

# Deep Generative Models

## Lecture 8: Normalizing Flows

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Aditya Grover

UCLA

# Recap of normalizing flow models

So far

- Transform simple to complex distributions via sequence of invertible transformations
- Directed latent variable models with marginal likelihood given by the change of variables formula
- Triangular Jacobian permits efficient evaluation of log-likelihoods

Plan for today

- Invertible transformations with diagonal Jacobians (NICE, Real-NVP)
- Autoregressive Models as Normalizing Flow Models
- Case Study: Probability density distillation for efficient learning and inference in Parallel Wavenet

## Designing invertible transformations

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- NICE or Nonlinear Independent Components Estimation (Dinh et al., 2014) composes two kinds of invertible transformations: additive coupling layers and rescaling layers
- Real-NVP (Dinh et al., 2017)
- Inverse Autoregressive Flow (Kingma et al., 2016)
- Masked Autoregressive Flow (Papamakarios et al., 2017)
- I-resnet (Behrmann et al, 2018)
- Glow (Kingma et al, 2018)
- MintNet (Song et al., 2019)
- And many more

## NICE - Additive coupling layers

Partition the variables  $\mathbf{z}$  into two disjoint subsets, say  $\mathbf{z}_{1:d}$  and  $\mathbf{z}_{d+1:n}$  for any  $1 \leq d < n$

- Forward mapping  $\mathbf{z} \mapsto \mathbf{x}$ :
  - $\mathbf{x}_{1:d} = \mathbf{z}_{1:d}$  (identity transformation)
  - $\mathbf{x}_{d+1:n} = \mathbf{z}_{d+1:n} + m_\theta(\mathbf{z}_{1:d})$  ( $m_\theta(\cdot)$  is a neural network with parameters  $\theta$ ,  $d$  input units, and  $n - d$  output units)
- Inverse mapping  $\mathbf{x} \mapsto \mathbf{z}$ :
  - $\mathbf{z}_{1:d} = \mathbf{x}_{1:d}$  (identity transformation)
  - $\mathbf{z}_{d+1:n} = \mathbf{x}_{d+1:n} - m_\theta(\mathbf{x}_{1:d})$
- Jacobian of forward mapping:

$$J = \frac{\partial \mathbf{x}}{\partial \mathbf{z}} = \begin{pmatrix} I_d & 0 \\ \frac{\partial \mathbf{x}_{d+1:n}}{\partial \mathbf{z}_{1:d}} & I_{n-d} \end{pmatrix}$$

$$\det(J) = 1$$

## NICE - Rescaling layers

- Additive coupling layers are composed together (with arbitrary partitions of variables in each layer)
- Final layer of NICE applies a rescaling transformation
- Forward mapping  $\mathbf{z} \mapsto \mathbf{x}$ :

$$x_i = s_i z_i$$

where  $s_i > 0$  is the scaling factor for the  $i$ -th dimension.

- Inverse mapping  $\mathbf{x} \mapsto \mathbf{z}$ :

$$z_i = \frac{x_i}{s_i}$$

- Jacobian of forward mapping:

$$J = \text{diag}(\mathbf{s})$$

$$\det(J) = \prod_{i=1}^n s_i$$

# Samples generated via NICE

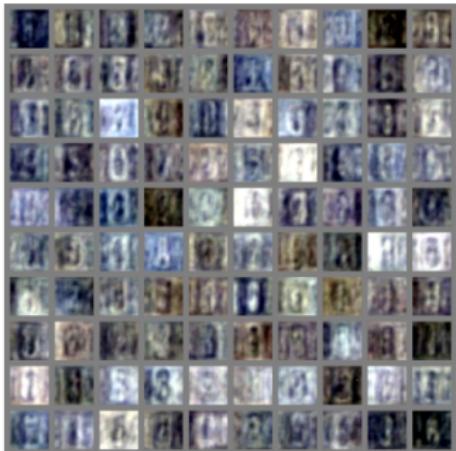


(a) Model trained on MNIST



(b) Model trained on TFD

## Samples generated via NICE



(c) Model trained on SVHN



(d) Model trained on CIFAR-10

# Real-NVP: Non-volume preserving extension of NICE

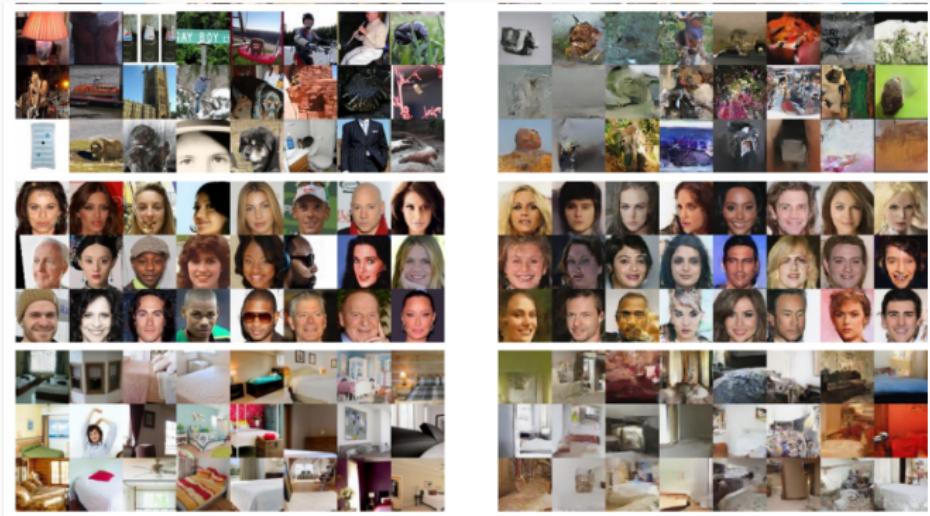
- Forward mapping  $\mathbf{z} \mapsto \mathbf{x}$ :
  - $\mathbf{x}_{1:d} = \mathbf{z}_{1:d}$  (identity transformation)
  - $\mathbf{x}_{d+1:n} = \mathbf{z}_{d+1:n} \odot \exp(\alpha_\theta(\mathbf{z}_{1:d})) + \mu_\theta(\mathbf{z}_{1:d})$
  - $\mu_\theta(\cdot)$  and  $\alpha_\theta(\cdot)$  are neural networks with parameters  $\theta$ ,  $d$  input units, and  $n - d$  output units [ $\odot$  denotes elementwise product]
- Inverse mapping  $\mathbf{x} \mapsto \mathbf{z}$ :
  - $\mathbf{z}_{1:d} = \mathbf{x}_{1:d}$  (identity transformation)
  - $\mathbf{z}_{d+1:n} = (\mathbf{x}_{d+1:n} - \mu_\theta(\mathbf{x}_{1:d})) \odot (\exp(-\alpha_\theta(\mathbf{x}_{1:d})))$
- Jacobian of forward mapping:

$$J = \frac{\partial \mathbf{x}}{\partial \mathbf{z}} = \begin{pmatrix} I_d & 0 \\ \frac{\partial \mathbf{x}_{d+1:n}}{\partial \mathbf{z}_{1:d}} & \text{diag}(\exp(\alpha_\theta(\mathbf{z}_{1:d}))) \end{pmatrix}$$

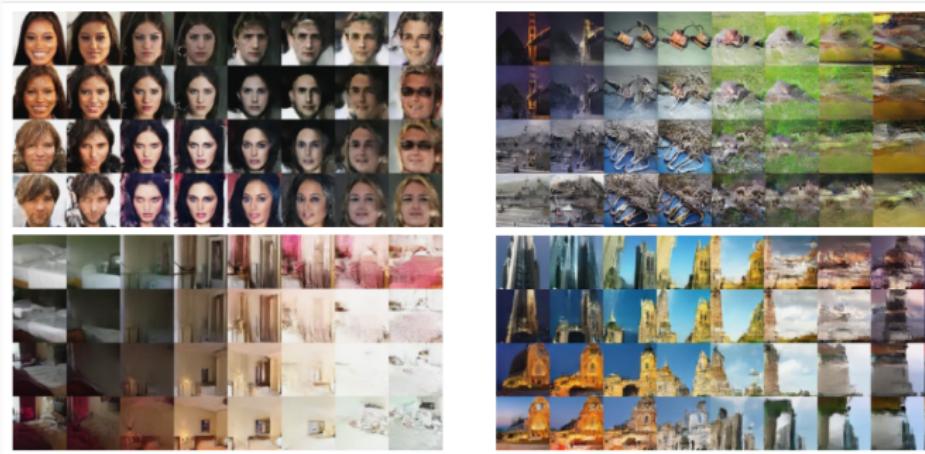
$$\det(J) = \prod_{i=d+1}^n \exp(\alpha_\theta(\mathbf{z}_{1:d})_i) = \exp \left( \sum_{i=d+1}^n \alpha_\theta(\mathbf{z}_{1:d})_i \right)$$

- **Non-volume preserving transformation** in general since determinant can be less than or greater than 1

# Samples generated via Real-NVP



# Latent space interpolations via Real-NVP



Using with four validation examples  $\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \mathbf{z}^{(3)}, \mathbf{z}^{(4)}$ , define interpolated  $\mathbf{z}$  as:

$$\mathbf{z} = \cos\phi(\mathbf{z}^{(1)}\cos\phi' + \mathbf{z}^{(2)}\sin\phi') + \sin\phi(\mathbf{z}^{(3)}\cos\phi' + \mathbf{z}^{(4)}\sin\phi')$$

with manifold parameterized by  $\phi$  and  $\phi'$ .

## Continuous Autoregressive models as flow models

- Consider a Gaussian autoregressive model:

$$p(\mathbf{x}) = \prod_{i=1}^n p(x_i | \mathbf{x}_{<i})$$

such that

$$p(x_i | \mathbf{x}_{<i}) = \mathcal{N}(\mu_i(x_1, \dots, x_{i-1}), \exp(\alpha_i(x_1, \dots, x_{i-1}))^2).$$

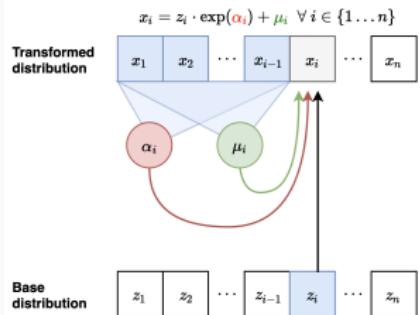
Here,  $\mu_i(\cdot)$  and  $\alpha_i(\cdot)$  are neural networks for  $i > 1$  and constants for  $i = 1$ .

- Sampler for this model:

- Sample  $z_i \sim \mathcal{N}(0, 1)$  for  $i = 1, \dots, n$
- Let  $x_1 = \exp(\alpha_1)z_1 + \mu_1$ . Compute  $\mu_2(x_1), \alpha_2(x_1)$
- Let  $x_2 = \exp(\alpha_2)z_2 + \mu_2$ . Compute  $\mu_3(x_1, x_2), \alpha_3(x_1, x_2)$
- Let  $x_3 = \exp(\alpha_3)z_3 + \mu_3$ . ...

- Flow interpretation:** transforms samples from the standard Gaussian  $(z_1, z_2, \dots, z_n)$  to those generated from the model  $(x_1, x_2, \dots, x_n)$  via invertible transformations (parameterized by  $\mu_i(\cdot), \alpha_i(\cdot)$ )

# Masked Autoregressive Flow (MAF)

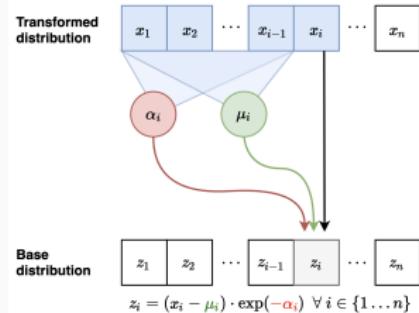


- Forward mapping from  $\mathbf{z} \mapsto \mathbf{x}$ :
  - Let  $x_1 = \exp(\alpha_1)z_1 + \mu_1$ . Compute  $\mu_2(x_1), \alpha_2(x_1)$
  - Let  $x_2 = \exp(\alpha_2)z_2 + \mu_2$ . Compute  $\mu_3(x_1, x_2), \alpha_3(x_1, x_2)$
- Sampling is sequential and slow (like autoregressive):  $O(n)$  time

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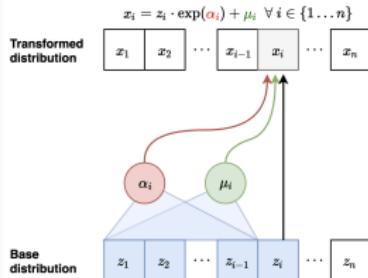
Figure adapted from Eric Jang's blog

# Masked Autoregressive Flow (MAF)



- Inverse mapping from  $\mathbf{x} \mapsto \mathbf{z}$ :
  - Compute **all**  $\mu_i, \alpha_i$  (can be done in parallel using e.g., MADE)
  - Let  $z_1 = (x_1 - \mu_1) / \exp(\alpha_1)$  (scale and shift)
  - Let  $z_2 = (x_2 - \mu_2) / \exp(\alpha_2)$
  - Let  $z_3 = (x_3 - \mu_3) / \exp(\alpha_3)$  ...
- Jacobian is lower diagonal, hence efficient determinant computation
- Likelihood evaluation is easy and parallelizable (like MADE)
- Layers with different variable orderings can be stacked

# Inverse Autoregressive Flow (IAF)



- Forward mapping from  $\mathbf{z} \mapsto \mathbf{x}$  (parallel):
  - Sample  $z_i \sim \mathcal{N}(0, 1)$  for  $i = 1, \dots, n$
  - Compute all  $\mu_i, \alpha_i$  (can be done in parallel)
  - Let  $x_1 = \exp(\alpha_1)z_1 + \mu_1$
  - Let  $x_2 = \exp(\alpha_2)z_2 + \mu_2 \dots$
- Inverse mapping from  $\mathbf{x} \mapsto \mathbf{z}$  (sequential):
  - Let  $z_1 = (x_1 - \mu_1) / \exp(\alpha_1)$ . Compute  $\mu_2(z_1), \alpha_2(z_1)$
  - Let  $z_2 = (x_2 - \mu_2) / \exp(\alpha_2)$ . Compute  $\mu_3(z_1, z_2), \alpha_3(z_1, z_2)$
- Fast to sample from, slow to evaluate model likelihoods (train)
- Note: Fast to evaluate likelihoods of a generated point (cache  $z_1, z_2, \dots, z_n$ )

# IAF is inverse of MAF

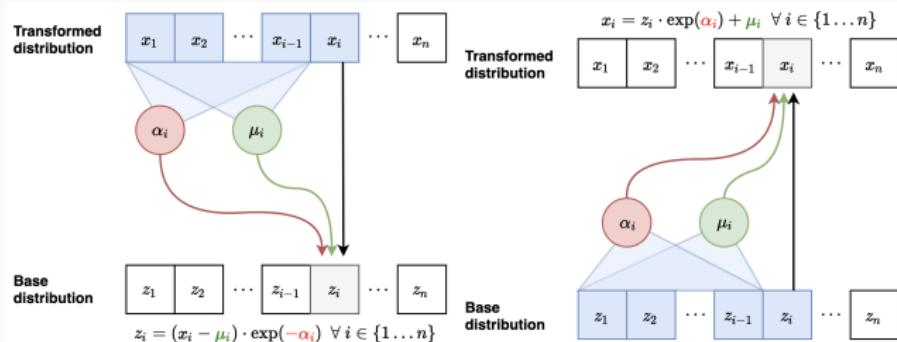


Figure 1: Inverse pass of MAF (left) vs. Forward pass of IAF (right)

- Interchanging  $z$  and  $x$  in the inverse transformation of MAF gives the forward transformation of IAF
- Similarly, forward transformation of MAF is inverse transformation of IAF

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Figure adapted from Eric Jang's blog

# IAF vs. MAF

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- Computational tradeoffs
  - MAF: Fast likelihood evaluation, slow sampling
  - IAF: Fast sampling, slow likelihood evaluation
- MAF more suited for training based on MLE, density estimation
- IAF more suited for real-time generation
- Can we get the best of both worlds?

- Two part training with a teacher and student model
- Teacher is parameterized by MAF. Teacher can be efficiently trained via MLE
- Once teacher is trained, initialize a student model parameterized by IAF. Student model cannot efficiently evaluate density for external datapoints but allows for efficient sampling
- **Key observation:** IAF can also efficiently evaluate densities of its own generations (via caching the noise variates  $z_1, z_2, \dots, z_n$ )

- **Probability density distillation:** Student distribution is trained to minimize the KL divergence between student ( $s$ ) and teacher ( $t$ )

$$D_{\text{KL}}(s, t) = E_{\mathbf{x} \sim s}[\log s(\mathbf{x}) - \log t(\mathbf{x})]$$

- Evaluating and optimizing Monte Carlo estimates of this objective requires:
  - Samples  $\mathbf{x}$  from student model (IAF)
  - Density of  $\mathbf{x}$  assigned by student model
  - Density of  $\mathbf{x}$  assigned by teacher model (MAF)
- All operations above can be implemented efficiently

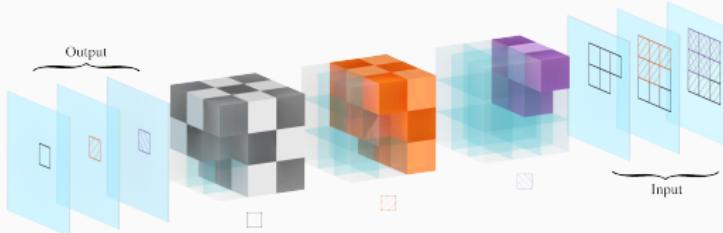
# Parallel Wavenet: Overall algorithm

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- Training
  - Step 1: Train teacher model (MAF) via MLE
  - Step 2: Train student model (IAF) to minimize KL divergence with teacher
- Test-time: Use student model for testing
- Improves sampling efficiency over original Wavenet (vanilla autoregressive model) by 1000x!

- MintNet: Building invertible neural networks with masked convolutions.
- A regular convolutional neural network is powerful, but it is not invertible and its Jacobian determinant is expensive.
- We can instead use masked convolutions like in autoregressive models to enforce ordering (like PixelCNN)
- Because of the ordering, the Jacobian matrix is triangular and the determinant is efficient to compute.
- If all the diagonal elements of the Jacobian matrix are (strictly) positive, the transformation is invertible.

- Illustration of a masked convolution with 3 filters and kernel size  $3 \times 3$ .



- Solid checkerboard cubes inside each filter represent unmasked weights, while the transparent blue blocks represent the weights that have been masked out.
- The receptive field of each filter on the input feature maps is indicated by regions shaded with the pattern (the colored square) below the corresponding filter.

# MintNet (Song et al., 2019)

- Uncurated samples on MNIST, CIFAR-10, and ImageNet 3232 datasets

6 4 2 7 0 6 1 6  
1 3 2 3 1 7 1 6  
8 1 7 6 2 0 1 9  
4 9 6 7 8 4 1 0  
7 7 9 0 4 1 1 2  
0 6 2 9 3 3 9 9  
5 9 5 0 0 8 4 5  
1 2 2 6 1 2 7 7

(a) MNIST



(b) CIFAR-10



(c) ImageNet-32×32

# Summary of Normalizing Flow Models

- Transform simple distributions into more complex distributions via change of variables
- Jacobian of transformations should have tractable determinant for efficient learning and density estimation
- Computational tradeoffs in evaluating forward and inverse transformations