda)$. If we had access to exact scores $\boldsymbol{\epsilon}^*(\mathbf{z}_\lambda, \mathbf{c})$ and $\boldsymbol{\epsilon}^*(\mathbf{z}_\lambda)$ (of $p(\mathbf{z}_\lambda|\mathbf{c})$ and $p(\mathbf{z}_\lambda)$, respectively), then the gradient of this implicit classifier would be $\nabla_{\mathbf{z}_\lambda} \log p^i(\mathbf{c}|\mathbf{z}_\lambda) = -\frac{1}{\sigma_\lambda}[\boldsymbol{\epsilon}^*(\mathbf{z}_\lambda, \mathbf{c}) - \boldsymbol{\epsilon}^*(\mathbf{z}_\lambda)]$, and classifier guidance with this implicit classifier would modify the score estimate into $\tilde{\boldsymbol{\epsilon}}^*(\mathbf{z}_\lambda, \mathbf{c}) = (1 + w)\boldsymbol{\epsilon}^*(\mathbf{z}_\lambda, \mathbf{c}) - w\boldsymbol{\epsilon}^*(\mathbf{z}_\lambda)$. Note the resemblance to Eq. (6), but also note that $\boldsymbol{\epsilon}^*(\mathbf{z}_\lambda, \mathbf{c})$ differs fundamentally from $\boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda, \mathbf{c})$. The former is constructed from the scaled classifier gradient $\boldsymbol{\epsilon}^*(\mathbf{z}_\lambda, \mathbf{c}) - \boldsymbol{\epsilon}^*(\mathbf{z}_\lambda)$; the latter is constructed from the estimate $\boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda, \mathbf{c}) - \boldsymbol{\epsilon}_\theta(\mathbf{z}_\lambda)$, and this expression is not in general the (scaled) gradient of any classifier, again because the score estimates are the outputs of unconstrained neural networks. The fact that Eq. (6) is as effective as classifier guidance despite this is an empirical finding that we report in Section 4.

4 Experiments

Our method is extremely simple to implement: during training we simply drop out the class label, and during sampling we simply mix the conditional and unconditional scores as in Eq. (6). Here, we report our results on 64×64 area-downsampled ImageNet [12]. We trained a model with architecture and hyperparameters identical to the 64×64 model in [3], and we jointly trained the model on unconditional generation with probability 0.1. We choose $\lambda_{\min} = -20$, $\lambda_{\max} = 20$, and $v = 0.3$. We consider implied-classifier weights $w \in \{0, 0.1, 0.2, \ldots, 5\}$ and calculate FID and Inception Scores with 50000 samples for each value using $T = 256$ sampling steps.

Figure 1 and Fig. 2 list our results: we obtain the best FID result with a small amount of guidance ($w = 0.1$) and the best IS result with strong guidance ($w \geq 4$). These results compare favorably to [3, 6] and are currently state-of-the-art for this data set as far as we are aware for models that use $T \approx 256$ steps (the ADM result uses 250 steps, and the CDM result is a two-stage model with 4000 steps each). Between these two extremes we see a clear trade-off between these two metrics of perceptual quality, with FID monotonically decreasing and IS monotonically increasing with guidance weight w.

Figure 3 shows randomly generated samples from our model for different levels of guidance: here we clearly see that increasing guidance has the effect of decreasing sample variety and increasing individual sample fidelity. Figure 4 shows samples from a similar model trained on 128×128 ImageNet.

Method	FID (↓)	IS (↑)
ADM [3]	2.07	-
CDM [6]	**1.48**	67.95
Ours, no guidance	1.80	53.71
Ours, with guidance		
$w = 0.1$	1.55	66.11
$w = 0.2$	2.04	78.91
$w = 0.3$	3.03	92.8
$w = 0.4$	4.30	106.2
$w = 0.5$	5.74	119.3
$w = 0.6$	7.19	131.1
$w = 0.7$	8.62	141.8
$w = 0.8$	10.08	151.6
$w = 0.9$	11.41	161
$w = 1.0$	12.6	170.1
$w = 2.0$	21.03	225.5
$w = 3.0$	24.83	250.4
$w = 4.0$	26.22	**260.2**

Figure 1: ImageNet 64x64 results

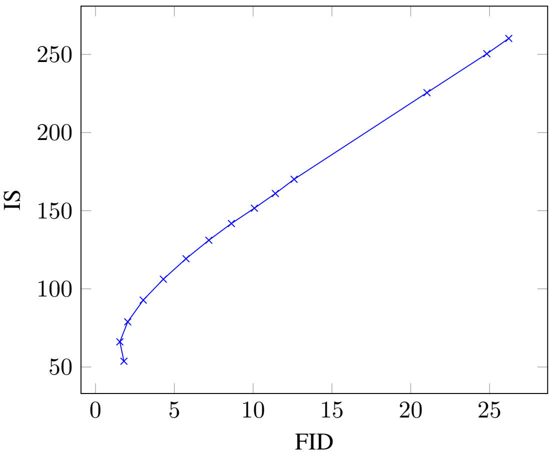
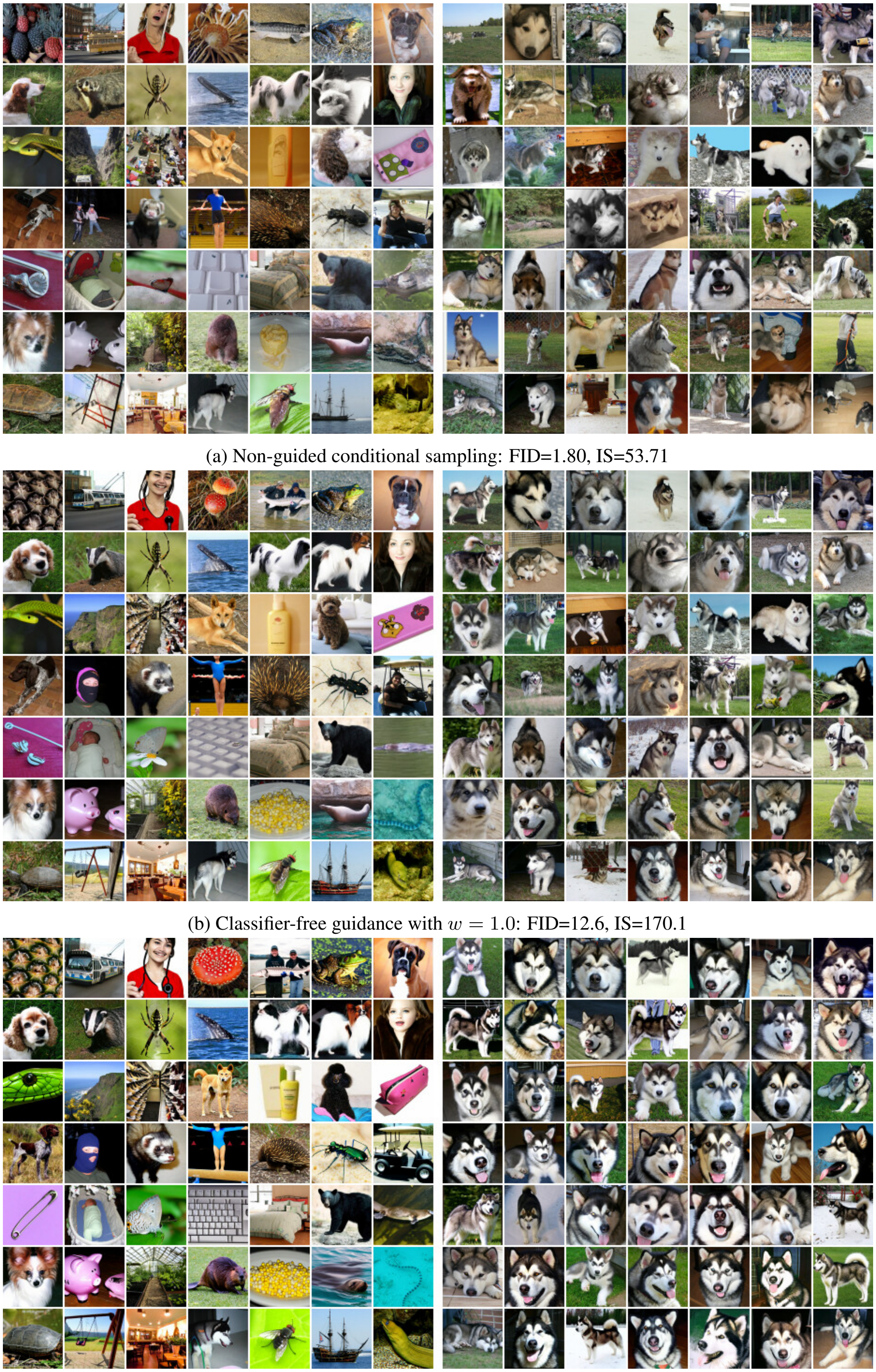


Figure 2: ImageNet 64x64 FID vs. IS



(a) Non-guided conditional sampling: FID=1.80, IS=53.71

(b) Classifier-free guidance with $w = 1.0$: FID=12.6, IS=170.1

(c) Classifier-free guidance with $w = 3.0$: FID=24.83, IS=250.4

Figure 3: Classifier-free guidance on ImageNet 64x64. Left: random classes. Right: single class (malamute). Same random seeds used for sampling in each subfigure.

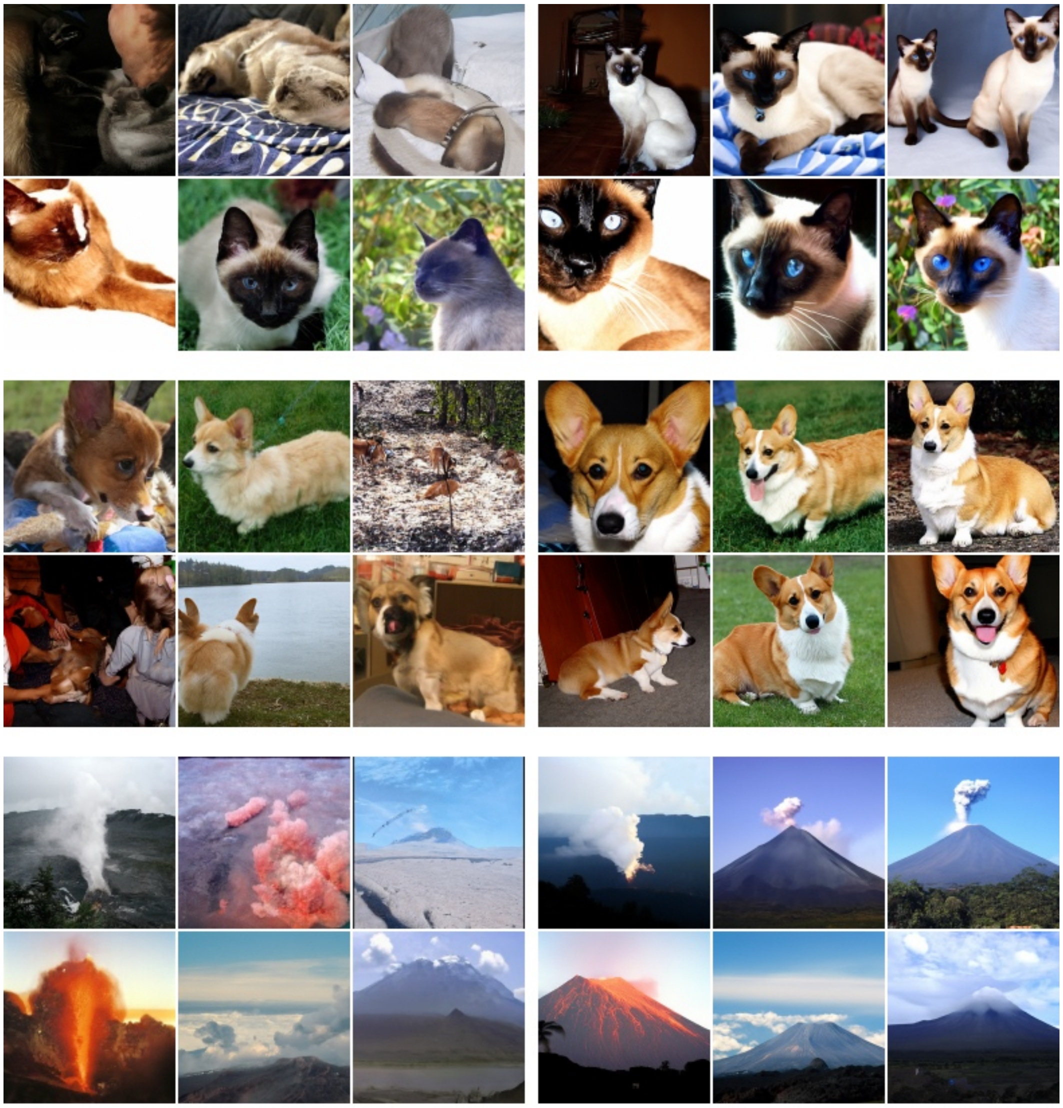


Figure 4: Classifier-free guidance on 128x128 ImageNet. Left: non-guided samples, right: guided samples with $w = 3.0$. Interestingly, strongly guided samples such as these display saturated colors.

5 Discussion

The most practical advantage of our classifier-free guidance method is its extreme simplicity: it is only a one-line change of code during training—to randomly drop out the class conditioning—and during sampling—to mix the conditional and unconditional score estimates. Classifier guidance, by contrast, complicates the training pipeline since it requires training an extra classifier. This classifier must be trained on noisy $\mathbf{z}_\lambda$, so it is not possible to plug in a standard pre-trained classifier.

Besides practical advantages, classifier-free guidance is able to trade off IS and FID like classifier guidance without needing an extra trained classifier, so we have demonstrated that guidance can be performed with a pure generative model. We confirm that it is possible to maximize Inception scores using classifier-free guidance (and improve FID score for a small amount of guidance), thus providing evidence that classifier-based sample quality metrics can be improved using methods that are not adversarial against ImageNet classifiers using classifier gradients. Our diffusion models are parameterized by unconstrained neural networks and therefore their score estimates do not necessarily form conservative vector fields, unlike classifier gradients [13]. Therefore, an unconditional-guided sampler follows step directions that do not resemble classifier gradients at all and thus cannot be interpreted as a gradient-based adversarial attack on a classifier; hence our results show that boosting the classifier-based IS and FID metrics can be accomplished with pure generative models with a sampling procedure that is not adversarial against image classifiers.

We also have arrived at an intuitive explanation for how guidance works: it decreases the unconditional likelihood of the sample while increasing the conditional likelihood. Classifier-free guidance accomplishes this by decreasing the unconditional likelihood with a *negative* score term, which to our knowledge has not yet been explored and may find uses in other applications.

A potential disadvantage of classifier-free guidance is sampling speed. Generally, classifiers can be smaller and faster than generative models, so classifier guided sampling may be faster than classifier-free guidance because the latter needs to run two forward passes of the diffusion model, one for conditional score and another for the unconditional score. The necessity to run multiple passes of the diffusion model might be mitigated by changing the architecture to inject conditioning late in the network, but we leave this exploration for future work.

Finally, any guidance method that increases sample fidelity at the expense of diversity must face the question of whether decreased diversity is acceptable. There may be negative impacts in deployed models, since sample diversity is important to maintain in applications where certain parts of the data are underrepresented in the context of the rest of the data. It would be an interesting avenue of future work to try to boost sample quality while maintaining sample diversity.

6 Conclusion

We have presented classifier-free guidance, a method to increase sample quality while decreasing sample diversity in diffusion models. Classifier-free guidance is classifier guidance without a classifier, and our results showing the effectiveness of classifier-free guidance confirm that pure generative diffusion models are capable of maximizing classifier-based sample quality metrics while entirely avoiding classifier gradients. We look forward to further explorations of classifier-free guidance in a wider variety of settings.

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