VFlow: More Expressive Generative Flows with Variational Data Augmentation

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Abstract

Generative flows are promising tractable models for density modeling that define probabilistic distributions with invertible transformations. However, tractability imposes architectural constraints on generative flows, making them less expressive than other types of generative models. In this work, we study a previously overlooked constraint that all the intermediate representations must have the same dimensionality with the original data due to invertibility, limiting the width of the network. We tackle this constraint by augmenting the data with some extra dimensions and jointly learning a generative flow for augmented data as well as the distribution of augmented dimensions under a variational inference framework. Our approach, VFlow, is a generalization of generative flows and therefore always performs better. Combining with existing generative flows, VFlow achieves a new state-of-the-art 2.98 bits per dimension on the CIFAR-10 dataset and is more compact than previous models to reach similar modeling quality.

1. Introduction

Generative flows (Dinh et al., 2014; 2017; Kingma & Dhariwal, 2018; Ho et al., 2019) are a promising class of generative models. They define a probability distribution $p(x)$ by applying an invertible transformation $x = f^{-1}(\epsilon)$ to some simple and known distribution $p(\epsilon)$. Stacking a sequence $f_1, \ldots, f_L$ of deep neural networks as the transformation, generative flows can model complicated high-dimensional data. Comparing with generative adversarial networks (GANs) (Goodfellow et al., 2014) and variational autoencoders (VAEs) (Kingma & Welling, 2014), generative flows are particularly attractive because their sampling process and density estimation are tractable. Due to these advantages, generative flows have been applied to a wide

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Figure 1. (a) Bottleneck problem in a Flow++ (Ho et al., 2019) for CIFAR-10. Dimensionality of the transformed data (red) limits the model capacity. (b) Our solution VFlow, where $D_Z$ is the dimensionality of the augmented random variable. Only the transformation step $f_1$ is shown due to space constraint.
range of problems including image generation (Kingma & Dhariwal, 2018), speech synthesis (Prenger et al., 2019), 3D point cloud generation (Yang et al., 2019), semi-supervised learning (Nalisnick et al., 2019), anomaly detection (Choi et al., 2018), and ray tracing (Müller et al., 2019).

However, tractability comes with a cost of model expressiveness. To be tractable, generative flows have more architectural constraints comparing with other non-invertible models, such as GANs and VAEs. One particular constraint is that the determinant of the Jacobian of \( f \) must be efficient to compute. While previous work typically adopts transformations with diagonal (Kingma & Dhariwal, 2018) or triangular Jacobian (Papamakarios et al., 2017), there has been lots of recent work developing transformations with free-form Jacobians, including invertible 1x1 convolution (Kingma & Dhariwal, 2018), continuous time flows (Chen et al., 2018; Grathwohl et al., 2019), invertible residual blocks (Behrmann et al., 2019; Chen et al., 2019), and emerging convolutions (Hoogeboom et al., 2019).

In this paper, we study another orthogonal architectural constraint, the bottleneck problem. To be invertible, all the transformation steps \( f_1, \ldots, f_L \) must output the same dimensionality with the input data \( x \), although each transformation (i.e., neural network) can have internal hidden layers of higher dimensionality. This contradicts with the commonly adopted wisdom of deep learning to learn overcomplete features, i.e., higher dimensional features than the data. As an example, Fig. 1(a) presents a state-of-the-art Flow++ (Ho et al., 2019) architecture. Although each transformation \( f_l \) has internal high-dimensional hidden layers (green), its input and output (red) still lie on the low-dimensional data space. This makes the generative flow highly inefficient because the high-dimensional features extracted within a transformation step cannot be reused by subsequent steps.

We propose VFlow as a solution to the bottleneck problem. VFlow augments the data \( x \) by extra dimensions \( z \), which are interpreted as latent variables. We develop a variational inference framework to learn a generative flow \( p(x; \theta) \) in the augmented data space jointly with the augmented data distribution \( q(z|x) \). We show that VFlow is a generalization of the vanilla generative flows, so the augmented dimensions always help. VFlow improves existing generative flows, and achieves a state-of-the-art 2.98 bits per dimension likelihood on the CIFAR-10 dataset.

On the efficiency side, the additional \( q(z|x) \) network and higher data dimensionality of VFlow only add marginal overhead to the vanilla generative flows. Meanwhile, VFlow can be more compact, since more information can be shared between individual transformation steps. Thus, each transformation step can be simpler by avoiding extracting high-dimensional features from scratch. We show that VFlow can be 2.6 times more compact than vanilla generative flows, while achieving similar model quality.

2. Backgrounds

In this section, we review the basics of generative flows and formally define the bottleneck problem.

2.1. Generative Flows

Given a distribution of \( D_X \)-dimensional data \( x \) on the space \( \mathbb{R}^{D_X} \), the task of generative modeling aims to learn a model distribution \( p(x; \theta) \) parameterized by \( \theta \) that approximates the data distribution. The model can be learned with the maximum likelihood principle

\[
\max_\theta \mathbb{E}_{\hat{p}(x)}[\log p(x; \theta)],
\]

where \( \hat{p}(x) \) is the empirical data distribution.

Generative flows define a sequence of invertible transformation steps \( f_1, \ldots, f_L \), that transform a datum \( x \) to some random variable \( \epsilon \).

\[
x \leftarrow f_1 \rightarrow h_1 \leftarrow f_2 \rightarrow h_2 \cdots \leftarrow f_L \rightarrow \epsilon,
\]

where \( \epsilon \) follows a simple factorized distribution that \( p_{\epsilon}(\epsilon) = \prod_i p_i(\epsilon_i) \), such as the standard normal distribution. For notational simplicity, we define \( h_0 = x \) and \( h_L = \epsilon \). Let \( f \) be the composition of all the \( L \) transformations, such that \( \epsilon = f(x; \theta) \), a generative flow defines the model distribution with the change-of-variables formula

\[
\log p(x; \theta) = \log p_{\epsilon}(\epsilon) + \log \left| \frac{\partial \epsilon}{\partial x} \right|,
\]

where \( \log \left| \frac{\partial \epsilon}{\partial x} \right| \) is the log-absolute-determinant of the Jacobian of \( f \). Samples from \( p(x; \theta) \) can be obtained by taking the inverse transformation from \( p_{\epsilon} \):

\[
\epsilon \sim p_{\epsilon}, \quad x = f^{-1}(\epsilon; \theta).
\]

One popular invertible transformation is the affine coupling layer (Dinh et al., 2017), where each transformation \( h_l = f_l(h_{l-1}; \theta) \) is defined as

\[
\begin{align*}
x_1, x_2 &= \text{split}(h_{l-1}), \\
y_1 &= x_1, \quad y_2 = \mu(x_1; \theta) + \exp(s(x_1; \theta)) \circ x_2,
\end{align*}
\]

\[
h_l = f_l(h_{l-1}; \theta) = \text{concat}(y_1, y_2),
\]

where \( \text{split}(\cdot) \) is any operation that splits the input into two halves, \( \text{concat}(\cdot) \) is its inverse operation, and \( \mu, s \) are neural networks with \( B \) hidden layers and \( D_H \) units per layer.

2.2. The Bottleneck Problem

Starting from the work on universal approximation theorems (Gybenko, 1989; Mhaskar, 1993) of multi-layer perceptrons, it is well known that network width plays an
We present VFlow, a variational data augmentation framework. The impact of network width is also verified empirically by recent works such as Wide ResNet (Zagoruyko & Komodakis, 2016) and EfficientNet (Tan & Le, 2019). Almost all existing non-invertible deep models, such as residual networks (He et al., 2016) and generative adversarial networks (Goodfellow et al., 2014) have features in a higher-dimensional space than the original data space.

However, for generative flows, all the transformed data $h_1, \ldots, h_L$ must have the same dimensionality $D_X$ with the input $x$ due to invertibility, as illustrated in Fig. 1. This architecture is ineffective for three reasons: (1) few features (green in Fig. 1) extracted within each transformation step can pass through the bottleneck (red in Fig. 1), so subsequent transformation steps must extract their own features from scratch; (2) for fixed dimensional $h_i$, the benefit of increasing the hidden layer size $D_H$ is limited. Unlike non-invertible deep networks, which can approximate arbitrary function with large $D_H$, the capacity of a single transformation step is intrinsically limited by architectural constraints, even with infinite $D_H$. For example, an affine coupling layer (Dinh et al., 2017) can only alter half of the dimensions, while an invertible residual block (Behrmann et al., 2019) has a bounded Lipschitz constant; (3) due to the limited capacity of a single transformation step, a sufficiently powerful generative flow need to have many transformation steps, which is expensive.

We refer to this issue as the bottleneck problem. To reflect the impact of the bottleneck width on model capacity, we denote a generative flow with $D$-dimensional bottleneck as a $D$-dimensional flow. Ideally, a $D_H$-dimensional flow completely eliminate the bottleneck.

3. VFlow

We present VFlow, a variational data augmentation framework and compare it with the vanilla generative flows.

3.1. Variational Data Augmentation

The bottleneck problem can be tackled by increasing the dimensionality of the original data, so that the dimensionality of the flow is also increased. To achieve this, we augment the data $x$ with an additional $D_Z$-dimensional random variable $z \in \mathbb{R}^{D_Z}$, and model the augmented data distribution $p(x, z; \theta)$ with a $(D_X + D_Z)$-dimensional flow. The new flow $p(x, z; \theta)$ is more powerful since its dimensionality can be adjusted freely by setting $D_Z$. The underlying invertible transformation becomes $\epsilon = f(x, z; \theta)$ where $\epsilon \in \mathbb{R}^{D_X + D_Z}$.

By modeling the augmented data distribution, the log marginal likelihood $\log p(x; \theta) = \log \int_z p(x, z; \theta)dz$ and optimization problem (1) become intractable in general. Thus, we resort to the variational methods and establish a lower bound of the marginal likelihood with a variational distribution of the augmented data $q(z|x; \phi)$:

$$\log p(x; \theta) \geq \mathbb{E}_{q(z|x; \phi)}[\log p(x, z; \theta) - \log q(z|x; \phi)],$$

which is known as evidence lower bound (ELBO) in variational inference literature. VFlow optimizes the following maximum ELBO objective as a surrogate of the maximum likelihood objective Eq. (1):

$$\max_{\theta, \phi} \mathbb{E}_{p(x)}[\log p(x, z; \theta) - \log q(z|x; \phi)].$$

After training, density estimation can be achieved with importance sampling

$$\log p(x; \theta) \approx \log \left( \frac{1}{S} \sum_{i=1}^{S} \frac{p(x, z_i; \theta)}{q(z_i; \phi)} \right),$$

where $z_1, \ldots, z_S \sim q(z|x; \phi)$ are the $S$ samples.

The augmented data distribution $q(z|x; \phi)$ is modeled with another conditional flow defined with an invertible transformation $z = g(\epsilon_q; x, \phi)$:

$$\log q(z|x; \phi) = \log p_\epsilon(\epsilon_q) - \log \left| \frac{\partial z}{\partial \epsilon_q} \right|,$$

where $\epsilon_q$ follows the same distribution $p_\epsilon$ with $\epsilon$. Given that $z = g(\epsilon_q; x, \phi)$ is differentiable reparameterization of $\epsilon_q$, the ELBO in Eq. (3) can be optimized with the reparameterization trick (Kingma & Welling, 2014). VFlow is illustrated in Fig. 1(b). By choosing different architectures for $p(x, z; \theta)$ and $q(z|x; \phi)$, VFlow can be combined with various existing generative flows (Kingma & Dhariwal, 2018; Ho et al., 2019; Chen et al., 2019), and improve their expressiveness and efficiency.

3.2. Connection to Vanilla Generative Flows

While VFlow tackles the bottleneck problem, it only maximizes a lower bound of the likelihood. It is thus worth studying whether the gain from increased dimensionality of the flow surpasses the gap between the marginal likelihood and the ELBO. We now show that VFlow is indeed better even it only optimizes a lower bound.

Define a flow family $\mathcal{P} = \{p(x; \theta) | \theta \in \Theta\}$ to be a set of generative flows, where $\Theta$ denotes the parameter space, i.e., the set of all possible values that $\theta$ can take. Popular flow families include Glow (Kingma & Dhariwal, 2018) and
Residual Flow (Chen et al., 2019). A flow family $\mathcal{P}$ can be further partitioned by the dimensionality: $\mathcal{P}_1 \cup \mathcal{P}_2 \cup \cdots = \mathcal{P}$, where $\mathcal{P}_D = \{p(x; \theta) | \theta \in \Theta_D\}$ is the subset of all $D$-dimensional flows, and $\Theta_D$ is the corresponding subset of parameters. While a vanilla generative flow can only model the data $x$ with a flow from $\mathcal{P}_{D_X \cup D_Z}$, VFlow can choose a flow from any $\mathcal{P}_{D_X + D_Z}$ such that $D_Z > 0$, to model the joint distribution of $(x, z)$. Similarly, let $\mathcal{Q}_D$ and $\Theta_D$ be the (partitioned) flow family and parameter space for $q(z|x; \phi)$. Recalling $p_e(\cdot)$ is a simple factorized distribution defined in Sec. 2.1, our analysis is based on the following mild assumptions:

**A1** (high-dimensional flow can emulate low-dimensional flow) For all $p(x; \theta_{D_X}) \in \mathcal{P}_{D_X}$ and $D_Z > 0$, there exists $p(x, z; \theta_{D_X + D_Z}) \in \mathcal{P}_{D_X + D_Z}$, such that for all $x$ and $z$,

$$p(x, z; \theta_{D_X + D_Z}) = p(x; \theta_{D_X}) p_e(z).$$

**A2** (the flow-family has an identity transformation) For all $D_Z > 0$, there exists $q(z|x; \phi) \in \mathcal{Q}_{D_Z}$, such that for all $x$ and $z$, $q(z|x; \phi) = p_e(z)$.

Assumptions A1 and A2 can be verified for most existing flow families (Kingma & Dhariwal, 2018; Chen et al., 2019). Consider the simplest case of a linear flow $\epsilon = x\theta_{D_X}$, where the weight matrix $\theta_{D_X}$ is orthonormal. Taking $\theta_{D_X + D_Z} = \begin{bmatrix} \theta_{D_X} & 0 \\ 0 & 1 \end{bmatrix}$ yields $p(x, z; \theta_{D_X + D_Z}) = p_e(x \theta_{D_X}) p_e(z)$, satisfying Assumption A1. Moreover, $q(z|x; \phi) = p_e(z)$, satisfying Assumption A2. We leave a detailed verification for Glow (Kingma & Dhariwal, 2018) and Residual Flow (Chen et al., 2019) in Appendix A.

The following theorem compares the maximum ELBO solution Eq. (4) of VFlow with the maximum likelihood solution Eq. (1) of vanilla generative flows.

**Theorem 1.** Under Assumptions A1 and A2, for any $D_X, D_Z > 0$, we have

$$\max_{\theta \in \Theta_{D_X}} \mathbb{E}_{p(x)}[\log p(x; \theta)]$$

$$\leq \max_{\theta \in \Theta_{D_X + D_Z}} \mathbb{E}_{p(x|q(z|x; \phi))} [\log p(x, z; \theta) - \log q(z|x; \phi)].$$

**Proof.**

$$\max_{\theta \in \Theta_{D_X}} \mathbb{E}_{p(x)}[\log p(x; \theta)]$$

$$= \max_{\theta \in \Theta_{D_X}} \mathbb{E}_{p(x|p_e(x))} [\log p(x; \theta) + \log p_e(z) - \log p_e(z)]$$

$$\leq \max_{\theta \in \Theta_{D_X + D_Z}} \mathbb{E}_{p(x|q(z|x; \phi))} [\log p(x, z; \theta) - \log p_e(z)] \quad (6)$$

$$\leq \max_{\theta \in \Theta_{D_X + D_Z}} \mathbb{E}_{p(x|q(z|x; \phi))} [\log p(x, z; \theta) - \log q(z|x; \phi)],$$

where the third line utilizes Assumption A1, and the last line utilizes Assumption A2.

**Remark 1:** Theorem 1 does not consider optimization issues, such as convergence speed. However, as we shall see in Appendix A, it is rather simple for a VFlow to mimic a vanilla generative flow by setting some parameters to zero, due to the residual structure of transformation steps. Therefore, we hypothesize that VFlow should still be better than vanilla generative flows under the same number of optimizer iterations. This is empirically verified in Fig. 6.

**Remark 2:** Variational inference-based models such as VAEs rely heavily on the quality of the variational posterior $q(z|x; \phi)$ to work well. Unlike VAE, VFlow is better than vanilla generative flows even with a trivial variational distribution $q(z|x) = p_e(z)$. This can be seen from Eq. (6).

**Remark 3:** After fitting a VFlow model, we can use it for sampling or density estimation. Sampling from VFlow is straightforward by discarding $z$ from the samples in the augmented space. Density estimation is slightly more complicated due to the importance sampling in Eq. (5). However according to Theorem 1, even the ELBO of VFlow is better than vanilla generative flows even with a trivial variational distribution $q(z|\theta)$.

3.3. Efficiency

While VFlow makes the model more expressive, its overhead is only marginal. The overhead arises from two parts: (1) the cost of computing $q(z|x; \phi)$ and (2) the increase of the cost for computing $p(x, z; \theta)$ due to the increase of the dimensionality. The first cost can be small by using a much smaller network for $q(z|x; \phi)$ than $p(x, z; \theta)$. As an extreme case, one can eliminate the cost by adopting $q(z|x; \phi) = p_e(z)$, according to Remark 2. The second cost is small because most computation of $p(x, z; \theta)$ is spent on the internal hidden layers (green layers in Fig. 1), whose time complexity is only related to the hidden layer size $D_H$ instead of the flow dimensionality $D_X + D_Z$.

On the other hand, VFlow can be more compact and efficient than a vanilla generative flow to achieve similar modeling quality, as it alleviates the ineffectiveness listed in Sec. 2.2 caused by the bottleneck problem.

3.4. Modeling Discrete Data

The discussion so far is limited to continuous data $x$. If the data follow a discrete distribution $P(x)$, an additional dequantization step is needed to convert the data from discrete to continuous. Ho et al. (2019) propose to bound the discrete density with a variational dequantization distribution.
Variational autoencoders (Kingma & Welling, 2014) can be understood as VFlows where both $p(x, z; \theta)$ and $q(z|x; \phi)$ are generative flows with a single affine coupling layer. Particularly, a Gaussian VAE $p(x, z; \theta) = \mathcal{N}(z; 0, I), \mathcal{N}(x; \mu(z), \exp(s(z))^2)$ is equivalent with

$$
\epsilon_Z \sim \mathcal{N}(0, I), \quad \epsilon_X \sim \mathcal{N}(0, I), \\
z = \epsilon_Z, \quad x = \mu(\epsilon_Z) + \exp(s(\epsilon_Z)) \circ \epsilon_X,
$$

which shares the same form with the affine coupling layer defined in Eq. (2), despite in the opposite direction. VFlows are more general than VAEs by not assuming the conditional independence $p(x, z) = p(z)p(x|z)$. Though it is possible for VAEs to implement both $p(z)$ and $p(x|z)$ with generative flows (Morrow & Chiu, 2020; Chen et al., 2017), the flow $p(x|z)$ is still $D_X$-dimensional, so the bottleneck problem persists. Another line of work implements $q(z|x)$ with generative flows (Kingma et al., 2016; Rezende & Mohamed, 2015) but leaves $p(x, z)$ unchanged. VFlow has identical $q(z|x)$ but more powerful $p(x, z)$ than these works. There are also a number of works combining VAEs with autoregressive models (Chen et al., 2017; Gulrajani et al., 2017). However they suffer from slow sampling due to the sequential nature of autoregressive models. Finally, while a powerful $q(z|x)$ is critical for VAEs, it is less important for VFlows, since $p(x, z)$ itself is powerful even with $q(z|x) = p_c(z)$, as discussed in Sec. 3.2.

5. Toy Data Experiments

We first evaluate VFlow on a toy $D_X = 2$ Checkerboard dataset (Behrmann et al., 2019), which is multimodal and its density is shown in Fig. 2(a). The baseline model is Glow (Kingma & Dhariwal, 2018), whose each transformation step consists of an affine coupling layer with 2 hidden layers and $D_H = 50$ hidden units per layer. VFlow further augments Glow with a conditional Glow $q(z|x; \phi)$ and various number of extra dimensions $D_Z$. All the models are trained 100,000 iterations with Adam (Kingma & Ba, 2015) and a batch size of 64, and each experiment is repeated by
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Figure 3. Visualization of learnt transformation on toy data. Top row: 2-step Glow. Bottom row: 2-step, 3-dimensional VFlow. Log-likelihood is shown in parenthesis. We sample $\epsilon$ and visualize the transformed density in $x$, $h_1$ and $\epsilon$ space. The density is estimated from samples by kernel density estimation, and we show the 50% probability contour / isosurface for each mode in different color.

Figure 4. Impact of the dimensionality on the toy dataset.

5 times with different random seeds. Model quality is measured with the log-likelihood $\log p(x)$ on a 1,000-sample test set. For VFlow, likelihood is evaluated with 100-sample importance sampling by Eq. (5).

We study the impact of the dimensionality of the flow $D_X + D_Z \in \{2, 4, 6, 8, 10\}$, where $D_X + D_Z = 2$ is the baseline Glow and $D_X + D_Z > 2$ is VFlow. To control the model size, we vary the total number of transformation steps $L \in \{2, 3, 4, 5, 10, 15, 20\}$. For baseline Glow, the $p$-network has all the $L_p = L$ transformation steps; and for VFlow, $p$-network has $L_p = L - 1$ transformation steps and $q$-network has one transformation step. The result is shown in Fig. 4. VFlow significantly outperforms Glow under similar model size. For example, a 3-step, 10-dimensional VFlow achieves $-3.51 \pm 0.01$ log-likelihood (Fig. 2(b)), outperforming the baseline 3-step Glow with $-3.67 \pm 0.03$ log-likelihood (Fig. 2(c)) by a large margin. The 3-layer, 10-dimensional VFlow even outperforms a much larger 20-step Glow, which achieves $-3.54 \pm 0.05$ log-likelihood (Fig. 2(d)), showing that the model can be much more compact by solving the bottleneck problem.

To further understand why the dimensionality is important, we visualize the learnt representation for a 2-step Glow and a 2-step VFlow, which has a single transformation step for both $p$ and $q$. To make visualization possible, $z$ is only one-dimensional, so $D_X + D_Z = 3$. Note that having odd number of dimensions is suboptimal because the affine coupling layer cannot split the data into two parts with equal number of dimensions. Moreover, affine coupling layer cannot represent the one-dimensional distribution $q(z|x)$, so we replace it with a Gaussian layer $\mathcal{N}(z; \mu(x), \sigma(x))$ without changing the architecture of $\mu(x)$ and $\sigma(x)$. The learnt transformations are visualized in Fig. 3. While Glow struggles to map different modes to the compact space of $\epsilon$, VFlow does a much better job. VFlow learns a pile of “pies” in the $\epsilon$ space, where each mode is a pie, and different
Table 1. Density modeling result on the CIFAR-10 dataset.

| Model                     | bpd |
|---------------------------|-----|
| Glow (Kingma & Dhariwal, 2018) | 3.35 |
| FFJORD (Grathwohl et al., 2019) | 3.40 |
| Residual Flow (Chen et al., 2019) | 3.28 |
| MintNet (Song et al., 2019) | 3.32 |
| Flow++ (Ho et al., 2019) | 3.08 |
| VFlow                     | 2.98 |

modes are directly distinguished by the extra dimension $z$.

By shifting the pies to different positions on the $x$-plane based on $z$, VFlow can easily handle the multi-modality of the data. Comparing with Glow which needs to map an irregular shape in the $\epsilon$ space to a square in the $x$ space, VFlow requires a much simpler transformation, because each mode is already a regular pie in the $\epsilon$ space.

6. Density Estimation of Images

In this section, we evaluate VFlow on the CIFAR-10 dataset for density estimation of images. VFlow augments a state-of-the-art generative flow, Flow++ (Ho et al., 2019) by introducing extra dimensions and another variational distribution $q(z|x)$. More specifically, the $p(x, z)$ network is similar with Flow++ shown in Fig. 1, and the main difference is the dimensionality of the flow. Variational dequantization is deployed according to Sec. 3.4. We choose the network architecture for $q(z|x)$ to be similar with the variational dequantization network $r(u|x)$ of Flow++. A detailed description of the model architecture is in Appendix B. While we only consider Flow++ for this section due to its impressive density estimation result, our variational data augmentation framework is general and can be combined with future advances of the model architecture.

The model size is controlled by three main hyper-parameters, (1) the dimensionality of the flow. For brevity, we refer to a $32 \times 32 \times C$-dimensional flow as a $C$-channel flow, where a 3-channel flow is the baseline Flow++; (2) the hidden layer size $D_H$; and (3) the number of hidden layers $B$ per transformation step, i.e., number of green layers in Fig. 1.

The model is trained with an Adam optimizer (Kingma & Ba, 2015) with a batch size 64 for 2,000 epochs. Following (Ho et al., 2019), the learning rate linearly warms up to 0.0012 during the first 2,000 training steps, and exponentially decays at a rate of 0.99999 per step starting from the 50,000-th step until it reaches 0.0003. All the experiments are run on 16 RTX 2080Ti GPUs.

The model quality is measured by bits per dimension (bpd) (Van Oord et al., 2016), defined as

$$bpd = \exp(-\frac{1}{N} \sum_{x \in \mathcal{X}} \log P(x; \theta)/D_X),$$

where $N$ is the size of the dataset $\mathcal{X}$. Bpd can be understood as the number of bits that a compression algorithm takes to encode an 8-bit RGB value. Therefore, smaller bpd implies higher likelihood and better modeling quality. The dataset is kept with its original 50000 / 10000 split. Without further notice, we report bpd on the test dataset, where the likelihood $P(x; \theta)$ is evaluated with importance sampling as Eq. (5) with $S = 4096$ samples.

6.1. Improving Existing Models

We compare a 6-channel VFlow with existing generative flows in Table 1, where the hyperparameters $D_H = 96$.
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Figure 6. Bpd on training (light) and testing (dark) dataset of Flow++ and VFlow under a 4-million parameter budget. Here bpd is only a upper bound because we evaluate it with ELBO as Eq. (7) instead of the marginal likelihood.

and $B = 10$ are set identical to Flow++. By augmenting the number of channels from 3 to 6, VFlow improves the bpd from 3.08 of Flow++ to 2.98. Samples from Flow++ and VFlow are shown in Fig. 5, where the image quality of VFlow is similar or slightly better than Flow++. Quantitatively, the Fréchet Inception Distance (Heusel et al., 2017) improves from 69.1 (Flow++) to 64.9 (VFlow). Therefore, VFlow not only improves the likelihood, but also improves the image quality. We emphasize that this study focuses on whether VFlow can improve existing models, and it is possible to generate more visually appealing images by combining VFlow with other architectures that have better image quality, such as Residual Flow (Chen et al., 2019).

6.2. Ablation Study under Fixed Parameter Budget

To further investigate the impact of the dimensionality, we vary the number of channels under a fixed 4 million parameter budget. As the dimensionality grows, we reduce the number of hidden layers $B$ to stay within the parameter budget. The training curve and final bpd are reported in Fig. 6 and Table 2 respectively, which clearly show that increased dimensionality is beneficial. Moreover, VFlow achieves better results at all stages of training. This supports Remark 1 in Sec. 3.2 that VFlow is still better even taken optimization issues into account. For this $D_H = 32$ network, a 6-channel VFlow, which has 24 channels on the $16 \times 16$ scale, is already sufficient to resolve the bottleneck problem. Going beyond 6 channels has marginal improvement on the model quality, while increasing the number of parameters.

Interestingly, Fig. 6 suggests that besides improved model capacity, the generalization gap of VFlow is also slightly smaller than Flow++. We suspect the additional randomness introduced by $z$ acts as an implicit regularization.

6.3. Parameter Efficiency

The last set of experiments aims for more compact models with similar model capacity. As shown by Table 3, we can reduce the number of parameters of the baseline Flow++ from 31.4 million to 11.9 million, which is a 2.6 times reduction. This reduction of model size is achieved by reducing the hidden layer size $D_H$ from 96 to 56. As we argued in Sec. 2.2, the excessive number of hidden units does not help much for a network with merely 3 channels. Increasing the dimensionality of the network (i.e., the bottleneck width) is much more efficient than increasing $D_H$. Therefore, VFlow is not only more expressive but also more compact than vanilla low-dimensional flows. We emphasize that the reduction of model size come solely from resolving the bottleneck problem. Even smaller models can be forged by combining with potentially more compact architectures, such as MintNet (Song et al., 2019).

7. Conclusions

We identify the bottleneck problem which limits the capacity of generative flows. To tackle this problem, we propose VFlow, a variational data augmentation framework that pads extra dimensions to the data with learnable variational distributions for the padded data. VFlow is a generalization of vanilla generative flows, and can be combined with existing generative flows to improve their expressiveness and compactness. In our experiments on the CIFAR-10 dataset, VFlow achieves a new state-of-the-art 2.98 bpd, or being 2.6 times more compact.

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A. Verification of Assumption A1 and A2

A1 For all $p(x; \theta_{D_X}) \in \mathcal{P}_{D_X}$ and $D_Z > 0$, there exists $p(x, z; \theta_{D_X+D_Z}) \in \mathcal{P}_{D_X+D_Z}$, such that for all $x$ and $z$,

$$p(x, z; \theta_{D_X+D_Z}) = p(x; \theta_{D_X})p_e(z).$$

A2 For all $D_Z > 0$, there exists $q(z|x; \phi) \in \mathcal{Q}_{D_Z}$, such that for all $x$ and $z$,

$$q(z|x; \phi) = p_e(z).$$

Let $x, z$ be row vectors, and $[x \ z]$ be the horizontal concatenation of $x$ and $z$. We first show that the following conditions are sufficient for Assumption A1 and A2.

B1 For all $\theta_{D_X} \in \Theta_{D_X}$ and $D_Z > 0$, there exists $\theta_{D_X+D_Z} \in \Theta_{D_X+D_Z}$, such that for all $l, x$ and $z$,

$$f_l([x \ z]; \theta_{D_X+D_Z}) = [f_l(x; \theta_{D_X}) \ z].$$

B2 For all $D_Z > 0$, there exists $\phi \in \Phi_{D_Z}$, such that for all $l, x$ and $z$,

$$g_l(\epsilon_q; x; \phi) = \epsilon_q.$$

Proof. Under condition B1,

$$f([x \ z]) = f_1(\ldots(f_L([x \ z])))) = f_1(\ldots(f_{L-1}([f_L(x) \ z]))) = f_1(\ldots(f_{L-2}([f_{L-1}(f_L(x)) \ z]))) = \ldots = [f_1(\ldots(f_L(x))) \ z].$$

Then,

$$p(x, z; \theta_{D_X+D_Z}) = p_e(f([x \ z]; \theta_{D_X+D_Z})) \left| \frac{\partial f([x \ z]; \theta_{D_X+D_Z})}{\partial [x \ z]} \right|$$

$$= p_e(f(x; \theta_{D_X})z) \left| \frac{\partial [f(x; \theta_{D_X}) \ z]}{\partial [x \ z]} \right|$$

$$= p_e(f(x; \theta_{D_X}))p_e(z) \left[ \frac{\partial f(x; \theta_{D_X})}{\partial x} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right]$$

$$= p_e(f(x; \theta_{D_X})) \left| \frac{\partial f(x; \theta_{D_X})}{\partial x} \right| p_e(z)$$

$$= p(x; \theta_{D_X})p_e(z).$$
Similarly, under condition B2,
\[
g(\epsilon_q; x, \phi) = g_1(\ldots (g_L(\epsilon_q))) = \epsilon_q.
\]
So
\[
q(z; x, \phi) = q(g(\epsilon_q; x, \phi)|x; \phi) = p_\epsilon(\epsilon_q) / |\partial z / \partial \epsilon_q| = p_\epsilon(\epsilon_q) / |I| = p_\epsilon(\epsilon_q).
\]

Therefore, we only need to verify condition B1 and B2 separately for each transformation step. For Glow (Kingma & Dhariwal, 2018) and Residual Flow (Chen et al., 2019), the transformations to verify includes affine coupling layer (Dinh et al., 2017), invertible 1×1 convolution (Kingma & Dhariwal, 2018), and invertible residual blocks (Behrmann et al., 2019). In this section we only verify condition B1 and B2 for fully-connected transformations, but they readily generalize to convolutional transformations.

### A.1. Invertible Residual Blocks

An invertible residual block (Behrmann et al., 2019) \( f_l(x; \theta_{D_X}) \) for \( D_X \)-dimensional input \( x \) is defined as
\[
a_1 = x\theta_{D_X}^{(1)}, \quad a_2 = n(a_1; \theta_{D_X}^{(2)}), \quad \Delta_x = a_2\theta_{D_X}^{(3)}, \quad f_l(x; \theta_{D_X}) = y = x + \Delta_x,
\]
where we explicitly write the first and last linear layer, and leave all the internal hidden layers as \( n(a_1; \theta_{D_X}^{(2)}) \). We construct a \( D_X + D_Z \)-dimensional invertible residual block \( f_l([x \quad z]; \theta_{D_X+D_Z}) \) as
\[
a_1 = [x \quad z]\theta_{D_X+D_Z}^{(1)}, \quad a_2 = n(a_1; \theta_{D_X+D_Z}^{(2)}), \quad [\Delta_x \quad 0] = a_2\theta_{D_X+D_Z}^{(3)},
\]
\[
f_l([x \quad z]; \theta_{D_X+D_Z}) = [x + \Delta_x \quad z + 0] = [f_l(x; \theta_{D_X}) \quad z],
\]
satisfying condition B1, where
\[
\theta_{D_X+D_Z}^{(1)} = \begin{bmatrix} \theta_{D_X}^{(1)} \\ 0 \end{bmatrix}, \quad \theta_{D_X+D_Z}^{(2)} = \theta_{D_X}^{(2)} + \Delta_x, \quad \theta_{D_X+D_Z}^{(3)} = \begin{bmatrix} \theta_{D_X}^{(3)} \\ 0 \end{bmatrix}.
\]

This construction is demonstrated by Fig. 7. Intuitively, due to the residual structure, we only need to output \( 0 \) for all the \( z \) dimensions. Similarly, condition B2 can be satisfied by taking \( \theta_{D_Z}^{(3)} = 0 \), so that all the residuals are zero and the network outputs identity.
A.2. Affine Coupling Layer

An affine coupling layer (Dinh et al., 2017) \( f_l(x; \theta_{D_X}) \) for \( D_X \)-dimensional input \( x \) is defined as

\[
x_1, x_2 = \text{split}(x), \quad y_1 = x_1, \quad y_2 = \mu(x_1; \theta_{D_X}) + \exp(s(x_1; \theta_{D_X})) \circ x_2, \quad f_l(x; \theta_{D_X}) = \text{concat}(y_1, y_2).
\]

The case of affine coupling layer is almost identical to the invertible residual block, because both transformations have residual structures. This can be seen by noticing when \( \mu(x_1; \theta_{D_X}) = s(x_1; \theta_{D_X}) = 0, f_l(x; \theta_{D_X}) = x \). We explicitly write out the first and last linear layers of \( \mu(\cdot) \) and \( s(\cdot) \):

\[
x_1, x_2 = \text{split}(x), \quad y_1 = x_1, \quad a_1 = x_1 \theta_D^{(a1)}, \quad a_2 = \mu'(a_1; \theta_{D_X}^{(a2)}), \quad a_3 = a_2 \theta_D^{(a3)}, \quad b_1 = x_1 \theta_D^{(b1)}, \quad b_2 = s'(b_1; \theta_{D_X}^{(b2)}), \quad b_3 = b_2 \theta_D^{(b3)}, \quad y_2 = a_3 + b_3 \circ x_2, \quad f_l(x; \theta_{D_X}) = \text{concat}(y_1, y_2).
\]

A \( D_X + D_Z \)-dimensional affine coupling layer has the form

\[
\begin{bmatrix}
x_1 \\
z_1 \\
x_2 \\
z_2
\end{bmatrix}
= \text{split}(\begin{bmatrix}x & z \end{bmatrix}), \quad y_1 = x_1,
\begin{bmatrix}
a_1 \\
a_2 \\
b_1 \\
b_2
\end{bmatrix}
= \begin{bmatrix}x_1 \theta_D^{(a1)} & x_1 \theta_D^{(a2)} & x_1 \theta_D^{(a3)} \\
\theta_D^{(a2)} & \theta_D^{(a3)} & \theta_D^{(b1)} & \theta_D^{(b2)} & \theta_D^{(b3)}
\end{bmatrix}, \quad \begin{bmatrix}a_3 \\
a_3 & u_3 & w_3 & z_2
\end{bmatrix}
= \begin{bmatrix}a_3 & u_3 & w_3 & z_2
\end{bmatrix},
\begin{bmatrix}
y_2 \\
y_2
\end{bmatrix}
= \text{concat}(\begin{bmatrix}y_1 & z_1 & y_2 \end{bmatrix}).
\]

We want the networks \( \mu(\cdot; \theta_{D_X+D_Z}) \) and \( s(\cdot; \theta_{D_X+D_Z}) \) to ignore the \( z_1 \) part from the input, and output zero for \( u_3, w_3 \), so that

\[
\begin{bmatrix}a_3 \\
u_3 \\
w_3
\end{bmatrix}
= \begin{bmatrix}a_3 & u_3 & w_3
\end{bmatrix}, \quad \begin{bmatrix}a_3 \\
u_3 & w_3 & z_2
\end{bmatrix}
= \begin{bmatrix}a_3 & u_3 & w_3 & z_2
\end{bmatrix},
\begin{bmatrix}
y_2 \\
y_2
\end{bmatrix}
= \begin{bmatrix}y_2 & \mu(x_1; \theta_{D_X}) + \exp(s(x_1; \theta_{D_X})) \circ x_2 & z_2
\end{bmatrix}, \quad f_l([x, z]; \theta_{D_X+D_Z}) = \begin{bmatrix}f_l(x; \theta_{D_X}) & z
\end{bmatrix},
\]

so condition B1 is satisfied. We can easily achieve this by setting

\[
\theta_D^{(a1)} = \begin{bmatrix}0 & 0
\end{bmatrix}, \quad \theta_D^{(a2)} = \begin{bmatrix}0 & 0
\end{bmatrix}, \quad \theta_D^{(a3)} = \begin{bmatrix}0 & 0
\end{bmatrix},
\theta_D^{(b1)} = \begin{bmatrix}0 & 0
\end{bmatrix}, \quad \theta_D^{(b2)} = \begin{bmatrix}0 & 0
\end{bmatrix}, \quad \theta_D^{(b3)} = \begin{bmatrix}0 & 0
\end{bmatrix}.
\]

Similarly, condition B2 can be satisfied by setting \( \theta_{D_Z}^{(a3)} = \theta_{D_Z}^{(b3)} = 0 \).

A.3. Invertible 1×1 Convolution

For fully-connected cases, invertible 1×1 convolution (Kingma & Dhariwal, 2018) degenerates to a regular matrix multiplication

\[
f_l(x; \theta_{D_X}) = x \theta_{D_X},
\]

where \( \theta_{D_X} \) is a non-singular matrix. We construct \( f_l(x; \theta_{D_X+D_Z}) \) such that

\[
\theta_{D_X+D_Z} = \begin{bmatrix}0 & 0
\end{bmatrix}.
\]

Clearly, \( \theta_{D_X+D_Z} \) is also non-singular, and \( f_l([x, z]; \theta_{D_X+D_Z}) = f_l(x; \theta_{D_X}) = z \). On the other hand, condition B2 can be satisfied by setting \( \theta_{D_Z} = I \).
We show the model architectures used in Sec. 6.1 and Sec. 6.3 in Table 4, where the architecture of VFlow is almost identical with the baseline Flow++, except we use both $f_{\text{checker}}$ and $f_{\text{channel}}$ for the $32 \times 32$ scale, while Flow++ uses only $f_{\text{checker}}$. Flow++ cannot use $f_{\text{channel}}$ for the $32 \times 32$ scale because there are odd number (3) of channels. The model architectures under 4-million-parameter budget used in Sec. 6.2 are listed in Table 5. In this experiment, we use a special affine coupling

\begin{table}[h]
\centering
\caption{Model architecture for improving existing models experiment and parameter efficiency experiment.}
\begin{tabular}{|c|c|c|c|c|}
\hline
Model & 3-channel Flow++ & 6-channel VFlow & 6-channel VFlow & 6-channel VFlow \\
\hline
Parameters & 31.4M & 37.8M & 16.5M & 11.9M \\
bpd & 3.08 & 2.98 & 3.03 & 3.08 \\
\hline
\end{tabular}
\end{table}
layer to mix \( z \) and \( x \) forcibly:

\[
\begin{align*}
& y_1 = z, \quad y_2 = \mu(z) + \exp(s(z)) \circ x, \quad f_{\text{affine}} = \text{concat}(y_1, y_2) \\
\end{align*}
\]

where \( \mu \) and \( s \) are \( \mathbb{R}^{D_z} \to \mathbb{R}^{D_x} \) functions. We empirically find that adding this special affine coupling layer accelerates the convergence for small networks. The building block with this affine coupling layer with \( B \) hidden layers and \( D_H \) hidden units is denoted as \( f_{\text{affine}}(B, D_H) \) in Table 3.

### Fixing Gradient Explosion

In our experiments, we find that the implementation of mixture-of-logistic attention coupling layer (Ho et al., 2019) sometimes produces huge gradients, leading the training to diverge. To see this, note that the mixture-of-logistic attention coupling layer for a given input \( x = (x_1, x_2) \) and the output \( y = (y_1, y_2) \) is defined by:

\[
\begin{align*}
\text{MixLogCDF}(x; \pi, \mu, s) &= \sum_{i=1}^{K} \pi_i \sigma((x - \mu_i) \cdot \exp(-s_i)), \quad \text{where} \quad \sum_{i=1}^{K} \pi_i = 1 \\
y_1 &= x_1, \quad y_2 = \sigma^{-1}\left(\text{MixLogCDF}(x_2; \pi\theta(x_1), \mu\theta(x_1), s\theta(x_1)) \circ \exp(a\theta(x_1)) + b\theta(x_1)\right)
\end{align*}
\]

where \( \sigma(x) = \frac{1}{1 + \exp(-x)} \) is the sigmoid function. However, the inverse sigmoid may cause gradient explosion. For example, if \( x = 1 - 10^{-N} \), then \( (\sigma^{-1}(x))' = \frac{1}{\sigma(1-x)} \approx 10^N \). If for each component, \( x - \mu_i \) is large and \( s_i \) is small, then \( (x - \mu_i) \cdot \exp(-s_i) \) is large, and \( \text{MixLogCDF}(x_2; \pi\theta(x_1), \mu\theta(x_1), s\theta(x_1)) \) will be close to 1, leading to gradient explosion of the inverse sigmoid function. For example, if \( \pi_1 = 1, x - \mu_i = 4 \) and \( s_1 = -1 \), we have \( \text{MixLogCDF} = \sigma((x - \mu_i) \cdot \exp(-s_i)) \approx 1 - 2 \cdot 10^{-5} \) and then the gradient can be very large. We fix this issue by scaling the input of the inverse sigmoid function to [0.05, 0.95]:

\[
y_2 = \sigma^{-1}(0.05 + 0.9 \times \text{MixLogCDF}(x_2; \pi\theta(x_1), \mu\theta(x_1), s\theta(x_1)) \circ \exp(a\theta(x_1)) + b\theta(x_1)).
\]

### C. Extra Experiments

We further study whether it is better to put more parameters on \( p(x, z) \) or \( q(z|x) \). Under a fixed 4 million total parameter budget, we vary the parameter allocation between \( p(x, z) \) or \( q(z|x) \), and list the corresponding result and model architecture in Table 6. The result implies that it is better to put most parameters on \( p(x, z) \), supporting our claim in Sec. 4 that the variational distribution of VFlow is not necessarily as complicated as those in VAEs.
Table 6. Parameter allocation between $p(x, z)$ and $q(z|x)$.

|                  | 6-channel VFlow | 6-channel VFlow | 6-channel VFlow |
|------------------|-----------------|-----------------|-----------------|
| **Total parameters** | 4.00M           | 4.05M           | 4.01M           |
| $q(z|x)$ parameters | 0.83M           | 0.64M           | 0.36M           |
| **bpd**          | 3.14            | 3.13            | 3.12            |

Architecture for $p(x, z)$: direction $(x, z) \rightarrow \epsilon$

| 32 × 32          | $f_{\text{affine}}(3, 32) \times 1$ | $f_{\text{affine}}(3, 32) \times 1$ | $f_{\text{affine}}(3, 32) \times 1$ |
|------------------|--------------------------------------|--------------------------------------|--------------------------------------|
|                   | $f_{\text{checker}}(8, 32, 4) \times 2$ | $f_{\text{checker}}(9, 32, 4) \times 2$ | $f_{\text{checker}}(10, 32, 4) \times 2$ |
|                   | $f_{\text{channel}}(8, 32, 4) \times 2$ | $f_{\text{channel}}(9, 32, 4) \times 2$ | $f_{\text{channel}}(10, 32, 4) \times 2$ |
|                   | SpaceToDepth                        | SpaceToDepth                        | SpaceToDepth                        |
| 16 × 16          | $f_{\text{checker}}(8, 32, 4) \times 2$ | $f_{\text{checker}}(9, 32, 4) \times 2$ | $f_{\text{checker}}(10, 32, 4) \times 2$ |
|                   | $f_{\text{channel}}(8, 32, 4) \times 3$ | $f_{\text{channel}}(9, 32, 4) \times 3$ | $f_{\text{channel}}(10, 32, 4) \times 3$ |

Architecture for $q(z|x)$: direction $\epsilon \rightarrow z$

| 32 × 32          | $g_{\text{checker}}(8, 32, 4) \times 4$ | $g_{\text{checker}}(6, 32, 4) \times 4$ | $g_{\text{checker}}(3, 32, 4) \times 4$ |
|------------------|--------------------------------------|--------------------------------------|--------------------------------------|
|                   | Sigmoid                              | Sigmoid                              | Sigmoid                              |

Architecture for $r(u|x)$: direction $\epsilon \rightarrow u$

| 32 × 32          | $f_{\text{checker}}(2, 32, 4) \times 4$ | $f_{\text{checker}}(2, 32, 4) \times 4$ | $f_{\text{checker}}(2, 32, 4) \times 4$ |
|------------------|--------------------------------------|--------------------------------------|--------------------------------------|
|                   | Sigmoid                              | Sigmoid                              | Sigmoid                              |