Invertible Normalizing Flows

ECE57000: Artificial Intelligence, Fall 2019

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Announcements

- Quiz moved to Friday
  - Same content (i.e., up to DCGANs, not today)

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 scores
    - Train separate image classifier
    - See if passing fakes to classifier produces a high confidence prediction

- Cannot use for classification or outlier detection

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

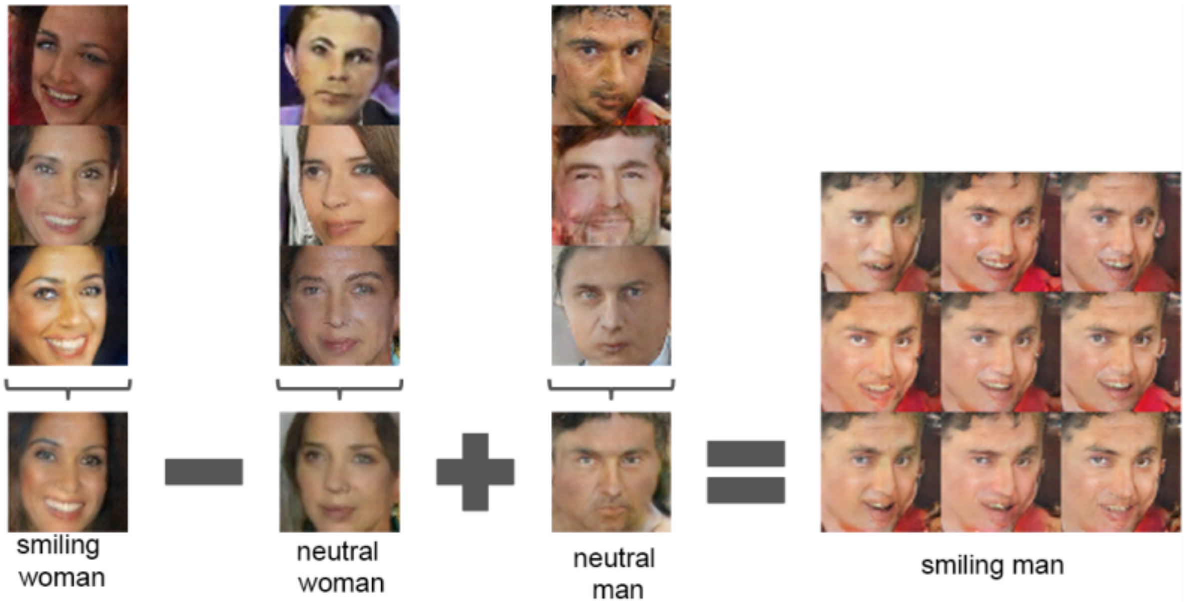
1. Assumptions on possible D and G
    1. Theory – All possible D and G
    2. Reality – Only functions defined by a neural network
2. Assumptions on optimality
    1. Theory – Both optimizations are solved perfectly
    2. Reality – The inner maximization is only solved approximately, and this interacts 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**

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->



<u>Normalizing flows</u> 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

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

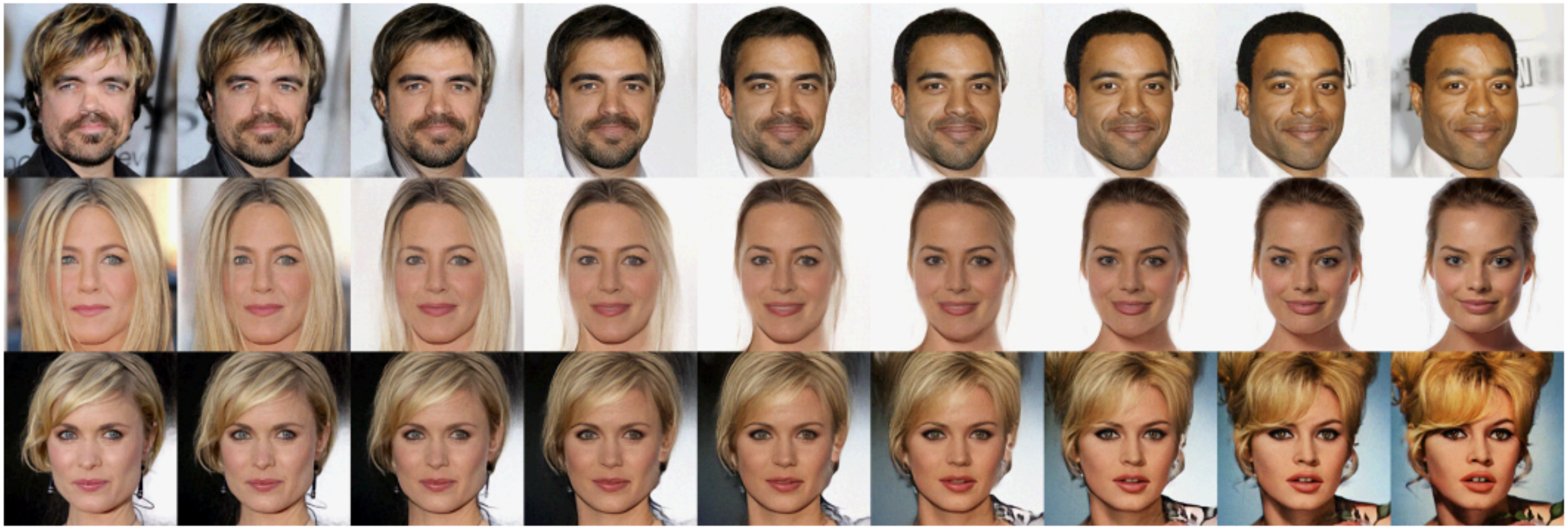


Figure 5: Linear interpolation in latent space between real images.

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

Transformations of real image along various features

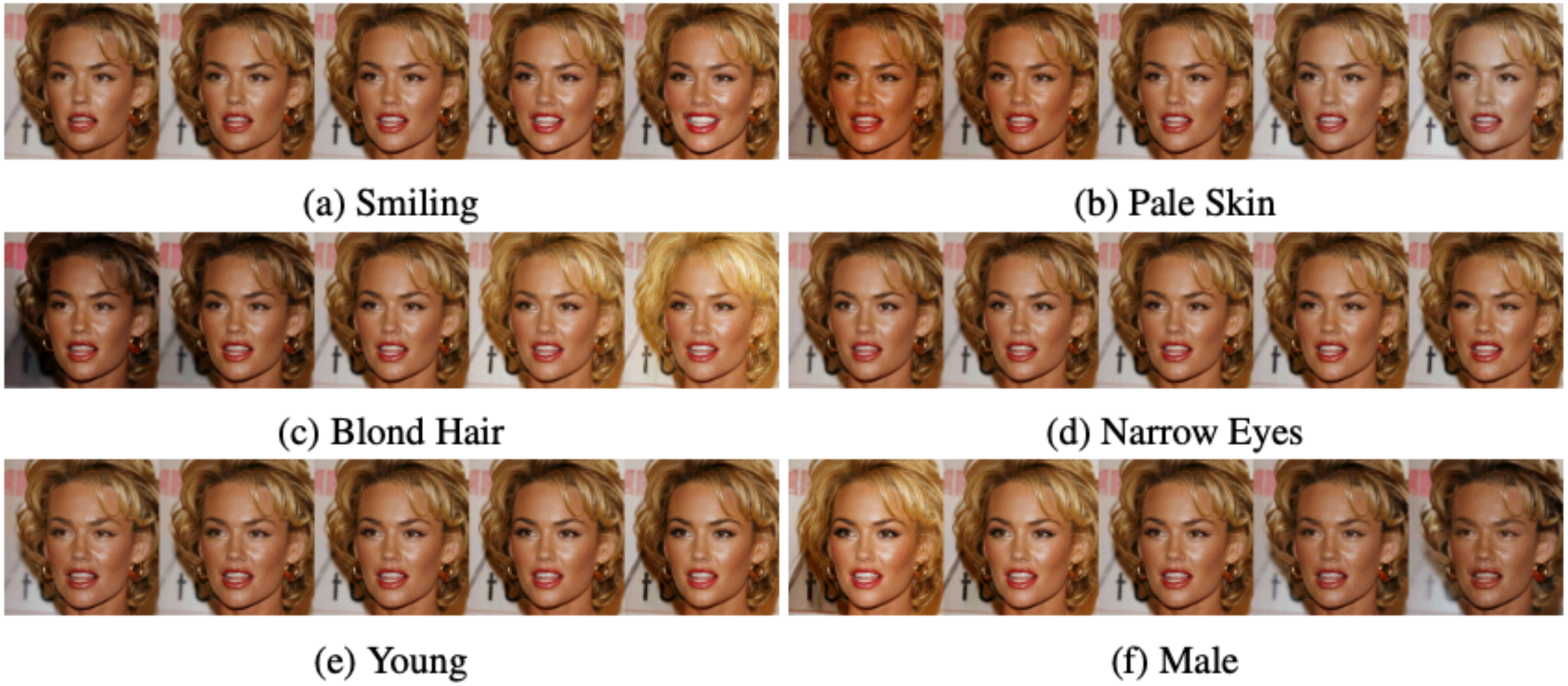


Figure 6: Manipulation of attributes of a face. Each row is made by interpolating the latent code of an image along a vector corresponding to the attribute, with the middle image being the original image

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

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

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

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

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

$$\frac{dF_x(a)}{da} = p_x(a)$$

$$\frac{dF_z\left(G^{-1}(a)\right)}{da} = \frac{dF_z\left(G^{-1}(a)\right)}{d\left(G^{-1}(a)\right)}\left(\frac{dG^{-1}(a)}{da}\right)$$

$$= p_z\left(G^{-1}(a)\right)\left(\frac{dG^{-1}(a)}{da}\right)$$

Derivation of change of variables using CDF function (Decreasing)

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

$$\frac{dF_x(a)}{da} = p_x(a)$$

$$-\frac{dF_z\left(G^{-1}(a)\right)}{da} = -\frac{dF_z\left(G^{-1}(a)\right)}{d\left(G^{-1}(a)\right)}\left(\frac{dG^{-1}(a)}{da}\right)$$

$$= -p_z\left(G^{-1}(a)\right)\left(\frac{dG^{-1}(a)}{da}\right)$$

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?

$$p_x(x) = p_z\big(F_v(x)\big)\left|\frac{dF_v(x)}{dx}\right|$$

$$p_x(x) = (1)|p_v(x)| = p_v(x)$$

Announcements

- Moved office hours from Thursday to Wed, 3:30pm—4:30pm

- Project submission instructions
  - https://www.davidinouye.com/course/ece57000-fall-2019/project/

- Quiz 6
  - Transposed convolution

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:

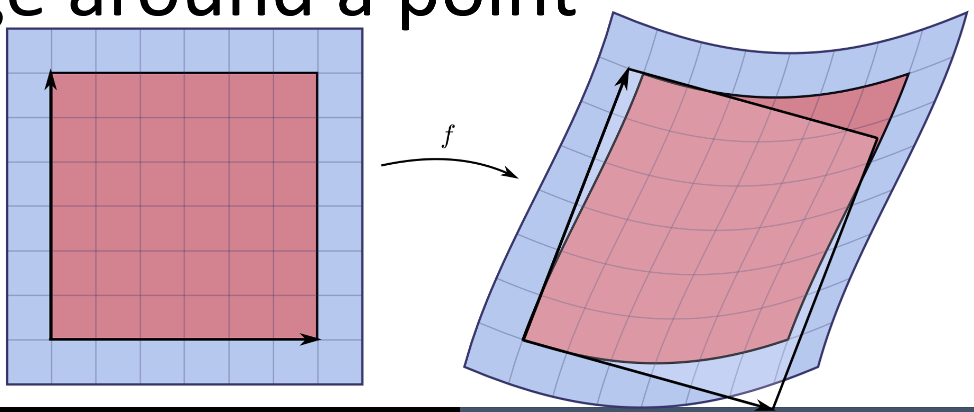
$$p_x(x) = |\det J_{G^{-1}}(x)|\, p_z\big(G^{-1}(x)\big)$$

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 expansion or shrinkage around a point



One useful identity for determinant of Jacobian of **invertible** function

- We can relate the Jacobian of a function to the Jacobian of the inverse in a natural way
- $J_{G^{-1}}(x) = J_{G^{-1}}\big(G(z)\big) = [J_G(z)]^{-1} = J_G(z)^{-1}$
- Using this we can come up with different ways of writing the change of variables formula

$$p_x(x) = |\det J_{G^{-1}}(x)|\, p_z\big(G^{-1}(x)\big)$$
$$p_x(x) = |\det J_G(z)|^{-1}\, p_z\big(G^{-1}(x)\big)$$
$$p_x(x) = |\det J_G(z)|^{-1}\, p_z(z)$$
$$p_z(z) = |\det J_G(z)| p_x(x)$$
$$p_z(z) = |\det J_G(z)| p_x\big(G(z)\big)$$

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 maximize likelihood of model $F_\theta = G^{-1}$

$$\arg\min_{F_\theta} -\log \prod_i \hat{p}_x(x_i;\theta)$$

$$\arg\min_{F_\theta} -\sum_i \left[\log p_z\big(F_\theta(x_i)\big) + \log\left|\det J_{F_\theta}(x_i)\right|\right]$$

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

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!

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

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

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

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

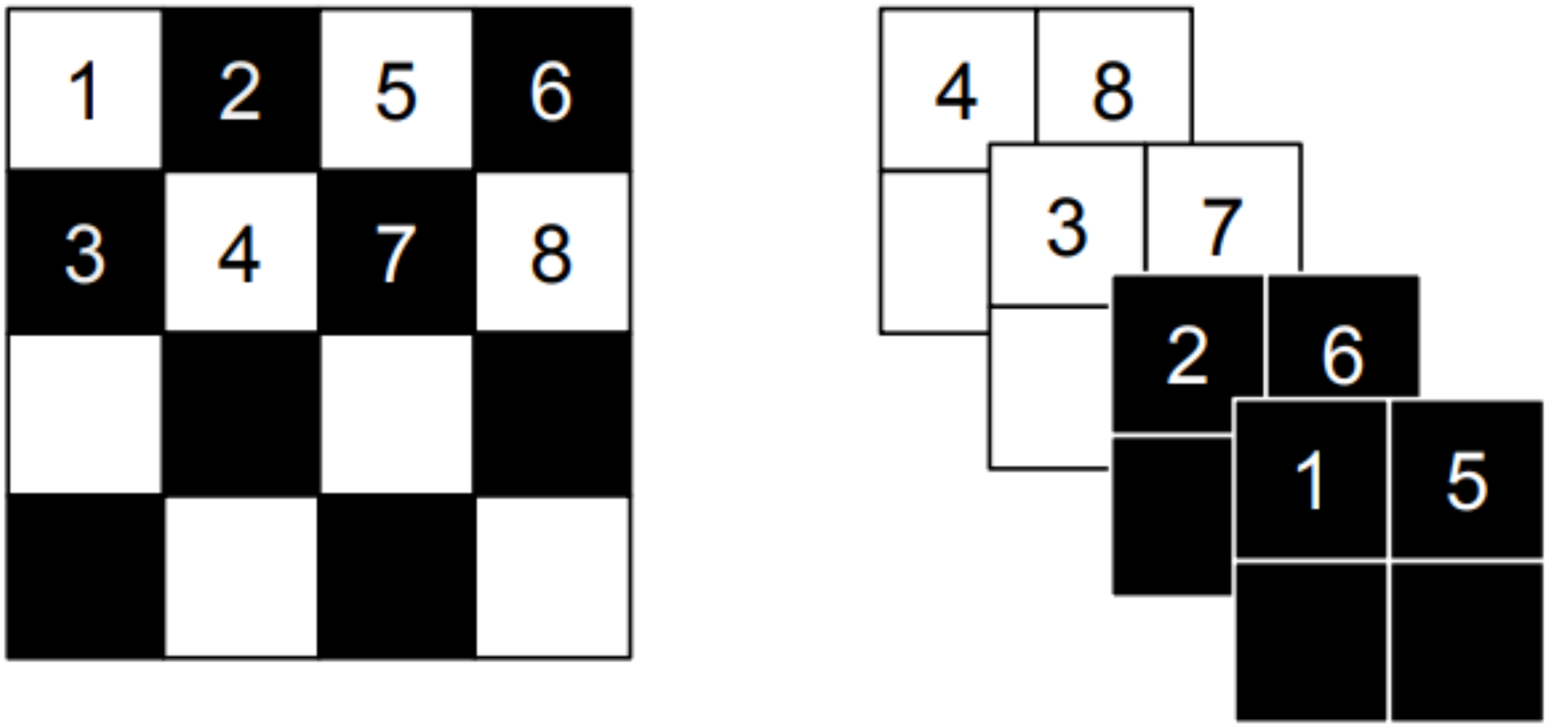
$$J_F = \begin{bmatrix} \exp(\alpha_1) & 0 & 0 \\ \frac{dz_2}{dx_1} & \exp(\alpha_2) & 0 \\ \frac{dz_3}{dx_1} & \frac{dz_3}{dx_2} & \exp(\alpha_3) \end{bmatrix}$$

What if we want parallel density estimation **and** sampling? (Real NVP https://arxiv.org/abs/1605.08803)

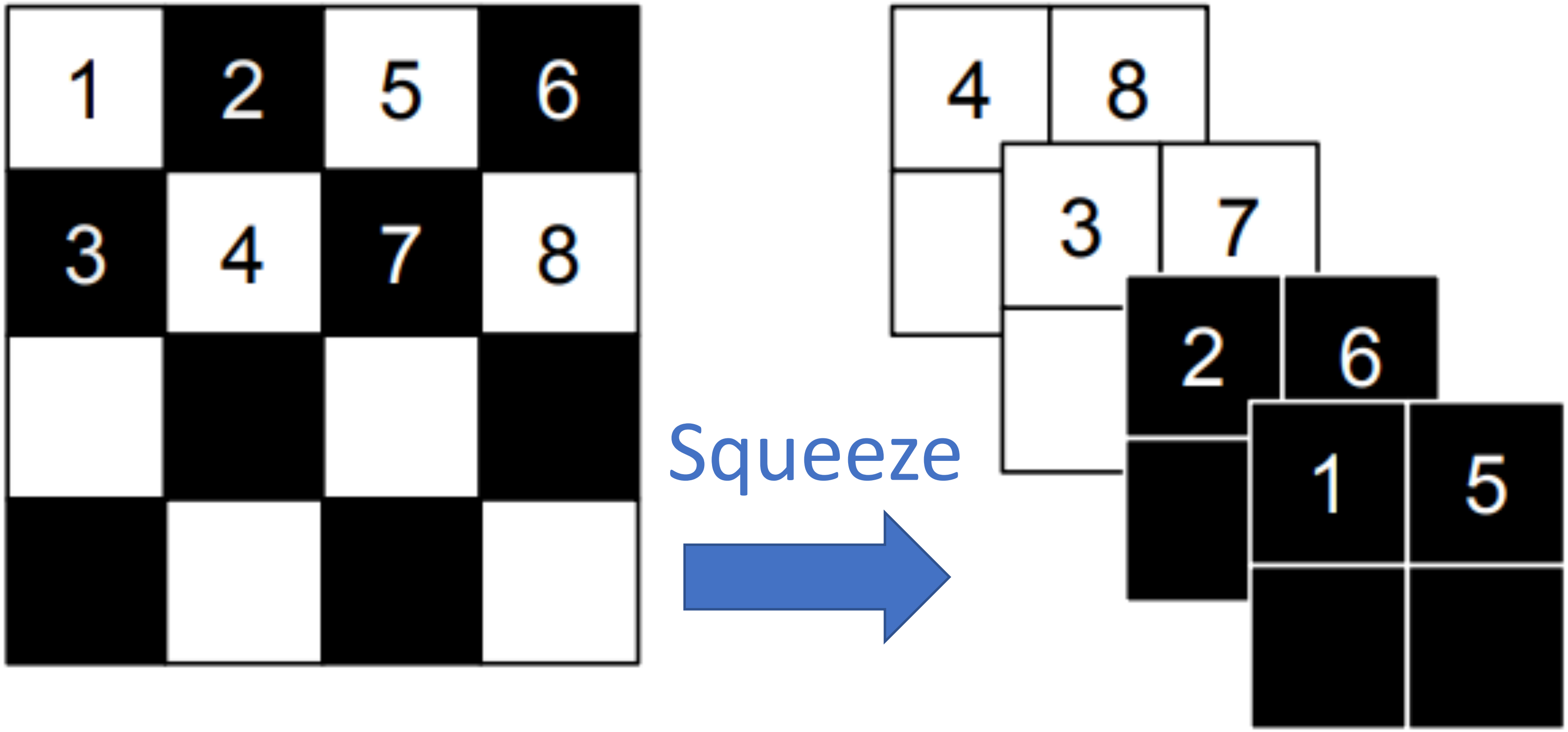
- Keep some set of features **fixed** and transform others
  - $z_{1:i-1} = x_{1:i-1}$
  - $z_{i:d} = \exp\big(f(x_{1:i-1})\big) \odot x_{i:d} + g(x_{1:i-1})$
- Reverse or shuffle coordinates and repeat
- What is Jacobian?

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

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



The squeeze operation trades off between spatial and channel dimensions



H x W x C

H/2 x W/2 x 4C

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

- Suppose an image has dimension $\mathrm{h} \times w \times c$
- Remember that a “1x1” convolution has kernel size of $1 \times 1 \times \boldsymbol{c}$
- Thus 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 $K \in \mathbb{R}^{c \times c}$
- Thus, a 1 x 1 convolution can also be seen as a linear transformation along the channel dimension

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.

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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