Lecture 10:

Parameter Learning for Bayes nets

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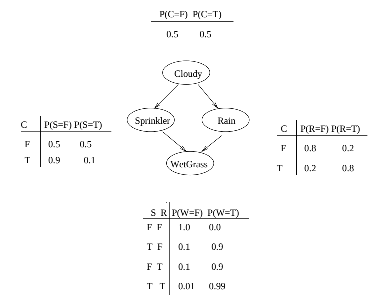
Learning graphical models

- Inference means computing $P(X_i|\theta, G)$
- Structure learning/ model selection = inferring G from data.
- Parameter learning/ estimation = inferring θ from data.



Parameter learning

- Assume G is known and fixed and is a DAG.
- Goal: estimate θ from a dataset of M independent, identically distributed (iid) training cases $D = (x^1, \ldots, x^M)$.
- In general, each training case $x^m = (x_1^m, \ldots, x_N^m)$ is a vector of values, one per node. (Think of a database with M rows and N columns.)
- We assume complete observability, i.e., every entry in the database is known (no missing values, no hidden variables).
- Initially we consider learning parameters for a single node.
- Then we consider how to learn parameters for a whole network.

Bayesian parameter estimation

- Bayesians treat the unknown parameters θ as a random variable, which can be estimated using Bayes rule:

$$p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})}$$

- This crucial equation can be written in words:

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{marginal likelihood}}$$

- For iid data, the likelihood is

$$p(D|\theta) = \prod_m p(x_m|\theta)$$

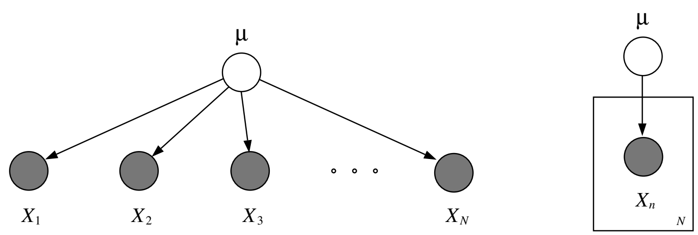
- The prior $p(\theta)$ encodes our prior knowledge about the domain.

Plates

- For iid (exchangeable) data, the likelihood is

$$p(D|\theta) = \prod_m p(x_m|\theta)$$

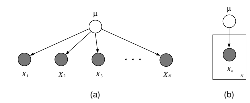
- We can represent this as a Bayes net with M nodes.
- “Plates” provide a more compact representation for repetitive structure, and are very common in Bayesian models.



(a) (b)

Plates

- “Plates” provide a compact representation for repetitive structure.
- The rules of plates are simple: repeat every structure in a box a number of times given by the integer in the corner of the box (e.g. N), updating the plate index variable (e.g. n) as you go.
- Duplicate every arrow going into the plate and every arrow leaving the plate by connecting the arrows to each copy of the structure.
- Plates are closely related to *probabilistic relational models*, and *object oriented Bayes nets*, which are forms of “syntactic sugar” for parameter tying (sharing).



Frequentist parameter estimation

- Two people with different priors $p(\theta)$ will end up with different estimates $p(\theta|D)$.
- Frequentists dislike this “subjectivity”.
- Frequentists think of the parameter as a fixed, unknown constant, not a random variable.
- Hence they have to come up with different estimators (ways of computing θ from data), instead of using Bayes' rule.
- These estimators have different properties, such as being “unbiased”, “minimum variance”, etc.
- A very popular estimator is the *maximum likelihood estimator*, which is simple and has good statistical properties.

Maximum likelihood estimation

- The log-likelihood is monotonically related to the likelihood:

$$\ell(\theta; D) = \log p(D|\theta) = \sum_m \log p(x^m|\theta)$$

- Idea of maximum likelihood estimation (MLE): pick the setting of parameters most likely to have generated the data we saw:

$$\hat{\theta}_{ML} = \mathrm{argmax}_\theta \;\ell(\theta; \mathcal{D})$$

- Often the MLE overfits the training data, so it is common to maximize a penalized log-likelihood instead:

$$\hat{\theta}_{MAP} = \mathrm{argmax}_\theta \;\ell(\theta; \mathcal{D}) - c(\theta)$$

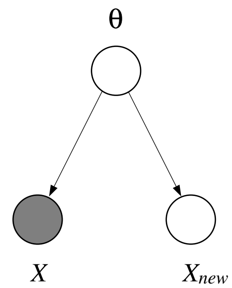
- This is equivalent to picking the mode of $P(\theta|D)$, where $c(\theta) = -\log p(\theta)$, since

$$\log p(\theta|D) = \log p(D|\theta) + \log p(\theta) + c$$

Integrate out or Optimize?

- $\hat{\theta}_{MAP}$ is not Bayesian (even though it uses a prior) since it is a point estimate.
- Consider predicting the future. A Bayesian will integrate out all uncertainty:

$$
\begin{aligned}
p(\mathbf{x}_{\text{new}}|\mathbf{X}) &= \int p(\mathbf{x}_{\text{new}}, \theta|\mathbf{X}) d\theta \\
&= \int p(\mathbf{x}_{\text{new}}|\theta, \mathbf{X}) p(\theta|\mathbf{X}) d\theta \\
&\propto \int p(\mathbf{x}_{\text{new}}|\theta) p(\mathbf{X}|\theta) p(\theta) d\theta
\end{aligned}
$$



- A frequentist will typically use a "plug-in" estimator such as ML/MAP:

$$p(\mathbf{x}_{\text{new}}|\mathbf{X}) = p(\mathbf{x}_{\text{new}}|\hat{\theta}), \quad \hat{\theta} = \arg\max_{\theta} p(\mathbf{X}|\theta)$$

Frequentist vs Bayesian

- This is a "theological" war.
- Advantages of Bayesian approach:
  - Mathematically elegant.
  - Works well when amount of data is much less than number of parameters (e.g., one-shot learning).
  - Easy to do incremental (sequential) learning.
  - Can be used for model selection (max likelihood will always pick the most complex model).
- Advantages of frequentist approach:
  - Mathematically/ computationally simpler.
- As $|D| \to \infty$, the two approaches become the same:

$$p(\theta|D) \to \delta(\theta, \hat{\theta}_{ML})$$

Example MLE: Bernoulli Trials

- We observe M iid coin flips: $\mathcal{D}$=H,H,T,H,...
- Model: $p(H) = \theta \quad p(T) = (1-\theta)$
- Likelihood:

$$
\begin{aligned}
\ell(\theta; \mathcal{D}) = \log p(\mathcal{D}|\theta) &= \log \prod_m \theta^{\mathbf{x}^m} (1-\theta)^{1-\mathbf{x}^m} \\
&= \log \theta \sum_m \mathbf{x}^m + \log(1-\theta) \sum_m (1-\mathbf{x}^m) \\
&= \log \theta N_{\text{H}} + \log(1-\theta) N_{\text{T}}
\end{aligned}
$$

- Take derivatives and set to zero:

$$
\begin{aligned}
\frac{\partial \ell}{\partial \theta} &= \frac{N_{\text{H}}}{\theta} - \frac{N_{\text{T}}}{1-\theta} \\
\Rightarrow \theta^*_{\text{ML}} &= \frac{N_{\text{H}}}{N_{\text{H}} + N_{\text{T}}}
\end{aligned}
$$

Sufficient statistics

- The counts $N_H = \sum_m x^m$ and $N_T = \sum_m (1 - x^m)$ are sufficient statistics of the data D.
- In general, $T(X)$ is a sufficient statistic for X if

$$T(x^1) = T(x^2) \Rightarrow L(\theta; x^1) = L(\theta; x^2)$$

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 $[\mathbf{x}^m = k]$):

$$\ell(\theta; \mathcal{D}) = \log p(\mathcal{D}|\theta) = \sum_m \log \prod_k \theta_1^{[\mathbf{x}^m = k]}$$
$$= \sum_m \sum_k [\mathbf{x}^m = k] \log \theta_k = \sum_k N_k \log \theta_k$$

- We need to maximize this subject to the constraint $\sum_k \theta_k = 1$, so we use a Lagrange multiplier.

Lagrange multipliers

- Constrained cost function:

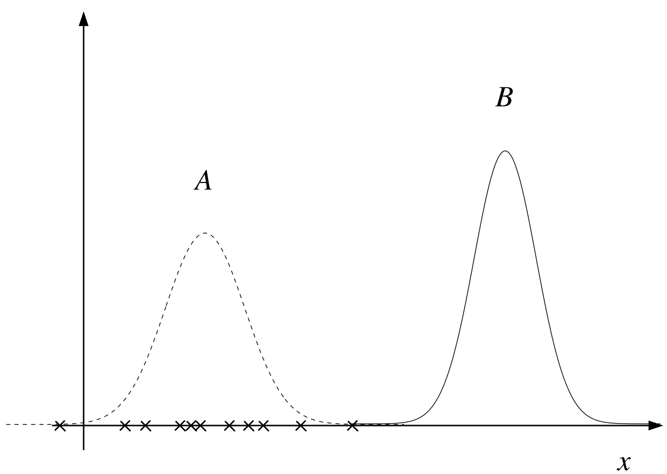
$$\tilde{l} = \sum_k N_k \log \theta_k + \lambda \left(1 - \sum_k \theta_k\right)$$

- Take derivatives wrt θ_k:

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

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

Example: Univariate Normal



Example: Univariate Normal

- We observe M iid real samples: $\mathcal{D}$=1.18,-.25,.78,...
- Model: $p(x) = (2\pi\sigma^2)^{-1/2} \exp\{-(x-\mu)^2/2\sigma^2\}$
- Log likelihood:

$$\begin{aligned}
\ell(\theta; \mathcal{D}) &= \log p(\mathcal{D}|\theta) \\
&= -\frac{M}{2} \log(2\pi\sigma^2) - \frac{1}{2} \sum_m \frac{(x^m - \mu)^2}{\sigma^2}
\end{aligned}$$

- Take derivatives and set to zero:

$$\begin{aligned}
\frac{\partial \ell}{\partial \mu} &= (1/\sigma^2) \textstyle\sum_m (x_m - \mu) \\
\frac{\partial \ell}{\partial \sigma^2} &= -\frac{M}{2\sigma^2} + \frac{1}{2\sigma^4} \textstyle\sum_m (x_m - \mu)^2 \\
\Rightarrow \mu_{\text{ML}} &= (1/M) \textstyle\sum_m x_m \\
\sigma^2_{\text{ML}} &= (1/M) \textstyle\sum_m (x_m - \mu_{\text{ML}})^2
\end{aligned}$$

Exponential Family

- For a numeric random variable $\mathbf{x}$

$$p(\mathbf{x}|\eta) = h(\mathbf{x})\exp\{\eta^\top T(\mathbf{x}) - A(\eta)\} \\ = \frac{1}{Z(\eta)} h(\mathbf{x})\exp\{\eta^\top T(\mathbf{x})\}$$

  is an exponential family distribution with *natural (canonical) parameter* η.
- Function $T(\mathbf{x})$ is a *sufficient statistic*.
- Function $A(\eta) = \log Z(\eta)$ is the log normalizer.
- Examples: Bernoulli, multinomial, Gaussian, Poisson, gamma,...
- A distribution $p(x)$ has finite sufficient statistics (independent of number of data cases) iff it is in the exponential family.

Multivariate Gaussian Distribution

- For a continuous vector random variable:

$$p(x|\mu,\Sigma) = |2\pi\Sigma|^{-1/2}\exp\left\{-\frac{1}{2}(\mathbf{x}-\mu)^\top\Sigma^{-1}(\mathbf{x}-\mu)\right\}$$

- Exponential family with:

$$\begin{aligned} \eta &= [\Sigma^{-1}\mu\ ;\ -1/2\Sigma^{-1}] \\ T(x) &= [\mathbf{x}\ ;\ \mathbf{x}\mathbf{x}^\top] \\ A(\eta) &= \log|\Sigma|/2 + \mu^\top\Sigma^{-1}\mu/2 \\ h(x) &= (2\pi)^{-d/2} \end{aligned}$$

- Note: a d-dimensional Gaussian is a d+d^2-parameter distribution with a d+d^2-component vector of sufficient statistics (but because of symmetry and positivity, parameters are constrained)

Moments

- We can easily compute moments of any exponential family distribution by taking the derivatives of the log normalizer $A(\eta)$.
- The q^{th} derivative gives the q^{th} centred moment.

$$\begin{aligned} \frac{dA(\eta)}{d\eta} &= \text{mean} \\ \frac{d^2A(\eta)}{d\eta^2} &= \text{variance} \\ &\cdots \end{aligned}$$

- When the sufficient statistic is a vector, partial derivatives need to be considered.

Moments

$$\begin{aligned} \frac{dA}{d\eta} &= \frac{d}{d\eta}\log Z(\eta) = \frac{1}{Z(\eta)}\frac{d}{d\eta}Z(\eta) \\ &= \frac{1}{Z(\eta)}\frac{d}{d\eta}\int h(\mathbf{x})\exp\{\eta T(\mathbf{x})\}dx \\ &= \frac{\int T(\mathbf{x})h(\mathbf{x})\exp\{\eta T(\mathbf{x})\}}{Z(\eta)} \\ &= ET(X) \\ \frac{d^2A}{d\eta^2} &= VarT(X) \end{aligned}$$

Moment vs canonical parameters

- The moment parameter μ can be derived from the natural (canonical) parameter

$$\frac{dA}{d\eta} = ET(X) \stackrel{\text{def}}{=} \mu$$

- Now $A(\eta)$ is convex since

$$\frac{d^2 A}{d\eta^2} = VarT(X) > 0$$

- Hence we can invert the relationship and infer the canonical parameter from the moment parameter:

$$\eta \stackrel{\text{def}}{=} \psi(\mu)$$

MLE for Exponential Family

- For iid data, the log-likelihood is

$$\begin{aligned}\ell(\eta; \mathcal{D}) &= \log \prod_m h(x^m) \exp\left(\eta^T T(x^m) - A(\eta)\right) \\ &= \left(\sum_m \log h(\mathbf{x}^m)\right) - MA(\eta) + \left(\eta^\top \sum_m T(\mathbf{x}^m)\right)\end{aligned}$$

- Take derivatives and set to zero:

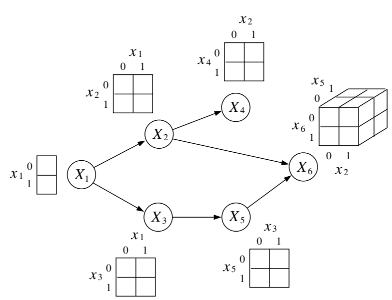
$$\begin{aligned}\frac{\partial \ell}{\partial \eta} &= \textstyle\sum_m T(\mathbf{x}^m) - M\frac{\partial A(\eta)}{\partial \eta} = 0 \\ \Rightarrow \frac{\partial A(\eta)}{\partial \eta} &= \frac{1}{M}\textstyle\sum_m T(\mathbf{x}^m) \\ \hat{\mu}_{\text{ML}} &= \frac{1}{M}\textstyle\sum_m T(\mathbf{x}^m)\end{aligned}$$

- This amounts to moment matching.
- We can infer the canonical parameters using $\hat{\eta}_{ML} = \psi(\hat{\mu}_{ML})$

MLE for general Bayes nets

- 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:

$$\log p(\mathcal{D}|\theta) = \log \prod_m \prod_i p(\mathbf{x}_i^m | \mathbf{x}_{\pi_i}, \theta_i) = \sum_i \sum_m \log p(\mathbf{x}_i^m | \mathbf{x}_{\pi_i}, \theta_i)$$

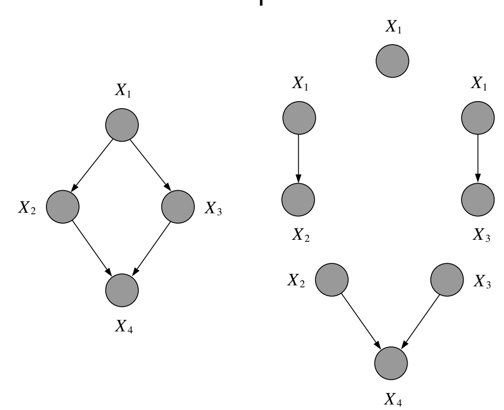


Example: A Directed Model

- 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.



(a) (b)

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

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

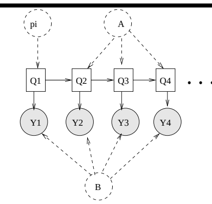
- The log-likelihood is

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

- Using a Lagrange multiplier to enforce so $\sum_j \theta_{ijk} = 1$ we get

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

Tied parameters

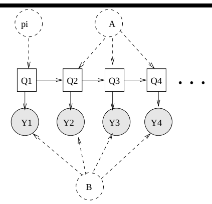


- Consider a time-invariant hidden Markov model (HMM)
  - State transition matrix $A(i,j) \stackrel{\text{def}}{=} P(X_t = j | X_{t-1} = i)$,
  - Discrete observation matrix $B(i,j) \stackrel{\text{def}}{=} P(Y_t = j | X_t = i)$
  - State prior $\pi(i) \stackrel{\text{def}}{=} P(X_1 = i)$.

  The joint is

$$P(X_{1:T}, Y_{1:T} | \theta) = P(X_1 | \pi) \prod_{t=2}^{T} P(X_t | X_{t-1}, A) \prod_{t=1}^{T} P(Y_t | X_t; B)$$

Learning a fully observed HMM



- The log-likelihood is

$$\ell(\theta; D) = \sum_m \log P(X_1 = x_1^m | \pi)$$
$$+ \sum_{t=2}^{T} P(X_t = x_t^m | X_{t-1} = x_{t-1}^m, A) + \sum_{t=1}^{T} P(Y_t = y_t^m | X_t = x_t^m, B)$$

- We can optimize each parameter (A, B, π) separately.

Learning a Markov chain transition matrix

- Define $A(i,j) = P(X_t = j | X_{t-1} = i)$.
- A is a stochastic matrix: $\sum_j A(i,j) = 1$
- Each row of A is multinomial distribution.
- So MLE is the fraction of transitions from i to j

$$\hat{A}_{ML}(i,j) = \frac{\# i \to j}{\sum_k \# i \to k} = \frac{\sum_m \sum_{t=2}^{T} I(X_{t-1}^m = i, X_t^m = j)}{\sum_m \sum_{t=2}^{T} I(X_{t-1}^m = i)}$$

- If the states X_t represent words, this is called a *bigram language model*.
- Note that $\hat{A}_{ML}(i,j) = 0$ if the particular i,j pair did not occur in the training data; this is called the *sparse data problem*.
- We will solve this later using a prior.

CPDs for continuous nodes

- So far we have considered the case where $p(y|x,\theta)$ can be represented as a multinomial (table).
- Now we consider the case where some nodes may be continuous.

X	Y	$p(Y\|X)$
$\mathbb{R}^n$	$\mathbb{R}^m$	regression
$\mathbb{R}^n$	$\{0,1\}$	binary classification
$\{0,1\}^n$	$\{0,1\}$	binary classification
$\mathbb{R}^n$	$\{1,\ldots,K\}$	multiclass classification
$\{1,\ldots,K\}$	$\mathbb{R}^n$	conditional density modeling

Learning a conditional Gaussian

- Consider an HMM with discrete states X_t but continuous observations $y_t \in \mathbb{R}^n$:

$$p(y_t|X_t = i) = \mathcal{N}(y_t; \mu_i, \Sigma_i)$$

- The MLE is the sample mean and sample variance of observations associated with each state (use X_t labels to partition the data):

$$\hat{\mu}_{ML}(i) = \frac{\sum_{m,t:X_t^m=i} \;\; y_t^m}{\sum_{m,t} y_t^m} = \frac{\sum_m \sum_{t=1}^T I(X_t^m = i) y_t^m}{\sum_m \sum_{t=1}^T y_t^m}$$

- Note that the MLE for Σ_i for states i with small numbers of observations is $\Sigma_i \to \infty I$.
- We will solve this later using a prior.