Invertible Normalizing Flows

ECE57000: Artificial Intelligence

David I. Inouye

GAN Limitation: Cannot compute density values

- Evaluation of GANs is challenging
  - Explicit density models could use test log likelihood
  - "I think this looks better than that"
  - Inception-based scores

- Cannot use for classification or outlier detection

GAN Limitation: Challenging to train because of careful balance between discriminator and generator

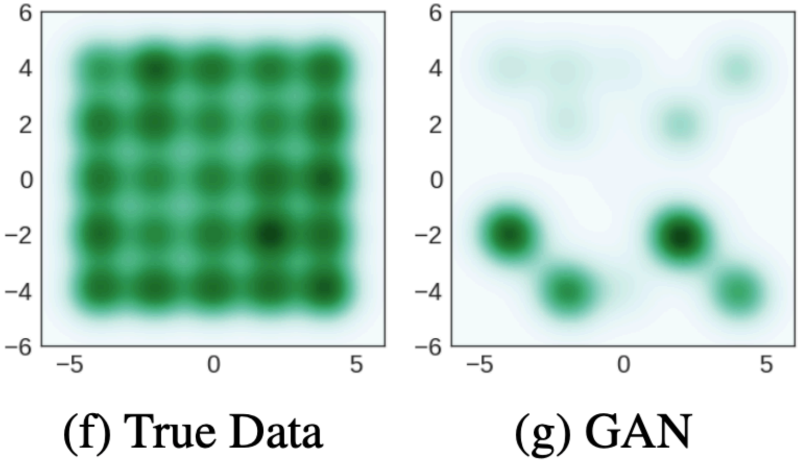
1. Assumptions on possible D and G
   1. Theory – All possible D and G
   2. Reality – Only functions defined by a neural network
2. Assumptions on optimality
   1. Theory – Both optimizations are solved perfectly
   2. Reality – The inner maximization is only solved approximately, and this interacts with outer minimization
3. Assumption on expectations
   1. Theory – Expectations over true distribution
   2. Reality – Empirical expectations over finite sample; for images, much of the high-dimensional space does not have samples

- **GANs can be very difficult/finicky to train**

Common problem with GANs: <u>Mode collapse</u> hinders diversity of samples

From: https://developers.google.com/machine-learning/gan/problems

- Wasserstein GANs
- Unrolled GANs
  - Trained on multiple discriminators simultaneously



Metz, L., Poole, B., Pfau, D., & Sohl-Dickstein, J. (2016). Unrolled generative adversarial networks. *arXiv preprint arXiv:1611.02163*.

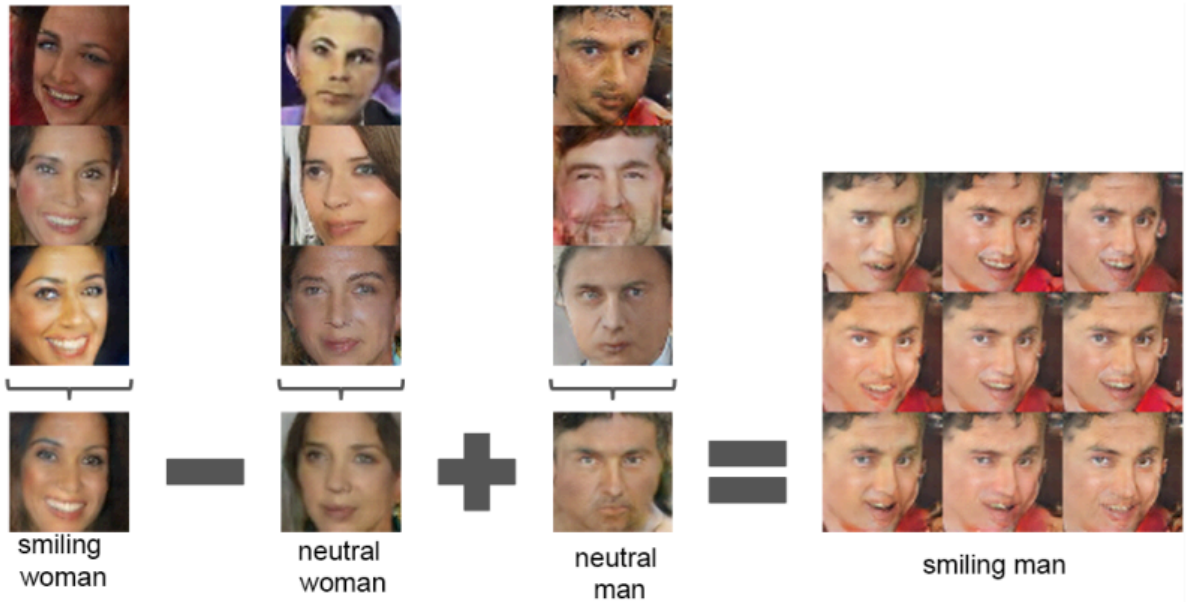
http://papers.nips.cc/paper/6923-veegan-reducing-mode-collapse-in-gans-using-implicit-variational-learning.pdf

https://software.intel.com/en-us/blogs/2017/08/21/mode-collapse-in-gans

GAN Limitation: Cannot go from observed to latent space, i.e. $x \to z$ not possible/easy

- Cannot manipulate an observed image in latent space
  - Cannot do the following, $x \to z,\ z' = z + 3,\ z' \to x'$
  - Rather, must start from fake image based on random z

All fake images->



Highly realistic random samples from powerful flow model (GLOW)

Figure 1: Synthetic celebrities sampled from our model; see Section 3 for architecture and method, and Section 5 for more results.

https://papers.nips.cc/paper/8224-glow-generative-flow-with-invertible-1x1-convolutions.pdf

Interpolation between **real images** using GLOW

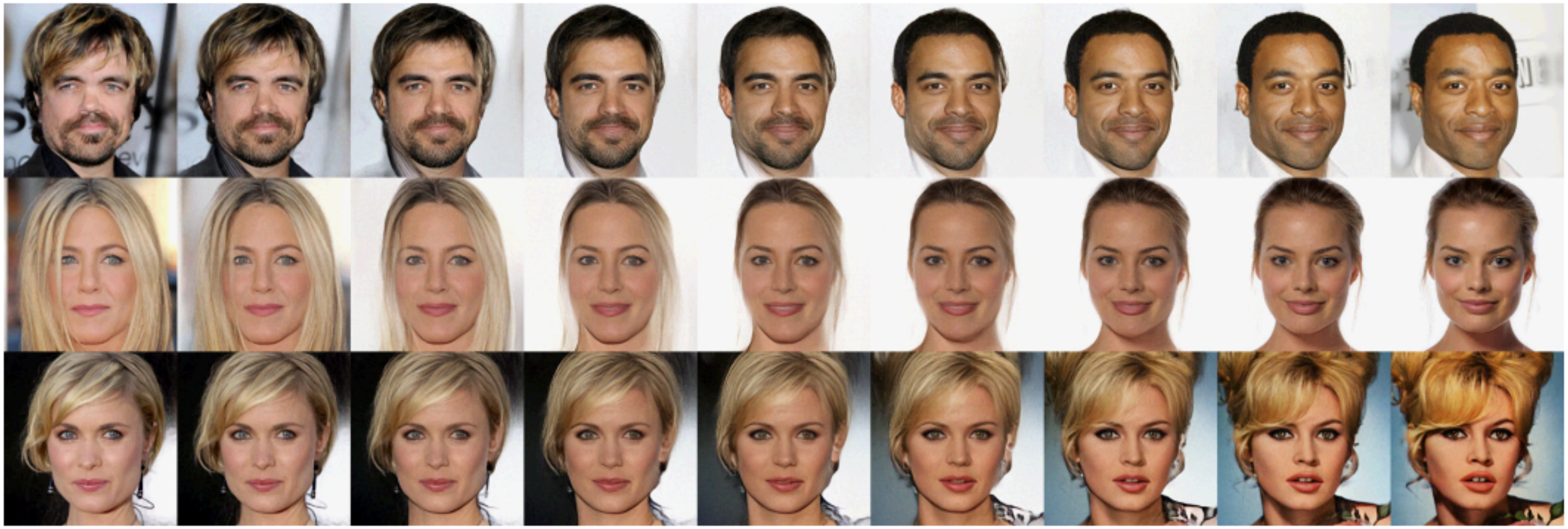
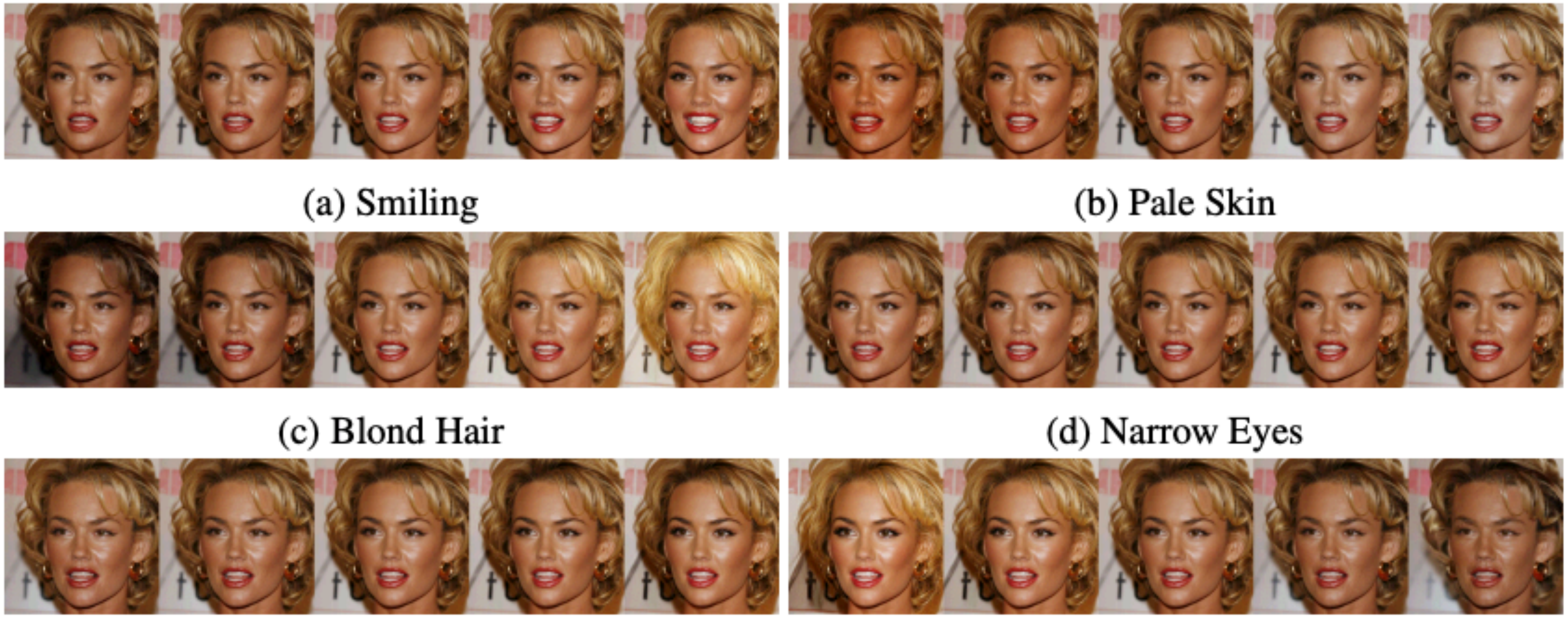


Figure 5: Linear interpolation in latent space between real images.

https://papers.nips.cc/paper/8224-glow-generative-flow-with-invertible-1x1-convolutions.pdf

Transformations of real image along various features



(a) Smiling (b) Pale Skin

(c) Blond Hair (d) Narrow Eyes

(e) Young (f) Male

Figure 6: Manipulation of attributes of a face. Each row is made by interpolating the latent code of an image along a vector corresponding to the attribute, with the middle image being the original image

https://papers.nips.cc/paper/8224-glow-generative-flow-with-invertible-1x1-convolutions.pdf

Normalizing flows use **invertible** deep models for the generator which allow more capabilities

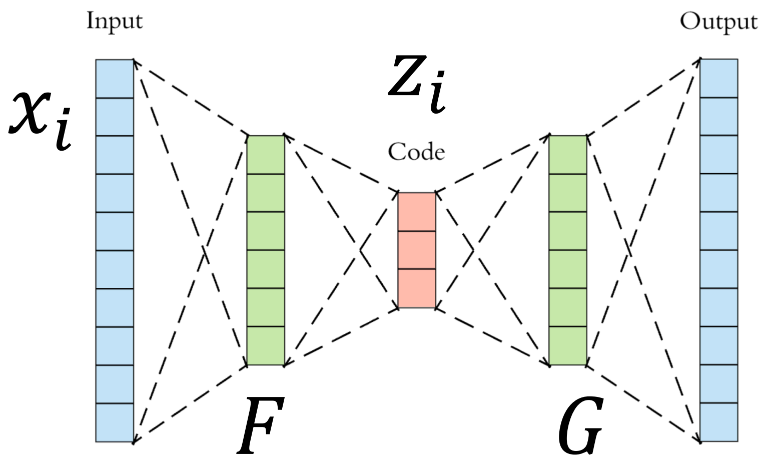
- Transforming between observed/input and latent space is easy
  - $x = G\,(z)$
  - $z = G^{-1}(x)$

- Simple sampling like GANs
  - $z \sim \text{SimpleDistribution}$
  - $x = G(z) \sim \hat{p}_g(x)$, which is estimated distribution

- **Exact density** is computable via change of variables
  - Standard maximum likelihood estimation can be used for training

Comparing VAEs and normalizing flows

VAE

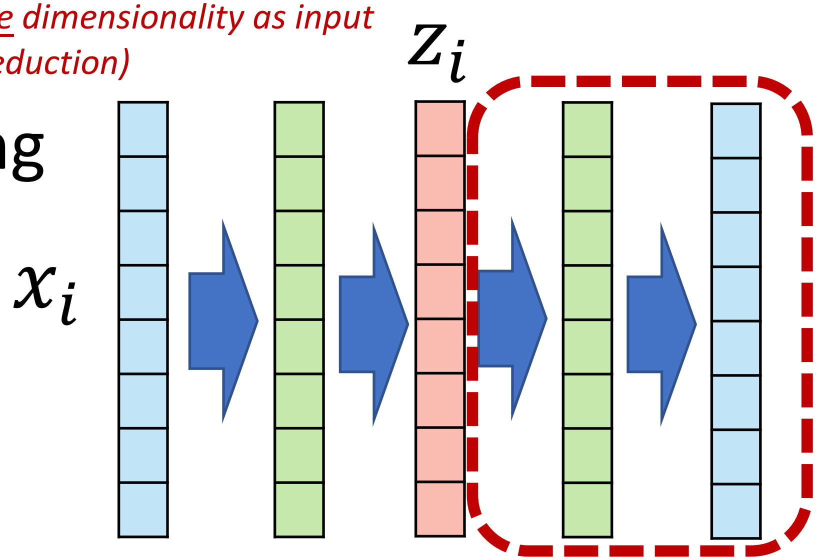


$$\tilde{x}_i \sim p(x_i|G(z_i))$$

$$L(x_i, \tilde{x}_i)$$

Latent code has <u>same</u> dimensionality as input (no dimensionality reduction)

Normalizing Flow



$F = G^{-1}$ $G = F^{-1}$

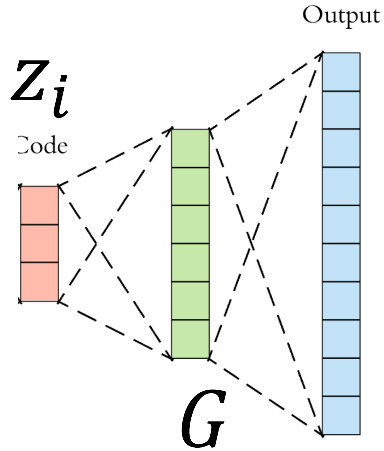
<u>*Implicit*</u> generator via $G = F^{-1}$
(only need to train encoder F)

$$\tilde{x}_i = G(F(x_i)) = G(G^{-1}(x_i)) = x_i$$

$$\Rightarrow L(x_i, \tilde{x}_i) = L(x_i, x_i) = 0$$

Comparing GANs and normalizing flows: Normalizing flows can use MLE training

GAN

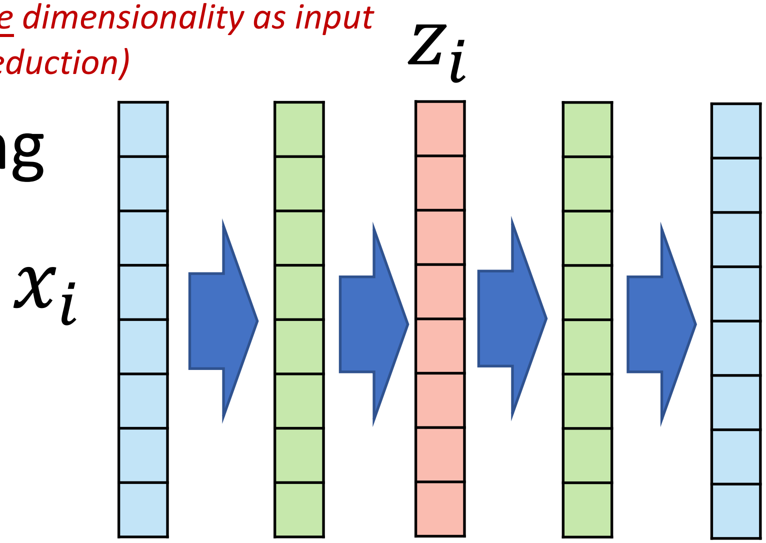


$$\tilde{x}_i = G(z_i)$$

Adversarial training to compare two sets of samples

Latent code has <u>same</u> dimensionality as input (no dimensionality reduction)

Normalizing Flow



$$F = G^{-1} \quad G = F^{-1}$$

$$\tilde{x}_i = G(z_i) = G\left(G^{-1}(x_i)\right) = x_i$$

MLE training since density function known

Back to maximum likelihood estimation (MLE): How can we compute the likelihood for normalizing flows?

- Suppose
  - $z \sim \text{Uniform}([0,1]), \text{i.e.}, p_z(z) = 1$ (latent space is uniform)
  - $G(\text{z}) = 2\text{z}$
  - Thus, $x = G(z) = 2z$.

- What is the density function of x, what is $p_x(x)$?

Change of variables formula gives p_x in terms of the p_z and the derivative of G^{-1}

- Key idea: Must conserve density **volume** (so that distribution sums to 1).
- $p_x(x)|dx| = p_z(z)|dz|$, this is like the preservation of volume/area/mass.
  - Intuition: We only have 1 unit of "dirt" to move around.
- Rearrange above equation to get formula

$$p_x(x) = \left|\frac{dz}{dx}\right| p_z(z) = \left|\frac{dG^{-1}(x)}{dx}\right| p_z\left(G^{-1}(x)\right)$$

Demo of change of variables

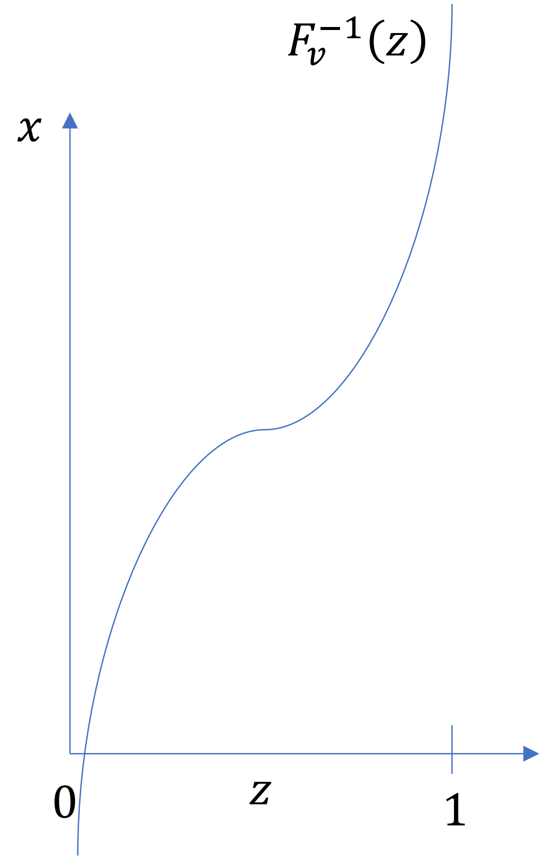
Derivation of change of variables using CDF function (Increasing)

- Assume $x = G(z)$, where $G(z)$ is an increasing function
- $F_x(a) = \Pr(x \le a) = \int_{-\infty}^{a} p_x(t)dt$
- $F_x(a) = \Pr(x \le a)$
- $= \Pr(G(z) \le a)$
- $= \Pr\left(z \le G^{-1}(a)\right) = F_z\left(G^{-1}(a)\right)$
- Now take the derivative of both sides with respect to a

- Left hand side: $\frac{dF_x(a)}{da} = p_x(a)$
- Right hand side: $\frac{dF_z\left(G^{-1}(a)\right)}{da} = \frac{dF_z\left(G^{-1}(a)\right)}{d\left(G^{-1}(a)\right)}\left(\frac{dG^{-1}(a)}{da}\right)$
- $= p_z\left(G^{-1}(a)\right)\left(\frac{dG^{-1}(a)}{da}\right)$
- $\Rightarrow p_x(a) = p_z\left(G^{-1}(a)\right)\left(\frac{dG^{-1}(a)}{da}\right)$
- You can do similarly for decreasing functions to get: $p_x(a) = p_z\left(G^{-1}(a)\right)\left|\frac{dG^{-1}(a)}{da}\right|$

Inverse transform sampling is based on change of variables

- $z \sim \text{Uniform}([0,1])$
- $v \sim \text{AnotherDistribution}$
- $x = F_v^{-1}(z)$, where F_v^{-1} is the inverse CDF for v
- What is the distribution of x?
- $p_x(x) = p_z\big(F_v(x)\big)\left|\frac{dF_v(x)}{dx}\right|$
- $p_x(x) = (1)|p_v(x)| = p_v(x)$



What about change of variables in higher dimensions?

- Let's again build a little intuition (see demo)
- Again, conservation of volume: Consider infinitesimal expansion or shrinkage of volume

$$\mathrm{p}(x_1, x_2)|dx_1 dx_2| = p(z_1, z_2)|dz_1 dz_2|$$

- Given that Jacobian is all mixed derivatives we get generalization for vector to vector invertible functions:

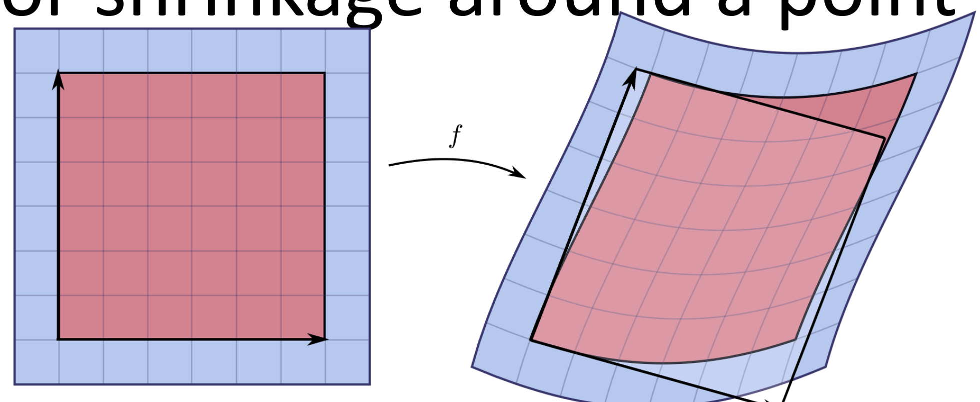
$$p_x(x) = |\det J_{G^{-1}}(x)|\, p_z\left(G^{-1}(x)\right)$$

What is the Jacobian again?
The best linear approximation at a point

- The Jacobian definition:

$$\frac{dz}{dx} = J_z(x) = \begin{bmatrix} \frac{\partial z_1}{\partial x_1} & \cdots & \frac{\partial z_1}{\partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial z_d}{\partial x_1} & \cdots & \frac{\partial z_d}{\partial x_d} \end{bmatrix} = \begin{bmatrix} \frac{\partial G^{-1}(x)_1}{\partial x_1} & \cdots & \frac{\partial G^{-1}(x)_1}{\partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial G^{-1}(x)_d}{\partial x_1} & \cdots & \frac{\partial G^{-1}(x)_d}{\partial x_d} \end{bmatrix}$$

- The determinant measures the local *linear* expansion or shrinkage around a point



The determinant Jacobian of compositions of functions is the product of determinant Jacobians

- Suppose $F(x) = F_2\big(F_1(x)\big)$
- The Jacobian expands like the chain rule

$$J_F(x) = J_{F_2}\big(F_1(x)\big)J_{F_1}(x) = J_{F_2}J_{F_1}$$

- If we take the determinant of the Jacobian, then it becomes a product of determinants

$$\det J_F = \det J_{F_2}J_{F_1} = \left(\det J_{F_2}\right)\left(\det J_{F_1}\right)$$

- This will be useful since each layer of our flows will be invertible

Okay, now back to learning flows: The log likelihood is the sum of determinant terms for each layer

- Simply optimize the minimize negative log likelihood where $F_\theta = G^{-1}$

$$\arg\min_{F_\theta} -\frac{1}{n}\sum_i \log p_x(x_i;\theta)$$

- $-\frac{1}{n}\sum_i \log p_z\big(F_\theta(x_i)\big)\big|\det J_{F_\theta}(x_i)\big|$
- $-\frac{1}{n}\sum_i\big[\log p_z\big(F_\theta(x_i)\big) + \log\big|\det J_{F_\theta}(x_i)\big|\big]$
- $-\frac{1}{n}\sum_i\left[\log p_z\big(F_\theta(x_i)\big) + \sum_\ell \log\left|\det J_{F_\theta^{(\ell)}}\left(z_i^{(\ell-1)}\right)\right|\right]$

$$\text{where } z_i^0 = x_i, \qquad \text{and} \quad z_i^\ell = F_\theta^{(\ell)}\big(z_i^{\ell-1}\big)$$

How do we create these invertible layers?

- Consider arbitrary invertible transformation F_θ
  - How often would $\left|\det J_{F_\theta}\right|$ need to be computed?

- High computation costs
  - Determinant costs roughly $O(d^3)$ even if Jacobian is already computed!
  - Would need to be computed every stochastic gradient iteration

How do we create these invertible layers? Independent transformation on each dimension

- $z_1 = F_1(x_1)$
- $z_2 = F_2(x_2)$
- $z_3 = F_3(x_3)$
- What is the Jacobian?

$$J_F = \begin{bmatrix} \frac{dF_1(x_1)}{dx_1} & 0 & 0 \\ 0 & \frac{dF_2(x_2)}{dx_2} & 0 \\ 0 & 0 & \frac{dF_3(x_3)}{dx_3} \end{bmatrix}$$

How do we create these invertible layers? Autoregressive Flows based on chain rule

- Forward - Density estimation (in **parallel**)
  - $z_1 = F_1(x_1)$
  - $z_2 = F_2(x_2|x_1)$
  - $z_3 = F_3(x_3|x_1, x_2)$
- Inverse – Sampling (conditioned on x so must be **sequential**)
  - $x_1 = F_1^{-1}(z_1)$
  - $x_2 = F_2^{-1}(z_2|x_1)$
  - $x_3 = F_3^{-1}(z_3|x_1, x_2)$
- What is the Jacobian and determinant?
  - Product of diagonal!

$$J_F = \begin{bmatrix} \frac{dF_1}{dx_1} & 0 & 0 \\ \frac{dF_2}{dx_1} & \frac{dF_2}{dx_2} & 0 \\ \frac{dF_3}{dx_1} & \frac{dF_3}{dx_2} & \frac{dF_3}{dx_3} \end{bmatrix}$$

Rezende, D., & Mohamed, S. (2015, June). Variational Inference with Normalizing Flows. In *International Conference on Machine Learning* (pp. 1530-1538).

How do we create these invertible layers? Inverse Autoregressive Flows based on chain rule

- Forward - Density estimation (**sequential**)
  - $z_1 = F_1(x_1)$
  - $z_2 = F_2(x_2|z_1)$
  - $z_3 = F_3(x_3|z_1, z_2)$
- Inverse – Sampling (**parallel**)
  - $x_1 = F_1^{-1}(z_1)$
  - $x_2 = F_2^{-1}(z_2|z_1)$
  - $x_3 = F_3^{-1}(z_3|z_1, z_2)$
- What is the Jacobian and determinant?
  - Product of diagonal!

$$J_F = \begin{bmatrix} \frac{dF_1}{dx_1} & 0 & 0 \\ \frac{dF_2}{dx_1} & \frac{dF_2}{dx_2} & 0 \\ \frac{dF_3}{dx_1} & \frac{dF_3}{dx_2} & \frac{dF_3}{dx_3} \end{bmatrix}$$

Kingma, D. P., Salimans, T., Jozefowicz, R., Chen, X., Sutskever, I., & Welling, M. (2016). Improved variational inference with inverse autoregressive flow. In *Advances in neural information processing systems* (pp. 4743-4751).

Scale-and-shift simple form of invertible functions (MAF https://arxiv.org/pdf/1705.07057.pdf)

- Forward – Density estimation (**parallel**)
  - $z_1 = \exp(\alpha_1) x_1 + \mu_1$
  - $z_2 = \exp(\alpha_2) x_2 + \mu_2,\ \alpha_2 = f_2(x_1),\ \mu_2 = g_2(x_1)$
  - $z_3 = \exp(\alpha_3) x_3 + \mu_3,\ \alpha_3 = f_3(x_1, x_2),\ \mu_3 = g_3(x_1, x_2)$
- What is the Jacobian and determinant?

$$J_F = \begin{bmatrix} \exp(\alpha_1) & 0 & 0 \\ \frac{dz_2}{dx_1} & \exp(\alpha_2) & 0 \\ \frac{dz_3}{dx_1} & \frac{dz_3}{dx_2} & \exp(\alpha_3) \end{bmatrix}$$

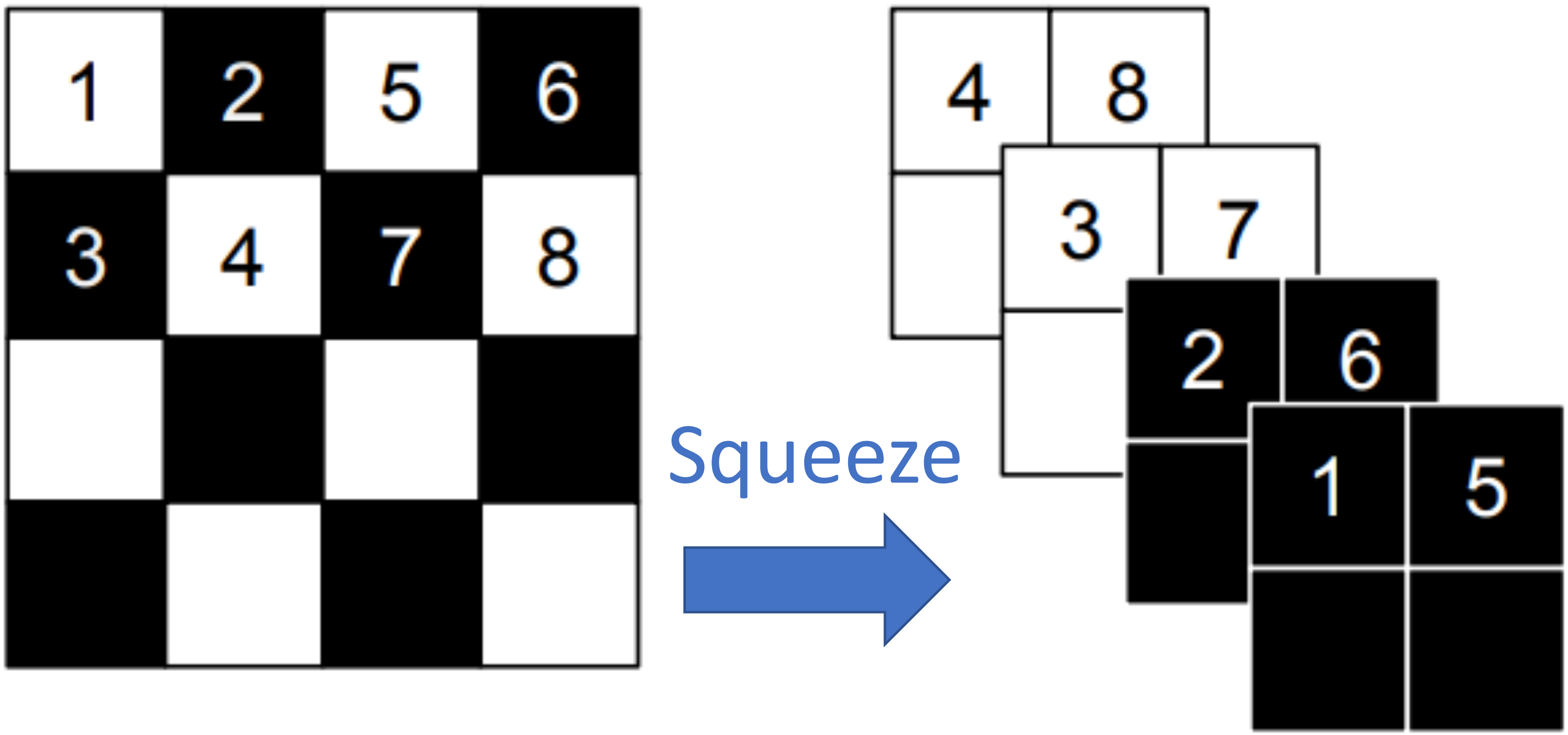
Coupling layers allow parallel density estimation **and** sampling

- Keep some set of features **fixed** and transform others
  - $z_{1:i-1} = x_{1:i-1}$
  - $z_{i:d} = \exp\left(f(x_{1:i-1})\right) \odot x_{i:d} + g(x_{1:i-1})$
- Reverse or shuffle coordinates and repeat
- What is Jacobian?

$$J_F = \begin{bmatrix} I & 0 \\ J_{cross} & \operatorname{diag}\left(\exp\left(f(x_{1:i-1})\right)\right) \end{bmatrix}$$

Dinh, L., Sohl-Dickstein, J., & Bengio, S. (2016). Density estimation using real nvp. *arXiv preprint arXiv:1605.08803*.

The squeeze operation trades off between spatial and channel dimensions



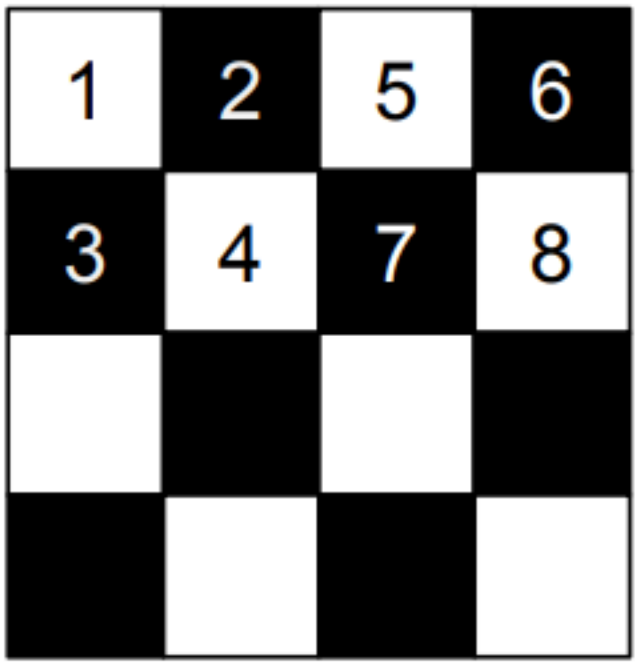
H x W x C

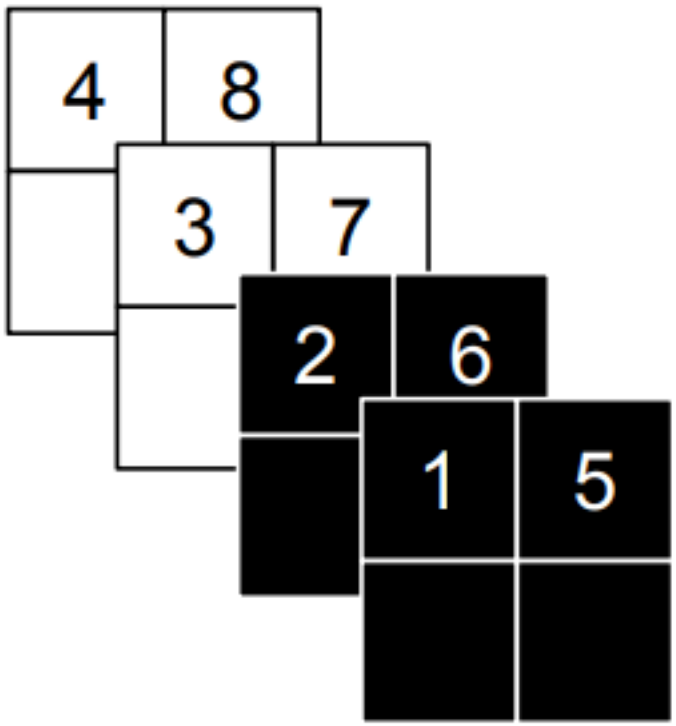
H/2 x W/2 x 4C

Dinh, L., Sohl-Dickstein, J., & Bengio, S. (2016). Density estimation using real nvp. *arXiv preprint arXiv:1605.08803*.

Checkboard or channel-wise masking can be used to separate fixed and non-fixed set of variables

White are **fixed, i.e.,** $x_{1:i-1}$, and black are **transformed**, $x_{i:d}$.



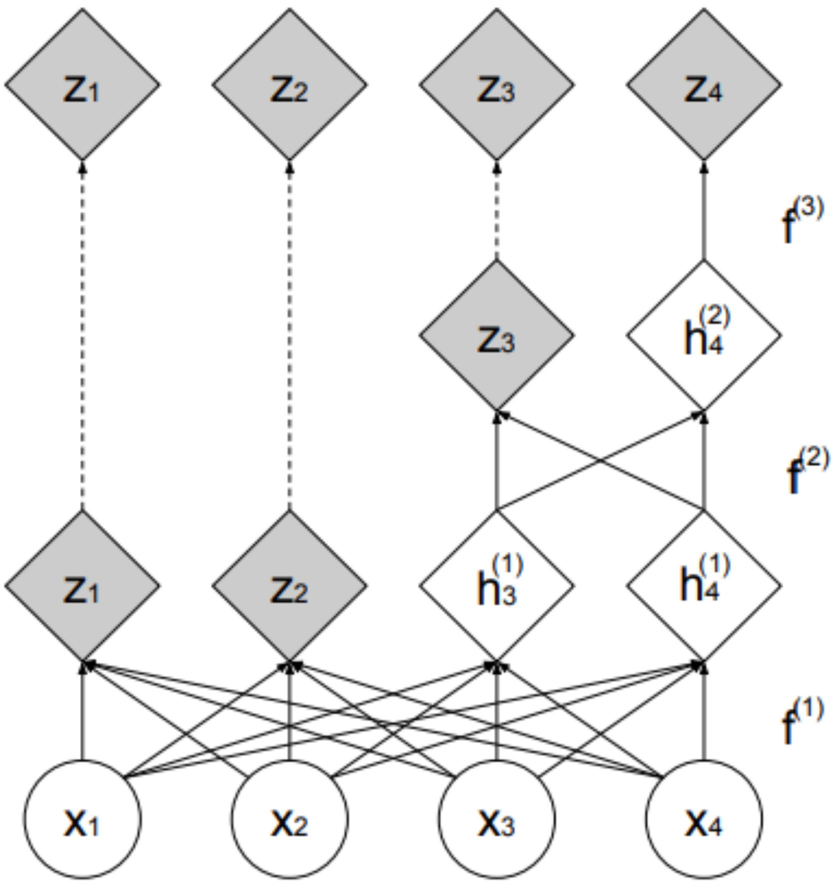


Dinh, L., Sohl-Dickstein, J., & Bengio, S. (2016). Density estimation using real nvp. *arXiv preprint arXiv:1605.08803*.

Hierarchical factorization is like an invertible dimensionality reduction method

- After each block, half of the dimensions are fixed and the rest pass through more transformations

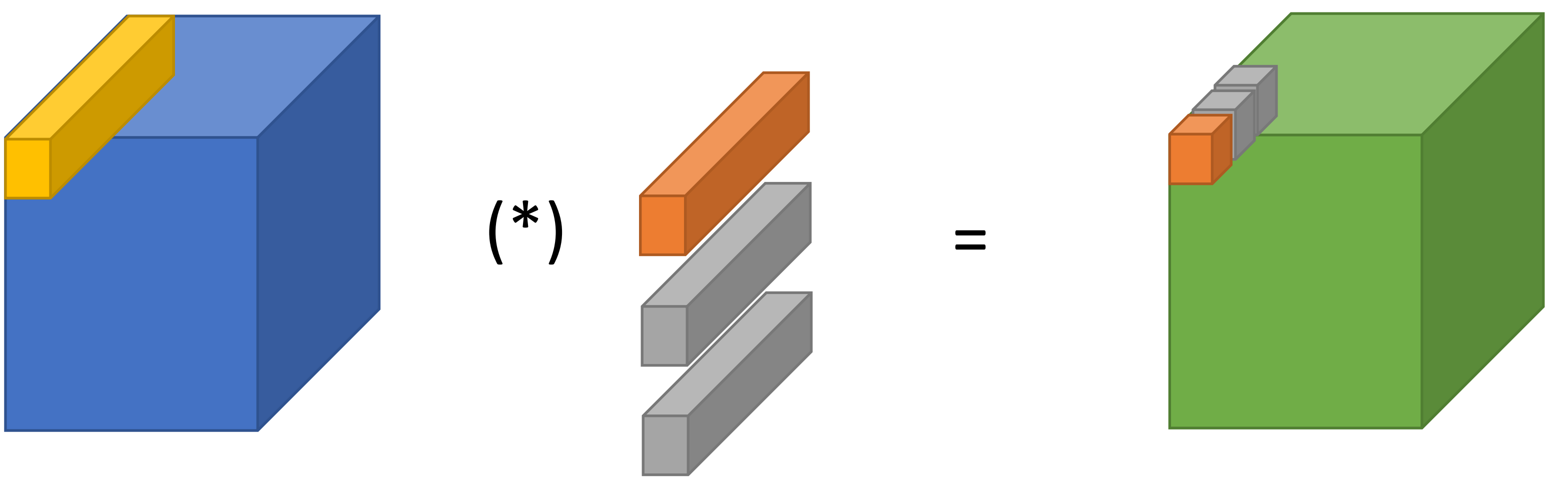
- Intuitively, the important part of the signal propagates deeper



Dinh, L., Sohl-Dickstein, J., & Bengio, S. (2016). Density estimation using real nvp. *arXiv preprint arXiv:1605.08803*.

GLOW: Convolutional flows 1 x 1 invertible convolutions are like fully connected layers for each pixel

- Image tensor: $\mathrm{h} \times w \times c$
- If we use c filters than we map from a $\mathrm{h} \times w \times c$ to another $\mathrm{h} \times w \times c$ image
- The number of parameters is a matrix $W \in \mathbb{R}^{c \times c}$
- 1x1 convolutions can be seen as a linear transform along the channel dimension (mixes the channel dimensions)



Highly realistic random samples from powerful flow model (GLOW)

Figure 1: Synthetic celebrities sampled from our model; see Section 3 for architecture and method, and Section 5 for more results.

https://papers.nips.cc/paper/8224-glow-generative-flow-with-invertible-1x1-convolutions.pdf

Similar concepts can be used to generate realistic audio (WaveGlow)

- Listen to some examples
  https://nv-adlr.github.io/WaveGlow

- Very similar concepts for audio generation