Acknowledgement: Partially based on slides by Eric Xing at CMU and Andrew McCallum at UMass Amherst
Today: learning undirected graphical models

1. Learning MRFs
   a. Feature-based (log-linear) representation of MRFs
   b. Maximum likelihood estimation
   c. Maximum entropy view

2. Getting around complexity of inference
   a. Using approximate inference (e.g., TRW) within learning
   b. Pseudo-likelihood

3. Conditional random fields
Recall: ML estimation in Bayesian networks

- Maximum likelihood estimation: \( \max_\theta \ell(\theta; D) \), where

\[
\ell(\theta; D) = \log p(D; \theta) = \sum_{x \in D} \log p(x; \theta) = \sum_{i} \sum_{\hat{x}_{pa(i)}} \sum_{x \in D: x_{pa(i)} = \hat{x}_{pa(i)}} \log p(x_i | \hat{x}_{pa(i)})
\]

- In Bayesian networks, we have the closed form ML solution:

\[
\theta_{ML}^{x_i | x_{pa(i)}} = \frac{N_{x_i, x_{pa(i)}}}{\sum_{\hat{x}_i} N_{\hat{x}_i, x_{pa(i)}}}
\]

where \( N_{x_i, x_{pa(i)}} \) is the number of times that the (partial) assignment \( x_i, x_{pa(i)} \) is observed in the training data

- We were able to estimate each CPD independently because the objective \textit{decomposes} by variable and parent assignment
Bad news for Markov networks

- The global normalization constant $Z(\theta)$ kills decomposability:

$$\theta_{ML} = \arg \max_\theta \log \prod_{x \in D} p(x; \theta)$$

$$= \arg \max_\theta \sum_{x \in D} \left( \sum_c \log \phi_c(x_c; \theta) - \log Z(\theta) \right)$$

$$= \arg \max_\theta \left( \sum_{x \in D} \sum_c \log \phi_c(x_c; \theta) \right) - |D| \log Z(\theta)$$

- The log-partition function prevents us from decomposing the objective into a sum over terms for each potential

- Solving for the parameters becomes much more complicated
What are the parameters?

- How do we parameterize $\phi_c(x_c; \theta)$? Use a log-linear parameterization:
  - Introduce weights $w \in \mathbb{R}^d$ that are used globally
  - For each potential $c$, a vector-valued feature function $f_c(x_c) \in \mathbb{R}^d$
  - Then, $\phi_c(x_c; w) = \exp(w \cdot f_c(x_c))$

- Example: discrete-valued MRF with only edge potentials, where each variable takes $k$ states
  - Let $d = k^2 |E|$, and let $w_{i,j,x_i,x_j} = \log \phi_{ij}(x_i, x_j)$
  - Let $f_{i,j}(x_i, x_j)$ have a 1 in the dimension corresponding to $(i, j, x_i, x_j)$ and 0 elsewhere

- The joint distribution is in the exponential family!
  $$p(x; w) = \exp\{w \cdot f(x) - \log Z(w)\},$$
  where $f(x) = \sum_c f_c(x_c)$ and $Z(w) = \sum_x \exp\{\sum_c w \cdot f_c(x_c)\}$

- This formulation allows for parameter sharing
Log-likelihood for log-linear models

$$
\theta^{ML} = \arg \max_{\theta} \left( \sum_{x \in D} \sum_{c} \log \phi_c(x_c; \theta) \right) - |D| \log Z(\theta)
$$

$$
= \arg \max_{w} \left( \sum_{x \in D} \sum_{c} w \cdot f_c(x_c) \right) - |D| \log Z(w)
$$

$$
= \arg \max_{w} w \cdot \left( \sum_{x \in D} \sum_{c} f_c(x_c) \right) - |D| \log Z(w)
$$

- The first term is linear in $w$
- The second term is also a function of $w$:

$$
\log Z(w) = \log \sum_{x} \exp \left( w \cdot \sum_{c} f_c(x_c) \right)
$$
Log-likelihood for log-linear models

\[
\log Z(\mathbf{w}) = \log \sum_x \exp \left( \mathbf{w} \cdot \sum_c f_c(x_c) \right)
\]

- \(\log Z(\mathbf{w})\) does not decompose
  - No closed form solution; even \textit{computing} likelihood requires inference
- Recall Problem 4 ("Exponential families") from Problem Set 2. Letting \(f(x) = \sum_c f_c(x_c)\), you showed that

\[
\nabla_\mathbf{w} \log Z(\mathbf{w}) = \mathbb{E}_{p(x;\mathbf{w})}[f(x)] = \sum_c \mathbb{E}_{p(x_c;\mathbf{w})}[f_c(x_c)]
\]

- Thus, the gradient of the log-partition function can be computed by \textit{inference}, computing marginals with respect to the current parameters \(\mathbf{w}\)
- We also claimed that the 2nd derivative of the log-partition function gives the second-order moments, i.e.

\[
\nabla^2 \log Z(\mathbf{w}) = \text{cov}[f(x)]
\]

- Since covariance matrices are always positive semi-definite, this proves that \(\log Z(\mathbf{w})\) is convex (so \(-\log Z(\mathbf{w})\) is concave)
Solving the maximum likelihood problem in MRFs

\[ \ell(w; D) = \frac{1}{|D|} w \cdot \left( \sum_{x \in D} \sum_{c} f_c(x_c) \right) - \log Z(w) \]

- First, note that the weights \( w \) are unconstrained, i.e. \( w \in \mathbb{R}^d \)
- The objective function is jointly concave. Apply any convex optimization method to learn!
- Can use gradient ascent, stochastic gradient ascent, quasi-Newton methods such as limited memory BFGS (L-BFGS)
- The gradient of the log-likelihood is:

\[
\frac{d}{dw_k} \ell(w; D) = \frac{1}{|D|} \sum_{x \in D} \sum_{c} (f_c(x_c))_k - \sum_{c} \mathbb{E}_{p(x_c; w)}[(f_c(x_c))_k]
\]

\[
= \sum_{c} \frac{1}{|D|} \sum_{x \in D} (f_c(x_c))_k - \sum_{c} \mathbb{E}_{p(x_c; w)}[(f_c(x_c))_k]
\]
The gradient of the log-likelihood

\[
\frac{\partial}{\partial w_k} \ell(w; D) = \sum_c \frac{1}{|D|} \sum_{x \in D} (f_c(x_c))_k - \sum_c \mathbb{E}_{p(x_c; w)} [(f_c(x_c))_k]
\]

- Difference of expectations!
- Consider the earlier pairwise MRF example. This then reduces to:

\[
\frac{\partial}{\partial w_{i,j}} \ell(w; D) = \left( \frac{1}{|D|} \sum_{x \in D} 1[x_i = \hat{x}_i, x_j = \hat{x}_j] \right) - p(\hat{x}_i, \hat{x}_j; w)
\]

- Setting derivative to zero, we see that for the maximum likelihood parameters \(w^{ML}\), we have

\[
p(\hat{x}_i, \hat{x}_j; w^{ML}) = \frac{1}{|D|} \sum_{x \in D} 1[x_i = \hat{x}_i, x_j = \hat{x}_j]
\]

for all edges \(ij \in E\) and states \(\hat{x}_i, \hat{x}_j\)

- Model marginals for each clique equal the empirical marginals!
- Called **moment matching**, and is a property of maximum likelihood learning in exponential families
Gradient ascent requires repeated marginal inference, which in many models is **hard**!

We will return to this shortly.
We can approach the modeling task from an entirely different point of view.

Suppose we know some expectations with respect to a (fully general) distribution $p(x)$:

(true) $\sum_x p(x)f_i(x)$,  
(empirical) $\frac{1}{|D|} \sum_{x \in D} f_i(x) = \alpha_i$

Assuming that the expectations are consistent with one another, 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:

$$\max_p H(p(x)) = -\sum_x p(x) \log p(x)$$

s.t.  
$$\sum_x p(x)f_i(x) = \alpha_i$$

$$\sum p(x) = 1$$  (strictly concave w.r.t. $p(x)$)
What does the MaxEnt solution look like?

To solve the MaxEnt problem, we form the Lagrangian:

\[
L = - \sum_x p(x) \log p(x) - \sum_i \lambda_i \left( \sum_x p(x) f_i(x) - \alpha_i \right) - \mu \left( \sum_x p(x) - 1 \right)
\]

Then, taking the derivative of the Lagrangian,

\[
\frac{\partial L}{\partial p(x)} = -1 - \log p(x) - \sum_i \lambda_i f_i(x) - \mu
\]

And setting to zero, we obtain:

\[
p^*(x) = \exp \left( -1 - \mu - \sum_i \lambda_i f_i(x) \right) = e^{-1-\mu} e^{-\sum_i \lambda_i f_i(x)}
\]

From the constraint \( \sum_x p(x) = 1 \) we obtain \( e^{1+\mu} = \sum_x e^{-\sum_i \lambda_i f_i(x)} = Z(\lambda) \)

We conclude that the maximum entropy distribution has the form (substituting \( w_i = -\lambda_i \))

\[
p^*(x) = \frac{1}{Z(w)} \exp(\sum_i w_i f_i(x))
\]
Equivalence of maximum likelihood and maximum entropy

- Feature constraints + MaxEnt $\Rightarrow$ exponential family!
- We have seen a case of convex duality:
  - In one case, we assume exponential family and show that ML implies model expectations must match empirical expectations
  - In the other case, we assume model expectations must match empirical feature counts and show that MaxEnt implies exponential family distribution
- Can show that one is the dual of the other, and thus both obtain the same value of the objective at optimality (no duality gap)
- Besides providing insight into the ML solution, this also gives an alternative way to (approximately) solve the learning problem
How can we get around the complexity of inference during learning?
Monte Carlo methods

Recall the original learning objective

\[
\ell(w; D) = \frac{1}{|D|} \mathbf{w} \cdot \left( \sum_{x \in D} \sum_{c} f_c(x_c) \right) - \log Z(w)
\]

Use any of the sampling approaches (e.g., Gibbs sampling) that we discussed in Lecture 9.

All we need for learning (i.e., to compute the derivative of \( \ell(w, D) \)) are **marginals** of the distribution.

No need to ever estimate \( \log Z(w) \).
Using approximations of the log-partition function

- We can substitute the original learning objective

\[ \ell(w; D) = \frac{1}{|D|} w \cdot \left( \sum_{x \in D} \sum_c f_c(x_c) \right) - \log Z(w) \]

with one that uses a tractable approximation of the log-partition function:

\[ \tilde{\ell}(w; D) = \frac{1}{|D|} w \cdot \left( \sum_{x \in D} \sum_c f_c(x_c) \right) - \log \tilde{Z}(w) \]

- Recall from Lecture 8 that we came up with a convex relaxation that provided an upper bound on the log-partition function,

\[ \log Z(w) \leq \log \tilde{Z}(w) \]

(e.g., tree-rewighted belief propagation, log-determinant relaxation)

- Using this, we obtain a lower bound on the learning objective

\[ \ell(w; D) \geq \tilde{\ell}(w; D) \]

- Again, to compute the derivatives we only need pseudo-marginals from the variational inference algorithm.
Alternatively, can we come up with a \textit{different} objective function (i.e., a different \textit{estimator}) which succeeds at learning while avoiding inference altogether?

Pseudo-likelihood method (Besag 1971) yields an exact solution if the data is generated by a model in our model family \( p(x; \theta^*) \) and \(|D| \to \infty\) (i.e., it is \textbf{consistent})

Note that, via the chain rule,

\[
p(x; w) = \prod_i p(x_i | x_1, \ldots, x_{i-1}; w)
\]

We consider the following approximation:

\[
p(x; w) \approx \prod_i p(x_i | x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n; w) = \prod_i p(x_i | x_{-i}; w)
\]

where we have added conditioning over additional variables
The pseudo-likelihood method replaces the likelihood,

\[
\ell(\theta; D) = \frac{1}{|D|} \log p(D; \theta) = \frac{1}{|D|} \sum_{m=1}^{|D|} \log p(x^m; \theta)
\]

with the following approximation:

\[
\ell_{PL}(w; D) = \frac{1}{|D|} \sum_{m=1}^{|D|} \sum_{i=1}^n \log p(x^m_i | x^m_{N(i)}; w)
\]

(we replaced \(x_{-i}\) with \(x_{N(i)}\), \(i\)'s Markov blanket)

For example, suppose we have a pairwise MRF. Then,

\[
p(x^m_i | x^m_{N(i)}; w) = \frac{1}{Z(x^m_{N(i)}; w)} e^{\sum_{j \in N(i)} \theta_{ij}(x^m_i, x^m_j)}, \quad Z(x^m_{N(i)}; w) = \sum_{\hat{x}_i} e^{\sum_{j \in N(i)} \theta_{ij}(\hat{x}_i, x^m_j)}
\]

More generally, and using the log-linear parameterization, we have:

\[
\log p(x^m_i | x^m_{N(i)}; w) = w \cdot \sum_{c : i \in c} f_c(x^m_c) - \log Z(x^m_{N(i)}; w)
\]
This objective only involves summation over $x_i$ and is tractable.

Has many small partition functions (one for each variable and each setting of its neighbors) instead of one big one.

It is still concave in $w$ and thus has no local maxima.

Assuming the data is drawn from a MRF with parameters $w^*$, can show that as the number of data points gets large, $w^{PL} \rightarrow w^*$.
Conditional random fields

- Recall from Lecture 4, a CRF is a Markov network on variables $\mathbf{X} \cup \mathbf{Y}$, which specifies the conditional distribution

$$P(y \mid x) = \frac{1}{Z(x)} \prod_{c \in C} \phi_c(x, y_c)$$

with partition function

$$Z(x) = \sum_{\hat{y}} \prod_{c \in C} \phi_c(x, \hat{y}_c).$$

- The feature functions now depend on $x$ in addition to $y$
- For each potential $c$, a vector-valued feature function $f_c(x, y_c) \in \mathbb{R}^d$
- Then, $\phi_c(x, y_c; w) = \exp(w \cdot f_c(x, y_c))$
Learning with conditional random fields

- Exact same as learning with MRFs, except that we have a different partition function for each data point

\[ \theta^{ML} = \arg \max_{\theta} \sum_{(x,y) \in D} \left( \sum_c \log \phi_c(x, y_c; \theta) - \log Z(x; \theta) \right) \]

\[ = \arg \max_w \mathbf{w} \cdot \left( \sum_{(x,y) \in D} \sum_c \mathbf{f}_c(x, y_c) \right) - \sum_{(x,y) \in D} \log Z(x; \mathbf{w}) \]