CLASSIFICATION-DENOISING NETWORKS

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Abstract

Image classification and denoising suffer from complementary issues of lack of robustness or partially ignoring conditioning information. We argue that they can be alleviated by unifying both tasks through a model of the joint probability of (noisy) images and class labels. Classification is performed with a forward pass followed by conditioning. Using the Tweedie-Miyasawa formula, we evaluate the denoising function with the score, which can be computed by marginalization and backpropagation. The training objective is then a combination of cross-entropy loss and denoising score matching loss integrated over noise levels. Numerical experiments on CIFAR-10 and ImageNet show competitive classification and denoising performance compared to reference deep convolutional classifiers/denoisers, and significantly improves efficiency compared to previous joint approaches. Our model shows an increased robustness to adversarial perturbations compared to a standard discriminative classifier, and allows for a novel interpretation of adversarial gradients as a difference of denoisers.¹

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1 INTRODUCTION: CLASSIFICATION AND DENOISING

026 Image classification and denoising are two cornerstone problems in computer vision and signal 027 processing. The former aims to associate a label $c \in \{1, ..., C\}$ to input images x. The latter involves recovering the image x from a noisy observation $y = x + \sigma \epsilon$. Before the 2010s, these two 029 problems were addressed with different kinds of methods but similar mathematical tools like wavelet decompositions, non-linear filtering and Bayesian modeling. Since the publication of AlexNet (Krizhevsky et al., 2012), deep learning (LeCun et al., 2015) and convolutional neural network 031 (CNNs) (LeCun et al., 1998) have revolutionized both fields. ResNets (He et al., 2016) and their 032 recent architectural and training improvements (Liu et al., 2022; Wightman et al., 2021) still offer 033 close to state-of-the-art accuracy, comparable with more recent methods like vision transformers 034 (Dosovitskiy et al., 2020) and visual state space models (Liu et al., 2024). In image denoising, CNNs 035 lead to significant improvements with the seminal work DnCNN (Zhang et al., 2017b) followed by FFDNet (Zhang et al., 2018) and DRUNet (Zhang et al., 2021). Importantly, deep image denoisers 037 are now at the core of deep generative models estimating the gradient of the distribution of natural 038 images (Song & Ermon, 2019), a.k.a. score-based diffusion models (Ho et al., 2020). 039

However, some unsolved challenges remain in both tasks. For one, classifiers tend to interpolate 040 their training set, even when the class labels are random (Zhang et al., 2016), and are thus prone 041 to overfitting. They also suffer from robustness issues such as adversarial attacks (Szegedy, 2013). 042 Conversely, deep denoisers seem to neither overfit nor memorize their training set when it is suffi-043 ciently large (Yoon et al., 2023; Kadkhodaie et al., 2023). On the other hand, when used to generate 044 images conditionally to a class label or a text caption, denoisers are known to occasionally ignore part of their conditioning information (Conwell & Ullman, 2022; Rassin et al., 2022), requiring ad-hoc 046 techniques like classifier-free guidance (Ho & Salimans, 2022) or specific architecture and synthesis 047 modifications (Chefer et al., 2023; Rassin et al., 2024). Another issue is that optimal denoisers should be conservative vector fields but DNN denoisers are only approximately conservative (Mohan et al., 048 2020), and enforcing this property is challenging (Saremi, 2019; Chao et al., 2023). 049

We introduce a conceptual framework which has the potential to address these issues simultaneously. We propose to learn a single model parameterizing the *joint* log-probability $\log p(\mathbf{y}, c)$ of noisy images \mathbf{y} and classes c. Both tasks are tackled with this common approach, aiming to combine their

¹We will release code upon acceptance.

strengths while alleviating their weaknesses. First, the model gives easy access to the conditional log-probability $\log p(c|\mathbf{y})$ by conditioning, allowing to classify images with a single forward pass. Second, we can obtain the marginal log-probability $\log p(\mathbf{y})$ by marginalizing over classes c, and compute its gradient with respect to the input \mathbf{y} with a backward pass. The denoised image can then be estimated using the Tweedie-Miyasawa identity (Robbins, 1956; Miyasawa et al., 1961; Raphan & Simoncelli, 2011). We can also perform class-conditional denoising similarly using $\nabla_{\mathbf{y}} \log p(\mathbf{y}|c)$.

060 Previous related works in learning joint energy-based models (Grathwohl et al., 2019) or gradient-061 based denoisers (Cohen et al., 2021; Hurault et al., 2021; Yadin et al., 2024) have faced two key 062 questions, respectively concerning the training objective and network architecture. Indeed, learning 063 a probability density over high-dimensional images is a very challenging problem due to the need 064 to estimate normalization constants, which has only been recently empirically solved with scorematching approaches (Song et al., 2021). Additionally, different architectures, and therefore inductive 065 biases, are used for both tasks: CNN classifiers typically have a feedforward architecture which maps 066 an image x to a logits vector $(\log p(c|\mathbf{x}))_{1 < c < C}$, while CNN denoisers have a UNet encoder/decoder 067 architecture which outputs a denoised image $\hat{\mathbf{x}}$ with the same shape as the input image \mathbf{x} . The joint 068 approach requires unifying these two architectures in a single one whose forward pass corresponds to 069 a classifier and forward plus backward pass corresponds to a denoiser, while preserving the inductive biases that are known to work well for the two separate tasks. 071

Here, we propose principled solutions to these questions. As a result of our unifying conceptual framework, we derive a new interpretation of adversarial classifier gradients as a difference of denoisers, which complements previous connections between adversarial robustness and denoising. Our approach also opens new research directions: having direct access to a log-probability density log $p(\mathbf{y}, c)$ can be expected to lead to new applications, such as out-of-distribution detection or improved interpretability compared to score-based models.

- 078 The contributions of this paper are the following:
 - We introduce a framework to perform classification, class-conditional and unconditional denoising with a single network parameterizing the joint distribution $p(\mathbf{y}, c)$. The two training objectives naturally combine in a lower-bound on the likelihood of the joint model. Further, our approach evidences a deep connection between adversarial classifier gradients and (conditional) denoising. Pursuing this line of research thus has the potential to improve both classifier robustness and denoiser conditioning.
 - We propose an architecture to parameterize the joint log-probability density of images and labels which we call GradResNet. It makes minimal modifications to a ResNet architecture to incorporate inductive biases from UNet architectures appropriate to denoising (when computing a backward pass), while preserving those for classification (in the forward pass).
 - We validate the potential of our method on the CIFAR-10 and ImageNet datasets. In particular, our method is significantly more efficient and scalable than previous approaches (Grathwohl et al., 2019; Yang & Ji, 2021; Yang et al., 2023). Additionally, we show that the denoising objective improves classification performance and robustness.

We motivate our approach through the perspectives of joint energy modeling and denoising score matching in Section 2. We then present our method in detail in Section 3, and evaluate it numerically in Section 4. We discuss our results in connection with the literature in Section 5. We conclude and evoke future research directions in Section 6.

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2 JOINT ENERGY-SCORE MODELS

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Consider a dataset of labeled images $(\mathbf{x}_i, c_i)_{1 \le i \le n}$ with images $\mathbf{x}_i \in \mathbb{R}^d$ and class labels $c_i \in \{1, \ldots, C\}$ of i.i.d. pairs sampled from a joint probability distribution $p(\mathbf{x}, c)$. Typical machine learning tasks then correspond to estimating conditional or marginal distributions: training a classifier amounts to learning a model of $p(c|\mathbf{x})$, while (conditional) generative modeling targets $p(\mathbf{x})$ or $p(\mathbf{x}|c)$. Rather than solving each of these problems separately, this paper argues for training a *single* model $p_{\theta}(\mathbf{x}, c)$ of the *joint* distribution $p(\mathbf{x}, c)$, following Hinton (2007); Grathwohl et al. (2019).

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Figure 1: Illustration of the generalization bounds $b + \frac{v}{n}$ in two idealized settings with stylized values for b and v. Left: bias-dominated setting with $b^{\text{gen}} = 5$, $b^{\text{dis}} = 1$, $v^{\text{gen}} = 20$, $v^{\text{dis}} = 100$. Right: variance-dominated setting with $b^{\text{gen}} = b^{\text{dis}} = 1$, $v^{\text{gen}} = 100$, $v^{\text{dis}} = 10000$.

The conditional and marginal distributions can then be recovered from the joint model with

$$p_{\theta}(c|\mathbf{x}) = \frac{p_{\theta}(\mathbf{x},c)}{\sum_{c=1}^{C} p_{\theta}(\mathbf{x},c)}, \qquad p_{\theta}(\mathbf{x}) = \sum_{c=1}^{C} p_{\theta}(\mathbf{x},c), \qquad p_{\theta}(\mathbf{x}|c) = \frac{p_{\theta}(\mathbf{x},c)}{p_{\theta}(c)}.$$
 (1)

We note that $p_{\theta}(c)$ is intractable to compute, but in the following we will only need the score of the conditional distribution $\nabla_{\mathbf{x}} \log p_{\theta}(\mathbf{x}|c)$, which is equal to $\nabla_{\mathbf{x}} \log p_{\theta}(\mathbf{x},c)$ independently of $p_{\theta}(c)$.

In Section 2.1, we motivate the joint approach and detail its potential benefits over separate modeling of the conditional distributions. We then extend this to the context of diffusion models in Section 2.2, which leads to an interpretation of adversarial gradients as a difference of denoisers.

132 2.1 Advantages of joint over conditional modeling

134 We first focus on classification. Models of the conditional distribution $p(c|\mathbf{x})$ derived from a model of the joint distribution $p(\mathbf{x}, c)$ are referred to as generative classifiers, as opposed to discriminative 135 classifiers which directly model $p(c|\mathbf{x})$. The question of which approach is better goes back at least 136 to Vapnik (1999). It was then generally believed that discriminative classifiers were better: quoting 137 Vapnik (1999), "when solving a given problem, try to avoid solving a more general problem as an 138 intermediate step". This has led the community to treat the modeling of $p(\mathbf{x})$ and $p(c|\mathbf{x})$ as two 139 separate problems, though there were some joint approaches (Ng & Jordan, 2001; Raina et al., 2003; 140 Ulusoy & Bishop, 2005; Lasserre et al., 2006; Ranzato et al., 2011). In the deep learning era, the joint 141 approach was revitalized by Grathwohl et al. (2019) with several follow-up works (Liu & Abbeel, 142 2020; Grathwohl et al., 2021; Yang & Ji, 2021; Yang et al., 2023). They showed the many benefits of 143 generative classifiers, such as better calibration and increased robustness to adversarial attacks. It was 144 also recently shown in Jaini et al. (2024) that generative classifiers are much more human-aligned in 145 terms of their errors, shape-vs-texture bias, and perception of visual illusions. We reconcile these apparently contradictory perspectives by updating the arguments in Ng & Jordan (2001) to the modern 146 setting. 147

Consider that we have a parametrized family $\{p_{\theta}(\mathbf{x}, c), \theta \in \mathbb{R}^m\}$ (for instance, given by a neural network architecture). Generative and discriminative classifiers are respectively trained to maximize likelihood or minimize cross-entropy:

$$\theta_n^{\text{gen}} = \arg\max_{\theta} \frac{1}{n} \sum_{i=1}^n \log p_{\theta}(\mathbf{x}_i, c_i), \qquad \theta_n^{\text{dis}} = \arg\max_{\theta} \frac{1}{n} \sum_{i=1}^n \log p_{\theta}(c_i | \mathbf{x}_i).$$
(2)

We measure the expected generalization error of the resulting classifiers in terms of the Kullback-Leibler divergence on a test point $\mathbf{x} \sim p(\mathbf{x})$:

$$\varepsilon(\theta) = \mathbb{E}_{\mathbf{x} \sim p(\mathbf{x})} [\mathrm{KL}(p(c|\mathbf{x}) \parallel p_{\theta}(c|\mathbf{x}))].$$
(3)

We show that it can be described with "bias" and "variance" constants b^{gen} , b^{dis} , v^{gen} , v^{dis} :

$$\mathbb{E}[\varepsilon(\theta_n^{\text{gen}})] = b^{\text{gen}} + \frac{v^{\text{gen}}}{2n} + o\left(\frac{1}{n}\right), \qquad \mathbb{E}[\varepsilon(\theta_n^{\text{dis}})] = b^{\text{dis}} + \frac{v^{\text{dis}}}{2n} + o\left(\frac{1}{n}\right), \qquad (4)$$

where the expected values average over the randomness of the training set. This is derived with standard arguments in Appendix D, where the constants are explicited as functions of p and $\{p_{\theta}\}$. The bias arises from model misspecification, while the variance measures the sample complexity of the model, as we detail below. We note that these results are only asymptotic, and the constants hidden in the little-o notation could be exponential in the dimension. Nevertheless, these results provide evidence of the two distinct regimes found by Ng & Jordan (2001), as illustrated in Figure 1.

168 Which approach is better then depends on the respective values of the bias and variance constants. 169 The bias is the asymptotic error when $n \to \infty$, and thus only depends on approximation properties. 170 It always holds that $b^{\text{dis}} \leq b^{\text{gen}}$, as discriminative classifiers directly model $p(c|\mathbf{x})$ and thus do not 171 pay the price of modeling errors on $p(\mathbf{x})$. The variance measures the number of samples needed to 172 reach this asymptotic error. In the case of zero bias, we have $v^{\text{gen}} \leq v^{\text{dis}}$ (and further $v^{\text{dis}} = m$ the 173 number of parameters): generative classifiers learn faster (with fewer samples) as they exploit the 174 extra information in $p(\mathbf{x})$ to estimate the parameters. With simple models with few parameters (e.g., 175 linear models, as in Ng & Jordan (2001)), we can expect the bias to dominate, which has led the 176 community to initially favor discriminative classifiers. On the other hand, with complex expressive models (e.g., deep neural networks) that have powerful inductive biases, we can expect the variance 177 to dominate. In this case, generative classifiers have the advantage, as can be seen in the recent 178 refocus of the community towards generative models and classifiers (Grathwohl et al., 2019; Jaini 179 et al., 2024). The success of self-supervised learning also indicates the usefulness of modeling $p(\mathbf{x})$ 180 to learn $p(c|\mathbf{x})$. 181

For similar reasons, a joint approach can also be expected to lead to benefits in conditional generative modeling. For instance, Dhariwal & Nichol (2021) found that conditional generative models could be improved by classifier guidance, and Ho & Salimans (2022) showed that these benefits could be more efficiently obtained with a single model.

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187 2.2 JOINT MODELING WITH DIFFUSION MODELS

188 The joint approach offers significant statistical advantages, but also comes with computational 189 challenges. Indeed, it requires to learn a model of a probability distribution over the high-dimensional 190 image \mathbf{x} , while in a purely discriminative model it only appears as a conditioning variable (the 191 probability distribution is over the discrete class label c). In Grathwohl et al. (2019), the generative 192 model is trained directly with maximum-likelihood and Langevin-based MCMC sampling, which 193 suffers from the curse of dimensionality and does not scale to large datasets such as ImageNet. We 194 revisit their approach in the context of denoising diffusion models, which have empirically resolved these issues. We briefly introduce them here, and explain the connections with adversarial robustness 195 in the context of generative classifiers. 196

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Diffusion models and denoising. In high-dimensions, computing maximum-likelihood parameters is typically intractable due to the need to estimate normalizing constants. As a result, Hyvärinen proposed to replace maximum-likelihood with score matching (Hyvärinen & Dayan, 2005), which removes the need for normalizing constants and is thus computationally feasible. However, its sample complexity is typically much larger as a result of this relaxation (Koehler et al., 2022). Song et al. (2021) showed that this computational-statistical tradeoff can be resolved by considering a diffusion process (Sohl-Dickstein et al., 2015; Ho et al., 2020; Song & Ermon, 2019; Kadkhodaie & Simoncelli, 2021), where maximum-likelihood and score matching become equivalent.

Denoising diffusion models consider the joint distribution $p_{\sigma}(\mathbf{y}, c)$ of noisy images \mathbf{y} together with class labels c for every noise level σ . Formally, the noisy image \mathbf{y} is obtained by adding Gaussian white noise of variance σ^2 to the clean image \mathbf{x} :

$$\mathbf{y} = \mathbf{x} + \sigma \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathrm{Id}).$$
 (5)

210 Note that the class label c becomes increasingly independent from y as σ increases.

Modeling $p(\mathbf{y})$ or $p(\mathbf{y}|c)$ by score matching then amounts to performing unconditional or classconditional denoising (Vincent, 2011), thanks to an identity attributed to Tweedie and Miyasawa (Robbins, 1956; Miyasawa et al., 1961; Raphan & Simoncelli, 2011):

$$\nabla_{\mathbf{y}} \log p(\mathbf{y}) = \frac{\mathbb{E}[\mathbf{x} \mid \mathbf{y}] - \mathbf{y}}{\sigma^2}, \qquad \nabla_{\mathbf{y}} \log p(\mathbf{y}|c) = \frac{\mathbb{E}[\mathbf{x} \mid \mathbf{y}, c] - \mathbf{y}}{\sigma^2}, \qquad (6)$$

see e.g. Kadkhodaie & Simoncelli (2021) for proof. Note that $\mathbb{E}[\mathbf{x} | \mathbf{y}]$ and $\mathbb{E}[\mathbf{x} | \mathbf{y}, c]$ are the best approximations of \mathbf{x} given \mathbf{y} (and c) in mean-squared error, and are thus the optimal unconditional and conditional denoisers. A joint model $p_{\theta}(\mathbf{y}, c)$ thus gives us access to unconditional and classconditional denoisers \mathcal{D}_{u} and \mathcal{D}_{c} ,

$$\mathcal{D}_{\rm u}(\mathbf{y}) = \mathbf{y} + \sigma^2 \nabla_{\mathbf{y}} \log p_{\theta}(\mathbf{y}), \qquad \qquad \mathcal{D}_{\rm c}(\mathbf{y}, c) = \mathbf{y} + \sigma^2 \nabla_{\mathbf{y}} \log p_{\theta}(\mathbf{y}|c), \qquad (7)$$

which can be trained to minimize mean-squared error:

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$$\min \mathbb{E}\Big[\|\mathbf{x} - \mathbf{y} - \sigma^2 \nabla_{\mathbf{y}} \log p_{\theta}(\mathbf{y})\|^2\Big], \qquad \min \mathbb{E}\Big[\|\mathbf{x} - \mathbf{y} - \sigma^2 \nabla_{\mathbf{y}} \log p_{\theta}(\mathbf{y}|c)\|^2\Big].$$
(8)

Adversarial gradients. In this formulation, the adversarial classifier gradients (on noisy images) can be interpreted as a scaled difference of conditional and unconditional denoisers:

$$\nabla_{\mathbf{y}} \log p_{\theta}(c|\mathbf{y}) = \nabla_{\mathbf{y}} \log p_{\theta}(\mathbf{y}|c) - \nabla_{\mathbf{y}} \log p_{\theta}(\mathbf{y}) = \frac{1}{\sigma^2} (\mathcal{D}_{c}(\mathbf{y},c) - \mathcal{D}_{u}(\mathbf{y})).$$
(9)

The adversarial gradient on clean images is obtained by sending the noise level $\sigma \to 0$, highlighting 230 potential instabilities. Equation (9) provides a novel perspective on adversarial robustness (which was 231 implicit in Ho & Salimans (2022)): adversarial gradients are the details in an infinitesimally noisy 232 image that are recovered when the denoiser is provided with the class information. Being robust to 233 attacks, which requires small adversarial gradients, thus requires the conditional denoiser to mostly 234 ignore the provided class information when it is inconsistent with the input image at small noise 235 levels. The denoising objective (8) thus directly regularizes the adversarial gradients. We discuss 236 other connections between additive input noise and adversarial robustness in Section 5.1. 237

Likelihood evaluation. We also note that modeling the log-probability rather than the score has several advantages in diffusion models. First, it potentially allows to evaluate likelihoods in a single forward pass, as done in Choi et al. (2022); Yadin et al. (2024). Second, it leads to generative classifiers that can be evaluated much more efficiently than recent approaches based on score diffusion models (Li et al., 2023; Clark & Jaini, 2023; Jaini et al., 2024).

244 3 ARCHITECTURE AND TRAINING 245

The previous section motivated the joint approach and led to a unification between classification and denoising tasks. We now focus on these two problems, and describe our parameterization of the joint log-probability density (Section 3.1), the GradResNet architecture (Section 3.2), and the training procedure (Section 3.3).

3.1 PARAMETERIZATION OF JOINT LOG-PROBABILITY

We want to parameterize the joint log-probability density $\log p(c, \mathbf{y})$ over (noisy) images $\mathbf{y} \in \mathbb{R}^d$ and image classes c using features computed by a neural network $f : \mathbb{R}^d \to \mathbb{R}^K$. In classification, the class logits are parameterized as a linear function of the features

$$\log p_{\theta}(c|\mathbf{y}) = (\mathbf{W}f(\mathbf{y}))_{c} - \operatorname{LogSumExp}_{c'}((\mathbf{W}f(\mathbf{y}))_{c'}),$$
(10)

with W a matrix of size $C \times K$ where C is the number of classes. We propose to parameterize the log-probability density of the noisy image distribution as a *quadratic* function of the features

$$\log p_{\theta}(\mathbf{y}) = -\frac{1}{2} (\mathbf{w}^{\mathrm{T}} f(\mathbf{y}))^2 - \log Z(\theta), \qquad (11)$$

where $\mathbf{w} \in \mathbb{R}^{K}$ and $Z(\theta)$ is a normalizing constant that depends only on the parameters θ . We thus have the following parameterization of the joint log-density

$$\log p_{\theta}(\mathbf{y}, c) = -\frac{1}{2} (\mathbf{w}^{\mathrm{T}} f(\mathbf{y}))^{2} + (\mathbf{W} f(\mathbf{y}))_{c} - \mathrm{LogSumExp}_{c'} ((\mathbf{W} f(\mathbf{y}))_{c'}) - \log Z(\theta).$$
(12)

Finally, the log-density of noisy images y conditioned on the class c can be simply accessed with log $p_{\theta}(\mathbf{y}|c) = \log p_{\theta}(\mathbf{y}, c) - \log p_{\theta}(c)$, where $\log p_{\theta}(c)$ is intractable but not needed in practice, as explained in Section 2. We chose the task heads to be as simple as possible, being respectively linear (for classification) and quadratic (for denoising) in the features. Preliminary experiments showed that additional complexity did not result in improved performance.



Figure 2: Left: ResNet BasicBlock with bias parameters, batch-normalization (BN) layers and ReLUs. Middle: GradResNet BasicBlock with bias-free convolutional layers, GELUs, and a single group-normalization (GN) layer. **Right:** Illustration of the proposed side connections.

3.2 GRADRESNET ARCHITECTURE

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We now specify the architecture of the neural network f_{θ} . As discussed in Section 2, realizing the 290 potential of the joint modeling approach requires that the modeling bias is negligible, or in other words, that the inductive biases of the architecture and training algorithm are well-matched to the 292 data distribution. Fortunately, we can rest on more than a decade of research on best architectures 293 for image classification and denoising. Architectures for these two tasks are however quite different, and the main difficulty lies in unifying them: in particular, we want the computational graph of the 295 gradient of a classifier network to be structurally similar to a denoising network.

296 In a recent work, Hurault et al. (2021) presented a gradient-based denoiser for Plug-and-Play image 297 restoration, and they found that "directly modeling [the denoiser] as [the gradient of] a neural network 298 (e.g., a standard network used for classification) leads to poor denoising performance". To remedy 299 this problem, we thus propose the following architectural modifications on a ResNet18 backbone:

300 **Smooth activation function:** Cohen et al. (2021) first proposed to use the gradient of a feedforward 301 neural network architecture as an image denoiser for Plug-and-Play image restoration. They write 302 "an important design choice is that all activations are continuously differentiable and smooth func-303 tions". We thus replace ReLUs with smooth GELUs, following recent improvements to the ResNet 304 architecture (Liu et al., 2022). 305

Normalization: Batch-normalization (loffe & Szegedy, 2015) is a powerful optimization technique, 306 but its major drawback is that it has different behaviors in train and eval modes, especially 307 for the backward pass. We hence replace batch-normalizations with group-normalizations (Wu 308 & He, 2018), leading to a marginal decrease in classification performance on ImageNet (Wu & He, 2018). Moreover, we found that reducing the number of normalization layers is beneficial for 310 denoising performance. While ResNets apply a normalization after each convolutional layer, we 311 apply a group-normalization at the end of each basic block (see Figure 2). 312

Bias removal: Mohan et al. (2020) have shown that removing all bias parameters in CNN denoisers 313 enable them to generalize across noise levels outside their training range. We decide to adopt this 314 modification, removing all biases of convolutional, linear, and group-norm layers. 315

Mimicking skip connections: The computational graph of the gradient of a feedforward CNN can 316 be viewed as a UNet, where the forward pass corresponds to the encoder (reducing image resolution), 317 and the backward pass corresponds to the decoder (going back to the input domain). Zhang et al. 318 (2021) show that integrating residual connections in the UNet architecture is beneficial for denoising 319 performance. In order to emulate these residual connections in our gradient denoiser, we add side 320 connections to our ResNet as illustrated in Figure 2 c). 321

With all these modification, we end up with a new architecture that we name *GradResNet*, which 322 is still close to the original ResNet architecture. As we will show in the numerical experiments in 323 Section 4, this architecture retains a strong accuracy and obtains competitive denoising results.

Table 1: CIFAR-10 experimental results. Training time is measured on a single NVIDIA A100 GPU, except for JEM, whose results and training time are taken from Grathwohl et al. (2019). Best results are highlighted in bold for each category of models.

Task	Architecture	Accuracy (%)	$\mathbf{PSNR}_{\sigma=15}$	$\mathbf{PSNR}_{\sigma=25}$	$\mathbf{PSNR}_{\sigma=50}$	Training time (h)
Classification	ResNet18	96.5	N.A.	N.A.	N.A.	0.7
	GradResNet	96.1	N.A.	N.A.	N.A.	0.7
Denoising	DnCNN	N.A.	32.05	29.07	25.23	0.8
	DRUNet	N.A.	32.12	29.20	25.52	0.9
	GradResNet	N.A.	32.21	29.28	25.51	1.3
Joint	JEM (WideResNet)	92.9	N.A.	N.A.	N.A.	36
	GradResNet	96.3	31.90	29.00	25.25	1.3

3.3 TRAINING

Training objectives. Our model of the joint log-distributions $\log p_{\theta}(\mathbf{y}, c)$ is the sum of two terms, $\log p_{\theta}(c|\mathbf{y})$ and $\log p_{\theta}(\mathbf{y})$. Our training objective is thus naturally a sum of two losses: a crossentropy loss for the class logits $\log p_{\theta}(c|\mathbf{y})$, and a denoising score matching loss for $\log p_{\theta}(\mathbf{y})$. Both objectives are integrated over noise levels σ . For simplicity, we do not add any relative weighting of the classification and denoising objectives. Our final training loss is thus

$$\ell(\theta) = \mathbb{E}\Big[-\log p_{\theta}(c|\mathbf{y}) + \left\|\sigma\nabla_{\mathbf{y}}\log p_{\theta}(\mathbf{y}) + \boldsymbol{\epsilon}\right\|^{2}\Big],\tag{13}$$

347 where the expectation is over $(\mathbf{x}, c) \sim p(\mathbf{x}, c), \epsilon \sim \mathcal{N}(0, \mathrm{Id})$, and $\sigma \sim p(\sigma)$ (described below). The 348 main advantage of the joint learning framework is that the two tasks (modeling $p(\mathbf{x})$ and $p(c|\mathbf{x})$) 349 naturally combine in a single task (modeling $p(\mathbf{x}, c)$), thus removing the need for tuning a Lagrange 350 multiplier trading off the two losses (where we interpret the denoising objective as a lower-bound 351 on the negative-log-likelihood (Song et al., 2021)). Finally, we note that although redundant, one 352 can also add a conditional denoising objective $\|\sigma \nabla_{\mathbf{y}} \log p_{\theta}(\mathbf{y}|c) + \boldsymbol{\epsilon}\|^2$, or use it to replace the 353 unconditional denoising objective. We have empirically found no difference between these choices. 354 Full experimental details can be found in Appendix A. 355

356 **Training distributions.** Data augmentation is used in both image classification and image denoising to reduce overfitting, but with different augmentation strategies. On the one hand, state of the 357 art image classification models, e.g. Liu et al. (2022), are trained with the sophisticated MixUp 358 (Zhang et al., 2017a) and CutMix (Yun et al., 2019) augmentations which significantly improve 359 classification performance but introduce visual artifacts and thus lead to non-natural images. On the 360 other hand, state-of-the-art denoisers like Restormer (Zamir et al., 2022) or Xformer (Zhang et al., 361 2023) use simple data-augmentation techniques like random image crops (without padding) and 362 random horizontal flips, which leave the distribution of natural images unchanged. We thus use these different data-augmentation techniques for each objective, and thus the two terms in our objective are 364 computed over different image distributions. Though this contradicts the assumptions behind the joint 365 modeling approach, we found that the additional data-augmentations on the classification objective 366 significantly boosted accuracy without hurting denoising performance. We also found beneficial to 367 use different noise level distributions $p(\sigma)$ for the two tasks. In both cases, σ is distributed as the 368 square of a uniform distribution, with $\sigma_{\min} = 1$ and $\sigma_{\max} = 100$ for denoising but $\sigma_{\max} = 20$ for classification (relative to image pixel values in [0, 255]). On the ImageNet dataset, for computational 369 efficiency, we set the image and batch sizes for the denoising objective according to a schedule 370 following Zamir et al. (2022), explicited in Appendix A. 371

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4 NUMERICAL RESULTS

375 4.1 CLASSIFICATION AND DENOISING VIA JOINT MODELING

377 With the proposed joint modeling framework, we can perform classification and denoising at the same time. Training and implementation details are given in Section 3 and Appendix A. We measure the

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Task	Architecture	Accuracy (%)	$\mathbf{PSNR}_{\sigma=15}$	$\mathbf{PSNR}_{\sigma=25}$	$\mathbf{PSNR}_{\sigma=50}$	Training time (h)
Classification	ResNet18	69.8	N.A.	N.A.	N.A.	96
Joint	GradResNet	68.6	34.59	31.94	27.17	208

Table 2: ImageNet experimental results. Training time is measured on a single NVIDIA A100 GPU.



Figure 3: Denoising experiment. **Top, left-to-right:** Original CIFAR-10 test image, noisy image $(\sigma = 50)$, denoised images with unconditional and conditional denoisers, and difference between them (magnified 500x). **Bottom, left-to-right:** Eigenvectors corresponding to the three largest (2.71,2.16, 2.03) and two lowest $(2.8 \times 10^{-5}, -1.9 \times 10^{-5})$ magnitude eigenvalues of the unconditional denoiser Jacobian. More examples are shown in Appendix C.

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classification accuracy and the denoising PSNR averaged over the test set, compared with baselines.
The classification baseline is a standard ResNet18 (He et al., 2016). As denoising baselines, we use
two standard architectures, DnCNN (Zhang et al., 2017b) and DRUNet (Zhang et al., 2021). All
baselines are trained with the same setup as our joint approach (but on a single objective).

404 Results are shown in Table 1 for CIFAR-10 (Krizhevsky et al., 2009) and in Table 2 for ImageNet 405 (Russakovsky et al., 2015). We obtain classification and denoising performances that are competitive 406 with the baselines. Importantly, our method provides a big computational advantage to the previous work JEM (Grathwohl et al., 2019), as can be seen from the training times in Table 1. JEM is 407 based on maximum-likelihood training, which is very challenging to scale in high dimensions (as the 408 authors of note, "training [...] can be quite unstable"), and therefore has been limited to 32×32 -sized 409 images, even in subsequent work (Yang et al., 2023). In contrast, denoising score matching is a 410 straightforward regression, which leads to a stable and lightweight training that scales much more 411 easily to ImageNet at full 224×224 resolution. 412

In Table 1, we report results for GradResNet trained on a single task to separate the impact of each objective. We remark that the denoising objective *improves* classification performance, confirming the arguments in Section 2.1. The classification objective however slightly degrades denoising performance. We also conduct several ablation experiments to validate our architecture choices in Table 3 in Appendix B. All our choices are beneficial for both classification and denoising performance, except for the removal for biases which very slightly affects denoising performance.

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4.2 ANALYZING THE LEARNED DENOISERS

On the top row of Figure 3, we show an example of a noisy image denoised using the learned
 unconditional and class-conditional denoisers. We also show the difference between the two denoised
 images scaled by a factor of 500. The two denoised images look very similar, suggesting that the
 class conditioning is not very informative here.

Importantly, as we removed all the bias terms from the convolutional layers, our denoisers are bias-free. Mohan et al. (2020) have shown that bias-free deep denoisers \mathcal{D} are locally linear operators, i.e., $\mathcal{D}(\mathbf{y}) = \nabla_{\mathbf{y}} \mathcal{D}(\mathbf{y}) \mathbf{y}$, where $\nabla_{\mathbf{y}} \mathcal{D}(\mathbf{y})$ is the Jacobian of the denoiser evaluated at \mathbf{y} . To study the effect of a denoiser on a noisy image \mathbf{y} , one can compute the singular value decomposition of the denoiser's Jacobian evaluated at \mathbf{y} (see Mohan et al. (2020) for details). The Jacobian of our unconditional denoiser is

$$\nabla_{\mathbf{y}} \mathcal{D}_{\mathbf{u}}(\mathbf{y}) = \mathrm{Id} + \sigma^2 \nabla_{\mathbf{y}}^2 \log p_{\theta}(\mathbf{y}), \tag{14}$$



Figure 4: Adversarial attacks on CIFAR-10 test set. The baseline is a ResNet18 trained for classification only, ours is a GradResNet trained for classification and denoising, and JEM is the method proposed by Grathwohl et al. (2019). Left: ℓ^{∞} PGD attack. Right: ℓ^2 PGD attack.

where ∇^2 denotes the Hessian. Since our denoiser is a gradient field, its Jacobian is symmetric, and can thus be diagonalized. The bottom row of Figure 3 shows the eigenvectors corresponding to the three largest and two lowest magnitude eigenvalues. Interestingly, eigenvectors corresponding to largest eigenvalues capture large scale features from the original image which are amplified by the denoiser. Conversely, lowest eigenvectors correspond to noisy images without shape nor structure that are discarded by the denoiser.

4.3 ADVERSARIAL ROBUSTNESS

In their seminal work on joint-modeling, Grathwohl et al. (2019) show that learning the joint distribution over images and classes leads to increased robustness to adversarial attacks. We perform projected gradient descent (PGD) adversarial attacks using the foolbox library (Rauber et al., 2020) on our baseline classifier and the classifier optimized for joint-modeling. Results are shown in Figure 4. We note that the proposed method increases adversarial robustness, but not as much as an MCMC-trained joint energy-based model (Grathwohl et al., 2019).

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5 DISCUSSION AND RELATED WORK

5.1 ROBUST CLASSIFIERS

Adversarial robustness. Adversarial robustness is deeply related to noise addition. Indeed, Gu 465 & Rigazio (2014) have shown that adding noise to adversarial attacks (referred to as randomized 466 smoothing) can mitigate their effect. Further, Lecuyer et al. (2019) and follow-ups (Li et al., 2019; 467 Cohen et al., 2019) showed that being robust to additive noise provably results in adversarial robust-468 ness using this strategy. This was recently shown to be practical in Maho et al. (2022). Note that 469 noise addition at test time (as opposed to only during training) is critical to obtain robustness (Carlini 470 & Wagner, 2017), an observation also made in Su & Kempe (2023). This appears in the instability of 471 the $\sigma \to 0$ limit in eq. (9), and indicates that robustness tests as in Figure 4 should be computed over 472 attack strength and noise levels.

Building classifiers that are robust to additive noise on the input image was considered in many works (note that this is separate from the issue of learning from noisy labels). Dodge & Karam (2017) found that fine-tuning standard networks on noisy images improve their robustness, but still falls short of human accuracy at large noise levels. A common benchmark (which also include corruptions beyond additive noise) was established in Hendrycks & Dietterich (2018). Effective approaches include carefully designing pooling operators (Li et al., 2020) and iterative distillation (Xie et al., 2020).

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Adversarial gradients and generative models. Several works use denoisers or other generative models to improve adversarial or noise robustness, e.g., by denoising input images as a pre-processing step (Roy et al., 2018), or by leveraging an off-the-shelf generative model to detect and "purify" adversarial examples (Song et al., 2017). Grathwohl et al. (2019) unified the generative model and the classifier in a single model and showed that joint modeling results in increased adversarial robustness. Our work goes one step further by also making the connection to noise robustness and denoising through diffusion models, warranting further work in this direction.

486 5.2 SAMPLING AND ARCHITECTURE OF GRADIENT DENOISERS

488 Gradient denoiser architectures. Several works have studied the question of learning the score as a gradient. Most similar to our setup is Cohen et al. (2021), where the authors introduce the GraDnCNN 489 architecture. When modeling directly the score with a neural network, Saremi (2019) show that the 490 learned score is not a gradient field unless under very restrictive conditions. Nonetheless, Mohan et al. 491 (2020) show that the learned score is approximately conservative (i.e., a gradient field), and Chao et al. 492 (2023) introduce an additional training objective to penalize the non-conservativity. Finally, Horvat 493 & Pfister (2024) demonstrate that the non-conservative component of the score is ignored during 494 sampling with the backward diffusion, though they find that a conservative denoiser is necessary for 495 other tasks such as dimensionality estimation. Our work provides several recommendations for the 496 design of gradient-based denoisers.

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498 **Sampling.** Preliminary experiments indicate that sampling from the distributions $p(\mathbf{x})$ and $p(\mathbf{x}|c)$ 499 learned by our model, e.g. with DDPM (Ho et al., 2020), is not on par with standard diffusion models. 500 Salimans & Ho (2021) noted that "specifying the score model by taking the gradient of an image classifier has so far not produced competitive results in image generation." While our changes to the 501 ResNet architecture significantly alleviate these issues, its gradient might not have the right inductive 502 biases to model the score function. Indeed, recent works (Salimans & Ho, 2021; Hurault et al., 503 2021; Yadin et al., 2024) rather model log-probabilities with (the squared norm of) a UNet, whose 504 gradient is then more complicated (its computational graph is not itself a UNet). Understanding the 505 inductive biases of these different approaches is an interesting direction for future work. After the 506 completion of this work, we became aware of a related approach by (Guo et al., 2023). They tackle 507 classification and denoising with a UNet network, and demonstrate competitive sampling results. 508 This complements our conceptual arguments for the joint approach, confirms its potential, and calls 509 for an explanation between the discrepancies in performance between the two architectures.

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511 **Conditioning.** We also note that the class information is used differently in classification and 512 conditional denoising. On the one hand, in classification, the class label is only used as an index 513 in the computed logits (which allows for fast evaluation of all class logits). On the other hand, conditional denoisers typically embed the class label as a continuous vector, which is then used to 514 modify gain and bias parameters in group-normalization layers (which is more expressive). This 515 raises the question whether these two different approaches could be unified in the joint framework. 516 An area where we expect the joint approach to lead to significant advances is in that of caption 517 conditioning, where the classifier $\log p(c|\mathbf{y})$ is replaced by a captioning model. Training a *single* 518 model on *both* objectives has the potential to improve the correspondence between generated images 519 and the given caption. Another type of conditioning is with the noise level σ , also known as the time 520 parameter t. In a recent work, Yadin et al. (2024) propose classification diffusion models (CDM). 521 They model the joint distribution over images and discrete noise levels with denoising score matching 522 and noise level classification. Both approaches are orthogonal and could be combined in future work.

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6 CONCLUSION

In this paper, we have shown that several machine-learning tasks and issues are deeply connected:
 classification, denoising, generative modeling, adversarial robustness, and conditioning are unified by
 our joint modeling approach. Our method is significantly more efficient than previous maximum likelihood approaches, and we have shown numerical experiments which give promising results on
 image (robust) classification and image denoising, though not yet in image generation.

531 We believe that exploring the bridges between these problems through the lens of joint modeling as 532 advocated in this paper are fruitful research directions. For instance, can we understand the different 533 inductive biases of ResNet and UNet architectures in the context of joint energy-based modeling? 534 Can we leverage the connection between adversarial gradients and denoising to further improve classifier robustness? We also believe that the joint approach holds significant potential in the case 536 where the class label c is replaced by a text caption. Indeed, modeling the distribution of captions p(c)is highly non-trivial and should be beneficial to conditional generative models for the same reasons than we used to motivate generative classifiers in Section 2.1. Finally, the joint approach yields a 538 model of the log-probability $\log p(\mathbf{y})$, as opposed to the score $\nabla_{\mathbf{y}} \log p(\mathbf{y})$. We thus expect that this model could be used to empirically probe properties of high-dimensional image distributions.

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A TRAINING AND IMPLEMENTATION DETAILS

786 **Experiments on CIFAR-10.** We implement the proposed network and the training script using the 787 PyTorch library (Paszke et al., 2019). We adapt the original ResNet18 (He et al., 2016) to 32×32 788 images by setting the kernel size of the first convolutional layer to 3 (originally 7) and the stride of the 789 first two convolutional layers to 1. We also remove the max-pooling layer. To train our GradResNet, 790 we use the AdamW optimizer with the default parameters except for the weight decay (0.05) and the 791 learning rate (3×10^{-4}) . We use a cosine annealing schedule for the learning rate, without warm-up. 792 We use a batch size of 64 for denoising and 128 for classification. The optimized loss is the sum of 793 the cross-entropy loss and the mean-squared denoising objective (eq. 13). We run the optimization 794 for 78k iterations, corresponding to 200 epochs for classification.

- For classification, we use for data-augmentation random horizontal flips, padded random crops with padding of 4 pixels, and MixUp (Zhang et al., 2017a) and CutMix (Yun et al., 2019) as implemented in torchvision.transforms with the default parameters. We also add Gaussian white noise scaled by σ that we draw from a squared uniform distribution in the range [0, 20]. For denoising, we simply use random flips. We add Gaussian noise with $\sigma \in [1, 100]$.
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801 Experiments on ImageNet. We use the standard ResNet18 architecture, but without the max-802 pooling layer. We set the learning rate to 2×10^{-4} and weight decay to 10^{-4} . We train the network for 803 400 epochs with a batch size of 512 for classification. We replace the random crop data augmentation 804 with random resized crops of size 224×224 . For denoising, we gradually change the image size and 805 batch size across training, following Zamir et al. (2022). That is, we compute the denoising loss over 806 image batches of size $64 \times 128 \times 128$ until epoch 150, then $40 \times 160 \times 160$ until epoch 260, then 807 $32 \times 192 \times 192$ until epoch 340, and $16 \times 224 \times 224$ until epoch 400. Smaller images are extracted by taking random crops of the chosen size. Both objectives are computed with Gaussian noise with σ 808 the square of a uniform distribution supported in [1, 70]. All other hyperparameters are the same as 809 for the CIFAR-10 dataset.

810 B ABLATION EXPERIMENTS

We present ablation experiments to validate our architecture choices of Section 3.2 in Table 3. Namely, we replace the GeLU non-linearity with the original ReLU, replace GroupNorm layers with the original BatchNorm, add biases to convolutional and GroupNorm layers, or remove side connections (see Figure 2).

Table 3: Ablation experiments on CIFAR-10 dataset.

Task	Architecture	Accuracy (%)	$\mathbf{PSNR}_{\sigma=15}$	$\mathbf{PSNR}_{\sigma=25}$	$\mathbf{PSNR}_{\sigma=50}$
	GradResNet	96.3	31.90	29.00	25.25
Joint	(ReLU)	92.0	29.59	24.90	17.11
	(BatchNorm)	11.9	24.33	20.84	18.06
	(Biases)	95.9	31.95	29.03	25.30
	(No side co.)	94.0	31.86	28.95	25.17

C DENOISING EXPERIMENTS

Additional denoising experiments are presented in Figure 5.

D BIAS-VARIANCE DECOMPOSITION OF THE GENERALIZATION ERROR

We sketch a derivation of the results. They can be rigorously proved under usual regularity conditions by a straightforward generalization of the proofs of asymptotic consistency, efficiency, and normality of the maximum-likelihood estimator (see, e.g., Hogg et al. (2013, Thereom 6.2.2)).

Given a function ℓ , a probability distribution $p(\mathbf{x})$, and i.i.d. samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$, consider the minimization problems

$$\theta_{\star} = \underset{\theta}{\operatorname{arg\,min}} \mathbb{E}[\ell(\theta, \mathbf{x})], \qquad \qquad \theta_n = \underset{\theta}{\operatorname{arg\,min}} \frac{1}{n} \sum_{i=1}^n \ell(\theta, \mathbf{x}_i). \tag{15}$$

We wish to estimate the fluctuations of the random parameters θ_n around the deterministic θ_{\star} when $n \to \infty$.

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The estimator θ_n is defined by

$$\sum_{i=1}^{n} \nabla_{\theta} \ell(\theta_n, \mathbf{x}_i) = 0.$$
(16)

A first-order Taylor expansion around θ_{\star} gives

$$\frac{1}{n}\sum_{i=1}^{n}\nabla_{\theta}\ell(\theta_{\star},\mathbf{x}_{i}) + \frac{1}{n}\sum_{i=1}^{n}\nabla_{\theta}^{2}\ell(\theta_{\star},\mathbf{x}_{i})(\theta_{n}-\theta_{\star}) = 0,$$
(17)

and thus

$$\theta_n = \theta_\star - \frac{1}{\sqrt{n}} \left(\frac{1}{n} \sum_{i=1}^n \nabla_\theta^2 \ell(\theta_\star, \mathbf{x}_i) \right)^{-1} \left(\frac{1}{\sqrt{n}} \sum_{i=1}^n \nabla_\theta \ell(\theta_\star, \mathbf{x}_i) \right).$$
(18)

By applying the law of large numbers to the first sum and the central limit theorem to the second sum (by definition of θ_* , $\mathbb{E}[\nabla_{\theta} \ell(\theta_*, \mathbf{x})] = 0$), it follows that as $n \to \infty$ we have

$$\theta_n \sim \mathcal{N}\left(\theta_\star, \frac{1}{n}\Sigma\right),$$
(19)

with a covariance

$$\Sigma = \mathbb{E} \Big[\nabla_{\theta}^2 \ell(\theta_{\star}, x) \Big]^{-1} \operatorname{Cov} [\nabla_{\theta} \ell(\theta_{\star}, \mathbf{x})] \mathbb{E} \Big[\nabla_{\theta}^2 \ell(\theta_{\star}, x) \Big]^{-1}.$$
(20)



Figure 5: Additional denoising experiments with $\sigma = 50$. See Figure 3 for details.

For the generative and discriminative modeling tasks, we have

$$\theta_{\star}^{\text{gen}} = \operatorname*{arg\,min}_{\theta} \mathbb{E}[-\log p_{\theta}(\mathbf{x}, c)], \qquad \theta_{n}^{\text{gen}} = \operatorname*{arg\,min}_{\theta} \frac{1}{n} \sum_{i=1}^{n} -\log p_{\theta}(\mathbf{x}_{i}, c_{i}), \quad (21)$$

$$\theta_{\star}^{\text{dis}} = \underset{\theta}{\arg\min} \ \mathbb{E}[-\log p_{\theta}(c|\mathbf{x})], \qquad \qquad \theta_{n}^{\text{dis}} = \underset{\theta}{\arg\min} \ \frac{1}{n} \sum_{i=1}^{n} -\log p_{\theta}(c_{i}|\mathbf{x}_{i}). \tag{22}$$

In this setting, eq. (20) yields

$$\Sigma^{\text{gen}} = \mathbb{E}\left[-\nabla_{\theta}^{2}\log p_{\theta_{\star}^{\text{gen}}}(\mathbf{x}, c)\right]^{-1} \operatorname{Cov}\left[-\nabla_{\theta}\log p_{\theta_{\star}^{\text{gen}}}(\mathbf{x}, c)\right] \mathbb{E}\left[-\nabla_{\theta}^{2}\log p_{\theta_{\star}^{\text{gen}}}(\mathbf{x}, c)\right]^{-1}, \quad (23)$$

$$\Sigma^{\rm dis} = \mathbb{E}\Big[-\nabla_{\theta}^2 \log p_{\theta_{\star}^{\rm dis}}(c|\mathbf{x})\Big]^{-1} \operatorname{Cov}\Big[-\nabla_{\theta} \log p_{\theta_{\star}^{\rm dis}}(c|\mathbf{x})\Big] \mathbb{E}\Big[-\nabla_{\theta}^2 \log p_{\theta_{\star}^{\rm dis}}(c|\mathbf{x})\Big]^{-1}.$$
 (24)

917 Note that we do not recover the Fisher information since expected values are with respect to the true distribution p, which is different from $p_{\theta_{\star}^{\text{gen}}}$ and $p_{\theta_{\star}^{\text{dis}}}$ under model misspecification.

These expressions can be plugged in a second-order Taylor expansion of the KL divergence: for any θ_n asymptotically normally distributed around θ_{\star} with covariance $\frac{1}{n}\Sigma$,

$$\mathbb{E}\left[\mathrm{KL}\left(p(c|\mathbf{x}) \| p_{\theta_n}(c|\mathbf{x})\right)\right] = \underbrace{\mathbb{E}\left[\mathrm{KL}\left(p(c|\mathbf{x}) \| p_{\theta_\star}(c|\mathbf{x})\right)\right]}_{b} + \frac{1}{2n}\underbrace{\mathrm{Tr}\left(\Sigma \mathbb{E}\left[-\nabla_{\theta}^2 \log p_{\theta_\star}(c|\mathbf{x})\right]\right)}_{v} + o\left(\frac{1}{n}\right).$$
(25)

Finally, we obtain

$$b^{\text{gen}} = \mathbb{E}\left[\text{KL}\left(p(c|\mathbf{x}) \| p_{\theta_{\star}^{\text{gen}}}(c|\mathbf{x})\right)\right], \qquad v^{\text{gen}} = \text{Tr}\left(\Sigma^{\text{gen}} \mathbb{E}\left[-\nabla_{\theta}^{2} \log p_{\theta_{\star}^{\text{gen}}}(c|\mathbf{x})\right]\right), \quad (26)$$

$$b^{\rm dis} = \mathbb{E}\Big[\mathrm{KL}\Big(p(c|\mathbf{x}) \,\Big\|\, p_{\theta^{\rm dis}_{\star}}(c|\mathbf{x})\Big)\Big], \qquad v^{\rm dis} = \mathrm{Tr}\Big(\Sigma^{\rm dis}\,\mathbb{E}\Big[-\nabla^2_{\theta}\log p_{\theta^{\rm dis}_{\star}}(c|\mathbf{x})\Big]\Big). \tag{27}$$

By definition of $\theta_{\star}^{\text{dis}}$, we have $b^{\text{dis}} \leq b^{\text{gen}}$ (since maximizing likelihood is equivalent to minimizing KL divergence). The variance terms can be compared when the model is well-specified, i.e., there exists θ_{\star} such that $p = p_{\theta_{\star}}$. In this case, we have $\theta_{\star}^{\text{gen}} = \theta_{\star}^{\text{dis}} = \theta_{\star}$, so that $b^{\text{gen}} = b^{\text{dis}} = 0$, and the variances simplify to

$$v^{\text{gen}} = \text{Tr}\left(\mathbb{E}\left[-\nabla_{\theta}^{2}\log p_{\theta_{\star}}(\mathbf{x}, c)\right]^{-1}\mathbb{E}\left[-\nabla_{\theta}^{2}\log p_{\theta_{\star}}(c|\mathbf{x})\right]\right) \le m,$$
(28)

$$v^{\rm dis} = {\rm Tr}({\rm Id}) = m, \tag{29}$$

using the Fisher information relationship

$$\mathbb{E}\Big[-\nabla_{\theta}^2 \log p_{\theta_{\star}}(c|\mathbf{x})\Big] = \operatorname{Cov}\Big[-\nabla_{\theta} \log p_{\theta_{\star}}(c|\mathbf{x})\Big],\tag{30}$$

and the decomposition

$$\mathbb{E}\left[-\nabla_{\theta}^{2}\log p_{\theta_{\star}}(\mathbf{x},c)\right] = \mathbb{E}\left[-\nabla_{\theta}^{2}\log p_{\theta_{\star}}(c|\mathbf{x})\right] + \underbrace{\mathbb{E}\left[-\nabla_{\theta}^{2}\log p_{\theta_{\star}}(\mathbf{x})\right]}_{\succeq 0}.$$
(31)

We thus have $v^{\text{gen}} \leq v^{\text{dis}}$ in the well-specified case.