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,

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

    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 saw how to write Gaussians as UGMs, today we focus on discrete x_j.

Discrete DAGs vs. Discrete UGMs

- 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 $\text{argmax}_x\, p(x)$.
  5. Compute univariate conditional $p(x_j|x_{j'})$.

- With discrete x_i, all of the above are easy in tree-structured graphs.
  - For DAGs, a tree-structured has at most one parent.
  - For UGMs, a tree-structured graph has no cycles.

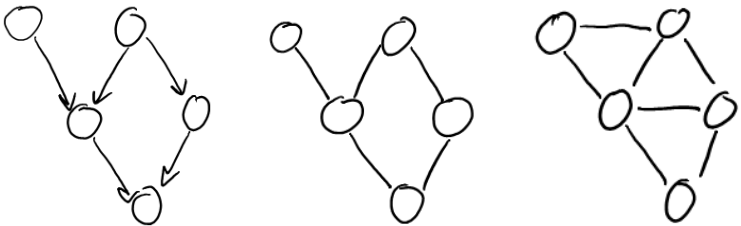
- With discrete x_i, the above may be harder for general graphs:
  - In DAGs the first two are easy, the others are NP-hard.
  - In UGMs all of these are NP-hard.

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:

$$p(x_1, x_2, \ldots, x_d)) = \prod_{j=1}^{d} p(x_j | x_{\text{pa}(j)}) = \prod_{j=1}^{d} \phi_j(x_j, x_{\text{pa}(j)}),$$

  which is a UGM with $Z = 1$.
- Graphically: we drop directions and "marry" parents (moralization).

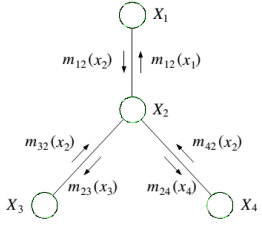


- May lose some condtional independences, but doesn't change computational cost.

Easy Cases: Chains, Trees and Forests

- The forward-backward still works for chain-structured UGMs:
  - We compute the forward messages M and the backwards messages V.
  - With both M and V we can compute [conditionally] decode/marginalize/sample.

- Belief propagation generalizes this to trees:
  - We start at an arbitrary "root", and pass messages away from it.
  - We also start from the leaves, passing messages towards the root.



https://www.quora.com/

Probabilistic-graphical-models-what-are-the-relationships-between-sum-product-algorithm-belief-propagation-and-junction-tree-

Easy Cases: Chains, Trees and Forests

- In pairwise UGM, belief propagation "message" from parent p to child c is gven by

$$M_{pc}(x_c) \propto \sum_{x_p} \phi_i(x_p)\phi_{pc}(x_p, x_c)M_{jp}(x_p)M_{kp}(x_p),$$

  assuming that parent p has parents j and k.

- Univariate marginals are proportional to $\phi_i(x_i)$ times all "incoming" messages.

- The "forward" and "backward" Markov chain messages are a special case.

- Replace $\sum_{x_i}$ with $\max_{x_i}$ for decoding.
  - "Sum-product" and "max-product" algorithms.

Exact Inference in UGMs

- Message passing is also favourable in some other graph structures.

- For example, computing Z in a simple 4-node cycle could be done using:

$$\begin{aligned} Z &= \sum_{x_4}\sum_{x_3}\sum_{x_2}\sum_{x_1} \phi_{12}(x_1,x_2)\phi_{23}(x_2,x_3)\phi_{34}(x_3,x_4)\phi_{14}(x_1,x_4) \\ &= \sum_{x_4}\sum_{x_3}\phi_{34}(x_3,x_4)\sum_{x_2}\phi_{23}(x_2,x_3)\sum_{x_1}\phi_{12}(x_1,x_2)\phi_{14}(x_1,x_4) \\ &= \sum_{x_4}\sum_{x_3}\phi_{34}(x_3,x_4)\sum_{x_2}\phi_{23}(x_2,x_3)M_{24}(x_2,x_4) \\ &= \sum_{x_4}\sum_{x_3}\phi_{34}(x_3,x_4)M_{34}(x_3,x_4) = \sum_{x_4} M_4(x_4). \end{aligned}$$

- Message-passing cost depends on graph structure and the order of the sums.

Exact Inference in UGMs

- To see the effect of the order, consider chain-structured UGM with a stupid order:

$$
\begin{aligned}
Z &= \sum_{x_5}\sum_{x_4}\sum_{x_3}\sum_{x_2}\sum_{x_1}\prod_{j=2}^{5}\phi(x_j, x_{j-1}) \\
&= \sum_{x_5}\sum_{x_3}\sum_{x_2}\sum_{x_4}\sum_{x_1}\prod_{j=2}^{5}\phi(x_j, x_{j-1}) \\
&= \sum_{x_5}\sum_{x_3}\sum_{x_2}\sum_{x_4}\prod_{j=3}^{5}\phi(x_j, x_{j-1})\underbrace{\sum_{x_1}\phi(x_2, x_1)}_{M_2(x_2)} \\
&= \sum_{x_5}\sum_{x_3}\sum_{x_2}\phi(x_3, x_2)\underbrace{\sum_{x_4}\phi(x_4, x_3)\phi(x_5, x_4)M_2(x_2)}_{M_{235}(x_2, x_3, x_5)}.
\end{aligned}
$$

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

Variable Order and Treewidth

- So cost of message passing depends on
  1. Graph structure.
  2. Variable order.

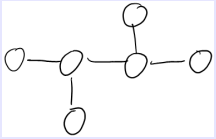
- Cost of message passing is given by $O(dk^{\omega+1})$.
  - Here, ω is the size of the largest message.
  - For trees, $\omega = 1$ so we get our usual cost of $O(dk^2)$.

- The minimum value of ω across orderings for a given graph is called treewidth.
  - In terms of graph: "minimum size of largest clique, minus 1, over all triangulations".
  - An m_1 by m_2 lattice has $\omega = \min\{m_1, m_2\}$.
    - For 28 by 28 MNIST digits it would cost $O(784 * 2^{29})$.
  - For some graphs $\omega = (d-1)$ so there is no gain over brute-force enumeration.

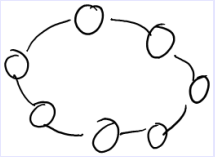
- Junction trees generalize belief propagation to general graphs (require ordering).
- Computing ω and the optimal ordering is NP-hard.
  - But various heuristic ordering methods exist.

Variable Order and Treewidth

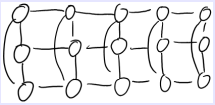
- Trees have $\omega = 1$, so with the right order inference costs $O(dk^2)$.



- A big loop has $\omega = 2$, so cost with the right ordering is $O(dk^3)$.



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



- Many graphs have high treewidth so we need approximate inference.

Outline

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

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

  where x_{-j}^k means "x_i^k for all i except 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 $p(x)$ 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 probability is given by

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

- Note that evaluating Z is hard but evaluating $\tilde{p}(x)$ is easy.
- And for decoding we only need unnormalized probabilities,

$$\operatorname*{argmax}_x p(x) \equiv \operatorname*{argmax}_x \frac{\tilde{p}(x)}{Z} \equiv \operatorname*{argmax}_x \tilde{p}(x),$$

so we can decoded based on $\tilde{p}$ without knowing Z.

ICM Issue 2: Efficiency

- Is coordinate optimization efficient for this problem?
- Consider a pairwise UGM,

$$p(x) \propto \left(\prod_{j=1}^{d} \phi_j(x_j) \right) \left(\prod_{(i,j) \in E} \phi_{ij}(x_i, x_j) \right).$$

or

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

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 problem where coordinate optimization is n-times faster.

Digression: Local Markov Property and Markov Blanket

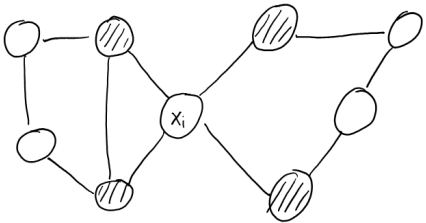
- In UGMs, conditional independence is determined by reachability.
  - $A \perp B \mid C$ if all paths from A to B are blocked by C.
- This implies a local Markov property,

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

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

- Graphically, ICM is efficient because update only depends on Markov blanket.
  - And even if graph is fully-connected, update only depends on edges to neighours.

Pseudo-Code for ICM

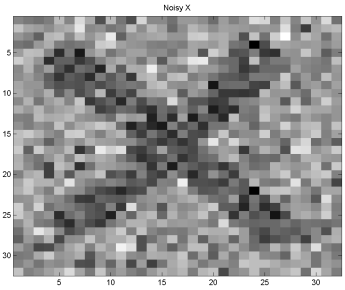
- Consider a pairwise UGM:

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

- 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.

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

- 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 values of 1 variable x_j.

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

$$p(x_j \mid x_{-j}) = p(x_j \mid x_{\mathrm{MB}(j)}).$$

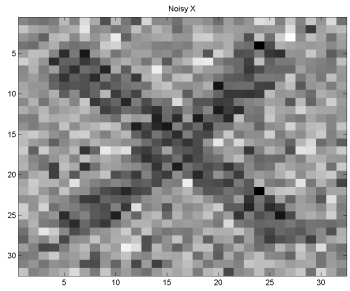
- For node i with 2 neighbours j and k, Gibbs sampling step would be:
  1. Compute $M_i(x_i) = \phi_i(x_i) \underbrace{\phi_{ij}(x_i, x_j)\phi_{ik}(x_i, x_k)}_{\text{edges in Markov blanket}}$ for all x_i.
  2. Sample x_i proportional to $M_i(x_i)$.

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 in Action: UGMs

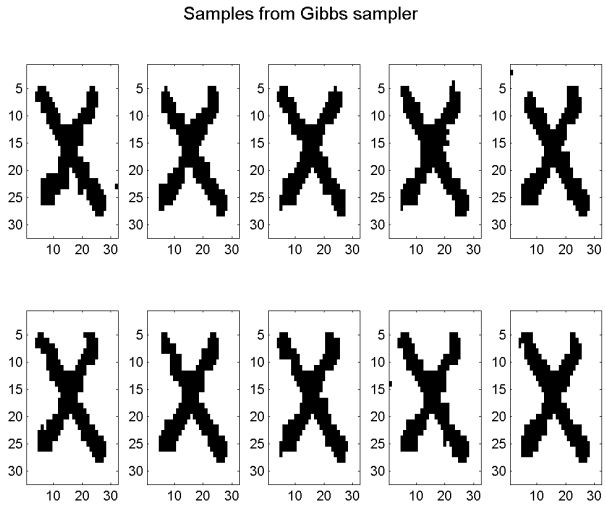
Back to image denoising...



(show videos)

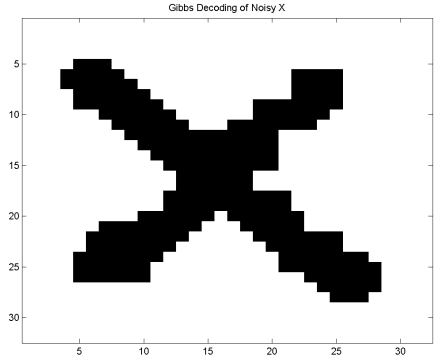
Gibbs Sampling in Action: UGMs

Gibbs samples after every $100d$ iterations:



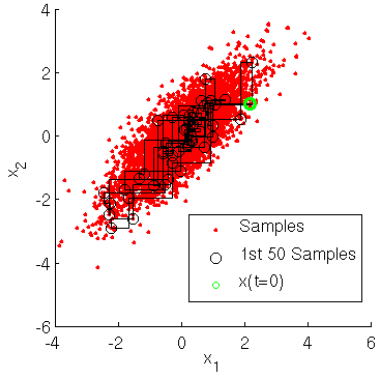
Gibbs Sampling in Action: UGMs

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

- 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.
  - If we pick a random j, we have the same transition distribution at each time.
  - If we cycle through the j, we consider dth sample as coming from 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.
- A sufficient condition for Gibbs sampling to converge to stationary:

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

  although weaker conditions exist.

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 $p(x)$.

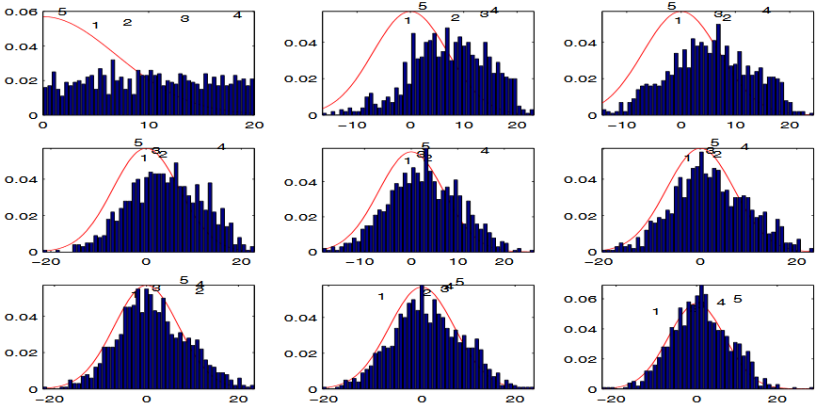
- So we can use it as a Markov Chain Monte Carlo (MCMC) method:
  - Design a Markov chain that has $\pi(x) = p(x)$.
  - Use these samples within a Monte Carlo estimator,

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

- 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

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



Summary

- Moralization of DAGs to do decoding/inference/sampling as a UGM.
- Markov blanket is set of nodes that make x_j independent of all others.

- Message passing can be used for inference in UGMs.
  - Belief propagation for trees.
  - Cost might be exponential for unfavourable graphs/ordering.

- 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.

Conditional Independence and Local Markov Property

- In UGMs, conditional independence is determined by reachability.
  - $A \perp B \mid C$ if all paths from A to B are blocked by C.
- The independence assumptions in DAGs were defined by

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

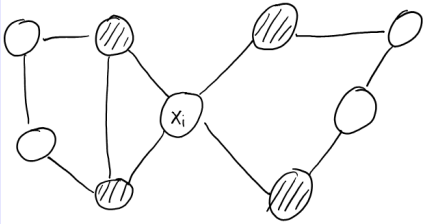
  that we're independent of previous non-parents given parents.
- In UGMs there is no order and we instead have a local Markov property,

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

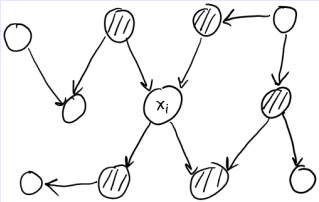
  that we're independent of all non-neighbours given neighbours in the graph.

Markov Blanket

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



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



Decomposable Graphical Models

- Probabilities whose conditonal independences that can be represented as DAGs *and* UGMs are called decomposable.
  - Includes chains, trees, and fully-connected graphs.

- These models allow some efficient operations in UGMs by writing them as DAGs:
  - Computing $p(x)$.
  - Ancestral sampling.
  - Fitting parameters independently.