Bayesian Learning

- Bayes Theorem
- MAP, ML hypotheses
- MAP learners
- Minimum description length principle
- Bayes optimal classifier
- Naive Bayes learner
- Bayesian belief networks

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 of hypothesis h
- $P(D)$ = prior probability of training data D
- $P(h|D)$ = probability of h given D
- $P(D|h)$ = probability of D given h

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}:

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

If assume $P(h_i) = P(h_j)$ then can further simplify, and choose the *Maximum likelihood* (ML) hypothesis

$$h_{ML} = \arg\max_{h_i \in H} P(D|h_i)$$

Bayes Theorem

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.

$$
\begin{array}{rl}
P(cancer) = & \qquad P(\neg cancer) = \\
P(+|cancer) = & \qquad P(-|cancer) = \\
P(+|\neg cancer) = & \qquad P(-|\neg cancer) =
\end{array}
$$

Basic Formulas for Probabilities

- *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

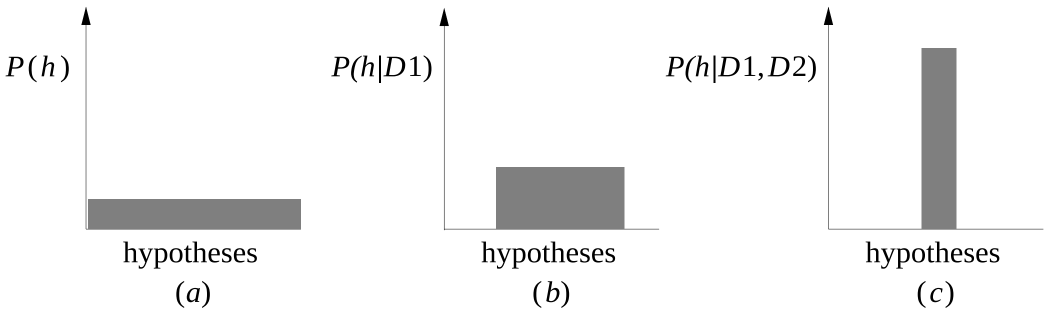
1. For each hypothesis h in H, calculate the posterior probability

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

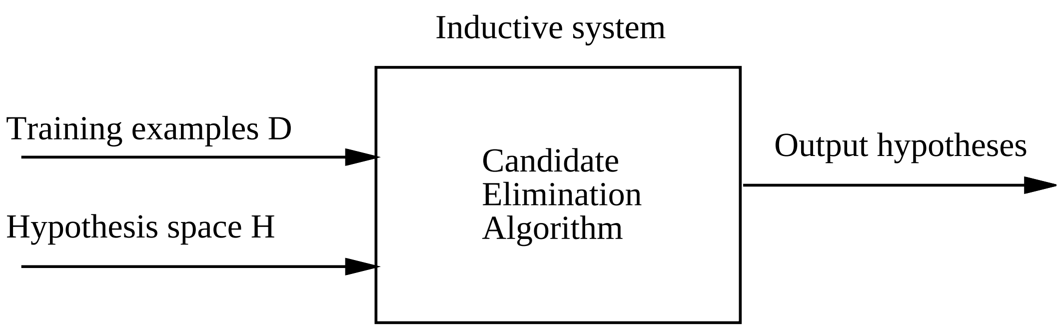
2. Output the hypothesis h_{MAP} with the highest posterior probability

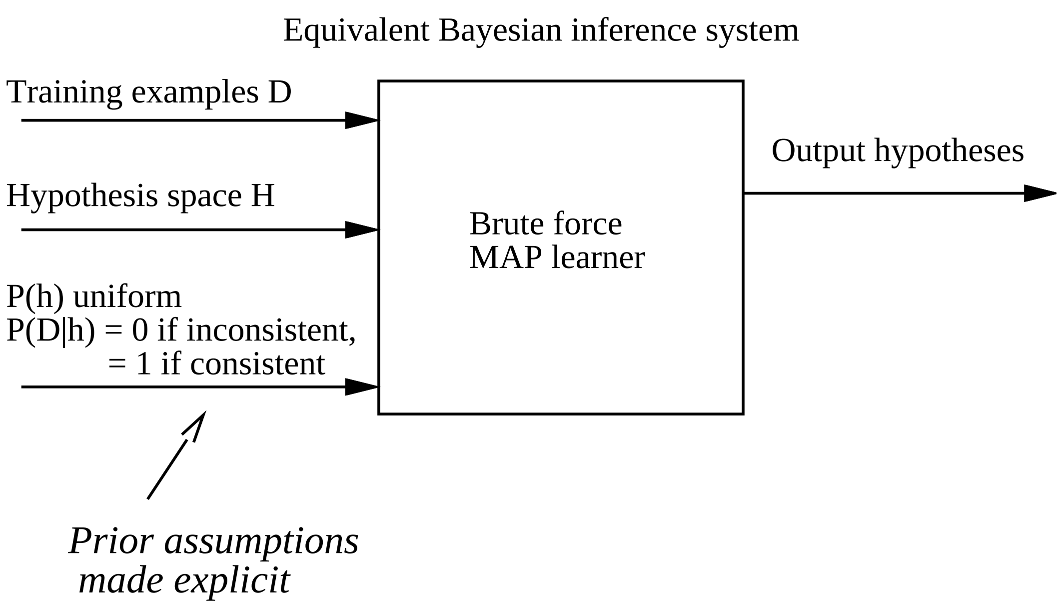
$$h_{MAP} = \operatorname*{argmax}_{h \in H} P(h|D)$$

Evolution of Posterior Probabilities

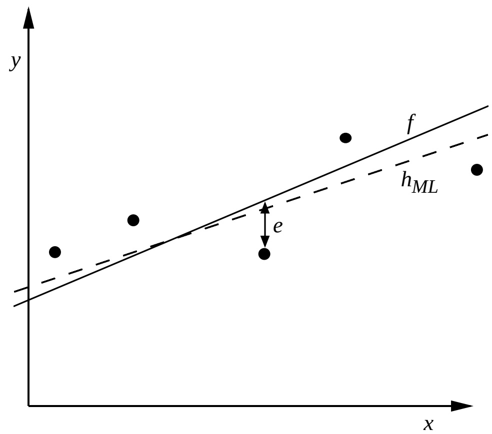


Characterizing Learning Algorithms by Equivalent MAP Learners





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:

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

Learning A Real Valued Function

$$
\begin{aligned}
h_{ML} &= \operatorname*{argmax}_{h \in H} p(D|h) \\
&= \operatorname*{argmax}_{h \in H} \prod_{i=1}^{m} p(d_i|h) \\
&= \operatorname*{argmax}_{h \in H} \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(\frac{d_i - h(x_i)}{\sigma})^2}
\end{aligned}
$$

Maximize natural log of this instead...

$$
\begin{aligned}
h_{ML} &= \operatorname*{argmax}_{h \in H} \sum_{i=1}^{m} \ln \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2}\left(\frac{d_i - h(x_i)}{\sigma}\right)^2 \\
&= \operatorname*{argmax}_{h \in H} \sum_{i=1}^{m} -\frac{1}{2}\left(\frac{d_i - h(x_i)}{\sigma}\right)^2 \\
&= \operatorname*{argmax}_{h \in H} \sum_{i=1}^{m} -\left(d_i - h(x_i)\right)^2 \\
&= \operatorname*{argmin}_{h \in H} \sum_{i=1}^{m} \left(d_i - h(x_i)\right)^2
\end{aligned}
$$

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 neural network to output a *probability* given x_i (not a 0 or 1)

In this case can show

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

Weight update rule for a sigmoid unit:

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

where

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

Minimum Description Length Principle

Occam's razor: prefer the shortest hypothesis

MDL: prefer the hypothesis h that minimizes

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

where $L_C(x)$ is the description length of x under encoding C

Example: H = decision trees, D = training data labels

- $L_{C_1}(h)$ is # bits to describe tree h
- $L_{C_2}(D|h)$ is # bits to describe D given h
  - Note $L_{C_2}(D|h) = 0$ if examples classified perfectly by h. Need only describe exceptions
- Hence h_{MDL} trades off tree size for training errors

Minimum Description Length Principle

$$\begin{aligned} h_{MAP} &= \arg\max_{h \in H} P(D|h)P(h) \\ &= \arg\max_{h \in H} \log_2 P(D|h) + \log_2 P(h) \\ &= \arg\min_{h \in H} -\log_2 P(D|h) - \log_2 P(h) \end{aligned} \tag{1}$$

Interesting fact from information theory:

The optimal (shortest expected coding length) code for an event with probability p is $-\log_2 p$ bits.

So interpret (1):

- $-\log_2 P(h)$ is length of h under optimal code
- $-\log_2 P(D|h)$ is length of D given h under optimal code

$\rightarrow$ prefer the hypothesis that minimizes

$$length(h) + length(misclassifications)$$

So far we've sought the most probable *hypothesis* given the data D (i.e., h_{MAP})

Given new instance x, what is its most probable *classification*?

- $h_{MAP}(x)$ is not the most probable classification!

Consider:

- Three possible hypotheses:

$$P(h_1|D) = .4,\ P(h_2|D) = .3,\ P(h_3|D) = .3$$

- Given new instance x,

$$h_1(x) = +,\ h_2(x) = -,\ h_3(x) = -$$

- What's most probable classification of x?

Bayes Optimal Classifier

Bayes optimal classification:

$$\arg\max_{v_j \in V} \sum_{h_i \in H} P(v_j|h_i)P(h_i|D)$$

Example:

$$\begin{array}{lll} P(h_1|D) = .4, & P(-|h_1) = 0, & P(+|h_1) = 1 \\ P(h_2|D) = .3, & P(-|h_2) = 1, & P(+|h_2) = 0 \\ P(h_3|D) = .3, & P(-|h_3) = 1, & P(+|h_3) = 0 \end{array}$$

therefore

$$\begin{aligned} \sum_{h_i \in H} P(+|h_i)P(h_i|D) &= .4 \\ \sum_{h_i \in H} P(-|h_i)P(h_i|D) &= .6 \end{aligned}$$

and

$$\arg\max_{v_j \in V} \sum_{h_i \in H} P(v_j|h_i)P(h_i|D) = -$$

Gibbs Classifier

Bayes optimal classifier provides best result, but can be expensive if many hypotheses.
Gibbs algorithm:

1. Choose one hypothesis at random, according to $P(h|D)$
2. Use this to classify new instance

Surprising fact: Assume target concepts are drawn at random from H according to priors on H. Then:

$$E[error_{Gibbs}] \leq 2E[error_{BayesOptimal}]$$

Naive Bayes Classifier

Along with decision trees, neural networks, nearest nbr, one of the most practical learning methods.

When to use

- Moderate or large training set available
- Attributes that describe instances are conditionally independent given classification

Successful applications:

- Diagnosis
- Classifying text documents

Naive Bayes Classifier

Assume target function $f : X \to V$, where each instance x described by attributes $\langle a_1, a_2 \dots a_n \rangle$.
Most probable value of $f(x)$ is:

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

Naive Bayes assumption:

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

which gives

Naive Bayes classifier: $v_{NB} = \operatorname*{argmax}_{v_j \in V} P(v_j) \prod_i P(a_i | v_j)$

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)

$$v_{NB} = \operatorname*{argmax}_{v_j \in V} \hat{P}(v_j) \prod_{a_i \in x} \hat{P}(a_i|v_j)$$

Bayesian Belief Networks

Interesting because:

- Naive Bayes assumption of conditional independence too restrictive
- But it's intractable without some such assumptions...
- Bayesian Belief networks describe conditional independence among *subsets* of variables

$\rightarrow$ allows combining prior knowledge about (in)dependencies among variables with observed training data

(also called Bayes Nets)

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

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

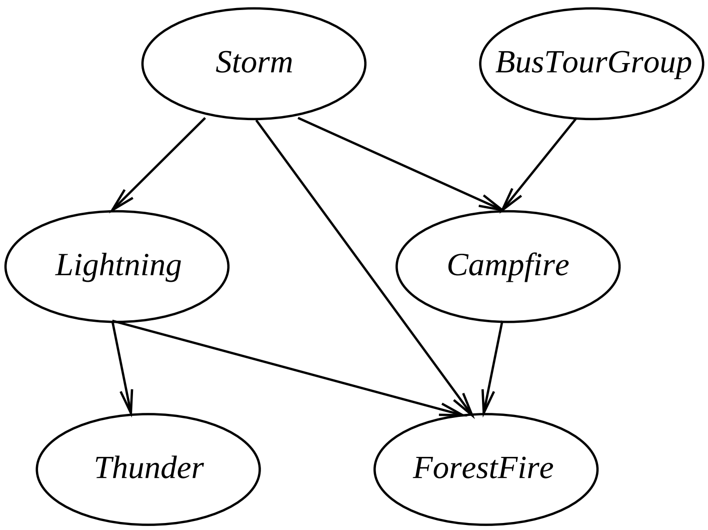
Example: $Thunder$ is conditionally independent of $Rain$, given $Lightning$

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

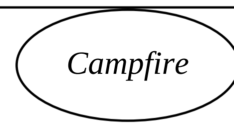
Naive Bayes uses cond. indep. to justify

$$\begin{aligned} P(X, Y|Z) &= P(X|Y, Z)P(Y|Z) \\ &= P(X|Z)P(Y|Z) \end{aligned}$$

Bayesian Belief Network



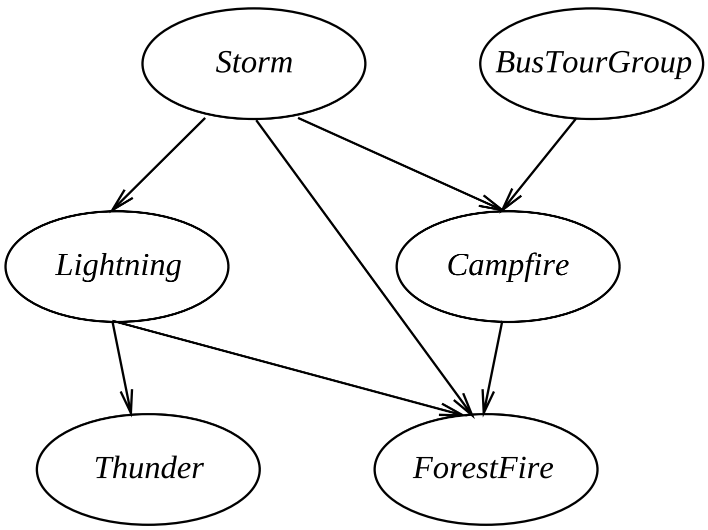
	S,B	$S,\neg B$	$\neg S,B$	$\neg S,\neg B$
C	0.4	0.1	0.8	0.2
$\neg C$	0.6	0.9	0.2	0.8



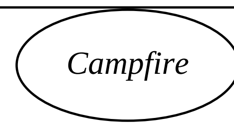
Network represents a set of conditional independence assertions:

- Each node is asserted to be conditionally independent of its nondescendants, given its immediate predecessors.
- Directed acyclic graph

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,

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

  where $Parents(Y_i)$ denotes immediate predecessors of Y_i in graph
- 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 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

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 $P(D|h)$

Gradient Ascent for Bayes Nets

Let w_{ijk} denote one entry in the conditional probability table for variable Y_i in the network

$$w_{ijk} = P(Y_i = y_{ij} | Parents(Y_i) = \text{the list } u_{ik} \text{ of values})$$

e.g., if $Y_i = Campfire$, then u_{ik} might be $\langle Storm = T, BusTourGroup = F \rangle$

Perform gradient ascent by repeatedly

1. update all w_{ijk} using training data D

$$w_{ijk} \leftarrow w_{ijk} + \eta \sum_{d \in D} \frac{P_h(y_{ij}, u_{ik} | d)}{w_{ijk}}$$

2. then, renormalize the w_{ijk} to assure

   - $\sum_j w_{ijk} = 1$
   - $0 \leq w_{ijk} \leq 1$

More on Learning Bayes Nets

EM algorithm can also be used. Repeatedly:

1. Calculate probabilities of unobserved variables, assuming h
2. Calculate new w_{ijk} to maximize $E[\ln P(D|h)]$ where D now includes both observed and (calculated probabilities of) unobserved variables

When structure unknown...

- Algorithms use greedy search to add/substract edges and nodes
- Active research topic

Summary: Bayesian Belief Networks

- Combine prior knowledge with observed data
- Impact of prior knowledge (when correct!) is to lower the sample complexity
- Active research area
  - Extend from boolean to real-valued variables
  - Parameterized distributions instead of tables
  - Extend to first-order instead of propositional systems
  - More effective inference methods
  - ...