Energy-Based Models

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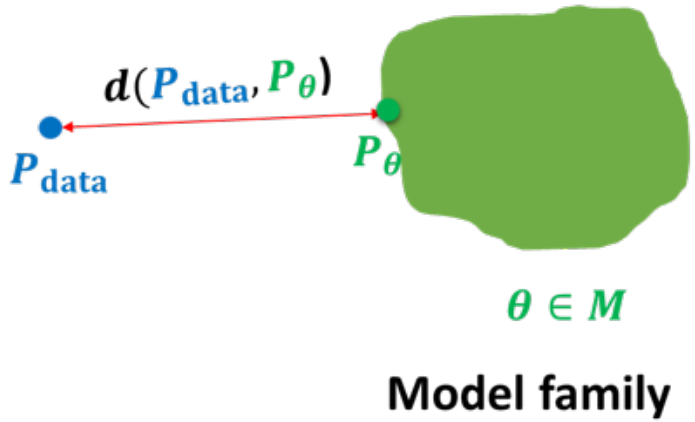
Lecture 11

Announcements

- Assignment 2 is due today
- Assignment 3 will be out today and due in two weeks
- Thank you for signing up for presentations

Summary

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



Story so far

- Representation: Latent variable vs. fully observed
- Objective function and optimization algorithm: Optimizing likelihood and its approximations (e.g., via variational inference) as well as other divergences (next few lectures)

Plan for today: Normalized vs. Energy-Based Models

Lecture Outline

1. Energy-Based Models
   - Motivation
   - Definitions
   - Exponential Families
   - Motivating Applications
2. Representation
   - Ising Models
   - Restricted Boltzmann Machines
   - Deep Boltzmann Machines
3. Learning
   - Likelihood-based learning
   - Markov Chain Monte Carlo
   - (Persistent) Contrastive Divergence

Parameterizing Probability Distributions

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

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)

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).

Parameterizing Probability Distributions

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

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)

Coming up with a non-negative function $g_\theta(\mathbf{x})$ is not hard. For example:

- $g_\theta(\mathbf{x}) = f_\theta(\mathbf{x})^2$ where f_θ is any neural network
- $g_\theta(\mathbf{x}) = \exp(f_\theta(\mathbf{x}))$ where f_θ is any neural network
- $\ldots$

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

Parameterizing Probability Distributions

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

$$p_\theta(x) = \frac{1}{Volume(g_\theta)} g_\theta(x) = \frac{1}{\int g_\theta(x)dx} g_\theta(x)$$

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

1. **Autoregressive:** Products of normalized objects $p_\theta(x)p_{\theta'(x)}(y)$:
$$\int_x \int_y p_\theta(x)p_{\theta'(x)}(y)dxdy = \int_x p_\theta(x) \underbrace{\int_y p_{\theta'(x)}(y)dy}_{=1} dx = \int_x p_\theta(x)dx = 1$$
2. **Latent variables:** Mixtures of normalized objects $\alpha p_\theta(x) + (1-\alpha)p_{\theta'}(x)$: $\int_x \alpha p_\theta(x) + (1-\alpha)p_{\theta'}(x)dx = \alpha + (1-\alpha) = 1$
3. **Flows:** Construct p via bijection from a simple distribution and track volume change.

How about using models where the "volume"/normalization constant is not easy to compute analytically?

Energy-Based Models

Energy-based models specify distributions of the form

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

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. Many common distributions ("exponential families") can be written this way.
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 Models

Energy-based models specify distributions of the form

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

Pros:

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

Cons: **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 $\mathbf{x}$.

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)

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

Applications of Energy-Based Models

Consider an energy-based model of the form:

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

Given $\mathbf{x}$, $\mathbf{x}'$ evaluating $p_\theta(\mathbf{x})$ or $p_\theta(\mathbf{x}')$ requires $Z(\theta)$. But evaluating $\frac{p_\theta(\mathbf{x})}{p_\theta(\mathbf{x}')}$ doesn't:

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

Given a trained energy-based model, many downstream applications are tractable:

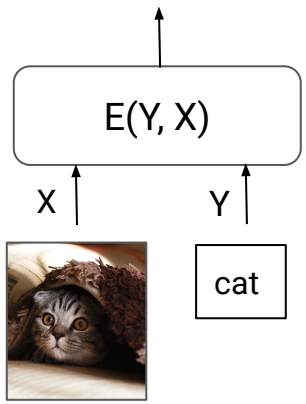
1. Anomaly detection: given new $\mathbf{x}'$, call anomaly if $\frac{p_\theta(\mathbf{x})}{p_\theta(\mathbf{x}')}$ exceeds threshold
2. Denoising & Imputation: using an optimization algorithm, find $\mathbf{x}'$ close to $\mathbf{x}$ with high $\frac{p_\theta(\mathbf{x})}{p_\theta(\mathbf{x}')}$. Also see Ising models example later.

Some applications remain intractable, most notably generation.

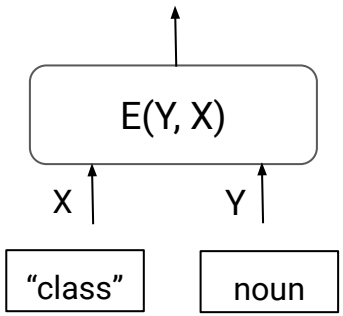
Applications of Conditional Energy-Based Models

A conditional energy model has an energy function $E(X, Y)$ over inputs X and outputs Y (categories, sentences, pixel-level predictions).

- Given a trained $E(X, Y)$, we can solve many prediction tasks without needing Z



object recognition



sequence labeling

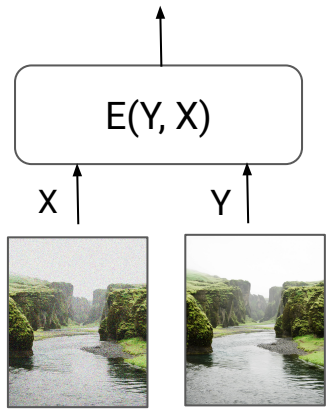


image restoration

- We can perform inference to find Y using optimization-based methods.
- There are also ways of training $E(X, Y)$ without requiring Z.
- Energy-based learning is a general framework generalizing many types of models that you know: regression, SVMs, CRFs, ranking models, etc.

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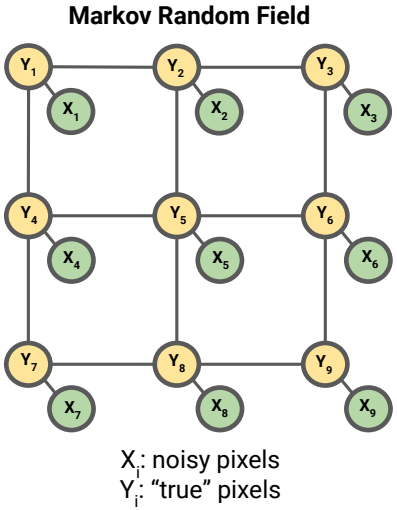
Ising Model

- 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 $\mathbf{y}$.



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

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

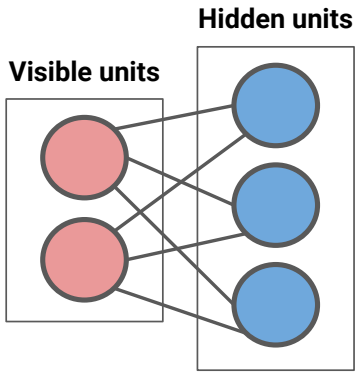
  - $\psi_i(x_i, y_i)$: the i-th corrupted pixel depends on the i-th original pixel
  - $\psi_{ij}(y_i, y_j)$: neighboring pixels tend to have the same value

- How did the original image $\mathbf{y}$ look like? Solution: maximize $p(\mathbf{y}|\mathbf{x})$. Efficient algorithms (based on graph cuts) exist.

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

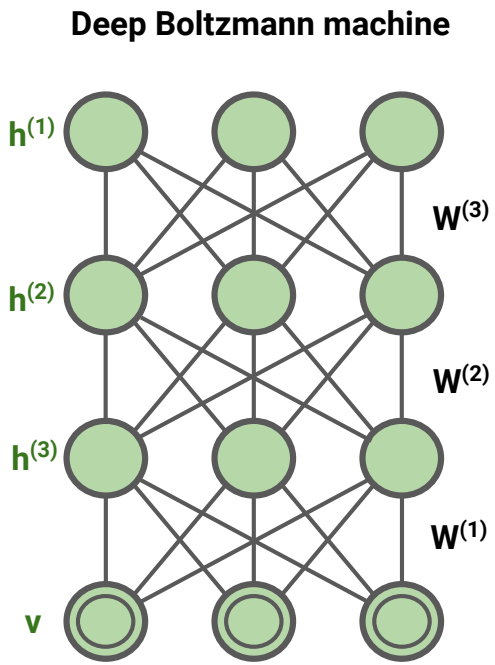
$$p_{W,b,c}(\mathbf{x},\mathbf{z}) = \frac{1}{Z}\exp\left(\mathbf{x}^T W\mathbf{z} + b\mathbf{x} + c\mathbf{z}\right) = \frac{1}{Z}\exp\left(\sum_{i=1}^{n}\sum_{j=1}^{m} x_i z_j w_{ij} + b\mathbf{x} + c\mathbf{z}\right)$$



- 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

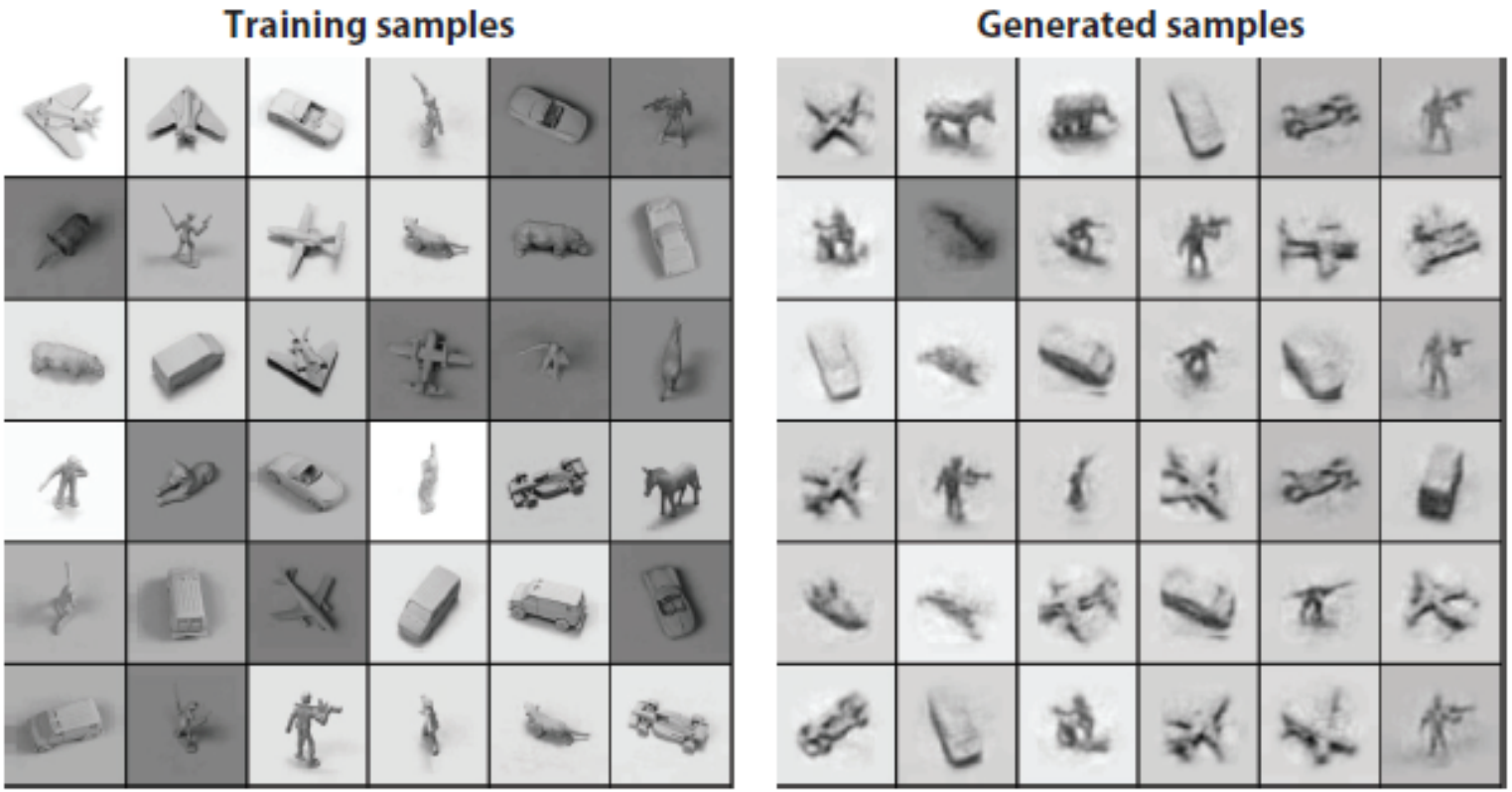
Deep Boltzmann Machines

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.

Boltzmann Machines: Samples



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Exponential Family Models

Energy-based models are closely related to *exponential family* models, such as:

$$p(x;\theta) = \frac{\exp(\theta^T f(x))}{Z(\theta)}.$$

Exponential families are

- Log-concave in their natural parameters θ. The partition function $Z(\theta)$ is also log-convex in θ.
- The vector $f(x)$ is called the vector of sufficient statistics; these "featurize" or "summarize" the data: two x's with the same $f(x)$ are equivalent.
- Maximizing the entropy $H(p)$ under the constraint $\mathbb{E}_p[f(x)] = \alpha$ (i.e. the sufficient statistics equal some value α) is an ExpFam.

Example: Gaussian: $f(x) = (x, x^2)$, $\theta = (\frac{\mu}{\sigma^2}, \frac{-1}{2\sigma^2})$. Also: Exponential, Binomial, Cauchy, Beta, Multinomial, Dirichlet, and many other distributions.

Exponential Families: Learning and Inference

Consider an exponential family model

$$p(x;\theta) = \frac{\exp(\theta^T f(x))}{Z(\theta)}.$$

Given a dataset D, we want to estimate θ via maximum likelihood. The log-likelihood is concave and equals.

$$\frac{1}{|D|}\log p(D;\theta) = \frac{1}{|D|}\sum_{x\in D}\theta^T f(x) - \log Z(\theta).$$

The first term is linear in θ and is easy to handle. The second term equals

$$\log Z(\theta) = \log \sum_x \exp(\theta^T f(x)).$$

Unlike the first term, this one does not decompose across x. It is not only hard optimize, but it is hard to even evaluate that term.

Exponential Families: Gradient-Based Learning

$$\frac{1}{|D|}\log p(D;\theta) = \frac{1}{|D|}\sum_{x\in D}\theta^T f(x) - \log Z(\theta).$$

Obtaining the gradient of the linear part is obviously easy. However,

$$\begin{aligned}
\nabla_\theta \log Z(\theta) &= \nabla_\theta \log \sum_x \exp(\theta^T f(x)) \\
&= \frac{1}{\sum_x \exp(\theta^T f(x))} \nabla_\theta \sum_x \exp(\theta^T f(x)) \\
&= \frac{1}{\sum_x \exp(\theta^T f(x))} \sum_x \exp(\theta^T f(x)) \cdot \nabla_\theta \theta^T f(x) \\
&= \frac{1}{\sum_x \exp(\theta^T f(x))} \sum_x \exp(\theta^T f(x)) \cdot f(x) \\
&= \mathbb{E}_{x\sim p}[f(x)].
\end{aligned}$$

Computing the expectation requires inference with respect to p. Inference in general is intractable, and therefore so is computing the gradient.

Exponential Families: Moment Matching

The log-likelihood is

$$\frac{1}{|D|}\log p(D;\theta) = \frac{1}{|D|}\sum_{x\in D}\theta^T f(x) - \log Z(\theta).$$

Taking the gradient, and using our expression for the gradient of the partition function, we obtain the expression

$$\nabla_\theta \frac{1}{|D|}\log p(D;\theta) = \frac{1}{|D|}\sum_{x\in D} f(x) - \mathbb{E}_{x\sim p}[f(x)]$$

This is the difference between the expectations of the natural parameters under the empirical (i.e. data) and the model distribution.

If f is also a function of θ, we can apply the rules of calculus to calculate the gradient, but it will have a similar form to the one above.

Approximate Learning Techniques in ExpFams

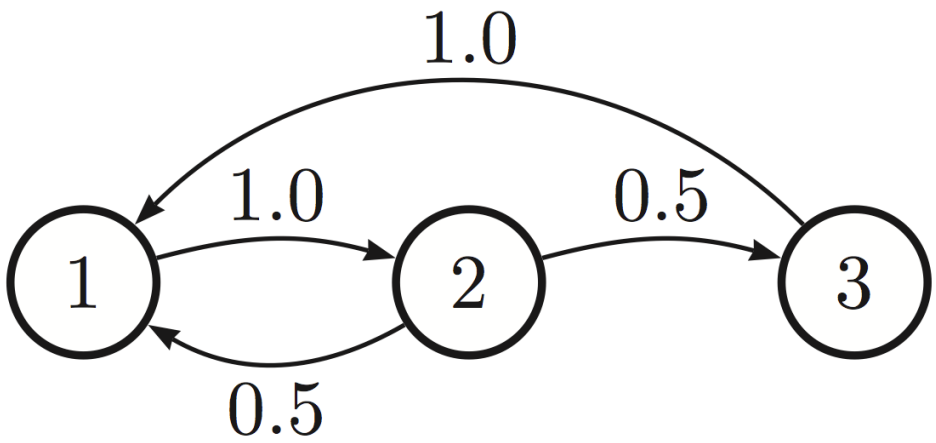
To compute gradients, we need to sample from the model. But this is hard!

We will look at two approximate methods:

1. **MCMC sampling** from the distribution at each step of gradient descent; we then approximate the gradient using Monte-Carlo.
2. **(Persistent) contrastive divergence**, a variant of MCMC sampling which re-uses the same Markov Chain between iterations.

Markov Chains: Definition

- A (discrete-time) Markov chain is a sequence of random variables $S_0, S_1, S_2, ...$ with $S_i \in \{1, 2, ..., d\}$, intuitively representing the state of a system.
- The initial state is distributed according to a probability $P(S_0)$
- All subsequent states are generated from $P(S_i \mid S_{i-1})$ that depends only on the previous random state.



Markov assumption: the probability $P(S_i \mid S_{i-1})$ is the same at every step i. The transition probabilities in the entire process depend only on the given state and not on how we got there.

Markov Chains: Stationary Distribution

If the initial state S_0 is drawn from a vector probabilities p_0, we may represent the probability p_t of ending up in each state after t steps as

$$p_t = T^t p_0 \qquad T \in \mathbb{R}^{d \times d} \text{ and } T_{ij} = P(S_{\text{new}} = i \mid S_{\text{prev}} = j).$$

The limit $\pi = \lim_{t \to \infty} p_t$ (when it exists) is called a stationary distribution of the Markov chain. It's an eigenvector of T.

A sufficent condition for π to exist is called detailed balance:

$$\pi(x')T(x \mid x') = \pi(x)T(x' \mid x) \text{ for all } x, x'$$

It is easy to show that such a π must form a stationary distribution. Just sum both sides of the equation over x and simplify:

$$\pi(x') = \sum_x \pi(x)T(x' \mid x) \text{ for all } x \text{ means } \pi \text{ is eigenvector of } T$$

Markov Chain Monte Carlo

The idea of MCMC will be to construct a Markov chain whose states will be joint assignments x to the variables in the model and whose stationary distribution will equal the model probability

$$p(x;\theta) = \frac{\exp(\theta^T f(x))}{Z(\theta)}.$$

An MCMC algorithm defines a transition operator T specifying a Markov chain, an initial variable assignment x_0 and performs the following steps.

1. Run the Markov chain from x_0 for B burn-in steps.
2. Run the Markov chain for N sampling steps and collect all the states that it visits.

Assuming B is sufficiently large, the latter collection of states will form samples from p. We may then use these samples for Monte Carlo integration (or in importance sampling).

Constructing MCMC Chains with Metropolis-Hastings

The MH method constructs a transition operator $T(x' \mid x)$ from two components:

- A transition kernel $Q(x' \mid x)$, specified by the user (something simple, like $x +$ noise)
- An acceptance probability for moves proposed by Q, specified by the algorithm as

$$A(x' \mid x) = \min\left(1, \frac{P(x')Q(x \mid x')}{P(x)Q(x' \mid x)}\right).$$

  - Encourages us to move towards more likely points in the distribution (e.g., consider formula for A when Q is uniform)
  - When Q suggests a move to a low-probability region, we do that a certain fraction of the time.

At each step of the Markov chain, we choose a new point x' according to Q. Then, we either accept this proposed change (with probability α), or with probability $1 - \alpha$ we remain at our current state.

Proof of Metropolis-Hastings Method

Given any Q the MH algorithm will ensure that P will be a stationary distribution of the resulting Markov Chain. More precisely, P will satisfy the detailed balance condition with respect to the MH Markov chain.

Suppose first that $A(x' \mid x) < 1$; then we can write:

$$A(x' \mid x) = \frac{P(x')Q(x \mid x')}{P(x)Q(x' \mid x)}$$
$$P(x')Q(x \mid x')A(x \mid x') = P(x)Q(x' \mid x)A(x' \mid x)$$
$$P(x')T(x \mid x') = P(x)T(x' \mid x),$$

which is simply the detailed balance condition. $T(x \mid x')$ is full transition operator of MH obtained by applying both Q and A.

If $A(x' \mid x) = 1$ and the above doesn't hold, then $\frac{P(x')Q(x|x')}{P(x)Q(x'|x)} > 1$ and $\frac{P(x)Q(x'|x)}{P(x')Q(x|x')} < 1$ and thus $A(x \mid x') < 1$ and same argument holds.

Gibbs Sampling

A special case of the Metropolis-Hastings methods is Gibbs sampling. We iterate through the variables one at a time; at each time step t, we:

1. Sample $x_i' \sim p(x_i \mid x_{-i}^t)$
2. Set $x^{t+1} = (x_1^t, ..., x_i', ..., x_n^t)$.
   - This is often easy, since we only need to condition x_i on small set of variables x_i directly depends on (its "Markov blanket").

Gibbs sampling can be seen as a special case of MH with proposal $Q(x_i', x_{-i} \mid x_i, x_{-i}) = P(x_i' \mid x_{-i})$. It is easy check that the acceptance probability simplifies to one.

(Persistent) Contrastive Divergence

(Persistent) Contrastive Divergence maximizes the log-likelihood using gradient descent and uses MCMC to take samples to compute gradients.

Starting at some θ_0, for $t = 1, 2, ..., T$:

1. Run MCMC chain to compute samples from $p(x; \theta_t)$
2. Use MCMC samples to compute gradient $\nabla \log p(\text{data}; \theta_t)$, e.g. using the formula we derived for ExpFams earlier.
3. Take a gradient step $\theta_{t+1} = \theta_t + \alpha \cdot \nabla \log p(\text{data}; \theta_t)$.

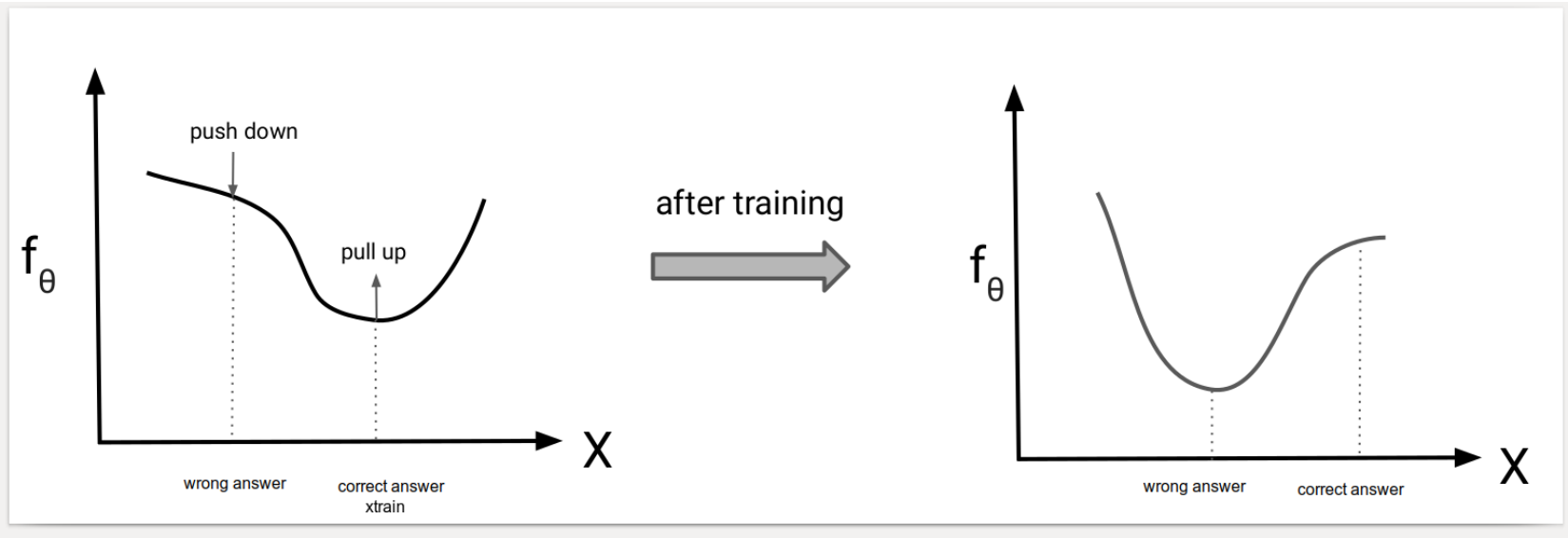
Persistent CD does not re-start MCMC chain in Step 1. Since $\theta_t \approx \theta_{t+1}$, old chain for $p(x; \theta_t)$ still produces good samples for $p(x; \theta_{t+1})$. We initialize new chain at old samples and run it for a few steps with the new θ_{t+1}.

MCMC 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 iterative approach based on Metropolis-Hastings MCMC:
  1. Initialize x^0 randomly, $t = 0$
  2. Let $x' = x^t$ + 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 2
- Works in theory, but can take a very long time to converge

Training Intuition



- Goal: maximize $\frac{f_\theta(x_{train})}{Z(\theta)}$. Increase numerator, decrease denominator.
- **Intuition**: because the model is not normalized, increasing the un-normalized probability $f_\theta(x_{train})$ by changing θ does **not** guarantees that 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.

Energy-Based Models: Pros and Cons

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

Pros:

1. Can plug in pretty much any function $f_\theta(\mathbf{x})$ you want
2. Can be combined with other model families
3. Can be combined with ideas from graphical models

Cons:

1. Sampling is hard
2. Evaluating likelihood (learning) is hard
3. Latent variable models are even harder