CPSC 540: Machine Learning

Boltzmann Machines

Mark Schmidt

University of British Columbia

Winter 2019

Last Time: Learning Log-Linear UGMs

- We discussed log-linear parameterization of UGMs,

$$\phi_j(s) = \exp(w_{j,s}), \quad \phi_{jk}(s, s') = \exp(w_{j,k,s,s'}), \quad \phi_{jkl}(s, s', s'') = \exp(w_{j,k,l,s,s',s''}).$$

- The likelihood of an example x given parameter w is given by

$$p(x \mid w) = \frac{\exp\left(w^T F(x)\right)}{Z},$$

and the feature functions $F(x)$ count the number of times we use each w_j.

- This leads to a convex NLL of the form

$$-\log p(x \mid w) = -w^T F(x) + \log(Z),$$

and gradient of the form

$$\nabla_w - \log p(x \mid w) = -F(x) + \mathbb{E}[F(x)],$$

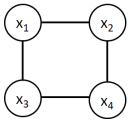
which (if you can do inference) can be optimzied with gradient descent methods.

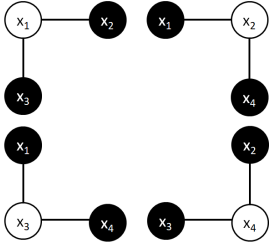
Approximate Learning: Alternate Objectives

- One way to avoid cost of inference is to change the objective:
  - Pseudo-likelihood (fast, convex, and crude):

$$p(x_1, x_2, \ldots, x_d) \approx \prod_{j=1}^{d} p(x_j \mid x_{-j}) = \prod_{j=1}^{d} p(x_j \mid x_{MB(j)}),$$

which turns learning into d single-variable problems (similar to DAGs).





Approximate Learning: Approximate Marginals

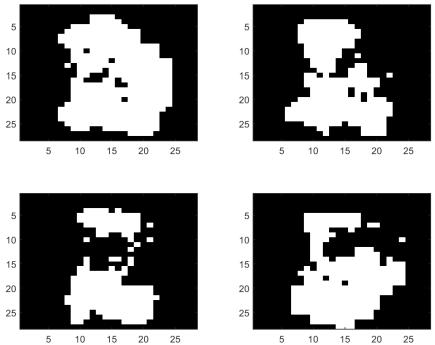
- Alternately, we can use approximate inference to use NLL:
  - Monte Carlo approximation of $\mathbb{E}[F_j(x)]$ given current parameters w:

$$\begin{aligned}\nabla f(w) &= -F(x) + \mathbb{E}[F(x)] \\ &\approx -F(x) + \underbrace{\frac{1}{t}\sum_{i=1}^{t} F(x^i)}_{\text{Monte Carlo approx}} .\end{aligned}$$

    - Simple method: generate lots of samples to approximate gradient given w, then update w (many samples per iteration, can grow batch to converge fast).
    - Younes algorithm: alternate between steps of Gibbs sampling and stochastic gradient, using 1 sample per iteration ("persistent contrastive divergence" in deep learning). (SG updates w, Gibbs updates x)
  - Deterministic variational approximations of $\mathbb{E}[F(x)]$ can alternately be used (later).

Pairwise UGM on MNIST Digits

- Samples from a lattice-structured pairwise UGM:



- Training: 100k stochastic gradient w/ Gibbs sampling steps with $\alpha_t = 0.01$.
- Samples are iteration 100k of Gibbs sampling with fixed w.

Structure Learning in UGMs

- Recall that in Ising UGMs, our edge potentials have the form

$$\phi_{ij}(x_i, x_j) = \exp(w_{ij} x_i x_j).$$

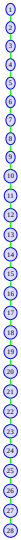
- If we set $w_{ij} = 0$, it sets $\phi_{ij}(x_i, x_j) = 1$ for all x_i and x_j.
  - Potential just "multiplies by 1", which is equivalent to removing the edge.

- L1-regularization of w_{ij} values performs structure learning in UGM.

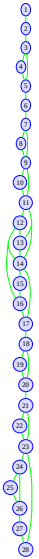
- For general log-linear, each edge has multiple parameters $w_{i,j,s,s'}$.
  - In this case we can use group L1-regularization for structure learning.
    - Each group will be all parameters $w_{i,j,\cdot,\cdot}$ associated with an edge (i, j).

Structure Learning on Rain Data

Large λ (and optimal tree):

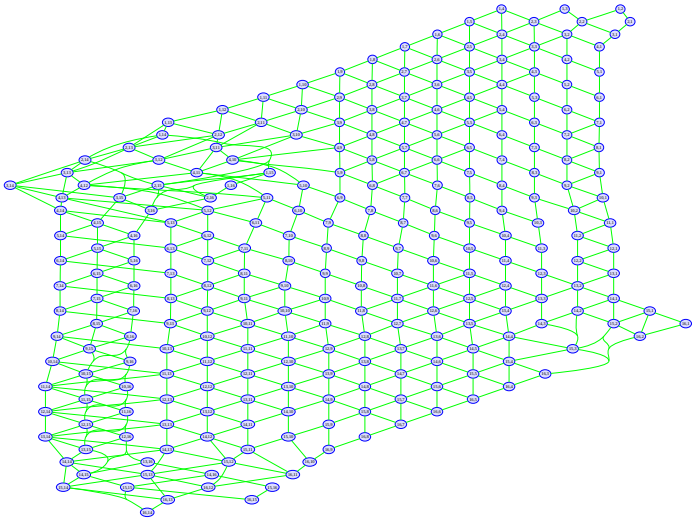


Small λ:



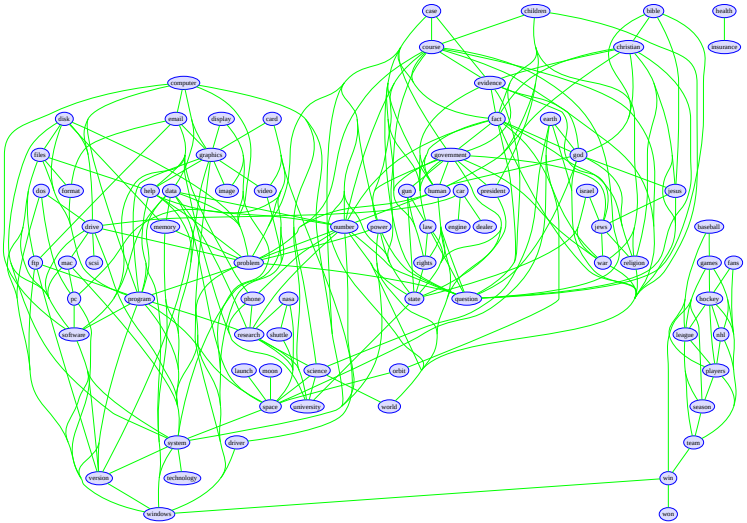
Structure Learning on USPS Digits

Structure learning of pairwise UGM with group-L1 on USPS digits:



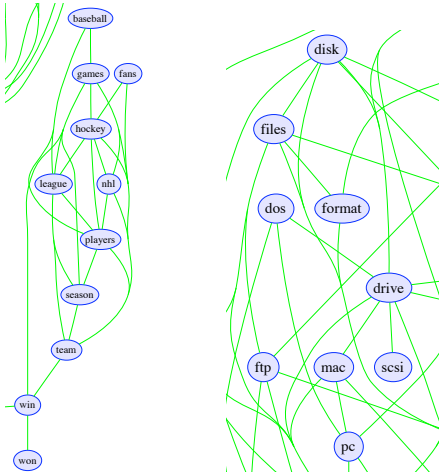
Structure Learning on News Words

Group-L1 on newsgroups data:



Structure Learning on News Words

Group-L1 on newsgroups data:



Outline

"THE REVOLUTION WILL NOT BE SUPERVISED" PROMISES FACEBOOK'S YANN LECUN IN KICKOFF AI SEMINAR

POSTED MARCH 6TH, 2018

« PRESS ROOM Facebook Twitter Print

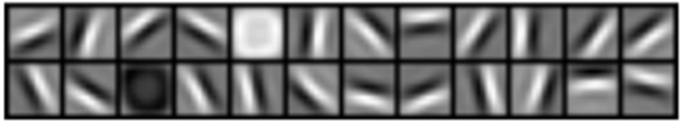
http://engineering.nyu.edu/news/2018/03/06/revolution-will-not-be-supervised-promises-facebooks-yann-lecun-kickoff-ai-seminar

Deep Density Estimation

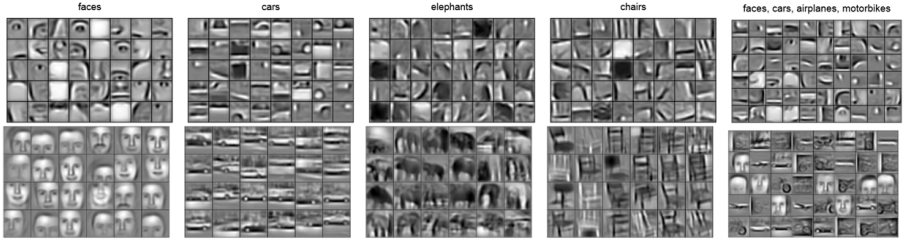
- In 340 we discussed deep learning methods for supervised learning.
- Does it make sense to talk about deep unsupervised learning?
- Standard argument:
  - Human learning seems to be mostly unsupervised.
  - Supervision gives limited feedback: bits in a class label vs. an image.
  - Could we learn unsupervised models with much less data?
- Deep belief networks started modern deep learning movement (2006).

Cool Pictures Motviation for Deep Learning

- First layer of z_i trained on 10 by 10 image patches:



- Visualization of second and third layers trained on specific objects:



http://www.cs.toronto.edu/~rgrosse/icml09-cdbn.pdf

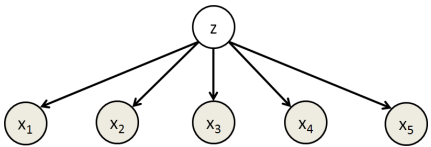
- Many classes use these particular images to motivate deep neural networks.
  - But they're not from a neural network; they're from a deep belief network.

Mixture of Independent Models

- Recall the mixture of independent models:

$$p(x) = \sum_{c=1}^{k} p(z = c) \prod_{j=1}^{d} p(x_j \mid z = c).$$

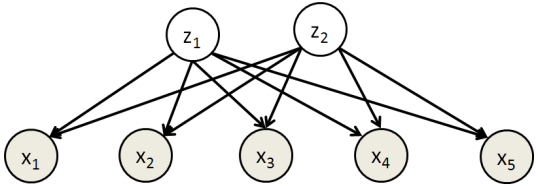
- Given z, each variable x_j comes from some "nice" distribution.



- This is enough to model *any* distribution.
  - Just need to know cluster of example x and distribution of x_j given z.
  - But not an efficient representation: number of cluster might need to be huge.

Latent DAG Model

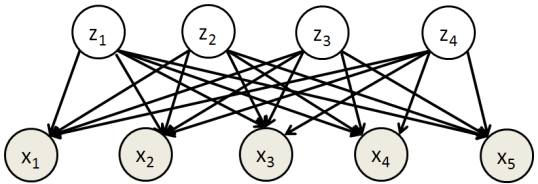
- Consider the following model with binary z_1 and z_2:



- Have we gained anything?
  - We have 4 clusters based on two hidden variables.
  - Each cluster shares a parent/part with 2 of the other clusters.

Latent DAG Model

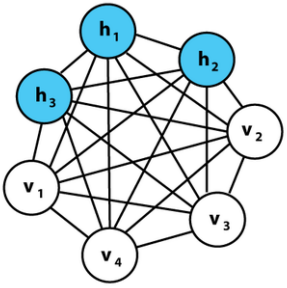
- Consider the following model:



- Now we have 16 clusters, in general we'll have 2^k with k hidden binary nodes.
  - This discrete latent-factors give combinatorial number of mixtures.
    - You can think of each z_c as a "part" that can be included or not ("binary PCA").
  - We'll assume $p(x_j \mid z_1, z_2, z_3, z_4)$ is a linear model (Gaussian, logistic, etc.).
    - Distributed representation where x is made of parts z.
    - With d visible x_j and k hidden z_j, we only have dk parameters.
  - Unfortunately, somewhat hard to use:
    - Combinatorial "explaining away" between z_c value when conditioning on x.
    - Restricted Boltzmann Machines are a similar undirected model...

Boltzmann Machines

- Boltzmann machines are UGMs with binary latent variables:

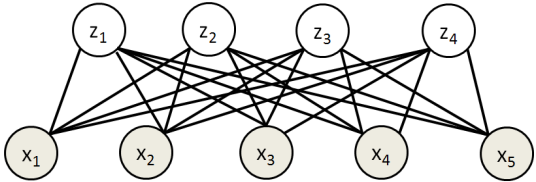


https://en.wikipedia.org/wiki/Boltzmann_machine

- Yet another latent-variable model for density estimation.
  - Hidden variables again give a combinatorial latent representation.
- Hard to do anything in this model, even if you know all the z (or x).

Restricted Boltzmann Machine

- By restricting graph structure, some things get easier:
  - Restricted Boltzmann machines (RBMs): edges only between the x_j and z_c.



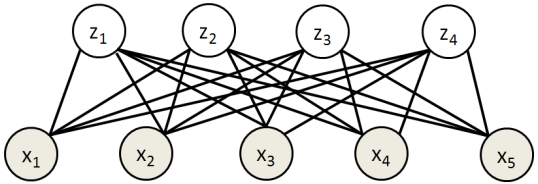
- Bipartite structure allows block Gibbs sampling given one type of variable:
  - Conditional UGM is disconnected.

- Given visible x, we can sample each z_c independently.
- Given hidden z, we can sample each x_j independently.

Restricted Boltzmann Machines

- The RBM graph structure leads to a joint distribution of the form

$$p(x,z) = \frac{1}{Z}\left(\prod_{j=1}^{d}\phi_j(x_j)\right)\left(\prod_{c=1}^{k}\phi_c(z_c)\right)\left(\prod_{j=1}^{d}\prod_{c=1}^{k}\phi_{jc}(x_j,z_c)\right).$$



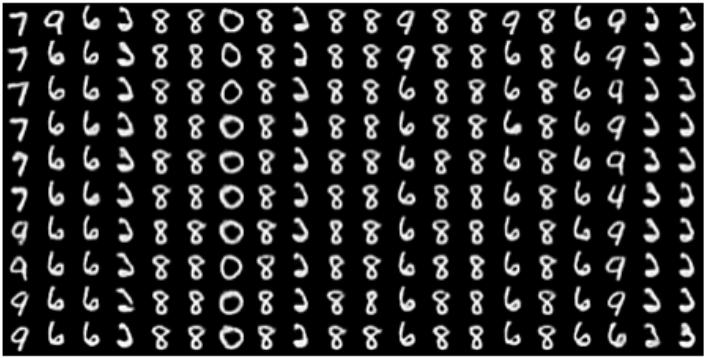
- RBMs usually use a log-linear parameterization like

$$p(x,z) \propto \exp\left(\sum_{j=1}^{d} x_j w_j + \sum_{c=1}^{k} z_c v_c + \sum_{j=1}^{d}\sum_{c=1}^{k} x_j w_{jc} z_c\right),$$

for parameters w_j, v_c, and w_{jc} (first term would be different for continuous x_j).

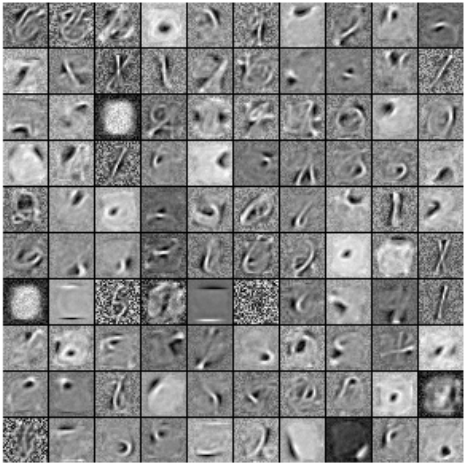
Generating Digits with RBMs

Here are the samples generated by the RBM after training. Each row represents a mini-batch of negative particles (samples from independent Gibbs chains). 1000 steps of Gibbs sampling were taken between each of those rows.



Generating Digits with RBMs

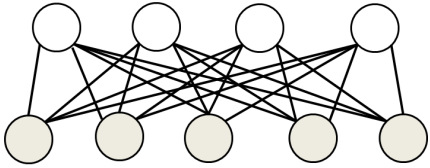
Visualizing each z_c's interaction parameters ($w_{\cdot c}$ values) as images:



http://deeplearning.net/tutorial/rbm.html

Learning UGMs with Hidden Variables

- For RBMs we have hidden variables:



- With hidden ("nuissance") variables z the observed likelihood has the form

$$p(x) = \sum_z p(x,z) = \sum_z \frac{\tilde{p}(x,z)}{Z}$$
$$= \frac{1}{Z} \underbrace{\sum_z \tilde{p}(x,z)}_{Z(x)} = \frac{Z(x)}{Z},$$

where $Z(x)$ is the partition function of the conditional UGM given x.

- $Z(x)$ is cheap in RBMs because the z are independent given x.

Learning UGMs with Hidden Variables

- This gives an observed NLL of the form

$$-\log p(x) = -\log(Z(x)) + \log Z,$$

where $Z(x)$ sums over hidden z values, and Z sums over z and x.

- The second term is convex but the first term is non-convex.
  - This is expected when we have hidden variables.

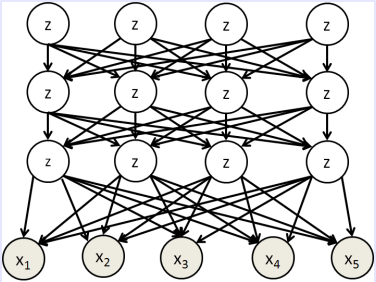
- With a log-linear parameterization, the gradient has the form

$$-\nabla \log p(x) = -\mathbb{E}_{z \mid x}[F(X, Z)] + \mathbb{E}_{z,x}[F(X, Z)].$$

- For RBMs, first term is cheap due to independence of z given x.
- We can approximate second term using block Gibbs sampling.
  - For other problems, you would also need to approximate first term.

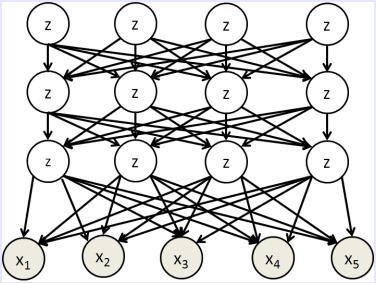
Deep Belief Networks

- Deep belief networks add are latent DAGs with more binary hidden layers:



- Data is at the bottom.
- First hidden layer could be "basic ingredients".
- Second hidden layer could be general "parts".
- Third hidden layer could be "abstract concept".

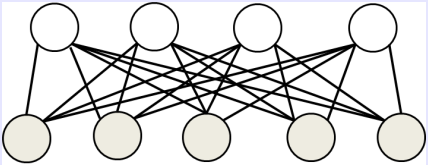
Deep Belief Networks



- If we were conditioning on *top* layer:
  - Sampling would be easy.
- But we're conditioning on the *bottom* layer:
  - Everything is hard.
  - There is combinatorial "explaining away".
- Common training method:
  - Greedy "layerwise" training as a restricted Boltzmann machine.

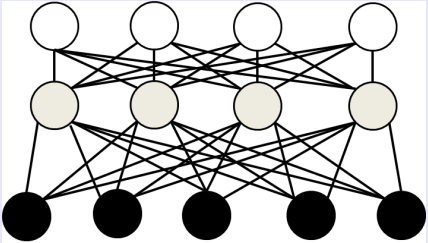
Greedy Layerwise Training of Stacked RBMs

- Step 1: Train an RBM (alternating between block Gibbs and stochastic gradient)



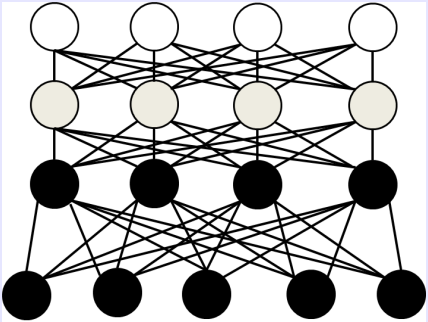
Greedy Layerwise Training of Stacked RBMs

- Step 1: Train an RBM (alternating between block Gibbs and stochastic gradient)
- Step 2:
  - Fix first hidden layer values.
  - Train an RBM.



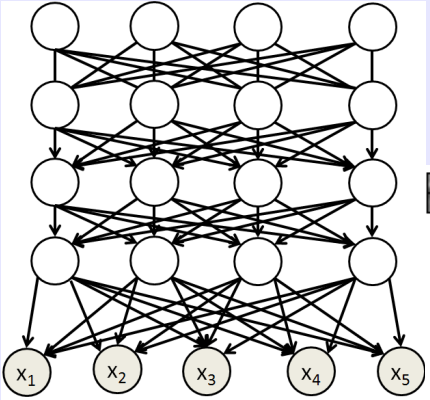
Greedy Layerwise Training of Stacked RBMs

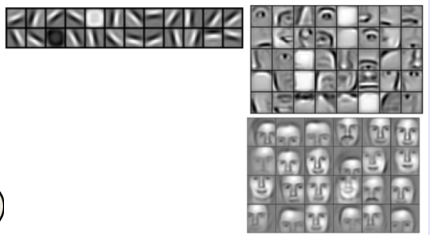
- Step 1: Train an RBM (alternating between block Gibbs and stochastic gradient)
- Step 2:
  - Fix first hidden layer values.
  - Train an RBM.
- Step 3:
  - Fix second hidden layer values.
  - Train an RBM.



Deep Belief Networks

- Keep top as an RBM.
- For the other layers, use DAG parameters that implement block sampling.
  - Can sample by running block Gibbs on top layer for a while, then ancestral sampling.

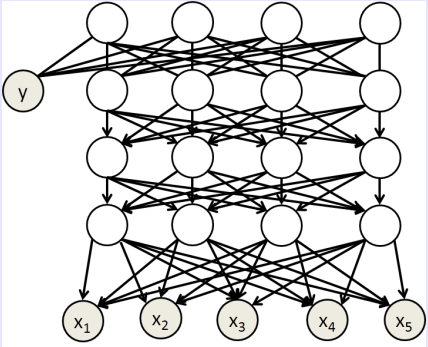




http://www.cs.toronto.edu/~rgrosse/icml09-cdbn.pdf

Deep Belief Networks

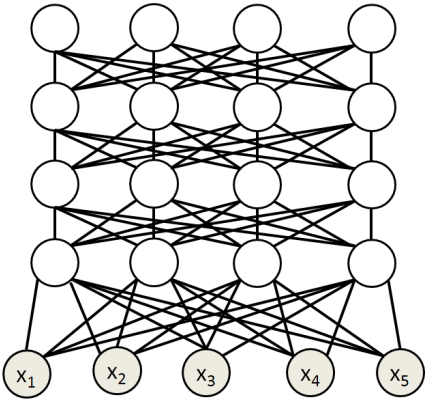
- Can add a class label to last layer.



- Can use "fine-tuning" as a feedforward neural network to refine weights.
  - `https://www.youtube.com/watch?v=KuPai0ogiHk`

Deep Boltzmann Machines

- Deep Boltzmann machines just keep as an undirected model.
  - Sampling is nicer: no explaning away within layers.
  - Variables in layer are independent given variables in layer above and below.



Deep Boltzmann Machines

- Performance of deep Boltzmann machine on NORB data:

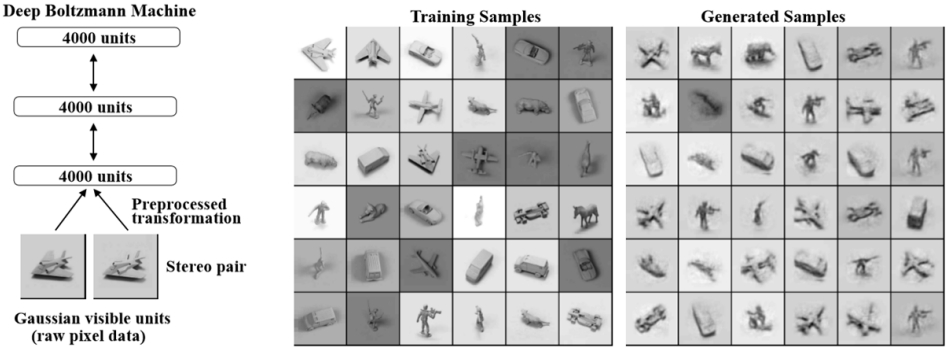


Figure 5: **Left:** The architecture of deep Boltzmann machine used for NORB. **Right:** Random samples from the training set, and samples generated from the deep Boltzmann machines by running the Gibbs sampler for 10,000 steps.

http://www.cs.toronto.edu/~fritz/absps/dbm.pdf

Summary

- Approximate UGM learning:
  1. Change objective function: pseudolikelihood.
  2. Approximate marginals: Monte Carlo or variational methods.
- Structure learning in UGMs with [group] L1-regularization.
- Boltzmann machines are UGMs with binary hidden variables.
  - Restricted Boltzmann machines only allow connections between hidden/visible.
- Deep belief networks and Boltzmann machines have layers of hidden variables.
- Next time: we'll use these tools for supervised learning.