Probabilistic Graphical Models

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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: $\max_\theta \ell(\theta; \mathcal{D})$, where

$$\ell(\theta;\mathcal{D}) = \log p(\mathcal{D};\theta) = \sum_{\mathbf{x}\in\mathcal{D}} \log p(\mathbf{x};\theta)$$
$$= \sum_i \sum_{\hat{\mathbf{x}}_{pa(i)}} \sum_{\substack{\mathbf{x}\in\mathcal{D}: \\ \mathbf{x}_{pa(i)}=\hat{\mathbf{x}}_{pa(i)}}} \log p(x_i \mid \hat{\mathbf{x}}_{pa(i)})$$

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

$$\theta^{ML}_{x_i|\mathbf{x}_{pa(i)}} = \frac{N_{x_i,\mathbf{x}_{pa(i)}}}{\sum_{\hat{x}_i} N_{\hat{x}_i,\mathbf{x}_{pa(i)}}}$$

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

- We were able to estimate each CPD independently because the objective **decomposes** by variable and parent assignment

Bad news for Markov networks

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

$$
\begin{aligned}
\theta^{ML} &= \arg\max_{\theta} \log \prod_{\mathbf{x} \in \mathcal{D}} p(\mathbf{x}; \theta) \\
&= \arg\max_{\theta} \sum_{\mathbf{x} \in \mathcal{D}} \left(\sum_{c} \log \phi_c(\mathbf{x}_c; \theta) - \log Z(\theta) \right) \\
&= \arg\max_{\theta} \left(\sum_{\mathbf{x} \in \mathcal{D}} \sum_{c} \log \phi_c(\mathbf{x}_c; \theta) \right) - |\mathcal{D}| \log Z(\theta)
\end{aligned}
$$

- 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 $\phi_c(\mathbf{x}_c; \theta)$? Use a log-linear parameterization:
  - Introduce **weights** $\mathbf{w} \in \mathbb{R}^d$ that are used globally
  - For each potential c, a vector-valued **feature function** $\mathbf{f}_c(\mathbf{x}_c) \in \mathbb{R}^d$
  - Then, $\phi_c(\mathbf{x}_c; \mathbf{w}) = \exp(\mathbf{w} \cdot \mathbf{f}_c(\mathbf{x}_c))$
- 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*!

$$p(\mathbf{x}; \mathbf{w}) = \exp\{\mathbf{w} \cdot \mathbf{f}(\mathbf{x}) - \log Z(\mathbf{w})\},$$

where $f(\mathbf{x}) = \sum_c f_c(\mathbf{x}_c)$ and $Z(\mathbf{w}) = \sum_{\mathbf{x}} \exp\{\sum_c \mathbf{w} \cdot f_c(\mathbf{x}_c)\}$

- This formulation allows for parameter sharing

Log-likelihood for log-linear models

$$\begin{aligned}
\theta^{ML} &= \arg\max_{\theta} \left(\sum_{\mathbf{x}\in\mathcal{D}} \sum_{c} \log \phi_c(\mathbf{x}_c;\theta) \right) - |\mathcal{D}| \log Z(\theta) \\
&= \arg\max_{\mathbf{w}} \left(\sum_{\mathbf{x}\in\mathcal{D}} \sum_{c} \mathbf{w}\cdot \mathbf{f}_c(\mathbf{x}_c) \right) - |\mathcal{D}| \log Z(\mathbf{w}) \\
&= \arg\max_{\mathbf{w}} \ \mathbf{w}\cdot \left(\sum_{\mathbf{x}\in\mathcal{D}} \sum_{c} \mathbf{f}_c(\mathbf{x}_c) \right) - |\mathcal{D}| \log Z(\mathbf{w})
\end{aligned}$$

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

$$\log Z(\mathbf{w}) = \log \sum_{\mathbf{x}} \exp\left(\mathbf{w}\cdot \sum_{c} \mathbf{f}_c(\mathbf{x}_c) \right)$$

Log-likelihood for log-linear models

$$\log Z(\mathbf{w}) = \log \sum_{\mathbf{x}} \exp\left(\mathbf{w} \cdot \sum_{c} \mathbf{f}_c(\mathbf{x}_c)\right)$$

- $\log Z(\mathbf{w})$ does not decompose
  - No closed form solution; even *computing* likelihood requires inference
- Letting $\mathbf{f}(\mathbf{x}) = \sum_c \mathbf{f}_c(\mathbf{x}_c)$, we will show (see blackboard) that:

$$\nabla_{\mathbf{w}} \log Z(\mathbf{w}) = \mathbb{E}_{p(\mathbf{x};\mathbf{w})}[\mathbf{f}(\mathbf{x})] = \sum_{c} \mathbb{E}_{p(\mathbf{x}_c;\mathbf{w})}[\mathbf{f}_c(\mathbf{x}_c)]$$

- Thus, the gradient of the log-partition function can be computed by *inference*, computing marginals with respect to the current parameters $\mathbf{w}$
- Similarly, you can show that 2nd derivative of the log-partition function gives the second-order moments, i.e.

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

- 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

$$\ell(\mathbf{w}; \mathcal{D}) = \frac{1}{|\mathcal{D}|} \mathbf{w} \cdot \left(\sum_{\mathbf{x} \in \mathcal{D}} \sum_c \mathbf{f}_c(\mathbf{x}_c) \right) - \log Z(\mathbf{w})$$

- First, note that the weights $\mathbf{w}$ are unconstrained, i.e. $\mathbf{w} \in \mathbb{R}^d$
- 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:

$$\begin{aligned} \frac{d}{dw_k} \ell(\mathbf{w}; \mathcal{D}) &= \frac{1}{|\mathcal{D}|} \sum_{\mathbf{x} \in \mathcal{D}} \sum_c (\mathbf{f}_c(\mathbf{x}_c))_k - \sum_c \mathbb{E}_{p(\mathbf{x}_c; \mathbf{w})}[(\mathbf{f}_c(\mathbf{x}_c))_k] \\ &= \sum_c \frac{1}{|\mathcal{D}|} \sum_{\mathbf{x} \in \mathcal{D}} (\mathbf{f}_c(\mathbf{x}_c))_k - \sum_c \mathbb{E}_{p(\mathbf{x}_c; \mathbf{w})}[(\mathbf{f}_c(\mathbf{x}_c))_k] \end{aligned}$$

The gradient of the log-likelihood

$$\frac{\partial}{\partial w_k}\ell(\mathbf{w};\mathcal{D}) = \sum_c \frac{1}{|\mathcal{D}|}\sum_{\mathbf{x}\in\mathcal{D}}(\mathbf{f}_c(\mathbf{x}_c))_k - \sum_c \mathbb{E}_{p(\mathbf{x}_c;\mathbf{w})}[(\mathbf{f}_c(\mathbf{x}_c))_k]$$

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

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

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

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

  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.

Maximum entropy (MaxEnt)

- 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 $p(\mathbf{x})$:

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

- 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:

$$\max_p H(p(\mathbf{x})) = -\sum_{\mathbf{x}} p(\mathbf{x}) \log p(\mathbf{x})$$

$$\text{s.t.} \qquad \sum_{\mathbf{x}} p(\mathbf{x}) f_i(\mathbf{x}) = \alpha_i$$

$$\sum p(\mathbf{x}) = 1 \quad \text{(strictly concave w.r.t. } p(\mathbf{x}))$$

What does the MaxEnt solution look like?

- To solve the MaxEnt problem, we form the Lagrangian:

$$L = -\sum_{\mathbf{x}} p(\mathbf{x}) \log p(\mathbf{x}) - \sum_i \lambda_i \left(\sum_{\mathbf{x}} p(\mathbf{x}) f_i(\mathbf{x}) - \alpha_i \right) - \mu \left(\sum_{\mathbf{x}} p(\mathbf{x}) - 1 \right)$$

- Then, taking the derivative of the Lagrangian,

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

- And setting to zero, we obtain:

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

- From the constraint $\sum_{\mathbf{x}} p(\mathbf{x}) = 1$ we obtain $e^{1+\mu} = \sum_{\mathbf{x}} e^{-\sum_i \lambda_i f_i(\mathbf{x})} = Z(\lambda)$
- We conclude that the maximum entropy distribution has the form (substituting $w_i = -\lambda_i$)

$$p^*(\mathbf{x}) = \frac{1}{Z(\mathbf{w})} \exp(\sum_i w_i f_i(\mathbf{x}))$$

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

$$\ell(\mathbf{w}; \mathcal{D}) = \frac{1}{|\mathcal{D}|}\mathbf{w} \cdot \left(\sum_{\mathbf{x}\in\mathcal{D}} \sum_{c} \mathbf{f}_c(\mathbf{x}_c)\right) - \log Z(\mathbf{w})$$

- 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 $\ell(\mathbf{w}, \mathcal{D})$) are **marginals** of the distribution
- No need to ever estimate $\log Z(\mathbf{w})$

Using approximations of the log-partition function

- We can substitute the original learning objective

$$\ell(\mathbf{w}; \mathcal{D}) = \frac{1}{|\mathcal{D}|}\mathbf{w} \cdot \Big(\sum_{\mathbf{x} \in \mathcal{D}} \sum_c \mathbf{f}_c(\mathbf{x}_c) \Big) - \log Z(\mathbf{w})$$

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

$$\tilde{\ell}(\mathbf{w}; \mathcal{D}) = \frac{1}{|\mathcal{D}|}\mathbf{w} \cdot \Big(\sum_{\mathbf{x} \in \mathcal{D}} \sum_c \mathbf{f}_c(\mathbf{x}_c) \Big) - \log \tilde{Z}(\mathbf{w})$$

- Recall from Lecture 7 that we came up with a *convex relaxation* that provided an upper bound on the log-partition function,

$$\log Z(\mathbf{w}) \leq \log \tilde{Z}(\mathbf{w})$$

  (e.g., tree-reweighted belief propagation, log-determinant relaxation)
- Using this, we obtain a *lower bound* on the learning objective

$$\ell(\mathbf{w}; \mathcal{D}) \geq \tilde{\ell}(\mathbf{w}; \mathcal{D})$$

- Again, to compute the derivatives we only need *pseudo-marginals* from the variational inference algorithm

Pseudo-likelihood

- Alternatively, can we come up with a *different* objective function (i.e., a different *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 $p(\mathbf{x}; \theta^*)$ and $|\mathcal{D}| \rightarrow \infty$ (i.e., it is **consistent**)
- Note that, via the chain rule,

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

- We consider the following approximation:

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

where we have added conditioning over additional variables

Pseudo-likelihood

- The pseudo-likelihood method replaces the likelihood,

$$\ell(\theta; \mathcal{D}) = \frac{1}{|\mathcal{D}|} \log p(\mathcal{D}; \theta) = \frac{1}{|\mathcal{D}|} \sum_{m=1}^{|\mathcal{D}|} \log p(\mathbf{x}^m; \theta)$$

  with the following approximation:

$$\ell_{PL}(\mathbf{w}; \mathcal{D}) = \frac{1}{|\mathcal{D}|} \sum_{m=1}^{|\mathcal{D}|} \sum_{i=1}^{n} \log p(x_i^m \mid x_{N(i)}^m; \mathbf{w})$$

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

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

$$p(x_i^m \mid x_{N(i)}^m; \mathbf{w}) = \frac{1}{Z(x_{N(i)}^m; \mathbf{w})} e^{\sum_{j \in N(i)} \theta_{ij}(x_i^m, x_j^m)}, \ Z(x_{N(i)}^m; \mathbf{w}) = \sum_{\hat{x}_i} e^{\sum_{j \in N(i)} \theta_{ij}(\hat{x}_i, x_j^m)}$$

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

$$\log p(x_i^m \mid x_{N(i)}^m; \mathbf{w}) = \mathbf{w} \cdot \sum_{c: i \in c} f_c(x_c^m) - \log Z(x_{N(i)}^m; \mathbf{w})$$

Pseudo-likelihood

- 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 $\mathbf{w}$ and thus has no local maxima
- Assuming the data is drawn from a MRF with parameters $\mathbf{w}^*$, can show that as the number of data points gets large, $\mathbf{w}^{PL} \to \mathbf{w}^*$

Conditional random fields

- Recall from Lecture 3, a CRF is a Markov network on variables $\mathbf{X} \cup \mathbf{Y}$, which specifies the conditional distribution

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

with partition function

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

- The feature functions now depend on $\mathbf{x}$ in addition to $\mathbf{y}$
- For each potential c, a vector-valued **feature function** $\mathbf{f}_c(\mathbf{x}, \mathbf{y}_c) \in \mathbb{R}^d$
- Then, $\phi_c(\mathbf{x}, \mathbf{y}_c; \mathbf{w}) = \exp(\mathbf{w} \cdot \mathbf{f}_c(\mathbf{x}, \mathbf{y}_c))$

Learning with conditional random fields

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

$$
\begin{aligned}
\theta^{ML} &= \arg\max_{\theta} \sum_{(\mathbf{x},\mathbf{y})\in\mathcal{D}} \left(\sum_{c} \log \phi_c(\mathbf{x}, \mathbf{y}_c; \theta) - \log Z(\mathbf{x}; \theta) \right) \\
&= \arg\max_{\mathbf{w}} \ \mathbf{w} \cdot \left(\sum_{(\mathbf{x},\mathbf{y})\in\mathcal{D}} \sum_{c} \mathbf{f}_c(\mathbf{x}, \mathbf{y}_c) \right) - \sum_{(\mathbf{x},\mathbf{y})\in\mathcal{D}} \log Z(\mathbf{x}; \mathbf{w})
\end{aligned}
$$