CPSC 540: Machine Learning

More Approximate Inference

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Last Time: Approximate Inference

- We've been discussing graphical models for density estimation,

$$p(x_1, x_2, \ldots, x_d) = \prod_{j=1}^{d} p(x_j \mid x_{\mathsf{pa}(j)}), \quad p(x_1, x_2, \ldots, x_d) \propto \prod_{c \in \mathcal{C}} \phi_c(x_c),$$

  where are natural and widely-used models for many phenomena.
  - These will also be among ingredients of more advanced models we'll see later.

- But most calculations involving graphical models are typically NP-hard.
  - We can convert to DAGs to UGMs, so we'll just study UGMs.

- We considered approximate inference in discrete UGMs:
  1. Iterated conditional mode (ICM) applies coordinate-wise optimization.
  2. Gibbs sampling applies coorrdinate-wise sampling.
     - A special case of Markov chain Monte Carlo (MCMC).

MCMC Implementation Issues

- Recall that key idea behind MCMC is designing Markov chain with

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

that stationary distribution is the target distribution that we want.

- We can use these samples within Monte Carlo methods:

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

- Typically, we 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.

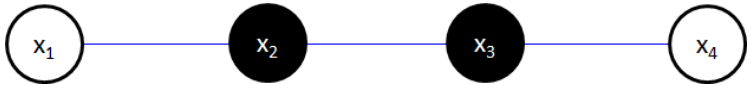
MCMC Implementation Issues

- 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.

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.

Closure of UGMs under Conditioning

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

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

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

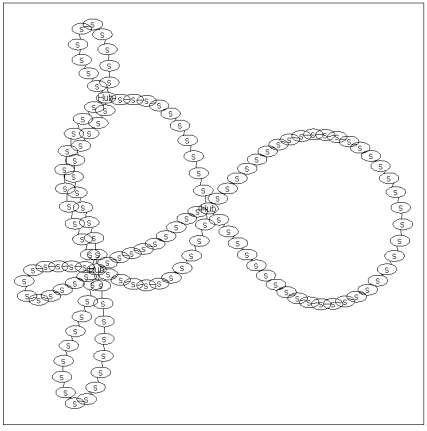
$$p(x_1, x_4 \mid x_2, x_3) = \frac{1}{Z'}\phi'_1(x_1)\phi'_4(x_4),$$

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

$$\phi'_1(x_1) = \phi_1(x_1)\phi_{12}(x_1, x_2), \quad \phi'_4(x_4) = \phi_4(x_4)\phi_{34}(x_3, x_4).$$

Inference in Conditional UGM

- Consider the following graph which could describe bus stops:



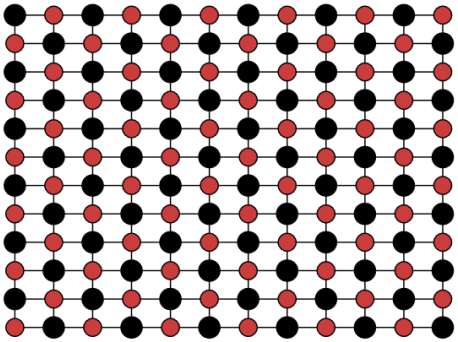
- If we condition on the "hubs", the graph forms a forest (and inference is easy).

Block-Structured Approximate Inference

- Basic approximate inference methods like ICM and Gibb sampling:
  - Update one x_j at a time.
  - Efficient because conditional UGM is 1 node.
- Better approximate inference methods use block updates:
  - Update a block of x_j values at once.
  - Efficient if conditional UGM allows exact inference.
- If we choose the blocks cleverly, this works substantially better.

Block-Structured Approximate Inference

- Consider a lattice-structure and the following two blocks ("red-black ordering"):

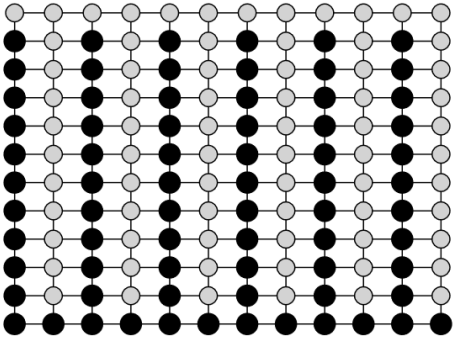


- Given black nodes, conditional UGM on red nodes is a disconnected graph.
  - "I can optimally update the red nodes given the black nodes" (and vice versa).

- Minimum number of blocks to disconnect the graph is graph colouring.

Block-Structured Approximate Inference

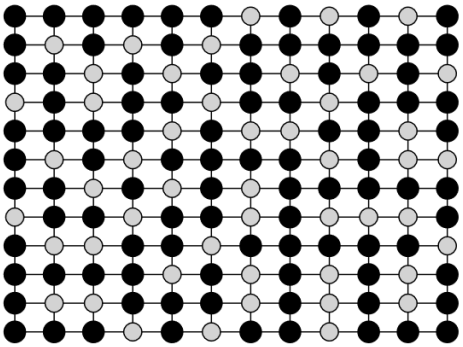
- We could also consider general forest-structured blocks:



- We can still optimally update the black nodes given the gray nodes.
  - This works much better than "one at a time".

Block-Structured Approximate Inference

- Or we could define a new tree-structured block on each iteration:

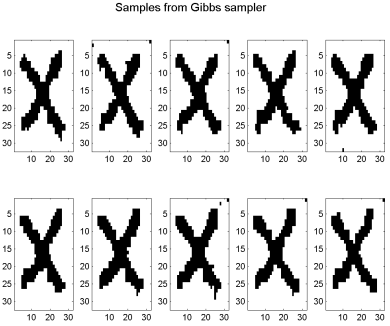


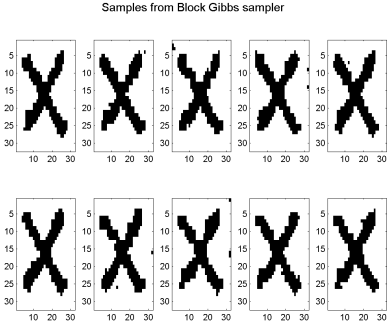
- The above block updates around two thirds of the nodes optimally.

(Here we're updating the black nodes.)

Block Gibbs Sampling in Action

- Gibbs vs. tree-structured block-Gibbs samples:





- We can also do tree-structured block ICM.
  - Harder to get stuck if you get update entire trees.

Block ICM Based on Graph Cuts

- Consider a binary pairwise UGMs with "attractive" potentials,

$$\log \phi_{ij}(1,1) + \log \phi_{ij}(2,2) \geq \log \phi_{ij}(1,2) + \log \phi_{ij}(2,1).$$

- In words: "neighbours prefer to have similar states".

- In this sitting exact decoding can be formulated as a max-flow min-cut problem.
  - Can be solved in polynomial time.

- This is widely-used computer vision:
  - Want neighbouring pixels/super-pixels/regions to be more likely to get same label.

Graph Cut Example: "GrabCut"

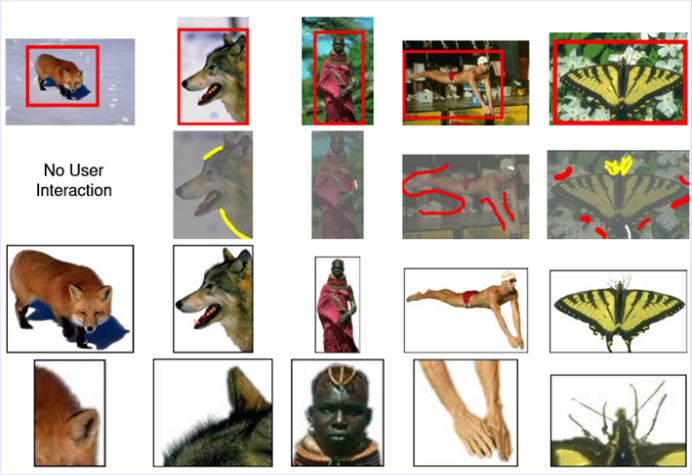
Figure 1: **Three examples of GrabCut.** The user drags a rectangle loosely around an object. The object is then extracted automatically.

http://cvg.ethz.ch/teaching/cvl/2012/grabcut-siggraph04.pdf

1. User draws a box around the object they want to segment.
2. Fit Gaussian mixture model to pixels inside the box, and to pixels outside the box.
3. Construct a pairwise UGM using:
   - $\phi_i(x_i)$ set to GMM probability of pixel i being in class x_i.
   - $\phi_{ij}(x_i, x_j)$ set to Ising potential times RBF based on spatial/colour distance.
     - Use $w_{ij} > 0$ so the model is "attractive".
4. Perform exact decoding in the binary attractive model using graph cuts.

Graph Cut Example: "GrabCut"

- GrabCut with extra user interaction:



http://cvg.ethz.ch/teaching/cvl/2012/grabcut-siggraph04.pdf

Alpha-Beta Swap and Alpha-Expansions: ICM with Graph Cuts

- If we have more than 2 states, we can't use graph cuts.
- Alpha-beta swaps are an approximate decoding method for "pairwise attractive",

$$\log \phi_{ij}(\alpha, \alpha) + \log \phi_{ij}(\beta, \beta) \geq \log \phi_{ij}(\alpha, \beta) + \log \phi_{ij}(\beta, \alpha).$$

  - Each step choose an α and β, optimally "swaps" labels among these nodes.
- Alpha-expansions are another variation based on a slightly stronger assumption,

$$\log \phi_{ij}(\alpha, \alpha) + \log \phi_{ij}(\beta_1, \beta_2) \geq \log \phi_{ij}(\alpha, \beta_1) + \log \phi_{ij}(\beta_2, \alpha).$$

  - Steps choose label α, and consider replacing the label of any node not labeled α.

Alpha-Beta Swap and Alpha-Expansions: ICM with Graph Cuts

- These don't find global optima in general, but make huge moves:

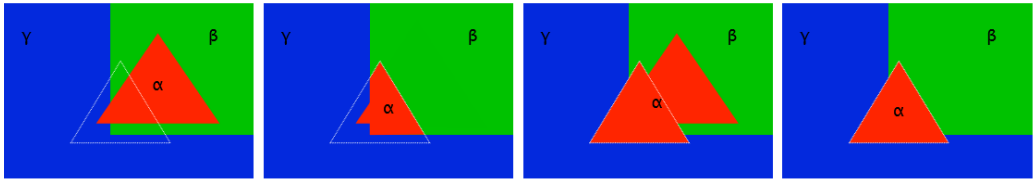


Figure 1: From left to right: Initial labeling, labeling after $\alpha\beta$-swap, labeling after α-expansion, labeling after α-expansion β-shrink. The optimal labeling of the α pixels is outlined by a white triangle, and is achieved from the initial labeling by one α-expansion β-shrink move.

- A somewhat-related MCMC method is Swendson-Wang algorithm.

Example: Photomontage

- Photomontage: combining different photos into one photo:

http://vision.middlebury.edu/MRF/pdf/MRF-PAMI.pdf

- Here, x_i corresponds to identity of original image at position i.

Example: Photomontage

- Photomontage: combining different photos into one photo:

http://vision.middlebury.edu/MRF/pdf/MRF-PAMI.pdf

Outline

Structured Prediction with Undirected Graphical Models

- Consider a pairwise UGM,

$$p(x) = \frac{1}{Z}\left(\prod_{j=1}^{d}\phi_j(x_j)\right)\left(\prod_{(j,k)\in E}\phi_{jk}(x_j, x_k)\right).$$

- We've been focusing on the case where the potential ϕ are known.
  - We've discussed decoding, inference, and sampling.
  - We've discussed [block-]coordinate approximate inference.

- We're now going to discuss learning the potentials ϕ from data.

- Unfortunately, Z makes this complicated compared to DAGs.
  - You can't fit each potential independently.

Naive Parameterization of UGMs

- We'll want to make the ϕ depend on a set of parameters w.
- As before, with n IID training x^i we can do MAP estimation,

$$w = \underset{w}{\text{argmin}} -\sum_{i=1}^{n} \log(p(x^i \mid w)) + \frac{\lambda}{2}\|w\|^2,$$

  where I've assumed an independent Gaussian prior on w.
- But how should the non-negative ϕ be related to w?
- A naive parameterization is to just directly treat potentials as parameters:

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

  so $w_{j,s}$ is "potential of node j being in state s".
  - And optimize subject to all parameters being non-negative.
  - This unfortunately leads to a non-convex optimizaiton.

Log-Linear Parameterization of UGMs

- Instead of using non-negative w, we can instead exponentiate w,

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

- This gives a log-linear model,

$$p(x \mid w) \propto \left(\prod_{j=1}^{d} \phi_j(x_j)\right)\left(\prod_{(j,k)\in E} \phi_{jk}(x_j, x_k)\right)$$
$$= \exp\left(\sum_{j=1}^{d} w_{j,x_j} + \sum_{(j,k)\in E} w_{j,k,x_j,x_k}\right),$$

and leads to a convex NLL.

- Normally, exponentiating to get non-negativity introduces local minima.

Parameter Tieing in UGMs

- So our log-linear parameterization has the form

$$\log \phi_j(s) = w_{j,s}, \quad \log \phi_{jk}(s, s') = w_{j,k,s,s'},$$

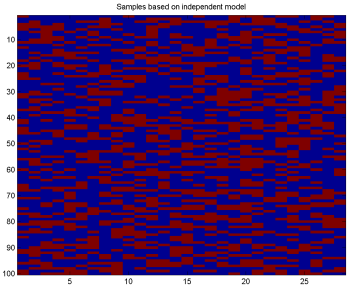
  which can represent any positive pairwise potentials.

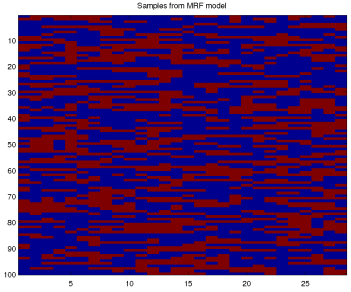
- There exist many common variations on parameter tieing:
  - We might want w_{j,x_j} to be the same for all j (all nodes use same potentials).
    - You can similarly tie the edge parameters across all edges.
    - This is similar to homogenous Markov chains.
  - In the Ising model we tied across states: $w_{j,k,1,1} = w_{j,k,2,2}$ and $w_{j,k,1,2} = w_{j,k,2,1}$.
  - We could also have special potentials for the boundaries.
    - Many language models are homogeneous, except for start/end of sentences.

Example: Ising Model of Rain Data

Independent model vs. chain-UGM model with tied nodes and Ising tied edges:

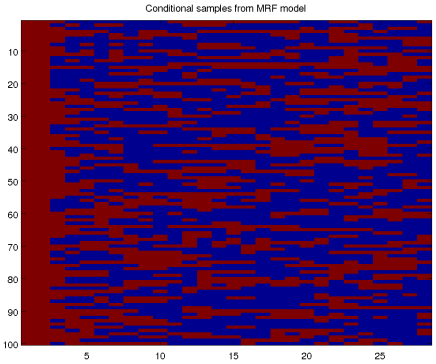
- For this dataset, using untied or general edges doesn't change likelihood much.





Example: Ising Model of Rain Data

Samples from Ising chain-UGM model if it rains on the first day:



Energy Function and Feature Vector Representation

- Recall that we use $\tilde{p}(x)$ for the unnormalized probability,

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

- In physics, the value $E(x) = -\log \tilde{p}(x)$ is called the energy function.

- With the log-linear parameterization, the energy function is linear,

$$-E(X) = \sum_i w_{j,x_j} + \sum_{(j,k)\in E} w_{j,k,x_j,x_k}.$$

- To account for parameter tieing, we often write

$$-E(x) = w^T F(x), \quad \text{or equivalently} \quad p(x) \propto \exp(w^T F(x)),$$

where feature function F counts number of times we use each parameter.

Example of Feature Function

- Consider the 2-node 1-edge UGM (1)–(2), where each state has 2 values.
- With no parameter tieing and $x = \begin{bmatrix} 1 & 2 \end{bmatrix}$, our parameter vector and features are

$$w = \begin{bmatrix} w_{1,1} \\ w_{1,2} \\ w_{2,1} \\ w_{2,2} \\ w_{1,2,1,1} \\ w_{1,2,1,2} \\ w_{1,2,2,1} \\ w_{1,2,2,2} \end{bmatrix}, \quad F(x) = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix},$$

so this gives

$$w^T F(x) = w_{1,1} + w_{2,2} + w_{1,2,1,2}.$$

UGM Training Objective Function

- With log-linear parameterization, NLL for IID training examples is

$$
\begin{aligned}
-\log p(X \mid w) &= -\sum_{i=1}^{n} \log p(x^i \mid w) = -\sum_{i=1}^{n} \log \left(\frac{\exp(w^T F(x^i))}{Z(w)} \right) \\
&= -\sum_{i=1}^{n} w^T F(x^i) + \sum_{i=1}^{n} \log Z(w) \\
&= -w^T F(X) + \log Z(w).
\end{aligned}
$$

  where the $F(X) = \sum_i F(x^i)$ are called the sufficient statistics of the dataset.
  - Given sufficient statistics $F(X)$, we can throw out the examples x^i.

    (only go through data once)
- Function $f(w)$ is convex (it's linear plus a big log-sum-exp function).
  - But notice that Z depends on w

.

Summary

- Conditioning in UGMs leads to a smaller/simpler UGM.
- Block approximate inference works better than single-variable methods.
  - Blocks could be defined by trees or to implement graph cuts.
- Log-linear parameterization can be used to learn UGMs:
  - Maximum likelihood is convex, but requires normalizing constant Z.
- Next time: measuring defense in the NBA.

Conditioning in UGMs

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

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

Other Graphical Models

- Factor graphs: we use a square between variables that appear in same factor.
  - Can distinguish between a 3-way factor and 3 pairwise factors.
- Chain-graphs: DAGs where each block can be a UGM.
- Ancestral-graph:
  - Generalization of DAGs that is closed under conditioning.
- Structural equation models (SEMs): generalization of DAGs that allows cycles.

Example: Ising Model of Rain Data

- E.g., for the rain data we could parameterize our node potentials using

$$\log(\phi_i(x_i)) = \begin{cases} w_1 & \text{no rain} \\ 0 & \text{rain} \end{cases}.$$

- Why do we only need 1 parameter?
  - Scaling $\phi_i(1)$ and $\phi(2)$ by constant doesn't change distribution.

- In general, we only need $(k-1)$ parameters for a k-state variable.
  - But if we're using regularization we may want to use k anyways (symmetry).

Example: Ising Model of Rain Data

- The Ising parameterization of edge potentials,

$$\log(\phi_{ij}(x_i, x_j)) = \begin{cases} w_2 & x_i = x_j \\ 0 & x_i \neq x_j \end{cases}.$$

- Applying gradient descent gives MLE of

$$w = \begin{bmatrix} 0.16 \\ 0.85 \end{bmatrix}, \quad \phi_i = \begin{bmatrix} \exp(w_1) \\ \exp(0) \end{bmatrix} = \begin{bmatrix} 1.17 \\ 1 \end{bmatrix}, \quad \phi_{ij} = \begin{bmatrix} \exp(w_2) & \exp(0) \\ \exp(0) & \exp(w_2) \end{bmatrix} = \begin{bmatrix} 2.34 & 1 \\ 1 & 2.34 \end{bmatrix},$$

  preference towards no rain, and adjacent days being the same.
- Average NLL of 16.8 vs. 19.0 for independent model.

Full Model of Rain Data

- We could alternately use fully expressive edge potentials

$$\log(\phi_{ij}(x_i, x_j)) = \begin{bmatrix} w_2 & w_3 \\ w_4 & w_5 \end{bmatrix},$$

  but these don't improve the likelihood much.

- We could fix one of these at 0 due to the normalization.
  - But we often don't do this when using regularization.

- We could also have special potentials for the boundaries.
  - Many language models are homogeneous, except for start/end of sentences.