CPSC 540: Machine Learning

Log-Linear Models

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Last Time: Approximate Inference

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

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

  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.

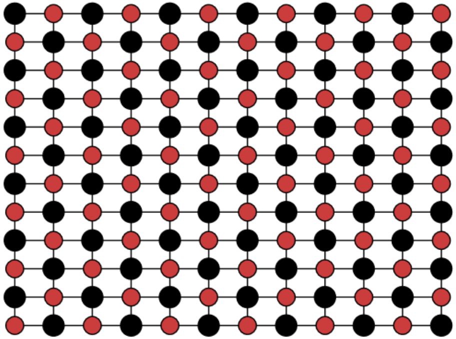
- We considered approximate inference in discrete UGMs:
  1. Iterated conditional mode (ICM) applies coordinate-wise optimization.
  2. Gibbs sampling applies coorrdinate-wise sampling.
     - A special case of Markov chain Monte Carlo (MCMC).

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"):

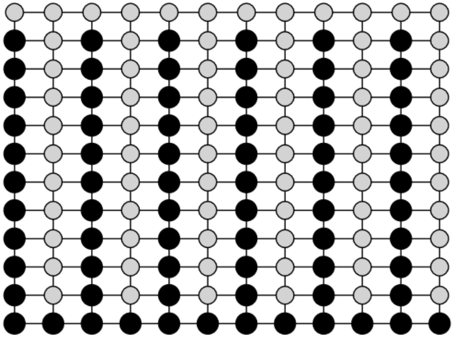


- Given black nodes, conditional UGM on red nodes is a disconnected graph.
  - "I can optimally update the red nodes given the black nodes" (and vice versa).
  - You can update $d/2$ of the nodes in parallel.

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

Block-Structured Approximate Inference

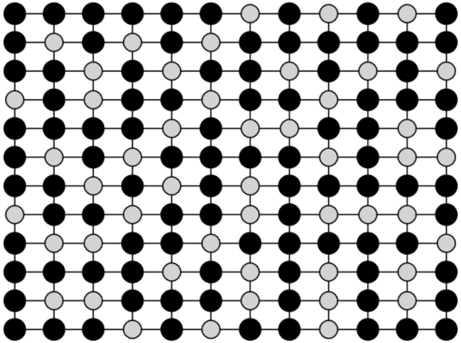
- We could also consider general forest-structured blocks:



- 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:

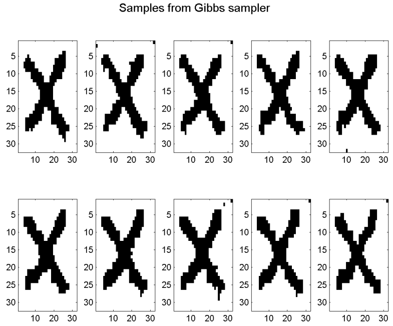


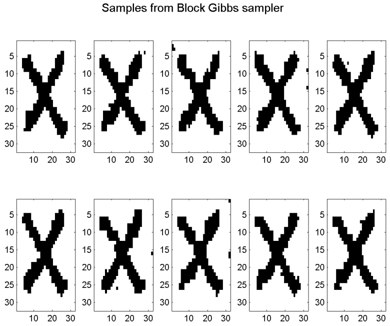
- The above block updates around two thirds of the nodes optimally.

(Here we're updating the black nodes.)

Block Gibbs Sampling in Action

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





- With block sampling, the samples are far less correlated.
- We can also do tree-structured block ICM.
  - Harder to get stuck if you get to 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 setting 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"

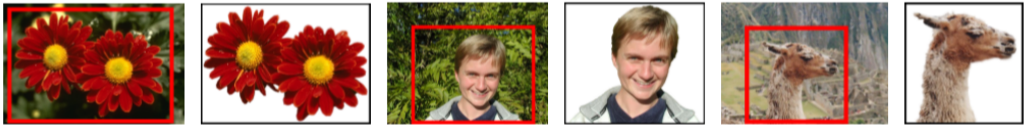


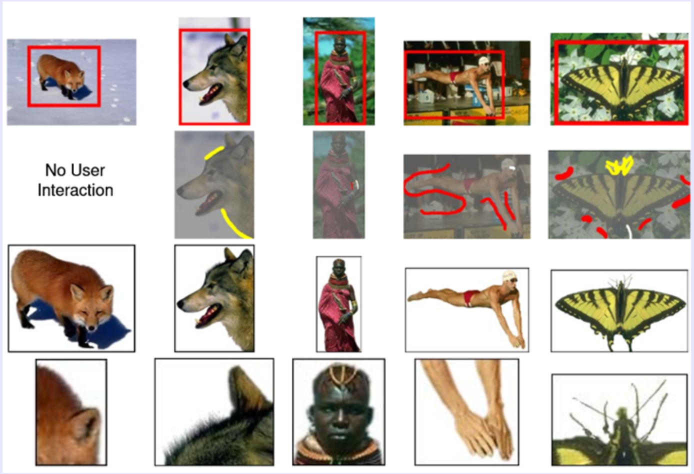
Figure 1: **Three examples of GrabCut.** The user drags a rectangle loosely around an object. The object is then extracted automatically.

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:



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:

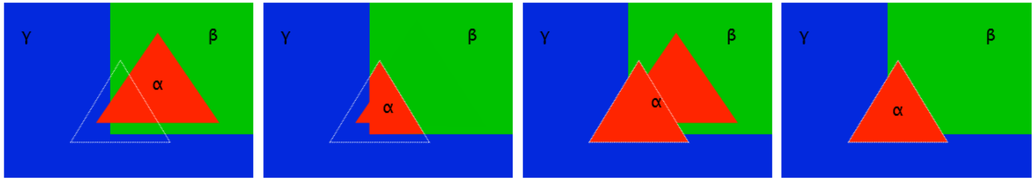
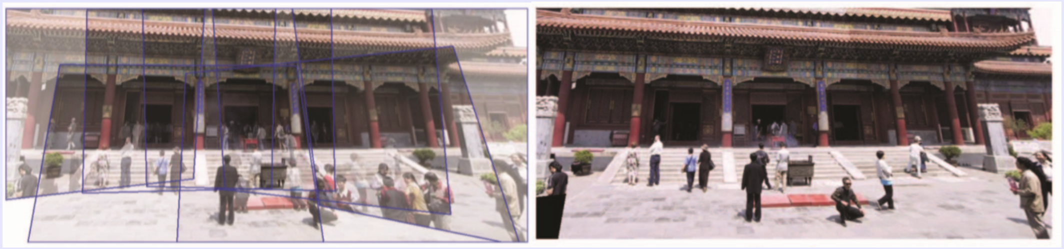


Figure 1: From left to right: Initial labeling, labeling after $\alpha\beta$-swap, labeling after α-expansion, labeling after α-expansion β-shrink. The optimal labeling of the α pixels is outlined by a white triangle, and is achieved from the initial labeling by one α-expansion β-shrink move.

- 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

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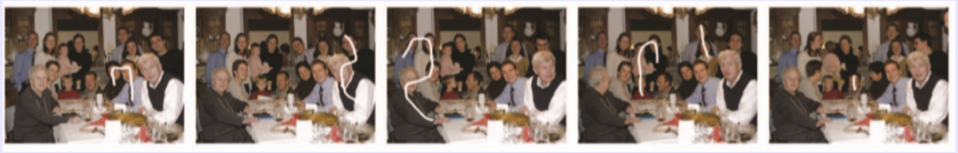
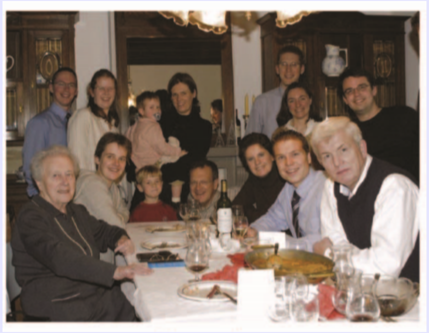




http://vision.middlebury.edu/MRF/pdf/MRF-PAMI.pdf

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 potentials 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.
- 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,

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

  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.

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,

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

- 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.
  - So we have potentials $\phi_1(x_1)$, $\phi_2(x_2)$, and $\phi_{12}(x_1, x_2)$ and want to have

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

- With no parameter tieing and $x = \begin{bmatrix} 2 & 1 \end{bmatrix}$, our parameter vector and features are

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

Example of Feature Function

- If we instead had Ising potentials (just measuring whether $x_1 = x_2$ we would have

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

where $w_{1,2,\text{same}}$ is the parameter specifying how much we want $x_1 = x_2$.

- With no parameter tieing and $x = \begin{bmatrix} 2 & 1 \end{bmatrix}$, our parameter vector and features are

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

UGM Training Objective Function

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

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

  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

.

Log-Linear UGM Gradient

- For 1 example x, we showed that NLL with log-linear parameterization is

$$f(w) = -w^T F(x) + \log Z(w).$$

- The partial derivative with respect to parameter w_j has a simple form

$$\begin{aligned}\nabla_{w_j} f(w) &= -F_j(x) + \sum_x \frac{\exp(w^T F(x))}{Z(w)} F_j(x) \\ &= -F_j(x) + \sum_x p(x \mid w) F_j(x) \\ &= -F_j(x) + \mathbb{E}[F_j(x)].\end{aligned}$$

- Observe that derivative of $\log(Z)$ is expected value of feature.

Log-Linear UGM Gradient

- For 1 example, gradient in log-linear UGM with respect to parameter w_j is

$$\nabla_{w_j} f(w) = -F_j(x) + \mathbb{E}[F_j(x)].$$

- Example of $\phi_{10}(3) = \exp(w_{10,3})$ (potential that feature 10 is in state 3).
  - Averaging over n examples, the gradient with no parameter tieing is given by

$$\nabla_{w_{10,3}} f(w) = -\underbrace{\frac{1}{n}\left[\sum_{i=1}^{n} I[x_{10}^i = 3]\right]}_{\text{frequency in data}} + \underbrace{p(x_{10} = 3)}_{\text{model ``frequency''}}.$$

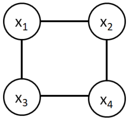
  - So if $\nabla_{w_{10,3}} f(w) = 0$, probabilities match frequencies in training data.
  - At MLE, you match the frequencies of all the potentials in the training data.
  - Typical training method: deterministic gradient descent methods (if have Z).
- But computing gradient requires inference (computing marginals like $p(x_{10} = 3)$).

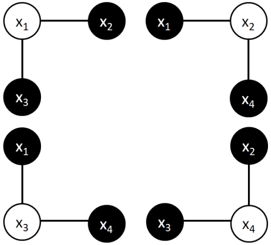
Approximate Learning: Alternate Objectives

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

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

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





Summary

- 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: the work that started the the modern deep learning movement.

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.

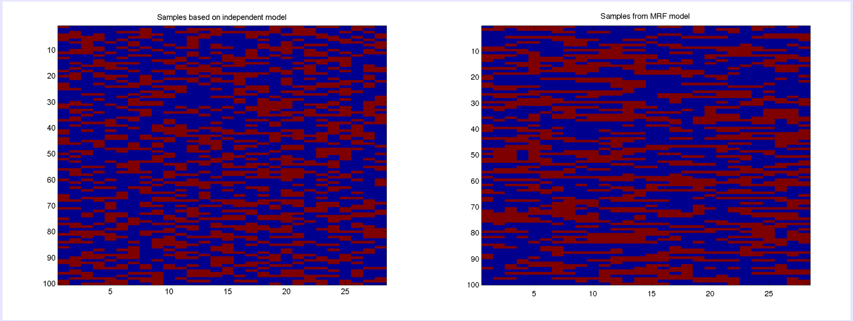
- We could fix one of these at 0 due to the normalization.
  - But we often don't do this when using regularization.

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

Example: Ising Model of Rain Data

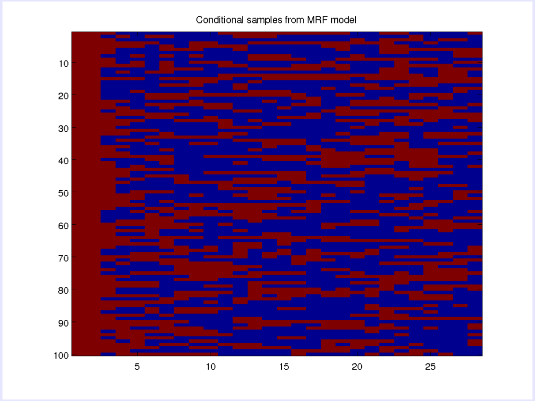
Independent model vs. chain-UGM model with tied nodes and Ising tied edges:

- 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:


Conditional samples from MRF model