SPATIAL DEPENDENCY NETWORKS: NEURAL LAYERS FOR IMPROVED GENERATIVE IMAGE MODELING

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Paper under double-blind review

ABSTRACT

How to improve generative modeling by better exploiting spatial regularities and coherence in images? To answer this question, we introduce a novel neural layer for building image generators (decoders) and apply it to variational autoencoders (VAEs). Our spatial dependency networks (SDNs) compute feature maps in a spatially coherent way, utilizing a sequential gating-based mechanism to distribute contextual information across 2D maps. Different SDN layers of a deep neural network represent spatial dependencies at different levels of abstraction. Augmenting the decoder of a hierarchical VAE by spatial dependencies considerably improves density estimation over baseline convolutional architectures and the state-of-the-art among the models of the same class. We show that SDN can be applied to larger images where we probe the learned distribution by synthesizing samples of high quality and coherence. In a vanilla VAE setting, we find that a powerful SDN decoder also improves learning of disentangled representations, indicating that neural architectures play an important role on this task. Our results suggest to favor SDNs over convolutional networks in various VAE settings.

1 INTRODUCTION

The abundance of data and computation are often identified as core facilitators of the deep learning revolution. In addition to this technological leap, historically speaking, most major algorithmic advancements critically hinged on the existence of inductive biases, incorporating prior knowledge in different ways. Main breakthroughs in image recognition (Cireşan et al., 2012; Krizhevsky et al., 2012) were preceded by the long standing pursuit for shift-invariant pattern recognition (Fukushima & Miyake, 1982) which catalysed the ideas of weight sharing and convolutions (Waibel et al., 1989; LeCun et al., 1989). Recurrent networks (exploiting temporal recurrence) and transformers (modeling the "attention" bias) revolutionized the field of natural language processing (Mikolov et al., 2011; Vaswani et al., 2017). Visual representation learning is also often based on priors e.g. independence of latent factors (Schmidhuber, 1992; Bengio et al., 2013) or invariance to input transformations (Becker & Hinton, 1992; Chen et al., 2020). Clearly, one promising strategy to move forward is to introduce more structure into learning algorithms, and more knowledge on the problems and the data we are dealing with.

Along this line of thought, we explore ways to improve generative modeling. The idea is to integrate into neural architectures assumptions on the holistic, spatially consistent nature of natural images: An image is meaningful only when there is a spatially coherent dependency interplay among its pixels. The hope is that, if equipped with a good spatial dependency model, learning algorithms will be biased to assign high likelihoods to, or to synthesize more coherent images. Popular generative models (Kingma & Welling, 2013; Goodfellow et al., 2014) typically contain a generator network (a decoder) which maps latent variables into images through a sequence of representations (stacks of feature maps), with increasing level of granularity. Crucially to our design decisions, we hypothesize that these feature maps should also be spatially coherent, as coarse representatives of the final image.

In the light of the above, to model specifically deep image generators, spatial dependency networks (SDNs; Figure 1) are proposed. As in convolutional networks (CNNs), the locality and equivariance to translation are exploited by design. On top of that, SDNs also explicitly model image-level spatial coherence and dependencies. As such, SDNs carry strong inductive bias to reflect the fact that most

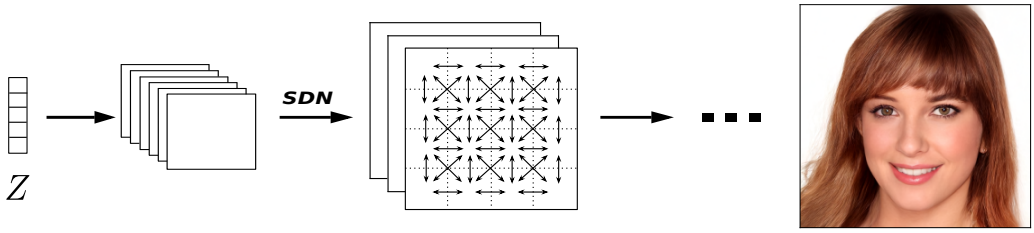

Figure 1: **SDN-based generator hallucinating a 'celebrity'.** Bi-directional arrows describe the network of direct dependencies within feature maps, created as a result of applying SDN layer. Non-neighboring feature vectors are indirectly dependent. Z is the latent code.

useful information in images is typically stored in the regularities of inter-pixel relations. Along the pipeline of a deep neural network, such regularities are represented at different levels of abstraction.

SDN is examined in two different settings. In the context of real-life-image density modeling, SDN-empowered hierarchical variational autoencoder (VAE) is shown to reach considerably higher test log-likelihoods than the baseline CNN-based architectures, and is able to synthesize perceptually appealing and coherent images even at high sampling temperatures. In a synthetic data setting, we observe that enhancing a non-hierarchical VAE with an SDN also facilitates learning of factorial latent codes, suggesting that unsupervised 'disentanglement' of representations can be bettered by using more powerful neural architectures, where SDN stands out as a good candidate model. The contributions and the contents of this paper can be summarized as follows.

CONTRIBUTIONS AND CONTENTS:

- The architecture of SDN is described and then contrasted to the convolutional networks, *de facto* standard choice in generative modeling, both experimentally and through discussion.
- As a result of applying SDN to IAF-VAE (Kingma et al., 2016), with modest modifications to the original architecture, SDN-VAE is introduced and evaluated on two different tasks: *(a)* density estimation, where the performance is considerably improved both upon the baseline and related approaches to non-autoregressive modeling, on CIFAR10 and ImageNet32 data sets; *(b)* image synthesis, where images of competitively high perceptual quality are generated based on CelebAHQ256 data set.
- By integrating SDN into a relatively simple, non-hierarchical VAE, trained on the synthetic 3D-Shapes data set, we demonstrate in another comparative analysis substantial improvements upon convolutional networks in terms of: *(a)* optimization of the evidence lower bound (ELBO); *(b)* learning of disentangled representations with respect to two popular metrics, when β-VAE (Higgins et al., 2016) is used as an objective function.
- The implementation of proposed architectures and of our experiments is disclosed in the frameworks of Pytorch (Paszke et al., 2019) and PytorchLightning (Falcon, 2019).

2 SDN ARCHITECTURE

The architectural design of SDN is motivated by our intent to improve modeling of spatial coherence and higher-order statistical correlations between pixels. Schematic overview of SDN is given in Figure 2. Technically speaking, SDN layer is a differentiable function which transforms input to output feature maps in a 3-stage procedure.

We first describe the stages of SDN in detail, then address practical and computational concerns, and finally contrast SDN to related architectures.

Project-in stage. Using a simple feature vector-wise affine transformation, input representation X^{L_k} at the layer L_k is transformed into an intermediate representation I^{L_k}:

$$I^{L_k}_{i,j} = X^{L_k}_{i,j}\mathbf{W}^{(1)} + \mathbf{B}^{(1)} \tag{1}$$

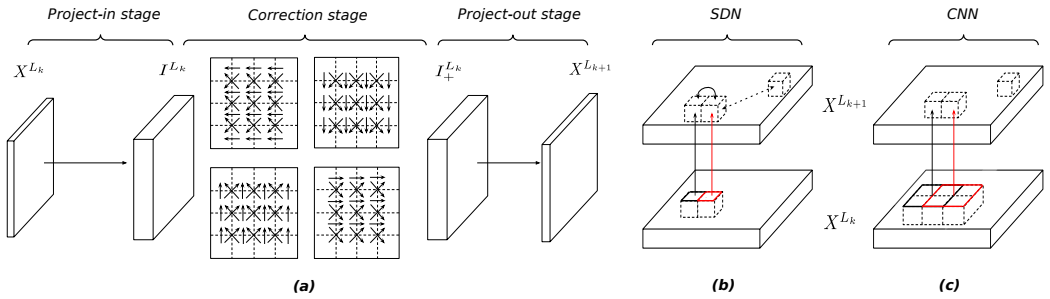

Figure 2: **SDN design.** **(a)** SDN layer as a 3-stage pipeline; **(b)** dependencies between the input X^{L_k} and the output $X^{L_{k+1}}$ modeled by an SDN, at the layer L_k. Solid arrows represent direct dependencies, and dashed indirect ones; **(c)** dependencies modeled by a 2×2 CNN.

where i and j are the corresponding 2D coordinates in X^{L_k} and I^{L_k}, $\mathbf{B}^{(\mathbf{1})}$ is a matrix of learnable biases and $\mathbf{W}^{(\mathbf{1})}$ is a learnable matrix of weights whose dimensions depend on the number of channels of X^{L_k} and I^{L_k}. In the absence of overfitting, it is advisable to increase the number of channels to enhance the memory capacity of I^{L_k} and enable unimpeded information flow in the correction stage. Notice that described transformation corresponds to the convolutional (CNN) operator with a kernel of size 1. If the scales between the input X^{L_k} and the output $X^{L_{k+1}}$ differ (e.g. if converting an 8x8 to a 16x16 tensor), in this stage we additionally perform upsampling by applying the corresponding transposed CNN operator, also known as 'deconvolution' (Zeiler & Fergus, 2014).

Correction stage. The elements of I^{L_k} are 'corrected' in a 4-step procedure. In each step, a unidirectional sweep through I^{L_k} is performed, in one of the 4 possible directions: *(i)* bottom-to-top; *(ii)* right-to-left; *(iii)* left-to-right; and *(iv)* top-to-bottom. During a single sweep, columns/rows are computed in parallel. The corresponding correction equations implement controlled updates of I^{L_k} using a gating mechanism, as done in popular recurrent units (Hochreiter & Schmidhuber, 1997; Cho et al., 2014). Specifically, we use a multiplicative update akin to the one found in GRUs (Cho et al., 2014), but adapted to the spatial setting. The procedure for the bottom-to-top sweep is given in Algorithm 1. The sweeps in the remaining 3 directions are performed analogously. With

Algorithm 1 Bottom-to-top sweep of the correction stage

Input: I^{L_k} – intermediate representation; N – the scale of I^{L_k};
Output: $I_+^{L_k}$ – corrected intermediate representation; # after all 4 sweeps
Complexity: $\mathcal{O}(N)$
$I^{L_k} = \tanh(I^{L_k})$ # done for the first direction only
$I^{L_k} = \textit{zero_padding}(I^{L_k})$ # done for the first direction only
for $i = 1$ **to** N and ($j = 1$ **to** N **in parallel**) **do**
  $r_{i,j,c} = \sigma([\mathbf{W^{r1}} I_{i,j}]_c + [\mathbf{W^{r2}} I_{i-1,j}]_c + [\mathbf{W^{r3}} I_{i-1,j-1}]_c) + [\mathbf{W^{r3}} I_{i-1,j+1}]_c + \mathbf{B^r})$ # reset gate
  $z_{i,j,c} = \sigma([\mathbf{W^{z1}} I_{i,j}]_c + [\mathbf{W^{z2}} I_{i-1,j}]_c + [\mathbf{W^{z3}} I_{i-1,j-1}]_c) + [\mathbf{W^{z3}} I_{i-1,j+1}]_c + \mathbf{B^z})$ # update gate
  $n_{i,j,c} = \tanh(r_{i,j,c}[\mathbf{W^{n1}} I_{i,j}]_c + [\mathbf{W^{n2}} I_{i-1,j}]_c + [\mathbf{W^{n3}} I_{i-1,j-1}]_c) + [\mathbf{W^{n3}} I_{i-1,j+1}]_c + \mathbf{B^n})$
  $I_{i,j,c} = z_{i,j,c} I_{i,j,c} + (1 - z_{i,j,c}) n_{i,j,c}$ # feature correction
end for

$\mathbf{W}^*$ we denote learnable weights, $\mathbf{B}^*$ are learnable biases, i is the height (growing bottom-to-top), j is the width and c is the channel dimension. Gating elements $r_{i,j,c}$ and $z_{i,j,c}$ control the correction contributions of the *a priori* value of $I_{i,j,c}$ and the proposed value $n_{i,j,c}$, respectively. For the borderline elements of I^{L_k}, missing neighbors are initialized to zeros (hence the zero padding).

Project-out stage. Corrected intermediate representation $I_+^{L_k}$ is then mapped to the output $X^{L_{k+1}}$, which has the same number of channels as the input X^{L_k}:

$$X_{i,j}^{L_{k+1}} = I_{+,i,j}^{L_k} \mathbf{W}^{(\mathbf{3})} + \mathbf{B}^{(\mathbf{3})} \tag{2}$$

where $\mathbf{W}^{(\mathbf{3})}$ is the stage-level learnable weight matrix and $\mathbf{B}^{(\mathbf{3})}$ is the corresponding bias matrix.

Scaling up. A valid concern in terms of scaling SDN to large images is the computational complexity of $\mathcal{O}(N)$, N being the scale of the output. We make two key observations:

a. one can operate with less than 4 directions per layer, alternating them across layers and thus achieving the same 'mixing' effect. This improves runtime with relatively minor sacrifice in performance;

b. in practice, we found it sufficient to apply SDN only at lower scales (e.g. up to 64x64 on CelebAHQ256), with little to no loss in performance. We speculate that this is due to redundancies in high-resolution images, which allows modelling of relevant spatial structure at lower scales;

Avoiding vanishing gradients. The problem of vanishing gradient might arise when SDN is plugged in a very deep neural network (such as the one discussed in Section 3). To remedy this, in our experiments we used the gated residual (Srivastava et al., 2015) variant of SDN, to which we refer to as ResSDN (shown in Figure 3).

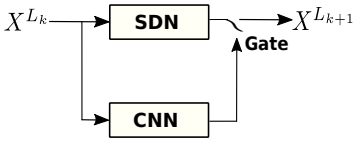

Figure 3: **Residual SDN (ResSDN).**

Comparison to CNNs. SDNs and CNNs are similar in the sense that both architectures exploit locality (a feature vector in SDN is corrected based on its direct neighbors) and equivariance to translation (achieved through parameter sharing within a one-directional pass). However, there are important differences in dependency modeling (depicted in Figures 2(b) and 2(c)). Firstly, when conditioned on the input X^{L_k}, CNN's output feature vectors are statistically independent: $p(X^{L_{k+1}}|X^{L_k}) = \prod_{i,j} p(X^{L_{k+1}}_{i,j}|X^{L_k})$, where i and j are feature map coordinates. In SDNs, all feature vectors are dependent, more formally: $p(X^{L_{k+1}}_{i,j}, X^{L_{k+1}}_{l,m}|X^{L_k}) \neq p(X^{L_{k+1}}_{i,j}|X^{L_k})p(X^{L_{k+1}}_{l,m}|X^{L_k})\ \forall (i,j) \neq (l,m)$. Secondly, in the observed one-layer setup, the unconditional dependency neighborhood is bounded by the size of the CNN's receptive field – a conceptual limitation not present in SDNs.

Related work. SDNs are perhaps most notably reminiscent of Multi-Dimensional RNNs (Graves et al., 2007), which were used for image segmentation (Graves et al., 2007; Stollenga et al., 2015) and recognition (Visin et al., 2015), but not in the context of generative modeling. Other existing methods worth noting, more central to generative modeling, are Spatial-LSTM (Theis & Bethge, 2015) and PixelRNN (Van Oord et al., 2016). These methods are designed for autoregressive density estimation, hence are conceptually very different e.g. because the generation ordering is fixed, such approaches are inherently one-directional.

3 SDN-VAE: An Improved Variational Autoencoder for Images

As a first use case, SDN is used in the SDN-VAE architecture. The basis of SDN-VAE is the IAF-VAE model (Kingma et al., 2016). Apart from integrating SDNs, we introduce additional modifications for improved performance, training stability, and reduced memory requirements. We first cover the basics of VAEs, then briefly summarize IAF-VAE and the related work. Finally, we elaborate on the novelties in the SDN-VAE design.

Background on VAEs. VAEs assume a latent variable generative model $p_\theta(X) = \int p_\theta(X, Z)dZ$ where θ are model parameters. When framed in the maximum likelihood setting, the marginal probability of data is intractable due to the integral in the above expression. VAEs take a variational approach, approximating posterior $q_\phi(Z|X)$ using a learnable function q with parameters ϕ. Following Kingma & Welling (2019), we can derive the following equality:

$$\log p_\theta(X) = \underbrace{\mathbb{E}_{q_\phi(Z|X)}\left[\log\left[\frac{p_\theta(X,Z)}{q_\phi(Z|X)}\right]\right]}_{\mathcal{L}_{\phi,\theta}(X)=ELBO} + \underbrace{\mathbb{E}_{q_\phi(Z|X)}\left[\log\left[\frac{q_\phi(Z|X)}{p_\theta(Z|X)}\right]\right]}_{KL(q_\phi(Z|X)||p_\theta(Z|X))\geq 0}. \tag{3}$$

$\mathcal{L}_{\phi,\theta}(X)$ is the evidence lower bound (ELBO), since it 'bounds' the marginal log-likelihood term $\log p_\theta(X)$, where the gap is defined by the KL-divergence term on the right. In VAEs, both q_ϕ and

p_θ are parametrized by deep neural networks. The model is learned via backpropagation, and a low variance approximation of the gradient $\nabla_{\phi,\theta}\mathcal{L}_{\phi,\theta}(X)$ can be computed via the *reparametrization trick* (Kingma & Welling, 2019).

Background on IAF-VAE. Main advancements of IAF-VAE in comparison to the vanilla VAE include: *(a)* leveraging on a hierarchical (ladder) network of stochastic variables (Sønderby et al., 2016) for increased expressiveness and improved training; *(b)* introducing inverse autoregressive flows to enrich simple isotropic Gaussian-based posterior with a normalizing flow; *(c)* utilizing a bi-directional inference procedure to encode latent variables through an encoder-decoder interplay; *(d)* introducing a ResNet block as a residual-based (He et al., 2016) instantiation of the ladder layer. For more details, we refer the reader to the original paper (Kingma et al., 2016).

Related work. BIVA (Maaløe et al., 2019) is an extension of IAF-VAE which adds skip connections across latent layers, and a stochastic bottom-up path. In our experiments, however, we were not able to improve performance in a similar way. Concurrently to our work, NVAE (Vahdat & Kautz, 2020) reported significant improvements upon the IAF-VAE baseline, by leveraging on many technical advancements including: batch normalization, depth-wise separable convolutions, mixed-precision, spectral normalization and residual parameterization of the approximate posterior. Both methods use the discretized mixture of logistics (Salimans et al., 2017).

SDN-VAE ARCHITECTURE

Our main contribution to the IAF-VAE architecture is the integration of ResSDN layers (Figure 3). We replace the convolutional layers on the top-down (generation) path of the IAF-VAE ResNet block, up to a particular scale: up to 32x32 for images of that resolution, and up to 64x64 for 256x256 images. For the convenience of the reader, we borrowed the scheme from the original paper and clearly marked the modifications (Figure 4).

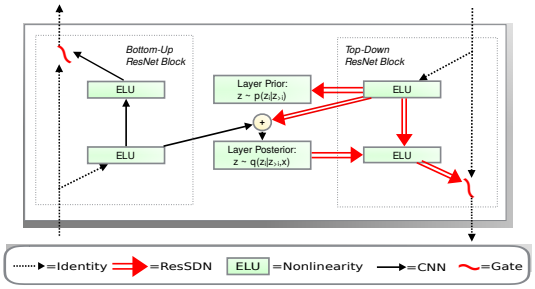

Figure 4: **SDN-VAE ResNet block as modified IAF-VAE ResNet block**. Two notable changes (marked in red) include applying: *(a)* ResSDN instead of convolutional networks on the top-down path; *(b)* gated rather than a sum residual; (figure adapted from Kingma et al. (2016))

Other notable modifications include: *(a)* gated residual instead of a sum residual in the ResNet block (Figure 4), for improved training stability; *(b)* more flexible observation model based on a discretized mixture of logistics instead of a discretized logistic distribution, for improved performance; and *(c)* mixed-precision (Micikevicius et al., 2018), which reduced memory requirements thus allowing training with larger batches. Without SDNs, we refer to this architecture as IAF-VAE+.

4 IMAGE DENSITY MODELING

Proposed SDN-VAE and the contributions of SDN layers to its performance were empirically evaluated on two different tasks: *(a)* density estimation, where SDN-VAE was in a quantitative fashion compared to the convolutional network baseline, and to the related state-of-the-art approaches; *(b)* image synthesis, where a learned distribution was analyzed in a qualitative way by sampling from it in different ways. Exact details of our experiments, additional ablation studies and additional results in image synthesis are documented in the Appendix sections A.1, A.2 and A.3 respectively.

Density estimation. From a set of i.i.d. images $\mathcal{D}_{train} = X_{1..N}$, the true probability density function $p(X)$ is estimated via a parametric model $p_\theta(X)$, whose parameters θ are learned using the maximum log-likelihood objective: $\arg\max_\theta \left[\log p_\theta(X) \approx \sum_{i=1}^{N} \log p_\theta(X_i)\right]$. The test log-likelihood is computed on an isolated set of images $\mathcal{D}_{test} = X_{1..K}$, to evaluate learned $p_\theta(X)$.

SDN-VAE and the competing methods were tested on CIFAR-10 (Krizhevsky et al., 2009), ImageNet32 (Van Oord et al., 2016), and CelebAHQ256 (Karras et al., 2017). Quantitative comparison is given in Table 1. IAF-VAE+ denotes our technically enhanced implementation of IAF-VAE, but without the SDN modules (recall Section 3).

Type	Method	CIFAR-10	ImageNet32	CelebAHQ256
VAE-based	**SDN-VAE (ours)**	(2.87)	(3.85)	(0.70)
	IAF-VAE+ (ours)	3.05	4.00	0.71
	IAF-VAE (Kingma et al., 2016)	3.11	X	X
	BIVA (Maaløe et al., 2019)	3.08	X	X
	NVAE (Vahdat & Kautz, 2020)	2.91	3.92	(0.70)
Flow-based	GLOW (Kingma & Dhariwal, 2018)	3.35	4.09	1.03
	FLOW++ (Ho et al., 2019)	3.08	3.86	X
	ANF (Huang et al., 2020)	3.05	3.92	0.72
	SurVAE (Nielsen et al., 2020)	3.08	4.00	X
Autoregressive*	PixelRNN (Van Oord et al., 2016)	3.00	3.86	X
	PixelCNN (Van den Oord et al., 2016)	3.03	3.83	X
	PixelCNN++ (Salimans et al., 2017)	2.92	X	X
	PixelSNAIL (Chen et al., 2018)	**2.85**	3.80	X
	SPN (Menick & Kalchbrenner, 2018)	X	3.85	**0.61**
	IT (Parmar et al., 2018)	2.90	**3.77**	X

Table 1: **Density estimation results.** Negative test log-likelihood is measured in *bits per dimension (BPD)* - lower is better. As in previous works, only the most successful runs are reported. Circled are the best runs among non-autoregressive models and bolded are the best runs overall.
* by autoregressive we refer to the methods based on $p(X) = \prod_{i=1} p(X_i|X_1, ..., X_{i-1})$ factorization.

Figure 5: **Linear interpolation between test images.** Given a pair of images from the test dataset (on the far right and far left), linear interpolation was performed on the layer 5 at a temperature of 0.9 (the sequence above) and on the layer 4 at a temperature of 1.0 (the sequence below).

Image synthesis. We additionally inspected the trained $p_\theta(X)$ by: *(a)* unconditionally generating samples from the prior, at different temperatures (Figure 6 left); *(b)* sampling in the neighborhood of an image not seen during training time (Figure 6 right); *(c)* interpolating between two images not seen during training time (Figure 5). All technical details on these experiments are in Appendix A.1. Additional images are given in Appendix A.3.

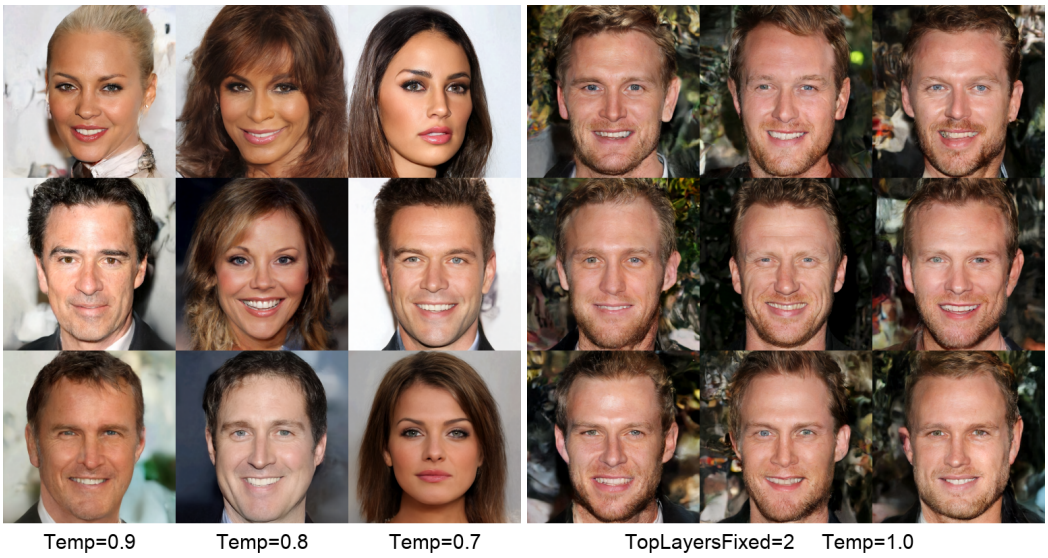

Figure 6: *(left)* **Unconditional sampling.** Samples were drawn from the SDN-VAE prior at varying temperatures; *(right)* **Sampling around a test image.** Conditioned on the top 2 layers of the latent code of the image in the center, the surrounding images were sampled at a temperature of 1.0.

Discussion. Our results clearly suggest that SDN-VAE is not only superior to the convolutional network baseline, but also to all previous related approaches for non-autoregressive density modeling. To further inspect whether the increase in performance is due to applying SDN or due to the implicit increase in the number of parameters, we conducted additional ablation studies (described in Appendix A.2). These results provide additional evidence that SDN is the cause of increased performance, as even convolutional networks with more parameters, increased receptive field or more depth lead to inferior performance.

In our image generation experiments we confirmed that SDN-VAE can be successfully scaled to large images. Generated samples are of exceptionally high quality. What is particularly challenging in VAE-based image generation, is sampling at high temperatures, however as shown in Figure 10 of our Appendix, SDN-VAE can successfully synthesize coherent images even in this case.

5 Learning Disentangled Representations

To study its performance impact in a more constrained setting, SDN was paired with a VAE architecturally much simpler than IAF-VAE. Apart from the implementation simplicity and shorter training time, a non-hierarchical VAE is more suitable for representation learning – there is a single stochastic vector and not a hierarchy of feature maps, which enables better control of the latent space. In particular, the gains in performance when using SDN were evaluated with respect to: *(a)* evidence lower bound (ELBO), as a proxy to measure how well an image distribution is approximated; *(b)* disentanglement of latent codes based on the corresponding metrics, to examine the effects of SDN decoder to the quality of learned latent representations.

Experiment setting. A relatively simple VAE architecture with a stack of convolutional networks in both the encoder and decoder (Higgins et al., 2016) was used as a baseline model. SDN decoder was constructed using a single non-residual, one-directional instance of SDN placed at the scale 32. The competing methods were evaluated on 3D-Shapes (Burgess & Kim, 2018), a synthetic dataset containing 64×64 images of scenes with rooms and objects of various colors and shapes. Following related literature (Locatello et al., 2019), there was no training-test split, so the reported ELBOs are measured on the training set. The exact hyperparameter and architecture details are provided in Appendix A.4.

Training with an unmodified VAE objective. Using the original VAE objective (Kingma & Welling, 2013), competing architectures were compared in terms of ELBO (Table 2). SDN leads to substantially better estimates which come from better approximation of the conditional log-likelihood term, as shown in more detail in Figure 12 in the Appendix A.5.

VAE	KLD [BPD$\times 10^{-3}$]	**ELBO** [BPD]
CNN	7.40 ± 0.07	4.44 ± 0.04
SDN	7.95 ± 0.07	$\mathbf{2.66 \pm 0.04}$

Table 2: **Density estimation on 3D-Shapes.**

Training with β-VAE objective. The same models were trained using β-VAE objective (Higgins et al., 2016). In the β-VAE algorithm, the 'disentanglement' of latent dimensions is controlled by an additional hyperparameter denoted as β, which effectively acts as a regularizer. Modified ELBO reads as: $\mathcal{L}_{\phi,\theta}(X, \beta) = \mathbb{E}_{q_\phi(Z|X)}[\log p_\theta(X|Z)] - \beta \, \mathrm{KL}(q_\phi(Z|X)||p_0(Z))$. To investigate the effects of SDN decoder on the shaping of the latent space, we measured disentanglement for different values of β, for two popular disentanglement metrics: β-VAE (Higgins et al., 2016) and FactorVAE (Kim & Mnih, 2018). The results are shown in Figure 7.

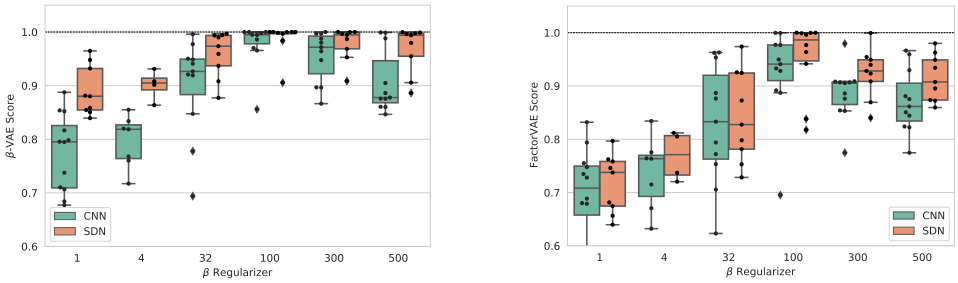

Figure 7: **β-VAE disentanglement results.** The plots compare the CNN and SDN-based VAE architectures, with respect to the β-VAE (left) and FactorVAE (right) disentanglement metrics.

Discussion. In a more constrained VAE setting, the beneficial effects of SDN to image modeling were confirmed. Perhaps surprisingly at first glance, we also found that improved VAE decoder facilitates factorization of latent codes. This may seem contradictory to the previous findings (Bowman et al., 2015; Chen et al., 2016; Razavi et al., 2019) which suggest that a powerful decoder hurts representation learning. However, the difference here is that SDN decoders do not leverage on teacher forcing. 'Posterior collapse' can happen only very early in the training, but this is in our case easily solved using β annealing (warm-up) procedure (Bowman et al., 2015). Our results indicate the importance of good neural architectures in learning disentangled representations.

6 Conclusions

Summary. This paper introduced a novel neural network architecture, specifically suitable for modeling image generators (decoders) in the context of deep generative modeling. The proposed SDN layer was analyzed in the context of: *(a)* a complex hierarchical VAE model, where we obtained state-of-the-art performance in non-autoregressive density modeling; *(b)* a vanilla VAE, resulting in improvements in both density modeling and representation learning.

Implications. SDN is a simple-to-use module which can be easily integrated into any deep neural network, and as demonstrated in the paper, it is favorable to convolutional networks in multiple settings. SDN-VAE can be used (unlike generative adversarial networks) for any density modeling task e.g. outlier detection. It is also favorable to autoregressive models in the settings where an explicit latent representation of data is needed, e.g. when the latent interpolation between test samples is necessary. We also provide an insight how VAE decoders can be changed for improved representation learning, suggesting an alternative way, and a concrete solution to tackle this important problem.

Limitations and future work. The main downside of SDN remains the computation time. However, we suspect that a more optimized implementation could substantially improve runtime performance. Another possible direction is to explore the applicability of SDN to other generative models such as generative adversarial networks (Goodfellow et al., 2014).

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A APPENDIX

A.1 DENSITY ESTIMATION – EXPERIMENT DETAILS

	CIFAR10	ImageNet32	CelebAHQ256
	$32^2 = 32$x32	32^2	256^2
# training samples	50K	1.281M	27K
# test samples	10K	50K	3K
Quantization	8 bits	8 bits	5 bits
Encoder/decoder depth	15	16	17
Deterministic #channels per layer	200	200	200
Stochastic #channels per layer	4	4	8
Scales	$8^2, 16^2, 32^2$	$4^2, 8^2, 16^2, 32^2$	$4^2, 8^2, 16^2, 32^2, 64^2, 128^2, 256^2$
SDN #channels per scale	120, 240, 260	424 for all	80, 160, 240, 320, 400, ~~SDN~~, ~~SDN~~
Layers per scale	5 for all	4 for all	2,2,2,2,2,3,4
Number of directions per SDN	2	3	2
Optimizer	Adamax	Adamax	Adamax
Learning rate	0.002	0.002	0.001
Learning rate annealing	Cosine	Cosine	Cosine
Batch size per GPU	32	32	4
Number of GPUs	8	8	8
GPU type	TeslaV100	TeslaV100	TeslaV100
GPU memory	32GB	32GB	32GB
Prior model	Gaussian	Gaussian	Gaussian
Posterior model	Gaussian	Gaussian	Gaussian
Posterior flow	1 IAF	1 IAF	1 IAF
Observation model	DML	DML	DML
DML Mixture components	5	10	30
Exponential Moving Average (EMA)	0.999	0.9995	0.999
Free bits	0.01	0.01	0.01
Number of importance samples	1024	1024	1024
Mixed-precision	Yes	Yes	Yes
Weight normalization	Yes	Yes	Yes
Horizontal flip data augmentation	Yes	No	Yes
Training time	45h	200h	90h

Table 3: **Experimental configurations for the density estimation tests.** DML is the discretized mixture of logistics (Salimans et al., 2017). Weight normalization, mixed-precision, free bits and Adamax are documented by Salimans & Kingma (2016); Micikevicius et al. (2018); Kingma et al. (2016); Kingma & Ba (2014) respectively. ~~SDN~~ means that SDN was not applied at the corresponding scale. The IAF (Kingma et al., 2016) contained 2 layers of masked 3x3 convolutional networks, with the context and number of CNN filters both of size 100. The importance sampling (Burda et al., 2015) was used for obtaining tighter lower bounds.

On configuring hyperparameters. Due to high computational demands, we only modestly optimized hyperparameters. In principle, our strategy was to scale up: (a) the number of deterministic and SDN filters; (b) batch size; (c) learning rate; (d) the number of SDN directions and (e) the number of DML components; as long as we found no signs of overfitting, had no memory or stability issues, and the training was not considerably slower. EMA coefficient values were taken from the previous related works (Kingma et al., 2016; Chen et al., 2018) – we tested 0.999 and 0.9995. We also swept through the values $\{2, 4, 8, 15\}$ for the number of latent stochastic filters, but saw no significant difference in the performance. Most extensively we explored the number of layers per scale, and found this to have relevant impact on runtime and over/underfitting, for both baseline and our architecture. We found that more downsampling improved runtime and reduced memory consumption, but made the tested models prone to overfitting.

A.2 Density Estimation – Ablation Studies

Additional ablation studies on SDN-VAE were conducted in order to explore in more detail whether the good performance on the density estimation experiments (Table 1) indeed comes from the proposed SDN layer. We used CIFAR-10 data on which both baseline and SDN-VAE models converged faster in comparison to two other data sets. Our main motivation was to understand whether the increase in performance comes from our architectural decisions or simply from the increase in the number of parameters. Namely, since ResSDN (from Figure 3) is a network with a larger number of parameters in comparison to the baseline 3x3 convolutional network, it would be justified to question if the increase in performance can be indeed attributed to ResSDN layers.

To that end, we designed multiple baseline blocks to replace CNN in the IAF-VAE+ architecture, by replicating the design protocol from Section 3 in which ResSDN was applied to create the SDN-VAE architecture. Baseline blocks are illustrated in Figure 8. The main idea is to explore whether possibly increased kernel of a CNN would be sufficient to model spatial dependencies, or whether a deeper network can bring the same performance to the basic VAE architecture.

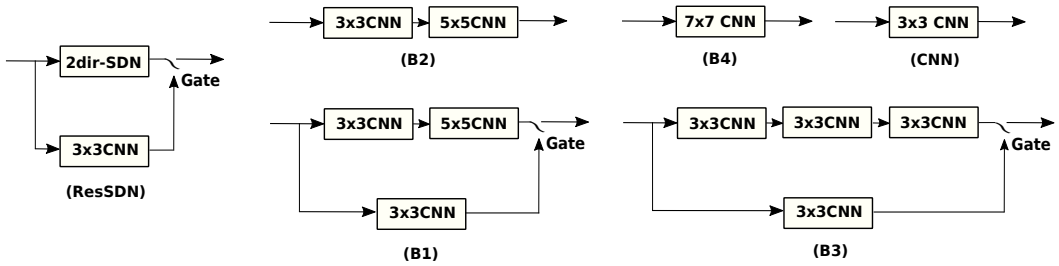


Figure 8: **ResSDN and baseline blocks.**

All baseline blocks were trained in the same setting as SDN-VAE i.e. all the parameters were kept fixed, except from the learning rate, which we halved after every 10 unsuccessful attempts to stabilize the training. IAF-VAE based on the CNN block was stable at the default learning rate of 0.002, B2 was stable at the learning rate of 0.001, while B4 and B1 were stable only at 0.0005. B2 was unstable. We also tested ResSDN at a learning rate of 0.001 to understand if there would be a drop in performance, but there wasn't any except from marginally slower convergence time.

The best runs in terms of evidence lower bound (ELBO) for each of the baseline blocks, along with our most successful run for SDN-VAE architecture are reported in Table 4. What we can observe is that the increase in capacity can indeed be correlated with good performance. However, even those VAE models which contained more parameters than the proposed SDN-VAE architecture were not able to converge to a higher ELBO. In fact, there exist a considerable performance gap between baseline blocks and the proposed ResSDN layer.

	Layer	Number of VAE parameters in millions	Time to reach best ELBO in hours	Time to reach best ELBO in iterations	**Best ELBO** in BPD
Baselines	CNN	42M	17h	140K	3.081
	B1	192M	21h	75K	3.080
	B2	104M		unstable	
	B3	126M	23h	90K	2.945
	B4	130M	22h	124K	3.120
Ours	ResSDN	121M	45h	60K	2.906

Table 4: **The comparison of ResSDN to the baselines from Figure 8.** We replaced CNN in the IAF-VAE+ architecture (from Section 3) with baseline blocks and compared the density estimation performance in terms of ELBO. The experiments were conducted on CIFAR-10 dataset.

A.3 IMAGE SYNTHESIS – ADDITIONAL RESULTS

Figure 9: **MSE-based nearest neighbors.** On the left, shown are images from Figure 6. On the right, shown are nearest neighbors in terms of mean squarred error (MSE), found in the training data set. There are no signs that generated samples are replicas of the training ones.

Figure 10: **Additional samples synthesized at different temperatures.** As we decrease the temperature, getting closer to the mean of the prior, the photographs become smoother i.e. more 'generic'.

Figure 11: **Sampling around a test image, for varying temperatures and number of fixed layers.** Presented is a 3x3 grid. In each grid there is a 3x3 sub-grid in which an image in the center is encoded, and the surrounding images are sampled conditioned on the specified number of layers from the encoded image and at the specified temperature. The text on the left hand side denotes the number of layers taken from an encoded image to condition sampling on. The text on the bottom denotes the temperature at which samples were drawn. Two key observations can be made: *(a)* lowering the temperature decreases the level of details, making photographs smoother; *(b)* Most of the information in SDN-VAE is encoded in the topmost layer. As we go further down the chain of the generator network, there is a gradual decrease in information content in latent stochastic variables.

A.4 LEARNING DISENTANGLED REPRESENTATIONS – EXPERIMENT DETAILS

The hyperparameter configuration is given in Table 5. In principle, we followed Higgins et al. (2016); Locatello et al. (2019) in configuring parameters. Notable changes include using of discretized logistics (Kingma et al., 2016) as the observation model and the Adamax optimizer. We also applied β-VAE annealing to avoid posterior collapse early in the training, an issue for both considered architectures. The base architecture was again taken from the same previous works. The exact description of architectures is given in Table 6 for the CNN-based VAE, and in Table 7 for the SDN-based VAE.

	3D Shapes $64^2 = 64 \times 64$
# data samples	448K
SDN #channels	200
Number of directions per SDN	1
Optimizer	Adamax
Learning rate	0.001
Batch size	128
Total number of training iterations	200k
Prior and posterior models	Gaussian
Observation model	Discretized Logistics

Table 5: **Configuration of disentangled representation learning experiments.**

Encoder	**Decoder**
4×4 conv, 32 ReLU, stride 2	FC, 256 ReLU
4×4 conv, 32 ReLU, stride 2	FC, $4 \times 4 \times 256$ ReLU
4×4 conv, 64 ReLU, stride 2	4×4 upconv, 64 ReLU, stride 2
4×4 conv, 64 ReLU, stride 2	4×4 upconv, 32 ReLU, stride 2
FC 256	4×4 upconv, 32 ReLU, stride 2
FC 2×10	4×4 upconv, 3 (number of channels) , stride 2

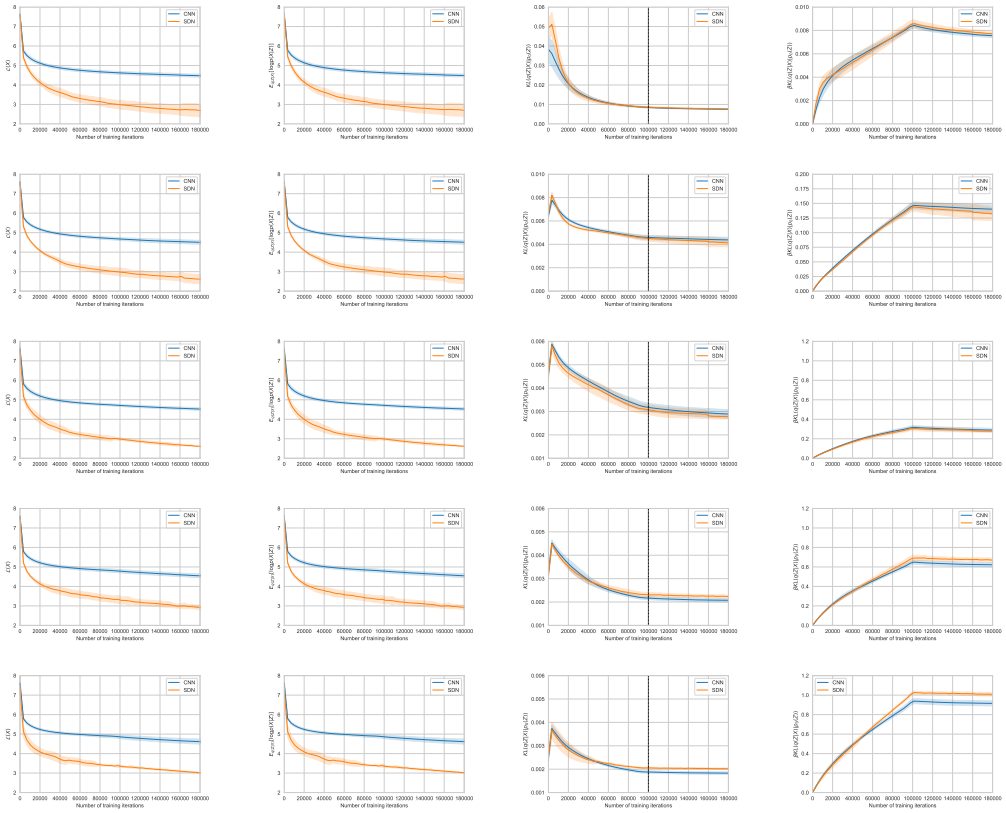
Table 6: **CNN-based vanilla VAE architecture.**

Encoder	**Decoder**
4×4 conv, 32 ReLU, stride 2	FC, 256 ReLU
4×4 conv, 32 ReLU, stride 2	FC, $4 \times 4 \times 256$ ReLU
4×4 conv, 64 ReLU, stride 2	4×4 upconv, 64 ReLU, stride 2
4×4 conv, 64 ReLU, stride 2	4×4 upconv, 32 ReLU, stride 2
FC 256	1dir-SDN with 200 channels
FC 2×10	4×4 upconv, 3 (number of channels) , stride 2

Table 7: **SDN-based vanilla VAE architecture.**

A.5 LEARNING DISENTANGLED REPRESENTATIONS – ADDITIONAL RESULTS

For the sake of completeness, we also provide learning curves for varying values of β and for different individual terms of β-VAE objective function. The plots are shown in Figure 12.



(a) (b) (c) (d)

Figure 12: **β-VAE learning curves for CNN and SDN-based VAE architectures.** Presented are the following quantities measured over the course of training: *(a)* evidence lower bound (ELBO); *(b)* conditional log-likelihood (reconstruction) term; *(c)* KL divergence term; *(d)* β-scaled KL divergence term; Top-to-bottom, the rows are related to $\beta = \{1, 32, 100, 300, 500\}$. Each pair ($\beta$ value, VAE architecture) is trained for 10 different random seeds. Linear β-annealing procedure was performed, where β was increased from 0 to its final value across the span of 100K training iterations (the end of the annealing procedure is denoted by the vertical line in the plots of the column (c)).