# Normalizing Flow Models

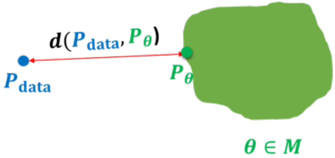
Stefano Ermon, Yang Song

Stanford University

Lecture 7

# Recap of likelihood-based learning so far:

$\mathbf{x}_i \sim P_{\text{data}}$
$i = 1, 2, \ldots, n$

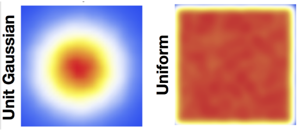



**Model family**

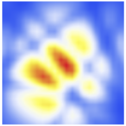
- Model families:
  - Autoregressive Models: $p_\theta(\mathrm{x}) = \prod_{i=1}^{n} p_\theta(x_i|\mathrm{x}_{<i})$
  - Variational Autoencoders: $p_\theta(\mathrm{x}) = \int p_\theta(\mathrm{x}, \mathrm{z})dz$
- Autoregressive models provide tractable likelihoods but no direct mechanism for learning features
- Variational autoencoders can learn feature representations (via latent variables z) but have intractable marginal likelihoods
- **Key question**: Can we design a latent variable model with tractable likelihoods? Yes!

# Simple Prior to Complex Data Distributions

- Desirable properties of any model distribution $p_\theta(x)$:
  - Easy-to-evaluate, closed form density (useful for training)
  - Easy-to-sample (useful for generation)
- Many simple distributions satisfy the above properties e.g., Gaussian, uniform distributions

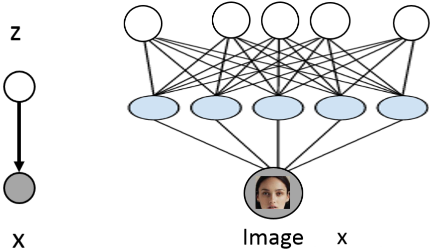



- Unfortunately, data distributions are more complex (multi-modal)



- **Key idea behind flow models**: Map simple distributions (easy to sample and evaluate densities) to complex distributions through an **invertible transformation**.

# Variational Autoencoder




A flow model is similar to a variational autoencoder (VAE):

1. Start from a simple prior: $z \sim \mathcal{N}(0, I) = p(z)$
2. Transform via $p(x \mid z) = \mathcal{N}(\mu_\theta(z), \Sigma_\theta(z))$
3. Even though $p(z)$ is simple, the marginal $p_\theta(x)$ is very complex/flexible. However, $p_\theta(x) = \int p_\theta(x, z) dz$ is expensive to compute: need to consider all z that could have generated x
4. What if we could easily "invert" $p(x \mid z)$ and compute $p(z \mid x)$ by design? How? Make $x = f_\theta(z)$ a deterministic and invertible function of z

# Continuous random variables refresher

- Let $X$ be a continuous random variable
- The cumulative density function (CDF) of $X$ is $F_X(a) = P(X \leq a)$
- The probability density function (pdf) of $X$ is $p_X(a) = F'_X(a) = \frac{dF_X(a)}{da}$
- Typically consider parameterized densities:
  - Gaussian: $X \sim \mathcal{N}(\mu, \sigma)$ if $p_X(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/2\sigma^2}$
  - Uniform: $X \sim \mathcal{U}(a, b)$ if $p_X(x) = \frac{1}{b-a} 1[a \leq x \leq b]$
  - Etc.
- If $\boldsymbol{X}$ is a continuous random vector, we can usually represent it using its **joint probability density function**:
  - Gaussian: if $p_X(\mathrm{x}) = \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \exp\left(-\frac{1}{2}(\mathrm{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathrm{x} - \boldsymbol{\mu})\right)$

# Change of Variables formula

- Let $Z$ be a uniform random variable $\mathcal{U}[0,2]$ with density $p_Z$. What is $p_Z(1)$? $\frac{1}{2}$
  - As a sanity check, $\int_0^2 \frac{1}{2} = 1$
- Let $X = 4Z$, and let $p_X$ be its density. What is $p_X(4)$?
- $p_X(4) = p(X = 4) = p(4Z = 4) = p(Z = 1) = p_Z(1) = 1/2$ **Wrong!**
- Clearly, $X$ is uniform in $[0, 8]$, so $p_X(4) = 1/8$
- To get correct result, need to use **change of variables formula**

# Change of Variables formula

- **Change of variables (1D case)**: If $X = f(Z)$ and $f(\cdot)$ is monotone with inverse $Z = f^{-1}(X) = h(X)$, then:

$$p_X(x) = p_Z(h(x))|h'(x)|$$

- Previous example: If $X = f(Z) = 4Z$ and $Z \sim \mathcal{U}[0, 2]$, what is $p_X(4)$?
  - Note that $h(X) = X/4$
  - $p_X(4) = p_Z(1)h'(4) = 1/2 \times |1/4| = 1/8$
- More interesting example: If $X = f(Z) = \exp(Z)$ and $Z \sim \mathcal{U}[0, 2]$, what is $p_X(x)$?
  - Note that $h(X) = \ln(X)$
  - $p_X(x) = p_Z(\ln(x))|h'(x)| = \frac{1}{2x}$ for $x \in [\exp(0), \exp(2)]$
- Note that the "shape" of $p_X(x)$ is different (more complex) from that of the prior $p_Z(z)$.

# Change of Variables formula

- **Change of variables (1D case)**: If $X = f(Z)$ and $f(\cdot)$ is monotone with inverse $Z = f^{-1}(X) = h(X)$, then:

$$p_X(x) = p_Z(h(x))|h'(x)|$$

- Proof sketch: Assume $f(\cdot)$ is monotonically increasing

$$F_X(x) = p[X \leq x] = p[f(Z) \leq x] = p[Z \leq h(x)] = F_Z(h(x))$$

Taking derivatives on both sides:

$$p_X(x) = \frac{dF_X(x)}{dx} = \frac{dF_Z(h(x))}{dx} = p_Z(h(x))h'(x)$$

- Recall from basic calculus that $h'(x) = [f^{-1}]'(x) = \frac{1}{f'(f^{-1}(x))}$. So letting $z = h(x) = f^{-1}(x)$ we can also write

$$p_X(x) = p_Z(z)\frac{1}{f'(z)}$$

# Geometry: Determinants and volumes

- Let $Z$ be a uniform random vector in $[0, 1]^n$
- Let $X = AZ$ for a square invertible matrix $A$, with inverse $W = A^{-1}$. How is $X$ distributed?
- Geometrically, the matrix $A$ maps the unit hypercube $[0, 1]^n$ to a parallelotope
- Hypercube and parallelotope are generalizations of square/cube and parallelogram/parallelopiped to higher dimensions

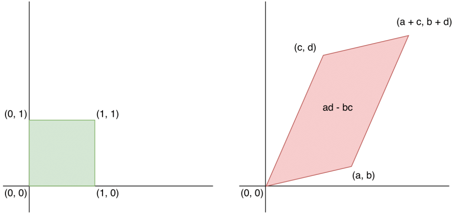
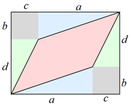



Figure: The matrix $A = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$ maps a unit square to a parallelogram

# Geometry: Determinants and volumes

- The volume of the parallelotope is equal to the absolute value of the determinant of the matrix $A$

$$\det(A) = \det\begin{pmatrix} a & c \\ b & d \end{pmatrix} = ad - bc$$




$(a+c)(b+d) - ab - 2bc - cd = ad - bc$

- Let $X = AZ$ for a square invertible matrix $A$, with inverse $W = A^{-1}$. $X$ is uniformly distributed over the parallelotope of area $|\det(A)|$. Hence, we have

$$\begin{aligned} p_X(\mathrm{x}) &= p_Z(W\mathrm{x}) / |\det(A)| \\ &= p_Z(W\mathrm{x}) |\det(W)| \end{aligned}$$

because if $W = A^{-1}$, $\det(W) = \frac{1}{\det(A)}$. Note similarity with 1D case formula.

# Generalized change of variables

- For linear transformations specified via $A$, change in volume is given by the determinant of $A$
- For non-linear transformations $\mathrm{f}(\cdot)$, the *linearized* change in volume is given by the determinant of the Jacobian of $\mathrm{f}(\cdot)$.
- **Change of variables (General case)**: The mapping between $Z$ and $X$, given by $\mathrm{f} : \mathbb{R}^n \mapsto \mathbb{R}^n$, is invertible such that $X = \mathrm{f}(Z)$ and $Z = \mathrm{f}^{-1}(X)$.

$$p_X(\mathrm{x}) = p_Z\left(\mathrm{f}^{-1}(\mathrm{x})\right)\left|\det\left(\frac{\partial \mathrm{f}^{-1}(\mathrm{x})}{\partial \mathrm{x}}\right)\right|$$

- Note 0: generalizes the previous 1D case $p_X(x) = p_Z(h(x))|h'(x)|$
- Note 1: unlike VAEs, $\mathrm{x}, \mathrm{z}$ need to be continuous and have the same dimension. For example, if $\mathrm{x} \in \mathbb{R}^n$ then $\mathrm{z} \in \mathbb{R}^n$
- Note 2: For any invertible matrix $A$, $det(A^{-1}) = det(A)^{-1}$

$$p_X(\mathrm{x}) = p_Z(\mathrm{z})\left|\det\left(\frac{\partial \mathrm{f}(\mathrm{z})}{\partial \mathrm{z}}\right)\right|^{-1}$$

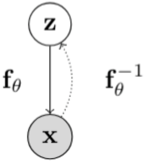
# Two Dimensional Example

- Let $Z_1$ and $Z_2$ be continuous random variables with joint density $p_{Z_1,Z_2}$.
- Let $u = (u_1, u_2)$ be a transformation
- Let $v = (v_1, v_2)$ be the inverse transformation
- Let $X_1 = u_1(Z_1, Z_2)$ and $X_2 = u_2(Z_1, Z_2)$ Then, $Z_1 = v_1(X_1, X_2)$ and $Z_2 = v_2(X_1, X_2)$

$$
\begin{aligned}
& p_{X_1,X_2}(x_1, x_2) \\
&= p_{Z_1,Z_2}(v_1(x_1, x_2), v_2(x_1, x_2)) \left| \det \begin{pmatrix} \frac{\partial v_1(x_1,x_2)}{\partial x_1} & \frac{\partial v_1(x_1,x_2)}{\partial x_2} \\ \frac{\partial v_2(x_1,x_2)}{\partial x_1} & \frac{\partial v_2(x_1,x_2)}{\partial x_2} \end{pmatrix} \right| \text{(inverse)} \\
&= p_{Z_1,Z_2}(z_1, z_2) \left| \det \begin{pmatrix} \frac{\partial u_1(z_1,z_2)}{\partial z_1} & \frac{\partial u_1(z_1,z_2)}{\partial z_2} \\ \frac{\partial u_2(z_1,z_2)}{\partial z_1} & \frac{\partial u_2(z_1,z_2)}{\partial z_2} \end{pmatrix} \right|^{-1} \text{(forward)}
\end{aligned}
$$

# Normalizing flow models

- Consider a directed, latent-variable model over observed variables $X$ and latent variables $Z$
- In a **normalizing flow model**, the mapping between $Z$ and $X$, given by $\mathrm{f}_\theta : \mathbb{R}^n \mapsto \mathbb{R}^n$, is deterministic and invertible such that $X = \mathrm{f}_\theta(Z)$ and $Z = \mathrm{f}_\theta^{-1}(X)$




- Using change of variables, the marginal likelihood $p(\mathrm{x})$ is given by

$$p_X(\mathrm{x}; \theta) = p_Z\left(\mathrm{f}_\theta^{-1}(\mathrm{x})\right) \left| \det\left( \frac{\partial \mathrm{f}_\theta^{-1}(\mathrm{x})}{\partial \mathrm{x}} \right) \right|$$

- Note: $\mathrm{x}, \mathrm{z}$ need to be continuous and have the same dimension.

# A Flow of Transformations

**Normalizing:** Change of variables gives a normalized density after applying an invertible transformation
**Flow:** Invertible transformations can be composed with each other

$$\mathrm{z}_m = \mathrm{f}_\theta^m \circ \cdots \circ \mathrm{f}_\theta^1(\mathrm{z}_0) = \mathrm{f}_\theta^m(\mathrm{f}_\theta^{m-1}(\cdots(\mathrm{f}_\theta^1(\mathrm{z}_0)))) \triangleq \mathrm{f}_\theta(\mathrm{z}_0)$$

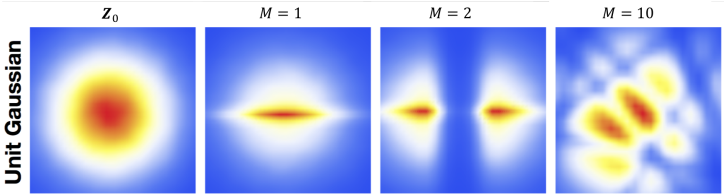
- Start with a simple distribution for $\mathrm{z}_0$ (e.g., Gaussian)
- Apply a sequence of $M$ invertible transformations to finally obtain $\mathrm{x} = \mathrm{z}_M$
- By change of variables

$$p_X(\mathrm{x};\theta) = p_Z\left(\mathrm{f}_\theta^{-1}(\mathrm{x})\right)\prod_{m=1}^{M}\left|\det\left(\frac{\partial(\mathrm{f}_\theta^m)^{-1}(\mathrm{z}_m)}{\partial \mathrm{z}_m}\right)\right|$$

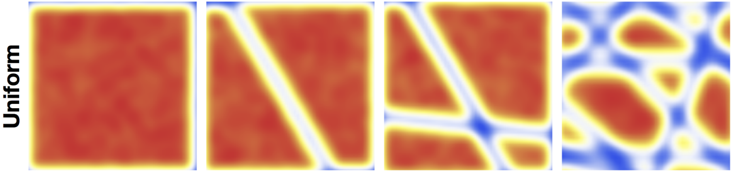
(Note: determininant of product equals product of determinants)

# Planar flows (Rezende & Mohamed, 2016)

- Base distribution: Gaussian




- Base distribution: Uniform




- 10 planar transformations can transform simple distributions into a more complex one

# Learning and Inference

- Learning via **maximum likelihood** over the dataset $\mathcal{D}$

$$\max_{\theta} \log p_X(\mathcal{D}; \theta) = \sum_{\mathrm{x} \in \mathcal{D}} \log p_Z\left(\mathrm{f}_\theta^{-1}(\mathrm{x})\right) + \log \left| \det \left( \frac{\partial \mathrm{f}_\theta^{-1}(\mathrm{x})}{\partial \mathrm{x}} \right) \right|$$

- **Exact likelihood evaluation** via inverse tranformation $\mathrm{x} \mapsto \mathrm{z}$ and change of variables formula
- **Sampling** via forward transformation $\mathrm{z} \mapsto \mathrm{x}$

$$\mathrm{z} \sim p_Z(\mathrm{z}) \quad \mathrm{x} = \mathrm{f}_\theta(\mathrm{z})$$

- **Latent representations** inferred via inverse transformation (no inference network required!)

$$\mathrm{z} = \mathrm{f}_\theta^{-1}(\mathrm{x})$$

# Desiderata for flow models

- Simple prior $p_Z(\mathrm{z})$ that allows for efficient sampling and tractable likelihood evaluation. E.g., isotropic Gaussian
- Invertible transformations with tractable evaluation:
  - Likelihood evaluation requires efficient evaluation of $\mathrm{x} \mapsto \mathrm{z}$ mapping
  - Sampling requires efficient evaluation of $\mathrm{z} \mapsto \mathrm{x}$ mapping
- Computing likelihoods also requires the evaluation of determinants of $n \times n$ Jacobian matrices, where $n$ is the data dimensionality
  - Computing the determinant for an $n \times n$ matrix is $O(n^3)$: prohibitively expensive within a learning loop!
  - **Key idea**: Choose tranformations so that the resulting Jacobian matrix has special structure. For example, the determinant of a triangular matrix is the product of the diagonal entries, i.e., an $O(n)$ operation

# Triangular Jacobian

$$\mathbf{x} = (x_1, \cdots, x_n) = \mathbf{f}(\mathbf{z}) = (f_1(\mathbf{z}), \cdots, f_n(\mathbf{z}))$$

$$J = \frac{\partial \mathbf{f}}{\partial \mathbf{z}} = \begin{pmatrix} \frac{\partial f_1}{\partial z_1} & \cdots & \frac{\partial f_1}{\partial z_n} \\ \cdots & \cdots & \cdots \\ \frac{\partial f_n}{\partial z_1} & \cdots & \frac{\partial f_n}{\partial z_n} \end{pmatrix}$$

Suppose $x_i = f_i(\mathbf{z})$ only depends on $\mathbf{z}_{\leq i}$. Then

$$J = \frac{\partial \mathbf{f}}{\partial \mathbf{z}} = \begin{pmatrix} \frac{\partial f_1}{\partial z_1} & \cdots & 0 \\ \cdots & \cdots & \cdots \\ \frac{\partial f_n}{\partial z_1} & \cdots & \frac{\partial f_n}{\partial z_n} \end{pmatrix}$$

has lower triangular structure. Determinant can be computed in **linear time**. Similarly, the Jacobian is upper triangular if $x_i$ only depends on $\mathbf{z}_{\geq i}$

# Planar flows (Rezende & Mohamed, 2016)

- Planar flow. Invertible transformation

$$x = f_\theta(z) = z + u h(w^T z + b)$$

  parameterized by $\theta = (w, u, b)$ where $h(\cdot)$ is a non-linearity
- Absolute value of the determinant of the Jacobian is given by

$$\left|\det \frac{\partial f_\theta(z)}{\partial z}\right| = \left|\det(I + h'(w^T z + b) u w^T)\right|$$
$$= \left|1 + h'(w^T z + b) u^T w\right|$$

(matrix determinant lemma)

- Need to restrict parameters and non-linearity for the mapping to be invertible. For example, $h = tanh()$ and $h'(w^T z + b)u^T w \geq -1$