Bayesian Learning

- Olive slides: Alpaydin
- Black slides: Mitchell.

Bayesian Learning

- Probabilistic approach to inference.
- Quantities of interest are governed by prob. dist. and optimal decisions can be made by reasoning about these prob.
- Learning algorithms that directly deal with probabilities.
- Analysis framework for non-probabilistic methods.

Two Roles for Bayesian Methods

Provides practical learning algorithms:

- Naive Bayes learning
- Bayesian belief network learning
- Combine prior knowledge (prior probabilities) with observed data
- Requires prior probabilities

Provides useful conceptual framework

- Provides "gold standard" for evaluating other learning algorithms
- Additional insight into Occam's razor

Bayes Theorem

$$P(h|D) = \frac{P(D|h)P(h)}{P(D)}$$

- $P(h)$ = prior probability that h holds, before seeing the training data
- $P(D)$ = prior probability of observing training data D
- $P(D|h)$ = probability of observing D in a world where h holds
- $P(h|D)$ = probability of h holding given observed data D

Choosing Hypotheses

$$P(h|D) = \frac{P(D|h)P(h)}{P(D)}$$

Generally want the most probable hypothesis given the training data

Maximum a posteriori hypothesis h_{MAP}:

$$\begin{aligned} h_{MAP} &= \arg\max_{h \in H} P(h|D) \\ &= \arg\max_{h \in H} \frac{P(D|h)P(h)}{P(D)} \\ &= \arg\max_{h \in H} P(D|h)P(h) \end{aligned}$$

Choosing Hypotheses

- If all hypotheses are equally probable a priori:

  $$P(h_i) = P(h_j), \forall h_i, h_j,$$

  then, h_{MAP} reduces to:

  $$h_{ML} \equiv \underset{h \in H}{\operatorname{argmax}} P(D|h).$$

  $\rightarrow$ Maximum Likelihood hypothesis.

Bayes Theorem: Example

Does patient have cancer or not?

> A patient takes a lab test and the result comes back positive. The test returns a correct positive result in only 98% of the cases in which the disease is actually present, and a correct negative result in only 97% of the cases in which the disease is not present. Furthermore, $.008$ of the entire population have this cancer.

$$\begin{aligned} P(cancer) &= & P(\neg cancer) &= \\ P(\oplus|cancer) &= & P(\ominus|cancer) &= \\ P(\oplus|\neg cancer) &= & P(\ominus|\neg cancer) &= \end{aligned}$$

How does $P(cancer|\oplus)$ compare to $P(\neg cancer|\oplus)$? (What is h_{MAP}?

Basic Probability Formulas

- *Product Rule*: probability $P(A \wedge B)$ of a conjunction of two events A and B:

  $$P(A \wedge B) = P(A|B)P(B) = P(B|A)P(A)$$

- *Sum Rule*: probability of a disjunction of two events A and B:

  $$P(A \vee B) = P(A) + P(B) - P(A \wedge B)$$

- *Theorem of total probability*: if events $A_1, \ldots, A_n$ are mutually exclusive with $\sum_{i=1}^{n} P(A_i) = 1$, then

  $$P(B) = \sum_{i=1}^{n} P(B|A_i)P(A_i)$$

Brute Force MAP Hypothesis Learner

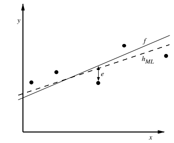
1. For each hypothesis h in H, calculate the posterior probability

$$P(h|D) = \frac{P(D|h)P(h)}{P(D)}$$

2. Output the hypothesis h_{MAP} with the highest posterior probability

$$h_{MAP} = \operatorname*{argmax}_{h \in H} P(h|D)$$

Learning A Real Valued Function



Consider any real-valued target function f

Training examples $\langle x_i, d_i \rangle$, where d_i is noisy training value

- $d_i = f(x_i) + e_i$
- e_i is random variable (noise) drawn independently for each x_i according to some Gaussian distribution with mean=0

Then the maximum likelihood hypothesis h_{ML} is the one that minimizes the sum of squared errors:

$$h_{ML} = \arg \min_{h \in H} \sum_{i=1}^{m} (d_i - h(x_i))^2$$

Setting up the Stage

- Probability density function:

$$p(x_0) \equiv \lim_{\epsilon \to 0} \frac{1}{\epsilon} P(x_0 \leq x < x_0 + \epsilon)$$

- ML hypothesis

$$h_{ML} = \operatorname*{argmax}_{h \in H} p(D|h)$$

- Training instances $\langle x_1, ..., x_m \rangle$ and target values $\langle d_1, ..., d_m \rangle$, where $d_i = f(x_i) + e_i$.
- Assume training examples are mutually independent given h,

$$h_{ML} = \operatorname*{argmax}_{h \in H} \prod_{i=1}^{m} p(d_i|h)$$

Note: $p(a, b|c) = p(a|b, c) \cdot p(b|c) = p(a|c) \cdot p(b|c)$

Derivation of ML for Func. Approx.

From $h_{ML} = \operatorname{argmax}_{h \in H} \prod_{i=1}^{m} p(d_i|h)$:

- Since $d_i = f(x_i) + e_i$ and $e_i \sim \mathcal{N}(0, \sigma^2)$, it must be:

$$d_i \sim \mathcal{N}(f(x_i), \sigma^2).$$

  - $x \sim \mathcal{N}(\mu, \sigma^2)$ means random variable x is normally distributed with mean μ and variance σ^2.

- Using pdf of $\mathcal{N}$:

$$h_{ML} = \operatorname*{argmax}_{h \in H} \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(d_i - \mu)^2}{2\sigma^2}}.$$

$$h_{ML} = \operatorname*{argmax}_{h \in H} \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(d_i - h(x_i))^2}{2\sigma^2}}.$$

Derivation of ML

$$h_{ML} = \underset{h \in H}{\operatorname{argmax}} \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(d_i - h(x_i))^2}{2\sigma^2}}.$$

- Get rid of constant factor $\frac{1}{\sqrt{2\pi\sigma^2}}$, and put on log:

$$\begin{aligned} h_{ML} &= \underset{h \in H}{\operatorname{argmax}} \ln \prod_{i=1}^{m} e^{-\frac{(d_i - h(x_i))^2}{2\sigma^2}} \\ &= \underset{h \in H}{\operatorname{argmax}} \sum_{i=1}^{m} \ln e^{-\frac{(d_i - h(x_i))^2}{2\sigma^2}} \\ &= \underset{h \in H}{\operatorname{argmax}} \sum_{i=1}^{m} -\frac{(d_i - h(x_i))^2}{2\sigma^2} \\ &= \underset{h \in H}{\operatorname{argmin}} \sum_{i=1}^{m} (d_i - h(x_i))^2 \end{aligned} \tag{1}$$

Least Square as ML

Assumptions

- Observed training values d_i generated by adding random noise to true target value, where noise has a normal distribution with zero mean.
- All hypotheses are equally probable (uniform prior).
  - Note: it is possible that $MAP \neq ML$!

Limitations

- Possible noise in x_i not accounted for.

Learning to Predict Probabilities

Consider predicting survival probability from patient data.

Training examples $\langle x_i, d_i \rangle$, where d_i is 1 or 0.

Want to train network to output a *probability* **given** x_i (not 0 or 1).

In this case we can show:

$$h_{ML} = \underset{h \in H}{\operatorname{argmax}} \sum_{i=1}^{m} d_i \ln h(x_i) + (1 - d_i) \ln(1 - h(x_i))$$

Weight update rule for a sigmoid unit:

$$w_{jk} \leftarrow w_{jk} + \Delta w_{jk}$$

where

$$\Delta w_{jk} = \eta \sum_{i=1}^{m} (d_i - h(x_i))\, x_{ijk}$$

Learning to Predict Probabilities: $P(D|h)$

- First start with $P(D|h)$, given $D = \{\langle x_1, d_1 \rangle, \ldots \langle x_m, d_m \rangle\}$.

$$P(D|h) = \prod_{i=1}^{m} P(x_i, d_i | h)$$

- Assuming $P(x_i|h) = P(x_i)$:

$$\begin{aligned} P(D|h) &= \prod_{i=1}^{m} P(x_i, d_i|h) \\ &= \prod_{i=1}^{m} P(d_i|h, x_i) P(x_i|h) \\ &= \prod_{i=1}^{m} P(d_i|h, x_i) P(x_i). \end{aligned} \tag{2}$$

Note: $P(A, B|C) = P(A|B, C) P(B|C)$

Learning to Predict Probabilities: $P(D|h)$

- h is the probability of $d_i = 1$ given the sample x_i, thus:
  - $P(d_i|h, x_i) = h(x_i)$ if $d_i = 1$
  - $P(d_i|h, x_i) = 1 - h(x_i)$ if $d_i = 0$
- Rewriting the above:

$$P(d_i|h, x_i) = h(x_i)^{d_i}(1 - h(x_i))^{1-d_i}$$

- Thus:

$$\begin{aligned} P(D|h) &= \prod_{i=1}^{m} P(d_i|h, x_i)P(x_i) \\ &= \prod_{i=1}^{m} h(x_i)^{d_i}(1 - h(x_i))^{1-d_i} P(x_i) \end{aligned}$$

Learning to Predict Probabilities: h_{ML}

$$\begin{aligned} h_{ML} &= \operatorname*{argmax}_{h \in H} \prod_{i=1}^{m} h(x_i)^{d_i}(1 - h(x_i))^{1-d_i} P(x_i) \\ &= \operatorname*{argmax}_{h \in H} \prod_{i=1}^{m} h(x_i)^{d_i}(1 - h(x_i))^{1-d_i} \qquad (3) \end{aligned}$$

since $P(x_i)$ is independent of h. Finally, taking $\ln$:

$$h_{ML} = \operatorname*{argmax}_{h \in H} \sum_{i=1}^{m} d_i \ln h(x_i) + (1 - d_i) \ln(1 - h(x_i)).$$

Note the similarity of the above to **entropy** (turn it into argmin, and compare to $-\sum_i p_i \log_2 p_i$).

Learning to Predict Probabilities: Gradient Descent

Letting $G(h, D) = h_{ML}$, and putting in a neural network with a sigmoid output unit $h(x_i)$:

$$\begin{aligned} \frac{\partial G(h,D)}{\partial w_{jk}} &= \sum_{i=1}^{m} \frac{\partial G(h,D)}{\partial h(x_i)} \frac{\partial h(x_i)}{\partial w_{jk}} \\ &= \sum_{i=1}^{m} \frac{\partial \sum_{p=1}^{m} d_p \ln h(x_p) + (1 - d_p) \ln(1 - h(x_p))}{\partial h(x_i)} \frac{\partial h(x_i)}{\partial w_{jk}} \\ &= \sum_{i=1}^{m} \frac{\partial d_i \ln h(x_i) + (1 - d_i) \ln(1 - h(x_i))}{\partial h(x_i)} \frac{\partial h(x_i)}{\partial w_{jk}} \\ &= \sum_{i=1}^{m} \frac{d_i - h(x_i)}{h(x_i)(1 - h(x_i))} \frac{\partial h(x_i)}{\partial w_{jk}} \\ &= \sum_{i=1}^{m} \frac{d_i - h(x_i)}{h(x_i)(1 - h(x_i))} \sigma'(x_i) x_{ijk} \\ &= \sum_{i=1}^{m} (d_i - h(x_i)) x_{ijk} \end{aligned}$$

Note: $\frac{d \ln(x)}{dx} = \frac{1}{x}$, and $\sigma'(x_i) = h(x_i)(1 - h(x_i))$.

Learning Probabilities: Weight Update

We want to **maximize** (not miminize), thus

$$\begin{aligned} \Delta w_{jk} &= \eta \frac{\partial G(h,D)}{\partial w_{jk}} \\ &= \eta \sum_{i=1}^{m} (d_i - h(x_i)) x_{ijk} \\ w_{jk} &\leftarrow w_{jk} + \Delta w_{jk} \end{aligned}$$

Following the above rule will produce (local minima in) h_{ML}.

Compare to backpropagation!

Minimum Description Length

Occam's razor: prefer the shortest hypothesis.

$$
\begin{aligned}
h_{MAP} &= \underset{h\in H}{\operatorname{argmax}} P(D|h)P(h) \\
h_{MAP} &= \underset{h\in H}{\operatorname{argmax}} \log_2 P(D|h) + \log_2 P(h) \\
h_{MAP} &= \underset{h\in H}{\operatorname{argmin}} -\log_2 P(D|h) - \log_2 P(h)
\end{aligned}
$$

Surprisingly, the above can be interpreted as h_{MAP} preferring shorter hypotheses, assuming a particular encoding scheme is used for the hypothesis and the data.

According to information theory, the shortest code length for a message occurring with probability p_i is $-\log_2 p_i$ bits.

MDL

$$h_{MAP} = \underset{h\in H}{\operatorname{argmin}} -\log_2 P(D|h) - \log_2 P(h)$$

- $L_C(i)$: description length of message i with respect to code C.
- $-\log_2 P(h)$: description length of h under optimal coding C_H for the hypothesis space H.

$$L_{C_H}(h) = -\log_2 P(h)$$

- $-\log_2 P(D|h)$: description length of training data D given hypothesis h, under optimal encoding $C_{D|H}$.

$$L_{C_{D|H}}(D|h) = -\log_2 P(D|h)$$

- Finally, we get:

$$h_{MAP} = \underset{h\in H}{\operatorname{argmin}} L_{C_{D|H}}(D|h) + L_{C_H}(h)$$

MDL

- MAP:

$$h_{MAP} = \underset{h\in H}{\operatorname{argmin}} L_{C_{D|H}}(D|h) + L_{C_H}(h)$$

- MDL: Choose h_{MDL} such that:

$$h_{MDL} = \underset{h\in H}{\operatorname{argmin}} L_{C_1}(h) + L_{C_2}(D|h)$$

  which is the hypothesis that minimizes the **combined length** of the hypotheis itself, and the data described by the hypothesis.

- $h_{MDL} = h_{MAP}$ if $C_1 = C_H$ and $C_2 = C_{D|H}$.

Bayes Optimal Classifier

- What is the most probable hypothesis given the training data, **vs.** What is the most probable classification?
- Example:
  - $P(h_1|D) = 0.4$, $P(h_2|D) = 0.3$, $P(h_3|D) = 0.3$.
  - Given a new instance x, $h_1(x) = 1$, $h_2(x) = 0$, $h_1(x) = 0$.
  - In this case, probability of x being positive is only 0.4.

Bayes Optimal Classification

If a new instance can take classification $v_j \in V$, then the probability $P(v_j|D)$ of correct classification of new instance being v_j is:

$$P(v_j|D) = \sum_{h_i \in H} P(v_j|h_i)P(h_i|D)$$

Thus, the optimal classification is

$$\operatorname*{argmax}_{v_j \in V} \sum_{h_i \in H} P(v_j|h_i)P(h_i|D).$$

Bayes Optimal Classifier

What is the assumption for the following to work?

$$P(v_j|D) = \sum_{h_i \in H} P(v_j|h_i)P(h_i|D)$$

Let's consider $H = \{h, \neg h\}$:

$$\begin{aligned}
P(v|D) &= P(v, h|D) + P(v, \neg h|D) \\
&= \frac{P(v, h, D)}{P(D)} + \frac{P(v, \neg h, D)}{P(D)} \\
&= \frac{P(v|h, D)P(h|D)P(D)}{P(D)} \\
&\quad + \frac{P(v|\neg h, D)P(\neg h|D)P(D)}{P(D)} \\
&\quad \{\text{if } P(v|h, D) = P(v|h), \text{ etc.}\} \\
&= P(v|h)P(h|D) + P(v|\neg h)P(\neg h|D)
\end{aligned}$$

Bayes Optimal Classifier: Example

- $P(h_1|D) = 0.4$, $P(h_2|D) = 0.3$, $P(h_3|D) = 0.3$.
- Given a new instance x, $h_1(x) = 1$, $h_2(x) = 0$, $h_1(x) = 0$.
  - $P(\ominus|h_1) = 0$, $P(\oplus|h_1) = 1$, etc.
  - $P(\oplus|D) = 0.4 + 0 + 0$,
    $P(\ominus|D) = 0 + 0.3 + 0.3 = 0.6$
  - Thus, $\operatorname{argmax}_{v \in O\{\oplus,\ominus\}} P(v|D) = \ominus$.
- Bayes optimal classifiers maximize the probability that a new instance is correctly classified, given the available data, hypothesis space H, and prior probabilities over H.
- Some oddities: The resulting hypotheis can be outside of the hypothesis space.

Gibbs Sampling

Finding $\operatorname{argmax}_{v \in V} P(v|D)$ by considering every hypothesis $h \in H$ can be infeasible. A less optimal, but error-bounded version is **Gibbs sampling**:

1. Randomly pick $h \in H$ with probability $P(h|D)$.
2. Use h to classify the new instance x.

The result is that missclassification rate is at most $2\times$ that of BOC.

Naive Bayes Classifier

Given attribute values $\langle a_1, a_2, ..., a_n \rangle$, give the classification $v \in V$:

$$v_{MAP} = \underset{v_j \in V}{\operatorname{argmax}} P(v_j | a_1, a_2, ..., a_n)$$

$$\begin{aligned} v_{MAP} &= \underset{v_j \in V}{\operatorname{argmax}} \frac{P(a_1, a_2, ..., a_n | v_j) P(v_j)}{P(a_1, a_2, ..., a_n)} \\ &= \underset{v_j \in V}{\operatorname{argmax}} P(a_1, a_2, ..., a_n | v_j) P(v_j) \end{aligned}$$

- Want to estimate $P(a_1, a_2, ..., a_n | v_j)$ and $P(v_j)$ from training data.

Naive Bayes

- $P(v_j)$ is easy to calculate: Just count the frequency.
- $P(a_1, a_2, ..., a_n | v_j)$ takes the number of posible instances $\times$ number of possible target values.
- $P(a_1, a_2, ..., a_n | v_j)$ can be approximated as

$$P(a_1, a_2, ..., a_n | v_j) = \prod_i P(a_i | v_j).$$

- From this naive Bayes classifier is defined as:

$$v_{NB} = \underset{v_j \in V}{\operatorname{argmax}} P(v_j) \prod_i P(a_i | v_j)$$

- Naive Bayes only takes number of distinct attribute values $\times$ number of distinct target values.

Naive Bayes Algorithm

Naive_Bayes_Learn($examples$)

For each target value v_j

$\hat{P}(v_j) \leftarrow$ estimate $P(v_j)$

For each attribute value a_i of each attribute a

$\hat{P}(a_i | v_j) \leftarrow$ estimate $P(a_i | v_j)$

Classify_New_Instance(x)

$$v_{NB} = \underset{v_j \in V}{\operatorname{argmax}} \hat{P}(v_j) \prod_i \hat{P}(x_i | v_j)$$

Naive Bayes: Example

Consider *PlayTennis* again, and new instance:

$$x = \langle Outlk = sun, Temp = cool, Humid = high, Wind = strong \rangle$$

$$V = \{Yes, No\}$$

Want to compute:

$$v_{NB} = \underset{v_j \in V}{\operatorname{argmax}} P(v_j) \prod_i P(x_i | v_j)$$

$$P(Y)\, P(sun|Y)\, P(cool|Y)\, P(high|Y)\, P(strong|Y) = .005$$

$$P(N)\, P(sun|N)\, P(cool|N)\, P(high|N)\, P(strong|N) = .021$$

Thus, $v_{NB} = No$

Naive Bayes: Subtleties

1. Conditional independence assumption is often violated

$$P(a_1, a_2 \ldots a_n|v_j) = \prod_i P(a_i|v_j)$$

- ...but it works surprisingly well anyway. Note don't need estimated posteriors $\hat{P}(v_j|x)$ to be correct; need only that

$$\underset{v_j \in V}{\operatorname{argmax}}\, \hat{P}(v_j) \prod_i \hat{P}(a_i|v_j) = \underset{v_j \in V}{\operatorname{argmax}}\, P(v_j) P(a_1 \ldots, a_n|v_j)$$

- Naive Bayes posteriors often unrealistically close to 1 or 0.

Naive Bayes: Subtleties

What if none of the training instances with target value v_j have attribute value a_i? Then

$$\hat{P}(a_i|v_j) = 0, \text{ and...}$$

$$\hat{P}(v_j) \prod_i \hat{P}(a_i|v_j) = 0$$

Typical solution is Bayesian estimate for $\hat{P}(a_i|v_j)$

$$\hat{P}(a_i|v_j) \leftarrow \frac{n_c + mp}{n + m}$$

where

- n is number of training examples for which $v = v_j$,
- n_c number of examples for which $v = v_j$ and $a = a_i$
- p is prior estimate for $\hat{P}(a_i|v_j)$
- m is weight given to prior (i.e. number of "virtual" examples)

Conditional Independence

Definition: X is *conditionally independent* of Y given Z if the probability distribution governing X is independent of the value of Y given the value of Z; that is, if

$$(\forall x_i, y_j, z_k)\; P(X = x_i|Y = y_j, Z = z_k) = P(X = x_i|Z = z_k)$$

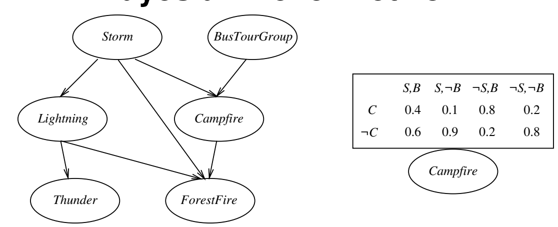
more compactly, we write

$$P(X|Y, Z) = P(X|Z)$$

Example: $Thunder$ is conditionally independent of $Rain$, given $Lightning$

$$P(Thunder|Rain, Lightning) = P(Thunder|Lightning)$$

Bayesian Belief Network

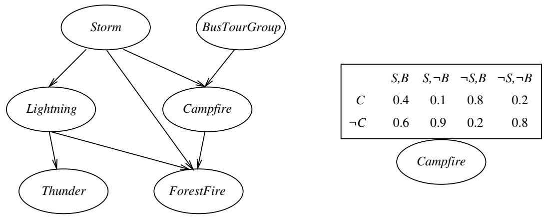


	S,B	S,¬B	¬S,B	¬S,¬B
C	0.4	0.1	0.8	0.2
¬C	0.6	0.9	0.2	0.8

Network represents a set of conditional independence assertions:

- Each node is asserted to be conditionally independent of its nondescendants, given its immediate predecessors.
- Directed acyclic graph.
- Each node has a conditional probability table: $P(Node|Parents(Node))$.
- BBN represents the joint probability $P(N_1, N_2, \ldots)$ in a compact form.

Bayesian Belief Network



	S,B	S,¬B	¬S,B	¬S,¬B
C	0.4	0.1	0.8	0.2
¬C	0.6	0.9	0.2	0.8

Represents joint probability distribution over all variables

- e.g., $P(Storm, BusTourGroup, \ldots, ForestFire)$
- in general,

$$P(Y_1 = y_1, \ldots, Y_n = y_n) = \prod_{i=1}^{n} P(Y_i = y_i | Parents(Y_i))$$

  where $Parents(Y_i)$ denotes immediate predecessors of Y_i in graph having the y values specified on the left.

- So, joint distribution is fully defined by graph, plus the $P(y_i|Parents(Y_i))$

Inference in Bayesian Networks

How can one infer the (probabilities of) values of one or more network variables, given observed values of others?

- Bayes net contains all the information needed for this inference.
- If only one variable with unknown value, easy to infer it.
- In general case, problem is NP hard.

In practice, can succeed in many cases:

- Exact inference methods work well for some network structures.
- Monte Carlo methods “simulate” the network randomly to calculate approximate solutions.

Monte Carlo for Inference in BBN

Want to calculate and arbitraty conditional probability.

1. Generate many random samples based on the given BBN.
   (a) Sample from $P(Storm)$ and $P(BusTourGroup)$.
   (b) Based on the outcome of previous step $outcome_1$, sample from $P(Lightening|Storm = outcome_1)$, $P(Campfire|Strom, BusTourGroup = outcome_1)$, etc.
   (c) Combine all the outcomes to form a single sample vector.
2. Estimate the particular conditional probability based on the samples you generated.

Learning of Bayesian Networks

Several variants of this learning task

- Network structure might be *known* or *unknown*
- Training examples might provide values of *all* network variables, or just *some*

If structure known and observe all variables

- Then it’s easy as training a Naive Bayes classifier

Learning Bayes Nets

Suppose structure known, variables partially observable

e.g., observe *ForestFire, Storm, BusTourGroup, Thunder*, but not *Lightning, Campfire*...

- Similar to training neural network with hidden units
- In fact, can learn network conditional probability tables using gradient ascent!
- Converge to network h that (locally) maximizes $P(D|h)$

Expectation Maximization (EM)

When to use:

- Data is only partially observable
- Unsupervised clustering (target value unobservable)
- Supervised learning (some instance attributes unobservable)

Some uses:

- Train Bayesian Belief Networks
- Unsupervised clustering (AUTOCLASS)
- Learning Hidden Markov Models

EM for Estimating k Means

Given:

- Instances from X generated by mixture of k Gaussian distributions
- Unknown means $\langle \mu_1, \ldots, \mu_k \rangle$ of the k Gaussians
- Don't know which instance x_i was generated by which Gaussian

Determine:

- Maximum likelihood estimates of $\langle \mu_1, \ldots, \mu_k \rangle$

Think of full description of each instance as $y_i = \langle x_i, z_{i1}, z_{i2} \rangle$, where

- z_{ij} is 1 if x_i generated by jth Gaussian
- x_i observable
- z_{ij} unobservable

EM for Estimating k Means

EM Algorithm: Pick random initial $h = \langle \mu_1, \mu_2 \rangle$, then iterate

E step: Calculate the expected value $E[z_{ij}]$ of each hidden variable z_{ij}, assuming the current hypothesis $h = \langle \mu_1, \mu_2 \rangle$ holds.

$$\begin{aligned} E[z_{ij}] &= \frac{p(x = x_i | \mu = \mu_j)}{\sum_{n=1}^{2} p(x = x_i | \mu = \mu_n)} \\ &= \frac{e^{-\frac{1}{2\sigma^2}(x_i - \mu_j)^2}}{\sum_{n=1}^{2} e^{-\frac{1}{2\sigma^2}(x_i - \mu_n)^2}} \end{aligned}$$

M step: Calculate a new maximum likelihood hypothesis $h' = \langle \mu'_1, \mu'_2 \rangle$, assuming the value taken on by each hidden variable z_{ij} is its expected value $E[z_{ij}]$ calculated above. Replace $h = \langle \mu_1, \mu_2 \rangle$ by $h' = \langle \mu'_1, \mu'_2 \rangle$.

$$\mu_j \leftarrow \frac{\sum_{i=1}^{m} E[z_{ij}]\ x_i}{\sum_{i=1}^{m} E[z_{ij}]}$$

EM Algorithm

Converges to local maximum likelihood h

and provides estimates of hidden variables z_{ij}

In fact, local maximum in $E[\ln P(Y|h)]$

- Y is complete (observable plus unobservable variables) data
- Expected value is taken over possible values of unobserved variables in Y

General EM Problem

Given:

- Observed data $X = \{x_1, \ldots, x_m\}$
- Unobserved data $Z = \{z_1, \ldots, z_m\}$
- Parameterized probability distribution $P(Y|h)$, where
  - $Y = \{y_1, \ldots, y_m\}$ is the full data $y_i = x_i \cup z_i$
  - h are the parameters

Determine:

- h that (locally) maximizes $E[\ln P(Y|h)]$

General EM Method

Define likelihood function $Q(h'|h)$ which calculates $Y = X \cup Z$ using observed X and current parameters h to estimate Z

$$Q(h'|h) \leftarrow E[\ln P(Y|h')|h, X]$$

EM Algorithm:

Estimation (E) step: Calculate $Q(h'|h)$ using the current hypothesis h and the observed data X to estimate the probability distribution over Y.

$$Q(h'|h) \leftarrow E[\ln P(Y|h')|h, X]$$

Maximization (M) step: Replace hypothesis h by the hypothesis h' that maximizes this Q function.

$$h \leftarrow \underset{h'}{\operatorname{argmax}}\, Q(h'|h)$$

Derivation of k-Means

- Hypothesis h is parameterized by $\theta = \langle \mu_1 ... \mu_k \rangle$.
- Observed data $X = \{\langle x_i \rangle\}$
- Hidden variables $Z = \{\langle z_{i1}, ..., z_{ik} \rangle\}$:
  - $z_{ik} = 1$ if input x_i is generated by th k-th normal dist.
  - For each input, k entries.
- First, start with defining $\ln p(Y|h)$.

Deriving $\ln P(Y|h)$

$$p(y_i|h') = p(x_i, z_{i1}, z_{i2}, \ldots, z_{ik}|h') = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}\sum_{j=1}^{k} z_{ij}(x_i-\mu_j')^2}$$

Note that the vector $\langle z_{i1}, \ldots, z_{ik} \rangle$ contains only a single 1 and all the rest are 0.

$$\begin{aligned}
\ln P(Y|h') &= \ln \prod_{i=1}^{m} p(y_i|h') \\
&= \sum_{i=1}^{m} \ln p(y_i|h') \\
&= \sum_{i=1}^{m} \left(\ln \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2\sigma^2} \sum_{j=1}^{k} z_{ij}(x_i - \mu_j')^2 \right)
\end{aligned}$$

Deriving $E[\ln P(Y|h)]$

Since $P(Y|h')$ is a linear function of z_{ij}, and since $E[f(z)] = f(E[z])$,

$$\begin{aligned}
E[\ln P(Y|h')] &= E\left[\sum_{i=1}^{m} \left(\ln \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2\sigma^2} \sum_{j=1}^{k} z_{ij}(x_i - \mu_j')^2 \right) \right] \\
&= \sum_{i=1}^{m} \left(\ln \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2\sigma^2} \sum_{j=1}^{k} E[z_{ij}](x_i - \mu_j')^2 \right)
\end{aligned}$$

Thus,

$$\begin{aligned}
Q(h'|h) &= Q(\langle \mu_1', \ldots, \mu_k' \rangle | h) \\
&= \sum_{i=1}^{m} \left(\ln \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2\sigma^2} \sum_{j=1}^{k} E[z_{ij}](x_i - \mu_j')^2 \right)
\end{aligned}$$

Finding $\mathrm{argmax}_{h'}\, Q(h'|h)$

With

$$E[z_{ij}] = \frac{e^{-\frac{1}{2\sigma^2}(x_i-\mu_j)^2}}{\sum_{n=1}^{2} e^{-\frac{1}{2\sigma^2}(x_i-\mu_n)^2}}$$

we want to find h' such that

$$\begin{aligned}
\operatorname*{argmax}_{h'} Q(h'|h) &= \operatorname*{argmax}_{h'} \sum_{i=1}^{m} \left(\ln \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2\sigma^2} \sum_{j=1}^{k} E[z_{ij}](x_i - \mu_j')^2 \right), \\
&= \operatorname*{argmin}_{h'} \sum_{i=1}^{m} \sum_{j=1}^{k} E[z_{ij}](x_i - \mu_j')^2,
\end{aligned}$$

which is minimized by

$$\mu_j \leftarrow \frac{\sum_{i=1}^{m} E[z_{ij}] x_i}{\sum_{i=1}^{m} E[z_{ij}]}.$$

Deriving the Update Rule

Set the derivative of the quantity to be minimized to be zero:

$$\begin{aligned}
& \frac{\partial}{\partial \mu_j'} \sum_{i=1}^{m} \sum_{j=1}^{k} E[z_{ij}](x_i - \mu_j')^2 \\
&= \frac{\partial}{\partial \mu_j'} \sum_{i=1}^{m} E[z_{ij}](x_i - \mu_j')^2 \\
&= 2 \sum_{i=1}^{m} E[z_{ij}](x_i - \mu_j') = 0
\end{aligned}$$

$$\begin{aligned}
\sum_{i=1}^{m} E[z_{ij}]x_i - \sum_{i=1}^{m} E[z_{ij}]\mu_j' &= 0 \\
\sum_{i=1}^{m} E[z_{ij}]x_i &= \mu_j' \sum_{i=1}^{m} E[z_{ij}] \\
\mu_j' &= \frac{\sum_{i=1}^{m} E[z_{ij}]x_i}{\sum_{i=1}^{m} E[z_{ij}]}
\end{aligned}$$

See Bishop (1995) *Neural Networks for Pattern Recognition*, Oxford U Press. pp. 63–64.

Losses and Risks

- Actions: α_i
- Loss of α_i when the state is C_k : λ_{ik}
- Expected risk (Duda and Hart, 1973)

$$R(\alpha_i \mid \mathbf{x}) = \sum_{k=1}^{K} \lambda_{ik} P(C_k \mid \mathbf{x})$$

$$\text{choose } \alpha_i \text{ if } R(\alpha_i \mid \mathbf{x}) = \min_k R(\alpha_k \mid \mathbf{x})$$

Losses and Risks: 0/1 Loss

$$\lambda_{ik} = \begin{cases} 0 \text{ if } i = k \\ 1 \text{ if } i \neq k \end{cases}$$

$$\begin{aligned} R(\alpha_i \mid \mathbf{x}) &= \sum_{k=1}^{K} \lambda_{ik} P(C_k \mid \mathbf{x}) \\ &= \sum_{k \neq i} P(C_k \mid \mathbf{x}) \\ &= 1 - P(C_i \mid \mathbf{x}) \end{aligned}$$

For minimum risk, choose the most probable class

Losses and Risks: Reject

$$\lambda_{ik} = \begin{cases} 0 & \text{if } i = k \\ \lambda & \text{if } i = K+1, \quad 0 < \lambda < 1 \\ 1 & \text{otherwise} \end{cases}$$

$$R(\alpha_{K+1} \mid \mathbf{x}) = \sum_{k=1}^{K} \lambda P(C_k \mid \mathbf{x}) = \lambda$$

$$R(\alpha_i \mid \mathbf{x}) = \sum_{k \neq i} P(C_k \mid \mathbf{x}) = 1 - P(C_i \mid \mathbf{x})$$

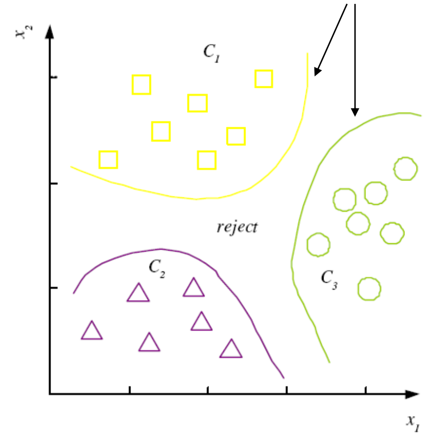
$$\begin{array}{ll} \text{choose } C_i & \text{if } P(C_i \mid \mathbf{x}) > P(C_k \mid \mathbf{x}) \;\; \forall k \neq i \text{ and } P(C_i \mid \mathbf{x}) > 1 - \lambda \\ \text{reject} & \text{otherwise} \end{array}$$

Discriminant Functions

$$\text{choose } C_i \text{ if } g_i(\mathbf{x}) = \max_k g_k(\mathbf{x})$$

$$g_i(\mathbf{x}), i = 1, \ldots, K$$

$$g_i(\mathbf{x}) = \begin{cases} -R(\alpha_i \mid \mathbf{x}) \\ P(C_i \mid \mathbf{x}) \\ p(\mathbf{x} \mid C_i) P(C_i) \end{cases}$$



K decision regions $\mathcal{R}_1, \ldots, \mathcal{R}_K$

$$\mathcal{R}_i = \{\mathbf{x} \mid g_i(\mathbf{x}) = \max_k g_k(\mathbf{x})\}$$

K=2 Classes

- Dichotomizer (K=2) vs Polychotomizer (K>2)
- $g(\mathbf{x}) = g_1(\mathbf{x}) - g_2(\mathbf{x})$

$$\text{choose} \begin{cases} C_1 \text{ if } g(\mathbf{x}) > 0 \\ C_2 \text{ otherwise} \end{cases}$$

- *Log odds:* $\log \frac{P(C_1 | \mathbf{x})}{P(C_2 | \mathbf{x})}$

Utility Theory

- Prob of state k given exidence $\mathbf{x}$: $P(S_k | \mathbf{x})$
- Utility of α_i when state is k: U_{ik}
- Expected utility:

$$EU(\alpha_i | \mathbf{x}) = \sum_k U_{ik} P(S_k | \mathbf{x})$$

$$\text{Choose } \alpha_i \text{ if } EU(\alpha_i | \mathbf{x}) = \max_j EU(\alpha_j | \mathbf{x})$$

Association Rules

- Association rule: $X \rightarrow Y$
- *People who buy/click/visit/enjoy X are also likely to buy/click/visit/enjoy Y.*
- A rule implies association, not necessarily causation.

Association measures

- Support ($X \rightarrow Y$):

$$P(X,Y) = \frac{\#\{\text{customers who bought } X \text{ and } Y\}}{\#\{\text{customers}\}}$$

- Confidence ($X \rightarrow Y$):

$$P(Y | X) = \frac{P(X,Y)}{P(X)} = \frac{\#\{\text{customers who bought } X \text{ and } Y\}}{\#\{\text{customers who bought } X\}}$$

- Lift ($X \rightarrow Y$):

$$= \frac{P(X,Y)}{P(X)P(Y)} = \frac{P(Y | X)}{P(Y)}$$

References