# CPSC 540: Machine Learning

## More DAGs, Undirected Graphical Models

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Winter 2017

# Admin

- Assignment 4:
  - Due March 20.

# Last Two Lectures: Directed and Undirected Graphical Models

- We've discussed the most common classes of graphical models:
  - DAG models represent probability as ordered product of conditionals,

$$p(x) = \prod_{j=1}^{d} p(x_j | x_{\mathsf{pa}(j)}),$$

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    and are also known as “Bayesian networks” and “belief networks”.

  - UGMs represent probability as product of non-negative potentials $\phi_c$,

$$p(x) = \frac{1}{Z} \prod_{c \in \mathcal{C}} \phi_c(x_c), \quad \text{with} \quad Z = \sum_x \prod_{c \in \mathcal{C}} \phi_c(x_c),$$

    and are also known as “Markov random fields” and ”Markov networks”.

- We saw how to write Gaussians as special cases, today we focus on discrete $x_j$.

# Last Time: Conditional Independence in UGMs

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- The independence assumptions in DAGs were defined by

$$p(x_j | x_{1:j-1}) = p(x_j | x_{\text{pa}(j)}),$$

that we're independent of previous non-parents given parents.

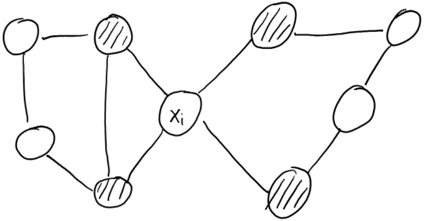
- In UGMs there is no order and we instead have a local Markov property,

$$p(x_j | x_{1:d}) = p(x_j | x_{\text{nei}(j)}),$$

that we're independent of all non-neighbours given neighbours in the graph.

# Markov Blanket

- Markov blanket is the set nodes that make you independent of all other nodes.

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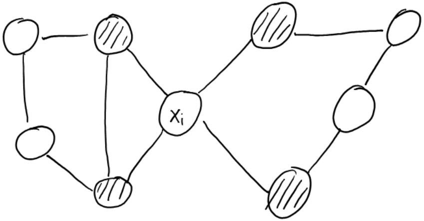
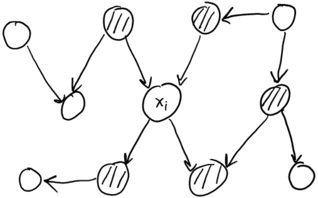



  - In UGMs the Markov blanket is the neighbours.
- Markov blanket in DAGs is all parents, children, and co-parents:



# Outline


1. Complexity of Inference in Graphical Models
2. ICM and Gibbs Sampling
3. Variational Inference

# Inference in Discrete Graphical Models

- Common inference tasks in graphical models:
  1. Compute $p(x)$ for an assignment to the variables $x$.
  2. Generate a sample $x$ from the distribution.
  3. Compute univariate marginals $p(x_j)$.
  4. Compute decoding $\text{argmax}_x\, p(x)$.
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  - For UGMs, a tree-structured graph has no cycles.

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- The above may be harder for general graphs:
  - In DAGs the first two are easy, the others are NP-hard.
  - In UGMs all of these are NP-hard.

# Moralization: Converting DAGs to UGMs

- To address the NP-hard problems, DAGs and UGMs use same techniques.
- We'll focus on UGMs, but we can convert DAGs to UGMs:

$$p(x) = \prod_{j=1}^{d} p(x_j | x_{\mathsf{pa}(j)}) = \prod_{j=1}^{d} \phi_j(x_j, x_{\mathsf{pa}(j)}).$$

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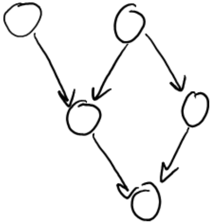

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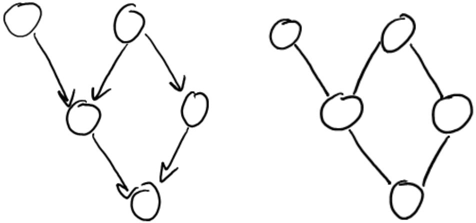

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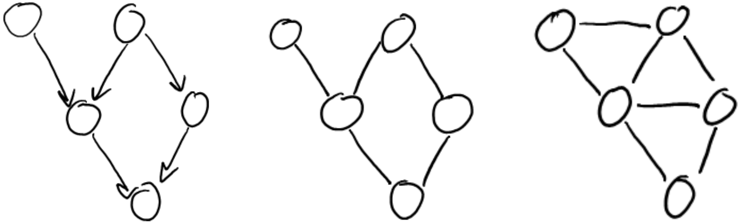

- May lose some condtional independences, but doesn't change computational cost.

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- Models that can be represented as DAGs or UGMs are called decomposable.
  - Includes chains, trees, and fully-connected graphs.
- These models allow some efficient operations.
  - E.g., we can write them as DAGs and do ancestral sampling.
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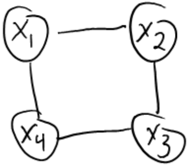
- We can perform the inference in general UGMs with message passing.
  - The algorithms for general graphs are almost identical....

# Exact Inference in UGMs

- For example, consider a UGM that is a simple 4-node cycle:




- We can compute $Z$ using

$$Z = \sum_{x_4} \sum_{x_3} \sum_{x_2} \sum_{x_1} \phi_{12}(x_1, x_2)\phi_{23}(x_2, x_3)\phi_{34}(x_3, x_4)\phi_{14}(x_1, x_4)$$

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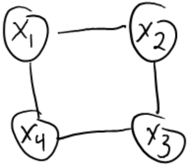


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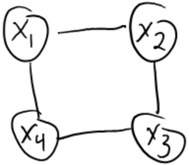


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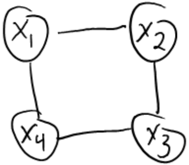


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\end{aligned}
$$

- So even though we have a chain, we have an $M$ with $k^3$ values instead of $k$.

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  - In the worst case, $\omega = (d-1)$ so there is no gain.
  - Computing $\omega$ and the optimal ordering is NP-hard.
    - But various heuristic ordering methods exist.

# Variable Order and Treewidth

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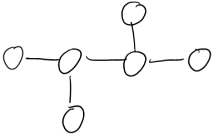

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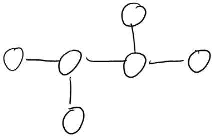
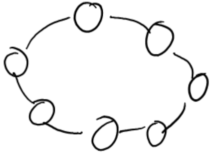


- A big loop has $\omega = 2$, so cost can be $O(dk^3)$.



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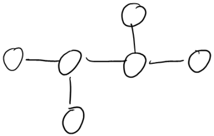

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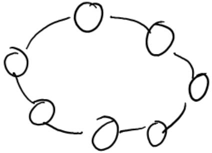
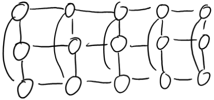


- The below grid-like structure has $\omega = 3$, so cost is $O(dk^4)$.



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- Belief propagation is generalization to trees:
  - We start at an arbitrary "root", and pass messages away from it.
  - We also start from the leaves, pass messages towards root.
- Generalization to general graphs is the junction tree method.
- Unfortunately, low tree width models are very restricted.
  - This has motivated a ton of work on approximate inference...

# Outline

1 Complexity of Inference in Graphical Models

2 ICM and Gibbs Sampling

3 Variational Inference

# Iterated Conditional Mode (ICM)

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- A special case of coordinate optimization.
- Iterations correspond to finding mode of conditional $p(x_j|x_{-j})$.

- 3 main issues:
  1. How can you optimize $p(x)$ if evaluating it is NP-hard?
  2. Is coordinate optimization efficient for this problem?
  3. Does it find the global optimum?

# ICM Issue 1: Intractable Objective

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  so we have $p(x) = \frac{\tilde{p}(x)}{Z}$.

- And for decoding we only need unnormalized probabilities,

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- To update $x_j$ we actually only need consider $\phi_c$ involving $x_j$
  - We only care about $x_{-j}$ in the Markov blanket (neighbours in the graph).

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or

$$\log p(x) = \sum_{j=1}^{d} \log \phi_j(x_j) + \sum_{(i,j)\in E} \log \phi_{ij}(x_i, x_j) + \text{constant}.$$

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which is a special case of

$$f(x) = \sum_{j=1}^{d} f_j(x_j) + \sum_{(i,j)\in E} f_{ij}(x_i, x_j),$$

which is one of our problems where coordinate optimization is efficient.

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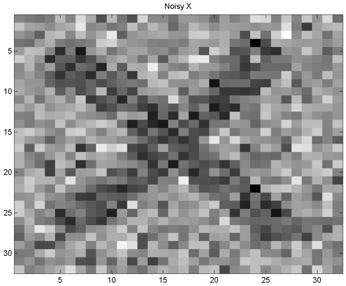
- There exist many globalization methods that can improve its performance:
  - Restarting with random initializations.
  - Simulated annealing, genetic algorithms, ant colony optimization, etc.
  - See the book/class of Holger Hoos on stochastic local search methods.

# ICM in Action

Consider using a UGM for image denoising:




We have

- Unary potentials $\phi_j$ for each position.
- Pairwise potentials $\phi_{ij}$ for neighbours on grid.
- Parameters are trained as CRF (later).

Goal is to produce a noise-free image (show video).

# Coordinate Sampling

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- In DAGs, ancestral sampling conditions on sampled values of parents,

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- In ICM, we approximately decode a UGM by iteratively maximizing an $x_{j_t}$,

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- We can approximately sample from a UGM by iteratively sampling an $x_{j_t}$,

$$x_j \sim p(x_j | x_{-j}),$$

and this coordinate-wise sampling algorithm is called Gibbs sampling.

# Gibbs Sampling

- Gibbs sampling starts with some $x$ and then repeats:
  1. Choose a variable $j$ uniformly at random.
  2. Update $x_j$ by sampling it from its conditional,

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- Analogy: sampling version of coordinate optimization:
  - Transformed $d$-dimensional sampling into $1$-dimensional sampling.

- Gibbs sampling is probably the most common multi-dimensional sampler.

# Gibbs Sampling

- For UGMs these conditionals needed for Gibbs sampling have a simple form,

$$p(x_j = c|x_{-j}) = \frac{p(x_j = c, x_{-j})}{\sum_{x_j = c'} p(x_j = c', x_{-j})} = \frac{\tilde{p}(x_j = c, x_{-j})}{\sum_{x_j = c'} \tilde{p}(x_j = c', x_{-j})},$$

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- And UGMs it further simplifies due to the local Markov property,

$$p(x_j|x_{-j}) = p(x_j|x_{\mathsf{MB}(j)}).$$

- Thus these iterations are very cheap:
  - We're just sampling a discrete variable given its Markov blanket.

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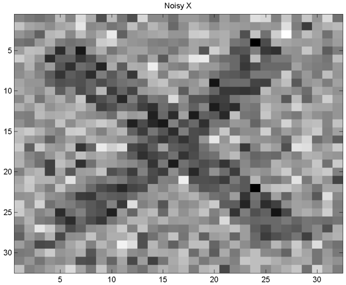
- Select random $j$ like $j = 2$.
- Sample variable $j$: $x^4 = \begin{bmatrix} 3 & \color{red}{2} & 1 & 1 \end{bmatrix}$.
- ...
- Use the samples to form Monte Carlo estimators.

# Gibbs Sampling in Action: UGMs

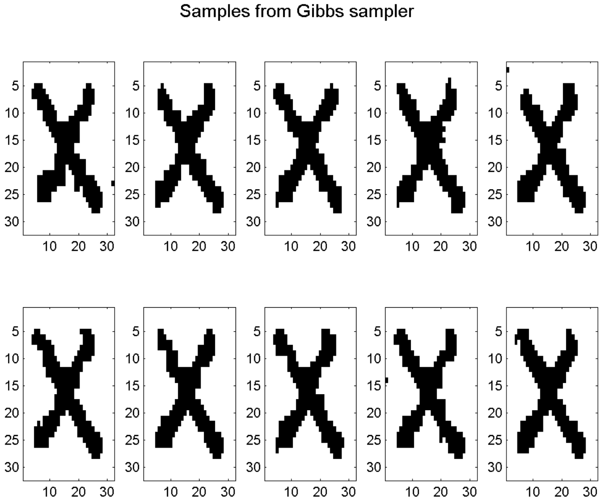
Back to image denoising...




(show videos)

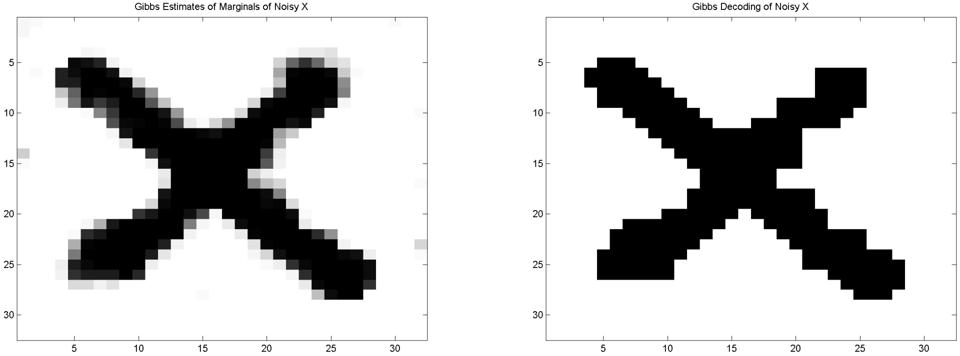
# Gibbs Sampling in Action: UGMs

Gibbs samples after every $100d$ iterations:



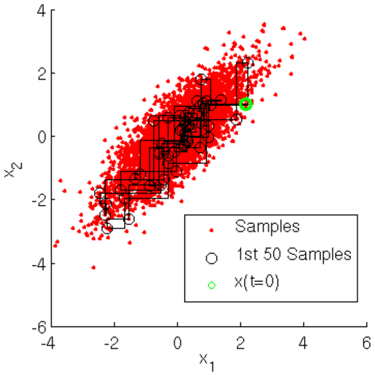
# Gibbs Sampling in Action: UGMs

Estimates of marginals and decoding based on Gibbs sampling:



# Gibbs Sampling in Action: Multivariate Gaussian

- Gibbs sampling works for general distributions.
  - E.g., sampling from multivariate Gaussian by univariate Gaussian sampling.




https://theclevermachine.wordpress.com/2012/11/05/mcmc-the-gibbs-sampler

# Gibbs Sampling and Markov Chains

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  - $p(x_j | x_{-j}) > 0$ is sufficient for Gibbs sampling.
  - A weaker condition is "irreducible and aperiodic".
- Invariant distribution $\pi$ of Gibbs sampling is the original distribution $p$.
  - If we stop it after a really long time, the final Gibbs sample will come from $p(x)$.
- A special case of Markov chain Monte Carlo (MCMC) methods.

# Markov Chain Monte Carlo (MCMC)

- Markov chain Monte Carlo (MCMC): given target $p$, design transitions such that

$$\frac{1}{n}\sum_{t=1}^{n} f(x^t) \to \sum_{x} f(x)p(x) \quad \text{and/or} \quad x^n \sim p,$$

  as $n \to \infty$.
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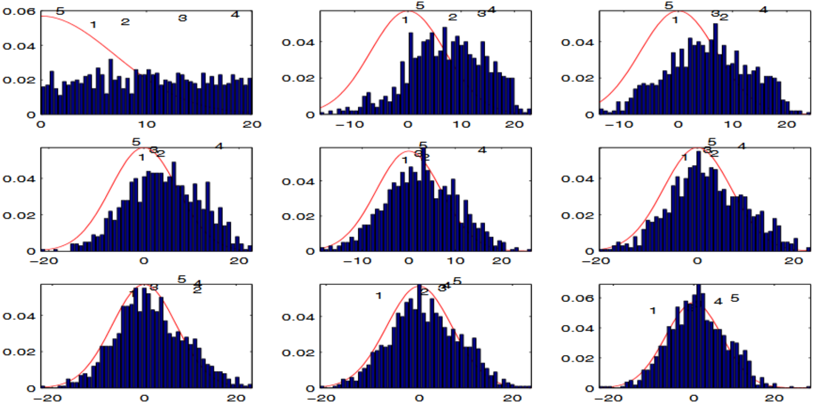
- It can very hard to diagnose if we reached invariant distribution.
  - Recent work showed that this is P-space hard (*not* polynomial-time).

# Markov Chain Monte Carlo

From top left to bottom right: histograms of 1000 independent Markov chains with a normal distribution as target distribution.



http://www.cs.ubc.ca/~arnaud/stat535/slides10.pdf

# Outline


1. Complexity of Inference in Graphical Models
2. ICM and Gibbs Sampling
3. Variational Inference

# Monte Carlo vs. Variational Inference

Two main strategies for approximate inference:

1. Monte Carlo methods:
   - Approximate $p$ with empirical distribution over samples,
     $$p(x) \approx \frac{1}{n}\sum_{i=1}^{n}\mathcal{I}[x^i = x].$$
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2. Variational methods:
    - Approximate $p$ with "closest" distribution $q$ from a tractable family,

$$p(x) \approx q(x).$$

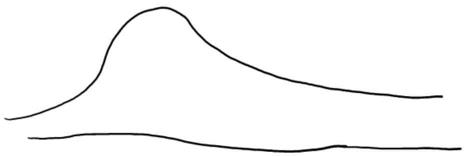
    - E.g., Gaussian, independent Bernoulli, or tree UGM.

(or mixtures of these simple distributions)

    - Turns inference into optimization.

# Variational Inference Illustration

- Approximate non-Gaussian $p$ by a Gaussian $q$:



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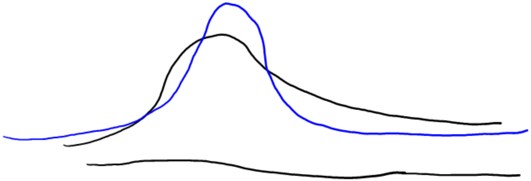

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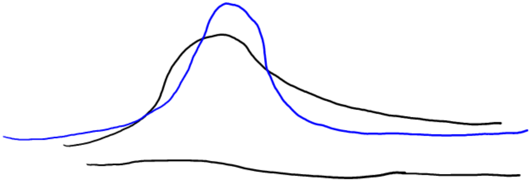
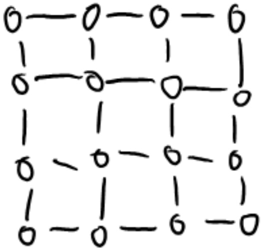


- Approximate loopy UGM by independent distribution



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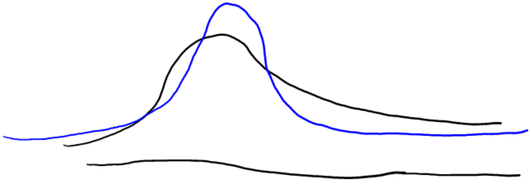

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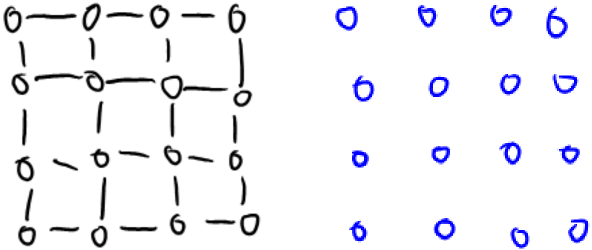

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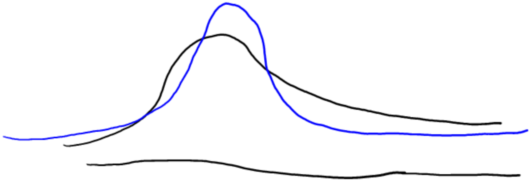
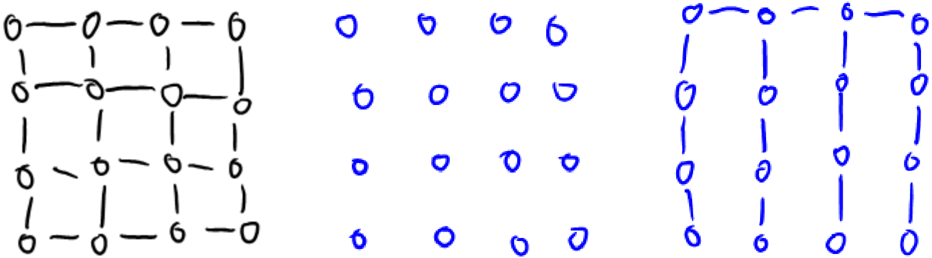


- Approximate loopy UGM by independent distribution or tree-structed UGM:



# Minimizing Reverse KL) Divergence

- Most common variational method:
  - Minimize (reverse) Kullback-Leibler (KL) divergence between $q$ and $p$,

$$\mathsf{KL}(q||p) = \sum_x q(x) \log \frac{q(x)}{p(x)}.$$

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which since KL is non-negative gives a lower bound on $\log(Z)$.

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- This is called the mean field approximation.

- Once you've fit $q$, you use the independent distribution instead of $p$.

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- Gibbs sampling is coordinate-wise sampling.
    - Special case of Markov chain Monte Carlo method.
- Variational methods approximate $p$ with a simpler distribution $q$.
    - Mean field approximation minimizes KL divergence with independent $q$.

Next time: deep graphical models and finally being able to model digits.