Deep Generative Models (Fall 2024)

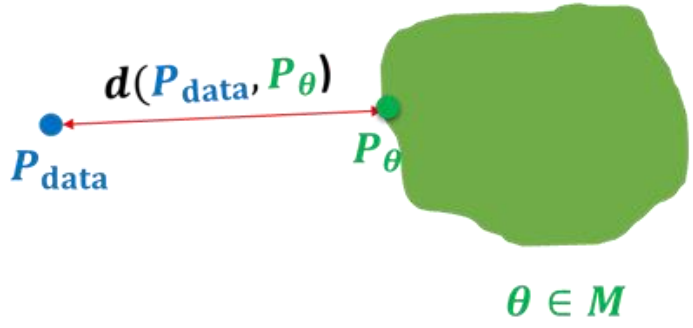
CS HUFS

Energy-Based Models

- Parameterizing probability distributions
- Energy-based model
- Applications of energy-based models
- Deep Boltzmann machines
- Learning and inference of energy-based models

Recap.

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



- Model families
  - Autoregressive Models: $p_\theta(\mathbf{x}) = \prod_{i=1}^{n} p_\theta(x_i \mid \mathbf{x}_{<i})$
  - Variational Autoencoders: $p_\theta(\mathbf{x}) = \int p(\mathbf{z})\, p_\theta(\mathbf{x} \mid \mathbf{z}) d\mathbf{z}$
  - Normalizing Flow Models: $p_\theta(\mathbf{x}) = p_z\left(\mathbf{f}_\theta^{-1}(\mathbf{x})\right)\left|\det\left(\frac{\partial \mathbf{f}_\theta^{-1}(\mathbf{x})}{\partial \mathbf{x}}\right)\right|$

Cons: Model architectures are restricted.

Recap.

$\mathbf{x}_i \sim P_{\text{data}}$
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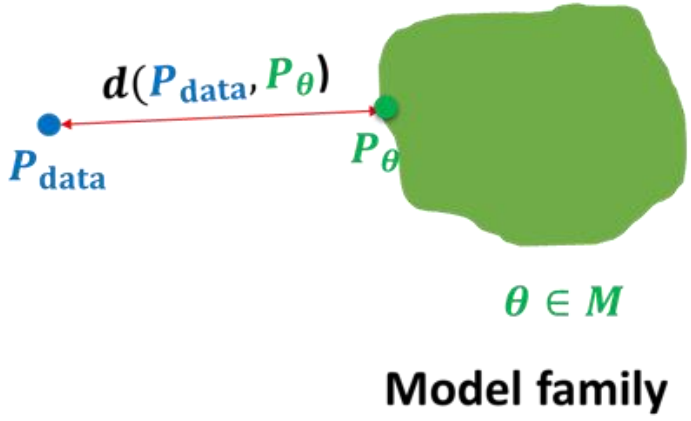
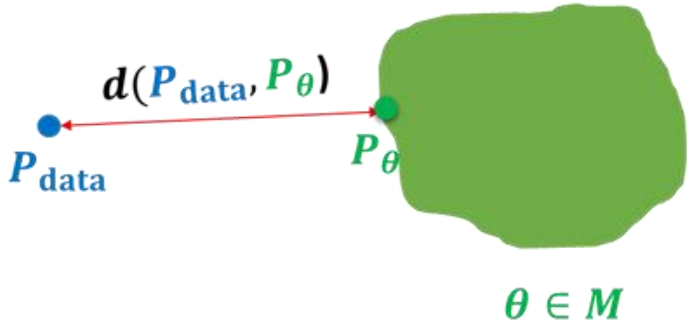


- Generative Adversarial Networks (GANs).
  - $\min_\theta \max_\phi E_{\mathbf{x}\sim p_{\text{data}}}[\log D_\phi(\mathbf{x})] + E_{\mathbf{z}\sim p(\mathbf{z})}[\log(1 - D_\phi(G_\theta(\mathbf{z})))]$.
  - Two sample tests. Can (approximately) optimize *f*-divergences (e.g. KL divergence, Jensen-Shannon divergence) or Wasserstein distance.
  - Very flexible model architectures. But likelihood is intractable, training is unstable, hard to evaluate, and has mode collapse issues.

Today's lecture

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



Energy-based models (EBMs).

- Very flexible model architectures.
- Stable training.
- Relatively high sample quality.
- Flexible composition.

Parameterizing probability distributions

Probability distributions $p(x)$ are a key building block in generative modeling.

1. non-negative: $p(x) \geq 0$
2. sum-to-one: $\sum_x p(x) = 1$ (or $\int p(x)dx = 1$ for continuous variables)

Coming up with a non-negative function $p_\theta(\mathbf{x})$ is not hard.
Given any function $f_\theta(\mathbf{x})$, we can choose

- $g_\theta(\mathbf{x}) = f_\theta(\mathbf{x})^2$
- $g_\theta(\mathbf{x}) = \exp(f_\theta(\mathbf{x}))$
- $g_\theta(\mathbf{x}) = |f_\theta(\mathbf{x})|$
- $g_\theta(\mathbf{x}) = \log(1 + \exp(f_\theta(\mathbf{x})))$
- etc.

Parameterizing probability distributions

Probability distributions $p(\mathbf{x})$ are a key building block in generative modeling.

1. non-negative: $p(\mathbf{x}) \geq 0$
2. sum-to-one: $\sum_{\mathbf{x}} p(\mathbf{x}) = 1$ (or $\int p(\mathbf{x}) d\mathbf{x} = 1$ for continuous variables)

Sum-to-one is key:

Total "volume" is fixed: increasing $p(x_{train})$ guarantees that x_{train} becomes relatively more likely (compared to the rest).

Problem:

- $g_\theta(\mathbf{x}) \geq 0$ is easy, but $g_\theta(\mathbf{x})$ might not sum-to-one.
- $\sum_{\mathbf{x}} g_\theta(\mathbf{x}) = Z(\theta) \neq 1$ in general, so $g_\theta(\mathbf{x})$ is not a valid probability mass function or density (for continuous case, $\int g_\theta(\mathbf{x}) d\mathbf{x} \neq 1$)

Parameterizing probability distributions

Problem: $g_\theta(\mathbf{x}) \geq 0$ is easy, but $g_\theta(\mathbf{x})$ might not be normalized

Solution:

$$p_\theta(\mathbf{x}) = \frac{1}{Z(\theta)} g_\theta(\mathbf{x}) = \frac{1}{\int g_\theta(\mathbf{x}) d\mathbf{x}} g_\theta(\mathbf{x}) = \frac{1}{Volume(g_\theta)} g_\theta(\mathbf{x})$$

Then by definition, $\int p_\theta(\mathbf{x}) d\mathbf{x} = \int \frac{g_\theta(\mathbf{x})}{Z(\theta)} d\mathbf{x} = \frac{Z(\theta)}{Z(\theta)} = 1$.

Example: choose $g_\theta(\mathbf{x})$ so that we know the volume *analytically* as a function of θ.

1. $g_{(\mu,\sigma)}(x) = e^{-\frac{(x-\mu)^2}{2\sigma^2}}$. **Volume** is: $\int e^{-\frac{(x-\mu)^2}{2\sigma^2}} dx = \sqrt{2\pi\sigma^2}$. $\rightarrow$ **Gaussian**
2. $g_\lambda(x) = e^{-\lambda x}$. **Volume** is: $\int_0^{+\infty} e^{-\lambda x} dx = \frac{1}{\lambda}$. $\rightarrow$ **Exponential**
3. $g_\theta(x) = h(x) \exp\{\theta \cdot T(x)\}$. **Volume** is $\exp\{A(\theta)\}$, where $A(\theta) = \log \int h(\mathbf{x}) \exp\{\theta \cdot T(\mathbf{x})\} d\mathbf{x}$. $\rightarrow$ **Exponential family**
   - Normal, Poisson, exponential, Bernoulli
   - beta, gamma, Dirichlet, Wishart, etc.

Function forms $g_\theta(\mathbf{x})$ need to allow *analytical* integration. Despite being restrictive, they are very useful as building blocks for more complex distributions.

Likelihood based learning

Problem: $g_\theta(\mathbf{x}) \geq 0$ is easy, but $g_\theta(\mathbf{x})$ might not be normalized
Solution:

$$p_\theta(\mathbf{x}) = \frac{1}{Volume(g_\theta)} g_\theta(\mathbf{x}) = \frac{1}{\int g_\theta(\mathbf{x}) d\mathbf{x}} g_\theta(\mathbf{x}) = \frac{1}{Z(\theta)} g_\theta(\mathbf{x})$$

Typically, choose $g_\theta(\mathbf{x})$ so that we know the volume *analytically*. More complex models can be obtained by combining these building blocks.

1. **Autoregressive:** Products of normalized objects $p_\theta(\mathbf{x}) p_{\theta'(\mathbf{x})}(\mathbf{y})$:

$$\int_{\mathbf{x}} \int_{\mathbf{y}} p_\theta(\mathbf{x}) p_{\theta'(\mathbf{x})}(\mathbf{y}) d\mathbf{x} d\mathbf{y} = \int_{\mathbf{x}} p_\theta(\mathbf{x}) \underbrace{\int_{\mathbf{y}} p_{\theta'(\mathbf{x})}(\mathbf{y}) d\mathbf{y}}_{=1} d\mathbf{x} = \int_{\mathbf{x}} p_\theta(\mathbf{x}) d\mathbf{x} = 1$$

2. **Latent variables:** Mixtures of normalized objects $\alpha p_\theta(\mathbf{x}) + (1-\alpha) p_{\theta'}(\mathbf{x})$:
$\int_{\mathbf{x}} \alpha p_\theta(\mathbf{x}) + (1-\alpha) p_{\theta'}(\mathbf{x}) d\mathbf{x} = \alpha + (1-\alpha) = 1$

How about using models where the "volume"/normalization constant of $g_\theta(\mathbf{x})$ is not easy to compute analytically?

Energy-based model

$$p_\theta(\mathbf{x}) = \frac{1}{\int \exp(f_\theta(\mathbf{x}))d\mathbf{x}} \exp(f_\theta(\mathbf{x})) = \frac{1}{Z(\theta)} \exp(f_\theta(\mathbf{x}))$$

The volume/normalization constant

$$Z(\theta) = \int \exp(f_\theta(\mathbf{x}))d\mathbf{x}$$

is also called the partition function. Why exponential (and not e.g. $f_\theta(\mathbf{x})^2$)?

1. Want to capture very large variations in probability. log-probability is the natural scale we want to work with. Otherwise need highly non-smooth f_θ.
2. Exponential families. Many common distributions can be written in this form.
3. These distributions arise under fairly general assumptions in statistical physics (maximum entropy, second law of thermodynamics).
   - $-f_\theta(\mathbf{x})$ is called the **energy**, hence the name.
   - Intuitively, configurations $\mathbf{x}$ with low energy (high $f_\theta(\mathbf{x})$) are more likely.

Energy-based model

$$p_\theta(\mathbf{x}) = \frac{1}{\int \exp(f_\theta(\mathbf{x}))d\mathbf{x}} \exp(f_\theta(\mathbf{x})) = \frac{1}{Z(\theta)} \exp(f_\theta(\mathbf{x}))$$

Pros:

1. extreme flexibility: can use pretty much any function $f_\theta(\mathbf{x})$ you want

Cons:

1. Sampling from $p_\theta(\mathbf{x})$ is hard
2. Evaluating and optimizing likelihood $p_\theta(\mathbf{x})$ is hard (learning is hard)
3. No feature learning (but can add latent variables)

Curse of dimensionality: The fundamental issue is that computing $Z(\theta)$ numerically (when no analytic solution is available) scales exponentially in the number of dimensions of $\mathbf{x}$.

Nevertheless, **some tasks do not require knowing** $Z(\theta)$

Applications of Energy-based models

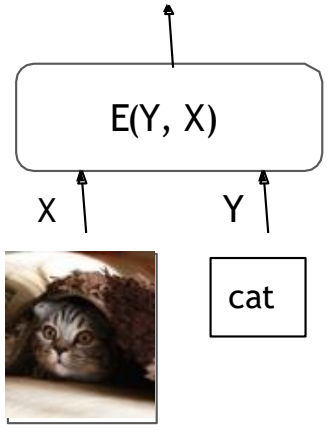
$$p_\theta(\mathbf{x}) = \frac{1}{\int \exp(f_\theta(\mathbf{x}))d\mathbf{x}} \exp(f_\theta(\mathbf{x})) = \frac{1}{Z(\theta)} \exp(f_\theta(\mathbf{x}))$$

- Given $\mathbf{x}$, $\mathbf{x}'$ evaluating $p_\theta(\mathbf{x})$ or $p_\theta(\mathbf{x}')$ requires $Z(\theta)$.
- However, their ratio

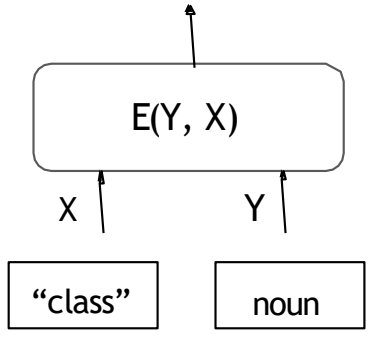
$$\frac{p_\theta(\mathbf{x})}{p_\theta(\mathbf{x}')} = \exp(f_\theta(\mathbf{x}) - f_\theta(\mathbf{x}'))$$

  does not involve $Z(\theta)$.
- This means we can easily check which one is more likely. Applications:
  1. anomaly detection
  2. denoising

Applications of Energy-based models



object recognition



sequence labeling

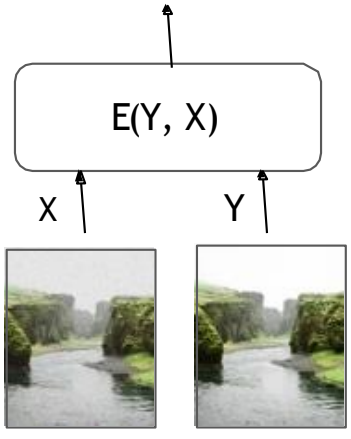
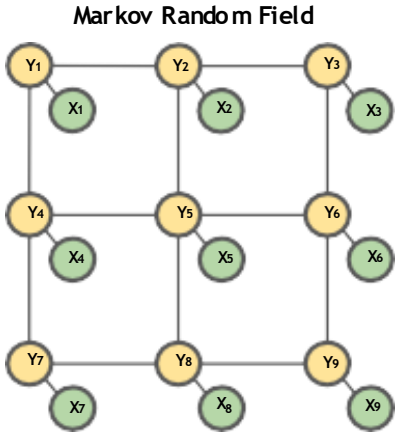


image restoration

Given a trained model, many applications require relative comparisons. Hence $Z(\theta)$ is not needed.

Example: Ising Model

- There is a true image $\mathbf{y} \in \{0,1\}^{3\times 3}$, and a corrupted image $\mathbf{x} \in \{0,1\}^{3\times 3}$. We know $\mathbf{x}$, and want to somehow recover $\mathbf{y}$.



X_i: noisy pixels
Y_i: "true" pixels

- We model the joint probability distribution $p(\mathbf{y}, \mathbf{x})$ as

$$p(\mathbf{y}, \mathbf{x}) = \frac{1}{Z} \exp\left(\sum_i \psi_i(x_i, y_i) + \sum_{(i,j)\in E} \psi_{ij}(y_i, y_j)\right)$$

  - $\psi_i(x_i, y_i)$: the i-th corrupted pixel depends on the i-th original pixel
  - $\psi_{ij}(y_i, y_j)$: neighboring pixels tend to have the same value

- How did the original image $\mathbf{y}$ look like? Solution: maximize $p(\mathbf{y}|\mathbf{x})$. Or equivalently, maximize $p(\mathbf{y}, \mathbf{x})$.

Example: Product of Experts

- Suppose you have trained several models $q_{\theta_1}(\mathbf{x})$, $r_{\theta_2}(\mathbf{x})$, $t_{\theta_3}(\mathbf{x})$. They can be different models (PixelCNN, Flow, etc.)
- Each one is like an *expert* that can be used to score how likely an input $\mathbf{x}$ is.
- Assuming the experts make their judgments indpendently, it is tempting to ensemble them as

$$p_{\theta_1}(\mathbf{x})q_{\theta_2}(\mathbf{x})r_{\theta_3}(\mathbf{x})$$

- To get a valid probability distribution, we need to normalize

$$p_{\theta_1,\theta_2,\theta_3}(\mathbf{x}) = \frac{1}{Z(\theta_1, \theta_2, \theta_3)} q_{\theta_1}(\mathbf{x})r_{\theta_2}(\mathbf{x})t_{\theta_3}(\mathbf{x})$$

- Note: similar to an AND operation (e.g., probability is zero as long as one model gives zero probability), unlike mixture models which behave more like OR

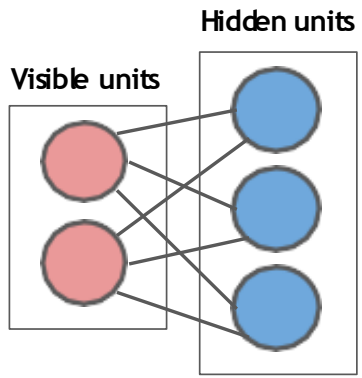
Example: Product of Experts

Image source: Du et al., 2020.

Example: Restricted Boltzmann machine (RBM)

- RBM: energy-based model with latent variables
- Two types of variables:
  1. $\mathbf{x} \in \{0,1\}^n$ are visible variables (e.g., pixel values)
  2. $\mathbf{z} \in \{0,1\}^m$ are latent ones
- The joint distribution is

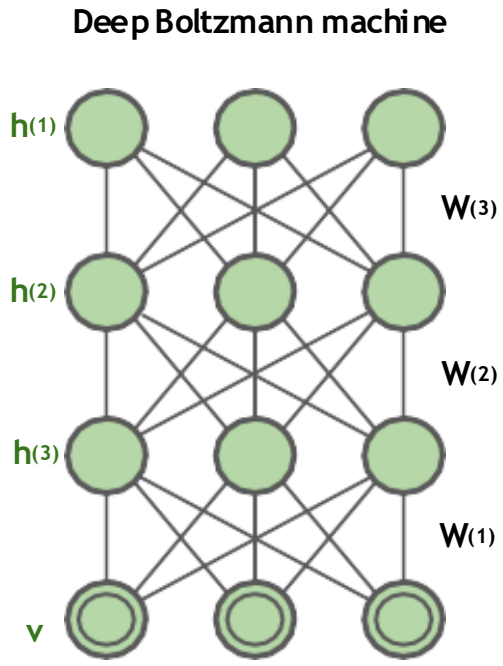
$$p_{W,b,c}(\mathbf{x},\mathbf{z}) = \frac{1}{Z}\exp\left(\mathbf{x}^T W\mathbf{z} + b\mathbf{x} + c\mathbf{z}\right) = \frac{1}{Z}\exp\left(\sum_{i=1}^{n}\sum_{j=1}^{m} x_i z_j w_{ij} + b\mathbf{x} + c\mathbf{z}\right)$$



- Restricted because there are no visible-visible and hidden-hidden connections, i.e., $x_i x_j$ or $z_i z_j$ terms in the objective

Example: Deep Boltzmann Machines

Stacked RBMs are one of the first deep generative models:



- Bottom layer variables **v** are pixel values. Layers above (**h**) represent "higher-level" features (corners, edges, etc).
- Early deep neural networks for *supervised learning* had to be pre-trained like this to make them work.

Deep Boltzmann Machines: samples

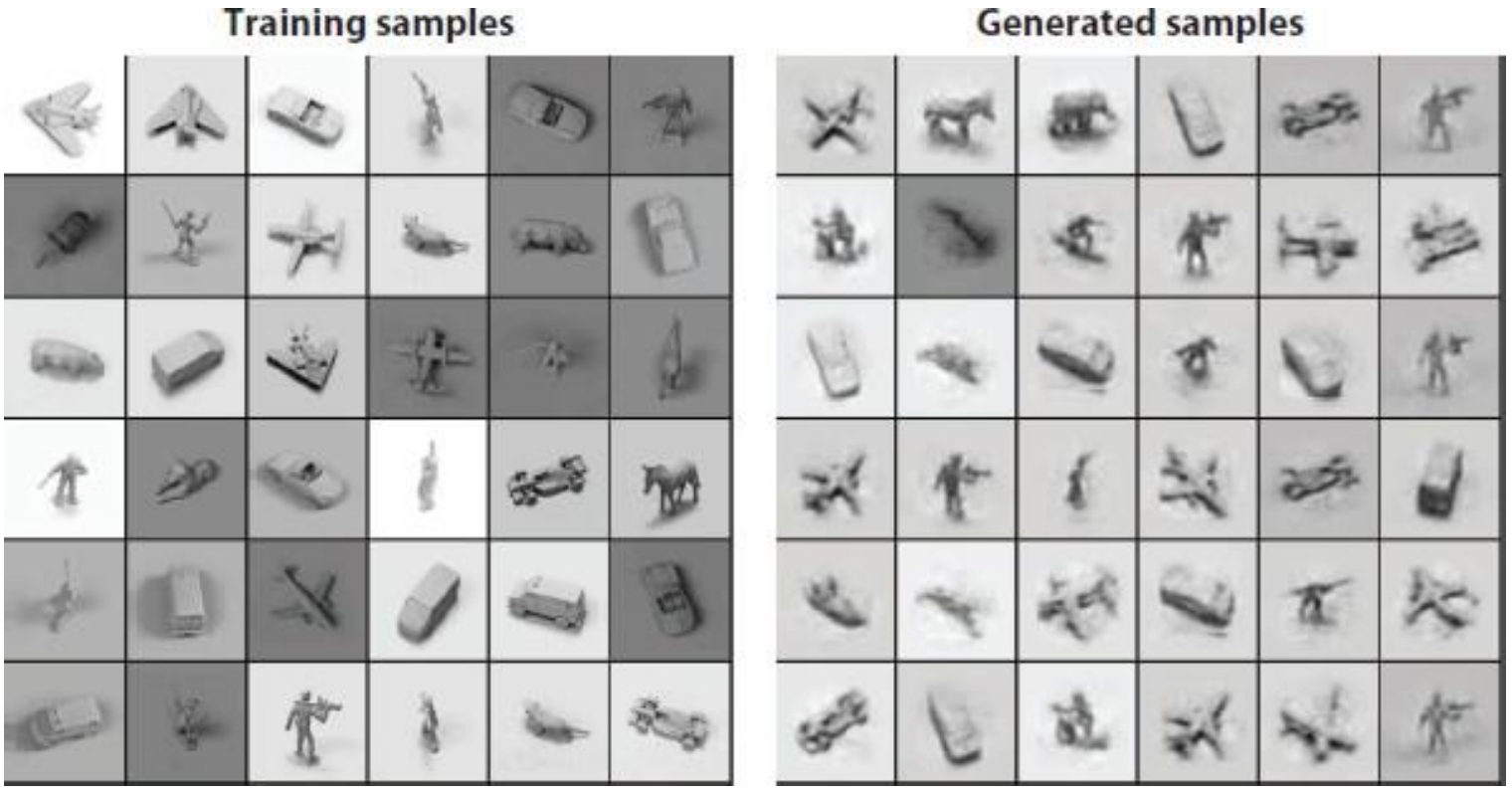


Image source: Salakhutdinov and Hinton, 2009.

Energy-based models: learning and inference

$$p_\theta(\mathbf{x}) = \frac{1}{\int \exp(f_\theta(\mathbf{x}))} \exp(f_\theta(\mathbf{x})) = \frac{1}{Z(\theta)} \exp(f_\theta(\mathbf{x}))$$

Pros:

1. can plug in pretty much any function $f_\theta(\mathbf{x})$ you want

Cons (lots of them):

1. Sampling is hard
2. Evaluating likelihood (learning) is hard
3. No feature learning

Curse of dimensionality: The fundamental issue is that computing $Z(\theta)$ numerically (when no analytic solution is available) scales exponentially in the number of dimensions of $\mathbf{x}$.

Computing the normalization constant is hard

- As an example, the RBM joint distribution is

$$p_{W,b,c}(\mathbf{x}, \mathbf{z}) = \frac{1}{Z} \exp\left(\mathbf{x}^T W \mathbf{z} + b\mathbf{x} + c\mathbf{z} \right)$$

where

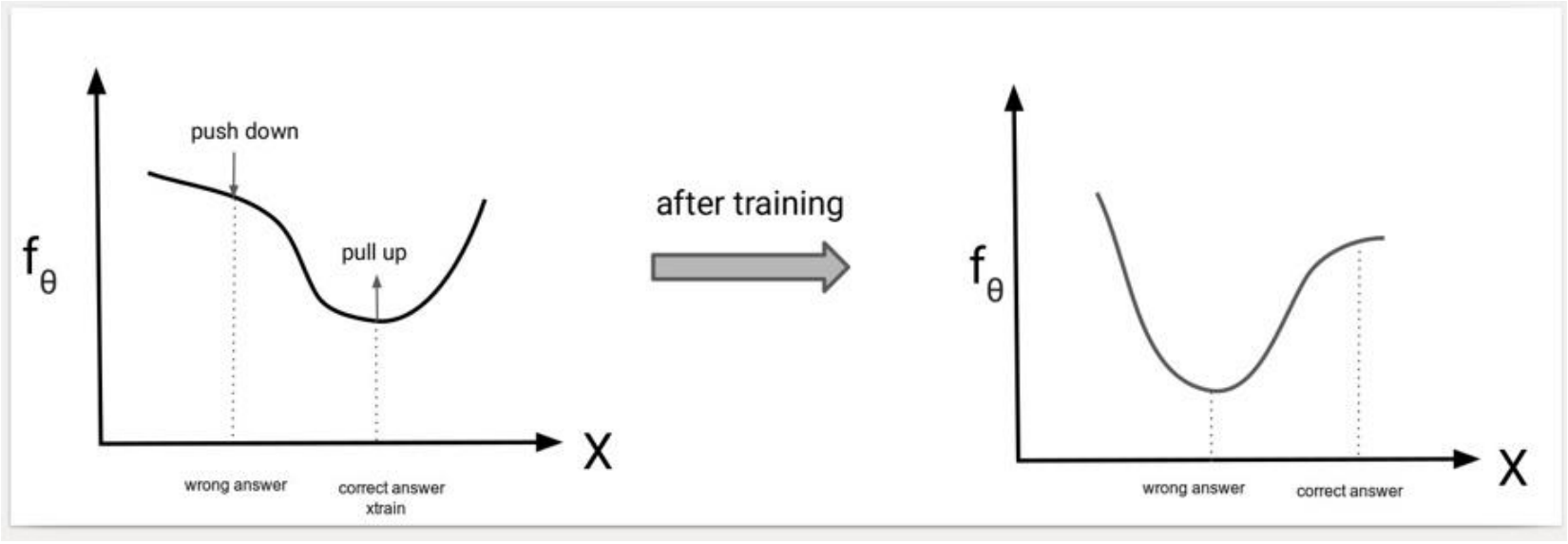
1. $\mathbf{x} \in \{0,1\}^n$ are visible variables (e.g., pixel values)
2. $\mathbf{z} \in \{0,1\}^m$ are latent ones

- The normalization constant (the "volume") is

$$Z(W, b, c) = \sum_{\mathbf{x} \in \{0,1\}^n} \sum_{\mathbf{z} \in \{0,1\}^m} \exp\left(\mathbf{x}^T W \mathbf{z} + b\mathbf{x} + c\mathbf{z} \right)$$

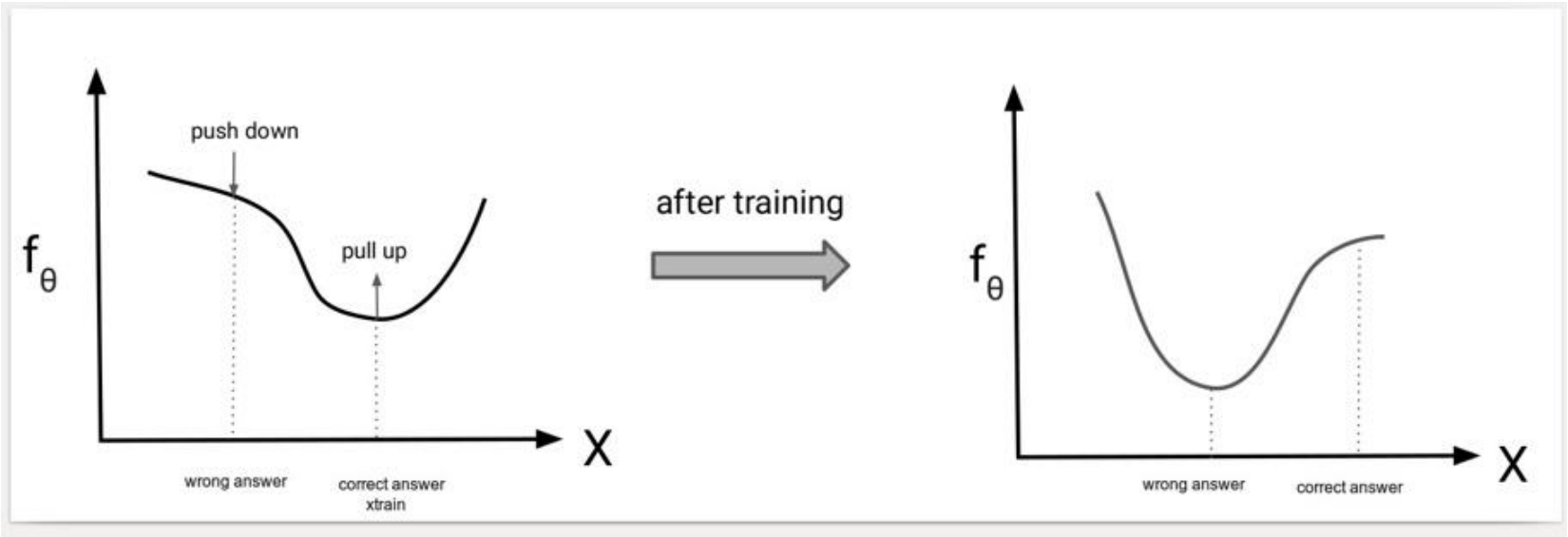
- **Note:** it is a well defined function of the parameters W, b, c, but no simple closed-form. Takes time exponential in n, m to compute. This means that *evaluating* the objective function $p_{W,b,c}(\mathbf{x}, \mathbf{z})$ for likelihood-based learning is hard.
- **Observation:** Optimizing the likelihood $p_{W,b,c}(\mathbf{x}, \mathbf{z})$ is difficult, but optimizing the un-normalized probability $\exp\left(\mathbf{x}^T W \mathbf{z} + b\mathbf{x} + c\mathbf{z} \right)$ (w.r.t. trainable parameters W, b, c) is easy.

Training intuition



- Goal: maximize $\frac{\exp\{f_\theta(\mathbf{x}_{train})\}}{Z(\theta)}$. Increase numerator, decrease denominator.
- **Intuition**: because the model is not normalized, increasing the un-normalized log-probability $f_\theta(\mathbf{x}_{train})$ by changing θ does **not** guarantee that $\mathbf{x}_{train}$ becomes relatively more likely (compared to the rest).
- We also need to take into account the effect on other "wrong points" and try to "push them down" to *also* make $Z(\theta)$ small.

Contrastive Divergence



- Goal: maximize $\frac{\exp\{f_\theta(x_{train})\}}{Z(\theta)}$
- **Idea**: Instead of evaluating $Z(\theta)$ exactly, use a Monte Carlo estimate.
- **Contrastive divergence algorithm**: sample $x_{sample} \sim p_\theta$, take step on $\nabla_\theta(f_\theta(x_{train}) - f_\theta(x_{sample}))$. Make training data more likely than typical sample from the model.

Contrastive Divergence

- Maximize log-likelihood: $\max_\theta f_\theta(x_{train}) - \log Z(\theta)$.
- Gradient of log-likelihood:

$$
\begin{aligned}
& \nabla_\theta f_\theta(x_{train}) - \nabla_\theta \log Z(\theta) \\
= \quad & \nabla_\theta f_\theta(x_{train}) - \frac{\nabla_\theta Z(\theta)}{Z(\theta)} \\
= \quad & \nabla_\theta f_\theta(x_{train}) - \frac{1}{Z(\theta)} \int \nabla_\theta \exp\{f_\theta(x)\} dx \\
= \quad & \nabla_\theta f_\theta(x_{train}) - \frac{1}{Z(\theta)} \int \exp\{f_\theta(x)\} \nabla_\theta f_\theta(x) dx \\
= \quad & \nabla_\theta f_\theta(x_{train}) - \int \frac{\exp\{f_\theta(x)\}}{Z(\theta)} \nabla_\theta f_\theta(x) dx \\
= \quad & \nabla_\theta f_\theta(x_{train}) - E_{x_{sample}}[\nabla_\theta f_\theta(x_{sample})] \\
\approx \quad & \nabla_\theta f_\theta(x_{train}) - \nabla_\theta f_\theta(x_{sample}),
\end{aligned}
$$

  where $x_{sample} \sim \exp\{f_\theta(x_{sample})\}/Z(\theta)$.
- How to sample?

Sampling from energy-based models

$$p_\theta(\mathbf{x}) = \frac{1}{\int \exp(f_\theta(\mathbf{x}))} \exp(f_\theta(\mathbf{x})) = \frac{1}{Z(\theta)} \exp(f_\theta(\mathbf{x}))$$

- No direct way to sample like in autoregressive or flow models. Main issue: cannot easily compute how likely each possible sample is
- However, we can easily compare two samples $\mathbf{x}, \mathbf{x}'$.
- Use an iterative approach called Markov Chain Monte Carlo (MCMC):
  1. Initialize x^0 randomly, $t = 0$
  2. Let $x' = x^t + \text{noise}$
     1. If $f_\theta(x') > f_\theta(x^t)$, let $x^{t+1} = x'$
     2. Else let $x^{t+1} = x'$ with probability $\exp(f_\theta(x') - f_\theta(x^t))$
  3. Go to step (on the next page)
- Works in theory, but can take a very long time to converge

Sampling from energy-based models

- For any continuous distribution $p_\theta(\mathbf{x})$, suppose we can compute its gradient (the **score function**) $\nabla_{\mathbf{x}} \log p_\theta(\mathbf{x})$.
- Let $\pi(\mathbf{x})$ be a prior distribution that is easy to sample from.
- Langevin MCMC.
  - $\mathbf{x}^0 \sim \pi(\mathbf{x})$
  - Repeat $\mathbf{x}^{t+1} \sim \mathbf{x}^t + \epsilon \nabla_{\mathbf{x}} \log p_\theta(\mathbf{x}^t) + \sqrt{2\epsilon}\, \mathbf{z}^t$ for $t = 0, 1, 2, \cdots, T-1$, where $\mathbf{z}^t \sim N(0, I)$.
  - If $\epsilon \to 0$ and $T \to \infty$, we have $\mathbf{x}^T \sim p_\theta(\mathbf{x})$.
- Note that for energy-based models, the score function is tractable

$$\nabla_{\mathbf{x}} \log p_\theta(\mathbf{x}) = \nabla_{\mathbf{x}} f_\theta(\mathbf{x}) - \underbrace{\nabla_{\mathbf{x}} \log Z(\theta)}_{=0}$$

$$= \nabla_{\mathbf{x}} f_\theta(\mathbf{x})$$

Modern energy-based models

Langevin sampling

Face samples

Image source: Nijkamp et al. 2019

Modern energy-based models

ImageNet samples

Image source: Du et al., 2019