10417-617 Deep Learning: Fall 2019

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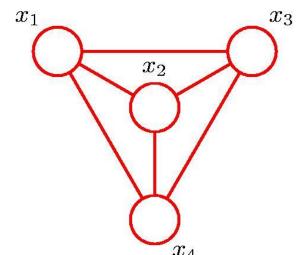
Machine Learning Department

Lecture 11:

Graphical models, directed and undirected

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:

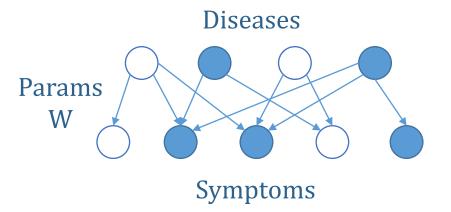
- **Bayesian networks**, also known as Directed Graphical Models (the links have a particular directionality indicated by the arrows)
- Markov Random Fields, also known as Undirected Graphical Models (the links do not carry arrows and have no directional significance).

Directed Graphs are useful for expressing causal relationships between random variables.

Your **symptoms**: fever + red spots.

Probability that you have measles?

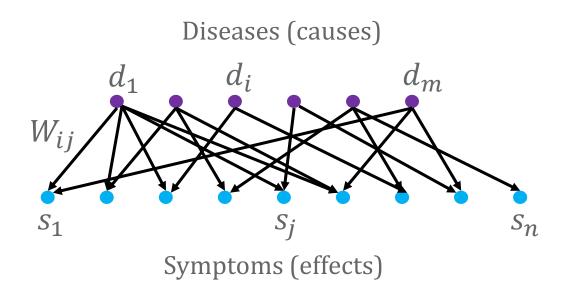




Bayesian network succinctly describes Pr[symptom| diseases]

Noisy-OR networks

 $d_i, s_j \in \{0,1\}$ $W_{ij} \ge 0$



Secondary Each d_i is on **independently** with prob. ρ Secondary When d_i is on, it **activates** s_j with probability $1 - \exp(-W_{ij})$.
Secondary s_j is **on** if one of d_i 's **activates** s_j

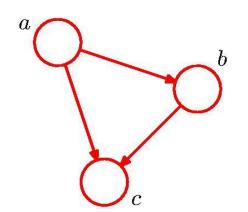
Directed Graphs are useful for expressing causal relationships between random variables.

"Deriving" Bayesian Networks as restrictions of arbitrary distributions:

An **arbitrary** joint distribution p(a,b,c) over three random variables a,b, and c can be written as

$$p(a,b,c) = p(c|a,b)p(a,b) = p(c|a,b)p(b|a)p(a)$$

Associate a graph with the decomposition:



- Node for each of the random variables.
- Add **directed** links to the graph from the nodes corresponding to the vars on which the distribution is conditioned.

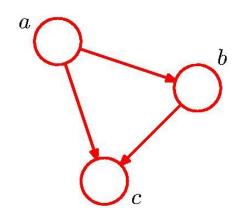
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Associate a graph with the decomposition:



Different ordering => different graphical representation.

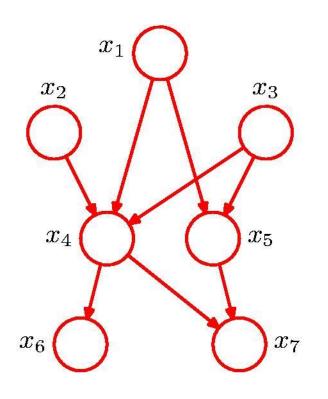
Joint distribution over K variables factorizes:

$$p(x_1,\ldots,x_K) = p(x_K|x_1,\ldots,x_{K-1})\ldots p(x_2|x_1)p(x_1)$$

Corresponding undirected graph is fully connected:

(as each lower-numbered node points to each higher-numbered node)

A graph that is **not** fully connected conveys information about the conditional independence structure of the distribution it encodes.



E.g. consider the graph on the left.

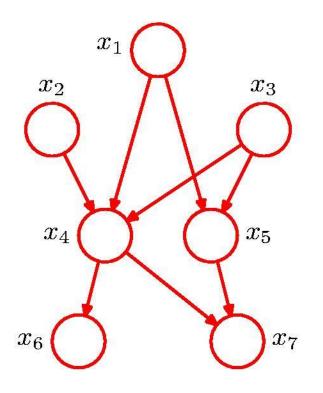
It encodes distributions over $x_1,...,x_7$ that can be written as the product:

$$p(x_1, \dots, x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)$$
$$p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)$$

Note the change from the previous slide: e.g. x_5 is **not** conditioned on all of $x_{1,} x_{2,} x_{3,} x_4$ but only on $x_{1,} x_{3,}$

The general case: factorization

The joint distribution defined by the graph is given by the product of a conditional distribution for each node conditioned on its parents:



$$p(\mathbf{x}) = \prod_{k=1}^{K} p(x_k | \mathbf{pa}_k)$$

where pa_k denotes a set of parents for the node x_k .

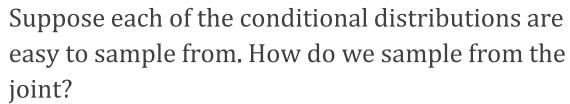
Each of the conditional distributions will typically have some parametric form. (e.g. product of Bernoullis in the noisy-OR case)

Important restriction: There must be **no directed cycles!** (i.e. graph is a DAG)

Crucial property: easy sampling

Consider a joint distribution over K random variables $p(x_1, x_2, ..., x_K)$ t factorizes as:

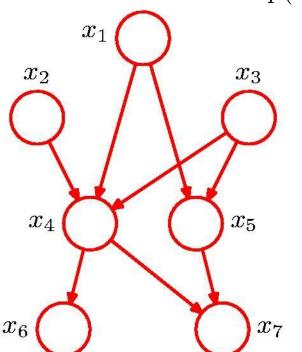
$$p(\mathbf{x}) = \prod_{k=1}^{N} p(x_k | \mathbf{pa}_k)$$



Start at the top and sample in order.

$$\hat{x}_1 \sim p(x_1)$$
 The parent variables are set to their sampled values $\hat{x}_4 \sim p(x_4|\hat{x}_1,\hat{x}_2,\hat{x}_3)$ $\hat{x}_5 \sim p(x_5|\hat{x}_1,\hat{x}_3)$

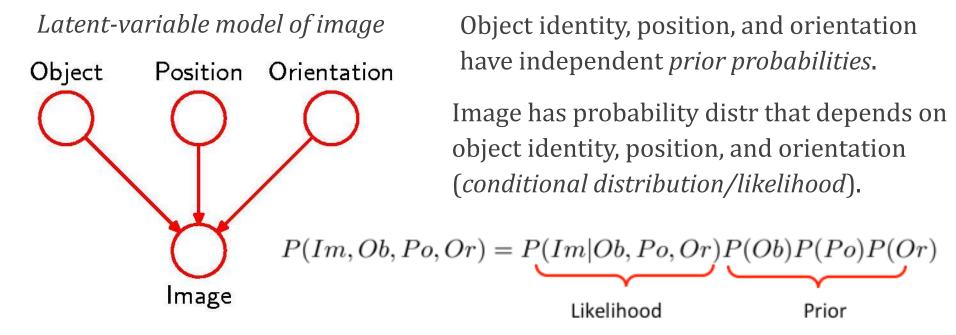
To obtain a sample from the marginal distribution, e.g. $p(x_2, x_5)$, sample from the full joint distribution, retain \hat{x}_2, \hat{x}_5 , discard the remaining values.



Typical deep learning application

Higher-up nodes will typically represent latent (hidden) random variables.

The role of latent variables is to allow modeling a **complicated** distribution over observed variables **constructed** from **simpler** conditional distributions.



Likelihood and prior are modeled by parametric distribution whose parameters are fitted throughout training.

Why restrict connectivity?

Why would we not want fully connected graphs?

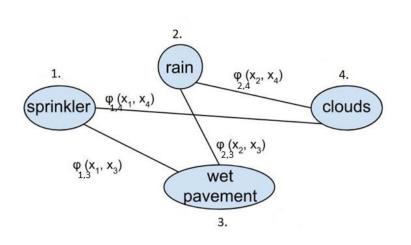
Restricts the richness of the class!!

Consider discrete joint distribution over n variables, where each variable takes one of k values.

To **fully** specify it in general, we need the values of probabilities of every possibly outcome – so we need to specify k^n values.

To specify the conditionals $p(x_1|x_2,x_3,...x_d)$ we need to specify k^d values. Hence, in a graph of in-degree at most d, we need to specify at most n $k^d \ll k^n$ values!!

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

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

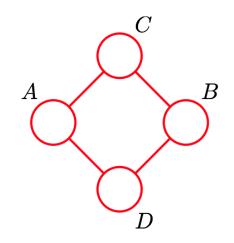
Typically the interactions are thought of as "soft constraints"

Unlike Bayesian networks, sampling is hard: partition function

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

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

Undirected graphical models or Markov Random Fields (MRFs)



More generally, we'd like to be able to define distribution in terms of "local" interactions.

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

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

For example, the joint distribution above factorizes as:

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

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.

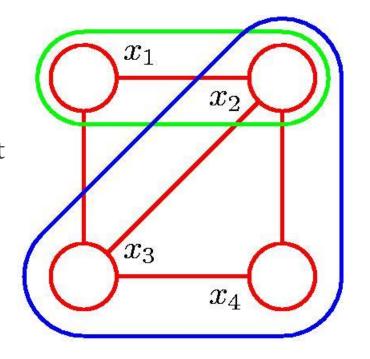
Maximal Clique: a clique such that it is not possible to include any other nodes in the set without it ceasing to be a clique.



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



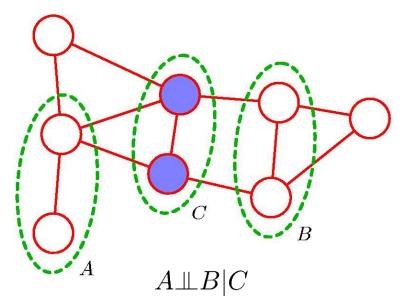
$${x_1, x_2, x_3}, {x_2, x_3, x_4}.$$



Why this odd parametrization?

- Why Markov Random Fields
 - Conditional independence (Hammersley-Clifford Theorem)

Conditional Independence

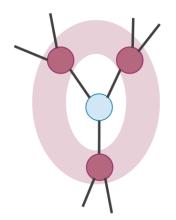


Nodes in A, B are independent, given a set of nodes C separating A, B

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

Equivalently:

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



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

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

Conditional Independence and Factorization

Surprisingly, converse holds too. 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.

Why this odd parametrization?

- Why Markov Random Fields
 - Conditional independence (Hammersley-Clifford)
 - Maximum entropy (Jaynes; sufficient statistics)

Jaynes principle: The distribution p that maximizes the entropy H(p), subject to the constraints $\mathbb{E}_p[\phi_C(x_C)] = \mu_C$, for some pre-specified values of μ_C has the form

$$p(x) \propto \exp\left(\sum_{C} w_{c} \phi_{C}(x_{C})\right)$$

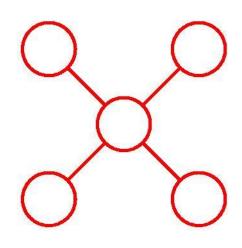
for some weights w_c depending on μ_C

Why this odd parametrization?

- Why Markov Random Fields
 - Conditional independence (Hammersley-Clifford)
 - Maximum entropy (Jaynes; sufficient statistics)
 - **❖** Encode "energy" as distribution

Energy interpretation

Rewriting the form of the distribution ever so slightly, we get:



$$p(\mathbf{x}) = \frac{1}{\mathcal{Z}} \prod_{C} \phi_C(x_C) = \frac{1}{\mathcal{Z}} \exp(-\sum_{C} E(x_c))$$

Thus, p is a distribution putting more mass on configurations that minimize a certain energy (Like a *sampling version* of loss minimization)

Configurations with high probabilities are those that find a *good balance* in satisfying the (possibly conflicting) influences of the clique potentials.

Why this odd parametrization?

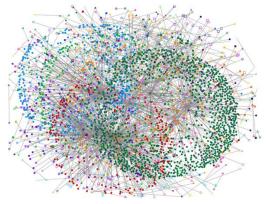
- Why Markov Random Fields
 - Conditional independence (Hammersley-Clifford)
 - Maximum entropy (Jaynes; sufficient statistics)
 - Encode "energy" as distribution
 - **❖** Interpretable, compact

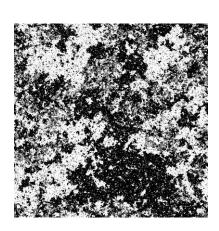
Can be misleading!

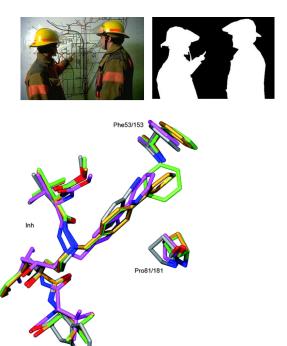
There are simple cases where variables far away in the graph are more strongly correlated than neighbors!!

Some applications







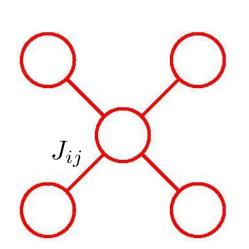


Simplest example: multivariate Gaussian

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



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

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

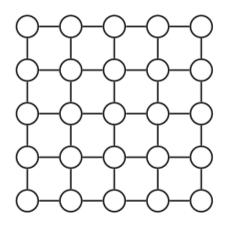
$$\mathbf{x}^T J \mathbf{x} = \sum_i J_{ii} x_i^2 + 2 \sum_{ij \in E} J_{ij} x_i x_j,$$

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

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

Discrete MRFs

MRFs with binary variables are sometimes called <u>Ising models</u> in statistical mechanics, and <u>Boltzmann machines</u> 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:

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

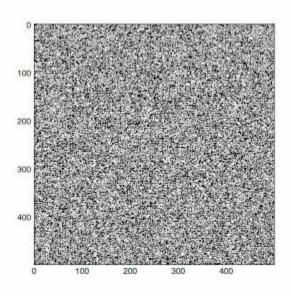
The conditional distribution is given by logistic (only depends on nbrhood!):

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

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

Example: Ferromagnetic Ising models

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

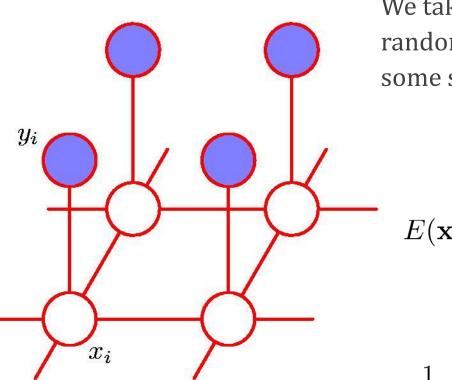


If $\theta_{ij} \geq 0$: the model is called ferromagnetic, and is used in physics to model the atomic structure (spins) of iron.

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 are likely to have the same sign $E(\mathbf{x},\mathbf{y}) = h \sum_i x_i - \beta \sum_{\{i,j\}} x_i x_j - \eta \sum_i x_i y_i$

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

Noisy and clean pixels are likely to have the same sign

Neighboring pixels

Modeling pros/cons of directed and undirected models

MRFs

- S Hard to draw samples (In fact, #P-hard provably, even in Ising models)
- Models independence structure directly
- Soft Captures soft constraints/energy

Bayesian networks

Second Easy to draw samples



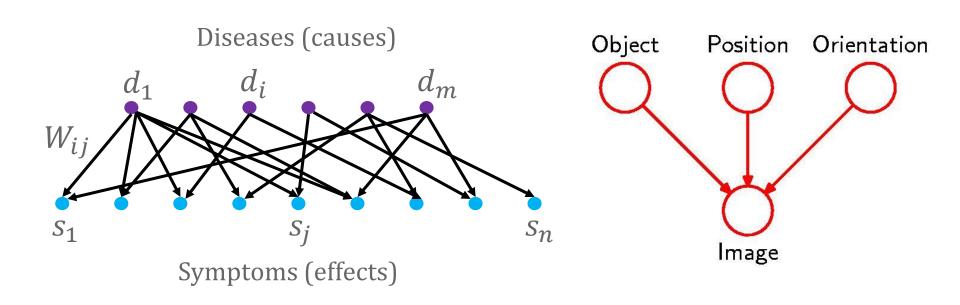
Models independence structure indirectly



S Captures "causal structure"

Latent variable models

More often than not, we need to model part of the data that is **not observable**. We already saw examples of this:



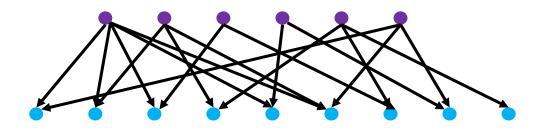
This is also a natural way to extract **features/representation**: the latent variables contain "meaningful" information.

Bayesian networks with latent variables

Simple, but powerful paradigm:

single-layer Bayesian networks, where top nodes are latent.

Latent variables Z



Observable variables X

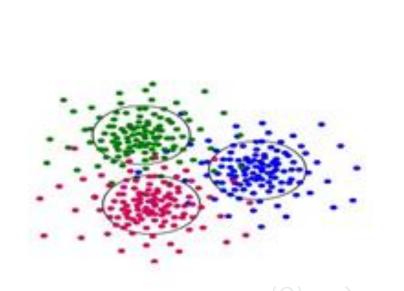
$$p_{\theta}(X,Z) = p_{\theta}(Z) p_{\theta}(X|Z)$$

Example 1: Mixture distributions

Mixture models: observables = points; latent = clustering

To draw a sample (X,Z):

Sample *Z* from a categorial distr. on K components with parameters $\{\pi_i\}$ Sample X from the corresponding component in the mixture.

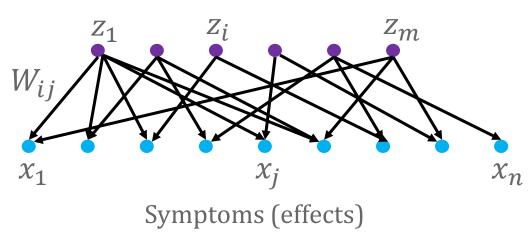


$$orall k: \pi_k \geqslant 0$$
 $\sum_{k=1}^K \pi_k = 1$ $p(\mathbf{x}) = \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{x}|oldsymbol{\mu}_k, oldsymbol{\Sigma}_k)$ Component Mixing coefficient

Example 2: Noisy-OR networks

 $x_i, z_j \in \{0, 1\}$ $W_{ij} \ge 0$



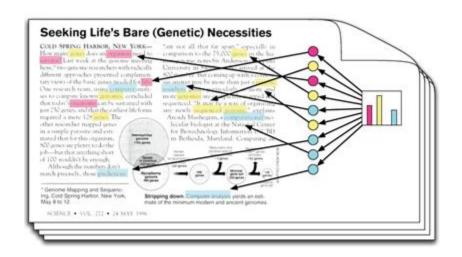


Sample each z_i is on **independently** with prob. ρ When z_i is on, it **activates** x_j with probability $1 - \exp(-W_{ij})$. So x_j is **on** if one of z_i 's **activates** x_j



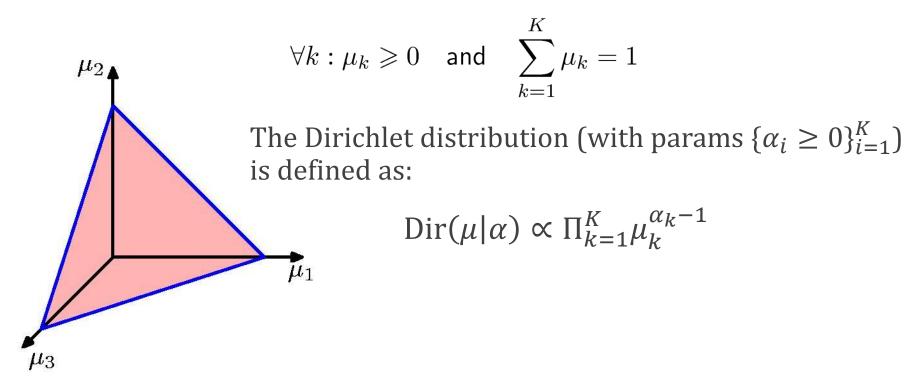
Example 3: Topic models (LDA)

Latent Dirichlet Allocation: famous model for modeling topic structure of documents of text. (Blei, Ng, Jordan '03)



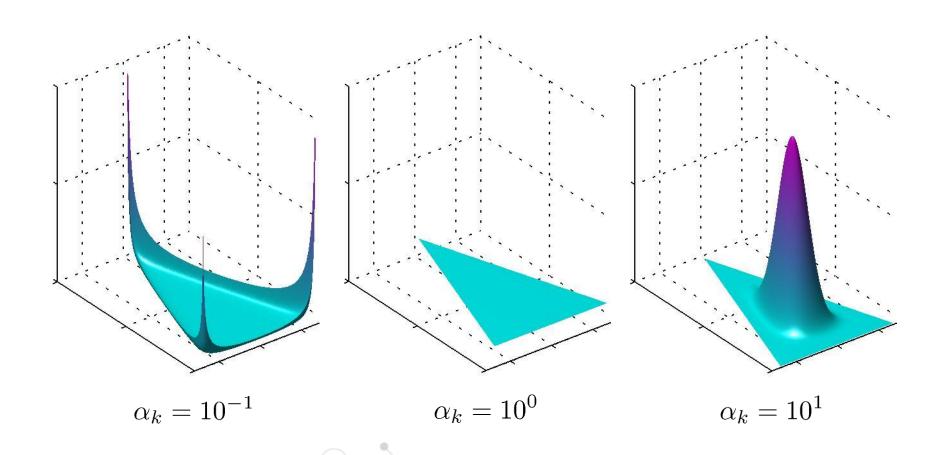
Dirichlet Distribution

Consider a distribution over simplex, namely over points $\{\mu_i\}_{i=1}^K$



Dirichlet Distribution

Plots of the Dirichlet distribution over three variables.

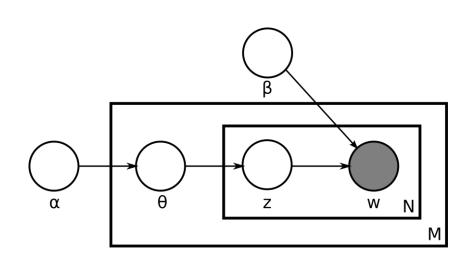


Example 3: Topic models (LDA)

Defines a distribution over documents, involving K topics.

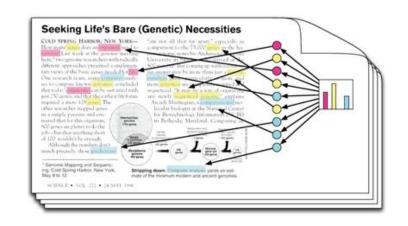
The **parameters** are: $\{\alpha_i\}_{i=1}^K$ (Dirichlet parameters) and matrix $\beta \in \mathbb{R}_+^{N \times K}$, where N is the size of the vocabulary.

The columns of β satisfy $\sum_{j=1}^{N} \beta_{ij} = 1$ (the distribution of words in a topic i)



To produce document:

- First, sample $\theta \sim \text{Dir}(\cdot | \alpha)$: this will be the topic proportion vector for the document.
- Each word in the document is generated in order, independently.
- ❖ To generate word i:
 - **Sample topic** z_i with categorical distribution with parameters θ
 - Sample word w_i with categorical distribution with parameters β_{z_i}



Example 3: Topic models (LDA)

"Arts"	"Budgets"	"Children"	"Education"
"Arts" NEW FILM SHOW MUSIC MOVIE PLAY MUSICAL BEST ACTOR FIRST YORK OPERA THEATER	"Budgets" MILLION TAX PROGRAM BUDGET BILLION FEDERAL YEAR SPENDING NEW STATE PLAN MONEY PROGRAMS	"Children" CHILDREN WOMEN PEOPLE CHILD YEARS FAMILIES WORK PARENTS SAYS FAMILY WELFARE MEN PERCENT	"Education" SCHOOL STUDENTS SCHOOLS EDUCATION TEACHERS HIGH PUBLIC TEACHER BENNETT MANIGAT NAMPHY STATE PRESIDENT
ACTRESS LOVE	GOVERNMENT CONGRESS	CARE LIFE	ELEMENTARY HAITI

The William Randolph Hearst Foundation will give \$1.25 million to Lincoln Center, Metropolitan Opera Co., New York Philharmonic and Juilliard School. "Our board felt that we had a real opportunity to make a mark on the future of the performing arts with these grants an act every bit as important as our traditional areas of support in health, medical research, education and the social services," Hearst Foundation President Randolph A. Hearst said Monday in announcing the grants. Lincoln Center's share will be \$200,000 for its new building, which will house young artists and provide new public facilities. The Metropolitan Opera Co. and New York Philharmonic will receive \$400,000 each. The Juilliard School, where music and the performing arts are taught, will get \$250,000. The Hearst Foundation, a leading supporter of the Lincoln Center Consolidated Corporate Fund, will make its usual annual \$100,000 donation, too.

The main algorithmic difficulty

Recall, sampling from Bayesian networks is easy.

But: sampling from the posterior distribution P(Z|X) is **hard**:

$$P(Diseases, Symptoms) = P(Diseases) P(Symptoms|Diseases)$$

Latent

Data

Simple, explicit

By Bayes rule, $P(\text{Diseases}|\text{Symptoms}) \propto P(\text{Diseases},\text{Symptoms})$

Up to normalizing const, simple...

Complicated partition function:

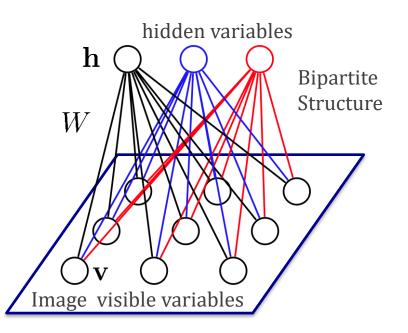
$$\sum_{\text{Diseases}} P(\text{Diseases, Symptoms})$$

Again, can be #P-hard to sample from!!

Restricted Boltzmann Machines

An **undirected** latent-variable model

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



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

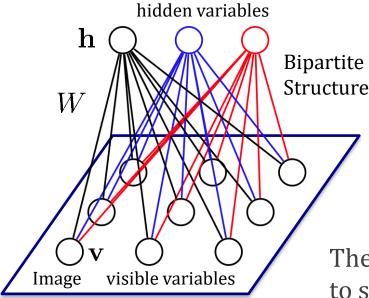
The energy of the joint configuration:

$$\begin{split} E(\mathbf{v},\mathbf{h};\theta) &= -\sum_{ij} W_{ij} v_i h_j - \sum_i b_i v_i - \sum_j a_j h_j \\ \theta &= \{W,a,b\} \text{ model parameters.} \end{split}$$

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

$$P_{\theta}(\mathbf{v}, \mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left(-E(\mathbf{v}, \mathbf{h}; \theta)\right) = \frac{1}{\mathcal{Z}(\theta)} \prod_{ij} e^{W_{ij}v_i h_j} \prod_{i} e^{b_i v_i} \prod_{j} e^{a_j h_j}$$
$$\mathcal{Z}(\theta) = \sum_{i} \exp\left(-E(\mathbf{v}, \mathbf{h}; \theta)\right)$$

Restricted Boltzmann Machines



Restricted: No interaction between hidden variables

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

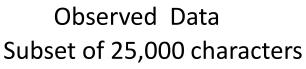
$$P(\mathbf{h}|\mathbf{v}) = \prod_{j} P(h_j|\mathbf{v}) \quad P(h_j = 1|\mathbf{v}) = \frac{1}{1 + \exp(-\sum_{i} W_{ij} v_i - a_j)}$$

Similarly:

Factorizes

$$P(\mathbf{v}|\mathbf{h}) = \prod_{i} P(v_i|\mathbf{h}) \quad P(v_i = 1|\mathbf{h}) = \frac{1}{1 + \exp(-\sum_{j} W_{ij} h_j - b_i)}$$

Restricted Boltzmann Machines





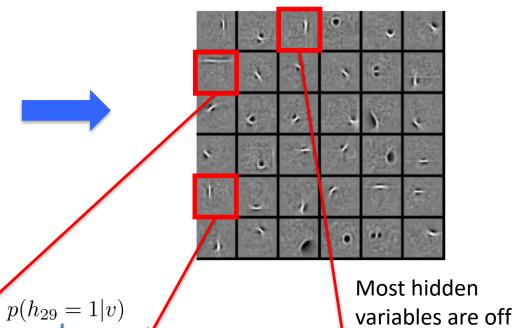
New Image:

$$= \sigma \bigg(0.99 \times \bigg)$$

 $p(h_7 = 1|v)$

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

Learned W: "edges"
Subset of 1000 features



+ 0.97 \times + 0.82 \times

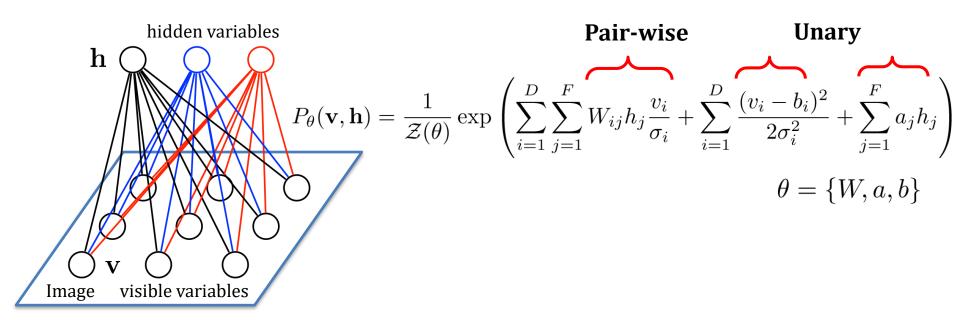
Logistic Function: Suitable for modeling binary images

Represent:



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

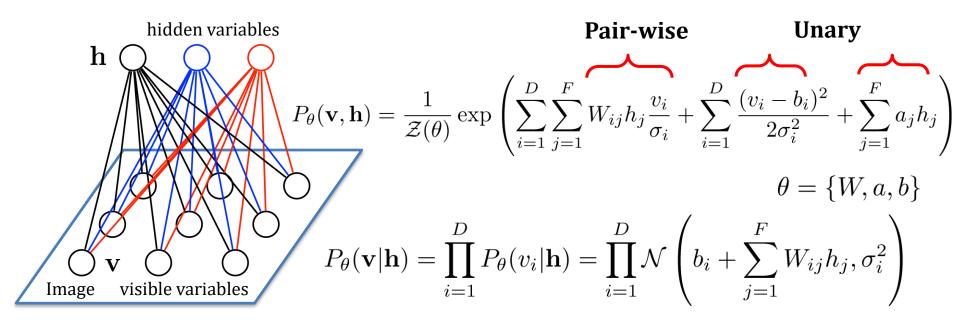
Gaussian Bernoulli RBMs



$$P(v_i = x | \mathbf{h}) = \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left(-\frac{(x - b_i - \sum_j W_{ij} h_j)^2}{2\sigma_i^2}\right) \quad \text{Gaussian}$$

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

Gaussian Bernoulli RBMs

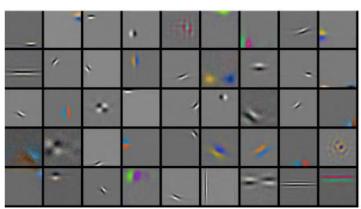


4 million unlabelled images





Learned features (out of 10,000)



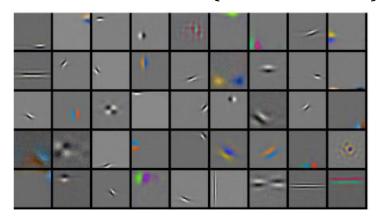
Gaussian Bernoulli RBMs

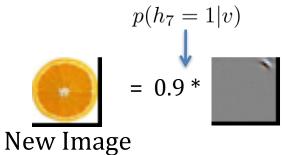
4 million **unlabelled** images

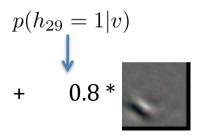




Learned features (out of 10,000)

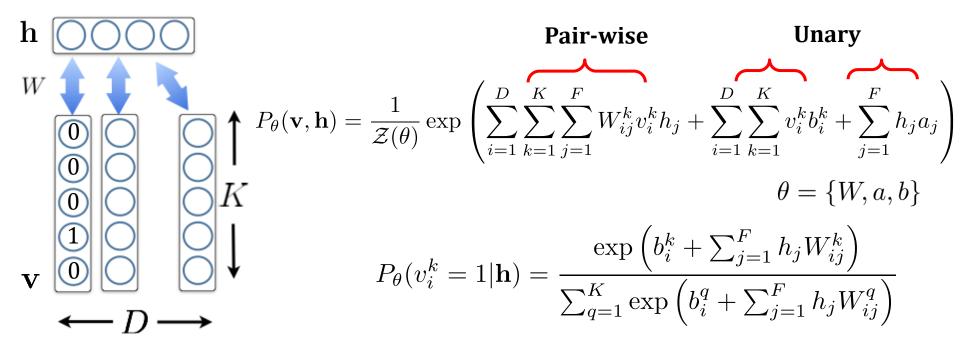








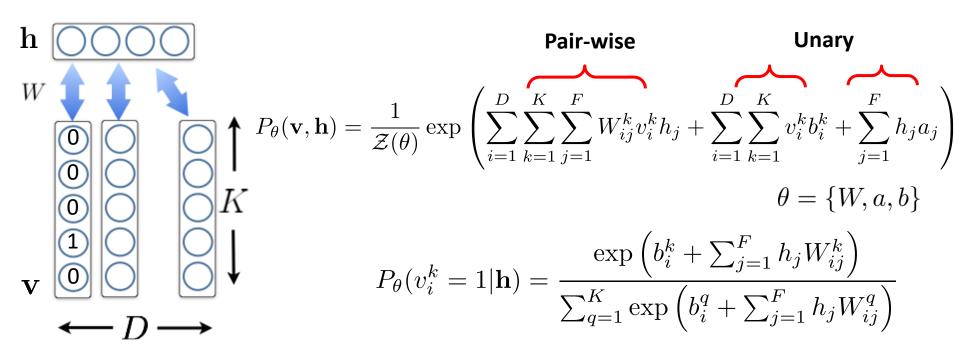
RBMs for Word Counts



Replicated Softmax Model: *undirected* topic model:

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

RBMs for Word Counts







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



russian russia moscow yeltsin soviet

Learned features: "topics"

clinton house president bill congress

computer system product software develop

trade country import world economy stock wall street point dow

RBMs for Word Counts

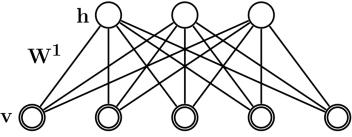
One-step reconstruction from the Replicated Softmax model.

Input	Reconstruction
chocolate, cake	cake, chocolate, sweets, dessert, cupcake, food, sugar, cream, birthday
nyc	nyc, newyork, brooklyn, queens, gothamist, manhattan, subway, streetart
dog	dog, puppy, perro, dogs, pet, filmshots, tongue, pets, nose, animal
flower, high, 花	flower, 花, high, japan, sakura, 日本, blossom, tokyo, lily, cherry
girl, rain, station, norway	norway, station, rain, girl, oslo, train, umbrella, wet, railway, weather
fun, life, children	children, fun, life, kids, child, playing, boys, kid, play, love
forest, blur	forest, blur, woods, motion, trees, movement, path, trail, green, focus
españa, agua, granada	españa, agua, spain, granada, water, andalucía, naturaleza, galicia, nieve

Collaborative Filtering

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

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

Bowling for Columbine

The People vs. Larry Flynt

Canadian Bacon La Dolce Vita

Friday the 13th

The Texas Chainsaw Massacre

Children of the Corn

Child's Play

The Return of Michael Myers

Independence Day

The Day After Tomorrow

Con Air

Men in Black II

Men in Black

Scary Movie

Naked Gun

Hot Shots!

American Pie

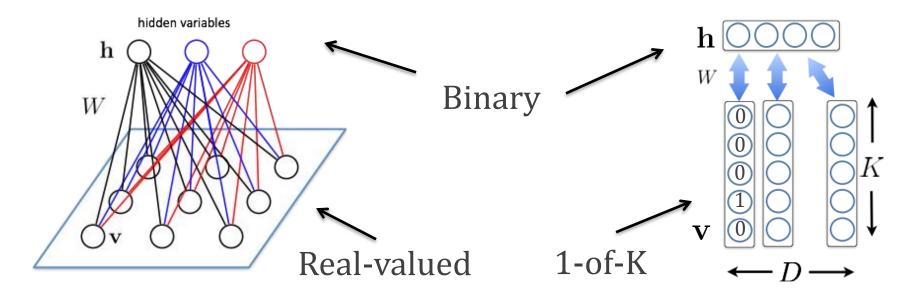
Police Academy

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

(Salakhutdinov, Mnih, Hinton, ICML 2007)

Different Data Modalities

Binary/Gaussian/Softmax RBMs: All have binary hidden variables but use them to model different kinds of data.



It is easy to infer the states of the hidden variables:

$$P_{\theta}(\mathbf{h}|\mathbf{v}) = \prod_{j=1}^{F} P_{\theta}(h_j|\mathbf{v}) = \prod_{j=1}^{F} \frac{1}{1 + \exp(-a_j - \sum_{i=1}^{D} W_{ij} v_i)}$$

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

RBM's

- S Hard to draw samples (In fact, #P-hard provably, even in Ising models)
- Second Easy to sample posterior distribution over latents



Directed models

S Easy to draw samples



Mard to sample posterior distribution over latents

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