Normalizing Flows

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Lecture 7

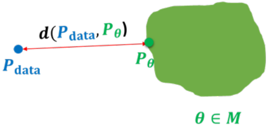
Announcements

- Assignment 1 is due on Wednesday.
- Project proposals are due in one and a half week.
- Assignment 2 will be released on Wednesday and will be due in two weeks.
- Please think about your preferred presentation topics.

Lecture Outline

1. Recap and Motivation for Normalizing Flows
2. Volume-Preserving Transformations
   - The Determinant
   - Change of Variables Formula
3. Normalizing Flows
   - Representation and Learning
   - Composing Simple Transformations
   - Triangular Jacobians

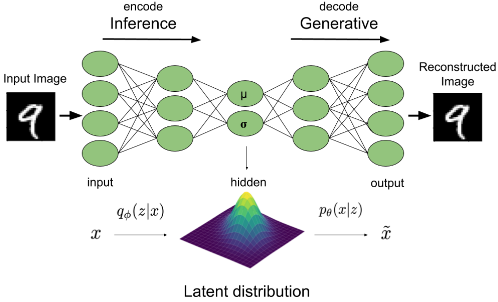
$\mathbf{x}_i \sim P_{\text{data}}$
$i = 1, 2, \ldots, n$



Model family

1. Autoregressive models: $p_\theta(\mathbf{x}) = \prod_{i=1}^{n} p_\theta(x_i|\mathbf{x}_{<i})$
    - Probability distributions factorize into a product of factors
    - We can efficiently represent p via *conditional independence* and/or *neural parameterizations*
2. Autoregressive models Pros:
    - It is computationally tractable to evaluate likelihoods
    - It is tractable to train $p(\mathbf{x})$ via maximum likelihood & gradient descent
3. Autoregressive models Cons:
    - They require choosing an ordering over variables
    - Generation is sequential (hence usually slow)
    - Cannot learn features in an unsupervised way

Recap: Latent Variable Models

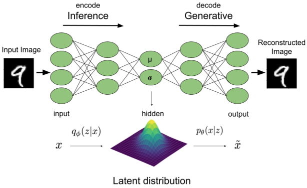


Variational Autoencoders: $p_\theta(\mathbf{x}) = \int p_\theta(\mathbf{x}, \mathbf{z}) d\mathbf{z}$

$$\mathcal{L}(\mathbf{x}; \theta, \phi) = E_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p(\mathbf{x}|\mathbf{z}; \theta)] - D_{KL}(q_\phi(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))$$

- Infinite mixture of Gaussians. Means are parametrized by deep net.
- Objective has a natural auto-encoder interpretation.

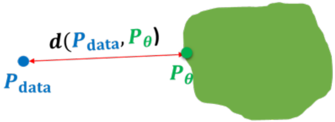
Recap: Latent Variable Models



1. Latent Variable Models Pros:
   - Naturally combine simple models into more flexible ones: $p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z}$ and $p(\mathbf{x}|\mathbf{z}), p(\mathbf{z})$ can be "simple".
   - Directed model permits efficient generation: $\mathbf{z} \sim p(\mathbf{z})$, $\mathbf{x} \sim p(\mathbf{x}|\mathbf{z};\theta)$
2. Latent Variable Models Cons:
   - Evaluating the log-likelihood is generally intractable
   - Hence, training via maximum-likelihood is intractable
   - Fundamentally, the challenge is that posterior inference $p(\mathbf{z} \mid \mathbf{x})$ is hard. Typically requires variational approximations

Can We Get Best of Both Worlds?

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



Model family

- 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! Use normalizing flows.

Simple Prior to Complex Data Distributions

- Desirable properties of any model distribution:
  - Analytic density
  - Easy-to-sample
- Many simple distributions satisfy the above properties e.g., Gaussian, uniform distributions
- Unfortunately, data distributions could be much more complex (multi-modal)
- **Key idea**: Map simple distributions (easy to sample and evaluate densities) to complex distributions (learned via data) using **invertible** change of variables transformations.

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Example: Change of Variables

- Let Z be a uniform random variable $\mathcal{U}[0,2]$ with density p_Z. What is $p_Z(1)$? $\frac{1}{2}$
- Let $X = 4Z$, and let p_X be its density. What is $p_X(4)$?
- $p_X(4) = p(X = 4) = p(4Z = 4) = p(Z = 1) = p_Z(1) = 1/2$
- **This is incorrect.** Clearly, X is uniform in $[0,8]$, so $p_X(4) = 1/8$
- Probability densities are not probability distributions (measures).
- Transformations expand the support of the distribution; we need to scale densities to preserve the *volume* of probability mass.

Change of Variables Formula in One Dimension

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 $X = 4Z$ and $Z \sim \mathcal{U}[0, 2]$, what is $p_X(4)$?
- Note that $h(X) = X/4$
- $p_X(4) = p_Z(1)h'(4) = 1/2 \times 1/4 = 1/8$
- We have expanded the support of the distribution by 4. Hence, we need to decrease the mass at each point by 4 to preserve the volume.
- Generalizes to higher dimensions via determinants of transformations

Change of Variables Formula: Intuition

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

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

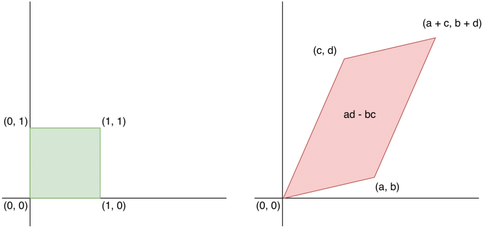
- We can understand this as follows:

$$\begin{aligned}\int p_Z(z)dz &= \int p_Z(z)\frac{dx}{dx}dz \\ &= \int p_Z(h(x))\left|\frac{dz}{dx}\right|dx \\ &= \int p_Z(h(x))\left|h'(x)\right|dx\end{aligned}$$

An integral is a sum of "infenitesimal rectangles" dz and dx. We adjust the "volume" of each dx around x because h changes it.

Review: Determinants and Volumes (in 2D)

Next, we would like to develop a notion of volume in higher dimensions.



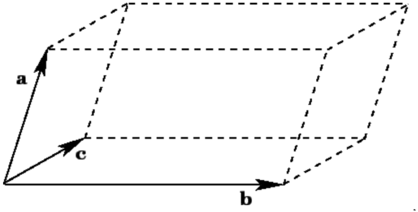
- Matrix $A = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$ maps a unit square to a parallelogram, e.g.:

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

- The volume of the parallelotope is equal to the determinant of A

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

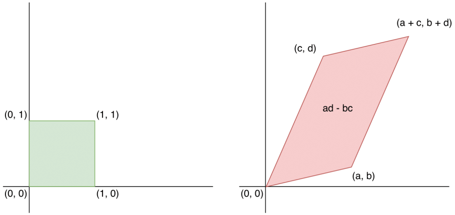
Review: Determinants and Volumes (in 3D)



- The volume formula still holds in 3D.
- Note that if two vectors are colinear, we get a plane, which has volume zero in 3D. The determinant is zero and the matrix is singular.

Review: Determinants and Volumes (in n-D)

- In general, 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



- Determinant $\det(A)$ still gives volume of the n-D shape.

Determinants and Volumes for Changing Variables

- 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?
- The volume of the parallelotope is equal to the determinant of the transformation A

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

- X is uniformly distributed over the parallelotope. Hence, we have

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

Change of Variables Formula (General Case)

- 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 $\mathbf{f}(\cdot)$.

The Jacobian

Consider a vector valued function $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$, with:

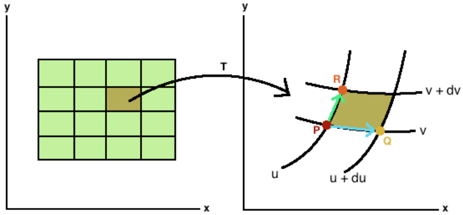
- $\mathbf{x} = (x_1, \cdots, x_n)$
- $\mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), \cdots, f_m(\mathbf{x}))$

The Jacobian is defined as:

$$J = \frac{\partial \mathbf{f}}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \cdots & \cdots & \cdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{pmatrix}$$

This generalizes the gradient to multi-variate functions.

Change of Variables Formula (General Case): Intuition



- We are interested in mapping a small volume between (v, u) and $(v + dv, u + du)$.
- For sufficiently small du, dv, the function can be linearized, and becomes the linear mapping specified by the Jacobian.

Change of Variables Formula (General Case)

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 1: $\mathbf{x}, \mathbf{z}$ 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, $det(A^{-1}) = det(A)^{-1}$

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

Change of Variables Formula (General Case): 2D 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 a transformation with inverse $v : \mathbb{R}^2 \to \mathbb{R}^2$.
- 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 $Z_2 = v_2(X_1, X_2)$

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

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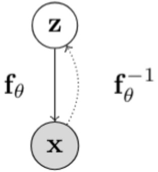
Normalizing Flow Models: Representation

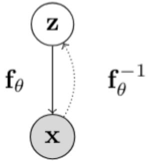
Consider a directed, latent-variable model over observed variables X and latent variables Z



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 $Z = \mathbf{f}_\theta^{-1}(X)$

Normalizing Flow Models: Learning

- 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 $Z = \mathbf{f}_\theta^{-1}(X)$



- We want to learn $p_X(\mathbf{x}; \theta)$ using the principle of maximum likelihood.
- 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 1: Unlike in VAEs, we compute the marginal likelihood exactly!
- Note 2: $\mathbf{x}, \mathbf{z}$ need to be continuous and have the same dimension.

Normalizing Flow Models: Constructing f.

We need to construct a density transformation that is:

- Invertible, so that we can apply the change of variables formula.
- Expressive, so that we can learn complex distributions.
- Computationally tractable, so that we can optimize and evaluate it.

One strategy:

- Start with a simple distribution for $\mathbf{z}_0$ (e.g., Gaussian)
- Apply sequence of M **simple** invertible transformations with $\mathbf{x} \triangleq \mathbf{z}_M$

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

- By change of variables

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

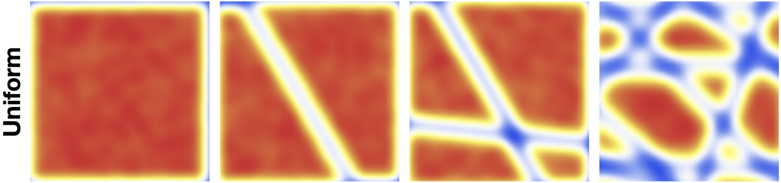
(Note: determininant of composition equals product of determinants)

Example: Planar Flows

Planar flow (Rezende and Mohamed, 2015). 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



Above, we visualize the transformation after 0, 1, 2, 10 recursive applications.

Example: Planar Flows

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

parameterized by $\theta = (\mathbf{w}, \mathbf{u}, b)$ where $h(\cdot)$ is a non-linearity

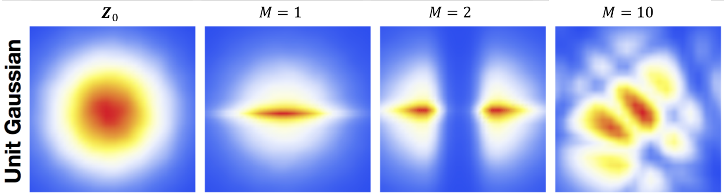
- Absolute value of the determinant of the Jacobian is given by

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

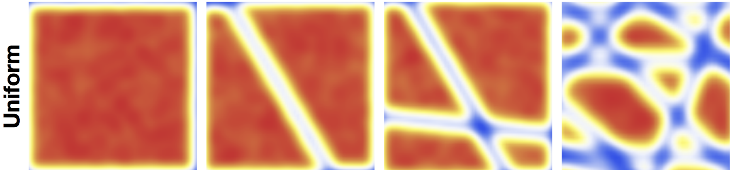
- Need to restrict parameters and non-linearity for the mapping to be invertible. For example, $h = tanh()$ and $h'(\mathbf{w}^T\mathbf{z} + b)\mathbf{u}^T\mathbf{w} \geq -1$

Example: Planar Flows

- Base distribution: Gaussian



- Base distribution: Uniform



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

Normalizing Flows: Recap

Normalizing: Change of variables gives a normalized density after applying an invertible transformation.
Flow: The function f makes the probability mass smoothly flow from a simple distribution over the space to one that is complex.

- Transformations need to be invertible, hence $\dim(X) = \dim(Z)$.
- Complex transformations can be composed from simple ones:

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

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

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

Normalizing Flows: Learning and Inference Recap

- **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!)

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

Challenges in Building Flow Models

To understand next steps, let's review the challenges posed by flow models.

- Complex, 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 $\mathbf{z}_{\geq i}$

Next lecture: Designing invertible transformations!