CPSC 540: Machine Learning

Approximate Inference

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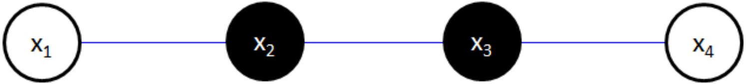
Last Lectures: Directed and Undirected Graphical Models

- We've discussed the most common classes of graphical models:
  - DAG models represent probability as ordered product of conditionals,
$$p(x) = \prod_{j=1}^{d} p(x_j \mid x_{\mathsf{pa}(j)}),$$
    and are also known as "Bayesian networks" and "belief networks".
  - UGMs represent probability as product of non-negative potentials ϕ_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 discused inference tasks (for both by converting to UGMs) in discrete x_j.
  - Cost of message passing is exponential in treewidth of graph.
  - Motivates considering approximate inference methods today.

Digression: Closure of UGMs under Conditioning

- UGMs are closed under conditioning:
  - If $p(x)$ is a UGM, then $p(x_A \mid x_B)$ can be written as a UGM (for partition A and B).

- Conditioning on x_2 and x_3 in a chain,



gives a UGM defined on x_1 and x_4 that is disconnected:

- Graphically, we "erase the black nodes and their edges".

- Notice that inference in the conditional UGM may be mucher easier.

Digression: Closure of UGMs under Conditioning

- Mathematically, a 4-node pairwise UGM with a chain structure assumes

$$p(x_1, x_2, x_3, x_4) \propto \phi_1(x_1)\phi_2(x_2)\phi_3(x_3)\phi_4(x_4)\phi_{12}(x_1, x_2)\phi_{23}(x_2, x_3)\phi_{34}(x_3, x_4).$$

- Conditioning on x_2 and x_3 gives UGM over x_1 and x_4 (tedious: bonus slide)

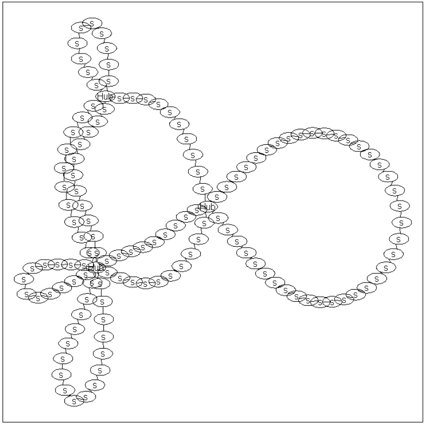
$$p(x_1, x_4 \mid x_2, x_3) = \frac{1}{Z'}\phi_1'(x_1)\phi_4'(x_4),$$

where new potentials "absorb" the shared potentials with observed nodes:

$$\phi_1'(x_1) = \phi_1(x_1)\phi_{12}(x_1, x_2), \quad \phi_4'(x_4) = \phi_4(x_4)\phi_{34}(x_3, x_4).$$

Simpler Inference in Conditional UGMs

- Consider the following graph which could describe bus stops:



- If we condition on the "hubs", the graph forms a forest (and inference is easy).
  - Simpler inference after conditioning is used many approximate inference methods.

Digression: Local Markov Property and Markov Blanket

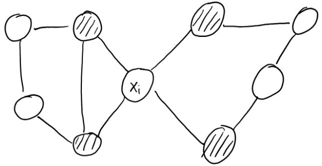
- Approximate inference methods often use conditional $p(x_j \mid x_{-j})$,
  - where x^k_{-j} means "x^k_i for all i except x^k_j": $x^k_1, x^k_2, \ldots, x^k_{j-1}, x^k_{j+1}, \ldots, x^k_d$.
- In UGMs, the conditional simplifies due to conditional independence,

$$p(x_j \mid x_{-j}) = p(x_j \mid x_{\mathsf{nei}(j)}),$$

  this local Markov property means conditional only depends on neighbours.
- We say that the neighbours of x_j are its "Markov blnkaet".

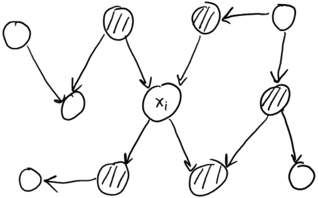
Digression: Local Markov Property and Markov Blanket

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



  - In UGMs the Markov blanket is the neighbours.

- Markov blanket in DAGs is all parents, children, and co-parents:



Iterated Conditional Mode (ICM)

- The iterated conditional mode (ICM) algorithm for approximate decoding:
  - On each iteration k, choose a variable j_k.
  - Optimize x_{j_k} with the other variables held fixed.

- So ICM is coordinate optimization.

- Iterations correspond to finding mode of conditional $p(x_j \mid x_{-j}^k)$,

$$x_j^{k+1} \leftarrow \max_c p(x_j = c \mid x_{-j}^k),$$

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

ICM Issue 1: Intractable Objective

- How can you optimize $p(x)$ coordinate-wise if evaluating it is NP-hard?
- Let's define the unnormalized probability $\tilde{p}$ as
$$\tilde{p}(x) = \prod_{c \in \mathcal{C}} \phi_c(x_c).$$
- So the normalized probability is given by
$$p(x) = \frac{\tilde{p}(x)}{Z}.$$
- In UGMs evaluating Z is hard but evaluating $\tilde{p}(x)$ is easy.
- And for decoding we only need unnormalized probabilities,
$$\underset{x}{\text{argmax}}\, p(x) \equiv \underset{x}{\text{argmax}} \frac{\tilde{p}(x)}{Z} \equiv \underset{x}{\text{argmax}}\, \tilde{p}(x),$$
so we can decode based on $\tilde{p}$ without knowing Z.

ICM Issue 2: Efficiency

- Is coordinate optimization efficient for this problem?

- Consider a pairwise UGM,
$$\tilde{p}(x) = \left(\prod_{j=1}^{d} \phi_j(x_j)\right)\left(\prod_{(i,j)\in E} \phi_{ij}(x_i, x_j)\right).$$
or
$$\log \tilde{p}(x) = \sum_{j=1}^{d} \log \phi_j(x_j) + \sum_{(i,j)\in E} \log \phi_{ij}(x_i, x_j),$$
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 the problems where coordinate optimization is n-times faster.

Pseudo-Code for ICM

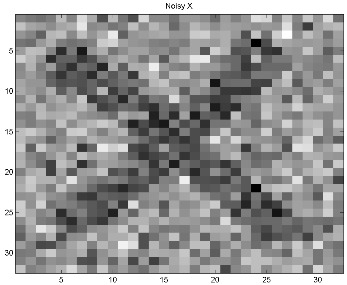
- Consider a pairwise UGM:

$$\tilde{p}(x_1, x_2, \dots, x_d) = \left(\prod_{i=1}^{d} \phi_i(x_i)\right)\left(\prod_{(i,j)\in E} \phi_{ij}(x_i, x_j)\right),$$

- For node i with 2 neighbours j and k, ICM update would be:
  1. Compute $M_i(x_i) = \phi_i(x_i)\underbrace{\phi_{ij}(x_i, x_j)\phi_{ik}(x_i, x_k)}_{\text{edges in Markov blanket}}$ for all x_i.
  2. Set x_i to the largest value of $M_i(x_i)$.

ICM in Action

Consider using a UGM for binary image denoising:



We have

- Unary potentials ϕ_j for each position.
- Pairwise potentials ϕ_{ij} for neighbours on grid.
- Parameters are trained as CRF (later).

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

ICM Issue 3: Non-Convexity

- Does it find the global optimum?
- Decoding is usually non-convex, so doesn't find global optimum.
- There exist many globalization methods that can improve its performance:
  - Restarting with random initializations.
  - Global optimization methods:
    - Simulated annealing, genetic algorithms, ant colony optimization, etc.

Outline

1 Iterated Conditional Mode

2 Gibbs Sampling

Coordinate Sampling

- What about approximate sampling?

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

$$x_j \sim p(x_j \mid x_{\mathsf{pa}(j)}).$$

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

$$x_j \leftarrow \max_{x_j} p(x_j \mid x_{-j}).$$

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

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

  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,

$$x_j \sim p(x_j \mid x_{-j}).$$

- 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 in Action

- Start with some initial value: $x^0 = \begin{bmatrix} 2 & 2 & 3 & 1 \end{bmatrix}$.
- Select random j like $j = 3$.
- Sample variable j: $x^1 = \begin{bmatrix} 2 & 2 & 1 & 1 \end{bmatrix}$.
- Select random j like $j = 1$.
- Sample variable j: $x^2 = \begin{bmatrix} 3 & 2 & 1 & 1 \end{bmatrix}$.
- Select random j like $j = 2$.
- Sample variable j: $x^3 = \begin{bmatrix} 3 & 2 & 1 & 1 \end{bmatrix}$.
- ...
- Use the samples to form a Monte Carlo estimator.

Gibbs Sampling

- For discrete x_j the conditionals needed for Gibbs sampling have a simple form,

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

  where we use unnormalized $\tilde{p}$ since Z is the same in numerator/denominator.
  - Note that this expression is easy to evaluate: just summing over values of x_j.

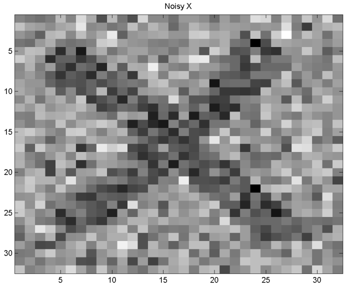
- And in UGMs it further simplifies to only depend on the Markov blanket,

$$p(x_j \mid x_{-j}) = p(x_j \mid x_{\text{MB}(j)}),$$

  since the other terms cancel in the numerator/denominator.

Gibbs Sampling in Action: UGMs

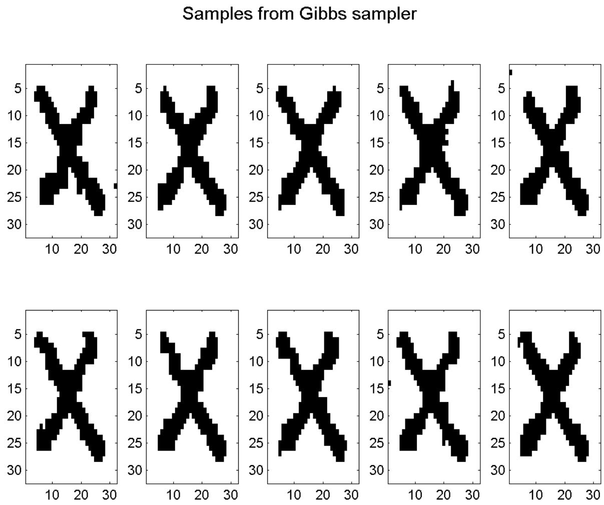
- For node i with 2 neighbours j and k, Gibbs sampling step would be:
  1. Compute $M_i(x_i) = \phi_i(x_i)\underbrace{\phi_{ij}(x_i, x_j)\phi_{ik}(x_i, x_k)}_{\text{edges in Markov blanket}}$ for all x_i.
  2. Sample x_i proportional to $M_i(x_i)$.



(show videos)

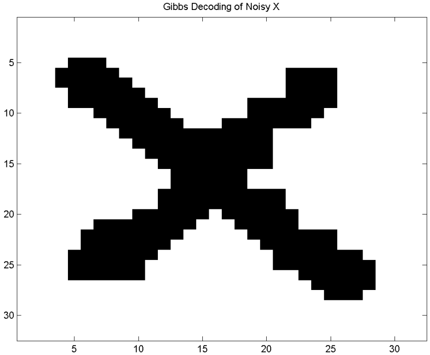
Gibbs Sampling in Action: UGMs

Gibbs samples after every $100d$ iterations:



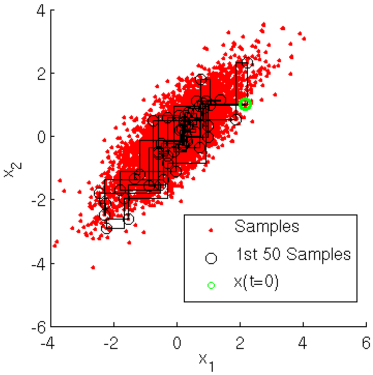
Gibbs Sampling in Action: UGMs

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

- Video: `https://www.youtube.com/watch?v=AEwY6QXWoUg`

Gibbs Sampling as a Markov Chain

- Why would Gibbs sampling work?
  - Key idea: Gibbs sampling generates a sample from a homogeneous Markov chain.

- The "Gibbs sampling Markov chain" for sampling from a 4-variable binary UGM:
  - The states are the possible configurations of the four variables:
    - $s = [0\ 0\ 0\ 0], s = [0\ 0\ 0\ 1], s = [0\ 0\ 1\ 0]$, etc.
  - The initial probability q is set to 1 for the initial state, and 0 for the others:
    - If you start at $s = [1\ 1\ 0\ 1]$, then $q(x^1 = [1\ 1\ 0\ 1]) = 1$ and $q(x^1 = [0\ 0\ 0\ 0]) = 0$.
  - The transition probabilities q are based on variable we choose and UGM:
    - If we are at $s = [1\ 1\ 0\ 1]$ and choose coordinate randomly we have:

$$q(x^{t+1} = [0\ 0\ 1\ 1] \mid x^t = [1\ 1\ 0\ 1]) = 0 \quad \text{(Gibbs only updates on variable)}$$

$$q(x^{t+1} = [1\ 0\ 0\ 1] \mid x^t = [1\ 1\ 0\ 1]) = \underbrace{\frac{1}{d}}_{\text{uniform}} \underbrace{p(x_2 = 0 \mid x_1 = 1, x_3 = 0, x_4 = 1)}_{\text{from UGM}}.$$

    - Not homogeneous if cycling through the j, but homogeneous over every d samples.

Gibbs Sampling as a Markov Chain

- Why would Gibbs sampling work?
  - Key idea: Gibbs sampling generates a sample from a homogeneous Markov chain.

- Previously we discussed stationary distribution of Markov chain:

$$\pi(s) = \sum_{s'} q(x^t = s \mid x^{t-1} = s')\pi(s'),$$

  with transition probabilities q (of the Gibbs sampling Markov chain).

- A sufficient condition for Gibbs Markov chain to have unique stationary:

$$p(x_j \mid x_{-j}) > 0 \quad \text{for all } j.$$

Markov Chain Monte Carlo (MCMC)

- Stationary distribution π of Gibbs sampling is the target distribution:

$$\pi(x) = p(x),$$

  so for large k a sample x^k will be distributed according to $p(x)$.

- Allows Gibbs sampling to be used in Markov Chain Monte Carlo (MCMC):
  - Design a Markov chain that has $\pi(x) = p(x)$.
  - Use these samples within a Monte Carlo estimator,

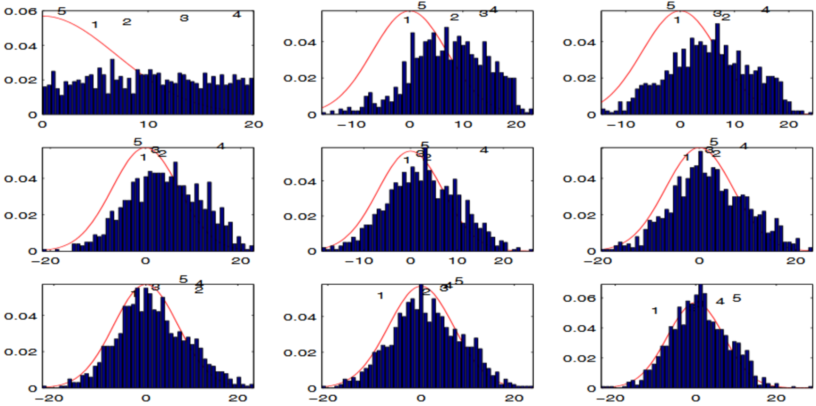
$$\mathbb{E}[g(x)] \approx \frac{1}{n}\sum_{t=1}^{n} g(x^i).$$

- Law of large numbers can be generalized to show this converges as $n \to \infty$.
  - But convergence rate is slower since we're generating dependent samples.

Markov Chain Monte Carlo

MCMC sampling from a Gaussian:

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



MCMC Implementation Issues

- Basic idea of Markov Chain Monte Carlo (MCMC) method:
  - Design a Markov chain that has $\pi(x) = p(x)$.
  - Use these samples within a Monte Carlo estimator,

$$\mathbb{E}[g(x)] \approx \frac{1}{n} \sum_{t=1}^{n} g(x^i).$$

- In practice, we often don't take all samples in our Monte Carlo estimate:
  - Burn in: throw away the initial samples when we haven't converged to stationary.
  - Thinning: only keep every k samples, since they will be highly correlated.

MCMC Implementation Issues

- Two common ways that MCMC is applied:
  1. Sample from a huge number of Markov chains for a long time, use final states.
     - Great for parallelization.
     - No need for thinning, if chains are independently initialized.
     - Need to worry about burn in.
  2. Sample from one Markov chain for a really long time, use states across time.
     - Less worry about burn in.
     - Need to worry about thinning.

- It can very hard to diagnose if we reached stationary distribution.
  - Recent work showed that this is P-space hard (*not* polynomial-time even if P=NP).
  - Various heuristics exist.

Summary

- Conditioning in UGMs leads to a smaller/simpler UGM.
- Iterated conditional mode is coordinate descent for decoding UGMs.
  - Fast but doesn't obtain global optimum in general.
- Gibbs sampling is coordinate-wise sampling.
  - Special case of Markov chain Monte Carlo method.
- Next time: reproducing the Spaceballs beaming experiment.

Conditioning in UGMs

- Conditioning on x_2 and x_3 in 4-node chain-UGM gives

$$
\begin{aligned}
p(x_1, x_4 | x_2, x_3) &= \frac{p(x_1, x_2, x_3, x_4)}{p(x_2, x_3)} \\
&= \frac{\frac{1}{Z}\phi_1(x_1)\phi_2(x_2)\phi_3(x_3)\phi_4(x_4)\phi_1(x_1, x_2)\phi_2(x_2, x_3)\phi_3(x_3, x_4)}{\sum_{x_1', x_4'} \frac{1}{Z}\phi_1(x_1')\phi_2(x_2)\phi_3(x_3)\phi_4(x_4')\phi_1(x_1', x_2)\phi_2(x_2, x_3)\phi_3(x_3, x_4')} \\
&= \frac{\frac{1}{Z}\phi_1(x_1)\phi_2(x_2)\phi_3(x_3)\phi_4(x_4)\phi_1(x_1, x_2)\phi_2(x_2, x_3)\phi_3(x_3, x_4)}{\frac{1}{Z}\phi_2(x_2)\phi_3(x_3)\phi_2(x_2, x_3)\sum_{x_1', x_4'} \phi_1(x_1')\phi_4(x_4')\phi_1(x_1', x_2)\phi_3(x_3, x_4')} \\
&= \frac{\phi_1(x_1)\phi_4(x_4)\phi_1(x_1, x_2)\phi_3(x_3, x_4)}{\sum_{x_1', x_4'} \phi_1(x_1')\phi_4(x_4')\phi_1(x_1', x_2)\phi_3(x_3, x_4')} \\
&= \frac{\phi_1'(x_1)\phi_4'(x_4)}{\sum_{x_1', x_4'} \phi_1'(x_1')\phi_4'(x_4')}
\end{aligned}
$$