**Abstract**

Flow-based generative models have recently become one of the most efficient approaches to model the data generation. Indeed, they are constructed with a sequence of invertible and tractable transformations. Glow [1] first introduced a simple type of generative flow using an invertible $1 \times 1$ convolution. However, the $1 \times 1$ convolution suffers from limited flexibility compared to the standard convolutions. In this paper, we propose a novel invertible $n \times n$ convolution approach that overcomes the limitations of the invertible $1 \times 1$ convolution. In addition, our proposed network is not only tractable and invertible but also uses fewer parameters than standard convolutions. The experiments on CIFAR-10, ImageNet, and Celeb-HQ datasets, have showed that our invertible $n \times n$ convolution helps to improve the performance of generative models significantly.

1 Introduction

Supervised deep learning models have recently achieved numerous breakthrough results in various applications. However, these methods usually require a huge number of annotated data which is highly expensive. In order to tackle the requirement of large annotations, generative models have become a feasible solution. The main objective of the generative models is to learn the hidden dependencies existing in the realistic data so that they can extract meaningful features and variable interactions to synthesize new realistic samples without human supervision or labeling. Generative models can be used in numerous applications such as anomaly detection, image inpainting, data

Figure 1: Reconstruction results using our proposed approach.

1Source code will be publicly available.
generation, super-resolution, etc. However, learning generative models is an extremely challenging process due to high-dimensional data.

There are two types of generative models extensively deployed in recent years, including likelihood-based methods [1–4] and Generative Adversarial Networks (GANs) [5]. Likelihood-based methods have three main categories: Autoregressive models [2], Variational autoencoders (VAEs) [6], and Flow-based models [1, 3, 4]. The flow-based generative model is constructed using a sequence of invertible and tractable transformations, the model explicitly learns the data distribution and therefore the loss function is simply a negative log-likelihood.

Flow-based model was first introduced in [4] and later extended in RealNVP [3]. These methods introduced an affine coupling layer that is invertible and tractable based on Jacobian determinant. As the design of the coupling layers, at each stage, only a subset of data is transformed while the rest is required to be fixed. Therefore, they may be limited at flexibility. To overcome this limitation, coupling layers are alternated with less complex transformations that manipulate on all dimensions of the data. In RealNVP [3], the authors use a fixed channel permutation using fixed checkerboard and channel-wise masks. Kingma et. al. [1] simplifies the architecture by replacing the reverse permutation operation on the channel ordering with invertible \(1 \times 1\) convolutions. However, the \(1 \times 1\) convolutions are not flexible enough in these scenarios. It is extremely hard to compute the inverse form of the standard \(n \times n\) convolutions, and this step usually produces highly computational costs. In this paper, we propose an approach to generalize an invertible \(1 \times 1\) convolution to a more general form of \(n \times n\) convolution. Firstly, we reformulate the standard convolution layer by shifting the inputs instead of the kernels. Then we propose an invertible shift function that is a tractable form of Jacobian determinant. Through the experiments on CIFAR-10 [7], ImageNet [8] and Celeb-HQ [9] datasets, we prove that our proposals are significantly and efficiently in high-dimensional data. Fig. 1 illustrates the advantages of our approach with high-resolution synthesized images.

1.1 Contributions of this Work

This work generalizes the invertible \(1 \times 1\) convolution to an invertible \(n \times n\) convolution by reformulating the convolution layer using our proposed invertible shift function. Our contributions can be summarized as follows:

- Firstly, by analyzing the standard convolution layer, we reformulate its equation into a form such that rather than shifting the kernels during convolution process, shifting the input give equivalent results.
- Secondly, we propose a novel invertible shift function that mathematically helps to reduce the computational cost of the standard convolution while keeping the range of the receptive fields. The determinant of the Jacobian matrix produced by this shift function can be computed efficiently.
- Thirdly, evaluations on several datasets on both objects and faces have showed the generalization of the proposed \(n \times n\) convolution using our proposed novel invertible shift function.

2 Related Work

The generative models can be divided into two groups, i.e. Generative Adversarial Networks and Flow-based Generative Models. In the first group, Generative Adversarial Networks [5] provides an appropriate solution to model the data generation. The discriminative model learns to distinguish the real data from the fake samples produced using a generative model. Two models are trained as they are playing a mini-max game. Meanwhile, in the second group, the Flow-based Generative Models [1, 3, 4] are constructed using a sequence of invertible and tractable transformations. Unlike GAN, the model explicitly learns the data distribution \(p(x)\) and therefore the loss function is efficiently employed with the log-likelihood.

In this section, we discuss several types of flow-based layers that are commonly used in flow-based generative models. An overview of several invertible functions is provided in the Table 1.
Table 1: Comparative invertible functions in several generative normalizing flows. All functions are easy to obtain reverse function and tractability of a Jacobian determinant. The symbols $\odot$, $/$ denote element-wise multiplication and division. $h, w$ denotes height and width of the input/output. $c, i, j$ are the depth channel index and spatial indices, respectively.

| Description          | Function                                           | Reverse Function                                          | Log-determinant       |
|----------------------|----------------------------------------------------|----------------------------------------------------------|-----------------------|
| ActNorm [1]          | $y = x \odot \gamma + \beta$                     | $x = (y - \beta) / \gamma$                              | $\sum \log |\gamma| $ |
| Affine Coupling [3]  | $x = [x_a, x_b]$                                    | $y = [y_a, y_b]$                                          | $\sum \log |s(x_b)| $ |
| $1 \times 1$ conv [1] | $y_{c,i,j} = Wx_{c,i,j}$                           | $x_{c,i,j} = W^{-1}y_{c,i,j}$                            | $h.w. \log |\det W| $ |
| Our Shift Function   | $y_{c,i,j} = \alpha_c x_{c,i,j} + \beta_c$       | $x_{c,i,j} = [y_{c,i,j} - \beta_c] / \alpha_c$          | $h.w. \sum_c \log |\alpha_c| $ |

**Coupling Layers:** NICE [4] and RealNVP [3] presented coupling layers with a normalizing flow by stacking a sequence of invertible bijective transformation functions. The bijective function is designed as an affine coupling layer which is a tractable form of Jacobian determinant. RealNVP can work in a multi-scale architecture to build a more efficient model for large inputs. To further improve the propagation step, the authors applied batch normalization and weight normalization during training.

**Inverse Autoregressive Convolution:** Germain et. al. [10] introduced autoregressive autoencoders by constructing an extension of a non-variational autoencoder that can estimate distributions and is straightforward to compute their Jacobian determinant. Masked autoregressive flow [11] is a type of normalizing flows, where the transformation layer is built as an autoregressive neural network. Inverse autoregressive flow [2] formulates the conditional probability of the target variable as an autoregressive model.

**Invertible $1 \times 1$ Convolution:** Kingma et. al. [1] proposed to simplify the architecture via invertible $1 \times 1$ convolutions. Learning a permutation matrix is a discrete optimization that is not amenable to gradient ascent. However, the permutation operation is simply a special case of a linear transformation with a square matrix. We can pursue this work with convolutional neural networks, as permuting the channels is equivalent to a $1 \times 1$ convolution operation with an equal number of input and output channels. Therefore, the authors replace the fixed permutation with learned $1 \times 1$ convolution operations.

**Activation Normalization:** [1] performs an affine transformation using scale and bias parameters per channel. This layer simply shifts and scales the activations, with data-dependent initialization that normalizes the activations given an initial minibatch of data. This allows scaling down the minibatch size to 1 (for large images) and scaling up the size of the model.

**Invertible $n \times n$ Convolution:** Since the invertible $1 \times 1$ convolution is not flexibility, Hoogeboom et. al. [12] proposed an invertible $n \times n$ convolutions generalized from the $1 \times 1$ convolutions. The authors presented two method to produce the invertible convolutions: (1) Emerging Convolution and (2) Invertible Periodic Convolutions. Emerging Convolution is obtained by chaining specific invertible autoregressive convolutions [2] and speedup this layer through the use of an accelerated parallel inversion module implemented in Cython. Invertible Periodic Convolutions transforms data to the frequency domain via Fourier transform, this alternative convolution has a tractable determinant Jacobian and inverse. However, these invertible $n \times n$ convolutions require more parameters, therefore, these have addition computational cost compared to our proposed method.

3 Background

3.1 Flow-based Generative Model

Let $x$ be a high-dimensional vector with unknown true distribution $x \sim p_X(x)$, $x \in X$, a simple prior probability distribution $p_Z$ on a latent variable $z \in Z$, a bijection $f : X \rightarrow Z$ , the change of variable formula defines a model distribution on $X$ as shown in Eqn. (1).

$$p_X(x) = p_Z(z) \left| \det \left( \frac{\partial f(x)}{\partial x} \right) \right|$$ (1)
Figure 2: Reformulating $n \times n$ convolution. We propose to shift inputs instead of kernels. The proposed invertible $n \times n$ convolution will be simplified as a combination of the invertible shift function $S$ and the invertible $1 \times 1$ convolution.

where $\frac{\partial f(x)}{\partial x}$ is the Jacobian of $f$ at $x$. The log-likelihood objective is then equivalent to minimizing:

$$
\mathcal{L}(\mathcal{X}) = - \mathbb{E}_{x \in \mathcal{X}} \log p_X(x) = - \mathbb{E}_{x \in \mathcal{X}} \left[ \log p_Z(z) + \log \left| \det \left( \frac{\partial f(x)}{\partial x} \right) \right| \right]
$$

(2)

Since the data $x$ is discrete data, we add a random uniform noise $u \in \mathcal{U}(0, a)$, where $a$ is determined by the discretization level of the data, to make $x$ be continuous data. The generative process can be defined as Eqn. (3).

$$
z \sim p_Z(z)$$

$$
x = f^{-1}(z)
$$

(3)

The bijection function $f$ is constructed from a sequence of invertible and tractability of Jacobian determinant transformations: $f = f_1 \circ f_2 \circ ... \circ f_K$ ($K$ is the number of transformations). Such a sequence of invertible transformations is also called a normalizing flow. Here, the Eqn. (2) can be written as in Eqn. (4).

$$
\mathcal{L}(\mathcal{X}) = - \mathbb{E}_{x \in \mathcal{X}} \log p_X(x) = - \mathbb{E}_{x \in \mathcal{X}} \left[ \log p_Z(z) + \sum_{k=1}^{K} \log \left| \det \left( \frac{\partial h_k}{\partial h_{k-1}} \right) \right| \right]
$$

(4)

where $h_k = f_1 \circ f_2 \circ ... \circ f_k(h_0)$ with $h_0 = x$.

3.2 Standard $n \times n$ Convolution

In this section, we revisit the standard $n \times n$ convolution. Let $X$ is an $C \times H \times W$ input, $W$ is a $D \times C \times K$ kernel, the convolution can be expressed as follows:

$$
Y = W \ast X = \left[ W_{:,1} \ W_{:,2} \ ... \ W_{:,K} \right] \ast X = \sum_{k=1}^{K} W_{:,k} \times X^k = \sum_{k=1}^{K} W_{:,k} \times S_k(X)
$$

(5)
where $X_{i:j,k}^k$ is a $C \times H \times W$ matrix that represents a spatially shifted version of input matrix $X$ with shift amount $(i_k, j_k)$. $W_{i:j,k}$ represents the $D \times C$ matrix corresponding to the kernel index $k$, the symbol $\ast$ denotes a convolution operator.

In Eqn. (5), the standard convolution is simply a sum of $1 \times 1$ convolutions on shifted inputs. The function $S_k$ maps the input $X$ to the corresponding shifted input $X_{i:j,k}^k$. The standard convolution uses the common shifted input with integer-valued shift amounts for index $k$. Fig. 2 illustrates our reformulated $n \times n$ convolution, if we can share the shifted inputs regardless of the kernel index, especially, $S_k(X) = S(X)$, the standard convolution will be simplified as the $1 \times 1$ convolution as shown in Eqn. (6). In this paper, we proposed an shift function $S$ which is an invertible and tractable form of the Jacobian determinant.

$$\sum_{k=1}^{K} W_{i:j,k} \times S_k(X) = \sum_{k=1}^{K} W_{i:j,k} \times S(X) = \left( \sum_{k=1}^{K} W_{i:j,k} \right) \times S(X)$$

(6)

4 Invertible $n \times n$ Convolution

In this section, we first introduce our proposed Invertible Shift Function and then present invertible $n \times n$ convolution in details.

4.1 Invertible Shift Function

The shift function $S$ will approximate all shifted input $X_{i:j,k}^k$ ($1 \leq k \leq K$). Here, we propose to design $S$ as a linear transformation per channel, specifically, we have learnable variables $\alpha_c, \beta_c$ ($1 \leq c \leq C$) are scale and translation parameters for each channel, respectively. The shift function $S$ can be formulated as follows:

$$S(X_{c,i,j}) = \alpha_c X_{c,i,j} + \beta_c$$

(7)

where $c, i,j$ are the depth channel index and spatial indices, respectively. The reverse function of $S$ can be easy to obtain:

$$X_{c,i,j} = \frac{S(X_{c,i,j}) - \beta_c}{\alpha_c}$$

(8)

Thank to Eqn. (7), the value of $S(X_{c,i,j})$ only depends on $X_{c,i,j}$, the Jacobian matrix will be in the form of the diagonal matrix as follows:

$$J = \frac{\partial S(X)}{\partial X} = \begin{bmatrix} \frac{\partial S(X_{1,1,1})}{\partial X_{1,1,1}} & \cdots & 0 \\ 0 & \frac{\partial S(X_{1,1,2})}{\partial X_{1,1,2}} & \cdots \\ \vdots & \vdots & \ddots \\ 0 & 0 & \cdots & \frac{\partial S(X_{c,H,W})}{\partial X_{c,H,W}} \end{bmatrix} = \begin{bmatrix} \alpha_1 & 0 & \cdots & 0 \\ 0 & \alpha_1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \alpha_c \end{bmatrix}$$

(9)

Therefore, the determinant of Eqn. (9) is the product of all elements in the diagonal of the matrix $J$ as in Eqn. (10).

$$\det \left( \frac{\partial S(X)}{\partial X} \right) = \prod_{c=1}^{C} \alpha_c^{H \times W}$$

$$\log \left| \det \left( \frac{\partial S(X)}{\partial X} \right) \right| = H \times W \times \sum_{c=1}^{C} \log |\alpha_c|$$

(10)

4.2 Invertible $n \times n$ Convolution

Kingma (1) proposed invertible $1 \times 1$ convolution is the smart way to learn the permutation matrix instead of the fixed permutation (4, 5). However, the $1 \times 1$ suffers from limited flexibility compared to the standard convolution. In particular, the receptive fields of $1 \times 1$ convolution is limited. When the network going deeper, the receptive fields of $1 \times 1$ convolutions are still small areas; these, therefore,
cannot generalize and model large objects of high-dimensional data. However, the $1 \times 1$ convolution has own advantages compared to the standard convolution. First, the $1 \times 1$ convolution allows the network to compress the data of the input volume to be smaller. Second, $1 \times 1$ suffers less over-fitting due to small kernel sizes. Therefore, in our proposal, we still take advantages of the $1 \times 1$ convolution. Specifically, we adopt the successfully invertible $1 \times 1$ convolution of Glow [1] in our design.

In the previous subsection, we proved that the shift function $S$ is invertible and tractability of Jacobian determinant. In Subsection 3.2, we indicated that if we can share shifted inputs regardless of the kernel index via the shift function $S$, we can simplify the standard $n \times n$ convolution to the composition of $S$ and $1 \times 1$ convolution. Therefore, the invertible $n \times n$ convolution will be equivalent to the combination of the invertible shift function $S$ and the invertible $1 \times 1$ convolution. Specifically, the input will be firstly forwarded to the shift function $S$ and then convoluted with the $1 \times 1$ filter.

Fig 3(a) illustrates our one step of flow. We adopt the common design of a flow step [1, 12] in our design. Our proposal can be easily to integrate to the multi-scale architecture designed by Dinh et. al. [3] (Fig 3(b)). By our proposal, we can generalize the invertible $1 \times 1$ convolution to the invertible $n \times n$ convolution through the shift function $S$. It can help to encourage the filters can learn the more efficient data representation and embed more useful latent features than the invertible $1 \times 1$ convolution used in Glow [1]. Besides, we use fewer parameters and have less inference time compared to the standard $n \times n$ convolutions.

5 Experiments

In this section, we present our experimental results on CIFAR-10, ImageNet and Celeb-HQ datasets. Firstly, in Subsection 5.1, we compare log-likelihood against the previous flow-based models, i.e. RealNVP [3], Glow [1], Emerging Convolution [12]. Finally, in Subsection 5.2, we show our qualitative results trained on the Celeb-HQ dataset.

5.1 Quantitative Experiments

We evaluate our invertible $n \times n$ convolution on CIFAR-10 (Fig. 4(a)), ImageNet (Fig. 4(b)) with $32 \times 32$ and $64 \times 64$ image sizes. We use bits per dimension as the criteria to evaluate models. We compare our method against RealNVP [3], Glow [1], and Emerging Convolution [12]. We adopt the network structures of Glow and replace all invertible $1 \times 1$ convolutions of Glow by our invertible $n \times n$ convolutions. For the data preprocessing, we follow the same process as in RealNVP [3].

The shift function $S$ will be not inverse if the $\alpha_c = 0 (\exists c \in [1...C])$. Hence, in the training process, we will first initialize $\alpha_c = 1$ and $\beta_c = 0 (1 \leq c \leq C)$. During the learning processing, we keep $\alpha_c (1 \leq c \leq C)$ be different 0 to guarantee that the shift function $S$ is inverse and tractability of
Jacobian determinant. Training models on high-dimensional data require large memory. To be able to train with large batch size, we simultaneously and distributively train the models on four GPUs via Horovod and TensorFlow frameworks.

**Hyperparameters:** In the CIFAR experiment, the depth of flow $K$ and the number of levels $L$ are set to 32 and 3, respectively. Meanwhile, the depth of flow in ImageNet experiments is set to 48, the numbers of levels of ImageNet $32 \times 32$ and ImageNet $64 \times 64$ experiments are set to 3 and 4, respectively. We use Adam optimizer [13] to optimize the networks where batch size and learning rate are set to 64 (per GPU) and 0.001, respectively. We choose Normal Distribution as the prior distribution $p_Z(z) \sim \mathcal{N}(z; 0, I)$ in all experiments.

Table 2 shows our experimental results. As the results, our proposal helps to improve the generative models on ImageNet $32 \times 32$ and ImageNet $64 \times 64$ datasets that are more challenging than CIFAR-10. Our proposed invertible $n \times n$ convolution provides a better generative capability than the stand-alone invertible $1 \times 1$ convolution. Since Emerging Convolution uses invertible auto-regressive convolution, our proposal is, therefore, less complicated and fast inference than Emerging Convolution. We take the advantages the invertible $1 \times 1$ convolution in our design, thus, we are also able to learn the permutation matrix via $1 \times 1$ convolution instead of the fixed permutation in RealNVP.

Table 2: Comparative results (bits per dimension) of proposed invertible $n \times n$ convolution compared to RealNVP, Glow, and Emerging Convolution

| Models          | CIFAR-10 | ImageNet $32 \times 32$ | ImageNet $64 \times 64$ |
|-----------------|----------|-------------------------|-------------------------|
| RealNVP         | 3.49     | 4.28                    | 3.98                    |
| Glow            | 3.35     | 4.09                    | 3.81                    |
| Emerging Conv   | **3.34** | 4.09                    | 3.81                    |
| **Ours**        | 3.50     | **3.96**                | **3.74**                |

5.2 Qualitative Experiments

CelebA-HQ dataset [9] has been selected to train the model using the architectures defined in the previous section with a higher resolution ($256 \times 256$ image sizes). The depth of flow $K$ and the number of levels $L$ are set to 32 and 6, respectively. Since high-dimensional data requires large memory, we reduce the batch size to 1 (per GPU) and train on eight GPUs. Fig. 4(c) shows the examples of Celeb-HQ datasets. We train our model on 5-bit images in order to improve visual quality with a slight trade-off of color fidelity. As the synthetic images are shown in Fig. 5, our model can generalize realistic images in high dimensional data.

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https://github.com/horovod/horovod
https://tensorflow.org
6 Conclusion

This paper has presented a novel invertible $n \times n$ convolution approach. By reformulating the convolution layer, we propose to use the shift function to shift inputs instead of kernels. We prove that our shift function is invertible and tractable in terms of calculating the Jacobian determinant. The method leverages the shift function and the invertible $1 \times 1$ convolution to generalize to the invertible $n \times n$ convolution. Through experiments, our proposal has been achieved the state-of-the-art results in quantitative measurement and able to generate realistic images with high-resolution.

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