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Ensemble Methods

Foundations and Algorithms




Zhi-Hua Zhou

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ENSEMBLE METHODS: FOUNDATIONS AND ALGORITHMS
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To my parents, wife and son.

Z.-H. Zhou

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Preface

Ensemble methods that train multiple learners and then combine them for use, with Boosting and Bagging as representatives, are a kind of state-of-the-art learning approach. It is well known that an ensemble is usually significantly more accurate than a single learner, and ensemble methods have already achieved great success in many real-world tasks.

It is difficult to trace the starting point of the history of ensemble methods since the basic idea of deploying multiple models has been in use in human society for a long time; however, it is clear that ensemble methods have become a hot topic since the 1990s, and researchers from various fields such as machine learning, pattern recognition, data mining, neural networks and statistics have explored ensemble methods from different aspects.

This book provides researchers, students and practitioners with an introduction to ensemble methods. The book consists of eight chapters which naturally constitute three parts.

Part I is composed of Chapter 1. Though this book is mainly written for readers with a basic knowledge of machine learning and pattern recognition, to enable readers who are unfamiliar with these fields to access the main contents, Chapter 1 presents some "background knowledge" of ensemble methods. It is impossible to provide a detailed introduction to all backgrounds in one chapter, and therefore this chapter serves mainly as a guide to further study. This chapter also serves to explain the terminology used in this book, to avoid confusion caused by other terminologies used in different but relevant fields.

Part II is composed of Chapters 2 to 5 and presents "core knowledge" of ensemble methods. Chapters 2 and 3 introduce Boosting and Bagging, respectively. In addition to algorithms and theories, Chapter 2 introduces multi-class extension and noise tolerance, since classic Boosting algorithms are designed for binary classification, and are usually hurt seriously by noise. Bagging is naturally a multi-class method and less sensitive to noise, and therefore, Chapter 3 does not discuss these issues; instead, Chapter 3 devotes a section to Random Forest and some other random tree ensembles that can be viewed as variants of Bagging. Chapter 4 introduces combination methods. In addition to various averaging and voting schemes, the Stacking method and some other combination methods as well as relevant methods such as mixture of experts are introduced. Chapter 5 focuses on ensemble diversity. After introducing the error-ambiguity and bias-variance

decompositions, many diversity measures are presented, followed by recent advances in information theoretic diversity and diversity generation methods.

Part III is composed of Chapters 6 to 8, and presents "advanced knowledge" of ensemble methods. Chapter 6 introduces ensemble pruning, which tries to prune a trained ensemble to get a better performance. Chapter 7 introduces clustering ensembles, which try to generate better clustering results by combining multiple clusterings. Chapter 8 presents some developments of ensemble methods in semi-supervised learning, active learning, cost-sensitive learning and class-imbalance learning, as well as comprehensibility enhancement.

It is not the goal of the book to cover all relevant knowledge of ensemble methods. Ambitious readers may be interested in *Further Reading* sections for further information.

Two other books [Kuncheva, 2004, Rokach, 2010] on ensemble methods have been published before this one. To reflect the fast development of this field, I have attempted to present an updated and in-depth overview. However, when writing this book, I found this task more challenging than expected. Despite abundant research on ensemble methods, a thorough understanding of many essentials is still needed, and there is a lack of thorough empirical comparisons of many technical developments. As a consequence, several chapters of the book simply introduce a number of algorithms, while even for chapters with discussions on theoretical issues, there are still important yet unclear problems. On one hand, this reflects the still developing situation of the ensemble methods field; on the other hand, such a situation provides a good opportunity for further research.

The book could not have been written, at least not in its current form, without the help of many people. I am grateful to Tom Dietterich who has carefully read the whole book and given very detailed and insightful comments and suggestions. I want to thank Songcan Chen, Nan Li, Xu-Ying Liu, Fabio Roli, Jianxin Wu, Yang Yu and Min-Ling Zhang for helpful comments. I also want to thank Randi Cohen and her colleagues at Chapman & Hall/CRC Press for cooperation.

Last, but definitely not least, I am indebted to my family, friends and students for their patience, support and encouragement.

Zhi-Hua Zhou
Nanjing, China

Notations

x	variable
$\boldsymbol{x}$	vector
$\mathbf{A}$	matrix
$\mathbf{I}$	identity matrix
$\mathcal{X}, \mathcal{Y}$	input and output spaces
$\mathcal{D}$	probability distribution
D	data sample (data set)
$\mathcal{N}$	normal distribution
$\mathcal{U}$	uniform distribution
$\mathcal{H}$	hypothesis space
H	set of hypotheses
$h(\cdot)$	hypothesis (learner)
$\mathfrak{L}$	learning algorithm
$p(\cdot)$	probability density function
$p(\cdot \mid \cdot)$	conditional probability density function
$P(\cdot)$	probability mass function
$P(\cdot \mid \cdot)$	conditional probability mass function
$\mathbb{E}_{\cdot \sim \mathcal{D}}[f(\cdot)]$	mathematical expectation of function $f(\cdot)$ to $\cdot$ under distribution $\mathcal{D}$. $\mathcal{D}$ and/or $\cdot$ is ignored when the meaning is clear
$var_{\cdot \sim \mathcal{D}}[f(\cdot)]$	variance of function $f(\cdot)$ to $\cdot$ under distribution $\mathcal{D}$
$\mathbb{I}(\cdot)$	indicator function which takes 1 if $\cdot$ is `true`, and 0 otherwise
$\texttt{sign}(\cdot)$	sign function which takes -1,1 and 0 when $\cdot < 0$, $\cdot > 0$ and $\cdot = 0$, respectively
$err(\cdot)$	error function
$\{\ldots\}$	set
$(\ldots)$	row vector

$(\ldots)^\top$	column vector
$\lvert\cdot\rvert$	size of data set
$\lVert\cdot\rVert$	L_2-norm

Contents

1

Introduction

1.1 Basic Concepts

One major task of machine learning, pattern recognition and data mining is to construct *good* **models** from **data sets**.

A "data set" generally consists of **feature vectors**, where each feature vector is a description of an object by using a set of **features**. For example, take a look at the synthetic *three-Gaussians* data set as shown in Figure 1.1. Here, each object is a data point described by the features x-coordinate, y-coordinate and shape, and a feature vector looks like (.5, .8, cross) or (.4, .5, circle). The number of features of a data set is called **dimension** or **dimensionality**; for example, the dimensionality of the above data set is three. Features are also called **attributes**, a feature vector is also called an **instance**, and sometimes a data set is called a **sample**.

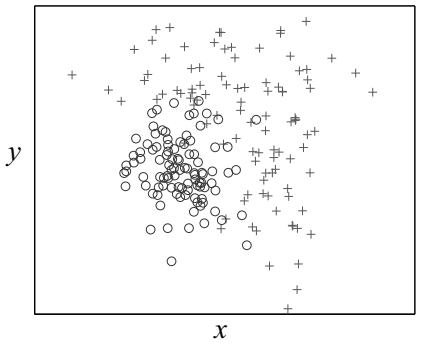


FIGURE 1.1: The synthetic *three-Gaussians* data set.

A "model" is usually a predictive model or a model of the structure of the data that we want to construct or discover from the data set, such as a decision tree, a neural network, a support vector machine, etc. The pro-

cess of generating models from data is called **learning** or **training**, which is accomplished by a **learning algorithm**. The learned model can be called a **hypothesis**, and in this book it is also called a **learner**. There are different learning settings, among which the most common ones are **supervised learning** and **unsupervised learning**. In supervised learning, the goal is to predict the value of a target feature on unseen instances, and the learned model is also called a **predictor**. For example, if we want to predict the shape of the *three-Gaussians* data points, we call "cross" and "circle" **labels**, and the predictor should be able to predict the label of an instance for which the label information is unknown, e.g., (.2, .3). If the label is *categorical*, such as shape, the task is also called **classification** and the learner is also called **classifier**; if the label is *numerical*, such as x-coordinate, the task is also called **regression** and the learner is also called **fitted regression model**. For both cases, the training process is conducted on data sets containing label information, and an instance with known label is also called an **example**. In **binary classification**, generally we use "positive" and "negative" to denote the two class labels. Unsupervised learning does not rely on label information, the goal of which is to discover some inherent distribution information in the data. A typical task is **clustering**, aiming to discover the cluster structure of data points. In most of this book we will focus on supervised learning, especially classification. We will introduce some popular learning algorithms briefly in Section 1.2.

Basically, whether a model is "good" depends on whether it can meet the requirements of the user or not. Different users might have different expectations of the learning results, and it is difficult to know the "right expectation" before the concerned task has been tackled. A popular strategy is to evaluate and estimate the performance of the models, and then let the user to decide whether a model is acceptable, or choose the best available model from a set of candidates. Since the fundamental goal of learning is **generalization**, i.e., being capable of generalizing the "knowledge" learned from training data to unseen instances, a good learner should generalize well, i.e., have a small **generalization error**, also called the **prediction error**. It is infeasible, however, to estimate the generalization error directly, since that requires knowing the **ground-truth** label information which is unknown for unseen instances. A typical empirical process is to let the predictor make predictions on **test data** of which the ground-truth labels are known, and take the **test error** as an estimate of the generalization error. The process of applying a learned model to unseen data is called **testing**. Before testing, a learned model often needs to be configured, e.g., tuning the parameters, and this process also involves the use of data with known ground-truth labels to evaluate the learning performance; this is called **validation** and the data is **validation data**. Generally, the test data should not overlap with the training and validation data; otherwise the estimated performance can be over-optimistic. More introduction on performance evaluation will be given in Section 1.3.

A formal formulation of the learning process is as follows: Denote $\mathcal{X}$ as the instance space, $\mathcal{D}$ as a distribution over $\mathcal{X}$, and f the *ground-truth* target function. Given a training data set $D = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_m, y_m)\}$, where the instances $\boldsymbol{x}_i$ are drawn ***i.i.d.*** (independently and identically distributed) from $\mathcal{D}$ and $y_i = f(\boldsymbol{x}_i)$, taking classification as an example, the goal is to construct a learner h which minimizes the generalization error

$$err(h) = \mathbb{E}_{\boldsymbol{x}\sim\mathcal{D}}[\mathbb{I}(h(\boldsymbol{x}) \neq f(\boldsymbol{x}))]. \tag{1.1}$$

1.2 Popular Learning Algorithms

1.2.1 Linear Discriminant Analysis

A **linear classifier** consists of a **weight vector** $\boldsymbol{w}$ and a **bias** b. Given an instance $\boldsymbol{x}$, the predicted class label y is obtained according to

$$y = \texttt{sign}(\boldsymbol{w}^\top \boldsymbol{x} + b). \tag{1.2}$$

The classification process is accomplished by two steps. First, the instance space is mapped onto a one-dimensional space (i.e., a line) through the weight vector $\boldsymbol{w}$; then, a point on the line is identified to separate the positive instances from negative ones.

To find the best $\boldsymbol{w}$ and b for separating different classes, a classical linear learning algorithm is *Fisher's linear discriminant analysis* (LDA). Briefly, the idea of LDA is to enable instances of different classes to be far away while instances within the same class to be close; this can be accomplished by making the distance between centers of different classes large while keeping the variance within each class small.

Given a two-class training set, we consider all the positive instances, and obtain the mean $\boldsymbol{\mu}_+$ and the covariance matrix Σ_+; similarly, we consider all the negative instances, and obtain the mean $\boldsymbol{\mu}_-$ and the covariance matrix Σ_-. The distance between the projected class centers is measured as

$$S_B(\boldsymbol{w}) = (\boldsymbol{w}^\top \boldsymbol{\mu}_+ - \boldsymbol{w}^\top \boldsymbol{\mu}_-)^2, \tag{1.3}$$

and the variance within classes is measured as

$$S_W(\boldsymbol{w}) = \boldsymbol{w}^\top \Sigma_+ \boldsymbol{w} + \boldsymbol{w}^\top \Sigma_- \boldsymbol{w}. \tag{1.4}$$

LDA combines these two measures by maximizing

$$J(\boldsymbol{w}) = S_B(\boldsymbol{w})/S_W(\boldsymbol{w}), \tag{1.5}$$

of which the optimal solution has a closed-form

$$\boldsymbol{w}^* = (\Sigma_+ + \Sigma_-)^{-1}(\boldsymbol{\mu}_+ - \boldsymbol{\mu}_-). \tag{1.6}$$

After obtaining $\boldsymbol{w}$, it is easy to calculate the bias b. The simplest way is to let b be the middle point between the projected centers, i.e.,

$$b^* = \boldsymbol{w}^\top(\boldsymbol{\mu}_+ + \boldsymbol{\mu}_-)/2, \tag{1.7}$$

which is optimal when the two classes are from normal distributions sharing the same variance.

Figure 1.2 illustrates the decision boundary of an LDA classifier.

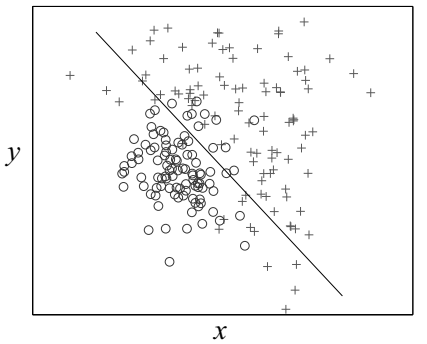


FIGURE 1.2: Decision boundary of LDA on the *three-Gaussians* data set.

1.2.2 Decision Trees

A decision tree consists of a set of tree-structured decision tests working in a *divide-and-conquer* way. Each non-leaf node is associated with a **feature test** also called a **split**; data falling into the node will be split into different subsets according to their different values on the feature test. Each leaf node is associated with a label, which will be assigned to instances falling into this node. In prediction, a series of feature tests is conducted starting from the root node, and the result is obtained when a leaf node is reached. Take Figure 1.3 as an example. The classification process starts by testing whether the value of the feature y-coordinate is larger than 0.73; if so, the instance is classified as "cross", and otherwise the tree tests whether the feature value of x-coordinate is larger than 0.64; if so, the instance is classified as "cross" and otherwise is classified as "circle".

Decision tree learning algorithms are generally recursive processes. In each step, a data set is given and a split is selected, then this split is used to divide the data set into subsets, and each subset is considered as the given data set for the next step. The key of a decision tree algorithm is how to select the splits.

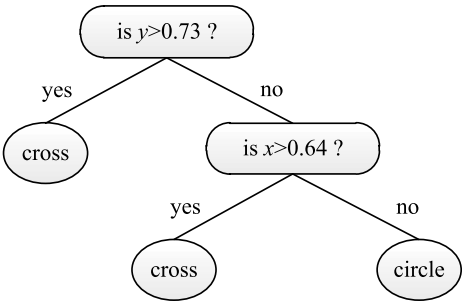


FIGURE 1.3: An example of a decision tree.

In the ID3 algorithm [Quinlan, 1998], the **information gain** criterion is employed for split selection. Given a training set D, the **entropy** of D is defined as

$$Ent(D) = -\sum_{y \in \mathcal{Y}} P(y|D) \log P(y|D). \tag{1.8}$$

If the training set D is divided into subsets $D_1, \ldots, D_k$, the entropy may be reduced, and the amount of the reduction is the information gain, i.e.,

$$G(D; D_1, \ldots, D_k) = Ent(D) - \sum_{i=1}^{k} \frac{|D_k|}{|D|} Ent(D_k). \tag{1.9}$$

Thus, the feature-value pair which will cause the largest information gain is selected for the split.

One problem with the information gain criterion is that features with a lot of possible values will be favored, disregarding their relevance to classification. For example, suppose we are dealing with binary classification and each instance has a unique "*id*", and if the "*id*" is considered as a feature, the information gain of taking this feature as split would be quite large since this split will classify every training instance correctly; however, it cannot generalize and thus will be useless for making prediction on unseen instances.

This deficiency of the information gain criterion is addressed in C4.5 [Quinlan, 1993], the most famous decision tree algorithm. C4.5 employs the **gain ratio**

$$P(D; D_1, \ldots, D_k) = G(D; D_1, \ldots, D_k) \cdot \left(-\sum_{i=1}^{k} \frac{|D_k|}{|D|} \log \frac{|D_k|}{|D|} \right)^{-1}, \tag{1.10}$$

which is a variant of the information gain criterion, taking **normalization** on the number of feature values. In practice, the feature with the highest gain ratio, among features with better-than-average information gains, is selected as the split.

CART [Breiman et al., 1984] is another famous decision tree algorithm, which uses **Gini index** for selecting the split maximizing the Gini

$$G_{gini}(D; D_1, \ldots, D_k) = I(D) - \sum_{i=1}^{k} \frac{|D_k|}{|D|} I(D_k), \tag{1.11}$$

where

$$I(D) = 1 - \sum_{y \in \mathcal{Y}} P(y \mid D)^2. \tag{1.12}$$

It is often observed that a decision tree, which is perfect on the training set, will have a worse generalization ability than a tree which is not-so-good on the training set; this is called **overfitting** which may be caused by the fact that some peculiarities of the training data, such as those caused by noise in collecting training examples, are misleadingly recognized by the learner as the underlying truth. To reduce the risk of overfitting, a general strategy is to employ **pruning** to cut off some tree branches caused by noise or peculiarities of the training set. **Pre-pruning** tries to prune branches when the tree is being grown, while **post-pruning** re-examines fully grown trees to decide which branches should be removed. When a validation set is available, the tree can be pruned according to the validation error: for pre-pruning, a branch will not be grown if the validation error will increase by growing the branch; for post-pruning, a branch will be removed if the removal will decrease the validation error.

Early decision tree algorithms, such as ID3, could only deal with categorical features. Later ones, such as C4.5 and CART, are enabled to deal with numerical features. The simplest way is to evaluate every possible split point on the numerical feature that divides the training set into two subsets, where one subset contains instances with the feature value smaller than the split point while the other subset contains the remaining instances.

When the height of a decision tree is limited to 1, i.e., it takes only one test to make every prediction, the tree is called a **decision stump**. While decision trees are nonlinear classifiers in general, decision stumps are a kind of linear classifiers.

Figure 1.4 illustrates the decision boundary of a typical decision tree.

1.2.3 Neural Networks

Neural networks, also called **artificial neural networks**, originated from simulating biological neural networks. The function of a neural network is determined by the model of **neuron**, the network structure, and the learning algorithm.

Neuron is also called **unit**, which is the basic computational component in neural networks. The most popular neuron model, i.e., the *McCulloch-Pitts* model (**M-P model**), is illustrated in Figure 1.5(a). In this model, input

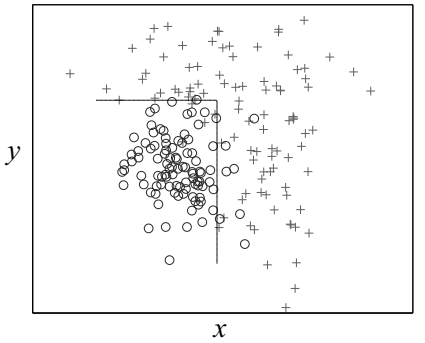


FIGURE 1.4: Decision boundary of a typical decision tree on the *three-Gaussians* data set.

signals are multiplied with corresponding **connection weights** at first, and then signals are aggregated and compared with a threshold, also called **bias** of the neuron. If the aggregated signal is larger than the bias, the neuron will be activated and the output signal is generated by an **activation function**, also called *transfer function* or *squashing function*.

Neurons are linked by weighted connections to form a network. There are many possible network structures, among which the most popular one is the **multi-layer feed-forward network**, as illustrated in Figure 1.5(b). Here the neurons are connected layer-by-layer, and there are neither in-layer connections nor cross-layer connections. There is an **input layer** which receives input feature vectors, where each neuron usually corresponds to one element of the feature vector. The activation function for input neurons is usually set as $f(x) = x$. There is an **output layer** which outputs labels, where each neuron usually corresponds to a possible label, or an element of a *label vector*. The layers between the input and output layers are called **hidden layers**. The hidden neurons and output neurons are functional units, and a popular activation function for them is the **sigmoid function**

$$f(x) = \frac{1}{1 + e^{-x}}. \tag{1.13}$$

Although one may use a network with many hidden layers, the most popular setting is to use one or two hidden layers, since it is known that a feed-forward neural network with one hidden layer is already able to approximate any continuous function, and more complicated algorithms are needed to prevent networks with many hidden layers from suffering from problems such as divergence (i.e., the networks do not converge to a stable state).

The goal of training a neural network is to determine the values of the connection weights and the biases of the neurons. Once these values are

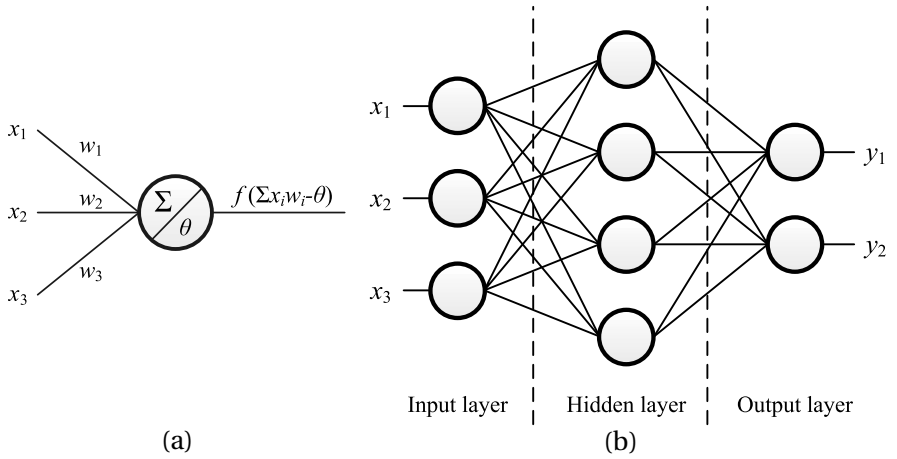


FIGURE 1.5: Illustration of (a) a neuron, and (b) a neural network.

decided, the function computed by the neural network is decided. There are many neural network learning algorithms. The most commonly applied idea for training a multi-layer feed-forward neural network is that, as long as the activation function is differentiable, the whole neural network can be regarded as a differentiable function which can be optimized by **gradient descent** method.

The most successful algorithm, **Back-Propagation (BP)** [Werbos, 1974, Rumelhart et al., 1986], works as follows. At first, the inputs are feed-forwarded from the input layer via the hidden layer to the output layer, at which the error is calculated by comparing the network output with the ground-truth. Then, the error will be back propagated to the hidden layer and the input layer, during which the connection weights and biases are adjusted to reduce the error. The process is accomplished by tuning towards the direction with the gradient. Such a process will be repeated in many rounds, until the training error is minimized or the training process is terminated to avoid overfitting.

1.2.4 Naïve Bayes Classifier

To classify a test instance $\boldsymbol{x}$, one approach is to formulate a probabilistic model to estimate the posterior probability $P(y \mid \boldsymbol{x})$ of different y's, and predict the one with the largest posterior probability; this is the ***maximum a posterior* (MAP)** rule. By *Bayes Theorem*, we have

$$P(y \mid \boldsymbol{x}) = \frac{P(\boldsymbol{x} \mid y)P(y)}{P(\boldsymbol{x})}\,, \tag{1.14}$$

where $P(y)$ can be estimated by counting the proportion of class y in the training set, and $P(\boldsymbol{x})$ can be ignored since we are comparing different y's on the same $\boldsymbol{x}$. Thus we only need to consider $P(\boldsymbol{x} \mid y)$. If we can get an accurate estimate of $P(\boldsymbol{x} \mid y)$, we will get the best classifier in theory from the given training data, that is, the **Bayes optimal classifier** with the **Bayes error rate**, the smallest error rate in theory. However, estimating $P(\boldsymbol{x} \mid y)$ is not straightforward, since it involves the estimation of exponential numbers of joint-probabilities of the features. To make the estimation tractable, some assumptions are needed.

The naïve Bayes classifier assumes that, given the class label, the n features are independent of each other within each class. Thus, we have

$$P(\boldsymbol{x} \mid y) = \prod_{i=1}^{n} P(x_i \mid y), \tag{1.15}$$

which implies that we only need to estimate each feature value in each class in order to estimate the conditional probability, and therefore the calculation of joint-probabilities is avoided.

In the training stage, the naïve Bayes classifier estimates the probabilities $P(y)$ for all classes $y \in \mathcal{Y}$, and $P(x_i \mid y)$ for all features $i = 1, \ldots, n$ and all feature values x_i from the training set. In the test stage, a test instance $\boldsymbol{x}$ will be predicted with label y if y leads to the largest value of

$$P(y \mid \boldsymbol{x}) \propto P(y) \prod_{i=1}^{n} P(x_i \mid y) \tag{1.16}$$

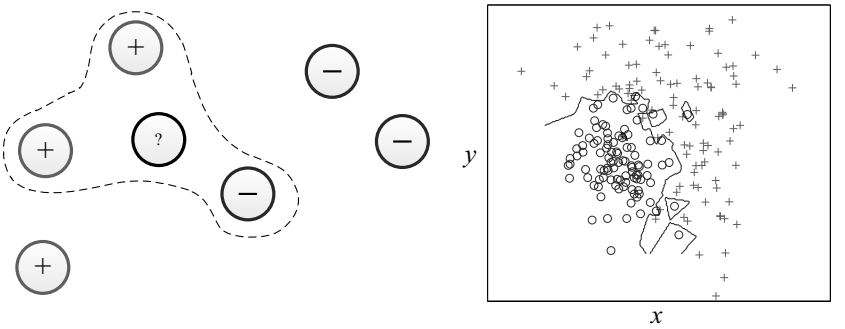
among all the class labels.

1.2.5 k-Nearest Neighbor

The k-nearest neighbor (kNN) algorithm relies on the principle that objects similar in the input space are also similar in the output space. It is a **lazy learning** approach since it does not have an explicit training process, but simply stores the training set instead. For a test instance, a k-nearest neighbor learner identifies the k instances from the training set that are closest to the test instance. Then, for classification, the test instance will be classified to the majority class among the k instances; while for regression, the test instance will be assigned the average value of the k instances. Figure 1.6(a) illustrates how to classify an instance by a 3-nearest neighbor classifier. Figure 1.6(b) shows the decision boundary of a 1-nearest neighbor classifier, also called the **nearest neighbor classifier**.

1.2.6 Support Vector Machines and Kernel Methods

Support vector machines (SVMs) [Cristianini and Shawe-Taylor, 2000], originally designed for binary classification, are **large margin classifiers**



(a) (b)

FIGURE 1.6: Illustration of (a) how a k-nearest neighbor classifier predicts on a test instance, and (b) the decision boundary of the nearest neighbor classifier on the *three-Gaussians* data set.

that try to separate instances of different classes with the maximum margin hyperplane. The **margin** is defined as the minimum distance from instances of different classes to the classification hyperplane.

Considering a linear classifier $y = \texttt{sign}(\boldsymbol{w}^\top \boldsymbol{x}+b)$, or abbreviated as $(\boldsymbol{w}, b)$, we can use the **hinge loss** to evaluate the fitness to the data:

$$\sum_{i=1}^{m} \max\{0, 1 - y_i(\boldsymbol{w}^\top \boldsymbol{x}_i + b)\}. \tag{1.17}$$

The Euclidean distance from an instance $\boldsymbol{x}_i$ to the hyperplane $\boldsymbol{w}^\top \boldsymbol{x} + b$ is

$$\frac{|\boldsymbol{w}^\top \boldsymbol{x}_i + b|}{\|\boldsymbol{w}\|}. \tag{1.18}$$

If we restrict $|\boldsymbol{w}^\top \boldsymbol{x}_i + b| \geq 1$ for all instances, the minimum distance to the hyperplane is $\|\boldsymbol{w}\|^{-1}$. Therefore, SVMs maximize $\|\boldsymbol{w}\|^{-1}$.

Thus, SVMs solve the optimization problem

$$\begin{aligned} (\boldsymbol{w}^*, b^*) = \arg\min_{\boldsymbol{w}, b, \xi_i} \frac{\|\boldsymbol{w}\|^2}{2} + C\sum_{i=1}^{m} \xi_i \\ s.t. \quad y_i(\boldsymbol{w}^\top \boldsymbol{x}_i + b) \geq 1 - \xi_i \ (\forall i = 1, \ldots, m) \\ \xi_i \geq 0 \ (\forall i = 1, \ldots, m)\,, \end{aligned} \tag{1.19}$$

where C is a parameter and ξ_i's are *slack variables* introduced to enable the learner to deal with data that could not be perfectly separated, such as data with noise. An illustration of an SVM is shown in Figure 1.7.

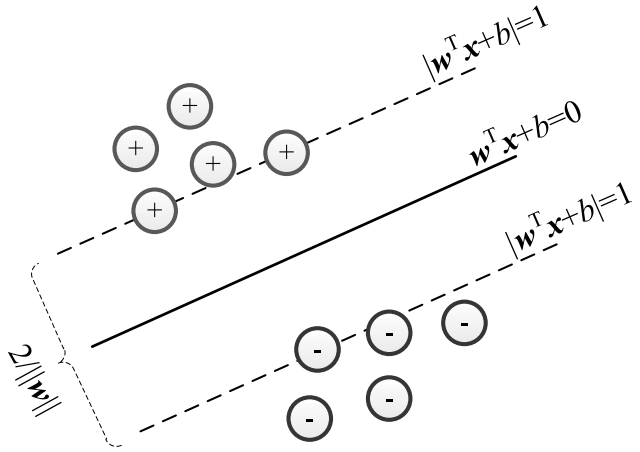


FIGURE 1.7: Illustration of SVM.

(1.19) is called the *primal* form of the optimization. The *dual* form, which gives the same optimal solution, is

$$\begin{aligned} \boldsymbol{\alpha}^* = \arg\max_{\boldsymbol{\alpha}} & \sum_{i=1}^{m} \alpha_i - \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j \langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle \\ s.t. \quad & \sum_{i=1}^{m} \alpha_i y_i = 0 \\ & \alpha_i \geq 0 \, (\forall i = 1, \ldots, m) \, , \end{aligned} \tag{1.20}$$

where $\langle \cdot, \cdot \rangle$ is the inner product. The solution $\boldsymbol{w}^*$ of the primal form is now presented as

$$\boldsymbol{w}^* = \sum_{i=1}^{m} \alpha_i^* y_i \boldsymbol{x}_i \, , \tag{1.21}$$

and the inner product between $\boldsymbol{w}^*$ and an instance $\boldsymbol{x}$ can be calculated as

$$\langle \boldsymbol{w}^*, \boldsymbol{x} \rangle = \sum_{i=1}^{m} \alpha_i^* y_i \langle \boldsymbol{x}_i, \boldsymbol{x} \rangle \, . \tag{1.22}$$

A limitation of the linear classifiers is that, when the data is intrinsically nonlinear, linear classifiers cannot separate the classes well. In such cases, a general approach is to map the data points onto a higher-dimensional feature space where the data linearly non-separable in the original feature space become linearly separable. However, the learning process may become very slow and even intractable since the inner product will be difficult to calculate in the high-dimensional space.

Fortunately, there is a class of functions, **kernel functions** (also called **kernels**), which can help address the problem. The feature space derived by kernel functions is called the **Reproducing Kernel Hilbert Space** (**RKHS**). An inner product in the RKHS equals kernel mapping of inner product of instances in the original lower-dimensional feature space. In other words,

$$K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \langle \phi(\boldsymbol{x}_i), \phi(\boldsymbol{x}_j) \rangle \tag{1.23}$$

for all $\boldsymbol{x}_i$'s, where ϕ is a mapping from the original feature space to a higher-dimensional space and K is a kernel. Thus, we can simply replace the inner products in the dual form of the optimization by the kernel.

According to *Mercer's Theorem* [Cristianini and Shawe-Taylor, 2000], every positive semi-definite symmetric function is a kernel. Popular kernels include the **linear kernel**

$$K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle \,, \tag{1.24}$$

the **polynomial kernel**

$$K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle^d \,, \tag{1.25}$$

where d is the degree of the polynomial, and the **Gaussian kernel** (or called **RBF kernel**)

$$K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \exp\left(-\frac{\|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2}{2\sigma^2}\right) \,, \tag{1.26}$$

where σ is the parameter of the Gaussian width.

The **kernel trick**, i.e., mapping the data points with a kernel and then accomplishing the learning task in the RKHS, is a general strategy that can be incorporated into any learning algorithm that considers only inner products between the input feature vectors. Once the kernel trick is used, the learning algorithms are called **kernel methods**. Indeed, SVMs are a special kind of kernel method, i.e., linear classifiers facilitated with kernel trick.

1.3 Evaluation and Comparison

Usually, we have multiple alternative learning algorithms to choose among, and a number of parameters to tune. The task of choosing the best algorithm and the settings of its parameters is known as **model selection**, and for this purpose we need to estimate the performance of the learner. By empirical ways, this involves design of experiments and statistical hypothesis tests for comparing the models.

It is unwise to estimate the generalization error of a learner by its **training error**, i.e., the error that the learner makes on the training data, since

training error prefers complex learners rather than learners that generalize well. Usually, a learner with very high complexity can have zero training error, such as a fully grown decision tree; however, it is likely to perform badly on unseen data due to overfitting. A proper process is to evaluate the performance on a validation set. Note that the labels in the training set and validation set are known *a priori* to the training process, and should be used together to derive and tune the final learner once the model has been selected.

In fact, in most cases the training and validation sets are obtained by splitting a given data set into two parts. While splitting, the properties of the original data set should be kept as much as possible; otherwise the validation set may provide misleading estimates, for an extreme example, the training set might contain only positive instances while the validation set contains only negative instances. In classification, when the original data set is split randomly, the class percentage should be maintained for both training and validation sets; this is called **stratification**, or *stratified sampling*.

When there is not enough labeled data available to create a separate validation set, a commonly used validation method is **cross-validation**. In k**-fold cross-validation**, the original data set is partitioned by stratified split into k equal-size disjoint subsets, $D_1, \ldots, D_k$, and then k runs of training-tests are performed. In the ith run, D_i is used as the validation set while the union of all the other subsets, i.e., $\bigcup_{j \neq i} D_j$, is used as the training set. The average results of the k runs are taken as the results of the cross-validation. To reduce the influence of randomness introduced by data split, the k-fold cross-validation can be repeated t times, which is called t**-times** k**-fold cross-validation**. Usual configurations include *10-times 10-fold cross-validation*, and *5-times 2-fold cross-validation* suggested by Dietterich [1998]. Extremely, when k equals the number of instances in the original data set, there is only one instance in each validation set; this is called **leave-one-out (LOO)** validation.

After obtaining the estimated errors, we can compare different learning algorithms. A simple comparison on average errors, however, is not reliable since the winning algorithm may occasionally perform well due to the randomness in data split. **Hypothesis test** is usually employed for this purpose.

To compare learning algorithms that are efficient enough to run 10 times, the $\mathbf{5 \times 2}$ **cv paired** t**-test** is a good choice [Dietterich, 1998]. In this test, we run 5-times 2-fold cross-validation. In each run of 2-fold cross-validation, the data set D is randomly split into two subsets D_1 and D_2 of equal size. Two algorithms a and b are trained on each set and tested on the other, resulting in four error estimates: $err_a^{(1)}$ and $err_b^{(1)}$ (trained on D_1 and tested on D_2) and $err_a^{(2)}$ and $err_b^{(2)}$ (trained on D_2 and tested on D_1). We have the error differences

$$d^{(i)} = err_a^{(i)} - err_b^{(i)} \qquad (i = 1, 2) \tag{1.27}$$

with the mean and the variance, respectively:

$$\mu = \frac{d^{(1)} + d^{(2)}}{2} , \tag{1.28}$$

$$s^2 = (d^{(1)} - \mu)^2 + (d^{(2)} - \mu)^2 . \tag{1.29}$$

Let s_i^2 denote the variance in the ith time 2-fold cross-validation, and $d_1^{(1)}$ denote the error difference in the first time. Under the null hypothesis, the 5×2 cv $\tilde{t}$-statistic

$$\tilde{t} = \frac{d_1^{(1)}}{\sqrt{\frac{1}{5}\sum_{i=1}^{5} s_i^2}} \sim t_5 , \tag{1.30}$$

would be distributed according to the *Student's t-distribution* with 5 degrees of freedom. We then choose a significance level α. If $\tilde{t}$ falls into the interval $[-t_5(\alpha/2), t_5(\alpha/2)]$, the null hypothesis is accepted, suggesting that there is no significant difference between the two algorithms. Usually α is set to 0.05 or 0.1.

To compare learning algorithms that can be run only once, the **McNemar's test** can be used instead [Dietterich, 1998]. Let err_{01} denote the number of instances on which the first algorithm makes a wrong prediction while the second algorithm is correct, and err_{10} denotes the inverse. If the two algorithms have the same performance, err_{01} is close to err_{10}, and therefore, the quantity

$$\frac{(|err_{01} - err_{10}| - 1)^2}{err_{01} + err_{10}} \sim \chi_1^2 \tag{1.31}$$

would be distributed according to the *χ^2-distribution*.

Sometimes, we evaluate multiple learning algorithms on multiple data sets. In this situation, we can conduct the **Friedman test** [Demšar, 2006]. First, we sort the algorithms on each data set according to their average errors. On each data set, the best algorithm is assigned rank 1, the worse algorithms are assigned increased ranks, and average ranks are assigned in case of ties. Then, we average the ranks of each algorithm over all data sets, and use the *Nemenyi post-hoc test* [Demšar, 2006] to calculate the *critical difference* value

$$CD = q_\alpha \sqrt{\frac{k(k+1)}{6N}} , \tag{1.32}$$

where k is the number of algorithms, N is the number of data sets and q_α is the *critical value* [Demšar, 2006]. A pair of algorithms are believed to be significantly different if the difference of their average ranks is larger than the critical difference.

The Friedman test results can be visualized by plotting the **critical difference diagram**, as illustrated in Figure 1.8, where each algorithm corresponds to a bar centered at the average rank with the width of critical difference value. Figure 1.8 discloses that the algorithm A is significantly better

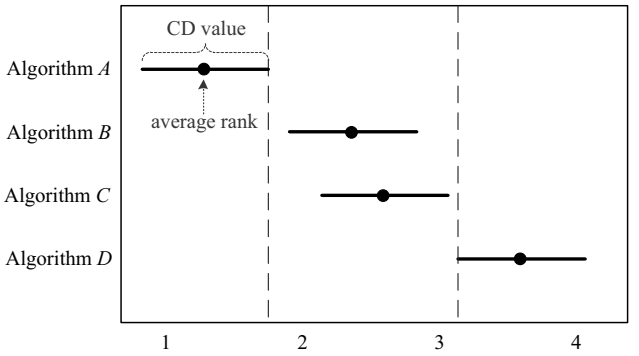


FIGURE 1.8: Illustration of critical difference diagram.

than all the other algorithms, the algorithm D is significantly worse than all the other algorithms, and the algorithms B and C are not significantly different, according to the given significance level.

1.4 Ensemble Methods

Ensemble methods train multiple learners to solve the same problem. In contrast to ordinary learning approaches which try to construct one learner from training data, ensemble methods try to construct a set of learners and combine them. Ensemble learning is also called **committee-based learning**, or learning **multiple classifier systems**.

Figure 1.9 shows a common ensemble architecture. An ensemble contains a number of learners called **base learners**. Base learners are usually generated from training data by a **base learning algorithm** which can be decision tree, neural network or other kinds of learning algorithms. Most ensemble methods use a single base learning algorithm to produce *homogeneous* base learners, i.e., learners of the same type, leading to **homogeneous ensembles**, but there are also some methods which use multiple learning algorithms to produce *heterogeneous* learners, i.e., learners of different types, leading to **heterogeneous ensembles**. In the latter case there is no single base learning algorithm and thus, some people prefer calling the learners **individual learners** or **component learners** to *base learners*.

The generalization ability of an ensemble is often much stronger than that of base learners. Actually, ensemble methods are appealing mainly because they are able to boost **weak learners** which are even just slightly better than random guess to **strong learners** which can make very accurate predictions. So, *base learners* are also referred to as *weak learners*.

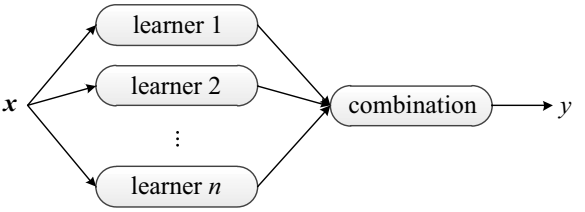


FIGURE 1.9: A common ensemble architecture.

It is difficult to trace the starting point of the history of ensemble methods since the basic idea of deploying multiple models has been in use in human society for a long time. For example, even earlier than the introduction of **Occam's razor**, the common basic assumption of scientific research which prefers simple hypotheses to complex ones when both fit empirical observations well, the Greek philosopher Epicurus (341 - 270 B.C.) introduced the **principle of multiple explanations** [Asmis, 1984] which advocated to keep all hypotheses that are consistent with empirical observations.

There are three threads of early contributions that led to the current area of ensemble methods; that is, **combining classifiers**, **ensembles of weak learners** and **mixture of experts**. *Combining classifiers* was mostly studied in the pattern recognition community. In this thread, researchers generally work on strong classifiers, and try to design powerful *combining rules* to get stronger combined classifiers. As the consequence, this thread of work has accumulated deep understanding on the design and use of different combining rules. *Ensembles of weak learners* was mostly studied in the machine learning community. In this thread, researchers often work on weak learners and try to design powerful algorithms to boost the performance from weak to strong. This thread of work has led to the birth of famous ensemble methods such as AdaBoost, Bagging, etc., and theoretical understanding on why and how weak learners can be boosted to strong ones. *Mixture of experts* was mostly studied in the neural networks community. In this thread, researchers generally consider a **divide-and-conquer** strategy, try to learn a mixture of parametric models jointly and use combining rules to get an overall solution.

Ensemble methods have become a major learning paradigm since the 1990s, with great promotion by two pieces of pioneering work. One is empirical [Hansen and Salamon, 1990], in which it was found that predictions made by the combination of a set of classifiers are often more accurate than predictions made by the best single classifier. A simplified illustration is shown in Figure 1.10. The other is theoretical [Schapire, 1990], in which it was proved that weak learners can be boosted to strong learners. Since strong learners are desirable yet difficult to get, while weak learners are easy to obtain in real practice, this result opens a promising direction of gener-

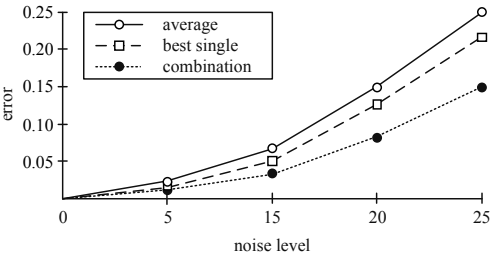


FIGURE 1.10: A simplified illustration of Hansen and Salamon [1990]'s observation: Ensemble is often better than the best single.

ating strong learners by ensemble methods.

Generally, an ensemble is constructed in two steps, i.e., generating the base learners, and then combining them. To get a good ensemble, it is generally believed that the base learners should be as *accurate* as possible, and as *diverse* as possible.

It is worth mentioning that generally, the computational cost of constructing an ensemble is not much larger than creating a single learner. This is because when we want to use a single learner, we usually need to generate multiple versions of the learner for model selection or parameter tuning; this is comparable to generating base learners in ensembles, while the computational cost for combining base learners is often small since most combination strategies are simple.

1.5 Applications of Ensemble Methods

The *KDD-Cup* [1] is the most famous data mining competition. Since 1997, it is held every year and attracts the interests of data mining teams all over the world. The competition problems cover a large variety of practical tasks, such as network intrusion detection (1999), molecular bioactivity & protein locale prediction (2001), pulmonary embolisms detection (2006), customer relationship management (2009), educational data mining (2010), music recommendation (2011), etc. In the past KDD-Cup competitions, among various techniques utilized in the solutions, ensemble methods have drawn the most attention and won the competitions for the most times. For example, in KDD-Cups of the last three years (2009-2011), all the first-place and second-place winners used ensemble methods.

[1] `http://www.sigkdd.org/kddcup/`.

Another famous competition, the *Netflix Prize*,[2] is held by the online DVD-rental service Netflix and seeks to improve the accuracy of predictions about how much someone is going to enjoy a movie based on their preferences; if one participating team improves Netflix's own algorithm by 10% accuracy, they would win the grand prize of $1,000,000. On September 21, 2009, Nexflix awarded the $1M grand prize to the team *BellKor's Pragmatic Chaos*, whose solution was based on combining various classifiers including asymmetric factor models, regression models, restricted Boltzmann machines, matrix factorization, k-nearest neighbor, etc. Another team, which achieved the winning performance but was defeated because the result was submitted 20 minutes later, even used *The Ensemble* as the team name.

In addition to the impressive results in competitions, ensemble methods have been successfully applied to diverse real-world tasks. Indeed, they have been found useful in almost all places where learning techniques are exploited. For example, computer vision has benefited much from ensemble methods in almost all branches such as object detection, recognition and tracking.

Viola and Jones [2001, 2004] proposed a general object detection framework by combining AdaBoost with a cascade architecture. Viola and Jones [2004] reported that, on a 466MHz machine, the face detector spent only 0.067 seconds for a 384×288 image; this is almost 15 times faster than state-of-the-art face detectors, while the detection accuracy is comparable. This framework was recognized as one of the most exciting breakthroughs in computer vision (especially, face detection) during the past decade.

Huang et al. [2000] designed an ensemble architecture for pose-invariant face recognition, particularly for recognizing faces with in-depth rotations. The basic idea is to combine a number of view-specific neural networks with a specially designed combination module. In contrast to conventional techniques which require pose information as input, this framework does not need pose information and it can even output pose estimation in addition to the recognition result. Huang et al. [2000] reported that this framework even outperformed conventional techniques facilitated with perfect pose information. A similar method was later applied to multi-view face detection [Li et al., 2001].

Object tracking aims to assign consistent labels to the target objects in consecutive frames of a video. By considering tracking as a binary classification problem, Avidan [2007] proposed *ensemble tracking*, which trains an ensemble online to distinguish between the object and the background. This framework constantly updates a set of weak classifiers, which can be added or removed at any time to incorporate new information about changes in object appearance and the background. Avidan [2007] showed

[2] http://www.netflixprize.com/.

that the ensemble tracking framework could work in a large variety of videos with various object size, and it runs very efficiently, at a few frames per second without optimization, hence can be used in online applications.

Ensemble methods have been found very appropriate to characterize computer security problems because each activity performed on computer systems can be observed at *multiple abstraction levels*, and the relevant information may be collected from *multiple information sources* [Corona et al., 2009].

Giacinto et al. [2003] applied ensemble methods to intrusion detection. Considering that there are different types of features characterizing the connection, they constructed an ensemble from each type of features independently, and then combined the outputs from these ensembles to produce the final decision. Giacinto et al. [2003] reported that, when detecting known attacks, ensemble methods lead to the best performance. Later, Giacinto et al. [2008] proposed an ensemble method for anomaly-based intrusion detection which is able to detect intrusions never seen before.

Malicious executables are programs designed to perform a malicious function without the owner's permission, and they generally fall into three categories, i.e., viruses, worms, and Trojan horses. Schultz et al. [2001] proposed an ensemble method to detect previously unseen malicious executables automatically, based on representing the programs using binary profiling, string sequences and hex dumps. Kolter and Maloof [2006] represented programs using n-grams of byte codes, and reported that boosted decision trees achieved the best performance; they also suggested that this method could be used as the basis for an operational system for detecting new malicious executables never seen before.

Ensemble methods have been found very useful in diverse tasks of computer aided medical diagnosis, particularly for increasing the diagnosis reliability.

Zhou et al. [2002a] designed a two-layered ensemble architecture for lung cancer cell identification, where the first layer predicts benign cases if and only if all component learners agree, and otherwise the case will be passed to the second layer to make a further decision among benign and different cancer types. Zhou et al. [2002a] reported that the two-layered ensemble results in a high identification rate with a low false-negative identification rate.

For early diagnosis of Alzheimer's disease, previous methods generally considered single channel data from the EEG (electroencephalogram). To make use of multiple data channels, Polikar et al. [2008] proposed an ensemble method where the component learners are trained on different data sources obtained from different electrodes in response to different stimuli and in different frequency bands, and their outputs are combined for the final diagnosis.

In addition to computer vision, computer security and computer aided medical diagnosis, ensemble methods have also been applied to many

other domains and tasks such as credit card fraud detection [Chan et al., 1999, Panigrahi et al., 2009], bankruptcy prediction [West et al., 2005], protein structure classification [Tan et al., 2003, Shen and Chou, 2006], species distributions forecasting [Araújo and New, 2007], weather forecasting [Maqsood et al., 2004, Gneiting and Raftery, 2005], electric load forecasting [Taylor and Buizza, 2002], aircraft engine fault diagnosis [Goebel et al., 2000, Yan and Xue, 2008], musical genre and artist classification [Bergstra et al., 2006], etc.

1.6 Further Readings

There are good textbooks on machine learning [Mitchell, 1997, Alpaydin, 2010, Bishop, 2006, Hastie et al., 2001], pattern recognition [Duda et al., 2000, Theodoridis and Koutroumbas, 2009, Ripley, 1996, Bishop, 1995] and data mining [Han and Kamber, 2006, Tan et al., 2006, Hand et al., 2001]. More introductory materials can be found in these books.

Linear discriminant analysis is closely related to **principal component analysis** (PCA) [Jolliffe, 2002], both looking for linear combination of features to represent the data. LDA is a supervised approach focusing on distinguishing between different classes, while PCA is an unsupervised approach generally used to identify the largest variability. Decision trees can be mapped to a set of "if-then" rules [Quinlan, 1993]. Most decision trees use splits like "$x \geq 1$" or "$y \geq 2$", leading to axis-parallel partitions of instance space. There are also exceptions, e.g., **oblique decision trees** [Murthy et al., 1994] which use splits like "$x+y \geq 3$", leading to non-axis-parallel partitions. The BP algorithm is the most popular and most successful neural network learning algorithm. It has many variants, and can also be used to train neural networks whose structures are different from feed-forward networks, such as **recurrent neural networks** where there are cross-layer connections. Haykin [1998] provides a good introduction to neural networks. Though the nearest neighbor algorithm is very simple, it works well in most cases. The error of the nearest neighbor classifier is guaranteed to be no worse than twice of the Bayes error rate on infinite data [Cover and Hart, 1967], and kNN approaches the Bayes error rate for some k value which is related to the amount of data. The distances between instances are not constrained to be calculated by the Euclidean distance, and the contributions from different neighbors can be weighted. More information on kNN can be found in [Dasarathy, 1991]. The naïve Bayes classifier based on the conditional independence assumption works well in most cases [Domingos and Pazzani, 1997]; however, it is believed that the performance can be improved further by relaxing the assumption, and therefore

many **semi-naïve Bayes classifiers** such as TAN [Friedman et al., 1997] and LBR [Zheng and Webb, 2000] have been developed. A particularly successful one is the AODE [Webb et al., 2005], which has incorporated ensemble mechanism and often beats TAN and LBR, especially on intermediate-size data sets. SVMs are rooted in the **statistical learning theory** [Vapnik, 1998]. More introductory materials on SVMs and kernel methods can be found in [Cristianini and Shawe-Taylor, 2000, Schölkopf et al., 1999].

Introductory materials on hypothesis tests can be found in [Fleiss, 1981]. Different hypothesis tests are usually based on different assumptions, and should be applied in different situations. The 10-fold cross-validation t-test was popularly used; however, Dietterich [1998] discloses that such a test underestimates the variability and it is likely to incorrectly detect a difference when no difference exists (i.e., the type I error), while the 5×2cv paired t-test is recommended instead.

The **No Free Lunch Theorem** [Wolpert, 1996, Wolpert and Macready, 1997] implies that it is hopeless to dream for a learning algorithm which is consistently better than other learning algorithms. It is important to notice, however, that the No Free Lunch Theorem considers the whole problem space, that is, all the possible learning tasks; while in real practice, we are usually only interested in a give task, and in such a situation, the effort of trying to find the best algorithm is valid. From the experience of the author of this book, for lots of tasks, the best off-the-shelf learning technique at present is ensemble methods such as Random Forest facilitated with **feature engineering** which constructs/generates usually an overly large number of new features rather than simply working on the original features.

[Kuncheva, 2004] and [Rokach, 2010] are books on ensemble methods. Xu and Amari [2009] discuss the relation between *combining classifiers* and *mixture of experts*. The *MCS* workshop (*International Workshop on Multiple Classifier Systems*) is the major forum in this area. Abundant literature on ensemble methods can also be found in various journals and conferences on machine learning, pattern recognition and data mining.

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