10417-617
Deep Learning: Fall 2020

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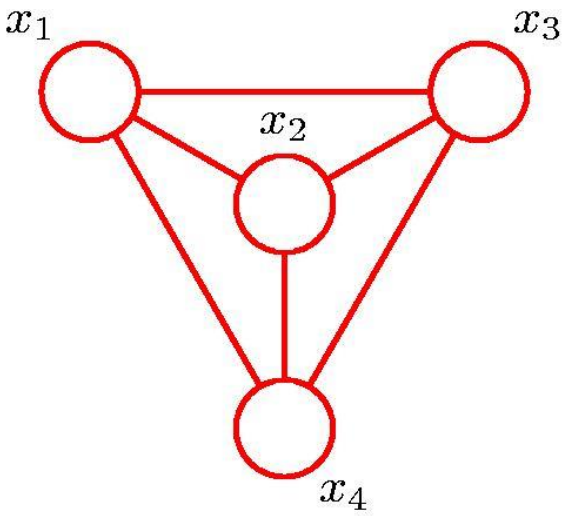
Lecture 12:
Markov Chains, applications to learning undirected models and RBMs

Graphical Models

Recall: graph contains a set of nodes connected by edges.



In a probabilistic graphical model, each node represents a random variable, links represent "probabilistic dependencies" between random variables.

Graph specifies how joint distribution over all random variables decomposes into a **product** of factors, each factor depending on a subset of the variables.

Two types of graphical models:

- **Bayesian networks**, also known as Directed Graphical Models (the links have a particular directionality indicated by the arrows)
- **Markov Random Fields**, also known as Undirected Graphical Models (the links do not carry arrows and have no directional significance).

Algorithmic pros/cons of latent-variable models (so far)

RBM's

- Hard to draw samples ✗

(In fact, #P-hard provably, even in Ising models)

- Easy to sample posterior distribution over latents ✓

Directed models

- Easy to draw samples ✓
- Hard to sample posterior distribution over latents ✗

(In fact, #P-hard even in mixtures)

Canonical tasks with graphical models

Inference

Given values for the parameters θ of the model, *sample/calculate* marginals (e.g. sample $p_\theta(x_1), p_\theta(x_4, x_5), p_\theta(z|x)$, etc.)

Learning

Find values for the parameters θ of the model, that give a *high likelihood* for the observed data. (e.g. canonical way is solving maximum likelihood optimization

$$\max_{\theta \in \Theta} \sum_{i=1}^{n} \log p(x_i)$$

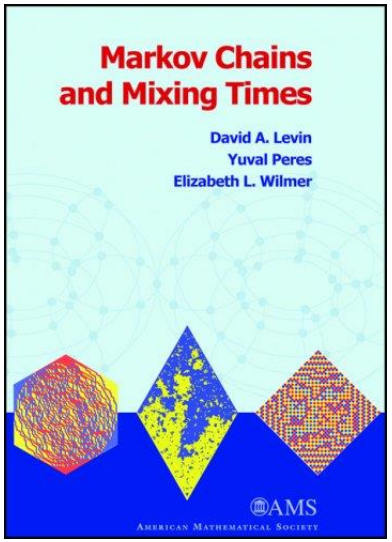
Other methods exist, e.g. method of moments (matching moments of model), but less used in deep learning practice.

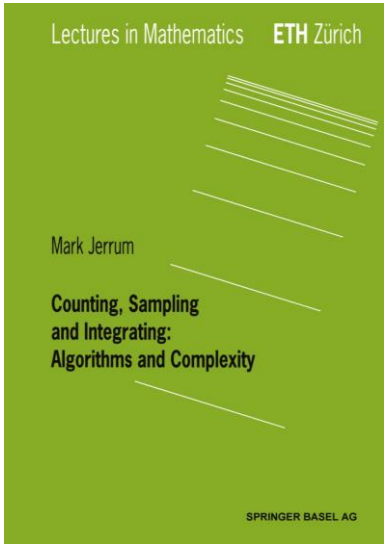
Algorithmic approaches

When faced with a difficult to calculate probabilistic quantity (partition function, difficult posterior), there are two families of approaches:

MARKOV CHAIN MONTE CARLO

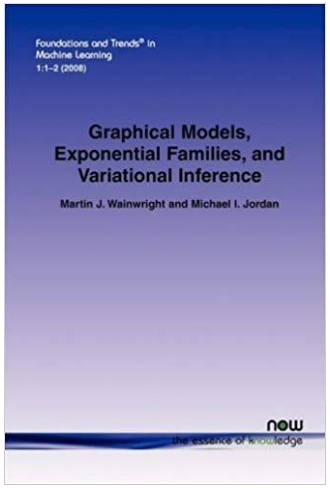
- Random walk w/ equilibrium distribution the one we are trying to sample from.





VARIATIONAL METHODS

- Based on solving an optimization problem.

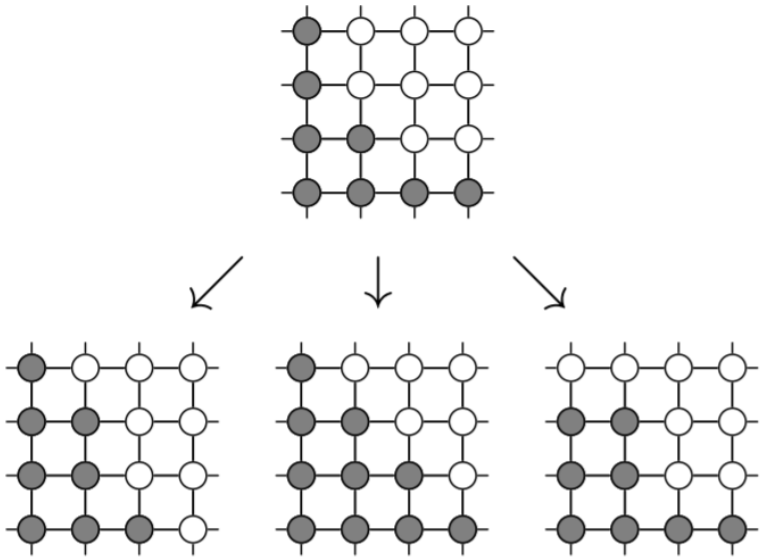


Part I: Intro to Markov Chains

Sampling via random walks

Goal: Sample from distribution given up to constant of proportionality.

Idea: explore domain via *random, local* moves



Hope: enough moves ⇒ the random process "forgets" starting point, follows the distr. we are trying to sample.

Sampling via random walks

Goal: Sample from distribution given up to constant of proportionality.

A set of random variables $(X_1, X_2, \dots, X_T)$ is **Markov** if
$\forall t: P(X_t|X_{<t}) = P(X_t|X_{t-1})$

It is homogeneous if $P(X_t|X_{t-1})$ doesn't depend on t.

We can describe a homogeneous Markov process on a discrete domain $\mathcal{X}$ by a **transition matrix** $T \in \mathbb{R}_+^{|\mathcal{X}|\times|\mathcal{X}|}: T_{ij} = P(X_{t+1} = j \,|X_t = i)$

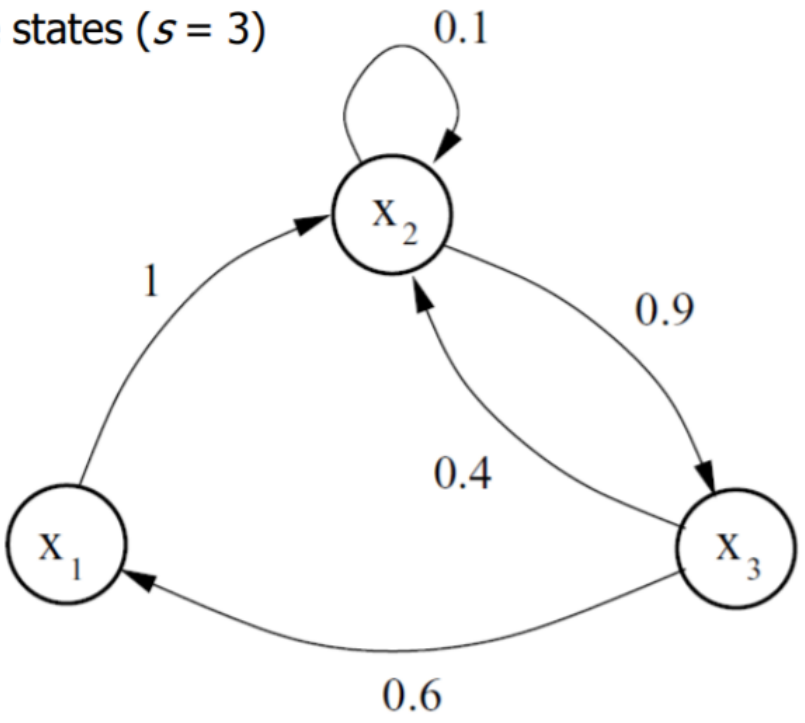
Clearly, $\forall i, \sum_j \; T_{ij} = 1$. We will also call such process a Markov Chain/ Markov random walk.

Example

Markov chain with three states ($s = 3$)

$$T = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0.1 & 0.9 \\ 0.6 & 0.4 & 0 \end{bmatrix}$$

Transition matrix



Transition graph

Stationary distribution

Stationary distribution: a distribution $\pi = (\pi_1, \dots \pi_{|\chi|})$ is stationary for a Markov walk if $\pi T = \pi$.

In other words: if we start with a sample of π and transition according to T, we end with a sample following π as well.

$$(0.22, 0.41, 0.37)\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0.1 & 0.9 \\ 0.6 & 0.4 & 0 \end{bmatrix} = (0.22, 0.41, 0.37)$$

Stationary distribution need not be unique: e.g. T is the identity matrix.

Many Markov Chains have unique stationary distributions: after taking many steps, starting with any distribution, we get to the same distribution

$$\forall p_0, \lim_{t\to\infty} p_0 T^t = \pi$$

In other words, eventually, the chain "forgets" the starting point.

Stationary distribution

Stationary distribution: a distribution $\pi = (\pi_1, \ldots \pi_{|\mathcal{X}|})$ is stationary for a Markov walk if $\pi T = \pi$.

Many Markov Chains have unique stationary distributions: after taking many steps, starting with any distribution, we get to the same distribution

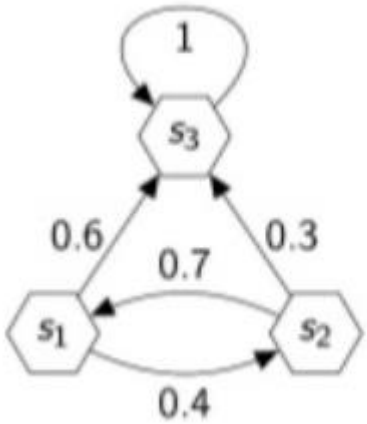
$$\forall p_0, \lim_{t \to \infty} p_0 T^t = \pi$$

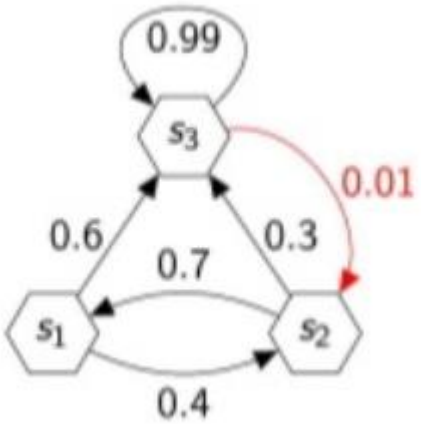
Name of the game: if we wish to sample from some π, design a Markov Chain which has π as stationary distribution.

If we run chain long enough (??), we can draw samples from something close to π

Conditions for having a unique stationary distribution

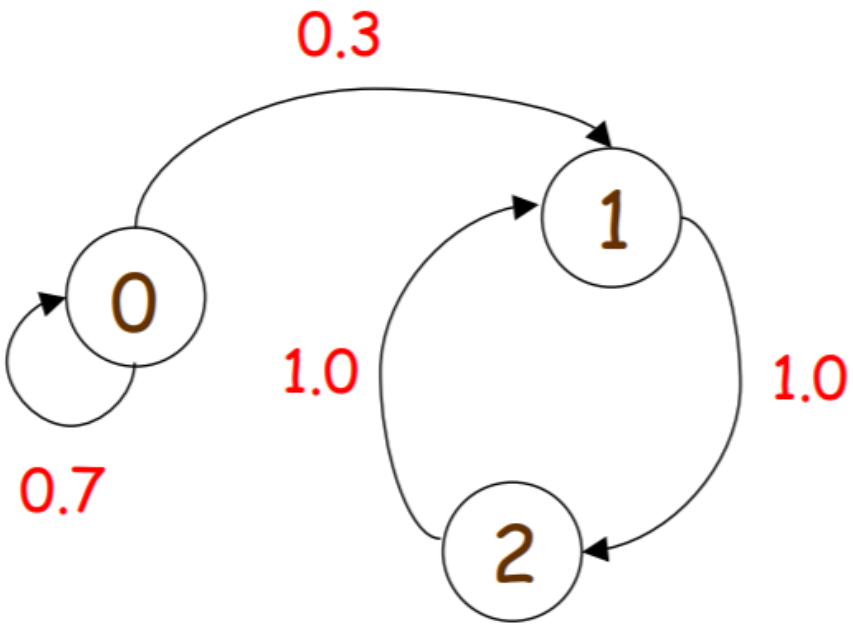
Potential problem: transition graph is not connected.





Conditions for having a unique stationary distribution

Potential problem: there are cycles in graph



Conditions for having a unique stationary distribution

These are all the possible problems!

Irreducibility: there is a path that transitions from any state to any other.
For each pairs of states (i,j), there is a positive probability, starting in state i, that the process will ever enter state j.

= Transition graph is connected;

Aperiodicity: random walk doesn't get trapped in cycles.
A state i is aperiodic if there exists n s.t., $\forall n' \geq n, P\left(X_{n'} = i \middle| X_0 = i\right) > 0$.
If all states are aperiodic, chain is called aperiodic.

Thm: for any *irreducible+aperiodic* Markov chain there is a unique π, s.t.

$$\forall p_0, \lim_{t \to \infty} p_0 T^t = \pi$$

Detailed balance

Useful sufficient condition for π to be a stationary distribution: detailed balance.

$$\pi_i T_{ij} = \pi_j T_{ji}, \forall (i,j)$$

Why?

$$\begin{aligned}(\pi T)_i = \sum_j \pi_j T_{ji} &= \textstyle\sum_j \pi_i T_{ij} \\ &= \pi_i \textstyle\sum_j T_{ij} \\ &= \pi_i\end{aligned}$$

Metropolis-Hastings

Suppose we are trying to sample from π defined over a domain of size m (think m is very large, like in Ising models), up to a constant of proportionality:

$$\pi_i = \frac{b(i)}{Z}, Z = \sum_{i=1}^{m} b(i)$$

Metropolis-Hastings: random walk assuming an "easy-to-sample from" transition kernel q(i,j), along with "corrections".

Metropolis-Hastings

Suppose we have an easy to sample from "transition kernel" q(i,j).

Consider the following random walk, for some $\alpha(i,j)$ we will pick:

$$\Pr(X_n = j \,|\, X_{n-1} = i) =$$

1., from state i go to state j with prob. $q(i,j)$

2., with prob $1-\alpha(i,j)$ go back to state i,
with prob $\alpha(i,j)$ stay in state j.

Then, we have:

$$P(X_{n+1} = j | X_n = i) = q(i,j)\alpha(i,j) \quad \forall j \neq i$$
$$P(X_{n+1} = i | X_n = i) = q(i,i) + \sum_{k \neq i} q(i,k)(1-\alpha(i,k))$$

Metropolis-Hastings

Observation

$$\pi_i P_{ij} = \pi_j P_{ji} \quad \forall j \neq i \Leftrightarrow \pi_i q(i,j)\alpha(i,j) = \pi_j q(j,i)\alpha(j,i) \quad \forall j \neq i \quad (*)$$

$$P_{ij} = P(X_{n+1} = j | X_n = i) = q(i,j)\alpha(i,j) \ \forall j \neq i$$

Claim:

$$\text{If } \alpha(i,j) = \min\left(\frac{\pi_j q(j,i)}{\pi_i q(i,j)}, 1\right) = \min\left(\frac{b(j)q(j,i)}{b(i)q(i,j)}, 1\right)$$

$$\Rightarrow (\pi_1, \ldots \pi_m) \text{ stationary distribution}$$

Note, this only depends on unnormalized distribution (b(i) values)

$$\text{If } \alpha(i,j) = \frac{\pi_j q(j,i)}{\pi_i q(i,j)} \Leftrightarrow \alpha(j,i) = 1$$

=> Detailed balance (*) holds

Gibbs sampling

Consider sampling a distribution over n variables $\boldsymbol{x} = (x_1, x_2, \dots, x_n)$, s.t. each of the conditional distributions $P(x_i|\boldsymbol{x}_{-i})$ is easy to sample. :

e.g. recall Ising models: $P_\theta(x_i = 1|\mathbf{x}_{-i}) = \dfrac{1}{1 + \exp(-\theta_i - \sum_{ij \in E} x_j \theta_{ij})}$,

A common way to do this is using **Gibbs sampling**:

Repeat:

Let current state be $\boldsymbol{x} = (x_1, x_2, \dots, x_n)$

Pick $i \in [n]$ uniformly at random.

Sample x $\sim P(X_i = x|\boldsymbol{x}_{-i})$

Update state to $\boldsymbol{y} = (x_1, x_2, \dots, x_{i-1}, x, x_{i+1}, \dots, x_n)$

Gibbs sampling

Repeat:

Let current state be $\boldsymbol{x} = (x_1, x_2, \dots, x_n)$

Pick $i \in [n]$ uniformly at random.

Sample x $\sim P(X_i = x | \boldsymbol{x}_{-i})$

Update state to $\boldsymbol{y} = (x_1, x_2, \dots, x_{i-1}, x, x_{i+1}, \dots, x_n)$

Why does it work? Metropolis-Hastings with appropriate kernel!

Let

$$
\begin{aligned}
q(\mathbf{x}, \mathbf{y}) &= q(\overbrace{(x_1, \dots, x_n)}^{\mathbf{x}}, \overbrace{(x_1, \dots, x_{i-1}, x, x_{i+1}, x_n)}^{\mathbf{y}}) \\
&\doteq \frac{1}{n} P(X_i = x | X_j = x_j, \forall j \neq i) \\
&= \frac{1}{n} \frac{P(\mathbf{y})}{P(X_j = x_j, \forall j \neq i)}
\end{aligned}
$$

Gibbs sampling

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Shouldn't we reject occasionally? **No**:

Claim:

$$\text{If } \alpha(i,j) = \min\left(\frac{\pi_j q(j,i)}{\pi_i q(i,j)},1\right) = \min\left(\frac{b(j)q(j,i)}{b(i)q(i,j)},1\right)$$

$$\Rightarrow (\pi_1,\ldots\pi_m) \text{ stationary distribution}$$

$$\frac{p(\mathbf{y})q(\mathbf{y},\mathbf{x})}{p(\mathbf{x})q(\mathbf{x},\mathbf{y})} = \frac{p(\mathbf{y})\frac{1}{n}\frac{P(\mathbf{x})}{P(Y_j=y_j,j\neq i)}}{p(\mathbf{x})\frac{1}{n}\frac{P(\mathbf{y})}{P(X_j=x_j,j\neq i)}}$$

Gibbs sampling

Why does it work? Metropolis-Hastings with appropriate kernel!

Let

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since $P(X_j = x_j, j \neq i) = P(Y_j = y_j, j \neq i)$

What governs "mixing time"

So far, we've only worried about designing chains s.t. $\forall p_0, \lim_{t\to\infty} p_0 T^t = \pi$

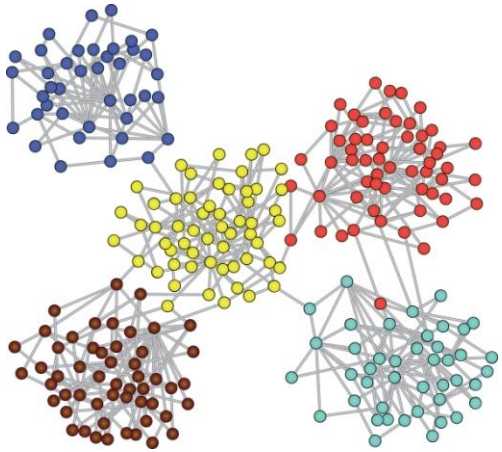
But, we're running this in practice, so want for sensible t, $\forall p_0,\ p_0 T^t \approx \pi$

(Appropriately formalized, this is called *mixing time*.)

There is no silver bullet for analyzing general transition T, but one common tool is *conductance*: which essentially says the transition graph doesn't have "bottlenecks".

The conductance of a subset S is defined as:

$$\phi(S) = \frac{\sum_{i\in S, j\notin S} T_{ij}}{\sum_{i\in S} \pi_i}$$



(e.g. how easy it is to leave S, given that we started in S)

(e.g. the colored sets have poor conductance)

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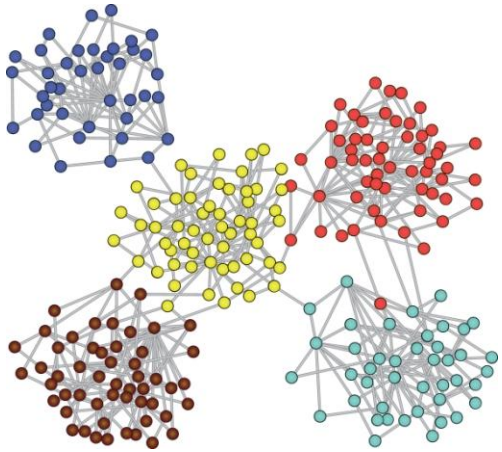

It's clear that sets of poor $\phi(S)$ impede mixing time:

If we start at S, even with the correct π, it'll take us long to leave S.

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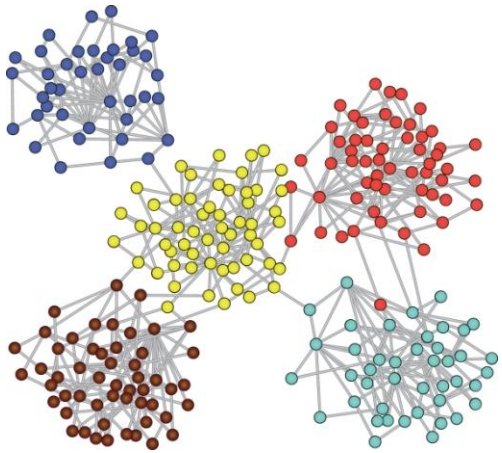

It's clear that sets of poor $\phi(S)$ impede mixing time:

The distribution is "multimodal": has S's that have large probability, but are difficult to transition between.

What governs "mixing time"

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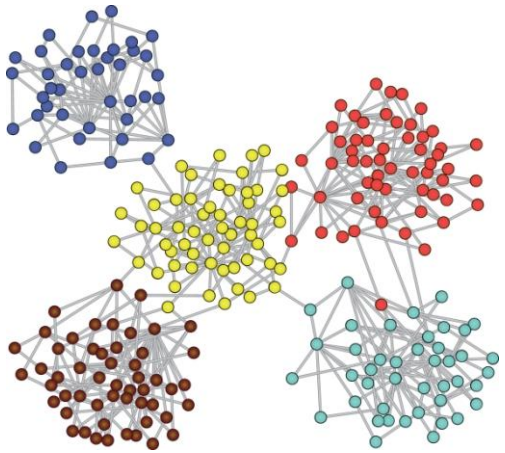

Conversely, if $\phi(S)$ is large for all S => mixing time is good!

What governs "mixing time"

So far, we've only worried about designing chains s.t. $\forall p_0, \lim_{t\to\infty} p_0 T^t = \pi$

But, we're running this in practice, so want for sensible t, $\forall p_0,\ p_0 T^t \approx \pi$

(Appropriately formalized, this is called *mixing time*.)

Note common misconception: random walk must visit each state in domain to mix.

This is of course not true! (There does however need to be a reasonable **probability** that some set of moves gets us anywhere in the domain.)

(Otherwise, what would be the point of running a Markov Chain as opposed to brute force calculation of the partition function…)

Part II: Learning Undirected Models and Restricted Boltzmann Machines (RBMs)

Warmup: learning fully observed undirected models

Goal: Learn distribution given up to constant of proportionality

$$p_\theta(x) \propto \exp(-E_\theta(x))$$

Recall our basic approach: maximum likelihood

Given data $x_1, x_2, \ldots, x_n$, solve the optimization problem

$$\max_{\theta \in \Theta} \sum_{i=1}^{n} \log p_\theta(x_i)$$

Expanding likelihoods: $\log\ p_\theta(x) = -E_\theta(x) - \log Z_\theta$

Our basic algorithm: gradient descent. Can we take gradients?

$\nabla_\theta E_\theta$ is typically easy (e.g. E_θ is an Ising model, neural network, etc.)

Warmup: learning fully observed undirected models

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Recall our basic approach: maximum likelihood

Given data $x_1, x_2, \ldots, x_n$, solve the optimization problem

$$\max_{\theta \in \Theta} \sum_{i=1}^{n} \log p_\theta(x_i)$$

$$\nabla_\theta \log Z_\theta = \frac{1}{Z_\theta} \nabla_\theta Z_\theta = \frac{1}{Z_\theta} \nabla_\theta \left(\int_x \exp\left(-E_\theta(x)\right) \right)$$

$$\frac{1}{Z_\theta} \int_x \exp\left(-E_\theta(x)\right) \nabla_\theta \left(-E_\theta(x)\right) = \mathbb{E}_{p_\theta}[-\nabla_\theta E_\theta(x)]$$

Warmup: learning fully observed undirected models

Goal: Learn distribution given up to constant of proportionality

$$p_\theta(x) \propto \exp(-E_\theta(x))$$

$$\nabla_\theta \left(\frac{1}{n} \sum_{i=1}^{n} \log p_\theta(x_i) \right) = \frac{1}{n} \left(\sum_i -\nabla_\theta E_\theta(x_i) \right) - \mathbb{E}_{p_\theta}[-\nabla_\theta E_\theta(x)]$$

$$\approx \mathbb{E}_{p_{data}}[-\nabla_\theta E_\theta(x)] - \mathbb{E}_{p_\theta}[-\nabla_\theta E_\theta(x)]$$

Goal of the algorithm: *Try to make the expectation of the energy match*

Warmup: learning fully observed undirected models

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$$p_\theta(x) \propto \exp(-E_\theta(x))$$

$$\nabla_\theta \left(\frac{1}{n} \sum_{i=1}^{n} \log p_\theta(x_i) \right) = \frac{1}{n} \left(\sum_i -\nabla_\theta E_\theta(x_i) \right) - \mathbb{E}_{p_\theta}[-\nabla_\theta E_\theta(x)]$$

$$\approx \mathbb{E}_{p_{data}}[-\nabla_\theta E_\theta(x)] - \mathbb{E}_{p_\theta}[-\nabla_\theta E_\theta(x)]$$

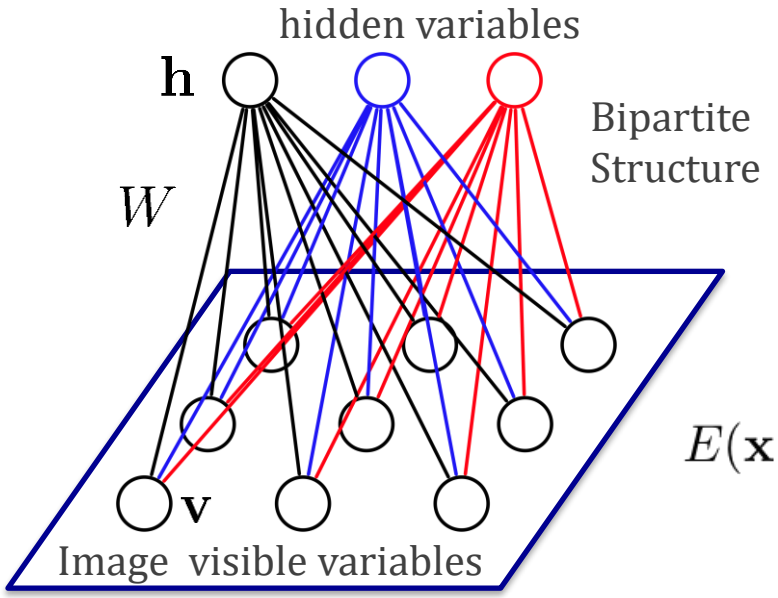
How does sampling come in: if we can sample from p_θ, and we draw samples $x_1, x_2, \ldots, x_m$ from p_θ, then:

$$\mathbb{E}_{p_\theta}[-\nabla_\theta E_\theta(x)] \approx \frac{1}{m}[-\nabla_\theta E_\theta(x_i)]$$

Restricted Boltzmann Machines

An **undirected** latent-variable model

We denote visible and hidden variables with vectors **v, h** respectively:



Visible variables $\mathbf{x} \in \{\mathbf{0}, \mathbf{1}\}^{\mathbf{D}}$
are connected to hidden variables $\mathbf{h} \in \{0, 1\}^{F}$

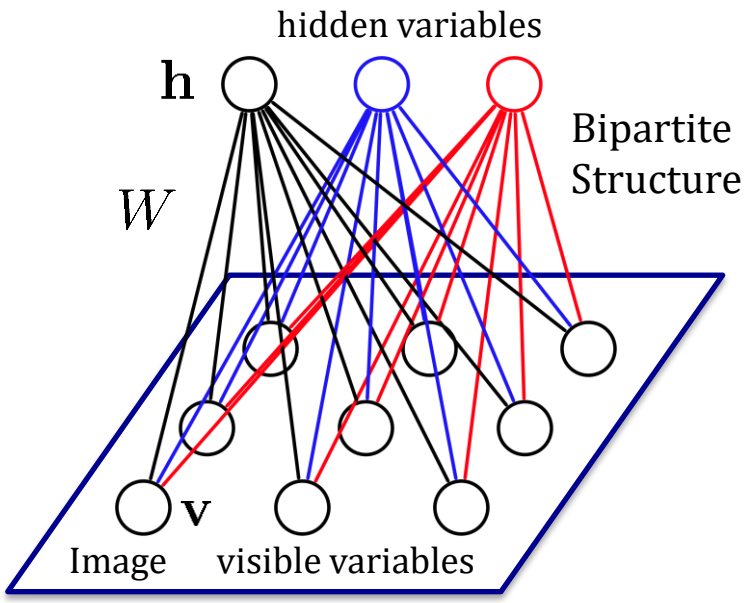
The energy of the joint configuration:

$$
\begin{aligned}
E(\mathbf{x}, \mathbf{h}) &= -\mathbf{h}^\top \mathbf{W}\mathbf{x} - \mathbf{c}^\top \mathbf{x} - \mathbf{b}^\top \mathbf{h} \\
&= -\sum_j \sum_k W_{j,k} h_j x_k - \sum_k c_k x_k - \sum_j b_j h_j
\end{aligned}
$$

Probability of the joint configuration:

$$p(\mathbf{x}, \mathbf{h}) = \exp(-E(\mathbf{x}, \mathbf{h}))/Z$$

Restricted Boltzmann Machines



The **posterior** over the hidden variables is easy to sample from!
(Conditional independence!)

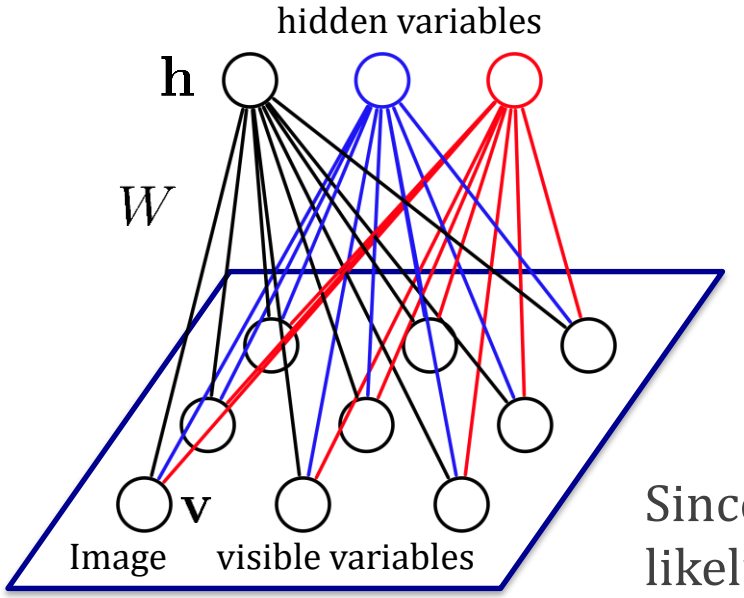
$$p(\mathbf{h}|\mathbf{x}) = \prod_j p(h_j|\mathbf{x}) \qquad p(h_j = 1|\mathbf{x}) = \frac{1}{1 + \exp(-(b_j + \mathbf{W}_j.\mathbf{x}))}$$

Factorizes

Similarly:

$$p(\mathbf{x}|\mathbf{h}) = \prod_k p(x_k|\mathbf{h}) \qquad p(x_k = 1|\mathbf{h}) = \frac{1}{1 + \exp(-(c_k + \mathbf{h}^\top \mathbf{W}_{.k}))}$$

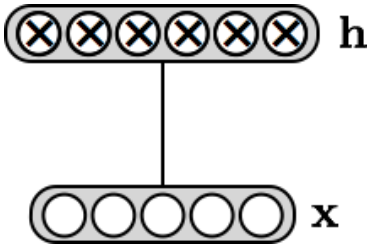
How to learn RBM's



Given data $x_1, x_2, \ldots, x_n$, solve

$$\max_{\theta \in \Theta} \sum_{i=1}^{n} \log p_\theta(x_i)$$

Since we have latent variables, we need to express the likelihood when we marginalize out the latents:



How to learn RBM's

$$p(\mathbf{x}) = \sum_{\mathbf{h} \in \{0,1\}^H} \exp(\mathbf{h}^\top \mathbf{W}\mathbf{x} + \mathbf{c}^\top \mathbf{x} + \mathbf{b}^\top \mathbf{h})/Z$$

How to learn RBM's

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\begin{aligned}
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&= \exp(\mathbf{c}^\top \mathbf{x}) \sum_{h_1\in\{0,1\}} \cdots \sum_{h_H\in\{0,1\}} \exp\left(\sum_j h_j \mathbf{W}_{j.}\mathbf{x} + b_j h_j\right)/Z
\end{aligned}
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&= \exp(\mathbf{c}^\top \mathbf{x}) \left(\sum_{h_1\in\{0,1\}} \exp(h_1 \mathbf{W}_{1.}\mathbf{x} + b_1 h_1)\right) \ldots \left(\sum_{h_H\in\{0,1\}} \exp(h_H \mathbf{W}_{H.}\mathbf{x} + b_H h_H)\right)/Z
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&= \exp(\mathbf{c}^\top \mathbf{x}) \left(1 + \exp(b_1 + \mathbf{W}_{1.}\mathbf{x})\right) \ldots \left(1 + \exp(b_H + \mathbf{W}_{H.}\mathbf{x})\right)/Z
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&= \exp(\mathbf{c}^\top \mathbf{x}) \exp(\log(1 + \exp(b_1 + \mathbf{W}_{1.}\mathbf{x}))) \ldots \exp(\log(1 + \exp(b_H + \mathbf{W}_{H.}\mathbf{x})))/Z
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&= \exp\left(\underbrace{\mathbf{c}^\top \mathbf{x} + \sum_{j=1}^{H} \log(1 + \exp(b_j + \mathbf{W}_{j.}\mathbf{x}))}_{= \mathrm{F}(\mathbf{x})}\right)/Z
\end{aligned}
$$

How to learn RBM's

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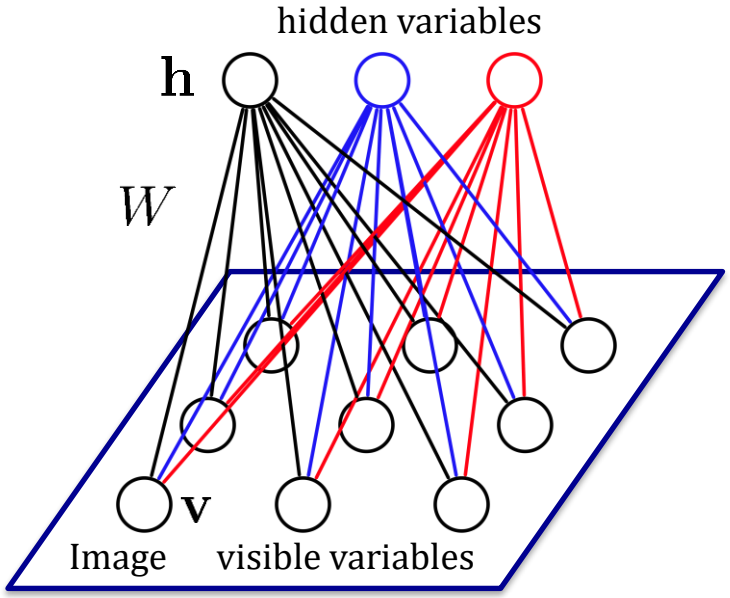
\end{aligned}
$$

$$= \exp\big(\mathrm{F}(\mathbf{x})\big)/Z$$

How to learn RBM's



Given data $x_1, x_2, \ldots, x_n$, solve

$$\max_{\theta \in \Theta} \sum_{i=1}^{n} \log p_\theta(x_i)$$

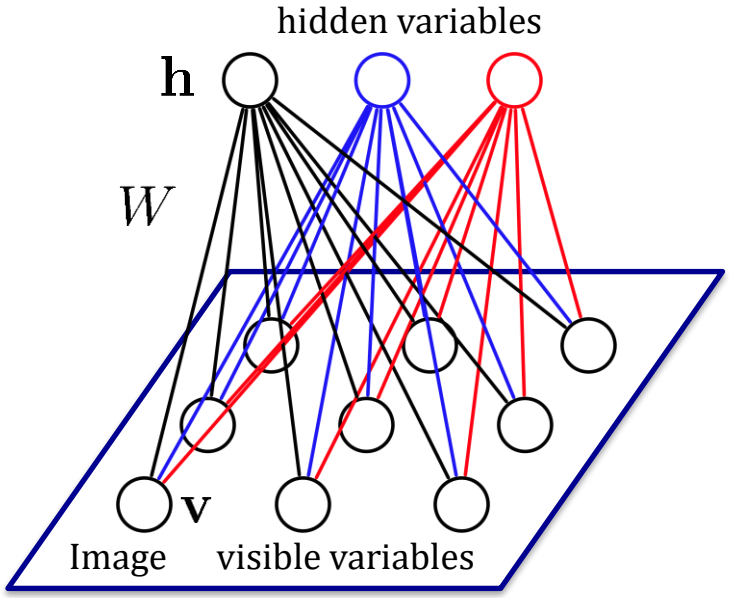
With this reduction, the undirected model calculations imply:

$$\nabla_\theta \left(\frac{1}{n} \sum_{i=1}^{n} \log p_\theta(x_i) \right) = \frac{1}{n} \left(\sum_i -\nabla_\theta F_\theta(x_i) \right) - \mathbb{E}_{p_\theta}[-\nabla_\theta F_\theta(x)]$$

$$\nabla_{\mathbf{W}_{ij}} \mathrm{F}_\theta(\mathbf{x}) = \nabla_{\mathbf{W}_{ij}} (\mathbf{c}^{\mathrm{T}}\mathbf{x} + \textstyle\sum_{j=1}^{H} \log\left(1 + \exp\left(\mathrm{b_j} + \mathbf{W_j}.\mathbf{x}\right)\right) = \frac{\exp\left(\mathrm{b_j} + \mathbf{W_j}.\mathbf{x}\right)}{1 + \exp\left(\mathrm{b_j} + \mathbf{W_j}.\mathbf{x}\right)} \mathbf{x}_\mathrm{i}$$

$$= \frac{1}{1 + \exp\left(-\left(\mathrm{b_j} + \mathbf{W_j}.\mathbf{x}\right)\right)} \mathbf{x}_\mathrm{i} = \mathrm{P}\left(\mathbf{h_j} = 1 \middle| \mathbf{x}\right) \mathbf{x}_\mathrm{i}$$

How to learn RBM's



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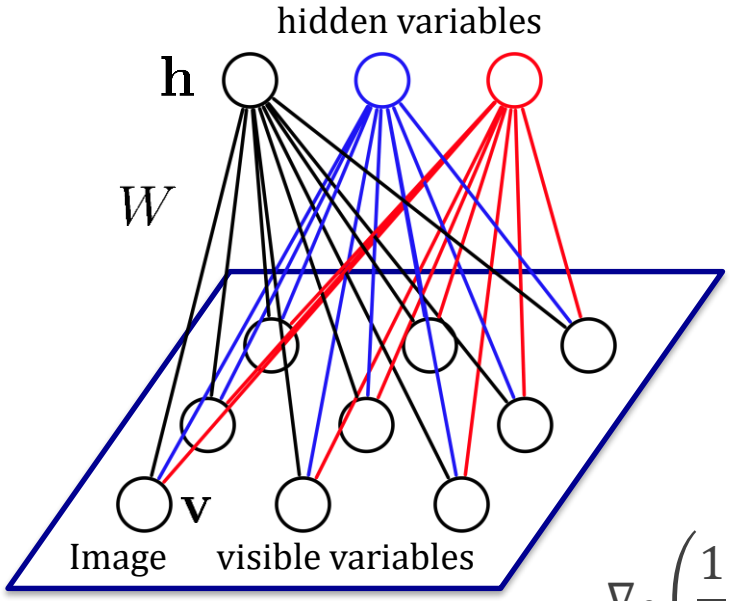
$$\nabla_{W_{ij}} F_\theta(\mathbf{x}) = P(\mathbf{h}_j = 1|\mathbf{x})\, \mathbf{x}\_i \quad \Rightarrow \quad \nabla_{\mathbf{W}} F_\theta(\mathbf{x}) = \mathbf{h}(\mathbf{x})\, \mathbf{x}^T$$

$$\nabla_{\boldsymbol{b}} F_\theta(\mathbf{x}) = \mathbf{h}(\mathbf{x})$$

$$\nabla_{\mathbf{c}} F_\theta(\mathbf{x}) = \mathbf{x}$$

$$\mathbf{h}(\mathbf{x}) \overset{\text{def}}{=} \begin{pmatrix} p(h_1 = 1|\mathbf{x}) \\ \cdots \\ p(h_H = 1|\mathbf{x}) \end{pmatrix} = \text{sigm}(\mathbf{b} + \mathbf{W}\mathbf{x})$$

How to learn RBM's



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The hard term is again: $\mathbb{E}_{p_\theta}[-\nabla_\theta E_\theta(x)]$ --- we need to draw samples from p_θ

We will draw samples using a Markov random walk: **Gibbs sampler**!

Gibbs sampling

Consider sampling a distribution over n variables $\boldsymbol{x} = (x_1, x_2, \dots, x_n)$, s.t. each of the conditional distributions $P(x_i|\boldsymbol{x}_{-i})$ is easy to sample. :

A common way to do this is using **Gibbs sampling**:

Repeat:

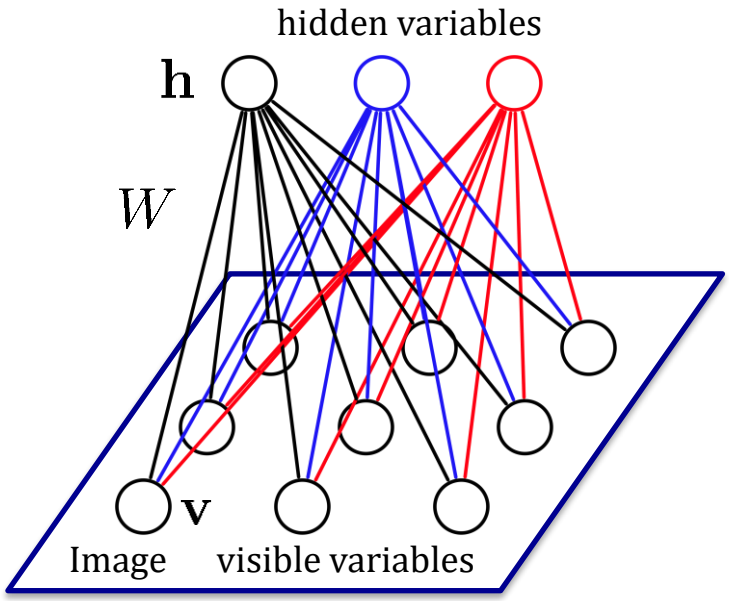
Let current state be $\boldsymbol{x} = (x_1, x_2, \dots, x_n)$

Pick $i \in [n]$ uniformly at random.

Sample x $\sim P(X_i = x|\boldsymbol{x}_{-i})$

Update state to $\boldsymbol{y} = (x_1, x_2, \dots, x_{i-1}, x, x_{i+1}, \dots, x_n)$

Gibbs sampling for RBM's

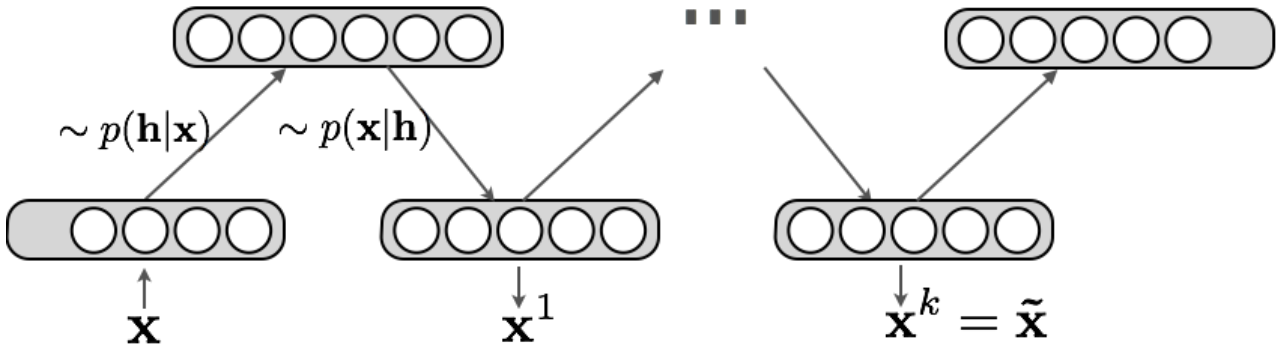


Repeat:

Sample $\mathbf{h} \sim P(\boldsymbol{h}|\boldsymbol{v})$

Sample $\mathbf{v} \sim P(\boldsymbol{v}|\boldsymbol{h})$

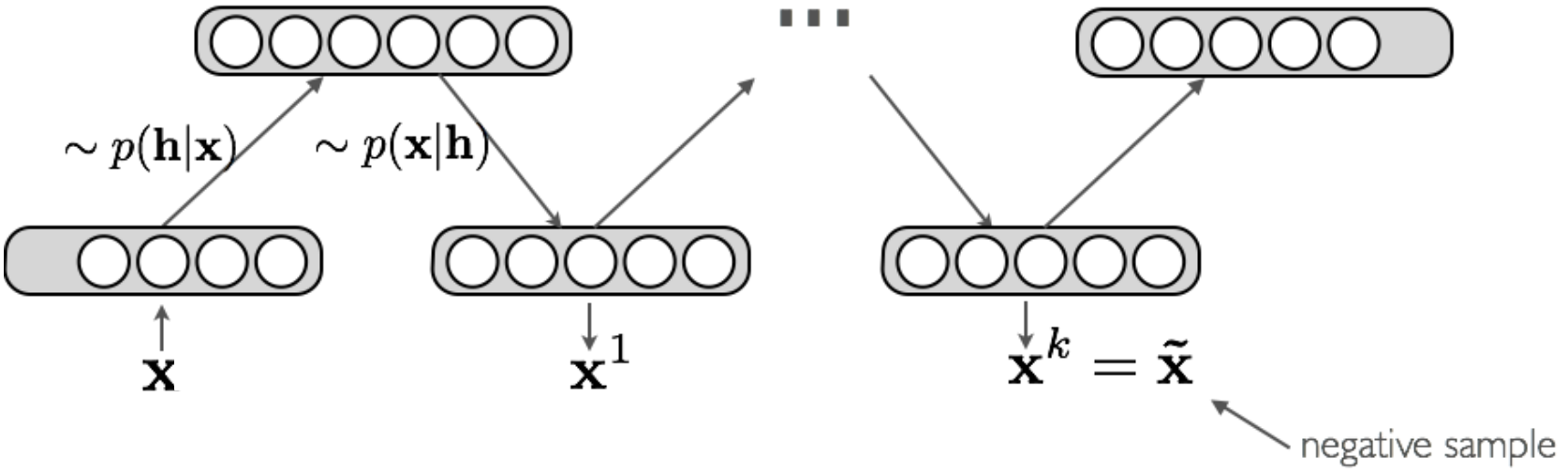
Pictorially:



Contrastive Divergence

Key idea behind Contrastive Divergence:

- Replace the expectation by a point estimate at $\tilde{\mathbf{x}}$
- Obtain the point $\tilde{\mathbf{x}}$ by Gibbs sampling
- Start sampling chain at $\mathbf{x}$



k is often taken to be just 1.

Hinton, Neural Computation, 2002

CD-k Algorithm

For each training example $\mathbf{x}$

- Generate a negative sample $\tilde{\mathbf{x}}$ using k steps of Gibbs sampling, starting at the data point $\mathbf{x}$
- Update model parameters:

$$\mathbf{W} \Longleftarrow \mathbf{W} + \alpha \left(\mathbf{h}(\mathbf{x}) \, \mathbf{x}^{\top} - \mathbf{h}(\tilde{\mathbf{x}}) \, \tilde{\mathbf{x}}^{\top} \right)$$

$$\mathbf{b} \Longleftarrow \mathbf{b} + \alpha \left(\mathbf{h}(\mathbf{x}) - \mathbf{h}(\tilde{\mathbf{x}}) \right)$$

$$\mathbf{c} \Longleftarrow \mathbf{c} + \alpha \left(\mathbf{x} - \tilde{\mathbf{x}} \right)$$

Gradients we derived before

- Go back to 1 until stopping criteria

Step size

CD-k Algorithm

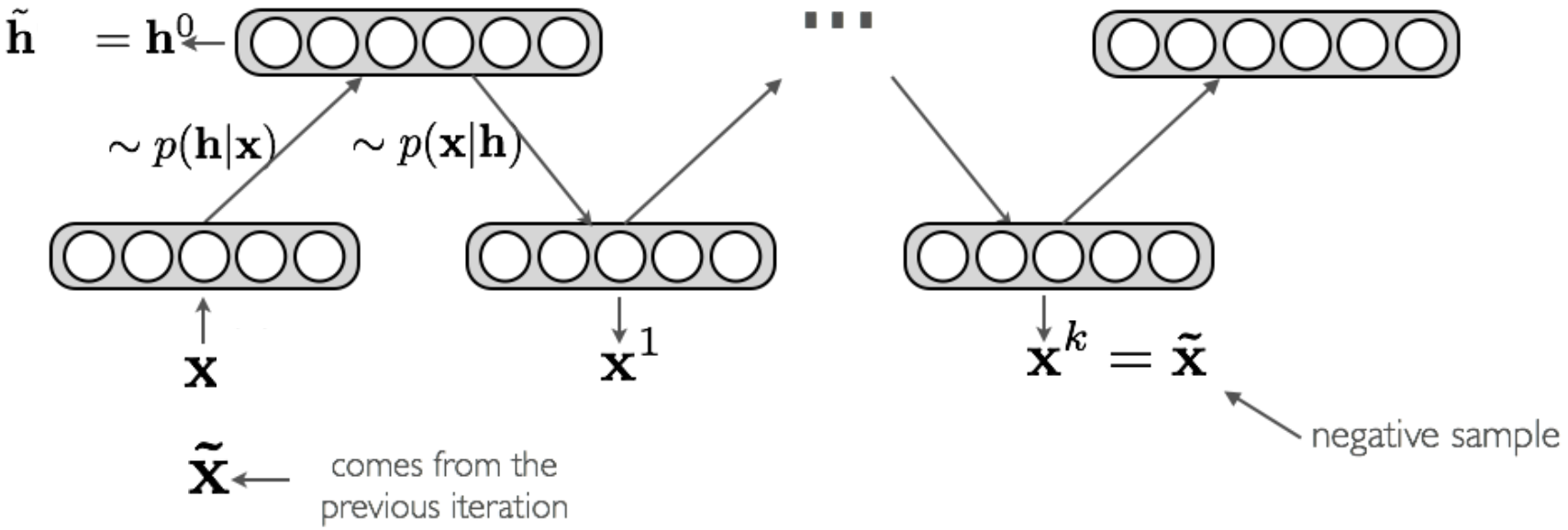
- CD-k: contrastive divergence with k iterations of Gibbs sampling

- In general, the bigger k is, the less biased the estimate of the gradient will be

- In practice, k=1 works well for learning good features and for pre-training

Persistent CD

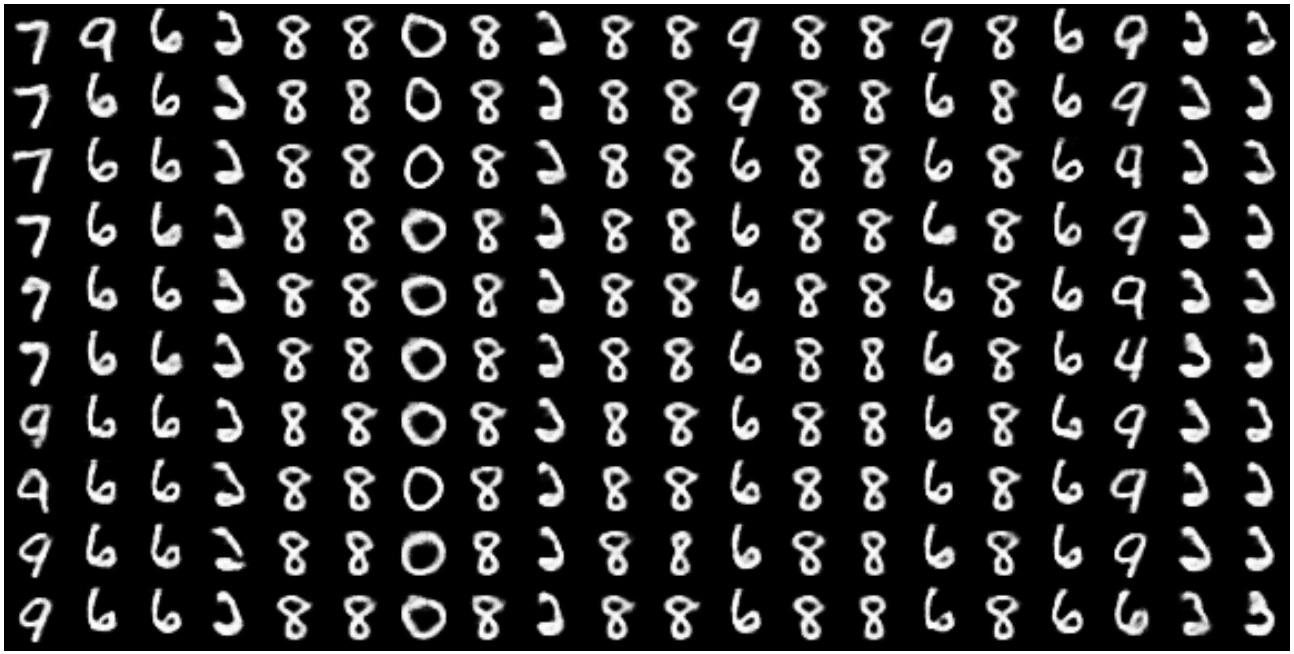
Idea: instead of initializing the chain to $\mathbf{x}$, initialize the chain to the negative sample of the last iteration



Tieleman, ICML, 2008

Example: MNIST

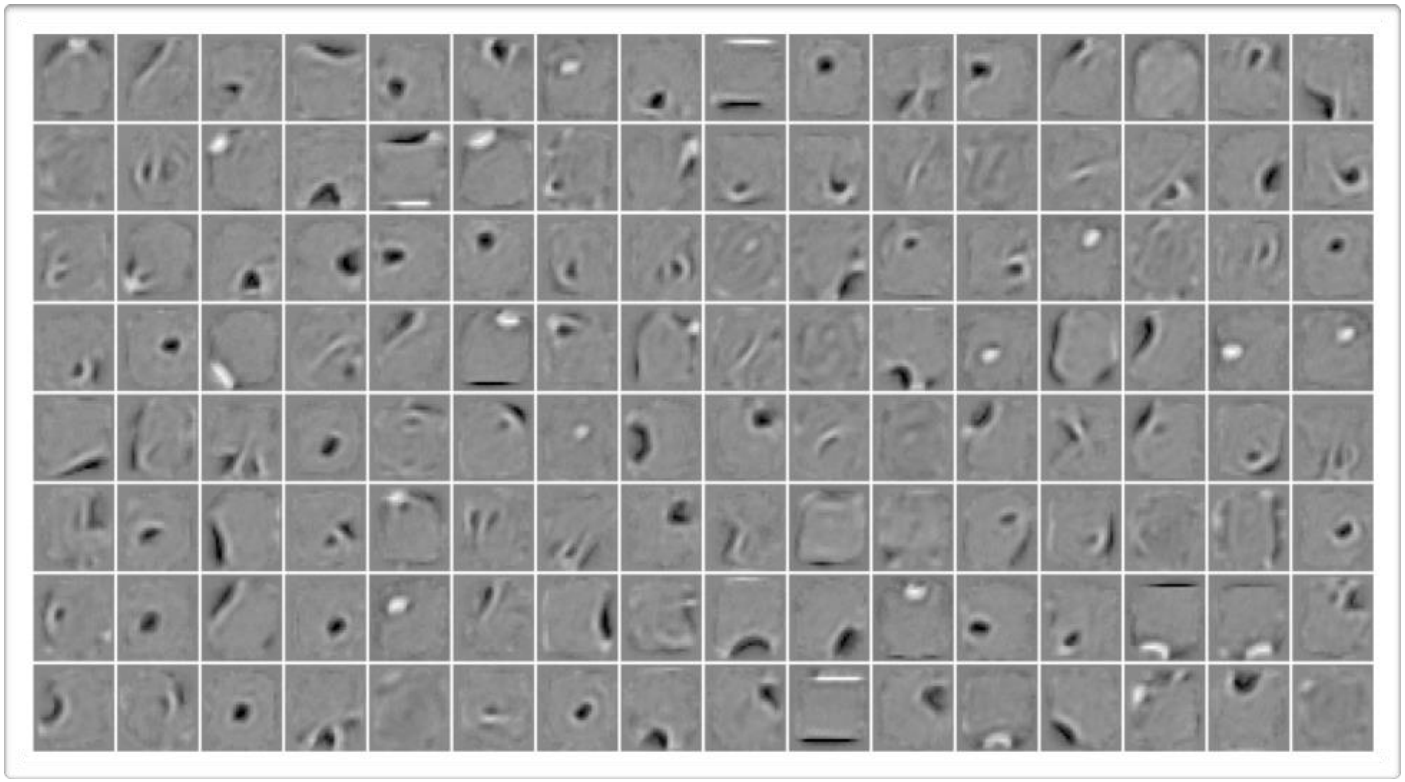
MNIST dataset:



Each row is small set of “initial points”, after which next row is gotten by running 1000 Gibbs steps.

Learned Features

MNIST dataset:



(Larochelle et al., JMLR 2009)

Tricks and Debugging

Unfortunately, it is not easy to debug training RBMs (e.g. using gradient checks)

We instead rely on approximate "tricks"

- we plot the average stochastic reconstruction $||\mathbf{x}^{(t)} - \tilde{\mathbf{x}}||^2$ and see if it tends to decrease
- for inputs that correspond to image, we visualize the connection coming into each hidden unit as if it was an image
- gives an idea of the type of visual feature each hidden unit detects
- we can also try to approximate the partition function Z and see whether the (approximated) NLL decreases

(Salakhutdinov, Murray, ICML 2008)