Normalizing Flow Models

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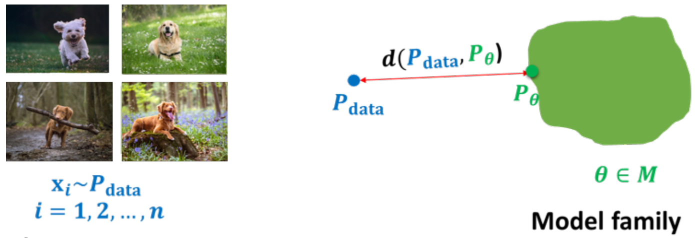
Lecture 7

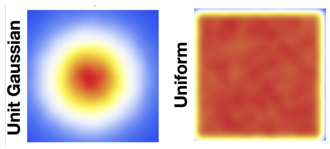
Recap of likelihood-based learning so far:



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

Simple Prior to Complex Data Distributions

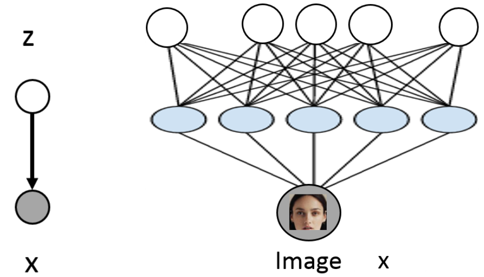
- Desirable properties of any model distribution $p_\theta(\mathbf{x})$:
  - Easy-to-evaluate, closed form density (useful for training)
  - Easy-to-sample (useful for generation)
- Many simple distributions satisfy the above properties e.g., Gaussian, uniform distributions



- 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: $\mathbf{z} \sim \mathcal{N}(0, I) = p(\mathbf{z})$
2. Transform via $p(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}(\mu_\theta(\mathbf{z}), \Sigma_\theta(\mathbf{z}))$
3. Even though $p(\mathbf{z})$ is simple, the marginal $p_\theta(\mathbf{x})$ is very complex/flexible. However, $p_\theta(\mathbf{x}) = \int p_\theta(\mathbf{x}, \mathbf{z}) d\mathbf{z}$ is expensive to compute: need to enumerate all $\mathbf{z}$ that could have generated $\mathbf{x}$
4. What if we could easily "invert" $p(\mathbf{x} \mid \mathbf{z})$ and compute $p(\mathbf{z} \mid \mathbf{x})$ by design? How? Make $\mathbf{x} = f_\theta(\mathbf{z})$ a deterministic and invertible function of $\mathbf{z}$, so for any $\mathbf{x}$ there is a unique corresponding $\mathbf{z}$ (no enumeration)

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 $p_X(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^n |\mathbf{\Sigma}|}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)$

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

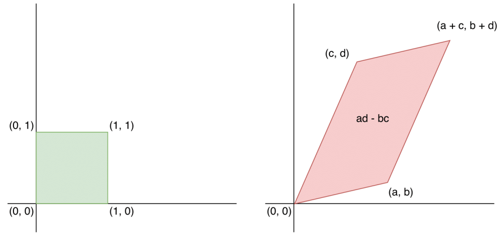
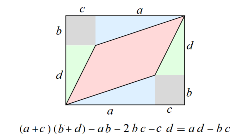


Figure: The matrix $A = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$ maps a unit square to a parallelogram

Geometry: Determinants and volumes

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

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



- 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

$$p_X(\mathbf{x}) = p_Z(W\mathbf{x}) \,/\, |\det(A)|$$
$$= p_Z(W\mathbf{x}) \, |\det(W)|$$

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

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

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

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

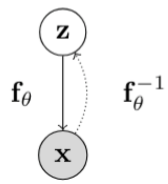
Two Dimensional Example

- Let Z_1 and Z_2 be continuous random variables with joint density p_{Z_1,Z_2}.
- Let $u : \mathbb{R}^2 \to \mathbb{R}^2$ be an invertible transformation. Two inputs and two outputs, denoted $u = (u_1, u_2)$
- Let $v = (v_1, v_2)$ be its 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 $Z_2 = v_2(X_1, X_2)$

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

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 $\mathbf{f}_\theta : \mathbb{R}^n \mapsto \mathbb{R}^n$, is deterministic and invertible such that $X = \mathbf{f}_\theta(Z)$ and $Z = \mathbf{f}_\theta^{-1}(X)$



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

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

- Note: $\mathbf{x}, \mathbf{z}$ 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

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

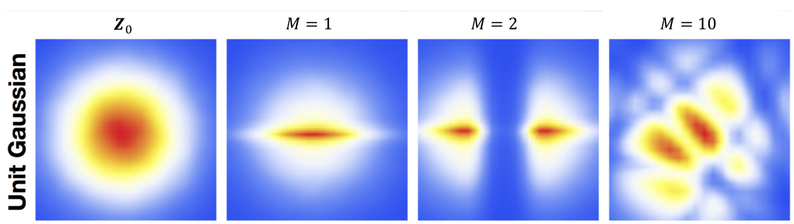
- Start with a simple distribution for $\mathbf{z}_0$ (e.g., Gaussian)
- Apply a sequence of M invertible transformations to finally obtain $\mathbf{x} = \mathbf{z}_M$
- By change of variables

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

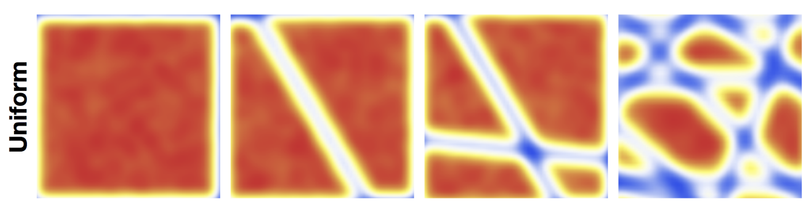
(Note: determininant of product equals product of determinants)

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 $\mathcal{D}$

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

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

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

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

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

Desiderata for flow models

- Simple prior $p_Z(\mathbf{z})$ that allows for efficient sampling and tractable likelihood evaluation. E.g., isotropic Gaussian
- Invertible transformations with tractable evaluation:
  - Likelihood evaluation requires efficient evaluation of $\mathbf{x} \mapsto \mathbf{z}$ mapping
  - Sampling requires efficient evaluation of $\mathbf{z} \mapsto \mathbf{x}$ 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

$$\mathbf{x} = \mathbf{f}_\theta(\mathbf{z}) = \mathbf{z} + \mathbf{u}h(\mathbf{w}^T\mathbf{z} + b)$$

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

$$\begin{aligned} \left|\det \frac{\partial \mathbf{f}_\theta(\mathbf{z})}{\partial \mathbf{z}}\right| &= \left|\det(I + h'(\mathbf{w}^T\mathbf{z} + b)\mathbf{u}\mathbf{w}^T)\right| \\ &= \left|1 + h'(\mathbf{w}^T\mathbf{z} + b)\mathbf{u}^T\mathbf{w}\right| \end{aligned}$$

(matrix determinant lemma)

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