Machine Learning (CS 567)

Fall 2008

Time: T-Th 5:00pm - 6:20pm
Location: GFS 118

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Class web page:
http://www-scf.usc.edu/~csci567/index.html

Lecture 11 Outline

- Bayesian Learning
  - Probability theory
  - Bayesian Classification

So far: Discriminative Learning

- We want to distuinguish between different classes based on examples of each class.
- Linear classifiers and decision trees generate separating planes between the classes.
- When a new instance needs to be classified, we check on which side of the decision boundaries it falls, and classify accordingly (deterministic).
- This is called discriminative learning, because we defined an explcit boundary that discriminates between the different classes.
- The classification algorithms studied so far (except logistic regression) fall into this category.

Next: *Generative* Learning

- A different idea: use the data to build a model for each of the different classes
- To classify a new instance, we match it against the different models, then decide which model it resembles more.
- This is called generative learning
- Note that we now categorize whether an instances is more or less likely to come from a given model.
- Also note that you can use these models to generate new data.

Learning Bayesian Networks: Naïve and non-Naïve Bayes

- Hypothesis Space
  - fixed size
  - stochastic
  - continuous parameters
- Learning Algorithm
  - direct computation
  - eager
  - batch

But first… basic probability theory

- Random variables
- Distributions
- Statistical formulae

Random Variables

- A random variable is a random number (or value) determined by chance, or more formally, drawn according to a probability distribution
  - The probability distribution can be estimated from observed data (e.g., throwing dice)
  - The probabiliy distribution can be synthetic
  - Discrete & continuous variables
- Typical random variables in Machine Learning Problems
  - The input data
  - The output data
  - Noise
- Important concept in learning: The data generating model
  - E.g., what is the data generating model for:
    i) Throwing dice
    ii) Regression
    iii) Classification
    iv) For visual perception

Why have Random Variables?

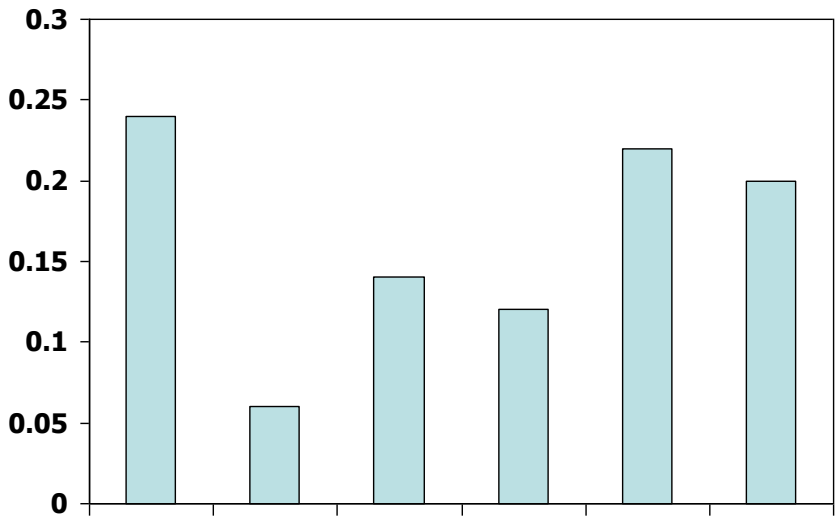
- Our goal is to predict our target variable
- We are not given the true (presumably deterministic) function
- We are only given observations
  - Can observe the number of times a dice lands on 4
  - Can estimate the probability, given the input, that the dice will land on 4
  - But we don't *know* where the dice will land
  - Can only make a guess to the most likely value of the dice, given the input.

Distributions

- The random variables only take on discrete values
  - E.g., throwing dice: possible values: $v_i \in \{1,2,3,4,5,6\}$
- The probabilies sum to 1

$$\sum_i P(v_i) = 1$$

- Discrete distributions are particularly important in classification
- Probability Mass Function or Frequency Function (normalized histogram)



A "non fair" dice

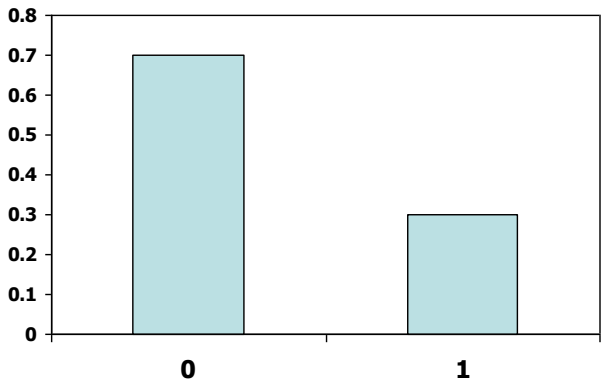
Classic Discrete Distributions (I)

Bernoulli Distribution

- A Bernoulli random variable takes on only two values, i.e., 0 and 1.
- $P(1)=p$ and $P(0)=1-p$ or in compact notation:

$$P(x) = \begin{cases} p^x(1-p)^{1-x}, \text{if} x = 0 \text{ or } x = 1 \\ 0, \text{otherwise} \end{cases}$$

- The performance of a fixed number of trials with fixed probability of success (p) on each trial is known as a *Bernoulli trial.*



P(**x**) for **p**=0.3

Classic Discrete Distributions (II)

Binomial Distribution

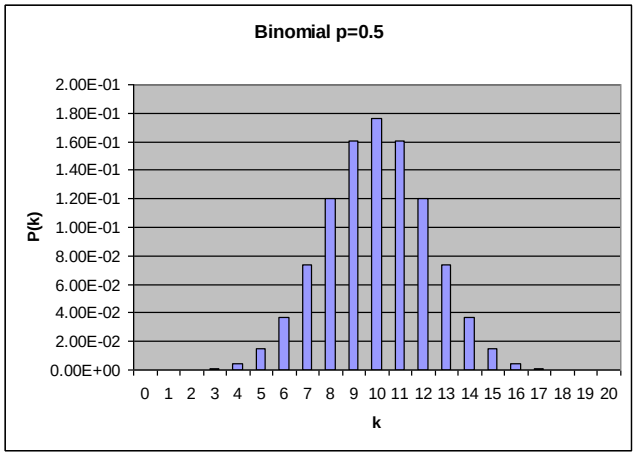
- Like Bernoulli distribution: binary input variables: 0 or 1, and probability $P(1)=p$ and $P(0)=1-p$
- What is the probability of k successes, $P(k)$, in a series of n independent trials? ($n>=k$)
- P(k) is a binomial random variable:

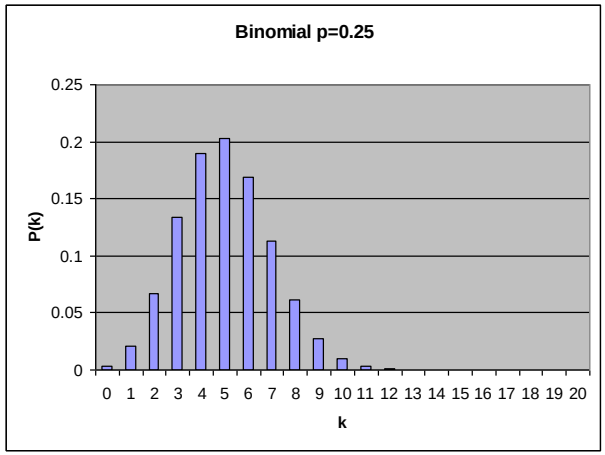
$$P(k) = \binom{n}{k} p^k (1-p)^{n-k} \text{ where } \binom{n}{k} = \frac{n!}{k!(n-k)!}$$

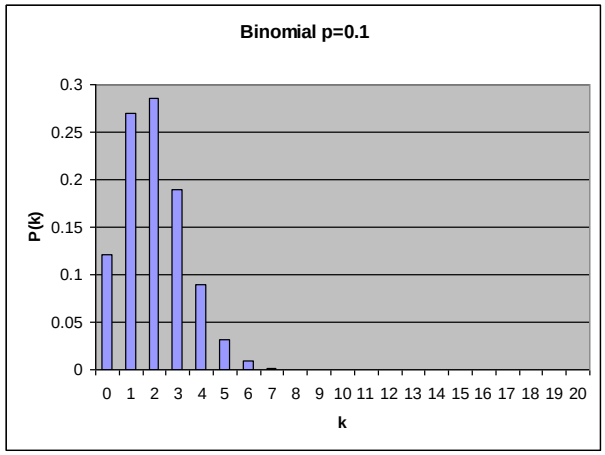
- Bernoulli distribution is a subset of the binomial distribution (i.e., $n=1$)

Classic Discrete Distributions (II)

Binomial Distribution







Classic Discrete Distributions (III)

Multinomial Distribution

- A generalization of the binomial distribution to multiple outputs (i.e., multiple classes an be categorized instead of just one class)
- n independent trials can result in one of r types of outcomes, where each outcome c_r has a probability $P(c_r)=p_r$(p_r=1).
- What is the probability $P(n_1,n_2,\ldots,n_r)$, i.e., the probability that in n trials, the frequency of the r classes is $(n_1,n_2,\ldots,n_r)$? This is a multinomial random variable:

$$P(n_1, n_2, \cdots, n_r) = \left(\begin{array}{c} n \\ n_1 n_2 \cdots n_r \end{array} \right) p_1^{n_1} p_2^{n_2} \cdots p_r^{n_r}$$

where

$$\left(\begin{array}{c} n \\ n_1 n_2 \cdots n_r \end{array} \right) = \frac{n!}{n_1! n_2! \cdots n_r!}$$

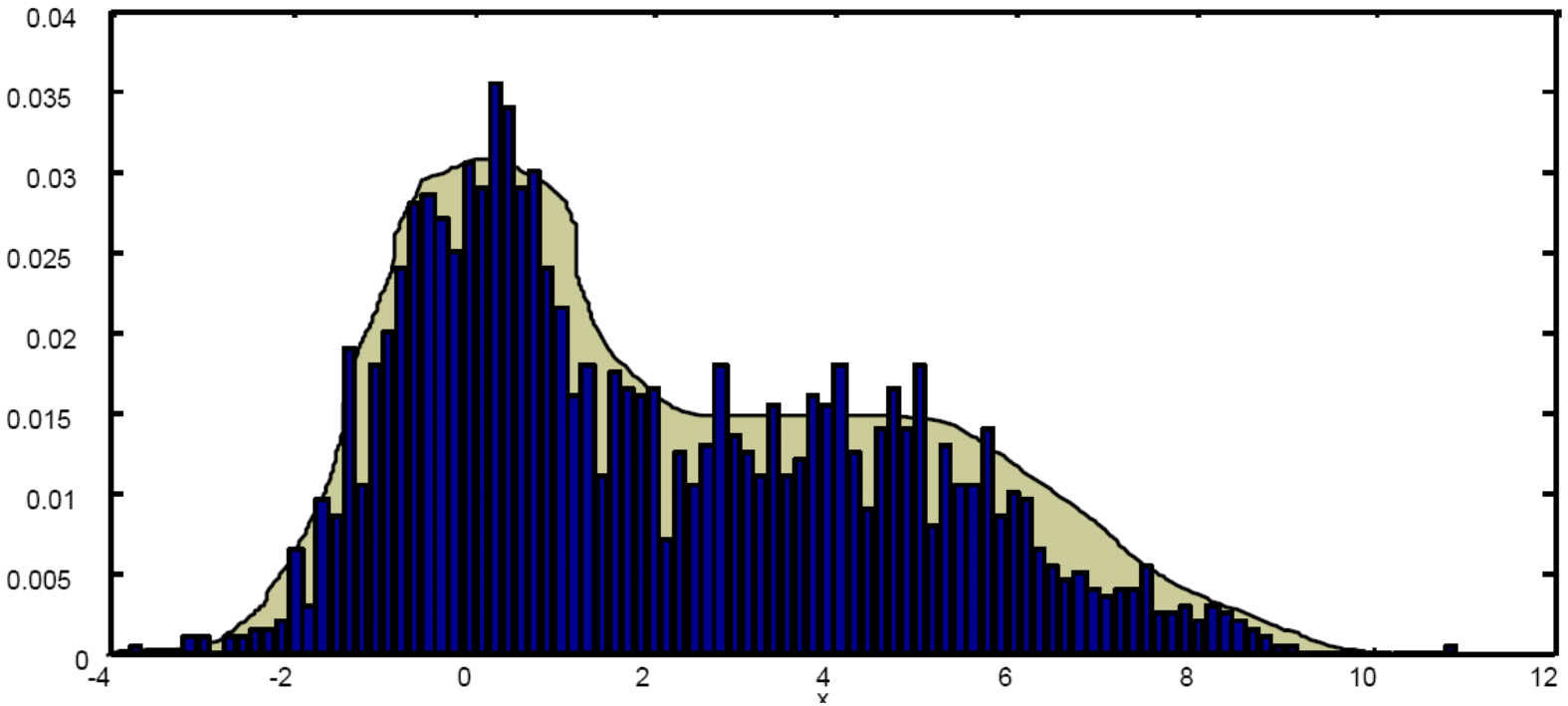
Continuous Probability Distributions

- The random variables take on real values.
- Continuous distributions are discrete distributions where the number of discrete values goes to infinity while the probability of each discrete value goes to zero.
- Probabilities become densities.
- Probability density integrates to 1.

$$\int_{-\infty}^{+\infty} p(x)dx = 1$$

Continuous Probability Distributions (cont'd)

- Probability Density Function p(x)



- Probability of an event:

$$P(a < x < b) = \int_a^b p(x)dx = 1$$

Classic Continuous Distributions (I)

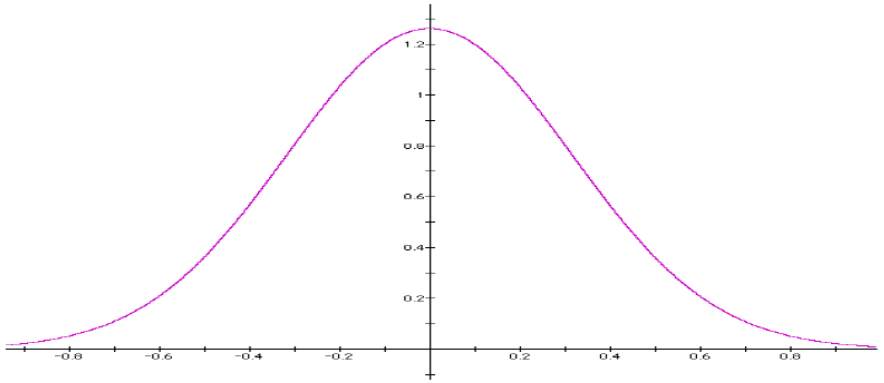
Normal Distribution

- The most used distribution

$$P(x) = \frac{1}{\sqrt{(2\pi)^d \|\Sigma\|}} \exp\left(-\frac{1}{2}(\mathbf{x}-\mu)^T \Sigma^{-1}(\mathbf{x}-\mu)\right)$$

- Also called Gaussian distribution after C.F.Gauss who proposed it
- Justified by the Central Limit Theorem:
  - Roughly: "if a random variable is the sum of a large number of independent random variables it is approximately normally distributed"
  - Many observed variables are the sum of several random variables
- Shorthand:

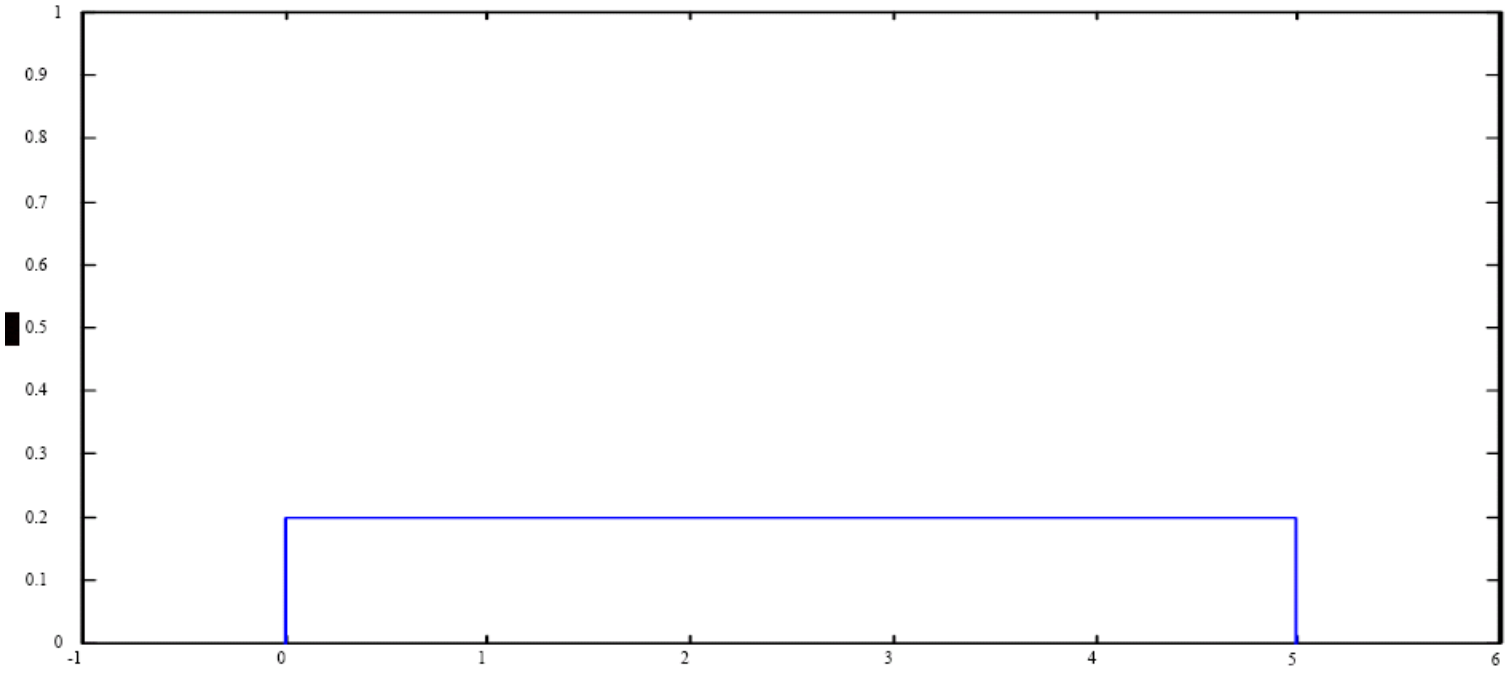
$$x \sim N(\mu, \Sigma)$$



Classic Continuous Distributions (II)

Uniform Distribution

- All data is equally probably within a bounded region R, p(x)=1/R



Expected Value

- The *expected value, mean* or *average* of the random variable x is defined by:

$$E[x] = \mu = \sum_{x \in \mathcal{X}} xP(x) = \sum_{i=1}^{m} v_i p_i.$$

- More generally, if $f(x)$ is any function of x, the expected value of f is defined by:

$$E[f(x)] = \sum_{x \in \mathcal{X}} f(x)P(x).$$

- This is also called the center of mass.
- Note that forming an expected values is *linear*, in that if α_1 and α_2 are arbitrary constants, then we have

$$E[\alpha_1 f_1(x) + \alpha_2 f_2(x)] = \alpha_1 E[f_1(x)] + \alpha_2 E[f_2(x)]$$

Expected Value

- General rules of thumb:

$$\begin{aligned} E[g(x)] &\neq g(E[x]) \\ E[\alpha x] &= \alpha E[x] \\ E[x+y] &= E[x] + E[y] \\ E\left[\sum_i \alpha_i x_i\right] &= \sum_i \alpha_i E[x_i] \end{aligned}$$

- In general:

$$E[x \cdot y] \neq E[x] \cdot E[y]$$

- Given a FINITE sample data, the Expectation is:

$$E[x] = \frac{1}{N} \sum_{i=1}^{N} \mathbf{x}_i$$

Variance and Standard Deviation

- Variance: $Var[x] = \sigma^2 = E\left[(x-\mu)^2\right] = \sum_{x \in \mathcal{X}} (x-\mu)^2 P(x)$
- σ is the *standard deviation* of x. The variance is never negative and approaches 0 as the probability mass is centered at one point.
- The standard deviation is a simple measure of how far values of x are likely to depart from the mean.
  - i.e., the standard or typical amount one should expect a randomly drawn value of x to deviate or differ from μ.

Sample variance and covariance

- Sample Variance

$$Var[x] = \frac{1}{N-1}\sum_{i=1}^{N}(x_i - E[x])^2$$

  - Why division by (N-1)? This is to obtain an unbiased estimate of the variance. (unbiased estimate: $E[\hat{x}] = x$)

- Covariance

$$Cov[x, y] = E\left[(x - E[x])(y - E[y])\right]$$

- Sample Covariance

$$Cov[x, y] = \frac{1}{N-1}\sum_{i=1}^{N}(x_i - E[x])(y_i - E[y])$$

$$Cov[\mathbf{x}] = \frac{1}{N-1}\sum_{i=1}^{N}(\mathbf{x}_i - E[\mathbf{x}])(\mathbf{x}_i - E[\mathbf{x}])^T$$

Biased vs. Unbiased variance

- Biased variance: $V = \frac{1}{n}\sum_{i=1}^{n}(x_i - X')^2$
- "Anti-biased" variance: $V^* = \frac{1}{n}\sum_{i=1}^{n}\left(x_i - X_i'\right)^2$

→ $(n-1)^2 V^* = n^2 V$

→ $\sqrt{V^* \cdot V} = \frac{1}{n-1}\sum_{i=1}^{n}\left(x_i - X'\right)^2$

Sample variance

s^2 is sample variance, σ^2 is true variance, μ is true mean

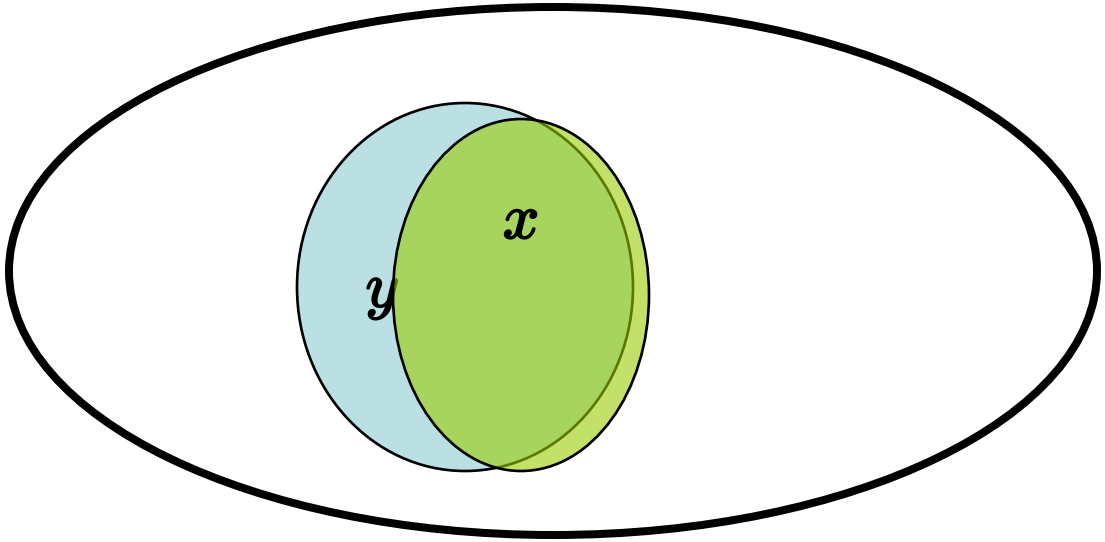
$$
\begin{aligned}
E[s^2] &= E\left[\frac{1}{n-1}\sum_{i=1}^{n}(x_i-\overline{x})^2\right] \quad \text{(where } \overline{x} = E[x] \text{ is the sample mean)} \\
&= \frac{1}{n-1}\sum_{i=1}^{n}(x_i-\overline{x})^2 \\
&= \frac{1}{n-1}\sum_{i=1}^{n}((x_i-\mu)-(\overline{x}-\mu))^2 \\
&= \frac{1}{n-1}\sum_{i=1}^{n}E\left[(x_i-\mu)^2\right] - 2E\left[(x_i-\mu)-(\overline{x}-\mu)\right] + E\left[(\overline{x}-\mu)^2\right] \\
&= \frac{1}{n-1}\sum_{i=1}^{n}\left[\sigma^2 - 2\left(\frac{1}{n}\sum_{j=1}^{n}E\left[(x_i-\mu)(x_j-\mu)\right]\right) + \frac{1}{n^2}\sum_{j=1}^{n}\sum_{k=1}^{n}E\left[(x_j-\mu)(x_k-\mu)\right]\right] \\
&= \frac{1}{n-1}\sum_{i=1}^{n}\left[\sigma^2 - \frac{2\sigma^2}{n} + \frac{\sigma^2}{n}\right] \\
&= \frac{1}{n-1}\sum_{i=1}^{n}\frac{(n-1)\sigma^2}{n} \\
&= \frac{(n-1)\sigma^2}{n-1} \\
&= \sigma^2
\end{aligned}
$$

Conditional Probability

- $P(x|y)$ is the probability of the occurrence of event x given that y occurred and is given as:

$$P(x|y) = \frac{P(x \cap y)}{P(y)}$$

- Knowing that y occurred reduces the sample space to y, and the part of it where x also occurred is (x,y)



Conditional Probability

- $P(x|y)$ is the probability of the occurrence of event x given that y occurred and is given as:

$$P(x|y) = \frac{P(x \bigcap y)}{P(y)}$$

- Knowing that y occurred reduces the sample space to y, and the part of it where x also occurred is (x,y)
- This is only defined if P(y)>0. Also, because $\bigcap$ is commutative, we have:

$$P(x \bigcap y) = P(x|y)P(y) = P(y|x)P(x)$$

Statistical Independence

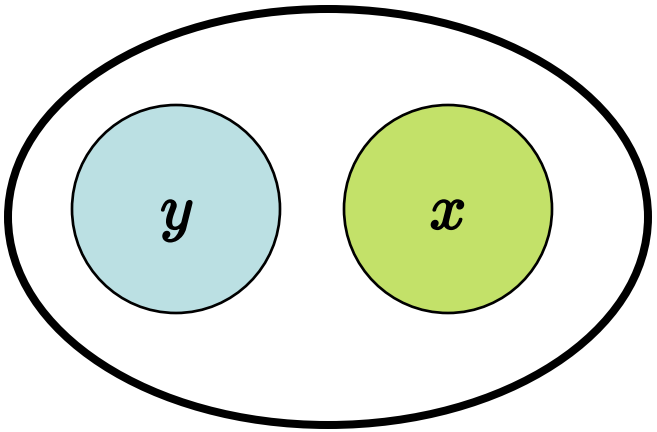
- If x and y are *independent* then we have

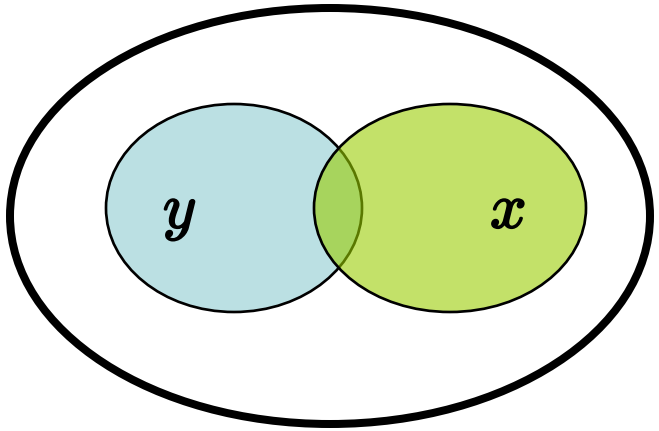
$$P(x|y) = P(x)$$

- From there it follows that

$$P(x \bigcap y) = P(x)P(y)$$

- In other words, knowing that y occurred does not change the probability that x occurs (and vice versa).





Bayes Rule

- Remember: $\boxed{P(x \bigcap y) = P(x|y)P(y) = P(y|x)P(x)}$
- Bayes Rule:

$$P(y|x) = \frac{P(x|y)P(y)}{P(x)}$$

- Interpretation
  - P(y) is the **PRIOR** knowledge about y
  - X is new evidence to be incorporated to update my belief about y.
  - P(x|y) is the **LIKELIHOOD** of x given that y was observed.
  - Both prior and likelihood can often be generated beforehand, e.g., by histogram statistics
  - P(x) is a normalizing factor, corresponding to the *marginal distribution* of x. Often it need not be evaluated explicitly, but it can become a great computational burden.

    "P(x) is an enumeration of all possible combinations of x, and the probability of their occurrence."
  - P(y|x) is the **POSTERIOR** probability of y, i.e., the belief in y after on discovers x.

Learning Bayesian Networks: Naïve and non-Naïve Bayes

- Hypothesis Space
  - fixed size
  - stochastic
  - continuous parameters
- Learning Algorithm
  - direct computation
  - eager
  - batch

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

Bayes Theorem

- Consider hypothesis space H

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

- $P(h)$ = prior prob. of hypothesis $h \in H$
- $P(D)$ = prior prob. of training data D
- $P(h|D)$ = probability of h given D
- $P(D|h)$ = probability of D given h

Choosing Hypotheses

Natural choice is most probable hypothesis given the training data, or *maximum a posteriori* hypothesis h_{MAP}:

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

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

$$h_{\text{ML}} = \text{argmax}_{h \in H} P(D|h)$$

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 98% of the cases in which the disease is actually present, and a correct negative result in 97% of the cases in which the disease is not present. Furthermore, .008 of the entire population have this cancer.

$P(\text{cancer}) = 0.008$ $P(\neg\text{cancer}) = 0.992$

$P(+|\text{cancer}) = 0.98$ $P(-|\text{cancer}) = 0.02$

$P(+|\neg\text{cancer}) = 0.03$ $P(-|\neg\text{cancer}) = 0.97$

Bayes Theorem: Example

P (cancer) = 0.008 P (¬cancer) = 0.992

P (+|cancer) = 0.98 P (-|cancer) = 0.02

P (+|¬cancer) = 0.03 P (-|¬cancer) = 0.97

A positive test result comes in for a patient.

What is the h_{MAP}?

P(+|cancer)P(cancer) = (0.98)*(0.008) = .0078

P(+|¬cancer)P(¬cancer) = (0.03)*(0.992) = .0298

h_{MAP}=¬cancer

Brute Force MAP Learner

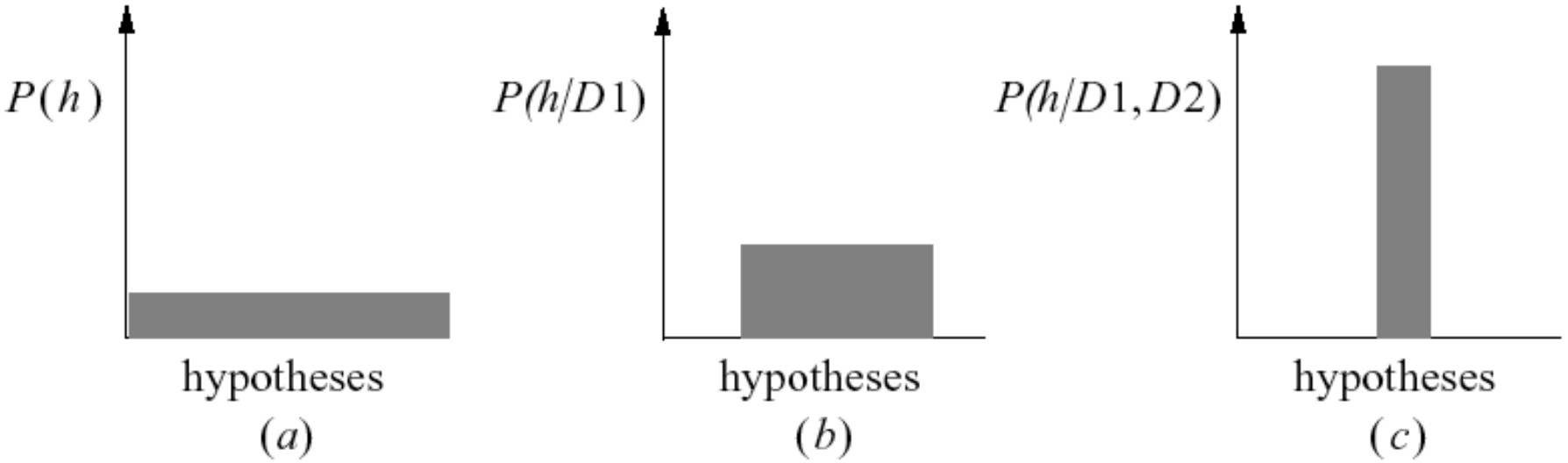
1. For each hypothesis h in H, calculate the posterior probability

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

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

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

Evolution of Posterior Probs



- As data is added, certainty of hypotheses increases.

Classifying New Instances

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

Given new instance $\mathbf{x}$, what is its most probable *classification*?

$h_{\text{MAP}}(\mathbf{x})$ is not the most probable classification!

Classification Example

Consider:

- Three possible hypotheses:
  $P(h_1|D) = .4$, $P(h_2|D) = .3$, $P(h_3|D) = .3$
- Given new instance x,
  $h_1(\mathbf{x}) = +$, $h_2(\mathbf{x}) = -$, $h_3(\mathbf{x}) = -$
- What's $h_{MAP}(\mathbf{x})$?
- What's most probable classification of $\mathbf{x}$?

Bayes Optimal Classifier

Bayes optimal classification:

$$\text{argmax}_{v \in V} \sum_{h \in H} P(v|h)P(h|D)$$

Example:

- $P(h_1|D) = .4$, $P(-|h_1) = 0$, $P(+|h_2) = 1$
- $P(h_2|D) = .3$, $P(-|h_2) = 1$, $P(+|h_3) = 0$
- $P(h_3|D) = .3$, $P(-|h_3) = 1$, $P(+|h_3) = 0$,

therefore

$$\sum_{h \in H} P(+|h)P(h|D) = 0.4$$

$$\sum_{h \in H} P(-|h)P(h|D) = 0.6$$

MAP class

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 one to classify new instance

Error of Gibbs

Noteworthy fact [Haussler 1994]: Assume target concepts are drawn at random from H according to priors on H. Then:

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

Suppose correctly, uniform prior distribution over H, then

- Pick any hypothesis consistent with the data, with uniform probability
- Its expected error no worse than twice Bayes optimal

Naive Bayes Classifier

Along with decision trees, neural networks, *k*NN, one of the most practical and most used 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

Naïve Bayes Assumption

- Suppose the features x_i are discrete
- Assume the x_i are conditionally independent given y.
- In other words, assume that:

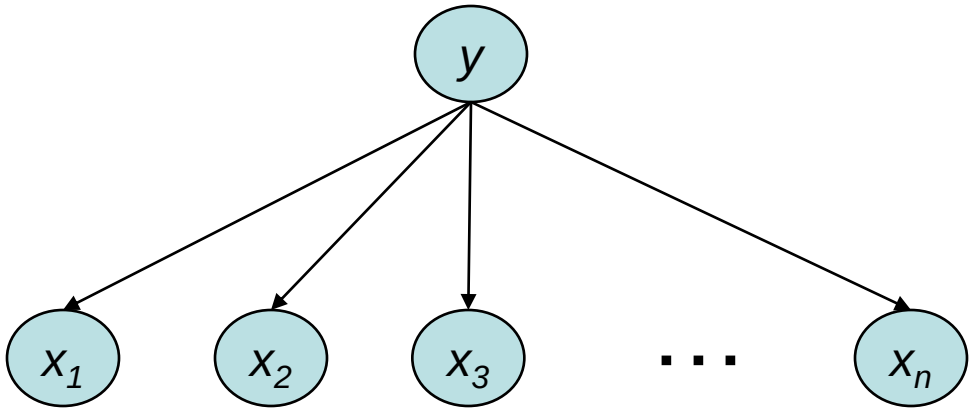
$$P(x_i|y) = P(x_i|y, x_j), \forall i, j$$

- Then we have:

$$P(x_1, x_2, \cdots, x_n|y) = P(x_1|y)P(x_2|y)\cdots P(x_n|y)$$

- For binary features, instead of $O(2^n)$ numbers to describe a model, we only need O(n)!

Graphical Representation of Naïve Bayes Model



- Each node contains a probability table
  - y: $P(y = k)$
  - x_j: $P(x_j = v \mid y = k)$ "class conditional probability"
- Interpret as a generative model
  - Choose the class k according to $P(y = k)$
  - Generate each feature *independently* according to $P(x_j = v \mid y = k)$
  - The feature values are *conditionally independent*
    $P(x_i, x_j \mid y) = P(x_i \mid y) \cdot P(x_j \mid y)$

Naïve Bayes Algorithm

Naïve_Bayes_Learn(examples)

For each target value y_j

$P(\hat{y}_j) \leftarrow$ estimate $P(y_j)$

For each attribute value x_i

$P(\hat{x}_i|y_j) \leftarrow$ estimate $P(x_i|y_j)$

Classify_New_Instance(**x**)

$y_{\text{NB}} = \text{argmax}_{y_j \in Y} P(y_j) \Pi_i P(x_i|y_j)$

Naïve Bayes: Example

- Consider the *PlayTennis* problem and new instance

<*Outlook* = *sun*, *Temp* = *cool*, *Humid* = *high*, *Wind* = *strong*>

Want to compute:

$$y_{\text{NB}} = \text{argmax}_{y_j \in Y} P(y_j) \Pi_i P(x_i | y_j)$$

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

- So, y_{NB} = *n*

Naïve Bayes: Subtleties

- Conditional independence assumption is often violated

$$P(x_1, x_2 \ldots x_n | y_j) = \Pi_i P(x_i | y_j)$$

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

$$\text{argmax}_{y_j \in Y} P(y_j|\mathbf{x}) = \text{argmax}_{y_j \in Y} P(y_j) \Pi_i P(x_i|y_j)$$

- See Domingos & Pazzani [1996] for analysis
- Naïve Bayes posteriors often unrealistically close to 1 or 0

Decision Boundary of naïve Bayes with binary features

- The parameters of the model are $\theta_{i,1}$ = P(x_i=1|y=1), $\theta_{i,0}$=P(x_i=1|y=0), θ_1 = P(y=1)
- What is the decision surface?

$$\frac{P(y=1|\mathbf{x})}{P(y=0|\mathbf{x})} = \frac{P(y=1)\Pi_{i=1}^{n} P(x_i|y=1)}{P(y=0)\Pi_{i=1}^{n} P(x_i|y=0)}$$

- Using the log trick, we get:

$$\log\frac{P(y=1|\mathbf{x})}{P(y=0|\mathbf{x})} = \log\frac{P(y=1)}{P(y=0)} + \sum_{i=1}^{n} \log\frac{(x_i|y=1)}{P(x_i|y=0)}$$

- Note that in the equation above, the x_i would be 1 or 0, depending on the values were present in the instance.

Decision Boundary of naïve Bayes with binary features

let:
$$w_o = \log \frac{P(y=1)}{P(y=0)}$$
$$w_{i,1} = \log \frac{P(x_i=1|y=1)}{P(x_i=1|y=0)}$$
$$w_{i,0} = \log \frac{P(x_i=0|y=1)}{P(x_i=0|y=0)}$$

- We can re-write the decision boundary as:

$$\log \frac{P(y=1|\mathbf{x})}{P(y=0|\mathbf{x})} = w_0 + \sum_{i=0}^{n} (w_{i,1}x_i + w_{i,0}(1-x_i))$$
$$= w_0 + \sum_{i=1}^{n} w_{i,0} + \sum_{i=1}^{n} (w_{i,1} - w_{i,0})x_i$$

- This is a *linear decision boundary!*

Representing $P(x_j|y)$

Many representations are possible

- Univariate Gaussian
  - if x_j is a continuous random variable, then we can use a normal distribution and learn the mean μ and variance σ^2
- Multinomial/Binomial
  - if x_j is a discrete random variable, $x_j \in \{v_1, ..., v_m\}$, then we construct a conditional probability table
- Discretization
  - convert continuous x_j into a discrete variable
- Kernel Density Estimates
  - apply a kind of nearest-neighbor algorithm to compute $P(x_j \mid y)$ in neighborhood of query point

Representing $P(x_j|y)$ – Discrete Values

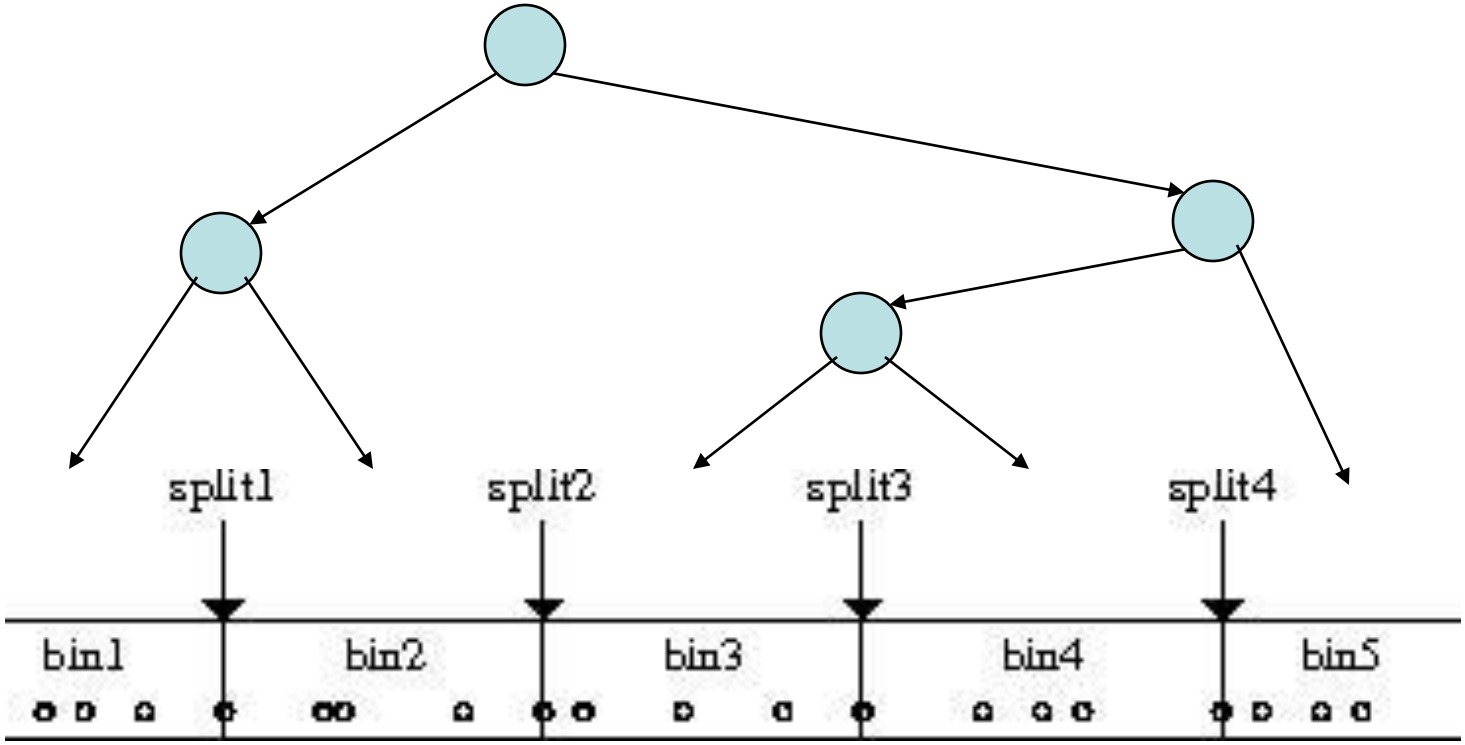
- Multinomial/Binomial
  - if x_j is a discrete random variable, $x_j \in \{v_1, \ldots, v_m\}$, then we construct the conditional probability table

	$y = 1$	$y=2$	...	$y=K$
$x_j = v_1$	$P(x_j = v_1 \mid y = 1)$	$P(x_j = v_1 \mid y = 2)$	...	$P(x_j = v_1 \mid y = K)$
$x_j = v_2$	$P(x_j = v_2 \mid y = 1)$	$P(x_j = v_2 \mid y = 2)$	...	$P(x_j = v_2 \mid y = K)$
...	...	...	...	...
$x_j = v_m$	$P(x_j = v_m \mid y = 1)$	$P(x_j = v_m \mid y = 2)$	...	$P(x_j = v_m \mid y = K)$

$$P(x_j = v_l|y = k) = \frac{\text{number of instances for which } x_j = v_l \text{ and } y = k}{\text{number of instances for which } y = k}$$

Discretization via Mutual Information

- Many discretization algorithms have been studied. One of the best is based on mutual information [Fayyad & Irani 93].
  - To discretize feature x_j, grow a decision tree considering only splits on x_j. Each leaf of the resulting tree will correspond to a single value of the discretized x_j.



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  - To discretize feature x_j, grow a decision tree considering only splits on x_j. Each leaf of the resulting tree will correspond to a single value of the discretized x_j.
  - Stopping rule (applied at each node). Stop when

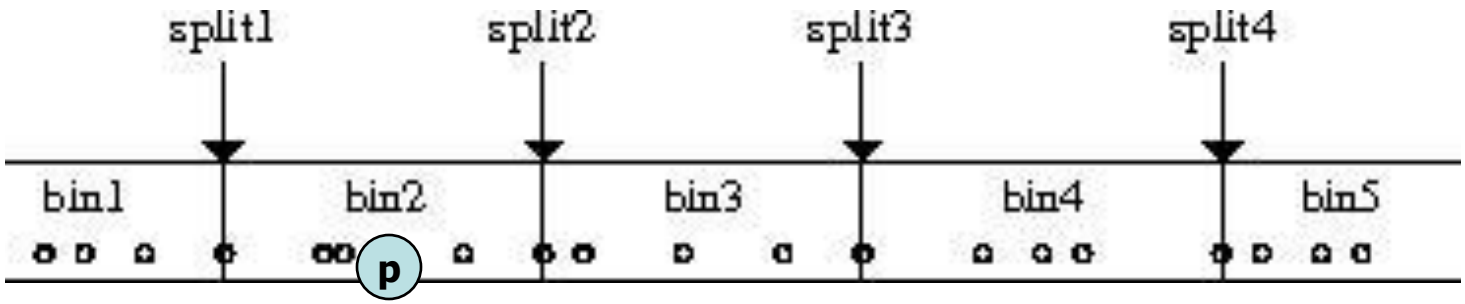
$$I(x_j; y) < \frac{\log_2(N-1)}{N} + \frac{\Delta}{N}$$

$$\Delta = \log_2(3^K - 2) - [K \cdot H(S) - K_l \cdot H(S_l) - K_r \cdot H(S_r)]$$

  - where S is the training data in the parent node; S_l and S_r are the examples in the left and right child. K, K_l, and K_r are the corresponding number of classes present in these examples. I is the mutual information, H is the entropy, and N is the number of examples in the node.

Discretization: Thermometer Encoding

- Many discretization algorithms have been studied. One of the best is based on mutual information [Fayyad & Irani 93].
  - An alternative encoding [Macskassy et al. 02] is similar to thermometer coding as used in neural networks [Gallant 93].
  - Rather than encode continuous values into *one* value, encode into $2v$ values, where v is the number of split points created.
  - Each encoded binary value represents whether the continuous value was greater or less-than-or-equal to one of the split points.



Encoding: {>split1,≤ split1, >split2,≤ split2, >split3,≤ split3, >split4,≤ split4}

p: { 1 , 0 , 0 , 1 , 0 , 1 , 0 , 1 }

Kernel Density Estimators

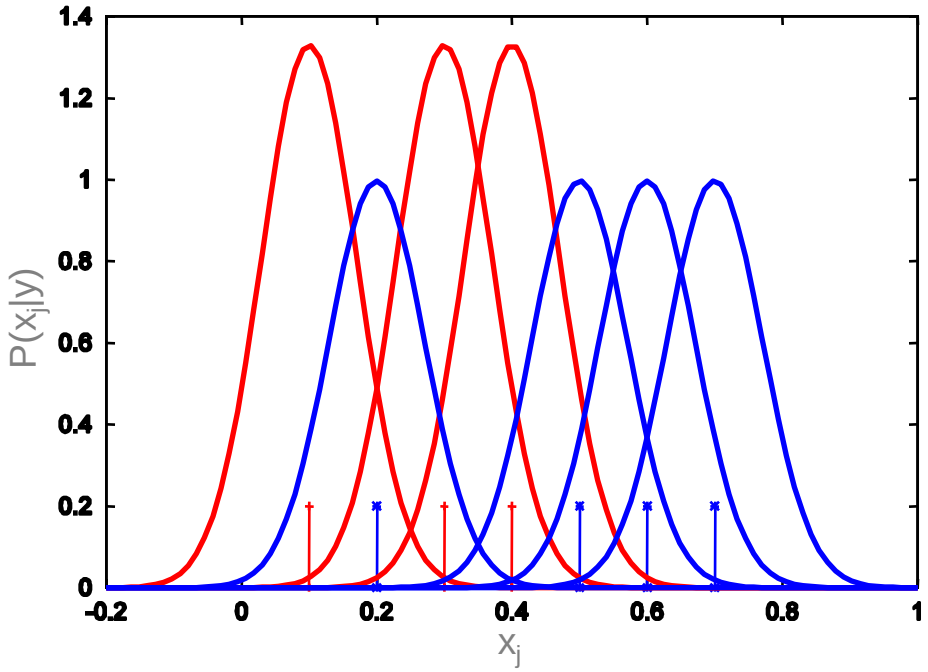
- Define $K(x_j, x_{i,j}) = \frac{1}{\sqrt{2\pi}\sigma} \exp - \left(\frac{x_j - x_{i,j}}{\sigma} \right)^2$ to be the Gaussian Kernel with parameter σ
- Estimate

$$P(x_j | y = k) = \frac{\sum_{\{i|y=k\}} K(x_j, x_{i,j})}{N_k}$$

where N_k is the number of training examples in class k.

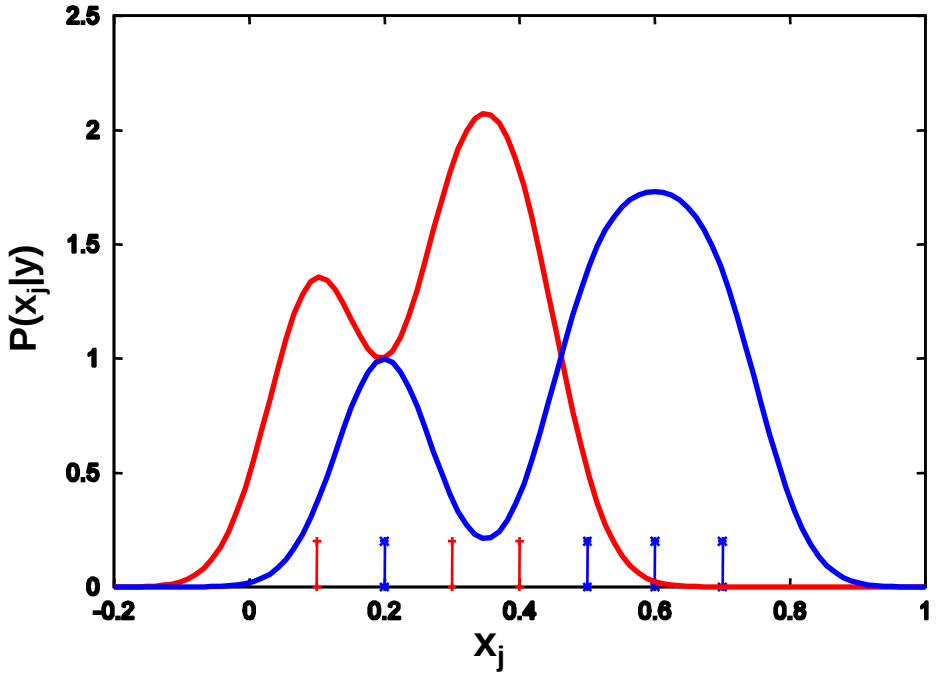
Kernel Density Estimators (2)

- This is equivalent to placing a Gaussian "bump" of height $1/N_k$ on each training data point from class k and then adding them up

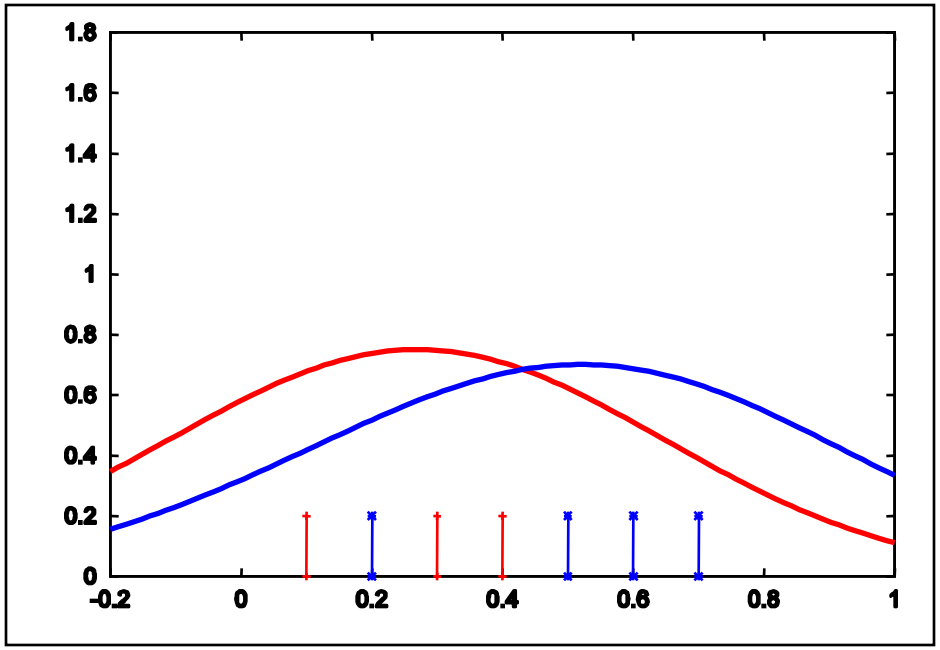


Kernel Density Estimators (3)

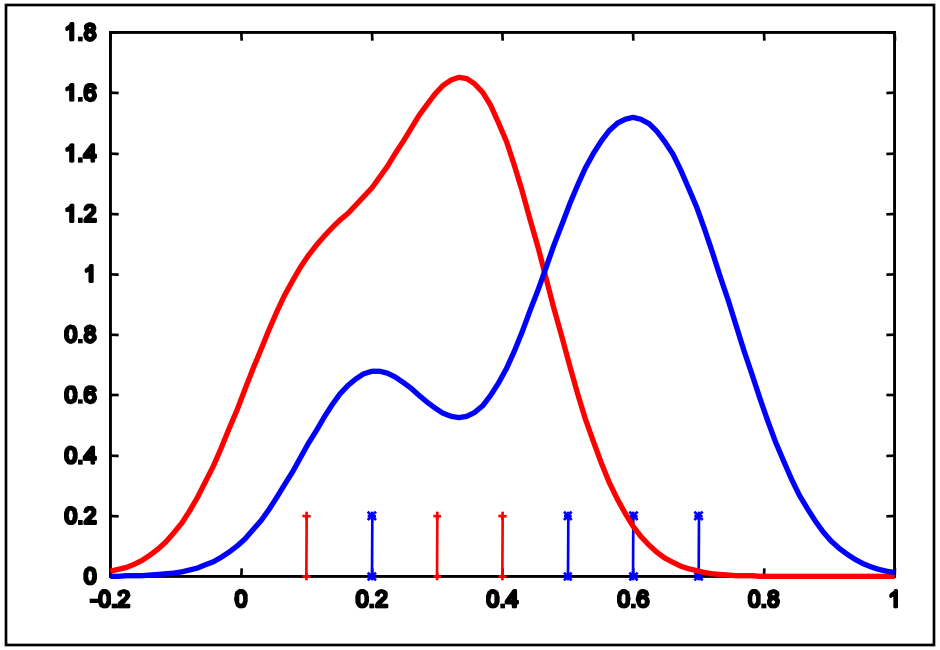
- Resulting probability density



The value chosen for σ is critical



σ=0.15???



σ=0.50

Learning the Probability Distributions by Direct Computation

- P(y=k) is just the fraction of training examples belonging to class k.
- For multinomial variables, P($x_j = v \mid y = k$) is the fraction of training examples in class k where $x_j = v$
- For Gaussian variables, $\hat{\mu}_{jk}$ is the average value of x_j for training examples in class k. $\hat{\sigma}_{jk}$ is the sample standard deviation of those points:

$$\hat{\sigma}_{jk} = \sqrt{\frac{1}{N_k} \sum_{\{i|y_i=k\}} (x_{i,j} - \hat{\mu}_{jk})^2}$$

Improved Probability Estimates via Laplace Corrections

- When we have very little training data, direct probability computation can give probabilities of 0 or 1. Such extreme probabilities are "too strong" and cause problems
- Suppose we are estimating a probability P(z) and we have n_0 examples where z is false and n_1 examples where z is true. Our direct estimate is

$$P(z=1) = \frac{n_1}{n_0 + n_1}$$

- Laplace Estimate. Add 1 to the numerator and 2 to the denominator

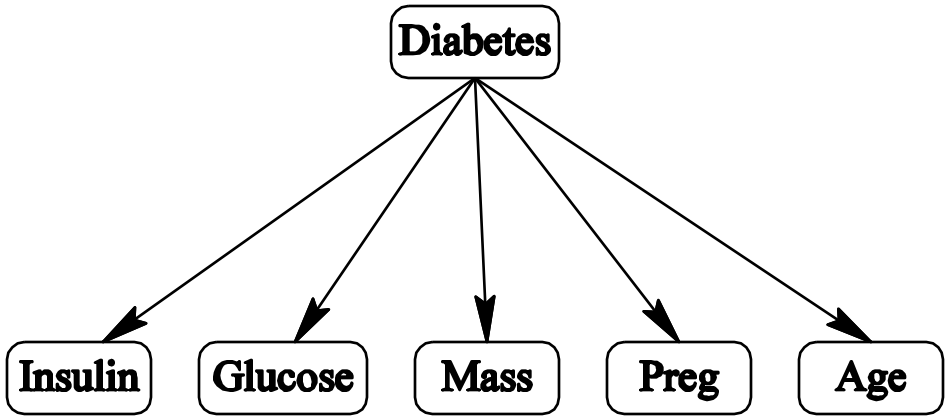
$$P(z=1) = \frac{n_1 + 1}{n_0 + n_1 + 2}$$

This says that in the absence of any evidence, we expect P(z) = 0.5, but our belief is weak (equivalent to 1 example for each outcome).

- Generalized Laplace Estimate. If z has K different outcomes, then we estimate it as

$$P(z=1) = \frac{n_1 + 1}{n_0 + \cdots + n_{K-1} + K}$$

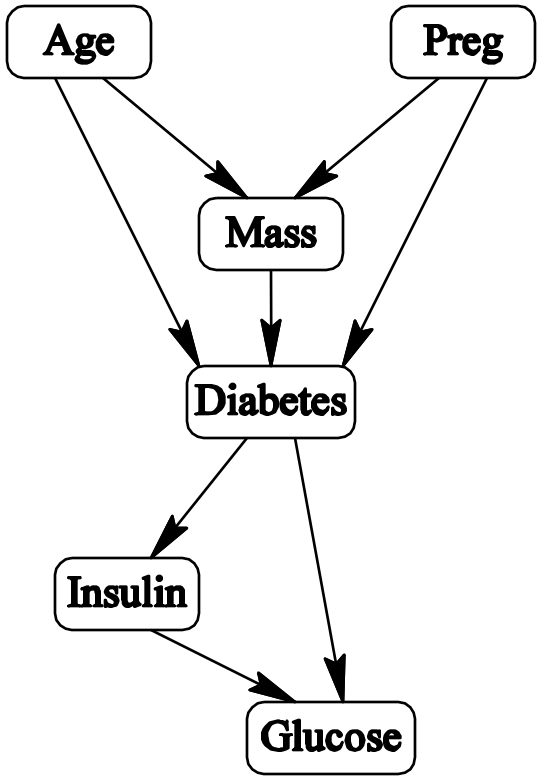
Naïve Bayes Applied to Diabetes Diagnosis



- Bayes nets and causality
  - Bayes nets work best when arrows follow the direction of causality
    - two things with a common cause are likely to be conditionally independent given the cause; arrows in the causal direction capture this independence
  - In a Naïve Bayes network, arrows are often not in the causal direction
    - diabetes does not cause pregnancies
    - diabetes does not cause age
  - But some arrows are correct
    - diabetes does cause the level of blood insulin and blood glucose

Non-Naïve Bayes

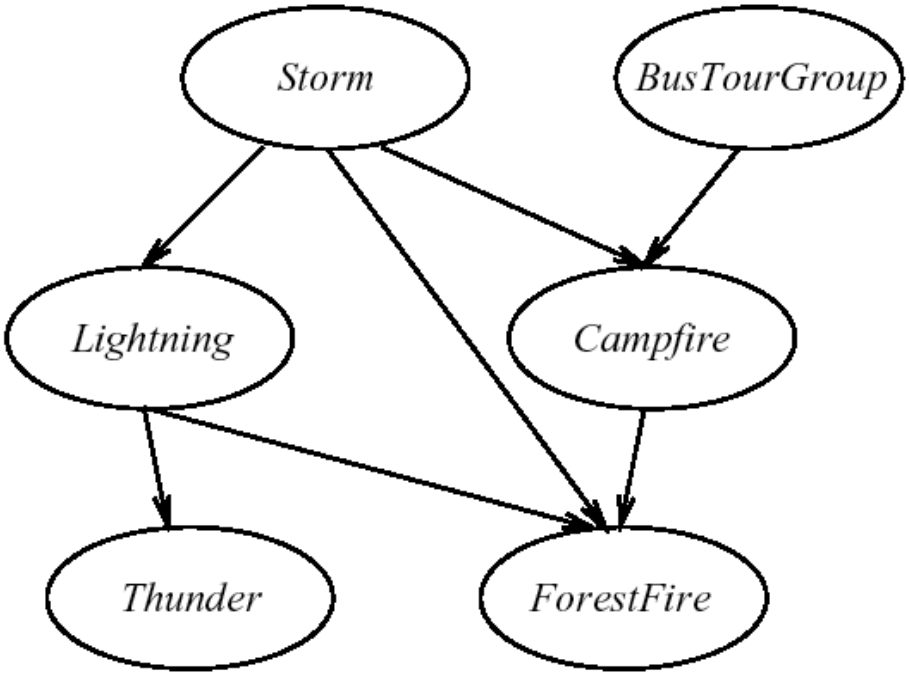
- Manually construct a graph in which all arcs are causal
- Learning the probability tables is still easy. For example, P(Mass | Age, Preg) involves counting the number of patients of a given age and number of pregnancies that have a given body mass
- Classification:



$$P(D = d|A, P, M, I, G) =$$

$$\frac{P(I|D = d)P(G|I, D = d)P(D = d|A, M, P)}{P(I, G)}$$

Bayesian Belief Network



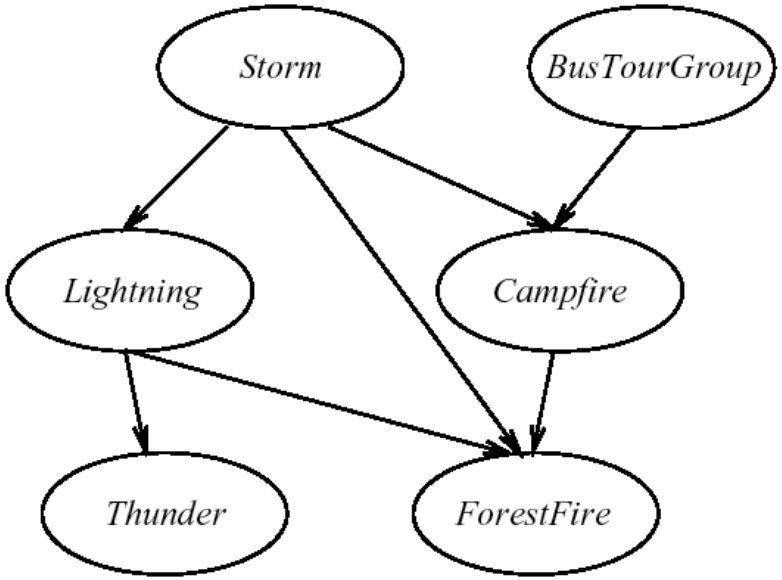
	S,B	$S,\neg B$	$\neg S,B$	$\neg S,\neg B$
C	0.4	0.1	0.8	0.2
$\neg C$	0.6	0.9	0.2	0.8

Campfire

Network represents a set of conditional ind. assertions:

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

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

Campfire

Represents joint probability distribution over all variables

- e.g., P(*Storm*, *BusTourGroup*, …, *ForestFire*)
- in general, $P(y_1, \ldots, y_n) = \Pi_{i=1}^{n} P(y_i|\text{Parents}(Y_i))$
  where Parents(Y_i) denotes immediate predecessors of Y_i in the graph
- Therefore, the joint distribution is fully defined by graph, plus the CPTS:

$$P(y_i|\text{Parents}(Y_i))$$

Inference in Bayesian Nets

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
- Easy if BN is a "polytree"
- In general case, problem is NP hard (#P-complete, Roth 1996).

Inference in Practice

In practice, can succeed in many cases

- Exact inference methods work well for some network structures (small "induced width")
- Monte Carlo methods "simulate" the network randomly to calculate approximate solutions
- Now used as a primitive in more advanced learning and reasoning scenarios. (e.g., in relational learning)

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 BNs

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

$$w_{ijk} = P(Y_i = y_{ij} | \text{Parents}(Y_i) = u_{jk} \text{ values})$$

e.g., if Y_i = *Campfire*, then u_{ik} might be

<*Storm* = *T*, *BusTourGroup* = *F*>

Perform gradient ascent by repeatedly:

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

$$w_{ijk} \leftarrow_{ijk} + \eta \frac{\Sigma_{d \in D} P_h(y_{ij}, u_{jk} | d)}{w_{ijk}}$$

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

$$\sum_j w_{ijk} = 1, \; o \leq w_{ijk} \leq 1$$

Unknown Structure

When structure unknown...

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

Somewhat like decision trees: searching for a discrete graph structure

Belief Networks

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

Naïve Bayes Summary

- Advantages of Bayesian networks
  - Produces stochastic classifiers
    - can be combined with utility functions to make optimal decisions
  - Easy to incorporate causal knowledge
    - resulting probabilities are easy to interpret
  - Very simple learning algorithms
    - if all variables are observed in training data
- Disadvantages of Bayesian networks
  - Fixed sized hypothesis space
    - may underfit or overfit the data
    - may not contain any good classifiers if prior knowledge is wrong
  - Harder to handle continuous features

Evaluation of Naïve Bayes

Criterion	LMS	Logistic	LDA	Trees	NNbr	Nets	NB
Mixed data	**no**	**no**	**no**	**yes**	**no**	**no**	**yes**
Missing values	**no**	**no**	**yes**	**yes**	**some**	**no**	**yes**
Outliers	**no**	**yes**	**no**	**yes**	**yes**	**yes**	**disc**
Monotone transformations	**no**	**no**	**no**	**yes**	**no**	**some**	**disc**
Scalability	**yes**	**yes**	**yes**	**yes**	**no**	**yes**	**yes**
Irrelevant inputs	**no**	**no**	**no**	**some**	**no**	**no**	**some**
Linear combinations	**yes**	**yes**	**yes**	**no**	**some**	**yes**	**yes**
Interpretable	**yes**	**yes**	**yes**	**yes**	**no**	**no**	**yes**
Accurate	**yes**	**yes**	**yes**	**no**	**no**	**yes**	**yes**

- Naïve Bayes is very popular, particularly in natural language processing and information retrieval where there are many features compared to the number of examples
- In applications with lots of data, Naïve Bayes does not usually perform as well as more sophisticated methods