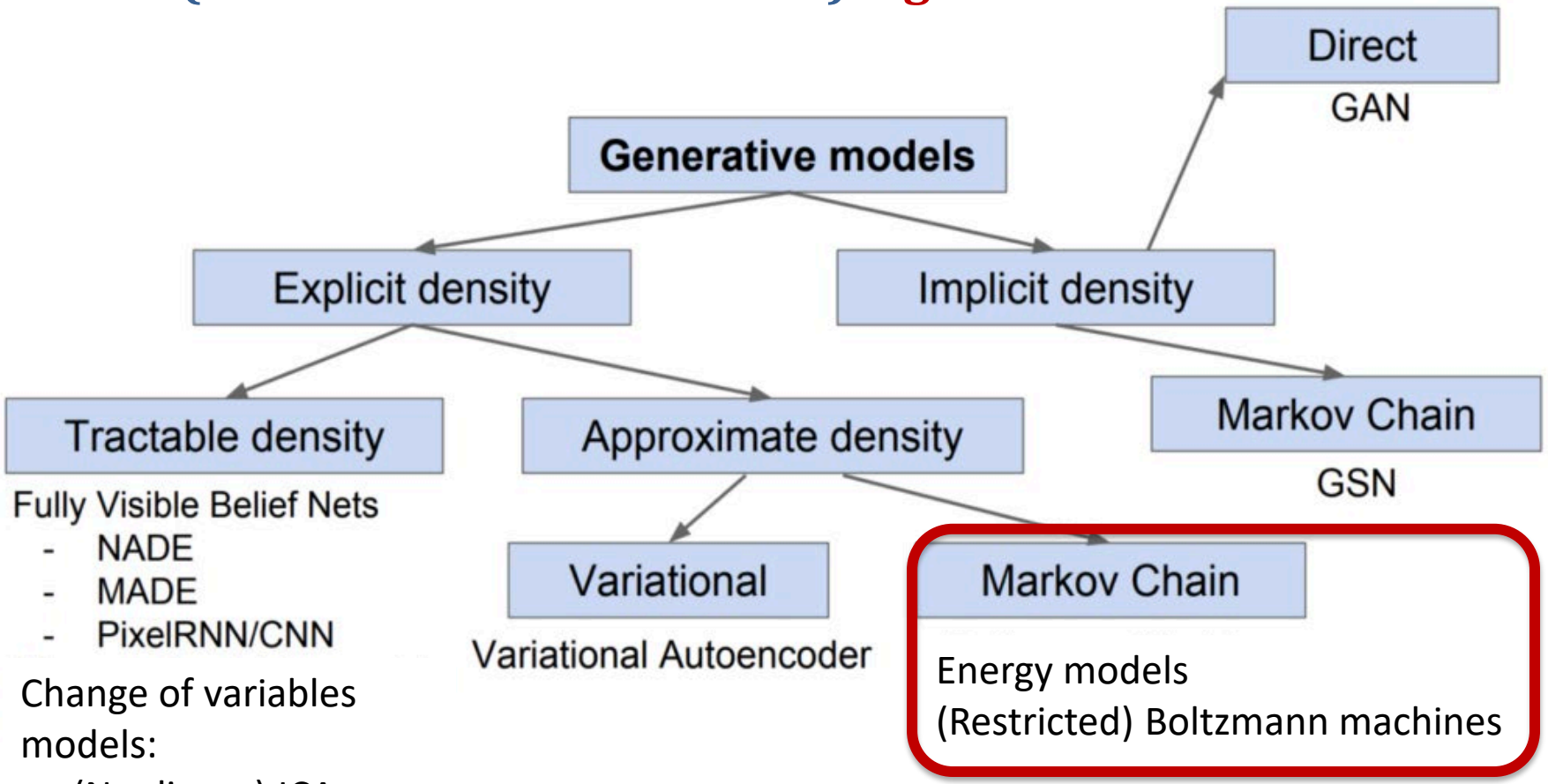
10707
Deep Learning: Spring 2021

Andrej Risteski

Machine Learning Department

Lecture 9+10:
Algorithmic techniques for intractable explicit density models: MCMC, energy models, RBMs

The distribution $p_\theta(x)$ does not have a tractable form, but we can approximate it by running a MCMC (Markov Chain Monte Carlo) algorithm.



Training explicit density models

Likelihood-based: maximize the likelihood of the data under the model (possibly with variational or MCMC approximations)

$$\max_{\theta} \sum_{\text{samples } x_i} \log p_\theta(x_i)$$

In the limit of infinite number of samples:

$$\max_{\theta} \mathbb{E}_{x\sim p} \log p_\theta(x) = -(\mathbb{E}_{x\sim p} \log \frac{1}{p_\theta(x)} + \mathbb{E}_{x\sim p} \log p(x) - \mathbb{E}_{x\sim p} \log p(x))$$

$$= -(\quad KL(p||p_\theta) \quad + \quad H(p))$$

Hence, we are minimizing KL divergence ($H(p)$ is a constant).

Training explicit density models

Likelihood-based: maximize the likelihood of the data under the model (possibly with variational or MCMC approximations)

Need to be able to evaluate

$\nabla \log p_\theta(x)$

In th ples:

$$\max_\theta \mathbb{E}_{x\sim p} \log p_\theta(x) = -(\mathbb{E}_{x\sim p} \log \frac{1}{p_\theta(x)} + \mathbb{E}_{x\sim p} \log p(x) - \mathbb{E}_{x\sim p} \log p(x))$$

$$= -(\quad KL(p||p_\theta) \quad + \quad H(p))$$

Hence, we are minimizing KL divergence ($H(p)$ is a constant).

Unnormalized density models

A frequent paradigm is for probabilistic models to have the form:

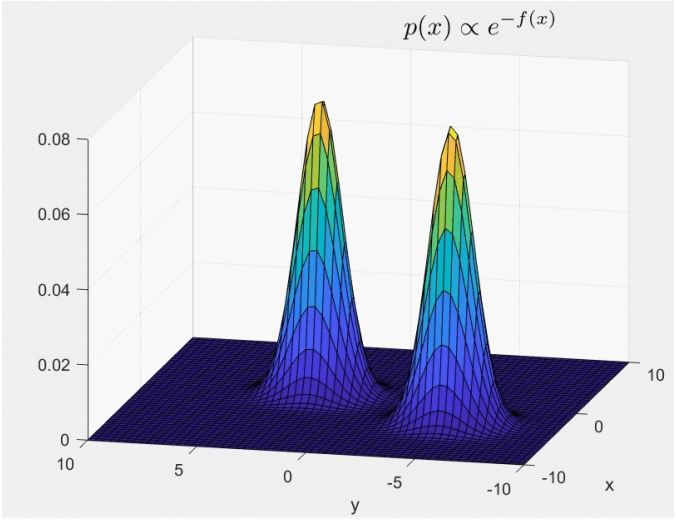
$$p_\theta(x) \propto \exp(-E_\theta(x))$$

where $E_\theta(x)$ has some easy to evaluate form.

It's an easy way to convert an energy E_θ to a probability distribution.

(The above distribution puts more mass on points with lower energy.)

Furthermore, by scaling $E_\theta(x)$ you can regulate the "sharpness" of the distribution.)



Unnormalized density models

A frequent paradigm is for probabilistic models to have the form:

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

where $E_\theta(x)$ has some easy to evaluate form.

To evaluate $p_\theta(x)$, we need to calculate $\int_x \exp(-E_\theta(x))$ or $\sum_x \exp(-E_\theta(x))$

How about gradient? Denoting above quantity Z_θ, we have:

$$\nabla \log p_\theta(x) = -\nabla E_\theta(x) + \nabla \log Z_\theta$$

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

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

We'd like to draw samples from p_θ

Interpretation of gradient descent for unnormalized density models

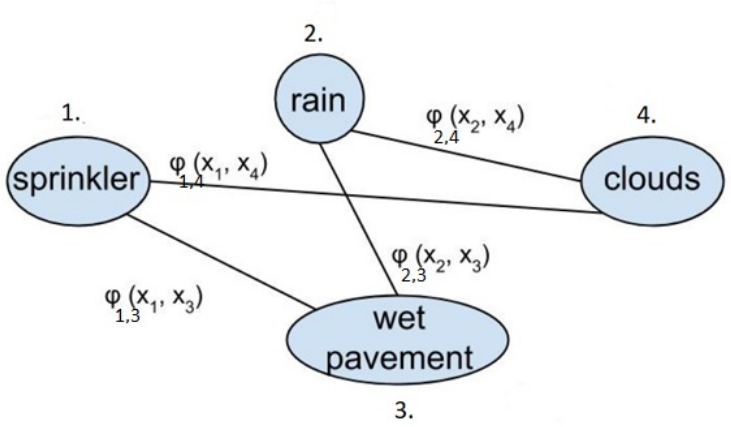
$$\nabla_\theta \left(\frac{1}{n} \sum_{i=1}^{n} \log p_\theta(x_i) \right) = \frac{1}{n} \left(\sum_i -\nabla_\theta E_\theta(x_i) \right) - \mathbb{E}_{p_\theta}[-\nabla_\theta E_\theta(x)]$$

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

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

Examples of unnormalized density models

Undirected graphical models or Markov Random Fields (MRFs)



A *pairwise* **undirected graphical model (MRF)** expresses a distribution as product of local potentials ϕ_{ij} (interactions), for example

$$p(x) = \frac{1}{Z}\Pi_{(i,j)\in E(G)}\phi_{ij}(x_i, x_j)$$

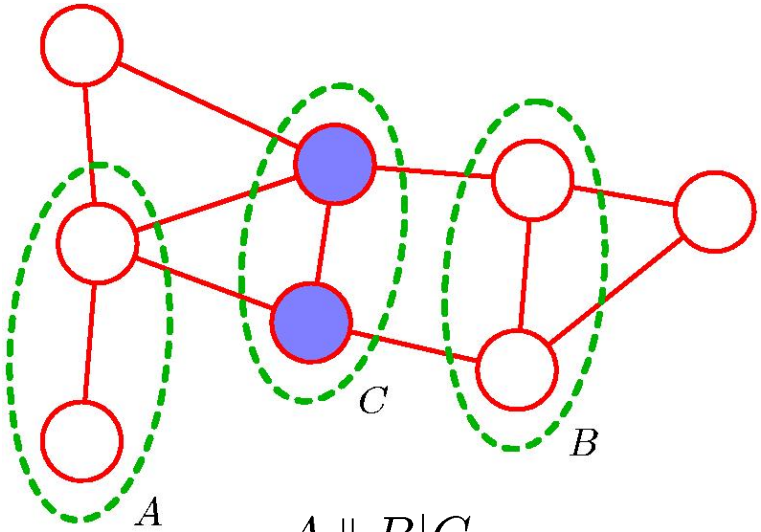
Encodes "*soft constraints*": the distribution tries to find a *good balance* in satisfying the (possibly conflicting) influences of the potentials.

Sampling from an MRF is hard: *partition function*

$$Z = \sum_{x} \Pi_{(i,j)\in E(G)}\phi_{ij}(x_i, x_j)$$ is intractable.

(In fact, there are simple cases where classical results in TCS show it is #P-hard to calculate.)

Conditional independence in MRFs



$A \perp\!\!\!\perp B | C$

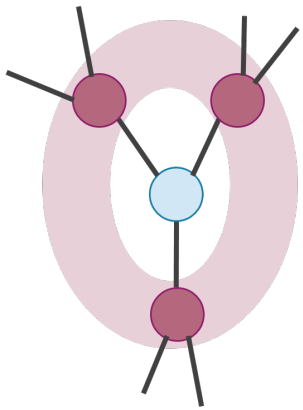
The independence structure of variables is "captured" by the graph.

Nodes in A, B are independent, given a set of nodes C separating A, B

$$p(x_A \mid x_C, x_B) = p(x_A|x_C)$$

Equivalently:

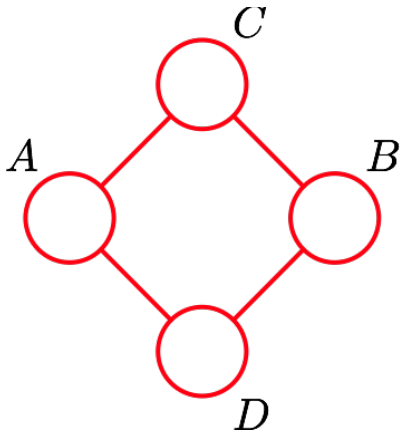
$$p(x_A, x_B \mid x_C) = p(x_A|x_C)\, p(x_B|x_C)$$



Special case: node is independent of the rest of the graph, given values of the neighbors

$$p(x_v \mid x_{N(v)}, x_{V/\{N(v),v\}}) = p(x_v|x_{N(v)})$$

Instance of a more general principle



More generally, we can describe the family of distributions whose conditional independence structure "tracks" a given (undirected) graph.

The way to formalize this is in terms of **maximal cliques** C (clique = fully connected subset of nodes) of the graph:

$$p(x) \propto \Pi_C \phi_C(x_C)$$

For example, the joint distribution above factorizes as:

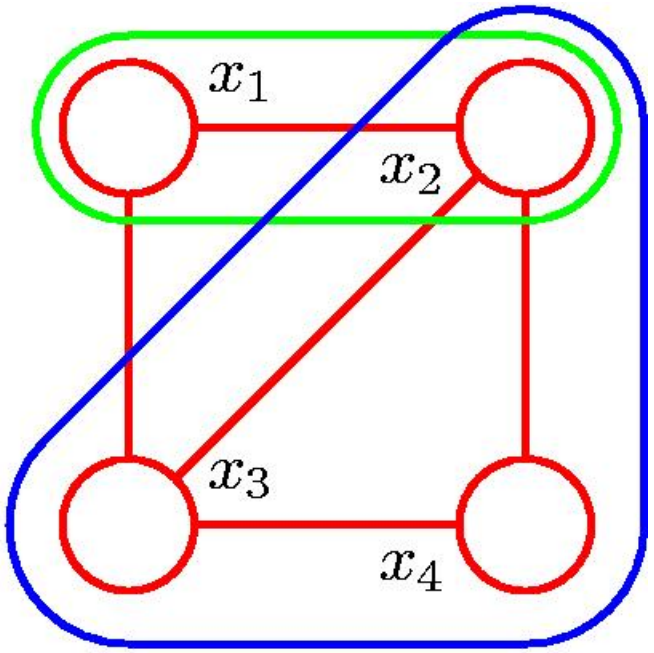
$$p(A,B,C,D) \propto \phi_{AC}(A,C)\phi_{BC}(B,C)\phi_{AC}(B,D)\phi_{AD}(A,D)$$

Maximal cliques

The subsets that are used to define the potential functions are represented by maximal cliques in the undirected graph.

Clique: a subset of nodes such that there exists an edge between all pairs of nodes in a subset.

Maximal Clique: a clique such that it is not possible to include any other nodes in the set without it ceasing to be a clique.



This graph has 5 cliques:

$$\{x_1, x_2\}, \{x_2, x_3\}, \{x_3, x_4\},$$
$$\{x_4, x_2\}, \{x_1, x_3\}.$$

Two maximal cliques:

$$\{x_1, x_2, x_3\}, \{x_2, x_3, x_4\}.$$

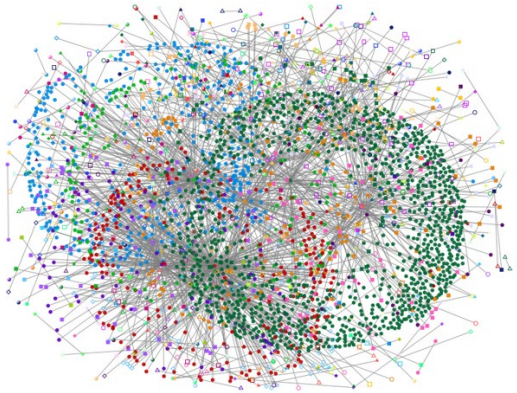
Hammersley-Clifford theorem

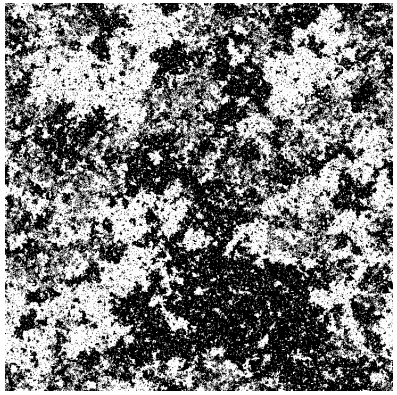
Consider the following sets of distributions:

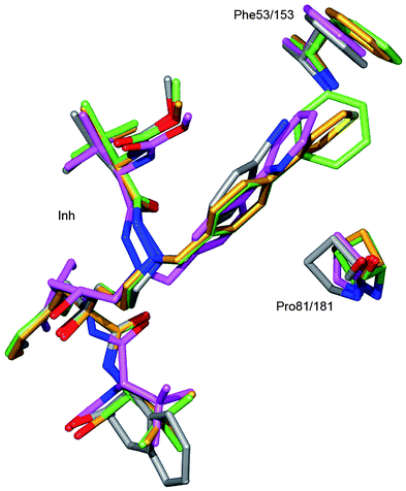
- The set of distributions consistent with the conditional independence relationships defined by the undirected graph.
- The set of distributions consistent with the factorization defined by potential functions on maximal cliques of the graph.

Hammersley-Clifford theorem: these two sets of distributions are the same.

Some applications





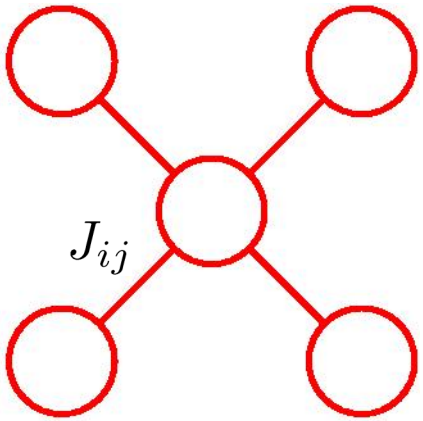


Example: multivariate Gaussian

Recall the multivariate Gaussian

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

The term inside the exponential is **quadratic**: namely, we can write



$$P(\mathbf{x}) = \frac{1}{\mathcal{Z}} \exp(-\frac{1}{2}\mathbf{x}^T J\mathbf{x} + \mathbf{g}^T\mathbf{x}),$$

where $J = \Sigma^{-1}, \quad \mu = J^{-1}\mathbf{g}.$

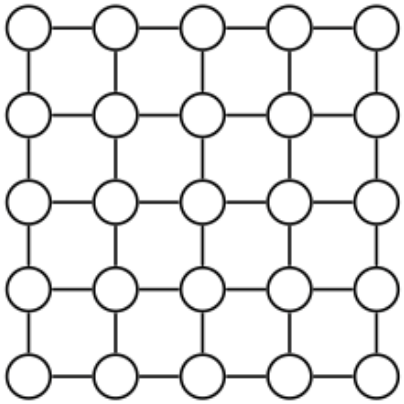
$$\mathbf{x}^T J\mathbf{x} = \sum_i J_{ii}x_i^2 + 2\sum_{ij\in E} J_{ij}x_i x_j,$$

Thus, the interactions are given by the precision matrix J.

(Note: precision mx being sparse **does not** imply the covariance mx is sparse.)

Example: Ising models

MRFs with binary variables are sometimes called Ising models in statistical mechanics, and Boltzmann machines in machine learning literature.



Denoting the binary valued variable at node j by $x_j \in \{\pm 1\}$, the **Ising model** for the joint probabilities is given by:

$$P_\theta(\mathbf{x}) = \frac{1}{\mathcal{Z}(\theta)} \exp\Big(\sum_{ij \in E} x_i x_j \theta_{ij} + \sum_{i \in V} x_i \theta_i\Big)$$

The conditional distribution is given by logistic (*only depends on nbrhood*!):

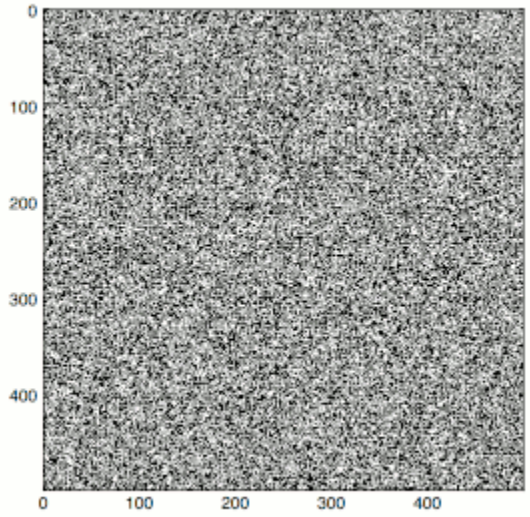
$$P_\theta(x_i = 1 | \mathbf{x}_{-i}) = \frac{1}{1 + \exp(-\theta_i - \sum_{ij \in E} x_j \theta_{ij})},$$

where x_{-i} denotes all nodes except for i.

If $\theta_{ij} \geq 0$: the nodes i,j, prefer to be the same. If $\theta_{ij} \leq 0$: they prefer to be different.

Example: Ferromagnetic Ising models

$$P_\theta(\mathbf{x}) = \frac{1}{\mathcal{Z}(\theta)} \exp\Big(\sum_{ij \in E} x_i x_j \theta_{ij} + \sum_{i \in V} x_i \theta_i \Big)$$

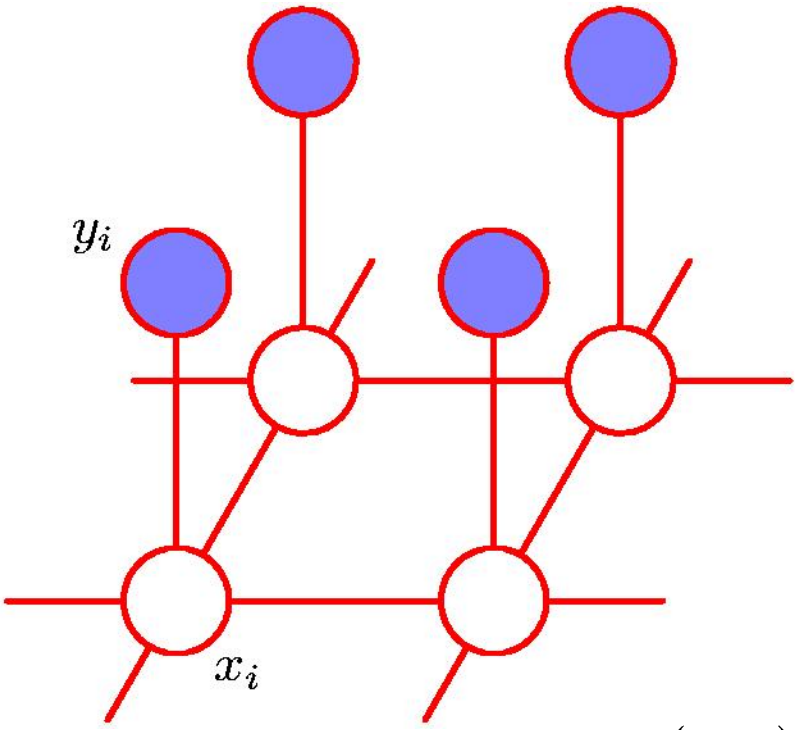


If $\theta_{ij} \geq 0$: the model is called ferromagnetic, and is used in physics to model the atomic structure (spins) of iron.

Example: Image Denoising

Noise removal from a binary image:

Let the observed noisy image be described by an array of binary pixel values: $y_j \in \{-1, +1\}$, i=1,...,D.



We take a noise-free image $x_j \in \{-1, +1\}$, randomly flip the sign of pixels with some small probability.

Bias term

Neighboring pixels are likely to have the same sign

$$E(\mathbf{x}, \mathbf{y}) = h \sum_i x_i - \beta \sum_{\{i,j\}} x_i x_j - \eta \sum_i x_i y_i$$

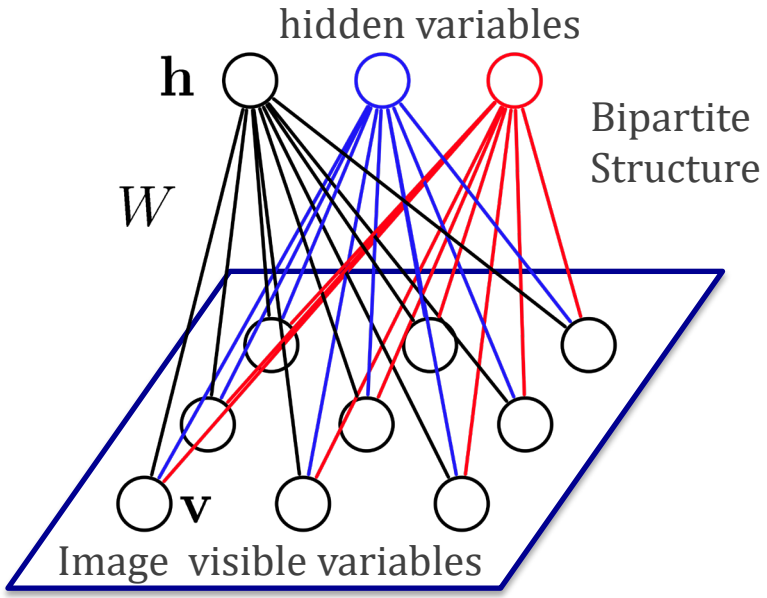
Noisy and clean pixels are likely to have the same sign

$$p(\mathbf{x}, \mathbf{y}) = \frac{1}{Z} \exp\{-E(\mathbf{x}, \mathbf{y})\}$$

Restricted Boltzmann Machines

A **latent-variable model**: some of the variables the distribution models are not observed (hidden).

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



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

The energy of the joint configuration:

$$E(\mathbf{v},\mathbf{h};\theta) = -\sum_{ij} W_{ij} v_i h_j - \sum_i b_i v_i - \sum_j a_j h_j$$

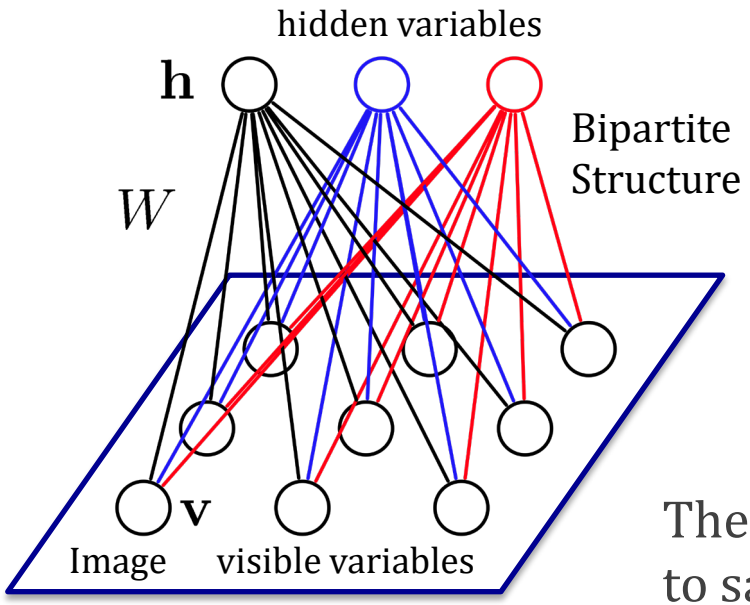
$\theta = \{W, a, b\}$ model parameters.

Probability of the joint configuration is given by the Boltzmann distribution:

$$P_\theta(\mathbf{v},\mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\big(-E(\mathbf{v},\mathbf{h};\theta)\big) = \frac{1}{\mathcal{Z}(\theta)} \prod_{ij} e^{W_{ij} v_i h_j} \prod_i e^{b_i v_i} \prod_j e^{a_j h_j}$$

$$\mathcal{Z}(\theta) = \sum_{\mathbf{h},\mathbf{v}} \exp\big(-E(\mathbf{v},\mathbf{h};\theta)\big)$$

Restricted Boltzmann Machines



Restricted: No interaction between hidden variables

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

$$P(\mathbf{h}|\mathbf{v}) = \prod_j P(h_j|\mathbf{v}) \qquad P(h_j = 1|\mathbf{v}) = \frac{1}{1 + \exp(-\sum_i W_{ij} v_i - a_j)}$$

Factorizes

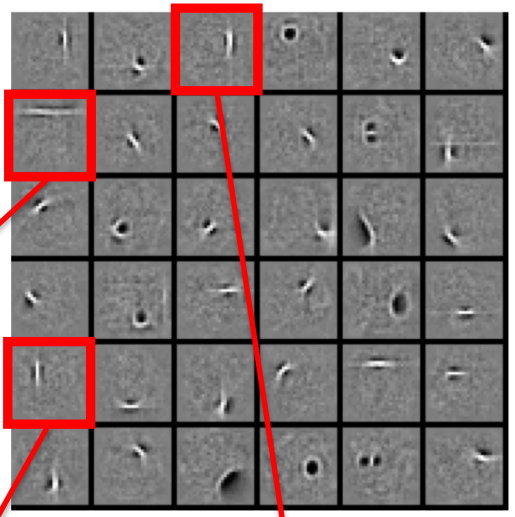
Similarly:

$$P(\mathbf{v}|\mathbf{h}) = \prod_i P(v_i|\mathbf{h}) \qquad P(v_i = 1|\mathbf{h}) = \frac{1}{1 + \exp(-\sum_j W_{ij} h_j - b_i)}$$

Example: learning alphabets using RBMs

Observed Data
Subset of 25,000 characters

Learned W: "edges"
Subset of 1000 features



New Image:

$$= \sigma\Big(0.99 \times \quad + \quad 0.97 \times \quad + \quad 0.82 \times \quad \cdots\Big)$$

$p(h_7 = 1|v)$ $p(h_{29} = 1|v)$

Most hidden variables are off

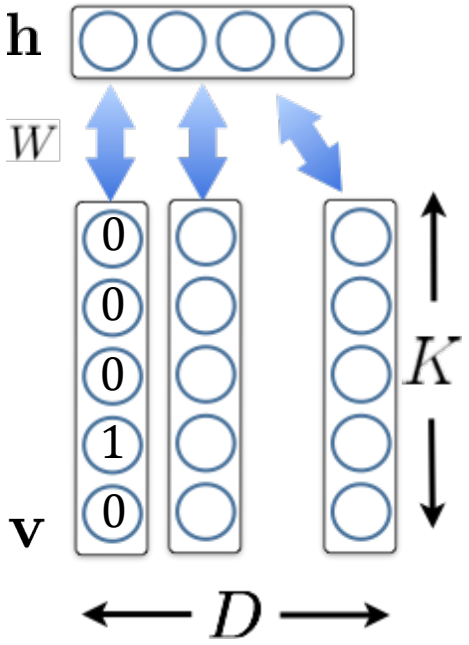
$$\sigma(x) = \frac{1}{1+\exp(-x)}$$

Logistic Function: Suitable for modeling binary images

Represent:

as $P(\mathbf{h}|\mathbf{v}) = [0,\ 0,\ 0.82,\ 0,\ 0,\ 0.99,\ 0,\ 0\ \ldots\ ]$

Example: inferring topic structure using RBMs



$$P_\theta(\mathbf{v}, \mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left(\sum_{i=1}^{D}\sum_{k=1}^{K}\sum_{j=1}^{F} W_{ij}^k v_i^k h_j + \sum_{i=1}^{D}\sum_{k=1}^{K} v_i^k b_i^k + \sum_{j=1}^{F} h_j a_j \right)$$

Pair-wise **Unary**

$$\theta = \{W, a, b\}$$

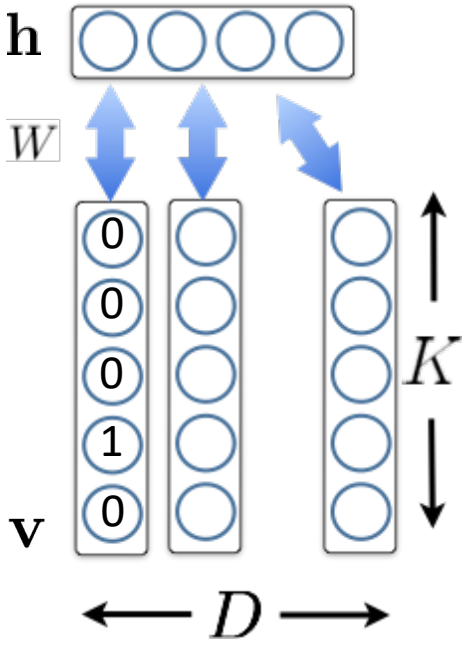
$$P_\theta(v_i^k = 1|\mathbf{h}) = \frac{\exp\left(b_i^k + \sum_{j=1}^{F} h_j W_{ij}^k\right)}{\sum_{q=1}^{K} \exp\left(b_i^q + \sum_{j=1}^{F} h_j W_{ij}^q\right)}$$

Replicated Softmax Model: *undirected* topic model:

- Stochastic 1-of-K visible variables.
- Stochastic binary hidden variables **h**
- Bipartite connections.

(Salakhutdinov & Hinton, NIPS 2010, Srivastava & Salakhutdinov, NIPS 2012)

Example: inferring topic structure using RBMs



Pair-wise Unary

$$P_\theta(\mathbf{v},\mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left(\sum_{i=1}^{D}\sum_{k=1}^{K}\sum_{j=1}^{F} W_{ij}^k v_i^k h_j + \sum_{i=1}^{D}\sum_{k=1}^{K} v_i^k b_i^k + \sum_{j=1}^{F} h_j a_j\right)$$

$$\theta = \{W, a, b\}$$

$$P_\theta(v_i^k = 1|\mathbf{h}) = \frac{\exp\left(b_i^k + \sum_{j=1}^{F} h_j W_{ij}^k\right)}{\sum_{q=1}^{K} \exp\left(b_i^q + \sum_{j=1}^{F} h_j W_{ij}^q\right)}$$

Reuters dataset:
804,414 **unlabeled** newswire stories
Bag-of-Words

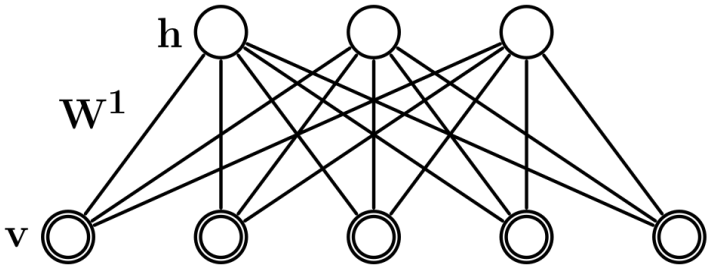
Learned features: ``topics''

russian	clinton	computer	trade	stock
russia	house	system	country	wall
moscow	president	product	import	street
yeltsin	bill	software	world	point
soviet	congress	develop	economy	dow

Example: movie predictions using RBMs

$$P_\theta(\mathbf{v}, \mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left(\sum_{ijk} W_{ij}^k v_i^k h_j + \sum_{ik} b_i^k v_i^k + \sum_j a_j h_j \right)$$

Binary hidden: user preferences



Multinomial visible: user ratings

Netflix dataset:
480,189 users
17,770 movies
Over 100 million ratings

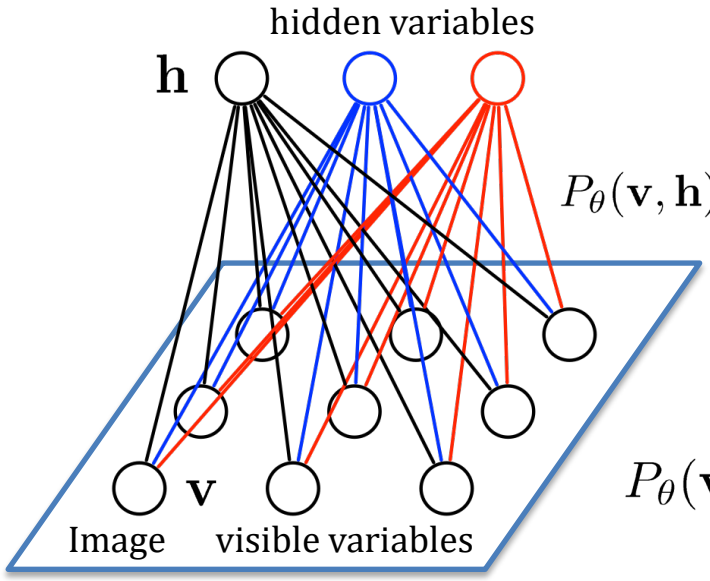
Learned features: ``genre''

Fahrenheit 9/11	Independence Day
Bowling for Columbine	The Day After Tomorrow
The People vs. Larry Flynt	Con Air
Canadian Bacon	Men in Black II
La Dolce Vita	Men in Black
Friday the 13th	Scary Movie
The Texas Chainsaw Massacre	Naked Gun
Children of the Corn	Hot Shots!
Child's Play	American Pie
The Return of Michael Myers	Police Academy

State-of-the-art performance on the Netflix dataset.

(Salakhutdinov, Mnih, Hinton, ICML 2007)

Example: RBMs for image data



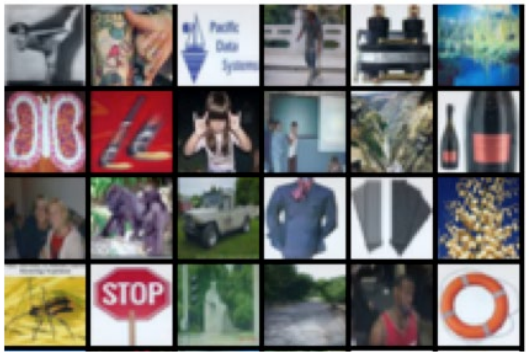
Pair-wise **Unary**

$$P_\theta(\mathbf{v},\mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left(\sum_{i=1}^{D}\sum_{j=1}^{F} W_{ij} h_j \frac{v_i}{\sigma_i} + \sum_{i=1}^{D} \frac{(v_i - b_i)^2}{2\sigma_i^2} + \sum_{j=1}^{F} a_j h_j\right)$$

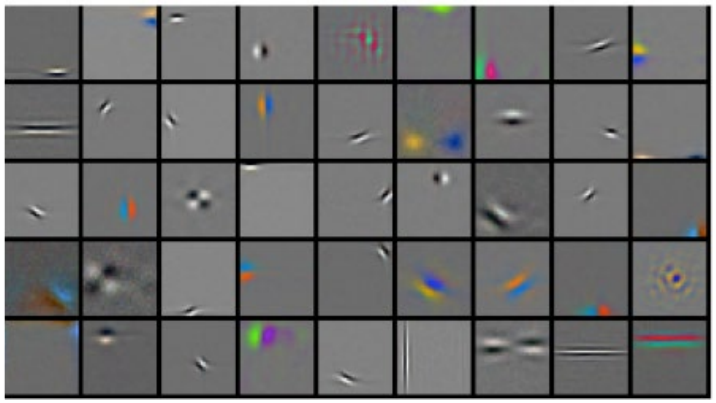
$$\theta = \{W, a, b\}$$

$$P_\theta(\mathbf{v}|\mathbf{h}) = \prod_{i=1}^{D} P_\theta(v_i|\mathbf{h}) = \prod_{i=1}^{D} \mathcal{N}\left(b_i + \sum_{j=1}^{F} W_{ij} h_j, \sigma_i^2\right)$$

4 million **unlabelled** images



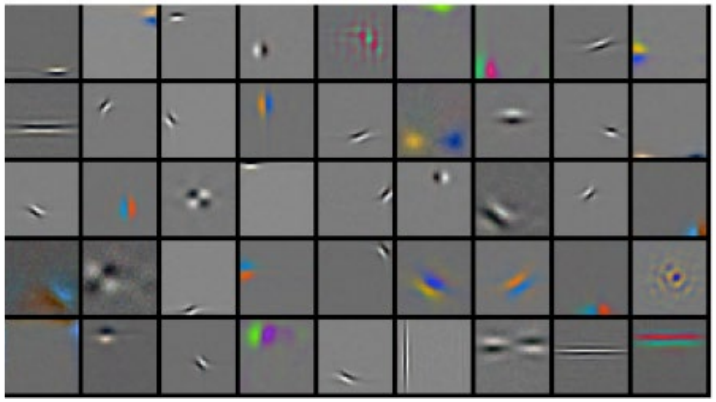
Learned features (out of 10,000)

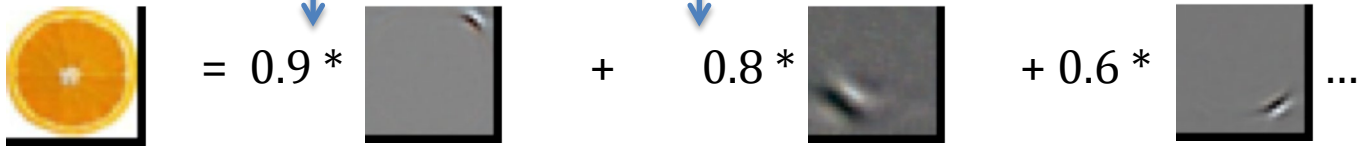


Example: RBMs for image data

4 million **unlabelled** images

Learned features (out of 10,000)





Continuous-space energy-based models (EBMs)

If the distribution $p_\theta(x) \propto \exp(-E_\theta(x))$ has as domain $\mathbb{R}^d$, an easy choice is E_θ is a neural net of some kind.

These have scaled up *only very recently* to real-life data, e.g. images.

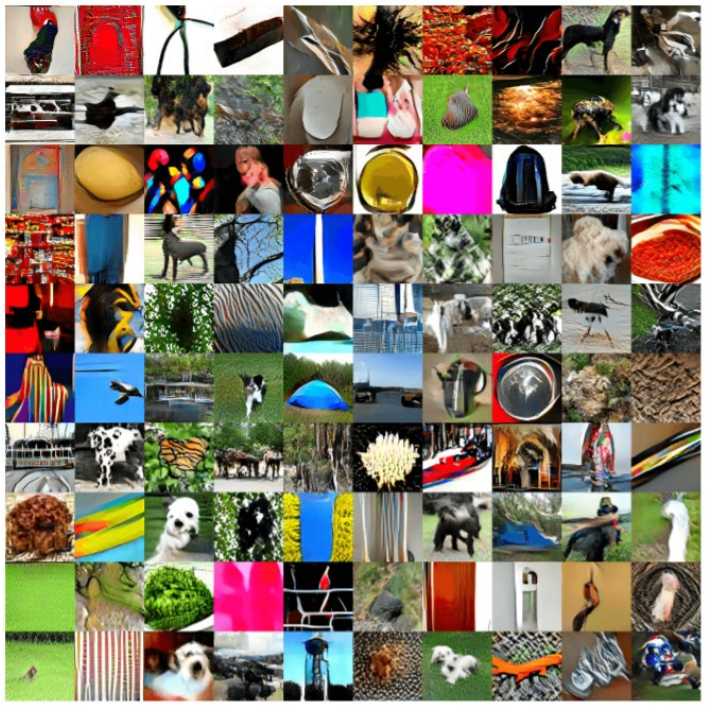


Figure 18: MCMC samples from conditional ImageNet128x128 models

Figure from (Du, Mordatch '20)

Example: denoising using EBMs

Figure 5: EBM image restoration on images in the **test** set via MCMC. The right column shows failure (approx. 10% objects change with ground truth initialization and 30% of objects change in salt/pepper corruption or inpainting. Bottom two rows shows worst case of change.)

Starting from a noised image, find the "closest" image via MCMC. (Stay tuned!) Indicates good coverage.

Example: image completion using EBMs

Figure 7: Illustration of image completions on conditional ImageNet model. Our models exhibit diversity in inpainting.

Testing overfitting via image completion.

Example: “logical” operators using energy functions

(Du, Li, Mordatch ’20)

Concept conjunction:

$$p(x|c_1 \text{ and } c_2 \ldots \text{and } c_n) := \Pi_i\, p(x|\, c_i) = e^{-\sum_i E_i(x)}$$

Concept disjunction:

$$p(x|c_1 \text{ or } c_2 \ldots \text{or } c_n)$$

$$:= \sum P(x|\, c_i) \propto^* \sum_i e^{-E_i(x)} = e^{\log \text{sum} \exp\left(-E_1(x),\ldots,-E_n(x)\right)}$$

Example: “logical” operators using energy functions

Figure 3: Combinations of different attributes on CelebA via concept conjunction. Each row adds an additional energy function. Images on the first row are conditioned on young, while images on the last row are conditioned on young, female, smiling, and wavy hair.

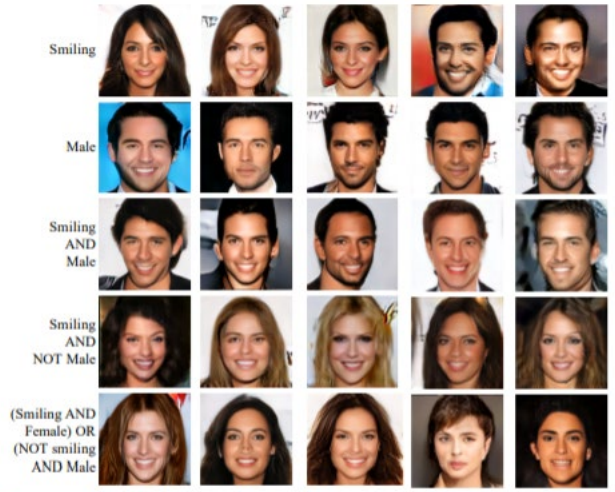


Figure 5: Examples of recursive compositions of disjunction, conjunction, and negation on the CelebA dataset.

Figure from (Du, Li, Mordatch ’20)

Basics of Markov Chains: tools for sampling from unnormalized densities

Preamble: some simple distributions to sample

Most univariate distributions:

Uniform[0,1]: np.random() (*Mersenne Twister based*)

Bernoulli(1/2): (*if np.random() < ½, output 1; else output 0*)

Bernoulli(p): (*if np.random() < p, output 1; else output 0*)

Standard univariate Gaussian: (*Box-Muller transform of uniform*)

…. (bruteforce transforms work in 1d)

Preamble: some simple distributions to sample

Extremely few multivariate distributions:

Product distributions: $P(x_1, x_2, \ldots, x_n) = \Pi_i P(x_i)$ (*sample coordinates independently*)

"Tractably factorized" distributions: $P(x_1, x_2, \ldots, x_n) = \Pi_i P(x_i | x_{<i})$ for which factors are some easy to sample distribution (e.g. Bernoulli, Gaussian, etc.)

Standard Gaussian (*product of standard univariate Gaussians*)

Any Gaussian: a sample from $\mathbf{y} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ can be generated as follows

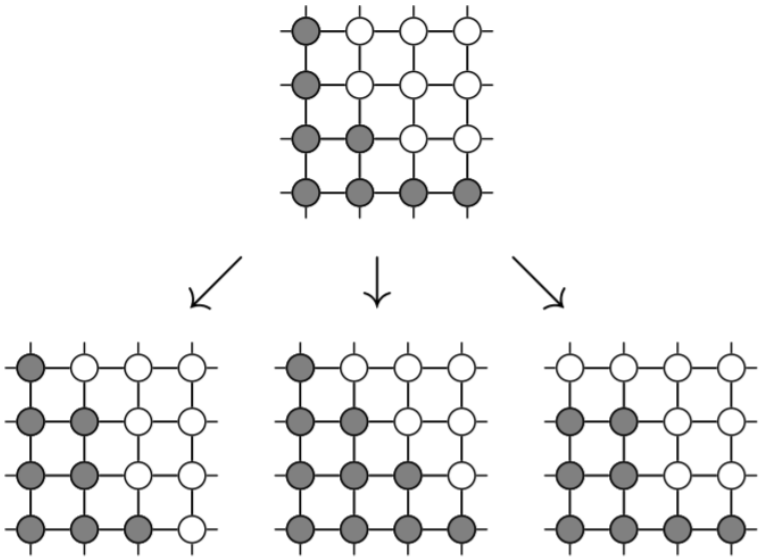
$$\text{Sample } \mathbf{x} \sim \mathcal{N}(0, \mathrm{I}) . \quad \text{Output } \boldsymbol{y} = \boldsymbol{\mu} + \boldsymbol{\Sigma}^{1/2} \boldsymbol{x} .$$

Random walks over discrete domains

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.

Definition: 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** $T \in \mathbb{R}_+^{|\mathcal{X}|\times|\mathcal{X}|}: T_{ij} = P(X_{t+1} = j \,|X_t = i)$

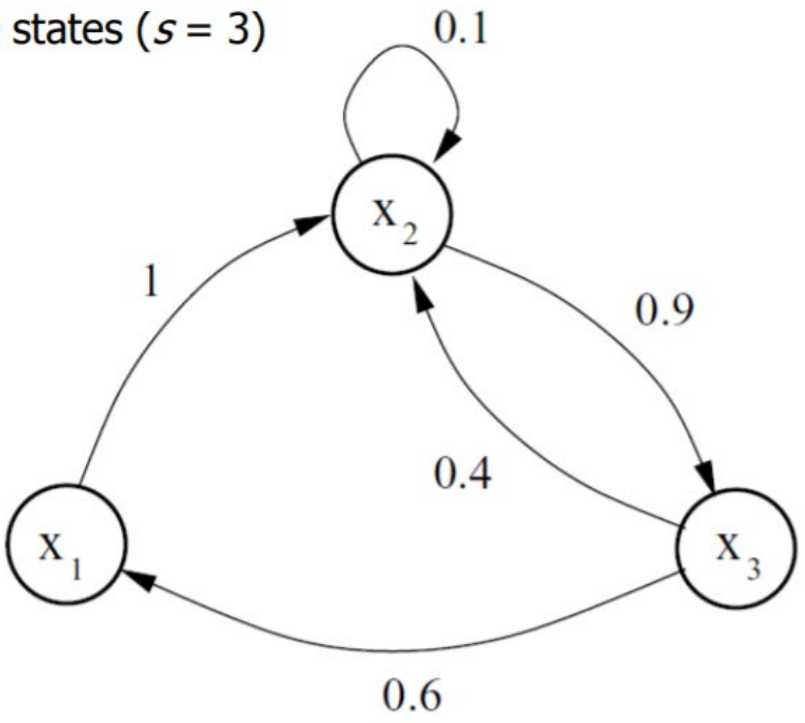
Clearly, $\forall i, \sum_j \; T_{ij} = 1$. We will also call such process a Markov Chain/ Markov random walk.

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

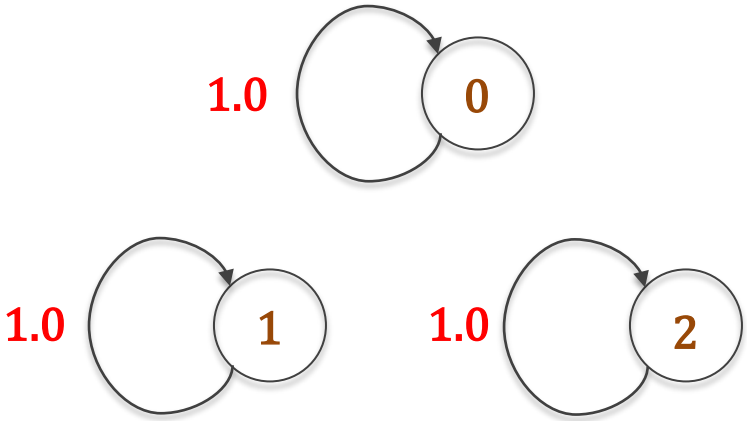
$$\forall p_0, \lim_{t \to \infty} p_0 T^t = \pi$$

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

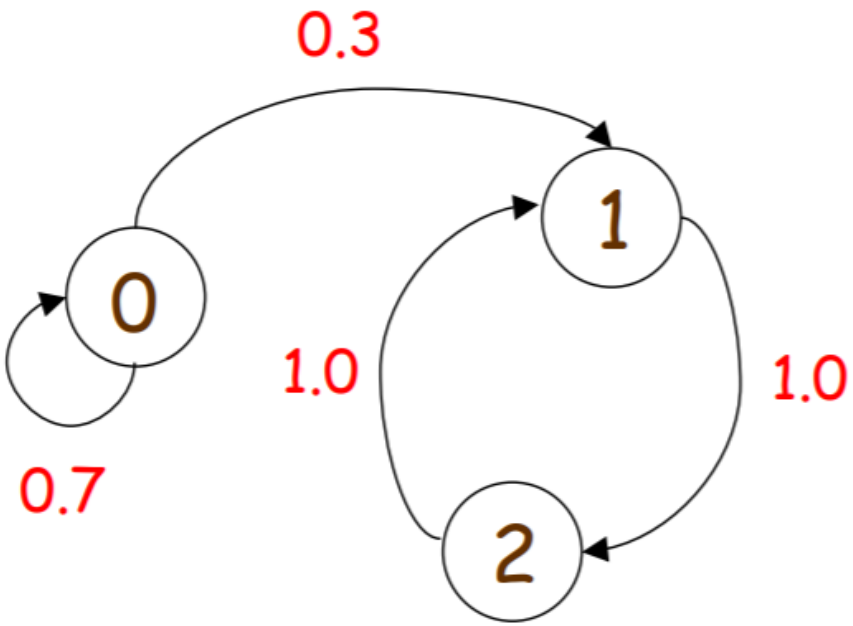
Conditions for having a unique stationary distribution

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.

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

Proof:

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

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:

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

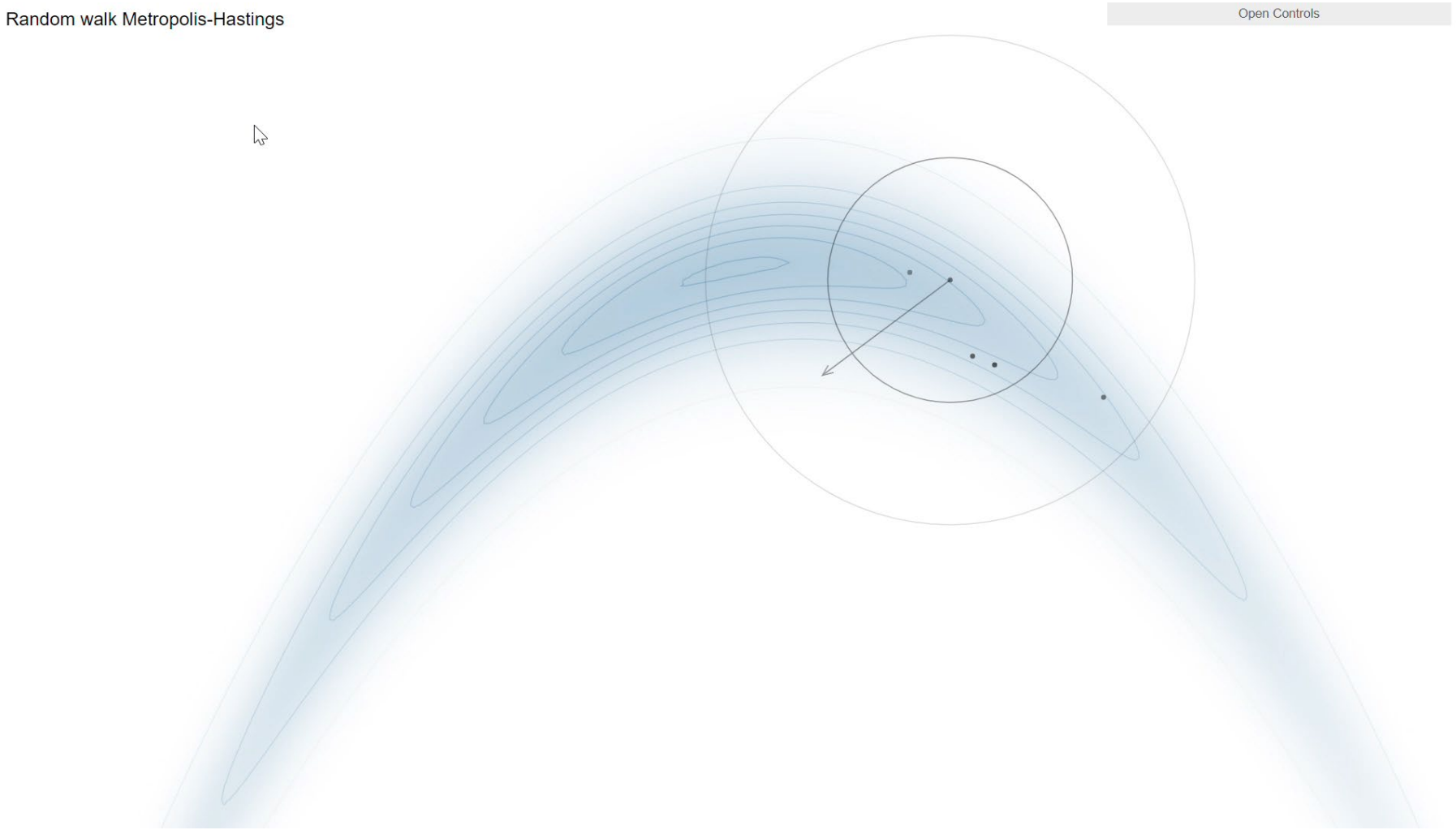
1., from state i go to state j with prob. $q(i,j)$

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



https://chi-feng.github.io/mcmc-demo/app.html

Metropolis-Hastings

Observation

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

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

Theorem

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

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

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

Proof:

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

=> Detailed balance (*) holds

Gibbs sampling

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

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

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

Repeat:

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

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

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

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

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

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

Let

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

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

Theorem

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

$\Rightarrow$ $(\pi_1,\ldots\pi_m)$ 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

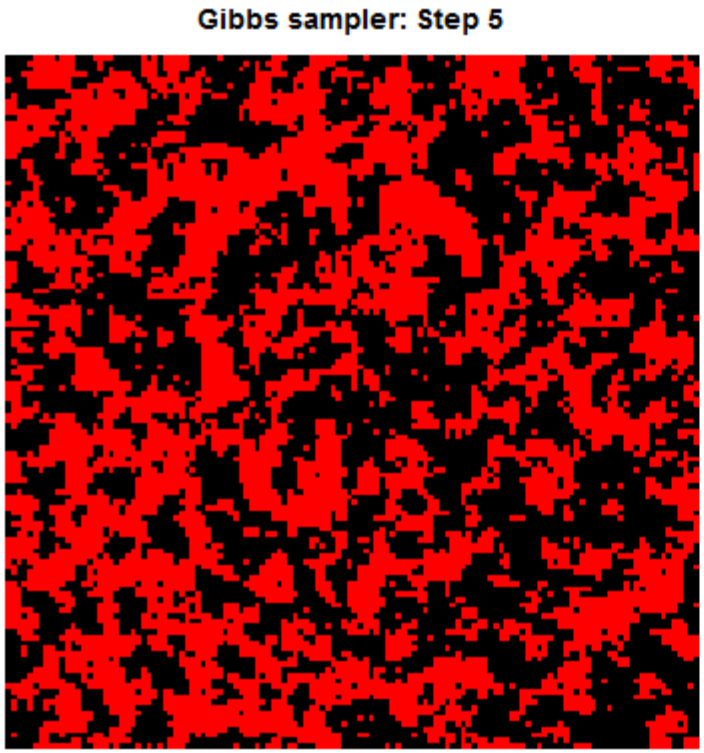
$$
\begin{aligned}
q(\mathbf{x},\mathbf{y}) &= q(\overbrace{(x_1,\ldots,x_n)}^{\mathbf{x}},\overbrace{(x_1,\ldots,x_{i-1},x,x_{i+1},x_n)}^{\mathbf{y}}) \\
&\doteq \frac{1}{n}P(X_i = x | X_j = x_j, \forall j \neq i) \\
&= \frac{1}{n}\frac{P(\mathbf{y})}{P(X_j = x_j, \forall j \neq i)}
\end{aligned}
$$

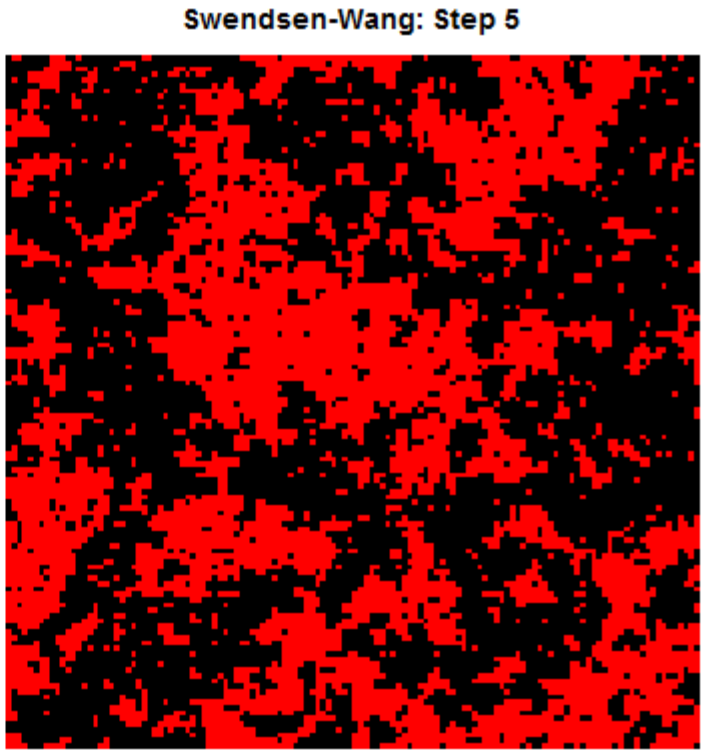
Shouldn't we reject occasionally? **No**:

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

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

Gibbs sampling





https://www.math.mcgill.ca/dstephens/MySite/index.html

What governs "mixing time"

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

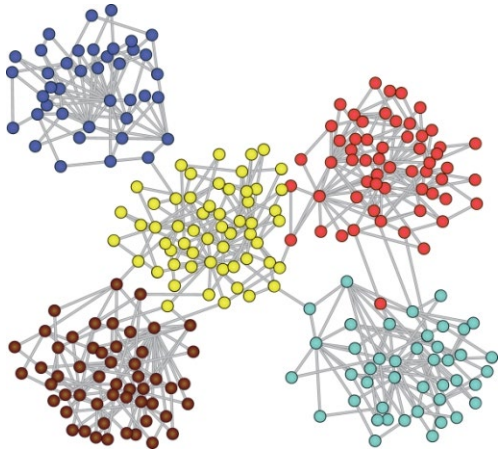
But, we're running this in practice, so want for sensible t, $\forall p_0,\ p_0 T^t \approx \pi$

(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)

What governs "mixing time"

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

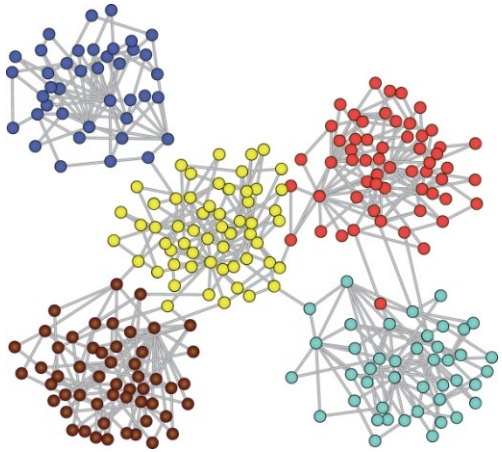
But, we're running this in practice, so want for sensible t, $\forall p_0,\ p_0 T^t \approx \pi$

(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:

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



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.

What governs "mixing time"

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

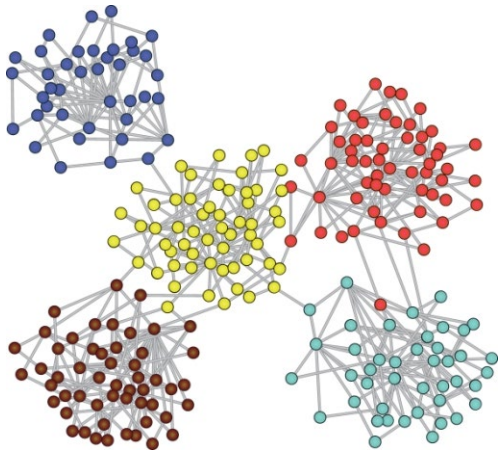
But, we're running this in practice, so want for sensible t, $\forall p_0,\ p_0 T^t \approx \pi$

(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:

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



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"

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

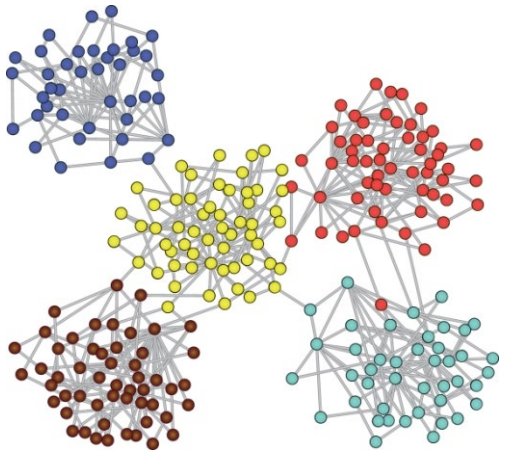
But, we're running this in practice, so want for sensible t, $\forall p_0,\ p_0 T^t \approx \pi$

(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:

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



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…)

Random walks over continuous domains (*Langevin dynamics*)

Langevin dynamics

Consider sampling from $p(x) = \frac{1}{Z}\exp\big(-f(x)\big)$ with support $\mathbb{R}^d$, f(x) is differentiable and we can efficiently take gradients. (e.g. f(x) is parametrized by a neural network).

A natural random walk:

Gradient descent Gaussian noise

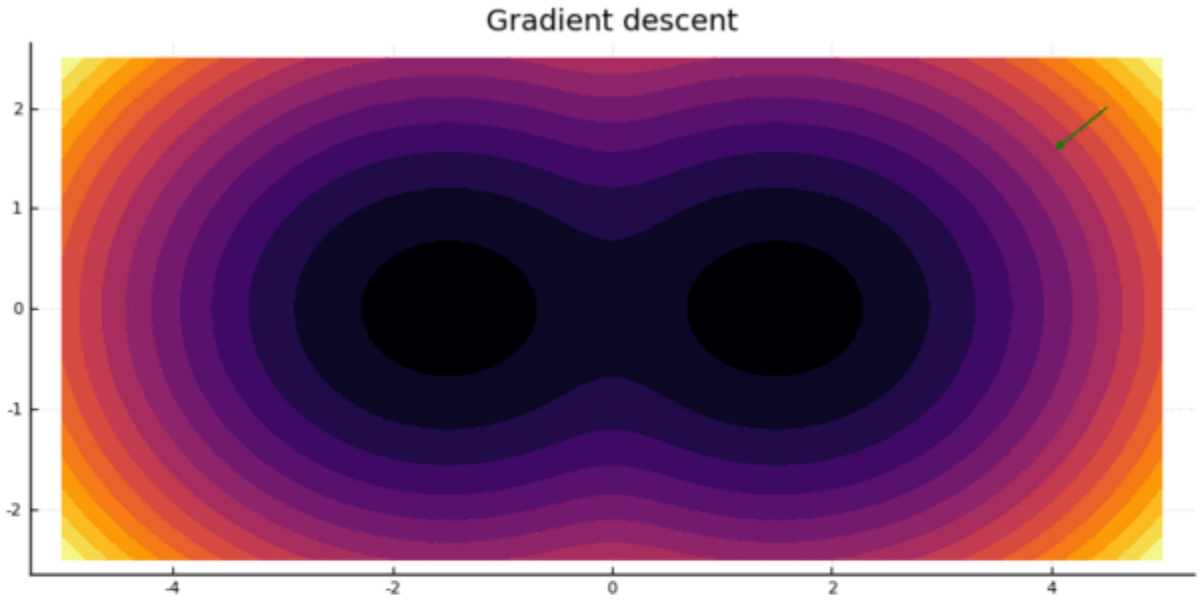
Limit (as $\eta \to 0$) of: $$x_{t+1} = x_t - \eta \nabla f(x_t) + \sqrt{2\eta}\xi_k$$

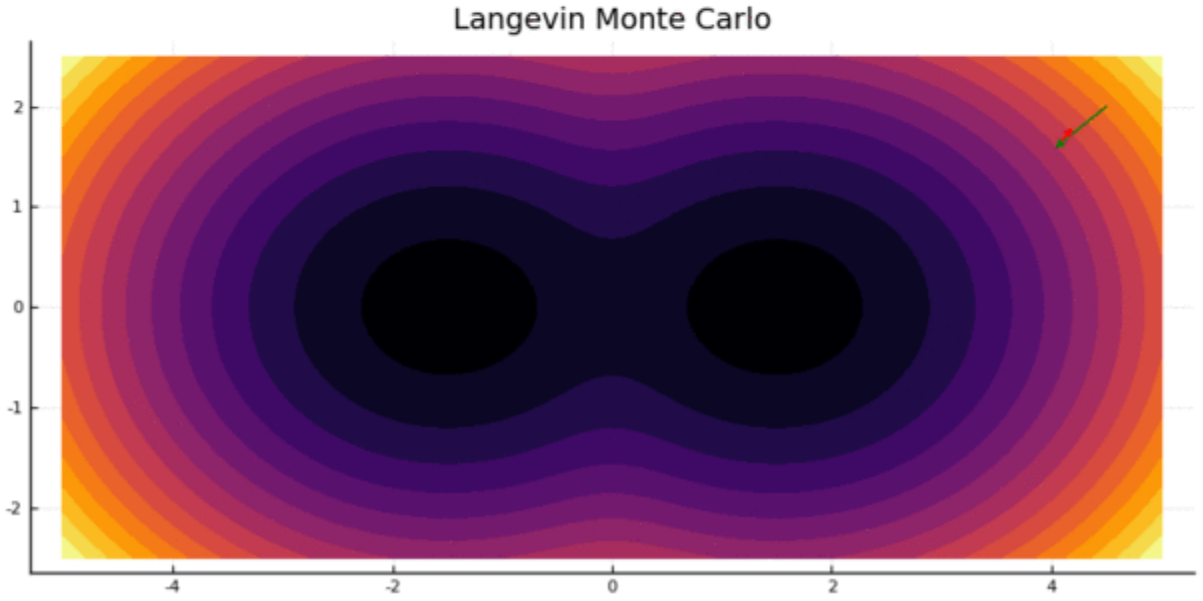
$$\xi_k \sim N(0, I)$$

Stationary (equilibrium) distr.

$$p(x) = \frac{1}{Z}\exp\big(-f(x)\big)$$

Langevin dynamics





The dichotomy

$$p(x) \propto e^{-f(x)}$$

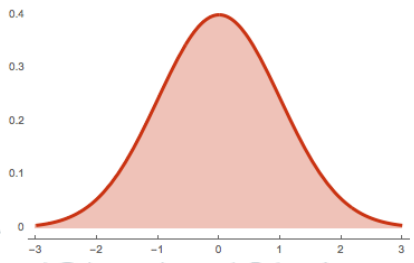
Log-concave distribution (f convex)

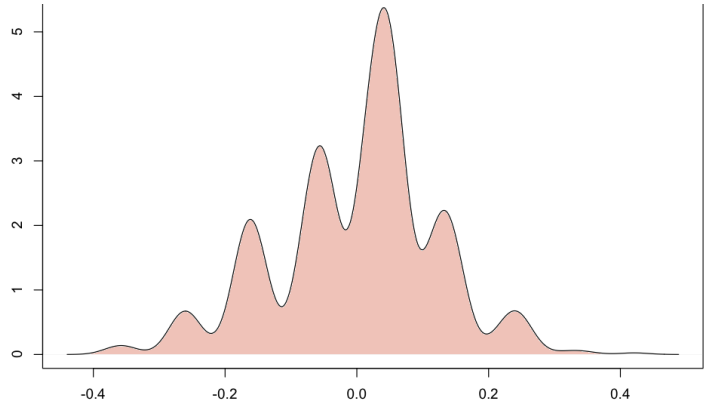
- Provable algorithms, but practically restrictive (unimodal)

Non-log-concave distributions

- #P-hard in the worst-case
- Common source of hardness: multimodality

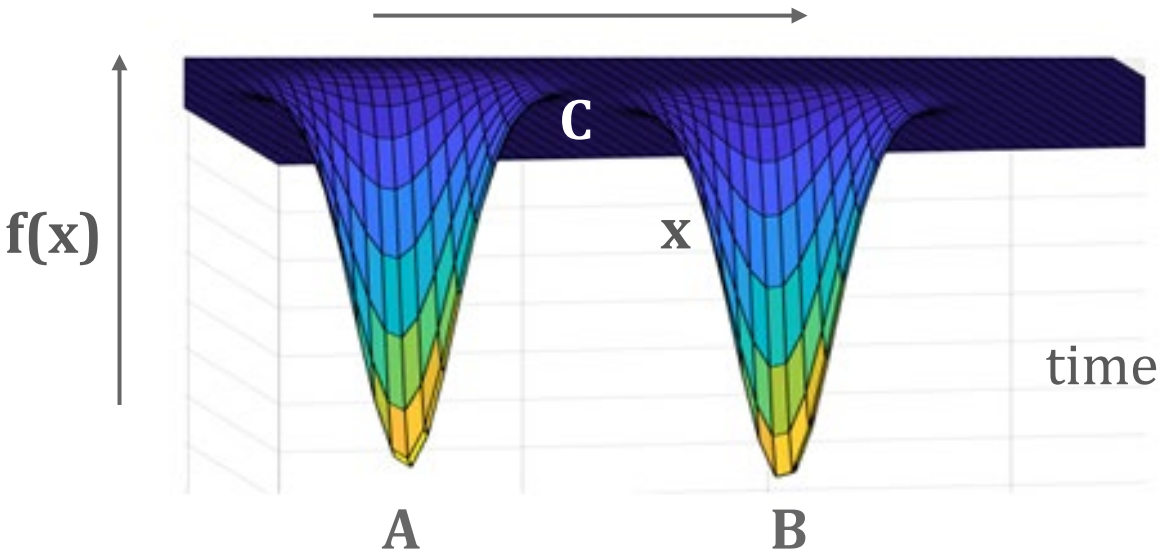
Parallel to optimization: if f is convex, minimizing f is easy. (All local minima are global ⇒ gradient descent works.)





Why multimodality is trouble

Sharp hills are hard to climb!



(Bovier '02,'04) ⇒ time to get from A to B (through C) can be exponential!

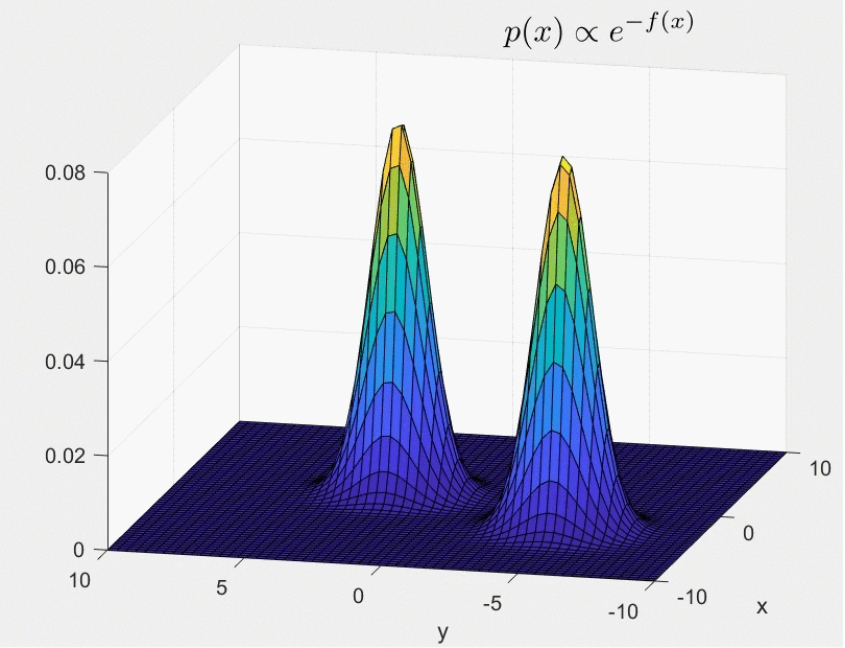
Recall, peaks of p = valleys of f

Potential solutions for multimodality

Unlike optimization,
scale (**temperature**) matters!

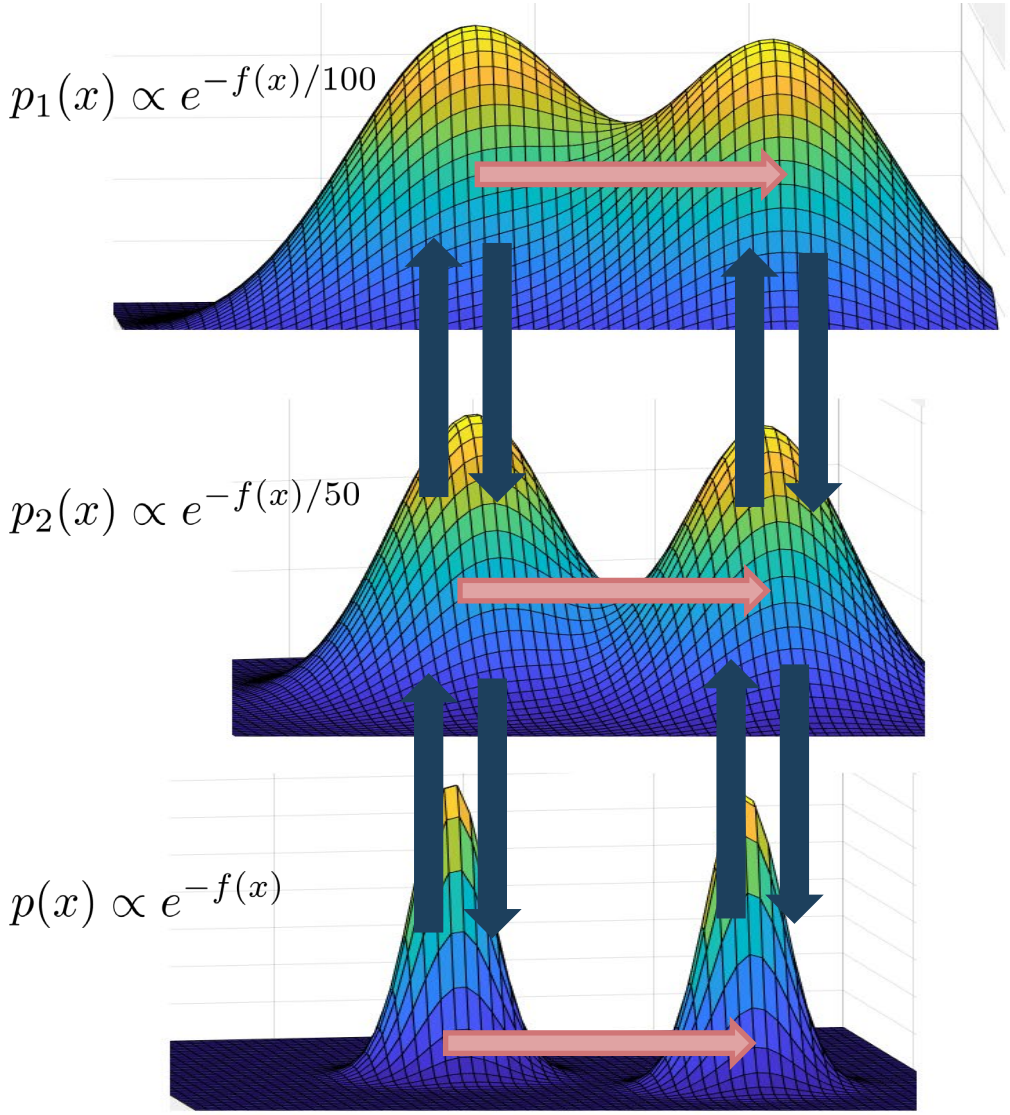
Sampling flatter distributions is easier!

Can we leverage this?



Tempering/annealing: run multiple chains at different temperatures, and use the fact that chains at higher temperatures move faster through landscape.

Tempering: flatten the hills



Algorithm: run multiple walks in parallel for **different temperatures**. **Swap** locations **occasionally** so lower-temp. chains explore space faster. (Occasionally = equilibrium distr. at each temperature is correct.)

Popular in practice, among other "annealing tricks" ((reverse) annealed importance sampling, tunneling…).

Little theory…

The tempering chain

- Markov Chain on state space: $\mathbb{R}^d \times [L]$. (L is # of temperatures)
- Let M_k be the Markov Chain corresponding to temperature k (i.e. with stationary distr. p_k)

<u>Tempering chain.</u>

Run k-th chain

Let current point be (x, k).

- With probability ½ ...

  Set next point ...

Swap points, perform
Metropolis-Hastings to
preserve stationary distr.

- With probability ½: pick ... set next point to (x,k') with probability $\min\left(\frac{p_{k'}(x)}{p_k(x)}, 1\right)$

The stationary distribution is $P(x,t) = \frac{1}{L} p_k(x)$

When does this work?

Each component a "**mode**"
"**Modes**" have same shape

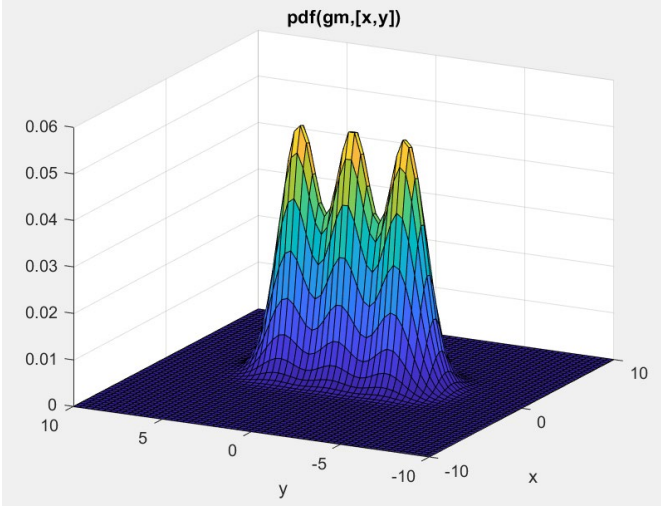
Unknown means!
(**gradient** access)

Thm [Ge-Lee-Risteski '18**]:**

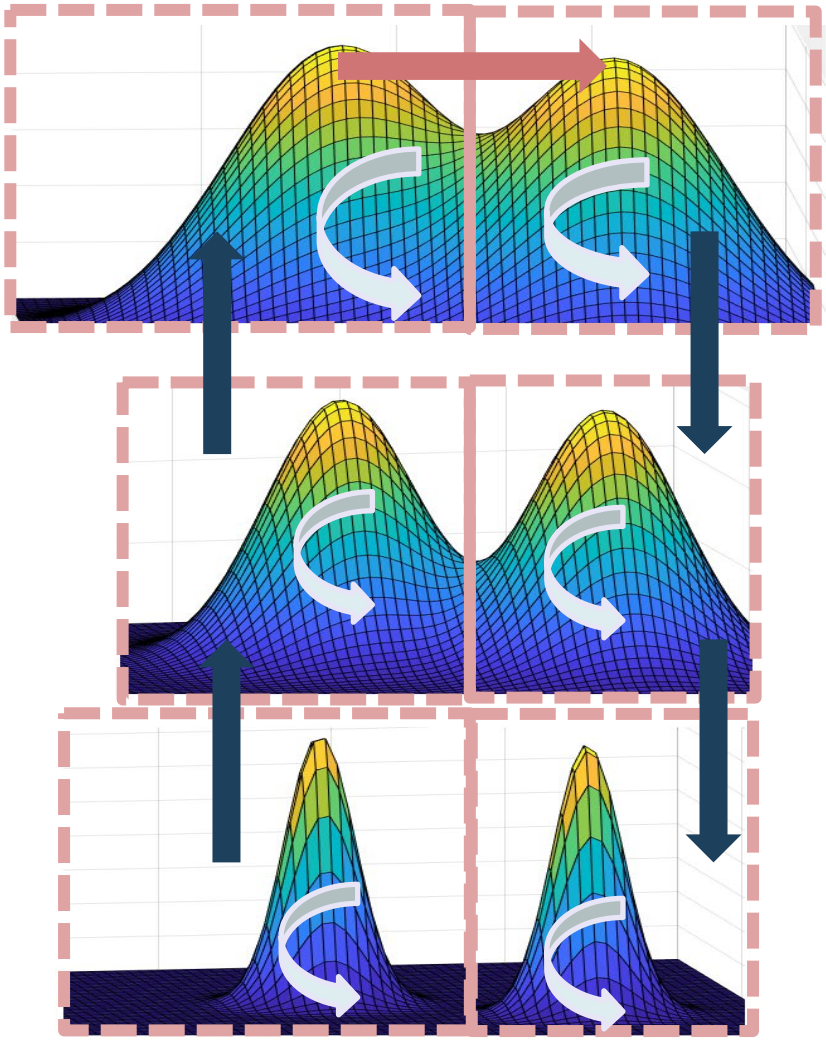
Let $p(x) \propto e^{-f(x)}$ be a **mixture** of **n shifts of a d-dim. log-concave distribution.**

Then, **Langevin + simulated tempering** run for time **poly(n, d)** samples from distribution close to **p**

Result is **robust**: works if p is **close** to a mixture (w/ degradation in runtime)



Why it works: take the road less hilly



Choose **highest temp.** s.t. walk converges fast. (Hills are flat)

Can partition space in **blocks** (≈ modes), s.t.

(1) Walk converges fast **inside each block**

(2) Blocks **aren't too small**

⇒ Fast convergence for tempering.

Intuition: Fast inside each mode.

Can get to highest temp. "parallel" mode.

Can get to any other mode at highest temp.

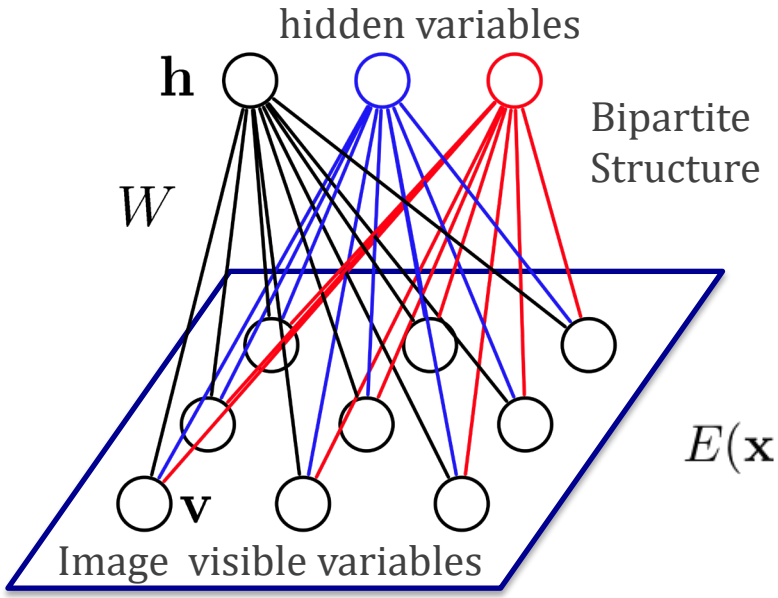
Can get to lowest temp. "parallel" mode.

Learning unnormalized density models using MCMC

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 $\mathbf{h} \in \{0, 1\}^{F}$

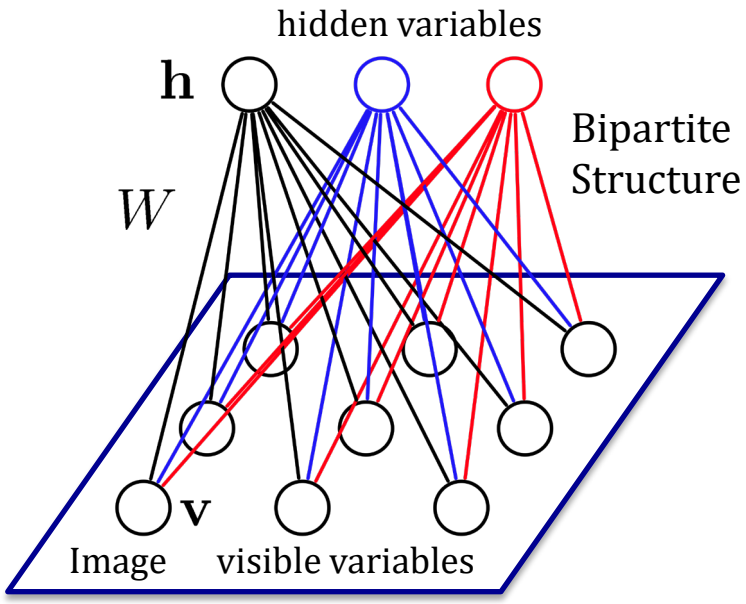
The energy of the joint configuration:

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

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!)

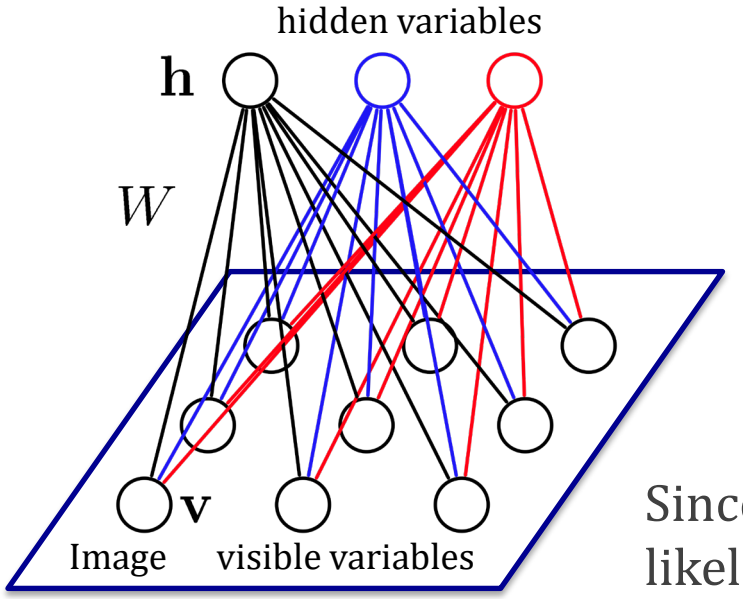
$$p(\mathbf{h}|\mathbf{x}) = \prod_j p(h_j|\mathbf{x}) \qquad p(h_j = 1|\mathbf{x}) = \frac{1}{1 + \exp(-(b_j + \mathbf{W}_j.\mathbf{x}))}$$

Factorizes

Similarly:

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

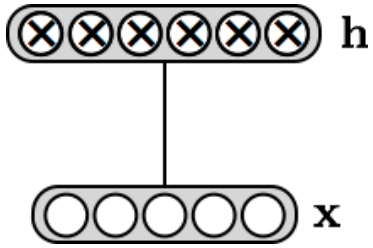
How to learn RBM's



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

$$
\begin{aligned}
p(\mathbf{x}) &= \sum_{\mathbf{h}\in\{0,1\}^H} \exp(\mathbf{h}^\top \mathbf{W}\mathbf{x} + \mathbf{c}^\top \mathbf{x} + \mathbf{b}^\top \mathbf{h})/Z \\
&= \exp(\mathbf{c}^\top \mathbf{x}) \sum_{h_1\in\{0,1\}} \cdots \sum_{h_H\in\{0,1\}} \exp\left(\sum_j h_j \mathbf{W}_{j.}\mathbf{x} + b_j h_j\right)/Z
\end{aligned}
$$

How to learn RBM's

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

How to learn RBM's

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

How to learn RBM's

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

How to learn RBM's

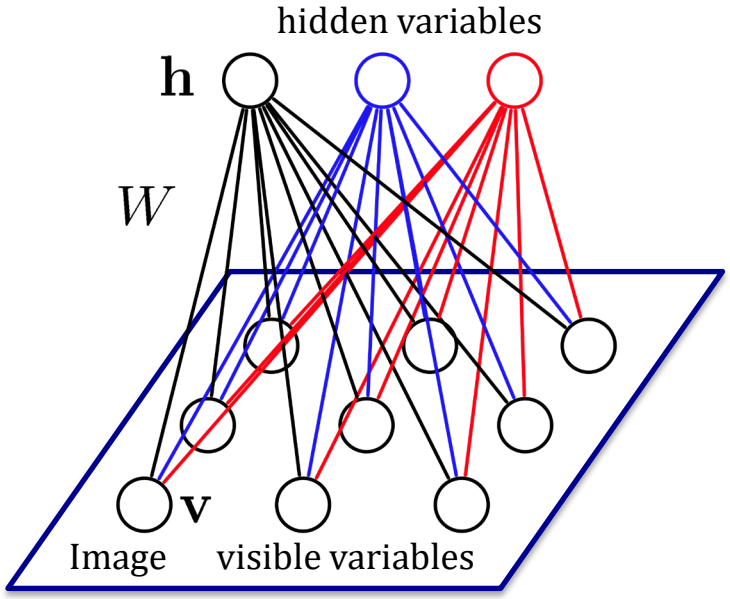
$$
\begin{aligned}
p(\mathbf{x}) &= \sum_{\mathbf{h}\in\{0,1\}^H} \exp(\mathbf{h}^\top \mathbf{W}\mathbf{x} + \mathbf{c}^\top \mathbf{x} + \mathbf{b}^\top \mathbf{h})/Z \\
&= \exp(\mathbf{c}^\top \mathbf{x}) \sum_{h_1\in\{0,1\}} \cdots \sum_{h_H\in\{0,1\}} \exp\left(\sum_j h_j \mathbf{W}_{j.}\mathbf{x}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

How to learn RBM's

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

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

How to learn RBM's



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

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

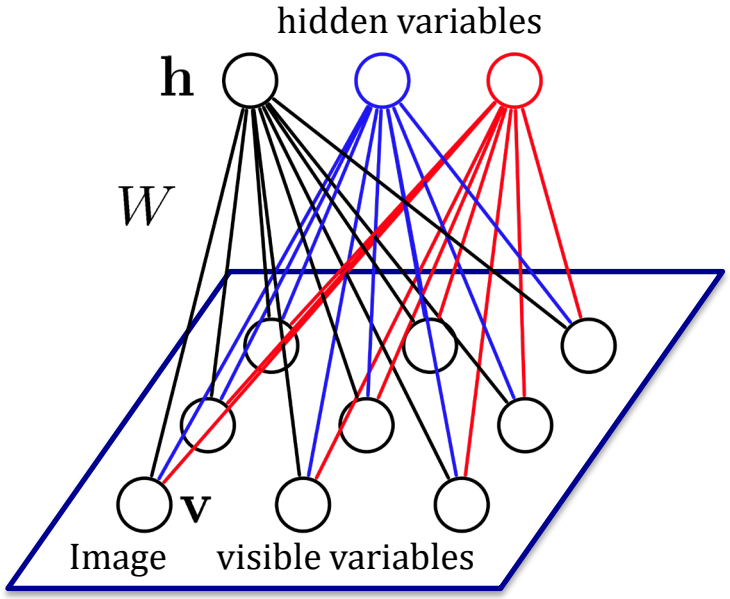
With this reduction, the undirected model calculations imply:

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

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

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

How to learn RBM's



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:

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

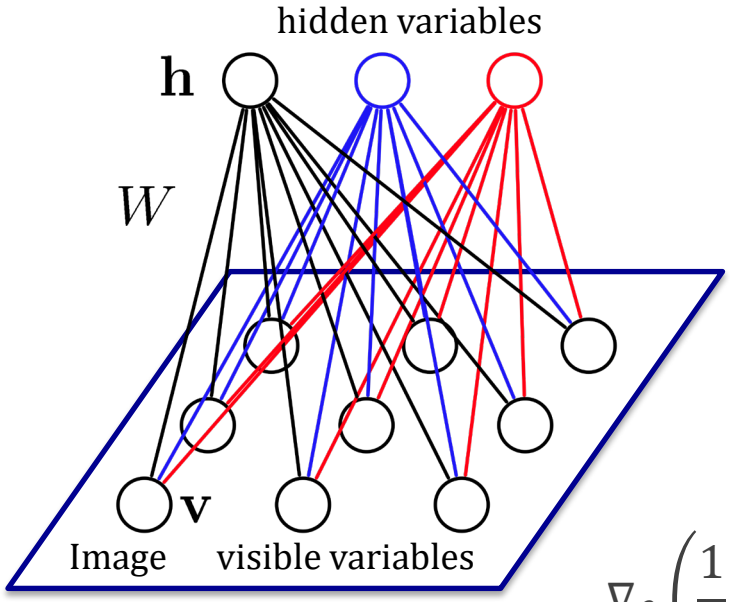
$$\nabla_{W_{ij}} F_\theta(\mathbf{x}) = P(\mathbf{h}_j = 1 | \mathbf{x})\, \mathbf{x}\_i \quad \Rightarrow \quad \nabla_{\mathbf{W}} F_\theta(\mathbf{x}) = \mathbf{h}(\mathbf{x})\, \mathbf{x}^T$$

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

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

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

How to learn RBM's



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

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

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

The hard term is again: $\mathbb{E}_{p_\theta}[-\nabla_\theta F_\theta(x)]$ --- 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:

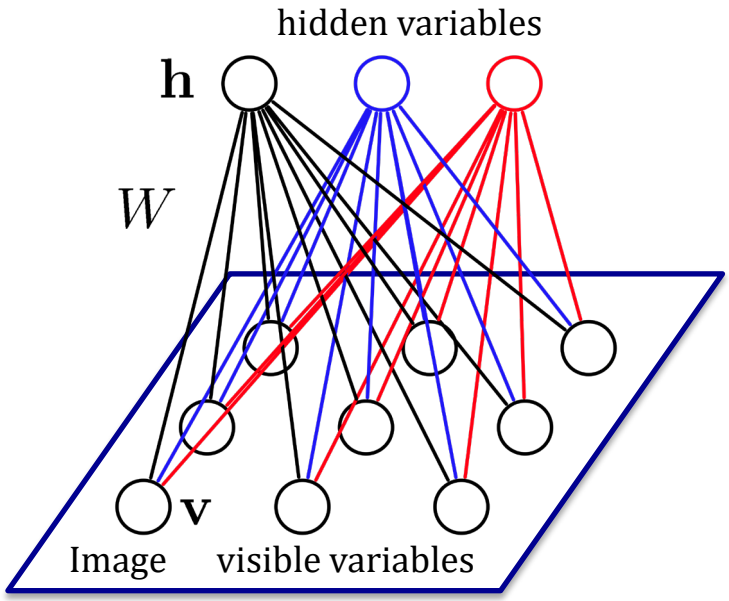
Let current state be $\boldsymbol{x} = (x_1, x_2, \dots, x_n)$

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

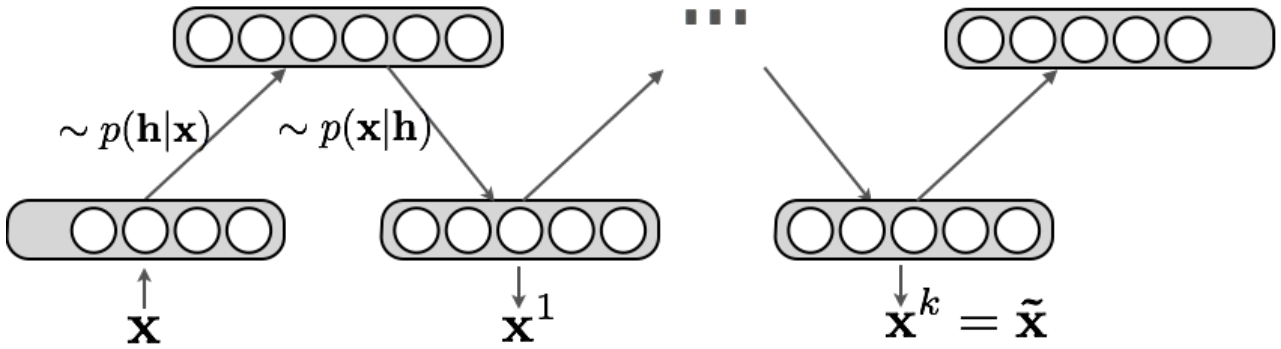


Repeat:

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

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

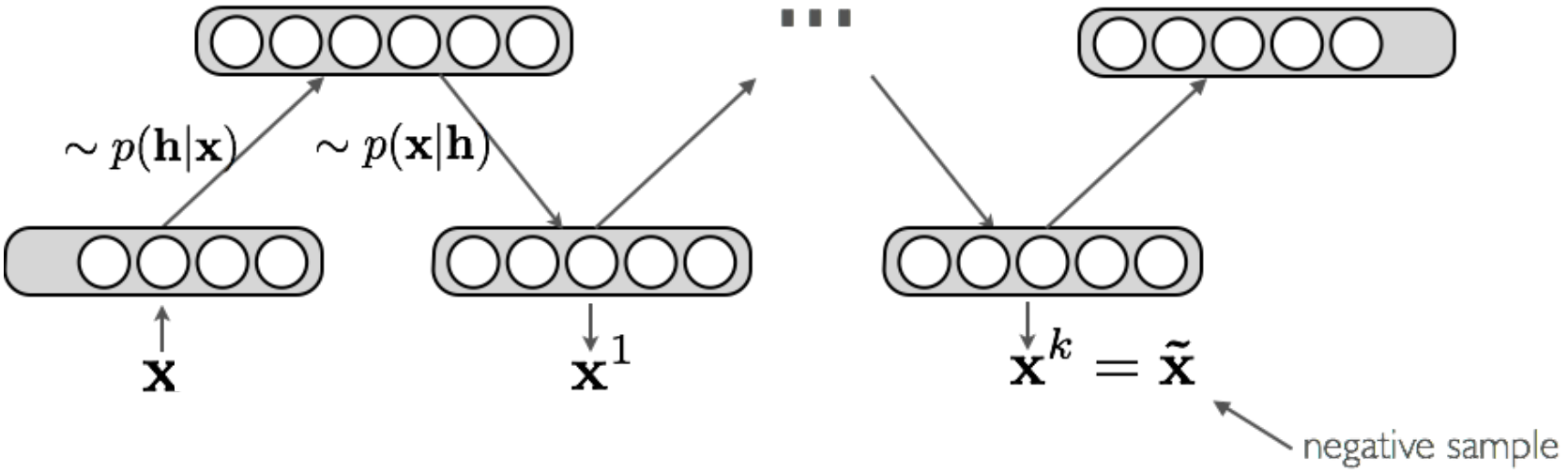
Pictorially:



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

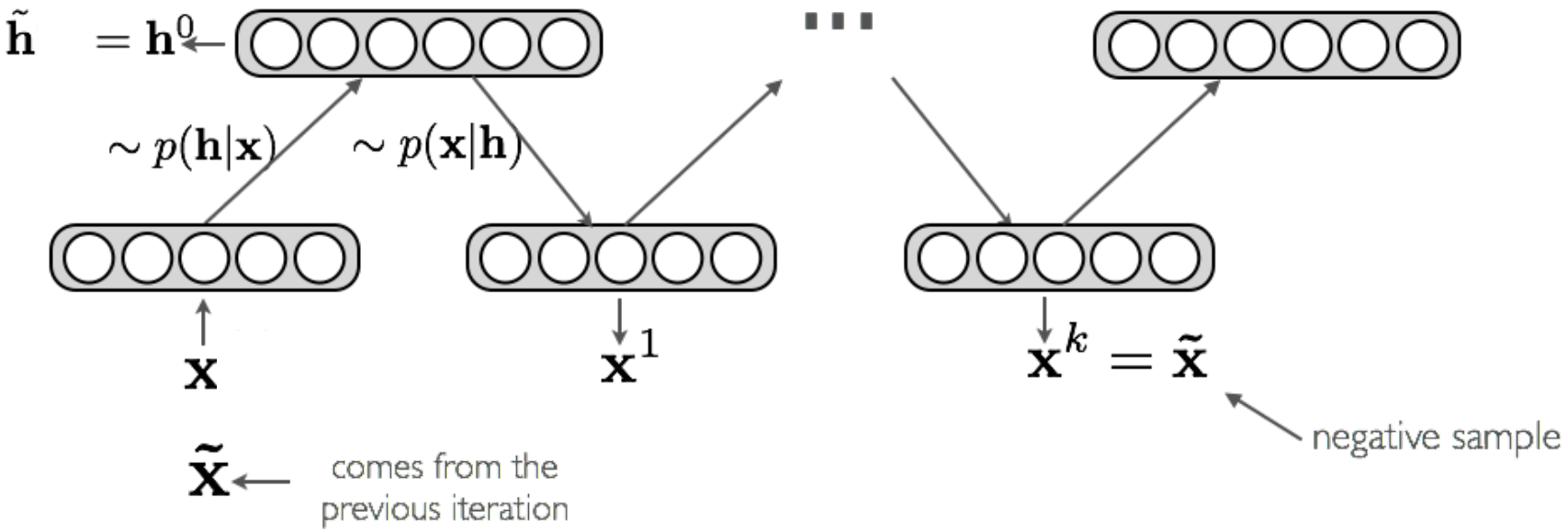
- CD-k: contrastive divergence with k iterations of Gibbs sampling

- 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

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)

Learning continuous-space EBMs

Let's assume $x \in \mathbb{R}^d$. An obvious way to produce the estimates $\mathbb{E}_{p_\theta}[-\nabla_\theta E_\theta(x)]$: sample approximately from p_θ using Langevin dynamics.

This was done recently: (Du, Mordatch '19), (Song, Ermon '19):

What's the difficulty?

Data is multimodal: Langevin might take long to mix.

Learning continuous-space EBMs

The algorithm from (Du, Mordatch '19)

Maintain buffer of previous samples to reduce mixing time

W/ some probability, start from random pt to encourage mode exploration

Langevin sampler

A bit of l2 regularization to ensure energy is somewhat smooth

Algorithm 1 Energy training algorithm

Input: data dist. $p_D(\mathbf{x})$, step size λ, number of steps K

$\mathcal{B} \leftarrow \varnothing$

while not converged **do**

$\mathbf{x}_i^+ \sim p_D$

$\mathbf{x}_i^0 \sim \mathcal{B}$ with 95% probability and $\mathcal{U}$ otherwise

▷ *Generate sample from q_θ via Langevin dynamics:*

for sample step $k = 1$ to K **do**

$\tilde{\mathbf{x}}^k \leftarrow \tilde{\mathbf{x}}^{k-1} - \nabla_{\mathbf{x}} E_\theta(\tilde{\mathbf{x}}^{k-1}) + \omega, \quad \omega \sim \mathcal{N}(0, \sigma)$

end for

$\mathbf{x}_i^- = \Omega(\tilde{\mathbf{x}}_i^k)$

▷ *Optimize objective $\alpha\mathcal{L}_2 + \mathcal{L}_{ML}$ wrt θ:*

$\Delta\theta \leftarrow \nabla_\theta \frac{1}{N} \sum_i \alpha(E_\theta(\mathbf{x}_i^+)^2 + E_\theta(\mathbf{x}_i^-)^2) + E_\theta(\mathbf{x}_i^+) - E_\theta(\mathbf{x}_i^-)$

Update θ based on $\Delta\theta$ using Adam optimizer

$\mathcal{B} \leftarrow \mathcal{B} \cup \tilde{\mathbf{x}}_i$

end while

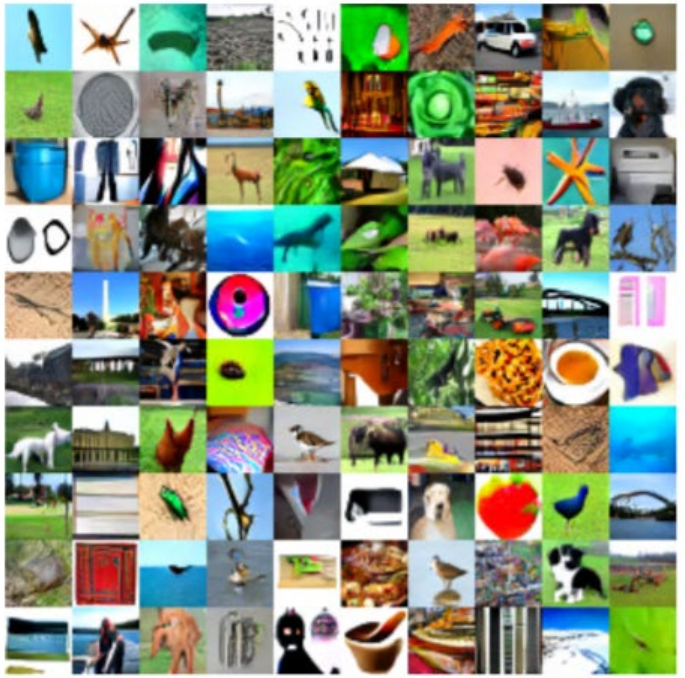


Figure 2: Conditional ImageNet32x32 EBM samples

Learning continuous-space EBMs

The algorithm from (Song, Ermon '19)

Not likelihood based, instead fit the **score** of the distribution:

$$\mathbb{E}_{p_{data}} ||\nabla_x \log p_{data}(x) - s_\theta(x)||^2$$

Turns out to be re-writeable (integration by parts) as:

$$\mathbb{E}_{p_{data}} \left[tr\left(\nabla s_\theta(x)\right) + \frac{1}{2}||s_\theta(x)||^2\right]$$

To alleviate multimodality, they use a variant of ***simulated tempering,*** which we saw last time.

They also use ***smoothing by convolving*** with Gaussians to account for points with bad estimates of $E_\theta(x)$.

Learning continuous-space EBMs

The algorithm from (Song, Ermon '19)

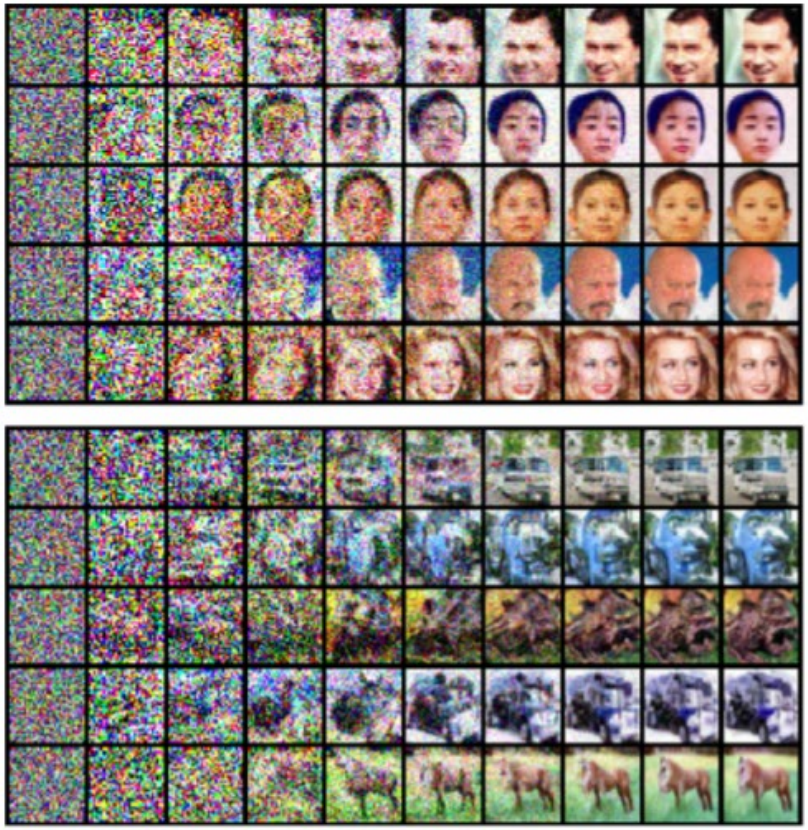


Figure 4: Intermediate samples of annealed Langevin dynamics.

Learning continuous-space EBMs

The algorithm from (Song, Ermon '19)

(a) MNIST (b) CelebA (c) CIFAR-10

Figure 5: Uncurated samples on MNIST, CelebA, and CIFAR-10 datasets.