Self-Supervised Variational Auto-Encoders

Abstract

Density estimation, compression, and data generation are crucial tasks in artificial intelligence. Variational Auto-Encoders (VAEs) constitute a single framework to achieve these goals. Here, we present a novel class of generative models, called *self-supervised Variational Auto-Encoder* (selfVAE), that utilizes deterministic and discrete transformations of data. This class of models allows performing both conditional and unconditional sampling while simplifying the objective function. First, we use a single self-supervised transformation as a latent variable, where a transformation is either downscaling or edge detection. Next, we consider a hierarchical architecture, i.e., multiple transformations, and we show its benefits compared to the VAE. The flexibility of selfVAE in data reconstruction finds a particularly interesting use case in data compression tasks, where we can trade-off memory for better data quality, and vice-versa. We present the performance of our approach on three benchmark image data (Cifar10, Imagenette64, and CelebA).

1. Introduction

The framework of variational autoencoders (VAEs) provides a principled approach for learning latent-variable models. As it utilizes a meaningful low-dimensional latent space with density estimation capabilities, it forms an attractive solution for generative modelling tasks. However, its performance in terms of the test log-likelihood and quality of generated samples is often disappointing, thus, many modifications were proposed. In general, one can obtain a tighter lower bound, and, thus, a more powerful and flexible model, by advancing over the following three components: the *encoder* (Rezende et al., 2014; van den Berg et al., 2018; Hoogeboom et al., 2020; Maaløe et al., 2016), the *prior* (or *marginal* over latents) (Chen et al., 2016; Habibian et al., 2019; Lavda et al., 2020; Lin and Clark, 2020; Tomczak and Welling, 2017) and the *decoder* (Gulrajani et al., 2016). Recent studies have shown that by employing deep hierarchical architectures and by carefully designing building blocks of the neural networks, VAEs can successfully model high-dimensional data and reach state-of-the-art test likelihoods (Zhao et al., 2017; Maaløe et al., 2019; Vahdat and Kautz, 2020).

In this work, we present a novel class of VAEs, called *self-supervised Variational Auto-Encoders*, where we introduce additional variables to VAEs that result from discrete and deterministic transformations of observed images. Since the transformations are deterministic, and they provide a specific aspect of images (e.g., contextual information through detecting edges or downscaling), we refer to them as *self-supervised representations*. The introduction of the discrete and deterministic variables allows to train deep hierarchical models efficiently by decomposing the task of learning a highly complex distribution into training smaller and conditional distributions. In this way, the model allows to integrate the prior knowledge about the data, but still enables to synthesize unconditional samples. Furthermore, the discrete and deterministic variables could be used to conditionally reconstruct data, which could be of great use in data compression and super-resolution tasks.

2. Our approach

Background   Let $\mathbf{x} \in \mathcal{X}^D$ be a vector of observable variables, where $\mathcal{X} \subseteq \mathbb{R}$ or $\mathcal{X} \subseteq \mathbb{Z}$, and $\mathbf{z} \in \mathbb{R}^M$ denote a vector of latent variables. Since calculating $p_\vartheta(\mathbf{x}) = \int p_\vartheta(\mathbf{x}, \mathbf{z})\mathrm{d}\mathbf{z}$ is computationally intractable for non-linear stochastic dependencies, a variational family of distributions could be used for approximate inference. Then, the following objective function could be derived, namely, the *evidence lower bound* (ELBO) (Jordan et al., 1999):

$$\ln p_\vartheta(\mathbf{x}) \geq \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \left[\ln p_\theta(\mathbf{x}|\mathbf{z}) + \ln p_\lambda(\mathbf{z}) - \ln q_\phi(\mathbf{z}|\mathbf{x}) \right], \tag{1}$$

where $q_\phi(\mathbf{z}|\mathbf{x})$ is the variational posterior (or the *encoder*), $p_\theta(\mathbf{x}|\mathbf{z})$ is the conditional likelihood function (or the *decoder*) and $p_\lambda(\mathbf{z})$ is the *prior* (or *marginal*), ϕ, θ and λ denote parameters.

The expectation is approximated by Monte Carlo sampling while exploiting the *reparameterization trick* in order to obtain unbiased gradient estimators. The models are parameterized by neural networks. This generative framework is known as *Variational Auto-Encoder* (VAE) (Kingma and Welling, 2013; Rezende et al., 2014).

Self-supervised representations   The idea of self-supervised learning is about utilizing original unlabeled data to create additional context information. It could be achieved in multiple manners, e.g., by adding noise to data (Vincent et al., 2008) or masking data during training (Zhang et al., 2017). Self-supervised learning could also be seen as turning an unsupervised model into a supervised by, e.g., treating predicting next pixels as a classification task (Hénaff et al., 2019; Oord et al., 2018). These are only a few examples of a quickly growing research line (Liu et al., 2020).

Here, we propose to use non-trainable transformations to obtain information about image data. Our main hypothesis is that since working with highly-quality images is challenging, we could alleviate this problem by additionally considering partial information about them. Fitting a model

Figure 1: The proposed approach.

to images of lower quality, and then enhancing them to match the target distribution seems to be overall an easier task (Chang et al., 2004; Gatopoulos et al., 2020). By incorporating compressed transformations (i.e., the self-supervised representations) that still contain global information, with the premise that it would be easier to approximate, the process of modelling a high-dimensional complex density breaks down into simpler tasks. In this way, the expressivity of the model will grow and gradually result into richer, better generations. A positive effect of the proposed framework is that the model allows us to integrate prior knowledge through the image transformations, without losing its unconditional generative functionality. Overall, we end up with a two-level VAE with three latent variables, where one is a data transformation that can be obtained in a self-supervised fashion. In Figure 1 a schematic representation of the proposed approach with downscaling is presented.

A number of exemplary image transformations are presented in Figure 4 (in the appendix). We can see that with these transformations, even though we discard a lot of information, the global structure is preserved. As a result, in practice the model should have the ability to extract a general concept of the data at the first stage, and add local information afterwards. In this work, we focus on downscaling (Figure 4.b, c & d in the appendix) and edge detection or *sketching* (Fig. 4.i in the appendix).

Model formulation In our model, we consider representations that result from *deterministic* and *discrete* transformations of an image. Formally, we introduce a transformation $d : \mathcal{X}^D \to \mathcal{X}^C$ that takes $\mathbf{x}$ and returns an image representation $\mathbf{y}$, e.g., a downscaled image. Since we lose information about the original image, $\mathbf{z}$ could be seen as a variable that compensates lost details in $\mathbf{x}$. Further we propose to introduce an additional latent variable, $\mathbf{u} \in \mathbb{R}^N$ to model $\mathbf{y}$ and $\mathbf{z}$. We can define the joint distribution of $\mathbf{x}$ and $\mathbf{y}$ as follows: $p(\mathbf{x}, \mathbf{y}) = p(\mathbf{y}|\mathbf{x})p(\mathbf{x})$, where $p(\mathbf{y}|\mathbf{x}) = \delta(\mathbf{y} - d(\mathbf{x}))$ due to the deterministic transformation $d(\cdot)$, where $\delta(\cdot)$ is the Kronecker delta. Thus, the empirical distribution is $\delta(\mathbf{y} - d(\mathbf{x}))p_{data}(\mathbf{x})$. However, since we are interested in decomposing the problem of modeling a complex distribution $p(\mathbf{x})$, we propose to model $p(\mathbf{x}|\mathbf{y})p(\mathbf{y})$ instead, and utilize the variational inference of the form $Q(\mathbf{u}, \mathbf{z}|\mathbf{x}, \mathbf{y}) = q(\mathbf{u}|\mathbf{y})q(\mathbf{z}|\mathbf{x})$ that yields:

$$\ln p(\mathbf{x}, \mathbf{y}) \geq \mathbb{E}_Q \big[\ln p_\theta(\mathbf{x}|\mathbf{y}, \mathbf{z}) + \ln p(\mathbf{z}|\mathbf{u}, \mathbf{y}) + \ln p(\mathbf{y}|\mathbf{u}) + \ln p(\mathbf{u}) - \ln q(\mathbf{z}|\mathbf{x}) - \ln q(\mathbf{u}|\mathbf{y}) \big]. \quad (2)$$

In the appendix (see Section B), we present the specific choices of the distributions. In order to highlight the self-supervised part in our model, we refer to it as the *self-supervised Variational Auto-Encoder* (or selfVAE for short).

Generation and Reconstruction in selfVAE As generative models, VAEs can be used to synthesize novel content through the following process: $\mathbf{z} \sim p(\mathbf{z}) \to \mathbf{x} \sim p(\mathbf{x}|\mathbf{z})$, but also to reconstruct a data sample $\mathbf{x}^*$ by using the following scheme: $\mathbf{z} \sim q(\mathbf{z}|\mathbf{x}^*) \to \mathbf{x} \sim p(\mathbf{x}|\mathbf{z})$.

Interestingly, our approach allows to utilize more operations regarding data generation and reconstruction. First, analogously to VAEs, the selfVAE allows to generate data by applying the following hierarchical sampling process (*generation*): $\mathbf{u} \sim p(\mathbf{u}) \to \mathbf{y} \sim p(\mathbf{y}|\mathbf{u}) \to \mathbf{z} \sim p(\mathbf{z}|\mathbf{u}, \mathbf{y}) \to \mathbf{x} \sim p(\mathbf{x}|\mathbf{y}, \mathbf{z})$. However, we can use the ground-truth $\mathbf{y}$ (i.e, $\mathbf{y}^* = d(\mathbf{x}^*)$), and sample or infer $\mathbf{z}$. Then, the generative process for the former (*conditional generation*) is: $\mathbf{z} \sim q(\mathbf{z}|\mathbf{x}^*) \to \mathbf{x} \sim p(\mathbf{x}|\mathbf{y}^*, \mathbf{z})$, and for the latter (*conditional reconstruction*): $\mathbf{u} \sim q(\mathbf{u}|\mathbf{y}^*) \to \mathbf{z} \sim p(\mathbf{z}|\mathbf{u}, \mathbf{y}^*), \to \mathbf{x} \sim p(\mathbf{x}|\mathbf{y}^*, \mathbf{z})$. If $\mathbf{y}$ is a downscaling transformation of the input image, selfVAE can be used in a manner similar to the super-resolution (Gatopoulos et al., 2020). Alternatively, we can sample (or generate) $\mathbf{y}$ instead, and choose to sample or infer $\mathbf{z}$. In this way, we can reconstruct an image in two ways, namely, *reconstruction 1*: $\mathbf{y}^* = d(\mathbf{x}^*) \to \mathbf{u} \sim q(\mathbf{u}|\mathbf{y}^*) \to \mathbf{y} \sim p(\mathbf{y}|\mathbf{u}) \to \mathbf{z} \sim p(\mathbf{z}|\mathbf{u}, \mathbf{y}) \to \mathbf{x} \sim p(\mathbf{x}|\mathbf{z}, \mathbf{y})$, and *reconstruction 2*: $\Big(\mathbf{y}^* = d(\mathbf{x}^*) \to \mathbf{u} \sim q(\mathbf{u}|\mathbf{y}^*) \to \mathbf{y} \sim p(\mathbf{y}|\mathbf{u})\Big)$, then $\mathbf{z} \sim q(\mathbf{z}|\mathbf{x}^*) \to \mathbf{x} \sim p(\mathbf{x}|\mathbf{y}, \mathbf{z})$.

The presented versions of generating and reconstructing images could be useful in the compression task. As we will see in the experiments, each option creates a different ratio of the reconstruction quality against the memory that we need to allocate to send information. However, every inferred variable needs to be sent, thus, more sampling corresponds to lower memory requirements.

Hierarchical self-supervised VAE The proposed approach can be further extended and generalized by introducing multiple transformations, in the way that it is illustrated in Figure 2. By incorporating a single (or multiple) self-supervised representation(s) of the data, the process of modelling a high-dimensional complex density breaks down into K simpler modeling tasks. Thus, we obtain a K-level VAE architecture, where the overall expressivity of the model grows even further and gradually results into generations of higher quality. Some transformations cannot be applied multiple times (e.g., edge detection), however, others could be used sequentially, e.g., downscaling.

a) Generative Model b) Inference Model

Figure 2: Hierarchical selfVAE.

We take K self-supervised data transformations $d_k(\cdot)$ that give K representations denoted by $\mathbf{y}_{1:K}$, and the following variational distributions:

$$Q(\mathbf{u}, \mathbf{z}|\mathbf{x}, \mathbf{y}_{1:K}) = q(\mathbf{u}|\mathbf{y}_K)q(\mathbf{z}_1|\mathbf{x}) \prod_{k=1}^{K-1} q(\mathbf{z}_{k+1}|\mathbf{y}_k), \tag{3}$$

that yields the following objective:

$$\ln p(\mathbf{x}, \mathbf{y}_{1:K}) \geq \mathbb{E}_Q \Big[\ln p_\theta(\mathbf{x}|\mathbf{y}_1, \mathbf{z}_1) + \sum_{k=1}^{K-1} \big(\ln p(\mathbf{z}_k|\mathbf{y}_k, \mathbf{z}_{k+1}) + \ln p(\mathbf{y}_k|\mathbf{y}_{k+1}, \mathbf{z}_{k+1}) \big) +$$

$$+ \ln p(\mathbf{z}_K|\mathbf{u}, \mathbf{y}_K) + \ln p(\mathbf{y}_K|\mathbf{u}) + \ln p(\mathbf{u}) - \ln q(\mathbf{u}|\mathbf{y}_K) - \ln q(\mathbf{z}_1|\mathbf{x}) - \sum_{k=1}^{K-1} \ln q(\mathbf{z}_{k+1}|\mathbf{y}_k) \Big]. \tag{4}$$

3. Experiments

Setup We evaluate the proposed model on CIFAR-10, Imagenette64[1] and CelebA. Encoders and decoders consist of building blocks composed of DenseNets (Huang et al., 2016), channel-wise attention (Zhang et al., 2018), and ELUs (Clevert et al., 2015) as activation functions. The dimensionality of all the latent variables were kept at $8 \times 8 \times 16 = 1024$ and all models were trained using AdaMax (Kingma and Ba, 2014) with data-dependent initialization (Salimans and Kingma, 2016). Regarding the selfVAEs, in CIFAR-10 we used an architecture with a single downscaled transformation (selfVAE-downscale), while on the remaining two datasets (CelebA and Imagenette64) we used a hierarchical 3-leveled selfVAE with downscaling, and a selfVAE with sketching. All models were employed with the bijective prior (RealNVP) comparable in terms of the number of parameters (the range of the weights of all models was from 32M to 42M). For more details, please refer to the appendix sections D and C. We approximate the negative log-likelihood using 512 IW-samples (Burda et al., 2015) and express the scores in bits per dimension (*bpd*). Additionally, for CIFAR-10, we use the *Fréchet Inception Distance* (FID) (Heusel et al., 2017).

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1. https://github.com/fastai/imagenette

Dataset	Model	*bpd* ↓	FID ↓
CIFAR-10	PixelCNN (van den Oord et al., 2016)	3.14	65.93
	GLOW (Kingma and Dhariwal, 2018)	3.35	65.93
	ResidualFlow (Chen et al., 2019)	3.28	46.37
	BIVA (Maaløe et al., 2019)	3.08	-
	NVAE (Vahdat and Kautz, 2020)	**2.91**	-
	DDPM (Ho et al., 2020)	3.75	**5.24** (**3.17***)
	VAE (ours)	3.51	41.36 (37.25*)
	selfVAE-downscale	3.65	34.71 (29.95*)
CelebA	RealNVP (Dinh et al., 2016)	3.02	-
	VAE (ours)	3.12	-
	selfVAE-sketch	3.24	-
	selfVAE-downscale-3lvl	**2.88**	-
Imagenette64	VAE (ours)	3.85	-
	selfVAE-downscale-3lvl	**3.70**	-

Table 1: Quantitative comparison on test sets from CIFAR-10, CelebA, and Imagenette64. *Measured on training set.

Quantitative results   We present the results of the experiments on the benchmark datasets in Table 1. First, we notice that on CIFAR-10 our implementation of the VAE is still lacking behind other generative models in terms of *bpd*, however, it is better or comparable in terms of FID. The selfVAE-downscale achieves worse *bpd* than the VAE. A possible explanation may lie in the small image size (32×32), as the benefits of breaking down the learning process in two or more steps are not obvious given the small target dimensional space. Nevertheless, the selfVAE-downscale achieves significantly better FID scores than the other generative models. This result could follow from the fact that downscaling allows to maintain context information about the original image and, as a result, a general coherence is of higher quality.

Interestingly, on the two other datasets, a three-level selfVAE-downscale achieves significantly better *bpd* scores than the VAE with the bijective prior. This indicates the benefit of employing a multi-leveled self-supervised framework against the VAE in higher-dimensional data, where the plain model fails to scale efficiently. It seems that the hierarchical structure of self-supervised random variables allows to encode the missing information more efficiently in $\mathbf{z}_k$, in contrast to the vanilla VAE, where all information about images must be coded in $\mathbf{z}$.

Qualitative results   We present generations on CIFAR-10 and Imagenette64 in Figure 6 and on CelebA in Figure 7, and reconstructions on CIFAR-10 and CelebA in Figure 3.[2] We first notice that the generations from selfVAE seem to be more coherent, in contrast with these from VAE that produces overall more contextless and distorted generations. This result seems to be in line with the FID scores. Especially for CelebA, we observe impressive synthesis quality, great sampling diversity and coherent generations (Figure 7). On the Imagenette64 dataset, we can also observe crisper generations for our method compared to

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2. In this paragraph, all results except Figure 3 are presented in the appendix.

Figure 3: Comparison on image reconstructions with different amount of sent information.

the VAE (Figure 6). Furthermore, the hierarchical selfVAE seems to be of a great potential for compression purposes. In contrast to the VAE, which is restricted to using a single way of reconstructing an image, the selfVAE allows four various options with different quality/memory ratios (Figure 3). In the selfVAE-sketch, we can retrieve the image with high accuracy by using only 16% of the original data, as it manages to encode all the texture of the image to $\mathbf{z}$ (Figure 8). This shows the advantage of choosing prior knowledge into the learning process. Lastly, the latents learn to add extra information, which defines the end result, and we can alter details of an image like facial expressions (Figure 9.ii).

4. Conclusion

In this paper, we showed that taking deterministic and discrete transformations results in coherent generations of high visual quality, and allows to integrate prior knowledge without loosing its unconditional generative functionality. The experimental results seem to confirm that hierarchical architectures perform better and allow to obtain both better *bpd* scores and better generations and reconstructions. In the experiments, we considered two classes of image transformations, namely, *downscaling* and edge detection (*sketching*). However, there is a vast of possible other transformations (see Figure 4), and we leave investigating them for future work. Moreover, we find the proposed approach interesting for the compression task. A similar approach with a multi-scale auto-encoder for image compression was proposed, e.g, by Mentzer et al. (2019) or Razavi et al. (2019). However, we still use a probabilistic framework and indicate that various non-trainable image transformations (not only multiple scales) could be of great potential.

References

Yuri Burda, Roger Grosse, and Ruslan Salakhutdinov. Importance weighted autoencoders. *arXiv*, 2015.

Hong Chang, Dit-Yan Yeung, and Yimin Xiong. Super-resolution through neighbor embedding. In *Proceedings of the 2004 IEEE Computer Society Conference on Computer Vision and Pattern Recognition, 2004. CVPR 2004.*, volume 1, pages I–I. IEEE, 2004.

Ricky T. Q. Chen, Jens Behrmann, David Duvenaud, and Jörn-Henrik Jacobsen. Residual flows for invertible generative modeling. *arXiv*, 2019.

Xi Chen, Diederik P. Kingma, Tim Salimans, Yan Duan, Prafulla Dhariwal, John Schulman, Ilya Sutskever, and Pieter Abbeel. Variational lossy autoencoder. *arXiv*, 2016.

Djork-Arné Clevert, Thomas Unterthiner, and Sepp Hochreiter. Fast and accurate deep network learning by exponential linear units (elus). *arXiv*, 2015.

Laurent Dinh, Jascha Sohl-Dickstein, and Samy Bengio. Density estimation using real nvp. *arXiv*, 2016.

Ioannis Gatopoulos, Maarten Stol, and Jakub M. Tomczak. Super-resolution variational auto-encoders. *arXiv.2006.05218*, 2020.

Ishaan Gulrajani, Kundan Kumar, Faruk Ahmed, Adrien Ali Taiga, Francesco Visin, David Vazquez, and Aaron Courville. Pixelvae: A latent variable model for natural images. *arXiv*, 2016.

Amirhossein Habibian, Ties van Rozendaal, Jakub M Tomczak, and Taco S Cohen. Video compression with rate-distortion autoencoders. In *Proceedings of the IEEE International Conference on Computer Vision*, pages 7033–7042, 2019.

Olivier J Hénaff, Aravind Srinivas, Jeffrey De Fauw, Ali Razavi, Carl Doersch, SM Eslami, and Aaron van den Oord. Data-efficient image recognition with contrastive predictive coding. *arXiv preprint arXiv:1905.09272*, 2019.

Martin Heusel, Hubert Ramsauer, Thomas Unterthiner, Bernhard Nessler, and Sepp Hochreiter. Gans trained by a two time-scale update rule converge to a local nash equilibrium. *arXiv*, 2017.

Jonathan Ho, Ajay Jain, and Pieter Abbeel. Denoising diffusion probabilistic models. *Advances in Neural Information Processing Systems*, 33, 2020.

Emiel Hoogeboom, Victor Garcia Satorras, Jakub M Tomczak, and Max Welling. The convolution exponential and generalized sylvester flows. *arXiv preprint arXiv:2006.01910*, 2020.

Gao Huang, Zhuang Liu, Laurens van der Maaten, and Kilian Q. Weinberger. Densely connected convolutional networks. *arXiv*, 2016.

Michael I. Jordan, Zoubin Ghahramani, and et al. An introduction to variational methods for graphical models. In *Machine Learning*, pages 183–233. MIT Press, 1999.

Diederik P. Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv*, 2014.

Diederik P. Kingma and Prafulla Dhariwal. Glow: Generative flow with invertible 1x1 convolutions. *arXiv*, 2018.

Diederik P Kingma and Max Welling. Auto-encoding variational bayes. *arXiv*, 2013.

Frantzeska Lavda, Magda Gregorová, and Alexandros Kalousis. Data-dependent conditional priors for unsupervised learning of multimodal data. *Entropy*, 22(8):888, 2020.

Shuyu Lin and Ronald Clark. Ladder: Latent data distribution modelling with a generative prior. *arXiv preprint arXiv:2009.00088*, 2020.

Xiao Liu, Fanjin Zhang, Zhenyu Hou, Zhaoyu Wang, Li Mian, Jing Zhang, and Jie Tang. Self-supervised learning: Generative or contrastive. *arXiv preprint arXiv:2006.08218*, 2020.

Lars Maaløe, Casper Kaae Sønderby, Søren Kaae Sønderby, and Ole Winther. Auxiliary deep generative models. *arXiv*, 2016.

Lars Maaløe, Marco Fraccaro, Valentin Liévin, and Ole Winther. Biva: A very deep hierarchy of latent variables for generative modeling. *arXiv*, 2019.

Fabian Mentzer, Eirikur Agustsson, Michael Tschannen, Radu Timofte, and Luc Van Gool. Practical full resolution learned lossless image compression. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 10629–10638, 2019.

Aaron van den Oord, Yazhe Li, and Oriol Vinyals. Representation learning with contrastive predictive coding. *arXiv preprint arXiv:1807.03748*, 2018.

Ali Razavi, Aaron van den Oord, and Oriol Vinyals. Generating diverse high-fidelity images with vq-vae-2. In *Advances in Neural Information Processing Systems*, pages 14866–14876, 2019.

Danilo Jimenez Rezende, Shakir Mohamed, and Daan Wierstra. Stochastic backpropagation and approximate inference in deep generative models. *arXiv*, 2014.

Tim Salimans and Diederik P. Kingma. Weight normalization: A simple reparameterization to accelerate training of deep neural networks. *arXiv*, 2016.

Tim Salimans, Andrej Karpathy, Xi Chen, and Diederik P. Kingma. Pixelcnn++: Improving the pixelcnn with discretized logistic mixture likelihood and other modifications. *arXiv*, 2017.

Wenzhe Shi, Jose Caballero, Ferenc Huszár, Johannes Totz, Andrew P. Aitken, Rob Bishop, Daniel Rueckert, and Zehan Wang. Real-time single image and video super-resolution using an efficient sub-pixel convolutional neural network. *arXiv*, 2016.

Jakub M Tomczak and Max Welling. Vae with a vampprior. *arXiv preprint arXiv:1705.07120*, 2017.

Arash Vahdat and Jan Kautz. Nvae: A deep hierarchical variational autoencoder. *arXiv*, 2020.

Rianne van den Berg, Leonard Hasenclever, Jakub M. Tomczak, and Max Welling. Sylvester normalizing flows for variational inference. *arXiv*, 2018.

Aaron van den Oord, Nal Kalchbrenner, and Koray Kavukcuoglu. Pixel recurrent neural networks. *arXiv*, 2016.

Pascal Vincent, Hugo Larochelle, Yoshua Bengio, and Pierre-Antoine Manzagol. Extracting and composing robust features with denoising autoencoders. In *Proceedings of the 25th international conference on Machine learning*, pages 1096–1103, 2008.

Richard Zhang, Phillip Isola, and Alexei A Efros. Split-brain autoencoders: Unsupervised learning by cross-channel prediction. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 1058–1067, 2017.

Yulun Zhang, Kunpeng Li, Kai Li, Lichen Wang, Bineng Zhong, and Yun Fu. Image super-resolution using very deep residual channel attention networks. *arXiv*, 2018.

Shengjia Zhao, Jiaming Song, and Stefano Ermon. Learning hierarchical features from deep generative models. In *International Conference on Machine Learning*, pages 4091–4099, 2017.

Appendix A. Non-trainable image transformations

In Figure 4, we present various examples of discrete and deterministic (and non-trainable) image transformations.

a) Original Image   b) Bicubic Interpolation x2   c) Bicubic Interpolation x3   d) Bicubic Interpolation x4   e) Gaussian Kernel (1x1)

f) 1 bit   g) 2 bits   h) 3 bits   i) Sketch   j) Greyscale

Figure 4: Examples of image transformations. All of these transformations preserve the global structure of the samples, but they disregard the high resolution details in different manners.

Appendix B. Specific choices of distributions in selfVAE

In this paper, we use the following distributions for the generative part of the selfVAE:

$$p(\mathbf{v}) = \mathcal{N}\left(\mathbf{v}|\mathbf{0}, \mathbf{1}\right)$$

$$p_\lambda\left(\mathbf{u}\right) = p(\mathbf{v}) \prod_{i=1}^{F} \left| \det \frac{\partial f_i(\mathbf{v}_{i-1})}{\partial \mathbf{v}_{i-1}} \right|^{-1}$$

$$p_{\theta_1}\left(\mathbf{y}|\mathbf{u}\right) = \sum_{i=1}^{I} \pi_i^{(\mathbf{u})} \mathrm{Dlogistic}\left(\mu_i^{(\mathbf{u})}, s_i^{(\mathbf{u})}\right)$$

$$p_{\theta_2}\left(\mathbf{z}|\mathbf{y}, \mathbf{u}\right) = \mathcal{N}\left(\mathbf{z}|\boldsymbol{\mu}_{\theta_2}(\mathbf{y}, \mathbf{u}), \mathrm{diag}\left(\boldsymbol{\sigma}_{\theta_2}(\mathbf{y}, \mathbf{u})\right)\right)$$

$$p_{\theta_3}\left(\mathbf{x}|\mathbf{z}, \mathbf{y}\right) = \sum_{i=1}^{I} \pi_i^{(\mathbf{z},\mathbf{y})} \mathrm{Dlogistic}\left(\mu_i^{(\mathbf{z},\mathbf{y})}, s_i^{(\mathbf{z},\mathbf{y})}\right)$$

where Dlogistic is defined as the discretized logistic distribution (Salimans et al., 2017), and we utilize a flow-based model for $p_\lambda\left(\mathbf{u}\right)$.

Further, we consider the following distributions for the variational part:

$$q_{\phi_1}\left(\mathbf{u}|\mathbf{y}\right) = \mathcal{N}\left(\mathbf{u}|\boldsymbol{\mu}_{\phi_1}(\mathbf{y}), \mathrm{diag}\left(\boldsymbol{\sigma}_{\phi_1}(\mathbf{y})\right)\right)$$

$$q_{\phi_2}\left(\mathbf{z}|\mathbf{x}\right) = \mathcal{N}\left(\mathbf{z}|\boldsymbol{\mu}_{\phi_2}(\mathbf{x}), \mathrm{diag}\left(\boldsymbol{\sigma}_{\phi_2}(\mathbf{x})\right)\right).$$

Appendix C. Datasets

CIFAR-10 The CIFAR-10 dataset is a well-known image benchmark data containing 60.000 training examples and 10.000 validation examples. From the training data, we put aside 15% randomly selected images as the test set. We augment the training data by using random horizontal flips and random affine transformations and normalize the data uniformly in the range (0, 1).

Imagenette64 Imagenette64[3] is a subset of 10 classes from the downscaled Imagenet dataset. We downscaled the dataset to 64px × 64px images. Similarly to CIFAR-10, e put aside 15% randomly selected training images as the test set. We used the same data augmentation as in CIFAR-10

CelebA The Large-scale CelebFaces Attributes (CelebA) Dataset consists of 202.599 images of celebrities. We cropped original images on the 40 vertical and 15 horizontal component of the top left corner of the crop box, which height and width were cropped to 148. Besides the uniform normalization of the image, no other augmentation was applied.

Appendix D. Neural Network Architecture

The choice of the NN architecture is crucial for the performance and the scalability of the overall framework, and usually architectures that showcased great performance in discriminate tasks (i.e. classification) are used in generative modelling tasks as well. However, the internal representations that the networks have to discover are fundamentally different, and little attention has been given into designing a NN specifically for an auto-encoder setting. For example, in classification tasks the network extracts specific representation of a particular object, in contrast with the generative models, where we aim for discovering the semantic structure of the data. Thus, as we argue that we can benefit from a carefully designed architecture, in this section we present our approach.

For building blocks of the network, we employed densely connected convolutional networks instead of residual ones. The motivation for this choice is that since DenseNets encourage feature reuse, it will help preserve visual information from the very first layer effectively, while requiring less trainable parameters. Thus, the network could discover easier generic graphical features and local pixel correlations. The concatenation of the filters will also alleviate the vanishing-gradient problem and allow us to build deep architectures. Additionally, exponential linear units (ELUs) are used everywhere as activation functions. In contrast to ReLUs, ELUs have negative values which allows them to push mean unit activations closer to zero, which speeds up the learning process. This is due to a reduced *bias shift effect*; bias that is introduced to the units from those of the previous layer which have a non-zero mean activation.

Typically, every convolution operation precedes a batch normalization layer, as they empirically exhibit a boost in performance in discriminate tasks. However, their performance is known to degrade for small batch sizes, as the variance of the activation noise that they contribute is inversely proportional to the number of data that is processed. This noise injection, in combination with their intensive memory demands, can be critical drawbacks when we process image data, especially high-dimensional ones. We instead use weight

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3. https://github.com/fastai/imagenette

normalization, where even though it separates the weight vector from its direction just like batch normalization, they do not make use of the variance. This allows them to get the desired output even in small mini-batches, while allocating a small proportion of memory. We empirically find out that indeed using weight normalization reduces the overfitting of the model. In addition, we used a data-dependant initialization of the model parameters, by sampling the first batch of the training set. This will allow the parameters to be adjusted by the output of the previous layers, taking into account and thus resulting into a faster learning process.

An important element of the auto-encoding scheme is the process of feature downscaling and upscaling. Despite its success in classification tasks, pooling is a fixed operation that replacing it with a stride-convolution layer can also be seen as generalization, as the scaling process is now learned. This will increase the models' expressibility with the cost of adding a negligible amount of learning parameters. For the upscaling operation, even though various methods have been proposed (Shi et al., 2016), we found out that the plain transposed convolution generalised better than the others, while requiring far less trainable parameters. Finally, inspired from the recent advantages on super-resolution neural network architectures, we used *channel-wise attention* blocks (CA) at the end of every DenseNet block (Zhang et al., 2018). The CA blocks will help the network to focus on more informative features, by exploiting the inter-dependencies among feature channels. Thus, it performs feature recalibration in a global way, where the per-channel summary statistics are calculated and then used to selectively emphasise informative feature-maps as well as suppress useless ones (e.g. redundant feature-maps). This is done through a global average pooling, that squeezes global spatial information into a channel statistical descriptor, followed by a gating mechanism, where it learns nonlinear interactions between the input channels.

The core building blocks and the network of an auto-encoding network are illustrated in Figure D.

Figure 5: Architecture of our autoencoder. On the right, there are some basic buildings block of the network. The notation as 'G' on the Conv2D channels indicate the growth rate of the densely connected network. The ϵ indicates a random variable drawn from a standard Gaussian, which helps us to make use of the *reparametrization* trick. Until **z**, we refer to this architecture as *Encoder NN* and thereafter as *Decoder NN*. The former and the later form the *building blocks* to every model that we train and evaluate.

Appendix E. Additional results

selfVAE - downscale   VAE

First level   Second level   Third level

Figure 6: Uncoditional generations on Imagenette64 and CIFAR-10.

Figure 7: Unconditional CelebA generations from (i) the three-level self-supervised VAE with downscaling, (ii) the self-supervised VAE employed with edge detection (sketches), (iii) the VAE with RealNVP prior.

Figure 8: Qualitative results illustrating all the reconstruction techniques on CelebA for selfVAE-sketch.

i) Image interpolation between two ground-truth samples though the latent variable **u**.

ii) Image generation given the latent variable **u** and sampling the latent codes of $\mathbf{z}_1, \mathbf{z}_2$.

Figure 9: Latent space interpolations and conditional generations of the selfVAEs.