#### LECTURE 13:

#### PARAMETER LEARNING IN UNDIRECTED MODELS

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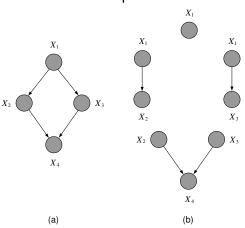
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#### Example: A Directed Model

• Consider the distribution defined by the DAGM:

$$p(\mathbf{x}|\theta) = p(\mathbf{x}_1|\theta_1)p(\mathbf{x}_2|\mathbf{x}_1,\theta_2)p(\mathbf{x}_3|\mathbf{x}_1,\theta_3)p(\mathbf{x}_4|\mathbf{x}_2,\mathbf{x}_3,\theta_4)$$

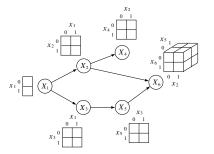
• This is exactly like learning four separate small DAGMs, each of which consists of a node and its parents.



# MLE FOR GENERAL BAYES NETS (K+F 13.1–13.2, J 9.1–9.2)

• If we assume the parameters for each CPD are globally independent, then the log-likelihood function decomposes into a sum of local terms, one per node:

$$\log p(\mathcal{D}|\theta) = \log \prod_{m} \prod_{i} p(\mathbf{x}_{i}^{m} | x_{\pi_{i}}, \theta_{i}) = \sum_{i} \sum_{m} \log p(\mathbf{x}_{i}^{m} | x_{\pi_{i}}, \theta_{i})$$



#### Example: Multinomial

- We observe M iid die rolls (K-sided):  $\mathcal{D}=3,1,K,2,...$
- Model:  $p(k) = \theta_k \quad \sum_k \theta_k = 1$
- Likelihood (for binary indicators  $[\mathbf{x}^m = k]$ ):

$$\ell(\theta; \mathcal{D}) = \log p(\mathcal{D}|\theta) = \sum_{m} \log \prod_{k} \theta_{k}^{[\mathbf{x}^{m} = k]}$$
$$= \sum_{m} \sum_{k} [\mathbf{x}^{m} = k] \log \theta_{k} = \sum_{k} N_{k} \log \theta_{k}$$

- ullet The counts  $N_k$  are the sufficient statistics.
- ullet We need to maximize this subject to the constraint  $\sum_k \theta_k = 1$ , so we use a Lagrange multiplier.

• Constrained cost function:

$$\tilde{l} = \sum_{k} N_k \log \theta_k + \lambda \left( 1 - \sum_{k} \theta_k \right)$$

• Take derivatives wrt  $\theta_k$ :

$$\begin{split} \frac{\partial \tilde{l}}{\partial \theta_k} &= \frac{N_k}{\theta_k} - \lambda = 0 \\ N_k &= \lambda \theta_k \\ \sum_k N_k &= M = \lambda \sum_k \theta_k = \lambda \\ \hat{\theta}_{k,ML} &= \frac{N_k}{M} \end{split}$$

•  $\hat{\theta}_{k,ML}$  if the fraction of times k occurs.

# MLE FOR UNDIRECTED GRAPHICAL MODELS (J 9.3)

- For directed graphical models, the log-likelihood decomposes into a sum of terms, one per family (node plus parents).
- ullet For undirected graphical models, the log-likelihood does not decompose, because the normalization constant Z is a function of all the parameters (c.f., EM)

$$P(\mathbf{X}) = \frac{1}{Z} \prod_{\text{cliques } c} \psi_c(\mathbf{x}_c) \qquad Z = \sum_{\mathbf{X}} \prod_{\text{cliques } c} \psi_c(\mathbf{x}_c)$$

• In general, we will need to do inference to learn params for undirected model, even in the fully observed case.

#### MLE FOR BAYES NETS WITH TABULAR CPDS

• Assume each CPD is represented as a table (multinomial) where

$$\theta_{ijk} \stackrel{\text{def}}{=} P(X_i = j | X_{\pi_i} = k)$$

• The sufficient statistics are just counts of family configurations

$$N_{ijk} \stackrel{\text{def}}{=} \sum_{m} I(X_i^m = j, X_{\pi_i}^m = k)$$

• The log-likelihood is

$$\ell = \log \prod_{m} \prod_{ijk} \theta_{ijk}^{N_{ijk}}$$
$$= \sum_{m} \sum_{ijk} N_{ijk} \log \theta_{ijk}$$

ullet Using a Lagrange multiplier to enforce so  $\sum_i heta_{ijk} = 1$  we get

$$\hat{\theta}_{ijk}^{ML} = \frac{N_{ijk}}{\sum_{j'} N_{ij'k}}$$

# LOG LIKELIHOOD FOR UNDIRECTED MODEL WITH TABULAR CLIQUE POTENTIALS

• In terms of the counts, the log likelihood is given by:

$$p(\mathcal{D}|\theta) = \prod_{n} \prod_{\mathbf{x}} p(\mathbf{x}|\theta)^{\delta(\mathbf{x},\mathbf{x}^n)}$$
$$\log p(\mathcal{D}|\theta) = \sum_{n} \sum_{\mathbf{x}} \delta(\mathbf{x},\mathbf{x}^n) \log p(\mathbf{x}|\theta)$$
$$\ell = \sum_{\mathbf{x}} n(\mathbf{x}) \log \left(\frac{1}{Z} \prod_{c} \psi_c(\mathbf{x}_c)\right)$$
$$= \sum_{c} \sum_{\mathbf{x}_c} n(\mathbf{x}_c) \log \psi_c(\mathbf{x}_c) - N \log Z$$

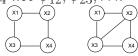
- ullet So the clique counts  $n(\mathbf{x}_c)$  are the sufficient statistics for our undirected model.
- ullet But now there is a nasty  $\log Z$  in the likelihood.

- $\bullet$  Log-likelihood:  $\ell = \sum_c \sum_{\mathbf{x}_c} n(\mathbf{x}_c) \log \psi_c(\mathbf{x}_c) N \log Z$
- First term.  $\frac{\partial \ell_1}{\partial \psi_c(x_c)} = n(x_c)/\psi_c(x_c)$
- Second term:

$$\frac{\partial \log Z}{\partial \psi_c(x_c)} = \frac{1}{Z} \frac{\partial}{\partial \psi_c(x_c)} \left( \sum_{\tilde{x}} \prod_d \psi_d(\tilde{x}_d) \right) 
= \frac{1}{Z} \sum_{\tilde{x}} \delta(\tilde{x}_c, x_c) \frac{\partial}{\partial \psi_c(x_c)} \left( \prod_d \psi_d(\tilde{x}_d) \right) 
= \sum_{\tilde{x}} \delta(\tilde{x}_c, x_c) \frac{1}{\psi_c(\tilde{x}_c)} \frac{1}{Z} \prod_d \psi_d(\tilde{x}_d) 
= \frac{1}{\psi_c(\tilde{x}_c)} \sum_{\tilde{x}} \delta(\tilde{x}_c, x_c) p(\tilde{x}) = \frac{p(x_c)}{\psi_c(x_c)}$$

#### MLE FOR UNDIRECTED GRAPHICAL MODELS

- Is the graph decomposable (triangulated)?
- Are all the clique potentials defined on maximal cliques (not subcliques)? e.g.,  $\psi_{123}$ ,  $\psi_{234}$  not  $\psi_{12}$ ,  $\psi_{23}$ , . . . .



• Are the clique potentials full tables (or Gaussians), or parameterized more compactly, e.g.,  $\psi_c(x_c) = exp(\sum_k w_k f_k(x_c))$ ?

| Decomposable? | Max. Cliques | Tabular | Method            |
|---------------|--------------|---------|-------------------|
| Yes           | Yes          | Yes     | Direct            |
| -             | _            | Yes     | IPF               |
| -             | _            | _       | Gradient ascent   |
| -             | _            | _       | Iterative scaling |

Derivative of log-likelihood

$$\frac{\partial \ell}{\partial \psi_c(\mathbf{x}_c)} = \frac{n(\mathbf{x}_c)}{\psi_c(\mathbf{x}_c)} - N \frac{p(\mathbf{x}_c)}{\psi_c(\mathbf{x}_c)}$$

• Hence, for the maximum likelihood parameters, we know that:

$$p_{ML}^*(\mathbf{x}_c) = \frac{n(\mathbf{x}_c)}{N} \stackrel{\text{def}}{=} q(\mathbf{x}_c) \stackrel{\text{def}}{=} \tilde{p}(\mathbf{x}_c)$$

In other words, at the maximum likelihood setting of the parameters, for each clique, the model marginals must be equal to the observed marginals (empirical counts).

• This doesn't tell us how to get the ML parameters, it just gives us a condition that must be satisfied when we have them.

#### MLE FOR DECOMPOSABLE UNDIRECTED MODELS

- Consider a chain  $X_1 X_2 X_3$ . The cliques are  $(X_1, X_2)$  and  $(X_2, X_3)$ ; the separator is  $X_2$ .
- The empirical marginals must equal the model marginals.
- $\bullet$  Let us guess that  $\hat{p}_{ML}(x_1,x_2,x_3) = \frac{\tilde{p}(x_1,x_2)\tilde{p}(x_2,x_3)}{\tilde{p}(x_2)}$
- We can verify this satisfies the conditions:

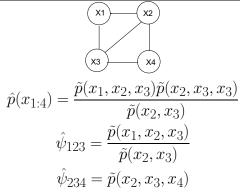
$$\hat{p}(x_1, x_2) = \sum_{x_3} \hat{p}(x_1, x_2, x_3) = \tilde{p}(x_1 | x_2) \sum_{x_3} \tilde{p}(x_2, x_3) = \tilde{p}(x_1, x_2)$$

and similarly  $\hat{p}(x_2, x_3) = \tilde{p}(x_2, x_3)$ .

ullet To compute the clique potentials, just equate them to the empirical marginals. Also, the separator must be divided into one of its neighbors. Then Z=1.

$$\hat{\psi}_{12}^{ML}(x_1, x_2) = \tilde{p}(x_1, x_2), \quad \hat{\psi}_{23}^{ML}(x_2, x_3) = \frac{\tilde{p}(x_2, x_3)}{\tilde{p}(x_2)} = \tilde{p}(x_3 | x_2)$$

#### MLE FOR DECOMPOSABLE UNDIRECTED MODELS



If the potentials were defined on non-maximal cliques (e.g.,  $\psi_{12}, \psi_{34}$ ), we could not equate empirical marginals on max-cliques with model parameters.

#### IPF FOR PAIRWISE MRFs

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while not converged for each node i for each neighbor j \in N_i m^t_{ij} = P(X_i, X_j | \theta^t) \text{ (inference)} c_{ij} = \text{normalize(empirical counts}(X_i, X_j)) \psi^{t+1}_{ij} = \psi^t_{ij} \times \frac{c_{ij}}{m^t_{ij}} \theta^{t+1} = \theta^t \setminus \psi^t_{ij} \cup \psi^{t+1}_{ij}
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If the graph is decomposable, we will converge after updating each potential once.

## ITERATIVE PROPORTIONAL FITTING (IPF)

• Let's go back to the derivative of the likelihood:

$$\frac{\partial \ell}{\partial \psi_c(\mathbf{x}_c)} = \frac{n(\mathbf{x}_c)}{\psi_c(\mathbf{x}_c)} - N \frac{p(\mathbf{x}_c)}{\psi_c(\mathbf{x}_c)}$$

• From this we can derive another relationship:

$$\frac{q(\mathbf{x}_c)}{\psi_c(\mathbf{x}_c)} = \frac{p(\mathbf{x}_c|\theta)}{\psi_c(\mathbf{x}_c)}$$

in which  $\psi_c$  appears implicitly in the model marginal  $p(\mathbf{x}_c|\theta)$ .

- ullet To solve for  $\psi_c$  is hard, because it appears on both sides of this implicit nonlinear equation.
- The idea of IPF is to hold  $\psi_c$  fixed on the right hand side (both in the numberator and denominator) and solve for it on the left hand side. We cycle through all cliques, then iterate:

$$\psi_c^{(t+1)}(\mathbf{x}_c) = \psi_c^{(t)}(\mathbf{x}_c) \frac{q(\mathbf{x}_c)}{p^{(t)}(\mathbf{x}_c)}$$

#### PROPERTIES OF IPF UPDATES

- IPF iterates a set of fixed-point equations.
- However, we can prove it is also a coordinate ascent algorithm (coordinates = parameters of clique potentials).
- Hence at each step, it will increase the log-likelihood, and it will converge to a global maximum.

IPF MINIMIZES KL DIVERGENCE

- IPF can also be seen to be coordinate ascent in the likelihood using the way of expressing likelihoods using KL divergences.
- First, we observe that maximizing the log likelihood is equivalent to minimizing the KL divergence (cross entropy) from the observed distribution to the model distribution:

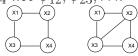
$$\max \ell \Leftrightarrow \min KL[q(\mathbf{x}) || p(\mathbf{x} | \theta)] = \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{p(\mathbf{x} | \theta)}$$

• Next, we use a property of KL divergence based on the conditional chain rule:  $p(\mathbf{x}) = p(\mathbf{x}_a)p(\mathbf{x}_b|\mathbf{x}_a)$ :

$$\begin{split} KL[q(\mathbf{x}_a,\mathbf{x}_b) \| p(\mathbf{x}_a,\mathbf{x}_b)] &= KL[q(\mathbf{x}_a) \| p(\mathbf{x}_a)] + \\ &\sum_{\mathbf{x}_a} q(\mathbf{x}_a) KL[q(\mathbf{x}_b | \mathbf{x}_a) \| p(\mathbf{x}_b | \mathbf{x}_a)] \end{split}$$

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|               |              |         |                   |

• Putting these two together, we see that:

$$KL[q(\mathbf{x})||p(\mathbf{x}|\theta)] = KL[q(\mathbf{x}_c)||p(\mathbf{x}_c|\theta)] + \sum_{\mathbf{x}_c} q(\mathbf{x}_c)KL[q(\mathbf{x}_{\tilde{c}}|\mathbf{x}_c)||p(\mathbf{x}_{\tilde{c}}|\mathbf{x}_c,\theta)]$$

But changing the clique potential has no effect on the conditional distribution, so the second term in unaffected. To minimize the first term, we set the marginal to the observed marginal, just as in IPF.

• In fact, we can interpret IPF updates as retaining the "old" conditional probabilities  $p^{(t)}(\mathbf{x}_{\tilde{c}}|\mathbf{x}_c)$  while replacing the "old" marginal probability  $p^{(t)}(\mathbf{x}_c)$  with the observed marginal  $q(\mathbf{x}_c)$ .

# CONSTRAINED CLIQUE POTENTIALS (J CH 19)

- ullet So far we have discussed the most general form of a graphical model in which maximal cliques are parametrized by general potential functions  $\psi_C(\mathbf{x}_C)$ .
- But for large cliques these general potentials are exponentially costly for inference and have exponential numbers of parameters that we must learn from limited data.
- One solution: change the graphical model to make cliques smaller.
   But this changes the dependencies, and may force us to make more independence assumptions than we would like.
- Another solution: keep the same graphical model, but use a less general parameterization of the clique potentials.
- This is the idea behind *feature-based models*. It is also the same idea behind *factor graphs* which we already saw.

- Consider a clique  $\mathbf{x}_C$  of random variables in a graphical model, e.g. three consecutive characters  $c_1c_2c_3$  in a string of English text.
- How would we build a model of  $p(c_1c_2c_3)$ ?
- The full joint clique potential would be huge:  $26^3 1$  parameters.
- However, we often know that some particular joint settings of the variables in a clique are quite likely or quite unlikely.
  e.g. ing, ate, ion, ?ed, qu?, jkx, zzz,...
- A "feature" is a function which is uniform over all joint settings except a few particulat ones on which it is high or low.
- For example, we might have  $f_{ing}(c_1c_2c_3)$  which is 1 if the string is 'ing' and 0 otherwise, and similar features for '?ed', etc.
- We can also define features when the inputs are continuous. Then the idea of a cell on which it is active disappears, but we might still have a compact parameterization of the feature.

# Combining Features

- Each feature has a weight which tells us how important it is and whether it increases or decreases the probability of the clique.
- This is a generalized exponential family distribution:

$$p(c_1c_2c_3) \propto \exp\{ \theta_{\texttt{ing}}f_{\texttt{ing}}(c_1c_2c_3) + \theta_{\texttt{?ed}}f_{\texttt{?ed}}(c_1c_2c_3) + \theta_{\texttt{qu}}f_{\texttt{qu}}(c_1c_2c_3) + \theta_{\texttt{zzz}}f_{\texttt{zzz}}(c_1c_2c_3) + \ldots \}$$

• In general, the features may be overlapping, unconstrained indicators of any function of the clique variables:

$$\psi_c(\mathbf{x}_c) \equiv \prod_{i \in I_C} \exp\{\theta_i f_i(\mathbf{x}_{Ci})\}$$
$$= \exp\left\{\sum_{i \in I_C} \theta_i f_i(\mathbf{x}_{Ci})\right\}$$

• How can we combine feature into a probability model?

- By exponentiating them, each feature function can be made into a "micropotential". We can multiply these micropotentials together to get a clique potential.
- ullet Example: a clique potential  $\psi(c_1,c_2,c_3)$  could be expressed as

$$\psi(c_1, c_2, c_3) = e^{\theta_{ing} f_{ing}} e^{\theta_{ing} f_{jed}} \dots$$
$$= \exp \left[ \sum_{i=1}^K \theta_i f_i(c_1, c_2, c_3) \right]$$

- This is still a potential over  $26^3$  possible settings, but only uses K parameters if there are K features.
- ullet By having one indicator function per combination of  $\mathbf{x}_C$ , we recover the standard tabular potential.

# FEATURE BASED MODEL

• We can multiply these clique potentials as usual:

$$p(\mathbf{x}|\theta) = \frac{1}{Z(\theta)} \prod_{C} \psi_{C}(\mathbf{x}_{C})$$

$$= \frac{1}{Z(\theta)} \prod_{C} \exp \left\{ \sum_{i \in I_{C}} \theta_{i} f_{i}(\mathbf{x}_{Ci}) \right\}$$

$$= \frac{1}{Z(\theta)} \exp \left\{ \sum_{C} \sum_{i \in I_{C}} \theta_{i} f_{i}(\mathbf{x}_{Ci}) \right\}$$

• However, in general we can forget about associating features with cliques and just use a simplified form:

$$p(\mathbf{x}|\theta) = \frac{1}{Z(\theta)} \exp\left\{\sum_{i} \theta_{i} f_{i}(\mathbf{x}_{Ci})\right\}$$

• This is just our friend the exponential model, with the features as sufficient statistics! We don't really need the graphical model at all.

i.e., At ML estimate, model expectations match empirical feature counts. (\*)  $\frac{\partial \log Z}{\partial \theta_i} = E f_i(X)$  (Jordan eqn 8.40).

# SOLUTION TO THE MAXENT PROBLEM

• To solve the maxent problem, we use Lagrange multipliers:

$$\begin{split} L &= -\sum_{\mathbf{x}} p(\mathbf{x}) \log p(\mathbf{x}) - \sum_{i} \theta_{i} \left( \sum_{\mathbf{x}} p(\mathbf{x}) f_{i}(\mathbf{x}) - \alpha_{i} \right) - \mu \left( \sum_{\mathbf{x}} p(\mathbf{x}) - 1 \right) \\ \frac{\partial L}{\partial p(\mathbf{x})} &= 1 + \log p(\mathbf{x}) - \sum_{i} \theta_{i} f_{i}(\mathbf{x}) - \mu \\ p^{*}(\mathbf{x}) &= e^{\mu - 1} \exp \left\{ \sum_{i} \theta_{i} f_{i}(\mathbf{x}) \right\} \\ Z(\theta) &\stackrel{\text{def}}{=} e^{1 - \mu} = \sum_{\mathbf{x}} \exp \left\{ \sum_{i} \theta_{i} f_{i}(\mathbf{x}) \right\} \text{ since } \sum_{x} p^{*}(x) = 1 \\ p(\mathbf{x}|\theta) &= \frac{1}{Z(\theta)} \exp \left\{ \sum_{i} \theta_{i} f_{i}(\mathbf{x}) \right\} \end{split}$$

- So feature constraints + maxent implies exponential family.
- Problem is convex, so solution is unique.

#### MAXIMUM ENTROPY

• We can approach the modeling problem from an entirely different point of view. *Begin* with some fixed feature expectations:

$$\sum_{\mathbf{x}} p(\mathbf{x}) f_i(\mathbf{x}) = \alpha_i$$

- Assuming expectations are consistent, there may exist many distributions which satisfy them. Which one should we select? The most uncertain or flexible one:
   i.e. the one with maximum entropy.
- This yields a new optimization problem:

$$\max \mathcal{H}[p(\mathbf{x})] = -\sum_{\mathbf{x}} p(\mathbf{x}) \log p(\mathbf{x})$$
subject to 
$$\sum_{\mathbf{x}} p(\mathbf{x}) f_i(\mathbf{x}) = \alpha_i$$
$$\sum_{\mathbf{x}} p(\mathbf{x}) = 1$$

#### Constraints from Data

- ullet Where do the constraints  $\alpha_i$  come from?
- Just as before, measure the empirical counts on the training data:

$$\alpha_i = \sum_{\mathbf{x}} \frac{n(\mathbf{x})}{N} f_i(\mathbf{x}) = \sum_{\mathbf{x}} \bar{p}(\mathbf{x}) f_i(\mathbf{x})$$

- This also ensures consistency automatically.
- Known as the "method of moments". (c.f. law of large numbers)
- We have seen a case of convex duality:
   In one case, we assume exponential family and show that ML implies feature expectations match observed counts.
   In the other case, we assume model expectations must match empirical feature counts and show that maxent implies exponential family distribution.

#### CONDITIONAL MAXENT MODELS

- So far we have focussed on maxent models for density estimation (unsupervised learning).
- We can also formulate such models for classification and regression (conditional density estimation).
- For classification, the simplest model is:

$$p(c|\mathbf{x}) = \frac{\exp \sum_{i} \theta_{ci} f_i(\mathbf{x})}{\sum_{c'} \exp \sum_{i} \theta_{c'i} f_i(\mathbf{x})}$$

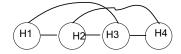
where each class gets its own set of weights  $\theta_{ci}$  over the features and we do the classification using softmax.

- If we use the "identity features"  $f_i(\mathbf{x}) = x_i$  then this is exactly equivalent to the *logistic regression* model we saw before.
- The model above is like doing logistic regression on the features. Now features can be very complex, nonlinear functions of the data.

# GENERATIVE VS DISCRIMINATIVE MODELS

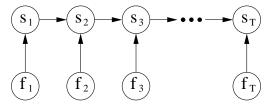
- An HMM is a model of how to *generate* observations  $o_t$  from hidden states  $h_t$ .
- Hence an HMM defines a joint distribution over hidden and observed variables,  $p(o_{1:t}|h_{1:t})p(h_{1:t})$ .
- An MEMM is a conditional model of hidden states given observations,  $p(h_{1:t}|o_{1:t})$ .
- Advantages of conditional models:
  - Do not need to waste parameters modeling observed inputs  $o_{1:t}$ .
  - Can incorporate arbitrary, nonlocal features of the input, without increasing complexity.





## MAXIMUM ENTROPY MARKOV MODEL (MEMM)

• We can combine local probabilistic classifiers together into a Markov chain, to get a *maximum entropy markov model*.



• A MEMM encodes a *conditional* density:

$$p(h_1^T | o_1^T) = \prod_t p(h_t | h_{t-1}, f_t(o_1^T))$$

whereas an HMM encodes a joint density

$$p(h_1^T, o_1^T) = \prod_t p(h_t | h_{t-1}) p(o_t | h_t)$$