

Non-Bayesian Composite Classifiers

K-NN, SVM, ANN and DT

An Introduction

Dr Muhammad Sarim

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- 2 Nearest Neighbor Classifier
 - k -Nearest Neighbor Classifier
 - Distance Functions
 - Feature Normalization
- 3 Linear Discriminant Functions
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- We have discussed parametric and non-parametric methods that learn classifiers by estimating the probabilities using training data.
- We will study new techniques that use training data to learn the classifiers directly without estimating any probabilistic structure.
- In particular, we will study the k -nearest neighbor classifier, linear discriminant functions and support vector machines, neural networks, and decision trees.

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The Nearest Neighbor Classifier

- Given the training data $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ as a set of n labeled examples, the *nearest neighbor classifier* assigns a test point \mathbf{x} the label associated with its closest neighbor in \mathcal{D} .

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- Closeness is defined using a distance function.
- Given the distance function, the nearest neighbor classifier partitions the feature space into cells consisting of all points closer to a given training point than to any other training points.

The Nearest Neighbor Classifier

- All points in such a cell are labeled by the class of the training point, forming a *Voronoi tessellation* of the space.

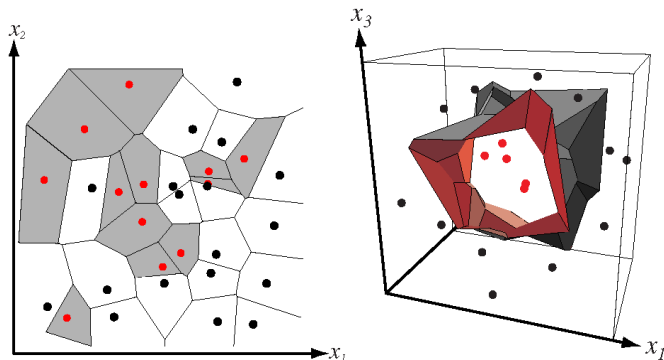


Figure: In two dimensions, the nearest neighbor algorithm leads to a partitioning of the input space into Voronoi cells, each labeled by the class of the training point it contains. In three dimensions, the cells are three-dimensional, and the decision boundary resembles the surface of a crystal.

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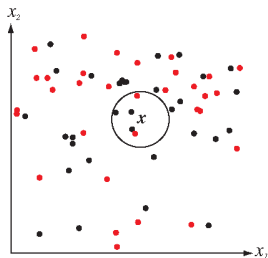


Figure: The k -nearest neighbor query forms a spherical region around the test point \mathbf{x} until it encloses k training samples, and it labels the test point by a majority vote of these samples. In the case for $k = 5$, the test point will be labeled as black.

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- The computational complexity of the nearest neighbor algorithm — both in space (storage) and time (search) — has received a great deal of analysis.
- In the most straightforward approach, we inspect each stored point one by one, calculate its distance to \mathbf{x} , and keep a list of the k closest ones.
- There are some parallel implementations and algorithmic techniques for reducing the computational load in nearest neighbor searches.

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 - computing partial distances using a subset of dimensions, and eliminating the points with partial distances greater than the full distance of the current closest points,
 - using search trees that are hierarchically structured so that only a subset of the training points are considered during search,
 - editing the training set by eliminating the points that are surrounded by other training points with the same class label.

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 - Triangle inequality: $D(\mathbf{x}, \mathbf{y}) + D(\mathbf{y}, \mathbf{z}) \geq D(\mathbf{x}, \mathbf{z})$
- If the second property is not satisfied, $D(\cdot, \cdot)$ is called a pseudometric.

Distance Functions

- A general class of metrics for d -dimensional patterns is the *Minkowski metric*

$$L_p(\mathbf{x}, \mathbf{y}) = \left(\sum_{i=1}^d |\mathbf{x}_i - \mathbf{y}_i|^p \right)^{1/p}$$

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- The *Manhattan* or *city block distance* is the L_1 norm

$$L_1(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^d |\mathbf{x}_i - \mathbf{y}_i|$$

Distance Functions

- The L_∞ norm is the maximum of the distances along individual coordinate axes

$$L_\infty(\mathbf{x}, \mathbf{y}) = \max_{i=1}^d |\mathbf{x}_i - \mathbf{y}_i|$$

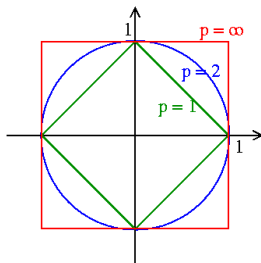


Figure: Each colored shape consists of points at a distance 1.0 from the origin, measured using different values of p in the Minkowski L_p metric.

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- We should be careful about scaling of the coordinate axes when we compute these metrics.
- When there is great difference in the range of the data along different axes in a multidimensional space, these metrics implicitly assign more weighting to features with large ranges than those with small ranges.
- *Feature normalization* can be used to approximately equalize ranges of the features and make them have approximately the same effect in the distance computation.

Feature Normalization

- The following methods can be used to independently normalize each feature.

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- *Linear scaling to unit range:*

Given a lower bound l and an upper bound u for a feature $x \in \mathbb{R}$,

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- *Linear scaling to unit variance:*

A feature $x \in \mathbb{R}$ can be transformed to a random variable with zero mean and unit variance as

$$\tilde{x} = \frac{x - \mu}{\sigma}$$

where μ and σ are the sample mean and the sample standard deviation of that feature, respectively.

Feature Normalization

- *Normalization using the cumulative distribution function:*
Given a random variable $x \in \mathbb{R}$ with cumulative distribution function $F_x(x)$, the random variable \tilde{x} resulting from the transformation $\tilde{x} = F_x(x)$ will be uniformly distributed in the $[0, 1]$ range.

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- *Rank normalization:*

Given the sample for a feature as $x_1, \dots, x_n \in \mathbb{R}$, first we find the order statistics $x^{(1)}, \dots, x^{(n)}$ and then replace each pattern's feature value by its corresponding normalized rank as

$$\tilde{x}_i = \frac{\text{rank}(x_i) - 1}{n - 1}$$

where x_i is the feature value for the i 'th pattern. This procedure uniformly maps all feature values to the $[0, 1]$ range.

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Linear Discriminant Functions

- A classifier that uses *discriminant functions* assigns a feature vector \mathbf{x} to class w_i if

$$g_i(\mathbf{x}) > g_j(\mathbf{x}) \quad \forall j \neq i$$

where $g_i(\mathbf{x})$, $i = 1, \dots, c$, are the discriminant functions for c classes.

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where $g_i(\mathbf{x})$, $i = 1, \dots, c$, are the discriminant functions for c classes.

- A discriminant function that is a linear combination of the components of \mathbf{x} is called a *linear discriminant function* and can be written as

$$g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0$$

where \mathbf{w} is the *weight vector* and w_0 is the *bias* (or threshold weight).

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The Two-Category Case

- For the two-category case, the decision rule can be written as

$$\text{Decide } \begin{cases} w_1 & \text{if } g(\mathbf{x}) > 0 \\ w_2 & \text{otherwise} \end{cases}$$

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- The equation $g(\mathbf{x}) = 0$ defines the decision boundary that separates points assigned to w_1 from points assigned to w_2 .
- When $g(\mathbf{x})$ is linear, the decision surface is a hyperplane whose orientation is determined by the normal vector \mathbf{w} and location is determined by the bias w_0 .

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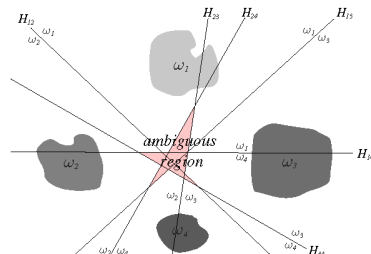
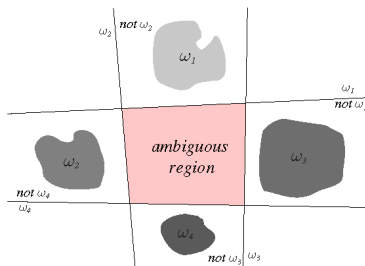
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- For example, we can pose the problem as c two-class problems, where the i 'th problem is solved by a linear discriminant that separates points assigned to w_i from those not assigned to w_i .
- Alternatively, we can use $c(c - 1)/2$ linear discriminants, one for every pair of classes.
- Also, we can use c linear discriminants, one for each class, and assign \mathbf{x} to w_i if $g_i(\mathbf{x}) > g_j(\mathbf{x})$ for all $j \neq i$.

The Multicategory Case

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Boundaries separate w_i from $\neg w_i$. Boundaries separate w_i from w_j .

Linear decision boundaries for a four-class problem devised as four two-class problems (left figure) and six pairwise problems (right figure). The pink regions have ambiguous category assignments.

The Multicategory Case

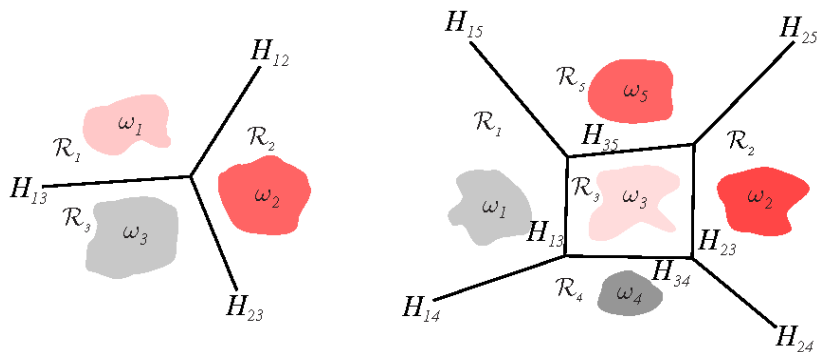


Figure: Linear decision boundaries produced by using one linear discriminant for each class. $\mathbf{w}_i - \mathbf{w}_j$ is the normal vector for the decision boundary that separates the decision region for class ω_i from class ω_j .

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Generalized Linear Discriminant Functions

- The linear discriminant function $g(\mathbf{x})$ can be written as

$$g(\mathbf{x}) = w_0 + \sum_{i=1}^d \mathbf{w}_i \mathbf{x}_i$$

where $\mathbf{w} = (\mathbf{w}_1, \dots, \mathbf{w}_d)^T$.

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- We can obtain the *quadratic discriminant function* by adding second-order terms as

$$g(\mathbf{x}) = w_0 + \sum_{i=1}^d \mathbf{w}_i \mathbf{x}_i + \sum_{i=1}^d \sum_{j=1}^d \mathbf{w}_{ij} \mathbf{x}_i \mathbf{x}_j$$

which result in more complicated decision boundaries (hyperquadrics).

Generalized Linear Discriminant Functions

- Adding higher-order terms gives the *generalized linear discriminant function*

$$g(\mathbf{x}) = \sum_{i=1}^{d'} \mathbf{a}_i y_i(\mathbf{x}) = \mathbf{a}^T \mathbf{y}$$

where \mathbf{a} is a d' -dimensional weight vector and d' functions $y_i(\mathbf{x})$ are arbitrary functions of \mathbf{x} .

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where \mathbf{a} is a d' -dimensional weight vector and d' functions $\mathbf{y}_i(\mathbf{x})$ are arbitrary functions of \mathbf{x} .

- The physical interpretation is that the functions $\mathbf{y}_i(\mathbf{x})$ map point \mathbf{x} in d -dimensional space to point \mathbf{y} in d' -dimensional space.

Generalized Linear Discriminant Functions

- Then, the discriminant $g(\mathbf{x}) = \mathbf{a}^T \mathbf{y}$ separates points in the transformed space using a hyperplane passing through the origin.

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- This mapping to a higher dimensional space brings problems and additional requirements for computation and data.
- However, certain assumptions can make the problem tractable.

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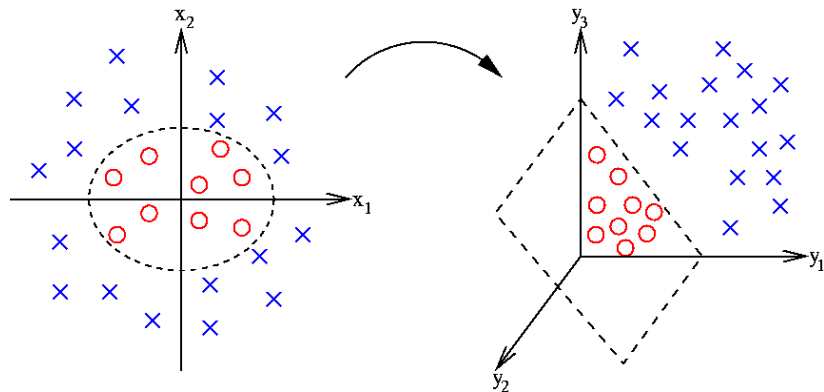


Figure: Mapping from \mathbb{R}^2 to \mathbb{R}^3 where points $(x_1, x_2)^T$ in the original space become $(y_1, y_2, y_3)^T = (x_1^2, \sqrt{2}x_1x_2, x_2^2)^T$ in the new space. The planar decision boundary in the new space corresponds to a non-linear decision boundary in the original space.

Generalized Linear Discriminant Functions

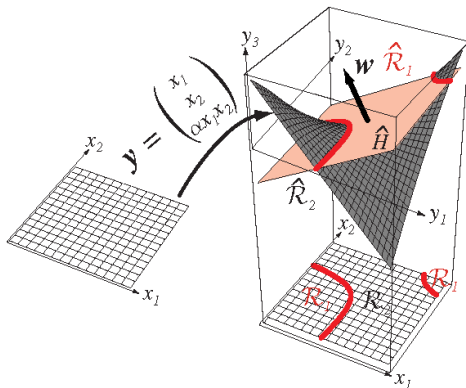


Figure: Mapping from \mathbb{R}^2 to \mathbb{R}^3 where points $(x_1, x_2)^T$ in the original space become $(y_1, y_2, y_3)^T = (x_1, x_2, \alpha x_1 x_2)^T$ in the new space. The decision regions $\hat{\mathcal{R}}_1$ and $\hat{\mathcal{R}}_2$ are separated by a plane in the new space where the corresponding regions \mathcal{R}_1 and \mathcal{R}_2 in the original space are separated by non-linear boundaries (\mathcal{R}_1 is also not connected).

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- We have seen that linear discriminant functions are optimal if the underlying distributions are Gaussians having equal covariance for each class.
- In the general case, the problem of finding linear discriminant functions can be formulated as a problem of optimizing a criterion function.
- Among all hyperplanes separating the data, there exists a unique one yielding the maximum margin of separation between the classes.

Support Vector Machines

- Given a set of training patterns and class labels as $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n) \in \mathbb{R}^d \times \{\pm 1\}$, the goal is to find a classifier function $f : \mathbb{R}^d \rightarrow \{\pm 1\}$ such that $f(\mathbf{x}) = y$ will correctly classify new patterns.

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- Support vector machines* are based on the class of hyperplanes

$$(\mathbf{w} \cdot \mathbf{x}) + b = 0, \quad \mathbf{w} \in \mathbb{R}^d, b \in \mathbb{R}$$

corresponding to decision functions

$$f(\mathbf{x}) = \text{sign}((\mathbf{w} \cdot \mathbf{x}) + b)$$

Support Vector Machines

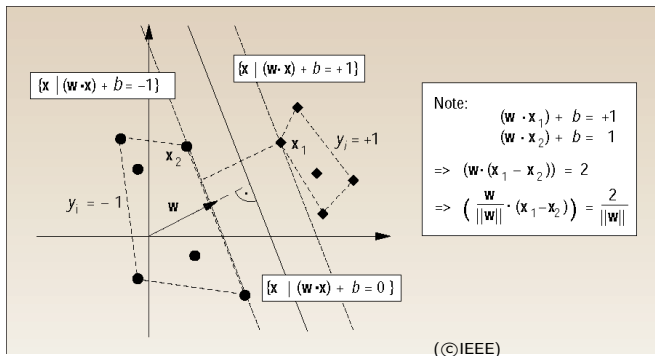


Figure: A binary classification problem of separating balls from diamonds. The optimal hyperplane is orthogonal to the shortest line connecting the convex hulls of the two classes (dotted), and intersects it half way between the two classes. There is a weight vector w and a threshold b such that the points closest to the hyperplane satisfy $|(w \cdot x_i) + b| = 1$ corresponding to $y_i((w \cdot x_i) + b) \geq 1$. The margin, measured perpendicularly to the hyperplane, equals $2/\|w\|$.

Support Vector Machines

- To construct the optimal hyperplane, we can define the following optimization problem:

$$\text{minimize } \frac{1}{2} \|\mathbf{w}\|^2$$

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- This constrained optimization problem is solved using Lagrange multipliers $\alpha_i \geq 0$ and the Lagrangian

$$L(\mathbf{w}, b, \alpha) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^n \alpha_i (y_i((\mathbf{w} \cdot \mathbf{x}_i) + b) - 1)$$

where L has to be minimized w.r.t the prime variables \mathbf{w} and b , and maximized w.r.t. the dual variables α_i .

Support Vector Machines

- The solution can be obtained using quadratic programming techniques where the solution vector

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- The support vectors lie on the margin and carry all relevant information about the classification problem (the remaining patterns are irrelevant).

Support Vector Machines

- Both the quadratic programming problem and the final decision function

$$f(\mathbf{x}) = \text{sign} \left(\sum_{i=1}^n \alpha_i y_i (\mathbf{x} \cdot \mathbf{x}_i) + b \right)$$

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- We can generalize this result to the non-linear case by mapping the original input space into some other space \mathcal{F} using a non-linear map $\Phi : \mathbb{R}^d \rightarrow \mathcal{F}$ and perform the linear algorithm in the \mathcal{F} space which only requires the dot products

$$k(\mathbf{x}, \mathbf{y}) = \Phi(\mathbf{x}) \Phi(\mathbf{y})$$

Support Vector Machines

- Even though \mathcal{F} may be high-dimensional, a simple *kernel* $k(\mathbf{x}, \mathbf{y})$ such as the following can be computed efficiently.

Table: Common kernel functions.

Polynomial	$k(\mathbf{x}, \mathbf{y}) = (\mathbf{x} \cdot \mathbf{y})^p$
Sigmoidal	$k(\mathbf{x}, \mathbf{y}) = \tanh(\kappa(\mathbf{x} \cdot \mathbf{y}) + \theta)$
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- Once a kernel function is chosen, we can substitute $\Phi(\mathbf{x}_i)$ for each training example \mathbf{x}_i , and perform the optimal hyperplane algorithm in \mathcal{F} .

Support Vector Machines

- This results in the non-linear decision function of the form

$$f(\mathbf{x}) = \text{sign} \left(\sum_{i=1}^n \alpha_i y_i k(\mathbf{x}, \mathbf{x}_i) + b \right)$$

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- In the original input space, the hyperplane corresponds to a non-linear decision function whose form is determined by the kernel.

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Support Vector Machines

- SVMs are quite popular because of their intuitive formulation using computational learning theory and their high performances in practical applications.
- However, we must be careful about certain issues such as the following during implementation.
- *Choice of kernel functions:* We can use training data to find the best performing kernel.
- *Computational requirements of the quadratic program:* Several algorithms exist for speeding up the optimization problem (see references).

Support Vector Machines

- *Extension to multiple classes:* We can train a separate SVM for each class, compute the output value using each SVM, and select the class that assigns the unknown pattern the furthest into the positive region.

Support Vector Machines

- *Extension to multiple classes:* We can train a separate SVM for each class, compute the output value using each SVM, and select the class that assigns the unknown pattern the furthest into the positive region.
- *Converting the output of an SVM to a posterior probability for post-processing:* We can fit a sigmoid model to the posterior probability $P(y = 1|f(\mathbf{x}))$ as

$$P(y = 1|f(\mathbf{x})) = \frac{1}{1 + \exp(a f(\mathbf{x}) + b)}$$

where the parameters a and b are learned using maximum likelihood estimation from a training set.

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- Kernel mappings can be used to obtain arbitrary decision regions.
- *Neural networks* try to learn the parameters of the nonlinear mapping at the same time as the linear discriminant.
- A neural network consists of an *input layer* , an *output layer* and usually one or more *hidden layers* that are interconnected by modifiable weights represented by links between layers.

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- The function of units is loosely based on properties of biological neurons, and hence they are sometimes called *neurons* .
- In pattern recognition applications, the input units represent the components of a feature vector and the output units give the values of the discriminant functions used for classification.

Neural Networks

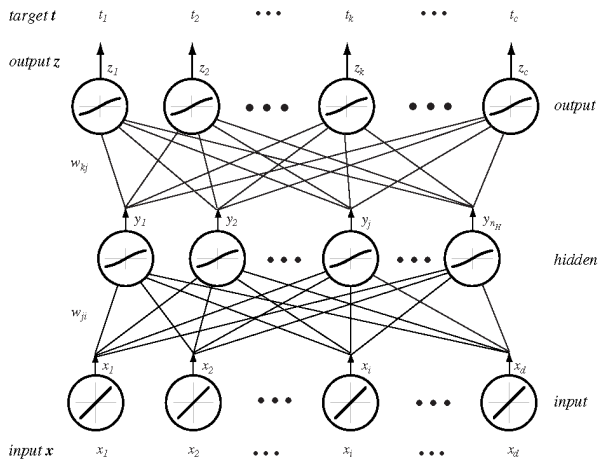


Figure: A $d - n_H - c$ fully connected three-layer network.

Feedforward Operation

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- The output corresponds to a nonlinear function of the input feature vector.

Neural Networks

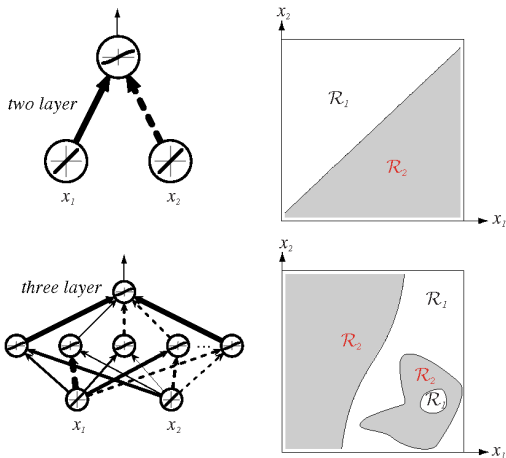


Figure: Whereas a two-layer network classifier can only implement a linear decision boundary, given an adequate number of hidden units, three or more layer networks can implement arbitrary decision boundaries.

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Neural Networks

- We can think of the network as computing discriminant functions and can classify the input according to which discriminant function is the largest.
- Theoretically, every decision (and every continuous function) can be implemented by a three-layer network given sufficient number of hidden units, proper nonlinearities and weights.
- However, this theorem does not tell us how we can learn the network structure, the nonlinear functions and the weights in practice.

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- It is based on the least-mean-squared algorithm where the error is proportional to the square of the difference between the actual output and the desired output.
- The dependence of the error on the hidden-to-output layer weights is straightforward.
- The backpropagation algorithm allows us to calculate an effective error for each hidden unit and derive a learning rule for the input-to-hidden weights.

Backpropagation Algorithm

- Using the notation of Figure 1, define the training error on a pattern to be the sum over output units of the squared difference between the desired output t_k and the actual output z_k as

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- The backpropagation learning rule changes the weights in a direction that reduces the error (gradient descent)

$$\Delta w_{pq} = -\eta \frac{\partial J}{\partial w_{pq}}$$

where η is the learning rate.

Backpropagation Algorithm

- For the hidden-to-output weights, the weight update rule becomes

$$\Delta w_{kj} = -\eta \frac{\partial J}{\partial net_k} \frac{\partial net_k}{\partial w_{kj}} = \eta(t_k - z_k)f'(net_k)y_j$$

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- For the input-to-hidden weights, the weight update rule becomes

$$\begin{aligned}\Delta w_{ji} &= -\eta \frac{\partial J}{\partial y_i} \frac{\partial y_i}{\partial net_j} \frac{\partial net_j}{\partial w_{ji}} \\ &= \eta \left(\sum_{k=1}^c w_{kj}(t_k - z_k)f'(net_k) \right) f'(net_j)x_i\end{aligned}$$

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- What happens when the classification problem involves *nominal* data, e.g., descriptions that are discrete and without any natural notion of similarity or even ordering?
- A common representation for this kind of data is a *list of attributes* (instead of vector of real numbers).

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- These nodes are similarly connected until terminal (*leaf*) nodes, which have no further links, are reached.

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- Each leaf node bears a class label and the pattern is assigned the label of the leaf node reached.

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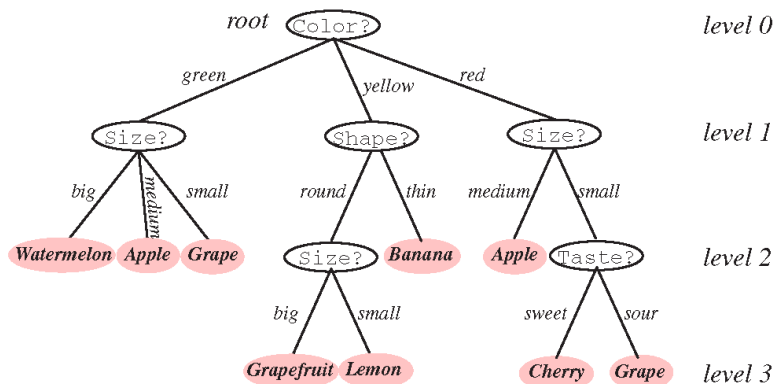


Figure: An example decision tree that uses the attributes {color, shape, taste, size}. Note that the same question can appear in different places in the tree and that different questions can have different numbers of branches. Moreover, different leaf nodes can be labeled by the same class.

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 - How can a class label be assigned to a leaf node?
 - How should missing data be handled?

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- For nonnumerical attributes, splitting questions have the form “is $x \in A$ ” where A is a subset of the possible values of x .

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 - They are capable of dealing with missing data.