BAYESIAN LEARNING

Bayesian reasoning provides a probabilistic approach to inference. It is based on the assumption that the quantities of interest are governed by probability distributions and that optimal decisions can be made by reasoning about these probabilities together with observed data

INTRODUCTION

Bayesian learning methods are relevant to study of machine learning for two different reasons.

1. First, Bayesian learning algorithms that calculate explicit probabilities for hypotheses, such as the naive Bayes classifier, are among the most practical approaches to certain types of learning problems
2. The second reason is that they provide a useful perspective for understanding many learning algorithms that do not explicitly manipulate probabilities.

Features of Bayesian Learning Methods

- Each observed training example can incrementally decrease or increase the estimated probability that a hypothesis is correct. This provides a more flexible approach to learning than algorithms that completely eliminate a hypothesis if it is found to be inconsistent with any single example
- Prior knowledge can be combined with observed data to determine the final probability of a hypothesis. In Bayesian learning, prior knowledge is provided by asserting (1) a prior probability for each candidate hypothesis, and (2) a probability distribution over observed data for each possible hypothesis.
- Bayesian methods can accommodate hypotheses that make probabilistic predictions
- New instances can be classified by combining the predictions of multiple hypotheses, weighted by their probabilities.
- Even in cases where Bayesian methods prove computationally intractable, they can provide a standard of optimal decision making against which other practical methods can be measured.

Practical difficulty in applying Bayesian methods

1. One practical difficulty in applying Bayesian methods is that they typically require initial knowledge of many probabilities. When these probabilities are not known in advance they are often estimated based on background knowledge, previously available data, and assumptions about the form of the underlying distributions.
2. A second practical difficulty is the significant computational cost required to determine the Bayes optimal hypothesis in the general case. In certain specialized situations, this computational cost can be significantly reduced.

BAYES THEOREM

Bayes theorem provides a way to calculate the probability of a hypothesis based on its prior probability, the probabilities of observing various data given the hypothesis, and the observed data itself.

Notations

- P(h) prior probability of h, reflects any background knowledge about the chance that h is correct
- P(D) prior probability of D, probability that D will be observed
- P(D|h) probability of observing D given a world in which h holds
- P(h|D) posterior probability of h, reflects confidence that h holds after D has been observed

Bayes theorem is the cornerstone of Bayesian learning methods because it provides a way to calculate the posterior probability P(h|D), from the prior probability P(h), together with P(D) and P(D|h).

Bayes Theorem:

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

- P(h|D) increases with P(h) and with P(D|h) according to Bayes theorem.
- P(h|D) decreases as P(D) increases, because the more probable it is that D will be observed independent of h, the less evidence D provides in support of h.

Maximum a Posteriori (MAP) Hypothesis

- In many learning scenarios, the learner considers some set of candidate hypotheses H and is interested in finding the most probable hypothesis h ∈ H given the observed data D. Any such maximally probable hypothesis is called a maximum a posteriori (MAP) hypothesis.
- Bayes theorem to calculate the posterior probability of each candidate hypothesis is h_{MAP} is a MAP hypothesis provided

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

- P(D) can be dropped, because it is a constant independent of h

Maximum Likelihood (ML) Hypothesis

- In some cases, it is assumed that every hypothesis in H is equally probable a priori ($P(h_i) = P(h_j)$ for all h_i and h_j in H).
- In this case the below equation can be simplified and need only consider the term P(D|h) to find the most probable hypothesis.

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

the equation can be simplified

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

P(D|h) is often called the likelihood of the data D given h, and any hypothesis that maximizes P(D|h) is called a maximum likelihood (ML) hypothesis

Example

- Consider a medical diagnosis problem in which there are two alternative hypotheses: (1) that the patient has particular form of cancer, and (2) that the patient does not. The available data is from a particular laboratory test with two possible outcomes: + (positive) and - (negative).

- We have prior knowledge that over the entire population of people only .008 have this disease. Furthermore, the lab test is only an imperfect indicator of the disease.
- 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. In other cases, the test returns the opposite result.
- The above situation can be summarized by the following probabilities:

$$P(cancer) = .008 \qquad P(\neg cancer) = 0.992$$
$$P(\oplus|cancer) = .98 \qquad P(\ominus|cancer) = .02$$
$$P(\oplus|\neg cancer) = .03 \qquad P(\ominus|\neg cancer) = .97$$

Suppose a new patient is observed for whom the lab test returns a positive (+) result. Should we diagnose the patient as having cancer or not?

$$P(\oplus|cancer)P(cancer) = (.98).008 = .0078$$
$$P(\oplus|\neg cancer)P(\neg cancer) = (.03).992 = .0298$$
$$\Rightarrow h_{MAP} = \neg cancer$$

The exact posterior probabilities can also be determined by normalizing the above quantities so that they sum to 1

$$P(cancer|\oplus) = \frac{0.0078}{0.0078 + 0.0298} = 0.21$$

$$P(\neg cancer|\oplus) = \frac{0.0298}{0.0078 + 0.0298} = 0.79$$

Basic formulas for calculating probabilities are summarized in Table

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- *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

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

- *Bayes theorem*: the posterior probability $P(h|D)$ of h given D

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

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

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

BAYES THEOREM AND CONCEPT LEARNING

What is the relationship between Bayes theorem and the problem of concept learning?

Since Bayes theorem provides a principled way to calculate the posterior probability of each hypothesis given the training data, and can use it as the basis for a straightforward learning algorithm that calculates the probability for each possible hypothesis, then outputs the most probable.

Brute-Force Bayes Concept Learning

Consider the concept learning problem

- Assume the learner considers some finite hypothesis space H defined over the instance space X, in which the task is to learn some target concept $c : X \rightarrow \{0,1\}$.
- Learner is given some sequence of training examples $((x_1, d_1) \ldots (x_m, d_m))$ where x_i is some instance from X and where d_i is the target value of x_i (i.e., $d_i = c(x_i)$).
- The sequence of target values are written as $D = (d_1 \ldots d_m)$.

We can design a straightforward concept learning algorithm to output the maximum a posteriori hypothesis, based on Bayes theorem, as follows:

BRUTE-FORCE MAP LEARNING algorithm:

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

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

In order specify a learning problem for the BRUTE-FORCE MAP LEARNING algorithm we must specify what values are to be used for P(h) and for P(D|h) ?

Let's choose P(h) and for P(D|h) to be consistent with the following assumptions:

- The training data D is noise free (i.e., $d_i = c(x_i)$)
- The target concept c is contained in the hypothesis space H
- Do not have a priori reason to believe that any hypothesis is more probable than any other.

What values should we specify for P(h)?

- Given no prior knowledge that one hypothesis is more likely than another, it is reasonable to assign the same prior probability to every hypothesis h in H.
- Assume the target concept is contained in H and require that these prior probabilities sum to 1.

$$P(h) = \frac{1}{|H|} \text{ for all } h \in H$$

What choice shall we make for P(D|h)?

- P(D|h) is the probability of observing the target values D = (d_1 . . .d_m) for the fixed set of instances (x_1 . . . x_m), given a world in which hypothesis h holds
- Since we assume noise-free training data, the probability of observing classification d_i given h is just 1 if $d_i = h(x_i)$ and 0 if $d_i \neq h(x_i)$. Therefore,

$$P(D|h) = \begin{cases} 1 & \text{if } d_i = h(x_i) \text{ for all } d_i \in D \\ 0 & \text{otherwise} \end{cases}$$

Given these choices for P(h) and for P(D|h) we now have a fully-defined problem for the above BRUTE-FORCE MAP LEARNING algorithm.

Recalling Bayes theorem, we have

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

Consider the case where h is inconsistent with the training data D

$$P(h|D) = \frac{0 \cdot P(h)}{P(D)} = 0$$

The posterior probability of a hypothesis inconsistent with D is zero

Consider the case where h is consistent with D

$$P(h|D) = \frac{1 \cdot \frac{1}{|H|}}{P(D)} = \frac{1 \cdot \frac{1}{|H|}}{\frac{|VS_{H,D}|}{|H|}} = \frac{1}{|VS_{H,D}|}$$

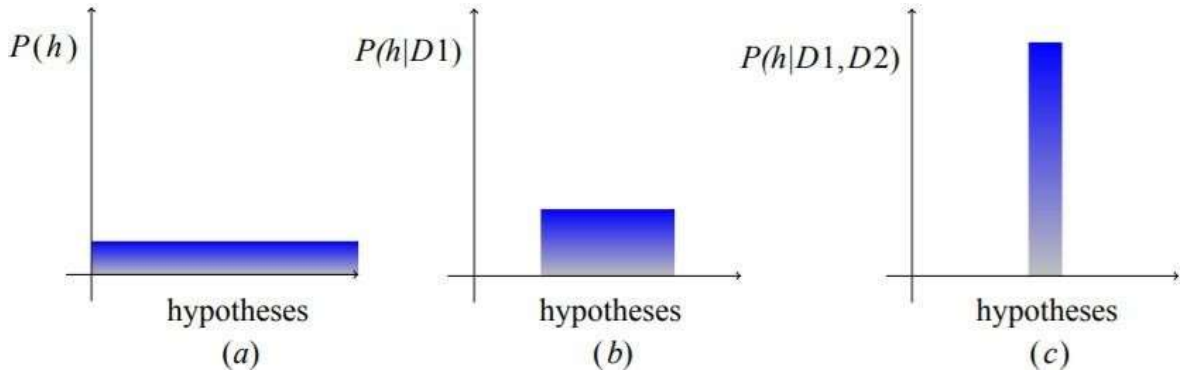
Where, $VS_{H,D}$ is the subset of hypotheses from H that are consistent with D

To summarize, Bayes theorem implies that the posterior probability P(h|D) under our assumed P(h) and P(D|h) is

$$P(D|h) = \begin{cases} \frac{1}{|V S_{H,D}|} & \text{if h is consistent with D} \\ 0 & \text{otherwise} \end{cases}$$

The Evolution of Probabilities Associated with Hypotheses

- Figure (a) all hypotheses have the same probability.
- Figures (b) and (c), As training data accumulates, the posterior probability for inconsistent hypotheses becomes zero while the total probability summing to 1 is shared equally among the remaining consistent hypotheses.



MAP Hypotheses and Consistent Learners

- A learning algorithm is a consistent learner if it outputs a hypothesis that commits zero errors over the training examples.
- Every consistent learner outputs a MAP hypothesis, if we assume a uniform prior probability distribution over H ($P(h_i) = P(h_j)$ for all i, j), and deterministic, noise free training data (P(D|h) =1 if D and h are consistent, and 0 otherwise).

Example:

- FIND-S outputs a consistent hypothesis, it will output a MAP hypothesis under the probability distributions P(h) and P(D|h) defined above.
- Are there other probability distributions for P(h) and P(D|h) under which FIND-S outputs MAP hypotheses? Yes.
- Because FIND-S outputs a maximally specific hypothesis from the version space, its output hypothesis will be a MAP hypothesis relative to any prior probability distribution that favours more specific hypotheses.

Note

- Bayesian framework is a way to characterize the behaviour of learning algorithms
- By identifying probability distributions P(h) and P(D|h) under which the output is a optimal hypothesis, implicit assumptions of the algorithm can be characterized (Inductive Bias)
- Inductive inference is modelled by an equivalent probabilistic reasoning system based on Bayes theorem

MAXIMUM LIKELIHOOD AND LEAST-SQUARED ERROR HYPOTHESES

Consider the problem of learning a *continuous-valued target function* such as neural network learning, linear regression, and polynomial curve fitting

A straightforward Bayesian analysis will show that under certain assumptions any learning algorithm that minimizes the squared error between the output hypothesis predictions and the training data will output a *maximum likelihood (ML) hypothesis*

- Learner L considers an instance space X and a hypothesis space H consisting of some class of real-valued functions defined over X, i.e., ($\forall$ h $\in$ H)[h : X $\rightarrow$ R] and training examples of the form $<x_i,d_i>$
- The problem faced by L is to learn an unknown target function f : X $\rightarrow$ R
- A set of m training examples is provided, where the target value of each example is corrupted by random noise drawn according to a Normal probability distribution with zero mean ($d_i = f(x_i) + e_i$)
- Each training example is a pair of the form (x_i ,d_i) where $d_i = f(x_i) + e_i$.
  - Here $f(x_i)$ is the noise-free value of the target function and e_i is a random variable representing the noise.
  - It is assumed that the values of the e_i are drawn independently and that they are distributed according to a Normal distribution with zero mean.
- The task of the learner is to *output a maximum likelihood hypothesis* or a *MAP hypothesis assuming all hypotheses are equally probable a priori.*

Using the definition of h_{ML} we have

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

Assuming training examples are mutually independent given h, we can write P(D|h) as the product of the various (d_i|h)

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

Given the noise e_i obeys a Normal distribution with zero mean and unknown variance σ^2 , each d_i must also obey a Normal distribution around the true targetvalue $f(x_i)$. Because we are writing the expression for P(D|h), we assume h is the correct description of f.
Hence, $\mu = f(x_i) = h(x_i)$

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

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

Maximize the less complicated logarithm, which is justified because of the monotonicity of function p

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

The first term in this expression is a constant independent of h, and can therefore be discarded, yielding

$$h_{ML} = \underset{h \in H}{argmax} \sum_{i=1}^{m} -\frac{1}{2\sigma^2}(d_i - h(x_i))^2$$

Maximizing this negative quantity is equivalent to minimizing the corresponding positive quantity

$$h_{ML} = \underset{h \in H}{argmin} \sum_{i=1}^{m} \frac{1}{2\sigma^2}(d_i - h(x_i))^2$$

Finally, discard constants that are independent of h.

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

Thus, above equation shows that the maximum likelihood hypothesis h_{ML} is the one that minimizes the sum of the squared errors between the observed training values d_i and the hypothesis predictions $h(x_i)$

Note:

Why is it reasonable to choose the Normal distribution to characterize noise?

- Good approximation of many types of noise in physical systems
- Central Limit Theorem shows that the sum of a sufficiently large number of independent, identically distributed random variables itself obeys a Normal distribution

Only noise in the target value is considered, not in the attributes describing the instances themselves

MAXIMUM LIKELIHOOD HYPOTHESES FOR PREDICTING PROBABILITIES

- Consider the setting in which we wish to learn a nondeterministic (probabilistic) function f : X → {0, 1}, which has two discrete output values.
- We want a function approximator whose output is the probability that f(x) = 1. In other words, learn the target function f ` : X → [0, 1] such that f ` (x) = P(f(x) = 1)

How can we learn f ` using a neural network?

- Use of brute force way would be to first collect the observed frequencies of 1's and 0's for each possible value of x and to then train the neural network to output the target frequency for each x.

What criterion should we optimize in order to find a maximum likelihood hypothesis for f' in this setting?

- First obtain an expression for P(D|h)
- Assume the training data D is of the form D = $\{(x_1, d_1) \ldots (x_m, d_m)\}$, where d_i is the observed 0 or 1 value for f (x_i).
- Both x_i and d_i as random variables, and assuming that each training example is drawn independently, we can write P(D|h) as

$$P(D \mid h) = \prod_{i=1}^{m} P(x_i, d_i \mid h) \qquad \text{equ (1)}$$

Applying the product rule

$$P(D \mid h) = \prod_{i=1}^{m} P(d_i \mid h, x_i) P(x_i) \qquad \text{equ (2)}$$

The probability $P(d_i|h, x_i)$

$$P(d_i|h, x_i) = \begin{cases} h(x_i) & \text{if } d_i = 1 \\ (1 - h(x_i)) & \text{if } d_i = 0 \end{cases} \qquad \text{equ (3)}$$

Re-express it in a more mathematically manipulable form, as

$$P(d_i|h, x_i) = h(x_i)^{d_i} (1 - h(x_i))^{1-d_i} \qquad \text{equ (4)}$$

Equation (4) to substitute for P(di |h, xi) in Equation (5) to obtain

$$P(D|h) = \prod_{i=1}^{m} h(x_i)^{d_i} (1 - h(x_i))^{1-d_i} P(x_i) \qquad \text{equ (5)}$$

We write an expression for the maximum likelihood hypothesis

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

The last term is a constant independent of h, so it can be dropped

$$h_{ML} = \underset{h \in H}{\operatorname{argmax}} \prod_{i=1}^{m} h(x_i)^{d_i} (1 - h(x_i))^{1-d_i} \qquad \text{equ (6)}$$

It easier to work with the log of the likelihood, yielding

$$h_{ML} = \underset{h \in H}{\operatorname{argmax}} \sum_{i=1}^{m} d_i \ln h(x_i) + (1 - d_i) \ln(1 - h(x_i)) \qquad \text{equ (7)}$$

Equation (7) describes the quantity that must be maximized in order to obtain the maximum likelihood hypothesis in our current problem setting

Gradient Search to Maximize Likelihood in a Neural Net

- Derive a weight-training rule for neural network learning that seeks to maximize G(h,D) using gradient ascent
- The gradient of G(h,D) is given by the vector of partial derivatives of G(h,D) with respect to the various network weights that define the hypothesis h represented by the learned network
- In this case, the partial derivative of G(h, D) with respect to weight w_{jk} from input k to unit j is

$$\begin{aligned} \frac{\partial G(h,D)}{\partial w_{jk}} &= \sum_{i=1}^{m} \frac{\partial G(h, D)}{\partial h(x_i)} \frac{\partial h(x_i)}{\partial w_{jk}} \\ &= \sum_{i=1}^{m} \frac{\partial (d_i \ln h(x_i) + (1 - d_i) \ln(1 - h(x_i)))}{\partial h(x_i)} \frac{\partial h(x_i)}{\partial w_{jk}} \\ &= \sum_{i=1}^{m} \frac{d_i - h(x_i)}{h(x_i)(1 - h(x_i))} \frac{\partial h(x_i)}{\partial w_{jk}} \qquad \text{equ (1)} \end{aligned}$$

- Suppose our neural network is constructed from a single layer of sigmoid units. Then,

$$\frac{\partial h(x_i)}{\partial w_{jk}} = \sigma'(x_i) x_{ijk} = h(x_i)(1 - h(x_i)) x_{ijk}$$

where x_{ijk} is the k^{th} input to unit j for the i^{th} training example, and d(x) is the derivative of the sigmoid squashing function.

- Finally, substituting this expression into Equation (1), we obtain a simple expression for the derivatives that constitute the gradient

$$\frac{\partial G(h, D)}{\partial w_{jk}} = \sum_{i=1}^{m} (d_i - h(x_i))\ x_{ijk}$$

Because we seek to maximize rather than minimize P(D|h), we perform gradient ascent rather than gradient descent search. On each iteration of the search the weight vector is adjusted in the direction of the gradient, using the weight update rule

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

Where,

$$\Delta w_{jk} = \eta \sum_{i=1}^{m} (d_i - h(x_i))\ x_{ijk} \qquad \text{equ (2)}$$

Where, η is a small positive constant that determines the step size of the i gradient ascent search

MINIMUM DESCRIPTION LENGTH PRINCIPLE

- A Bayesian perspective on Occam's razor
- Motivated by interpreting the definition of h_{MAP} in the light of basic concepts from information theory.

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

which can be equivalently expressed in terms of maximizing the $\log_2$

$$h_{MAP} = \underset{h \in H}{argmax}\ \log_2 P(D|h) + \log_2 P(h)$$

or alternatively, minimizing the negative of this quantity

$$h_{MAP} = \underset{h \in H}{argmin}\ -\log_2 P(D|h) - \log_2 P(h) \qquad \text{equ (1)}$$

This equation (1) can be interpreted as a statement that short hypotheses are preferred, assuming a particular representation scheme for encoding hypotheses and data

- $-\log_2 P(h)$: the description length of h under the optimal encoding for the hypothesis space H, $L_{CH}(h) = -\log_2 P(h)$, where C_H is the optimal code for hypothesis space H.
- $-\log_2 P(D \mid h)$: the description length of the training data D given hypothesis h, under the optimal encoding from the hypothesis space H: $L_{CH}(D|h) = -\log_2 P(D|\ h)$, where $C_{D|h}$ is the optimal code for describing data D assuming that both the sender and receiver know the hypothesis h.
- Rewrite Equation (1) to show that h_{MAP} is the hypothesis h that minimizes the sum given by the description length of the hypothesis plus the description length of the data given the hypothesis.

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

Where, C_H and $C_{D|h}$ are the optimal encodings for H and for D given h

The Minimum Description Length (MDL) principle recommends choosing the hypothesis that minimizes the sum of these two description lengths of equ.

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

Minimum Description Length principle:

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

Where, codes C_1 and C_2 to represent the hypothesis and the data given the hypothesis

The above analysis shows that if we choose C_1 to be the optimal encoding of hypotheses C_H, and if we choose C_2 to be the optimal encoding $C_{D|h}$, then $h_{MDL} = h_{MAP}$

Application to Decision Tree Learning

Apply the MDL principle to the problem of learning decision trees from some training data.
What should we choose for the representations C1 and C2 of hypotheses and data?

- For C_1: C_1 might be some obvious encoding, in which the description length grows with the number of nodes and with the number of edges
- For C_2: Suppose that the sequence of instances $(x_1 . . . x_m)$ is already known to both the transmitter and receiver, so that we need only transmit the classifications $(f(x_1) . . . f(x_m))$.
- Now if the training classifications $(f(x_1) . . . f(x_m))$ are identical to the predictions of the hypothesis, then there is no need to transmit any information about these examples. The description length of the classifications given the hypothesis ZERO
- If examples are misclassified by h, then for each misclassification we need to transmit a message that identifies which example is misclassified as well as its correct classification
- The hypothesis h_{MDL} under the encoding C_1 and C_2 is just the one that minimizes the sum of these description lengths.

NAIVE BAYES CLASSIFIER

- The naive Bayes classifier applies to learning tasks where each instance x is described by a conjunction of attribute values and where the target function f (x) can take on any value from some finite set V.
- A set of training examples of the target function is provided, and a new instance is presented, described by the tuple of attribute values (a_1, a_2.. .a_m).
- The learner is asked to predict the target value, or classification, for this new instance.

The Bayesian approach to classifying the new instance is to assign the most probable target value, V_{MAP}, given the attribute values (a_1, a_2.. .a_m) that describe the instance

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

Use Bayes theorem to rewrite this expression as

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

$$= \underset{v_j \in V}{\operatorname{argmax}} P(a_1, a_2 \ldots a_n | v_j) P(v_j) \qquad \textbf{equ (1)}$$

- The naive Bayes classifier is based on the assumption that the attribute values are conditionally independent given the target value. Means, the assumption is that given the target value of the instance, the probability of observing the conjunction (a_1, a_2.. .a_m), is just the product of the probabilities for the individual attributes:

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

Substituting this into Equation (1),

Naive Bayes classifier:

$$\mathbf{V_{NB} = \underset{v_j \in V}{\operatorname{argmax}} P(v_j) \prod_i P(a_i | v_j)} \qquad \text{equ (2)}$$

Where, V_{NB} denotes the target value output by the naive Bayes classifier

An Illustrative Example

- Let us apply the naive Bayes classifier to a concept learning problem i.e., classifying days according to whether someone will play tennis.
- The below table provides a set of 14 training examples of the target concept ***PlayTennis***, where each day is described by the attributes Outlook, Temperature, Humidity, and Wind

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

- Use the naive Bayes classifier and the training data from this table to classify the following novel instance:

  < Outlook = sunny, Temperature = cool, Humidity = high, Wind = strong >

- Our task is to predict the target value ***(yes or no)*** of the target concept ***PlayTennis*** for this new instance

$$V_{NB} = \underset{v_j \in \{yes, no\}}{\operatorname{argmax}} P(v_j) \prod_i P(a_i | v_j)$$

$$V_{NB} = \underset{v_j \in \{yes, no\}}{\operatorname{argmax}} P(v_j)\, P(\text{Outlook=sunny}|v_j)\, P(\text{Temperature=cool}|v_j)\, P(\text{Humidity=high}|v_j)\, P(\text{Wind=strong}|v_j)$$

The probabilities of the different target values can easily be estimated based on their frequencies over the 14 training examples

- P(P1ayTennis = yes) = 9/14 = 0.64
- P(P1ayTennis = no) = 5/14 = 0.36

Similarly, estimate the conditional probabilities. For example, those for Wind = strong

- P(Wind = strong | PlayTennis = yes) = 3/9 = 0.33
- P(Wind = strong | PlayTennis = no) = 3/5 = 0.60

Calculate V_{NB} according to Equation (1)

$$P(yes)\ P(sunny|yes)\ P(cool|yes)\ P(high|yes)\ P(strong|yes) = .0053$$
$$P(no)\ P(sunny|no)\ P(cool|no)\ P(high|no)\ P(strong|no) = .0206$$

Thus, the naive Bayes classifier assigns the target value ***PlayTennis* = *no*** to this new instance, based on the probability estimates learned from the training data.

By normalizing the above quantities to sum to one, calculate the conditional probability that the target value is ***no***, given the observed attribute values

$$\frac{.0206}{(.0206 + .0053)} = .795$$

Estimating Probabilities

- We have estimated probabilities by the fraction of times the event is observed to occur over the total number of opportunities.
- For example, in the above case we estimated P(Wind = strong | Play Tennis = no) by the fraction n_c/n where, n = 5 is the total number of training examples for which PlayTennis = no, and $n_c = 3$ is the number of these for which Wind = strong.
- When $n_c = 0$, then n_c/n will be zero and this probability term will dominate the quantity calculated in Equation (2) requires multiplying all the other probability terms by this zero value
- To avoid this difficulty we can adopt a Bayesian approach to estimating the probability, using the ***m-estimate*** defined as follows

***m* -estimate of probability:**

$$\frac{n_c + mp}{n + m}$$

- p is our prior estimate of the probability we wish to determine, and m is a constant called the equivalent sample size, which determines how heavily to weight p relative to the observed data
- Method for choosing p in the absence of other information is to assume uniform priors; that is, if an attribute has k possible values we set p = 1 /k.

BAYESIAN BELIEF NETWORKS

- The naive Bayes classifier makes significant use of the assumption that the values of the attributes $a_1 \ldots a_n$ are conditionally independent given the target value v.
- This assumption dramatically reduces the complexity of learning the target function

A Bayesian belief network describes the probability distribution governing a set of variables by specifying a set of conditional independence assumptions along with a set of conditional probabilities
Bayesian belief networks allow stating conditional independence assumptions that apply to subsets of the variables

Notation

- Consider an arbitrary set of random variables $Y_1 \ldots Y_n$, where each variable Yi can take on the set of possible values $V(Y_i)$.
- The joint space of the set of variables Y to be the cross product $V(Y_1)$ x $V(Y_2)$ x. . . $V(Y_n)$.
- In other words, each item in the joint space corresponds to one of the possible assignments of values to the tuple of variables $(Y_1 \ldots Y_n)$. The probability distribution over this joint' space is called the joint probability distribution.
- The joint probability distribution specifies the probability for each of the possible variable bindings for the tuple $(Y_1 \ldots Y_n)$.
- A Bayesian belief network describes the joint probability distribution for a set of variables.

Conditional Independence

Let X, Y, and Z be three discrete-valued random variables. X is conditionally independent of Y given Z if the probability distribution governing X is independent of the value of Y given a value for Z, that is, if

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

Where,

$$x_i \in V(X),\ y_j \in V(Y),\ \text{and}\ z_k \in V(Z).$$

The above expression is written in abbreviated form as

$$P(X \mid Y, Z) = P(X \mid Z)$$

Conditional independence can be extended to sets of variables. The set of variables $X_1 \ldots X_l$ is conditionally independent of the set of variables $Y_1 \ldots Y_m$ given the set of variables $Z_1 \ldots Z_n$ if

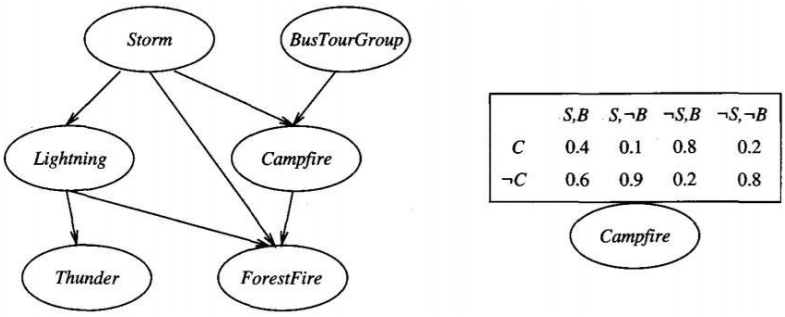
$$P(X_1 \ldots X_l | Y_1 \ldots Y_m, Z_1 \ldots Z_n) = P(X_1 \ldots X_l | Z_1 \ldots Z_n)$$

The naive Bayes classifier assumes that the instance attribute A_1 is conditionally independent of instance attribute A_2 given the target value V. This allows the naive Bayes classifier to calculate $P(A_l, A_2 \mid V)$ as follows,

$$\begin{aligned} P(A_1, A_2|V) &= P(A_1|A_2, V)P(A_2|V) \\ &= P(A_1|V)P(A_2|V) \end{aligned}$$

Representation

A Bayesian belief network represents the joint probability distribution for a set of variables. Bayesian networks (BN) are represented by directed acyclic graphs.



The Bayesian network in above figure represents the joint probability distribution over the boolean variables *Storm, Lightning, Thunder, ForestFire, Campfire,* and *BusTourGroup*

A Bayesian network (BN) represents the joint probability distribution by specifying a set of *conditional independence assumptions*

- BN represented by a directed acyclic graph, together with sets of local conditional probabilities
- Each variable in the joint space is represented by a node in the Bayesian network
- The network arcs represent the assertion that the variable is conditionally independent of its non-descendants in the network given its immediate predecessors in the network.
- A ***conditional probability table*** **(CPT)** is given for each variable, describing the probability distribution for that variable given the values of its immediate predecessors

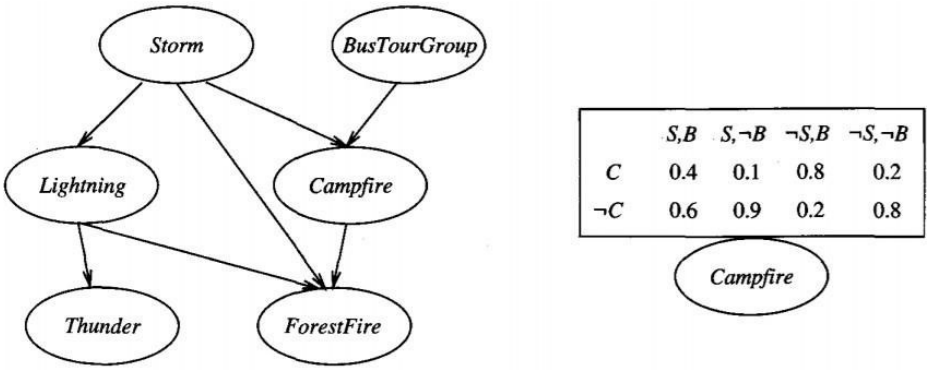
The joint probability for any desired assignment of values ($y_1, \ldots, y_n$) to the tuple of network variables ($Y_1 \ldots Y_m$) can be computed by the formula

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

Where, Parents(Y_i) denotes the set of immediate predecessors of Y_i in the network.

Example:

Consider the node ***Campfire***. The network nodes and arcs represent the assertion that ***Campfire*** is conditionally independent of its non-descendants ***Lightning*** and ***Thunder***, given its immediate parents Storm and ***BusTourGroup***.



This means that once we know the value of the variables ***Storm*** and ***BusTourGroup***, the variables ***Lightning*** and ***Thunder*** provide no additional information about ***Campfire***

The conditional probability table associated with the variable ***Campfire.*** The assertion is

P(Campfire = True | Storm = True, BusTourGroup = True) = 0.4

Inference

- Use a Bayesian network to infer the value of some target variable (e.g., ForestFire) given the observed values of the other variables.
- Inference can be straightforward if values for all of the other variables in the network are known exactly.
- A Bayesian network can be used to compute the probability distribution for any subset of network variables given the values or distributions for any subset of the remaining variables.
- An arbitrary Bayesian network is known to be NP-hard

Learning Bayesian Belief Networks

Affective algorithms can be considered for learning Bayesian belief networks from training data by considering several different settings for learning problem

- First, the network structure might be given in advance, or it might have to be inferred from the training data.
- Second, all the network variables might be directly observable in each training example, or some might be unobservable.
  - In the case where the network structure is given in advance and the variables are fully observable in the training examples, learning the conditional probability tables is straightforward and estimate the conditional probability table entries
  - In the case where the network structure is given but only some of the variable values are observable in the training data, the learning problem is more difficult. The learning problem can be compared to learning weights for an ANN.

Gradient Ascent Training of Bayesian Network

The gradient ascent rule which maximizes P(D|h) by following the gradient of ***ln P(D|h)*** with respect to the parameters that define the conditional probability tables of the Bayesian network.

Let w_{ijk} denote a single entry in one of the conditional probability tables. In particular w_{ijk} denote the conditional probability that the network variable Y_i will take on the value y_i, given that its immediate parents U_i take on the values given by u_{ik}.

The gradient of ***ln P(D|h)*** is given by the derivatives $\frac{\partial \ln P(D|h)}{\partial w_{ijk}}$ for each of the w_{ijk}.
As shown below, each of these derivatives can be calculated as

$$\frac{\partial \ln P(D|h)}{\partial w_{ij}} = \sum_{d \in D} \frac{P(Y_i = y_{ij}, U_i = u_{ik}|d)}{w_{ijk}} \qquad \textbf{equ(1)}$$

Derive the gradient defined by the set of derivatives $\frac{\partial P_h(D)}{\partial w_{ijk}}$ for all ***i, j,*** and ***k***. Assuming the training examples ***d*** in the data set D are drawn independently, we write this derivative as

$$\frac{\partial \ln P_h(D)}{\partial w_{ijk}} = \frac{\partial}{\partial w_{ijk}} \ln \prod_{d \in D} P_h(d)$$

$$= \sum_{d \in D} \frac{\partial \ln P_h(d)}{\partial w_{ijk}}$$

$$= \sum_{d \in D} \frac{1}{P_h(d)} \frac{\partial P_h(d)}{\partial w_{ijk}}$$

We write the abbreviation $P_h(D)$ to represent $P(D|h)$.

This last step makes use of the general equality $\frac{\partial \ln f(x)}{\partial x} = \frac{1}{f(x)} \frac{\partial f(x)}{\partial x}$. We can now introduce the values of the variables Y_i and $U_i = Parents(Y_i)$, by summing over their possible values $y_{ij'}$ and $u_{ik'}$.

$$\frac{\partial \ln P_h(D)}{\partial w_{ijk}} = \sum_{d \in D} \frac{1}{P_h(d)} \frac{\partial}{\partial w_{ijk}} \sum_{j',k'} P_h(d|y_{ij'}, u_{ik'}) P_h(y_{ij'}, u_{ik'})$$

$$= \sum_{d \in D} \frac{1}{P_h(d)} \frac{\partial}{\partial w_{ijk}} \sum_{j',k'} P_h(d|y_{ij'}, u_{ik'}) P_h(y_{ij'}|u_{ik'}) P_h(u_{ik'})$$

This last step follows from the product rule of probability . Now consider the rightmost sum in the final expression above. Given that $w_{ijk} \equiv P_h(y_{ij}|u_{ik})$, the only term in this sum for which $\frac{\partial}{\partial w_{ijk}}$ is nonzero is the term for which $j' = j$ and $i' = i$. Therefore

$$\frac{\partial \ln P_h(D)}{\partial w_{ijk}} = \sum_{d \in D} \frac{1}{P_h(d)} \frac{\partial}{\partial w_{ijk}} P_h(d|y_{ij}, u_{ik}) P_h(y_{ij}|u_{ik}) P_h(u_{ik})$$

$$= \sum_{d \in D} \frac{1}{P_h(d)} \frac{\partial}{\partial w_{ijk}} P_h(d|y_{ij}, u_{ik}) w_{ijk} P_h(u_{ik})$$

$$= \sum_{d \in D} \frac{1}{P_h(d)} P_h(d|y_{ij}, u_{ik}) P_h(u_{ik})$$

Applying Bayes theorem to rewrite $P_h(d|y_{ij}, u_{ik})$, we have

$$\frac{\partial \ln P_h(D)}{\partial w_{ijk}} = \sum_{d \in D} \frac{1}{P_h(d)} \frac{P_h(y_{ij}, u_{ik}|d) P_h(d) P_h(u_{ik})}{P_h(y_{ij}, u_{ik})}$$

$$= \sum_{d \in D} \frac{P_h(y_{ij}, u_{ik}|d) P_h(u_{ik})}{P_h(y_{ij}, u_{ik})}$$

$$= \sum_{d \in D} \frac{P_h(y_{ij}, u_{ik}|d)}{P_h(y_{ij}|u_{ik})}$$

$$= \sum_{d \in D} \frac{P_h(y_{ij}, u_{ik}|d)}{w_{ijk}} \qquad \text{equ (2)}$$

Thus, we have derived the gradient given in Equation (1). There is one more item that must be considered before we can state the gradient ascent training procedure. In particular, we require that as the weights w_{ijk} are updated they must remain valid probabilities in the interval [0,1]. We also require that the sum $\sum_j w_{ijk}$ remains 1 for all i, k. These constraints can be satisfied by updating weights in a two-step process. First we update each w_{ijk} by gradient ascent

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

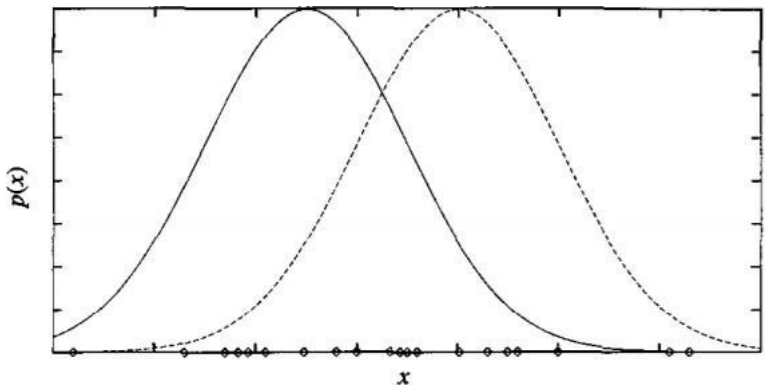
where η is a small constant called the learning rate. Second, we renormalize the weights w_{ijk} to assure that the above constraints are satisfied.
this process will converge to a locally maximum likelihood hypothesis for the conditional probabilities in the Bayesian network.

THE EM ALGORITHM

The EM algorithm can be used even for variables whose value is never directly observed, provided the general form of the probability distribution governing these variables is known.

Estimating Means of k Gaussians

- Consider a problem in which the data D is a set of instances generated by a probability distribution that is a mixture of k distinct Normal distributions.



- This problem setting is illustrated in Figure for the case where k = 2 and where the instances are the points shown along the x axis.
- Each instance is generated using a two-step process.
  - First, one of the k Normal distributions is selected at random.
  - Second, a single random instance x_i is generated according to this selected distribution.
- This process is repeated to generate a set of data points as shown in the figure.

- To simplify, consider the special case
  - The selection of the single Normal distribution at each step is based on choosing each with uniform probability
  - Each of the k Normal distributions has the same variance σ^2, known value.
- The learning task is to output a hypothesis h = (μ_1 , . . . ,μ_k) that describes the means of each of the k distributions.
- We would like to find a maximum likelihood hypothesis for these means; that is, a hypothesis ***h*** that maximizes p(D |h).

$$\mu_{ML} = \underset{\mu}{\operatorname{argmin}} \sum_{i=1}^{m} (x_i - \mu)^2 \qquad (1)$$

In this case, the sum of squared errors is minimized by the sample mean

$$\mu_{ML} = \frac{1}{m} \sum_{i=1}^{m} x_i \qquad (2)$$

- Our problem here, however, involves a mixture of k different Normal distributions, and we cannot observe which instances were generated by which distribution.
- Consider full description of each instance as the triple (x_i, z_{i1}, z_{i2}),
  - where x_i is the observed value of the ith instance and
  - where z_{i1} and z_{i2} indicate which of the two Normal distributions was used to generate the value x_i
- In particular, z_{ij} has the value 1 if x_i was created by the j^{th} Normal distribution and 0 otherwise.
- Here x_i is the observed variable in the description of the instance, and z_{il} and z_{i2} are hidden variables.
- If the values of z_{il} and z_{i2} were observed, we could use following Equation to solve for the means p_1 and p_2
- Because they are not, we will instead use the EM algorithm

EM algorithm

Step 1: 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.

Step 2: 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 in Step 1. Then replace the hypothesis $h = \langle \mu_1, \mu_2 \rangle$ by the new hypothesis $h' = \langle \mu'_1, \mu'_2 \rangle$ and iterate.

Let us examine how both of these steps can be implemented in practice. Step 1 must calculate the expected value of each z_{ij}. This $E[z_{ij}]$ is just the probability that instance x_i was generated by the jth Normal distribution

$$E[z_{ij}] = \frac{p(x = x_i|\mu = \mu_j)}{\sum_{n=1}^{2} p(x = x_i|\mu = \mu_n)}$$

$$= \frac{e^{-\frac{1}{2\sigma^2}(x_i-\mu_j)^2}}{\sum_{n=1}^{2} e^{-\frac{1}{2\sigma^2}(x_i-\mu_n)^2}}$$

Thus the first step is implemented by substituting the current values $\langle \mu_1, \mu_2 \rangle$ and the observed x_i into the above expression.

In the second step we use the $E[z_{ij}]$ calculated during Step 1 to derive a new maximum likelihood hypothesis $h' = \langle \mu'_1, \mu'_2 \rangle$.
maximum likelihood hypothesis in this case is given by

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

INSTANCE BASED LEARNING

INTRODUCTION

- Instance-based learning methods such as nearest neighbor and locally weighted regression are conceptually straightforward approaches to approximating real-valued or discrete-valued target functions.
- Learning in these algorithms consists of simply storing the presented training data. When a new query instance is encountered, a set of similar related instances is retrieved from memory and used to classify the new query instance
- Instance-based approaches can construct a different approximation to the target function for each distinct query instance that must be classified

Advantages of Instance-based learning

1. Training is very fast
2. Learn complex target function
3. Don't lose information

Disadvantages of Instance-based learning

- The cost of classifying new instances can be high. This is due to the fact that nearly all computation takes place at classification time rather than when the training examples are first encountered.

- In many instance-based approaches, especially nearest-neighbor approaches, is that they typically consider all attributes of the instances when attempting to retrieve similar training examples from memory. If the target concept depends on only a few of the many available attributes, then the instances that are truly most "similar" may well be alarge distance apart.

k- NEAREST NEIGHBOR LEARNING

- The most basic instance-based method is the K- Nearest Neighbor Learning. This algorithm assumes all instances correspond to points in the n-dimensional space R^n.
- The nearest neighbors of an instance are defined in terms of the standard Euclidean distance.
- Let an arbitrary instance x be described by the feature vector

  $$((a_1(x), a_2(x), \ldots\ldots\ldots, a_n(x))$$

  Where, $a_r(x)$ denotes the value of the r^{th} attribute of instance x.

- Then the distance between two instances x_i and x_j is defined to be $d(x_i , x_j)$
  Where,

$$d(x_i, x_j) \equiv \sqrt{\sum_{r=1}^{n} (a_r(x_i) - a_r(x_j))^2}$$

- In nearest-neighbor learning the target function may be either discrete-valued or real-valued.

Let us first consider learning ***discrete-valued target functions*** of the form

$$f : \Re^n \rightarrow V.$$

Where, V is the finite set $\{v_1, \ldots v_s\}$

The k- Nearest Neighbor algorithm for approximation a **discrete-valued target function** is given below:

Training algorithm:

- For each training example $\langle x, f(x) \rangle$, add the example to the list *training_examples*

Classification algorithm:

- Given a query instance x_q to be classified,
  - Let $x_1 \ldots x_k$ denote the k instances from *training_examples* that are nearest to x_q
  - Return

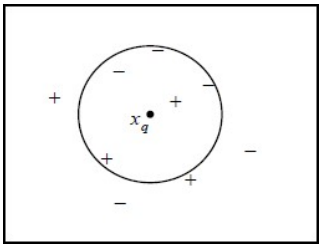
$$\hat{f}(x_q) \leftarrow \underset{v \in V}{\operatorname{argmax}} \sum_{i=1}^{k} \delta(v, f(x_i))$$

where $\delta(a, b) = 1$ if $a = b$ and where $\delta(a, b) = 0$ otherwise.

The value $\hat{f}(x_q)$ returned by this algorithm as its estimate of $f(x_q)$ is just the most common value of f among the k training examples nearest to x_q.

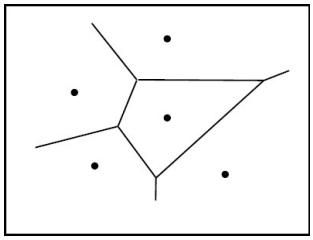
- If k = 1, then the 1- Nearest Neighbor algorithm assigns to $\hat{f}(x_q)$ the value f(xi). Where x_i is the training instance nearest to x_q.
- For larger values of k, the algorithm assigns the most common value among the k nearest training examples.

- Below figure illustrates the operation of the k-Nearest Neighbor algorithm for the case where the instances are points in a two-dimensional space and where the target function is Boolean valued.



- The positive and negative training examples are shown by "+" and "-" respectively. A query point x_q is shown as well.
- The 1-Nearest Neighbor algorithm classifies x_q as a positive example in this figure, whereas the 5-Nearest Neighbor algorithm classifies it as a negative example.

- Below figure shows the shape of this **decision surface** induced by 1- Nearest Neighbor over the entire instance space. The decision surface is a combination of convex polyhedra surrounding each of the training examples.



- For every training example, the polyhedron indicates the set of query points whose classification will be completely determined by that training example. Query points outside the polyhedron are closer to some other training example. This kind of diagram is often called the ***Voronoi diagram*** of the set of training example

The K- Nearest Neighbor algorithm for approximation a **real-valued target function** is given below $f : \Re^n \rightarrow \Re$

Training algorithm:

- For each training example $\langle x, f(x) \rangle$, add the example to the list *training_examples*

Classification algorithm:

- Given a query instance x_q to be classified,
  - Let $x_1 \ldots x_k$ denote the k instances from *training_examples* that are nearest to x_q
  - Return

$$\hat{f}(x_q) \leftarrow \frac{\sum_{i=1}^{k} f(x_i)}{k}$$

Distance-Weighted Nearest Neighbor Algorithm

- The refinement to the k-NEAREST NEIGHBOR Algorithm is to weight the contribution of each of the k neighbors according to their distance to the query point x_q, giving greater weight to closer neighbors.
- For example, in the k-Nearest Neighbor algorithm, which approximates discrete-valued target functions, we might weight the vote of each neighbor according to the inverse square of its distance from x_q

Distance-Weighted Nearest Neighbor Algorithm for approximation a discrete-valued target functions

Training algorithm:

- For each training example $\langle x, f(x) \rangle$, add the example to the list *training_examples*

Classification algorithm:

- Given a query instance x_q to be classified,
  - Let $x_1 \ldots x_k$ denote the k instances from *training_examples* that are nearest to x_q
  - Return

$$\hat{f}(x_q) \leftarrow \underset{v \in V}{\operatorname{argmax}} \sum_{i=1}^{k} w_i \delta(v, f(x_i))$$

where

$$w_i \equiv \frac{1}{d(x_q, x_i)^2}$$

Distance-Weighted Nearest Neighbor Algorithm for approximation a Real-valued target functions

Training algorithm:

- For each training example $\langle x, f(x) \rangle$, add the example to the list *training_examples*

Classification algorithm:

- Given a query instance x_q to be classified,
  - Let $x_1 \ldots x_k$ denote the k instances from *training_examples* that are nearest to x_q
  - Return

$$\hat{f}(x_q) \leftarrow \frac{\sum_{i=1}^{k} w_i f(x_i)}{\sum_{i=1}^{k} w_i}$$

where

$$w_i \equiv \frac{1}{d(x_q, x_i)^2}$$

Terminology

- **Regression** means approximating a real-valued target function.
- **Residual** is the error $f(x) - \hat{f}(x)$ in approximating the target function.
- **Kernel function** is the function of distance that is used to determine the weight of each training example. In other words, the kernel function is the function K such that $w_i = K(d(x_i, x_q))$

LOCALLY WEIGHTED REGRESSION

- The phrase "**locally weighted regression**" is called **local** because the function is approximated based only on data near the query point, **weighted** because the contribution of each training example is weighted by its distance from the query point, and **regression** because this is the term used widely in the statistical learning community for the problem of approximating real-valued functions.

- Given a new query instance x_q, the general approach in locally weighted regression is to construct an approximation $\hat{f}$ that fits the training examples in the neighborhood surrounding x_q. This approximation is then used to calculate the value $\hat{f}(x_q)$, which is output as the estimated target value for the query instance.

Locally Weighted Linear Regression

- Consider locally weighted regression in which the target function ***f*** is approximated near x_q using a linear function of the form

$$\hat{f}(x) = w_0 + w_1 a_1(x) + \cdots + w_n a_n(x)$$

Where, $a_i(x)$ denotes the value of the i^{th} attribute of the instance x

- Derived methods are used to choose weights that minimize the squared error summed over the set D of training examples using gradient descent

$$E \equiv \frac{1}{2} \sum_{x \in D} (f(x) - \hat{f}(x))^2$$

Which led us to the gradient descent training rule

$$\Delta w_j = \eta \sum_{x \in D} (f(x) - \hat{f}(x)) a_j(x)$$

Where, η is a constant learning rate

- Need to modify this procedure to derive a local approximation rather than a global one. The simple way is to redefine the error criterion E to emphasize fitting the local training examples. Three possible criteria are given below.

1. Minimize the squared error over just the k nearest neighbors:

$$E_1(x_q) \equiv \frac{1}{2} \sum_{x \in k \text{ nearest nbrs of } x_q} (f(x) - \hat{f}(x))^2 \qquad \textbf{equ(1)}$$

2. Minimize the squared error over the entire set D of training examples, while weighting the error of each training example by some decreasing function K of its distance from x_q :

$$E_2(x_q) \equiv \frac{1}{2} \sum_{x \in D} (f(x) - \hat{f}(x))^2 \; K(d(x_q, x)) \qquad \textbf{equ(2)}$$

3. Combine 1 and 2:

$$E_3(x_q) \equiv \frac{1}{2} \sum_{x \in k \text{ nearest nbrs of } x_q} (f(x) - \hat{f}(x))^2 \; K(d(x_q, x)) \qquad \textbf{equ(3)}$$

If we choose criterion three and re-derive the gradient descent rule, we obtain the following training rule

$$\Delta w_j = \eta \sum_{x \in k \text{ nearest nbrs of } x_q} K(d(x_q, x))\ (f(x) - \hat{f}(x))\ a_j(x)$$

The differences between this new rule and the rule given by Equation (3) are that the contribution of instance x to the weight update is now multiplied by the distance penalty **$K(d(x_q, x))$,** and that the error is summed over only the k nearest training examples.

RADIAL BASIS FUNCTIONS

- One approach to function approximation that is closely related to distance-weighted regression and also to artificial neural networks is learning with radial basis functions
- In this approach, the learned hypothesis is a function of the form

$$\hat{f}(x) = w_0 + \sum_{u=1}^{k} w_u K_u(d(x_u, x)) \qquad \textbf{equ (1)}$$

- Where, each x_u is an instance from X and where the kernel function $K_u(d(x_u, x))$ is defined so that it decreases as the distance d(xu, x) increases.
- Here k is a user provided constant that specifies the number of kernel functions to be included.
- *f* is a global approximation to f (x), the contribution from each of the $K_u(d(x_u, x))$ terms is localized to a region nearby the point x_u.

Choose each function $K_u(d(x_u, x))$ to be a Gaussian function centred at the point x_u with some variance σ_u^2

$$K_u(d(x_u, x)) = e^{\frac{1}{2\sigma_u^2} d^2(x_u, x)}$$

- The functional form of equ(1) can approximate any function with arbitrarily small error, provided a sufficiently large number k of such Gaussian kernels and provided the width σ^2 of each kernel can be separately specified
- The function given by equ(1) can be viewed as describing a two layer network where the first layer of units computes the values of the various $K_u(d(x_u, x))$ and where the second layer computes a linear combination of these first-layer unit values

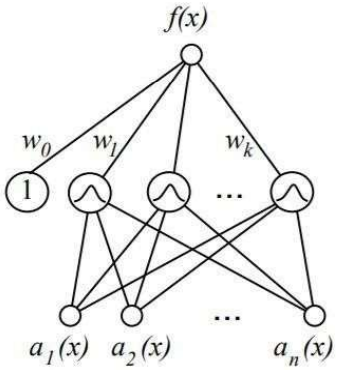
Example: Radial basis function (RBF) network

Given a set of training examples of the target function, RBF networks are typically trained in a two-stage process.

1. First, the number k of hidden units is determined and each hidden unit u is defined by choosing the values of x_u and σ_u^2 that define its kernel function $K_u(d(x_u, x))$
2. Second, the weights w, are trained to maximize the fit of the network to the training data, using the global error criterion given by

$$E \equiv \frac{1}{2}\sum_{x \in D}(f(x) - \hat{f}(x))^2$$

Because the kernel functions are held fixed during this second stage, the linear weight values w, can be trained very efficiently



Several alternative methods have been proposed for choosing an appropriate number of hidden units or, equivalently, kernel functions.

- One approach is to allocate a Gaussian kernel function for each training example $(x_i, f(x_i))$, centring this Gaussian at the point x_i.
  Each of these kernels may be assigned the same width σ^2. Given this approach, the RBF network learns a global approximation to the target function in which each training example $(x_i, f(x_i))$ can influence the value of $\hat{f}$ only in the neighbourhood of x_i.
- A second approach is to choose a set of kernel functions that is smaller than the number of training examples. This approach can be much more efficient than the first approach, especially when the number of training examples is large.

Summary

- Radial basis function networks provide a global approximation to the target function, represented by a linear combination of many local kernel functions.
- The value for any given kernel function is non-negligible only when the input x falls into the region defined by its particular centre and width. Thus, the network can be viewed as a smooth linear combination of many local approximations to the target function.
- One key advantage to RBF networks is that they can be trained much more efficiently than feedforward networks trained with BACKPROPAGATION.

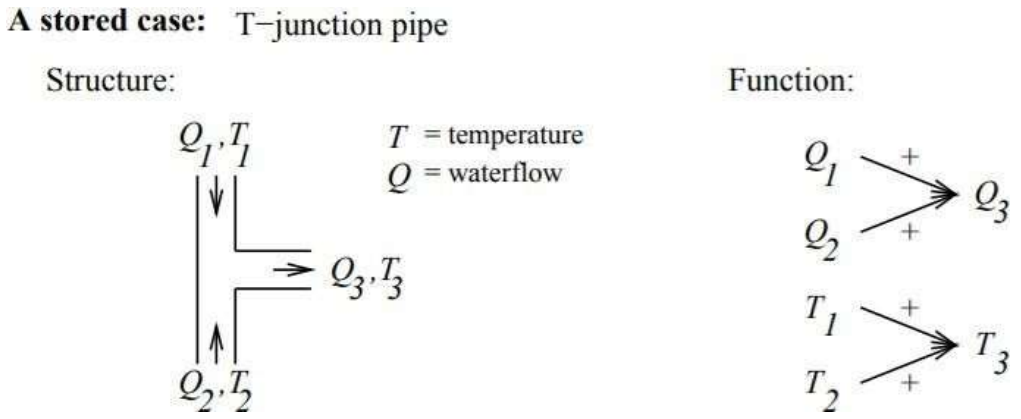
CASE-BASED REASONING

- Case-based reasoning (CBR) is a learning paradigm based on lazy learning methods and they classify new query instances by analysing similar instances while ignoring instances that are very different from the query.
- In CBR represent instances are not represented as real-valued points, but instead, they use a ***rich symbolic*** representation.
- CBR has been applied to problems such as conceptual design of mechanical devices based on a stored library of previous designs, reasoning about new legal cases based on previous rulings, and solving planning and scheduling problems by reusing and combining portions of previous solutions to similar problems

A prototypical example of a case-based reasoning

- The CADET system employs case-based reasoning to assist in the conceptual design of simple mechanical devices such as water faucets.
- It uses a library containing approximately 75 previous designs and design fragments to suggest conceptual designs to meet the specifications of new design problems.
- Each instance stored in memory (e.g., a water pipe) is represented by describing both its structure and its qualitative function.
- New design problems are then presented by specifying the desired function and requesting the corresponding structure.

The problem setting is illustrated in below figure



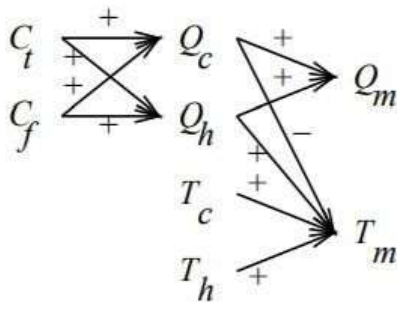
- The function is represented in terms of the qualitative relationships among the water- flow levels and temperatures at its inputs and outputs.
- In the functional description, an arrow with a "+" label indicates that the variable at the arrowhead increases with the variable at its tail. A "-" label indicates that the variable atthe head decreases with the variable at the tail.
- Here Q_c refers to the flow of cold water into the faucet, Q_h to the input flow of hot water,and Q_m to the single mixed flow out of the faucet.
- T_c, T_h, and T_m refer to the temperatures of the cold water, hot water, and mixed water respectively.
- The variable C_t denotes the control signal for temperature that is input to the faucet, andC_f denotes the control signal for waterflow.
- The controls C_t and C_f are to influence the water flows Q_c and Q_h, thereby indirectly influencing the faucet output flow Q_m and temperature T_m.

A problem specification: Water faucet

Structure:

?

Function:



- CADET searches its library for stored cases whose functional descriptions match the design problem. If an exact match is found, indicating that some stored case implementsexactly the desired function, then this case can be returned as a suggested solution to thedesign problem. If no exact match occurs, CADET may find cases that match various subgraphs of the desired functional specification.