PATTERN CLASSIFICATION AND SCENE ANALYSIS

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to C. A. Rosen

PREFACE

Our purpose in writing this book has been to give a systematic account of major topics in pattern recognition, a field concerned with machine recognition of meaningful regularities in noisy or complex environments. Stimulated by the development of the digital computer, pattern recognition blossomed in the early 1960's and has enjoyed more than a decade of vigorous growth. Contributions to the growth have come from many disciplines, including statistics, communication theory, switching theory, control theory, operations research, biology, psychology, linguistics, and computer science. Readers who sample the literature will soon appreciate the color and vigor that this has lent the field.

This diversity also presents serious problems to anyone writing a book on the subject. No single theory of pattern recognition embraces all of the important topics because each domain of application has unique characteristics that mold and shape the appropriate approach. The most prominent domain-independent theory is classification theory, the subject of Part I of this book. Based on statistical decision theory, it provides formal mathematical procedures for classifying patterns once they have been represented abstractly as vectors.

Attempts to find domain-independent procedures for constructing these vector representations have not yielded generally useful results. Instead, every problem area has acquired a collection of procedures suited to its special characteristics. Of the many areas of interest, the pictorial domain has received by far the most attention. Furthermore, work in this area has progressed from picture classification to picture analysis and description. Part II of this book is devoted to a systematic presentation of these topics in visual scene analysis.

Since the theories and techniques of pattern recognition are largely mathematical in nature, we should say something about the level of mathematical rigor in our exposition. In a word, it is low. We have been far more concerned with providing insight and understanding than with establishing rigorous mathematical foundations. The presence of many illustrative examples, plausibility arguments, and discussions of the behavior of solutions

reflects this concern. Concomitantly, we have avoided the use of measure theory, and we have tried to avoid preoccupation with such fine points as modes of convergence for sequences of random variables, justification for the use of delta functions, and possibilities of pathological cases. We do assume general knowledge of a number of basic topics in applied mathematics, including probability theory and linear algebra; an acquaintance with Fourier transforms would also be helpful in Chapter 8. The required mathematical maturity is that of a typical first-year graduate student in computer science, electrical engineering, or statistics.

Since pattern recognition appears to be a rather specialized topic, it is perhaps worthwhile to draw attention to the pedagogic flexibility of a course on the subject. Drawing as it does from several branches of mathematics as well as the other disciplines we mentioned, pattern recognition provides a nearly ideal vehicle for the presentation of a variety of topics within a single framework. Students with no long-term interest in pattern recognition per se are still likely to acquire knowledge and develop skills that will serve them well in other settings.

We have taught graduate courses based on the material in this book at the University of California, Berkeley, and at Stanford University. Each part of the book can be covered moderately well in independent, one-quarter, three-hour courses, and quite thoroughly in a one-semester course. For an abridged treatment, we recommend selecting a few topics from most of the chapters in preference to treating some chapters thoroughly and others not at all. As always, the interests of the instructor must dictate the final choice of material.

We also hope that this book will prove useful to the practicing professional, and to this end we have tried to make the material in it as accessible as possible. We have taken care to use standard notation whenever we could, and have included a comprehensive index. Each chapter concludes with bibliographical and historical remarks and a hopefully useful list of references. Although the lengths of these lists perhaps lend the book an air of scholarliness, the published literature is too extensive to allow us to be complete, and we make no claims in this regard.

While writing this book we benefitted from associations with many individuals and organizations. We would like first to thank the Information Systems Branch of the Office of Naval Research for its sponsorship under Contract N0014-68-C-0266. The Department of Electrical Engineering and Computer Sciences at Berkeley and the Computer Science Department at Stanford afforded us opportunities to test this material in the classroom. The Artificial Intelligence Center of Stanford Research Institute, under the enthusiastic leadership of Dr. Charles A. Rosen and Dr. Bertram Raphael, provided an ideal environment in which to work. Although we cannot mention

everyone who has helped us with their comments, we would like especially to thank Dr. Nils J. Nilsson for his many suggestions for improving the manuscript. In addition, we feel indebted to Dr. Thomas O. Binford, Dr. Thomas M. Cover, Mr. Claude L. Fennema, Dr. Gabriel F. Groner, Mr. David J. Hall, Dr. Martin E. Hellman, Dr. Michael A. Kassler, and Dr. John H. Munson for their thoughtful comments. We want also to thank Dr. Richard C. Singleton for his work in producing the pictorial examples in Chapter 8. Finally, it is a pleasure to acknowledge the cheerful help of Katharine L. Spence in typing several drafts of the manuscript.

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Part I

PATTERN CLASSIFICATION

Chapter 1

INTRODUCTION

1.1 MACHINE PERCEPTION

Since the advent of the digital computer there has been a constant effort to expand the domain of computer applications. Some of the motivation for this effort comes from important practical needs to find more efficient ways of doing things. Some of the motivation comes from the sheer challenge of building or programming a machine to do things that machines have never done before. Both of these motives are found in that area of artificial intelligence that we shall call machine perception.

At present, the ability of machines to perceive their environment is very limited. A variety of transducers are available for converting light, sound, temperature, etc., to electrical signals. When the environment is carefully controlled and the signals have a simple interpretation, as is the case with the standard computer input devices, the perceptual problems become trivial. But as we move beyond having a computer read punched cards or magnetic tapes to having it read hand-printed characters or analyze biomedical photographs, we move from problems of sensing the data to much more difficult problems of interpreting the data.

The apparent ease with which vertebrates and even insects perform perceptual tasks is at once encouraging and frustrating. Psychological and physiological studies have given us a great many interesting facts about animal perception, but no understanding sufficient for us to duplicate their performance with a computer. The problem area has a certain unique fascination to it because perception is something everyone experiences but no one really understands. Introspection has not proved as helpful in discovering the nature of perception as one might hope, apparently because most everyday perceptual processes are carried out below the conscious level. Paradoxically, we are all expert at perception, but none of us knows much about it.

The lack of a complete theory of perception has not prevented people from trying to solve more modest problems. Many of these involve pattern

classification—the assignment of a physical object or event to one of several prespecified categories. Extensive study of classification problems has led to an abstract mathematical model that provides the theoretical basis for classifier design. Of course, in any specific application one ultimately must come to grips with the special characteristics of the problem at hand. Of the various problem areas, the domain of pictorial problems has received by far the most attention. The purpose of this book is to give a systematic account of those principles of pattern classification and those techniques of pictorial scene analysis that seem to have the widest applicability and interest.

1.2 AN EXAMPLE

To illustrate some of the types of problems we shall address, let us consider the following imaginary and somewhat fanciful example. Suppose that a lumber mill producing assorted hardwoods wants to automate the process of sorting finished lumber according to species of tree. As a pilot project, it is decided to try first to distinguish birch lumber from ash lumber using optical sensing. A system to perform this very specific task might well have the form shown in Figure 1.1. The camera takes a picture of the lumber and passes the picture on to a *feature extractor*, whose purpose is to reduce the data by measuring certain "features" or "properties" that distinguish pictures of birch lumber from pictures of ash lumber. These features (or, more precisely, the values of these features) are then passed to a *classifier* that evaluates the evidence presented and makes a final decision about the lumber type.

Let us consider how the feature extractor and classifier might be designed. Suppose somebody at the lumber mill tells us that birch is often lighter colored than ash. Then brightness becomes an obvious feature, and we might attempt to classify the lumber merely by seeing whether or not the average brightness x exceeds some critical value x_0. To choose x_0, we could obtain some samples of the different types of wood, make brightness measurements, and inspect the results. Suppose that we do this, and obtain the histograms

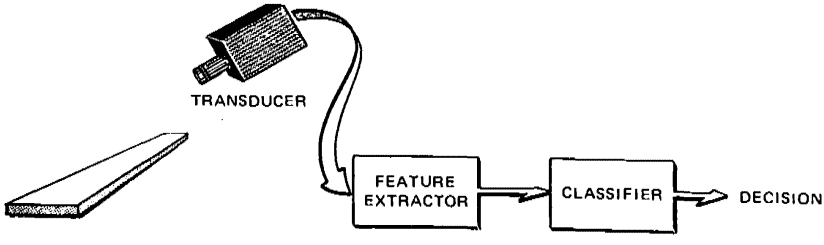

FIGURE 1.1. A pattern classification system.

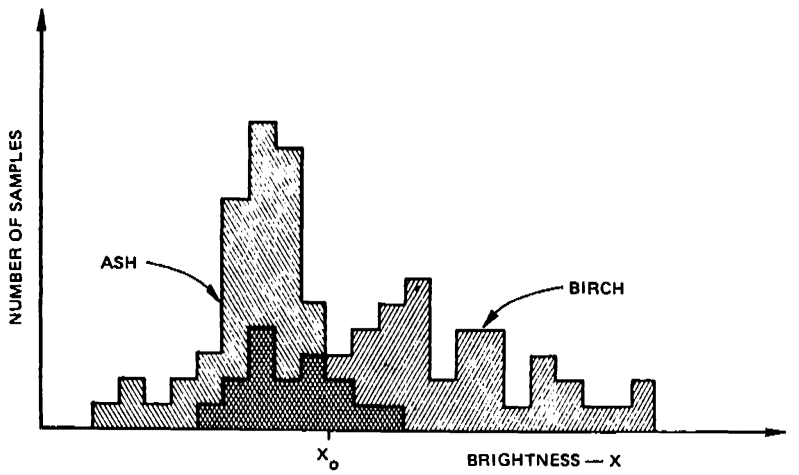

FIGURE 1.2. Histograms for the brightness feature.

shown in Figure 1.2. These histograms bear out the statement that birch is usually lighter than ash, but it is clear that this single criterion is not infallible. No matter how we choose x_0, we can not reliably separate birch from ash by brightness alone.

In our search for other features, we might try to capitalize on the observation that ash typically has a more prominent grain pattern than birch. This feature is much more difficult to measure than average brightness, but it is reasonable to assume that we can obtain a measure of grain prominence from the magnitude and frequency of occurrence of light-to-dark transitions in the picture. Now we have two features for classifying lumber, the brightness x_1 and the grain prominence x_2. The feature extractor has thus reduced each picture to a point or *feature vector* $\mathbf{x}$ in a two-dimensional feature space, where

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}.$$

Our problem now is to partition the feature space into two regions, where all the points in one region correspond to birch, and all points in the other correspond to ash. Suppose that we measure the feature vectors for our samples and obtain the scattering of points shown in Figure 1.3. This plot suggests the following rule for classifying the data: Classify the lumber as ash if its feature vector falls above the line AB, and as birch otherwise.

While this rule appears to do a good job of separating our samples, we have no guarantee that it will perform as well on new samples. It would certainly be prudent to obtain some more samples and see how many are

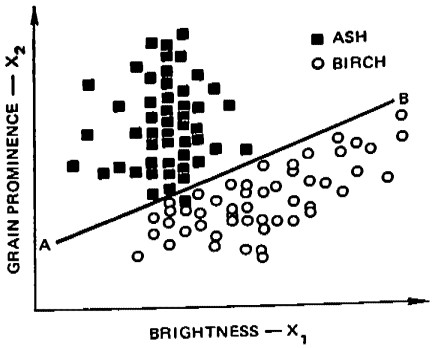

FIGURE 1.3. Scatter diagram for the feature vectors.

correctly classified. This suggests that our problem has a statistical component, and that perhaps we should look for a classification procedure that minimizes the probability of error.

Without forgetting this idea, we should remember that we chose a simple problem for a pilot project. A more realistic problem might involve sorting many different classes of lumber. To separate oak from birch and ash, we might well require less obvious features, such as "straightness-of-grain." With more categories and more features, the graphical approach to designing the classifier will probably have to be abandoned. To proceed further, we shall need whatever theoretical help we can get.

1.3 THE CLASSIFICATION MODEL

The preceding example contains many of the elements of the most commonly used abstract model for pattern recognition, the classification model. This model contains three parts: a transducer, a feature extractor, and a classifier The transducer senses the input and converts it into a form suitable for machine processing. The feature extractor (also called the receptor, property filter, attribute detector, or preprocessor) extracts presumably relevant information from the input data. The classifier uses this information to assign the input data to one of a finite number of categories.

A discussion of transducer specification or design lies outside the province of this book. However, we shall be concerned with both feature extraction and classification. From a theoretical viewpoint, the line between these topics is arbitrary. An ideal feature extractor would make the job of the classifier trivial, and an omnipotent classifier would not need the help of a feature extractor. The distinction is forced upon us for practical, not theoretical reasons, but the distinction is important nevertheless.

Generally speaking, the problem of feature extraction is much more problem dependent than the problem of classification. A good feature extractor for sorting lumber would probably be of little use for identifying fingerprints or classifying photomicrographs of blood cells. Nevertheless, a substantial body of techniques has been developed for extracting useful information from pictures. Part II of this book is devoted to an exposition of these techniques and their properties.

The problem of classification is basically one of partitioning the feature space into regions, one region for each category. Ideally, one would like to arrange this partitioning so that none of the decisions is ever wrong. When this cannot be done, one would like to minimize the probability of error, or, if some errors are more costly than others, the average cost of errors. In this case, the problem of classification becomes a problem in statistical decision theory, a subject that has many applications to pattern classification. Part I of this book is concerned with these and related topics in classification theory.

1.4 THE DESCRIPTIVE APPROACH

There are many problems in pattern recognition and machine perception for which the classification model is clearly inappropriate. For example, in analyzing a picture of bubble-chamber particle tracks, one wants a description, rather than just a classification, of the picture. Such a description should contain information about both the individual parts of the picture and about the relations among the parts. Ideally, it should directly reflect the structure present in the original scene.

Consider, for example, the simple scene shown in Figure 1.4. It is possible that a simple classification such as "office scene" or "telephone present" would be adequate for some purposes. A more complete analysis would include an identification of all the major objects present—the telephone, note pad, cup, pencils, eraser, etc. An even more complete analysis would indicate the relations between these objects, and might result in a description such as "(Two pencils on top of a pad) in front of (a cup to the left of (an eraser in front of a telephone))."

The problem of analyzing a visual scene and producing a structural description has proved to be quite difficult. A generally accepted formalization of the problem, analogous to the classification model, has yet to emerge from the work that has been done to date. Attempts have been made to borrow concepts from the theory of formal languages and to produce a linguistic model for scene analysis. Here the scene is viewed as a statement in a language whose grammar defines the allowed structural relations. With

FIGURE 1.4. A simple scene.

this formulation, scene analysis is viewed as the process of using a picture grammar to parse the scene, producing a description of the scene as a composition of related subscenes.

The linguistic model does not exhaust the ways of using known structural relations among the elements of a picture to guide its analysis and produce a useful description. Some of the most interesting procedures that have been developed are ad hoc and heuristic; a unifying conceptual framework encompassing all of these methods has not yet been developed. The procedures themselves can be described, however, and this general topic of descriptive approaches to scene analysis concludes Part II.

1.5 SUMMARY OF THE BOOK BY CHAPTERS

The orientation of Part I of this book is primarily statistical. Chapter 2 states the classification problem in decision-theoretic terms, and derives the general form for an optimal classifier. This solution is obtained under the assumption that all of the probability distributions involved are known. The remainder

of Part I is concerned with ways of proceeding when the probabilistic structure is not known.

In Chapter 3 we assume that everything is known except for some parameters of the distributions. Both maximum likelihood and Bayesian procedures for estimating parameters from samples are described. If none of the standard ways of parameterizing unknown distributions is suitable, one can resort to nonparametric techniques. These procedures, which are discussed in Chapter 4, exchange the need for knowledge of the forms of the distributions for the need for a large number of samples.

In Chapter 5 we parameterize the classifier and study ways of using samples to determine the classifier directly. These techniques have their origin in Fisher's linear discriminant, and include the well known perceptron and relaxation procedures, minimum-squared-error methods, stochastic approximation, the method of potential functions, and linear programming techniques. Chapter 6 concludes Part I with a discussion of various techniques for unsupervised learning and clustering.

Chapter 7 begins Part II with a discussion of procedures for representing pictures, and for performing such basic operations as sharpening, smoothing, template matching, and partitioning a picture into homogeneous regions. Chapter 8 develops the concept of spatial filtering, and interprets some of these operations in the frequency domain. Chapter 9 is concerned with a great variety of procedures for describing lines and shapes in pictures. Topological, linear, and metric properties of shape are described, together with a number of descriptive techniques based on these properties.

Chapters 10 and 11 present important mathematical background relevant to pictures of three-dimensional objects. Chapter 10 develops the equations for perspective transformation, and shows how they can be usefully employed in scene analysis. Chapter 11 treats the subject of projective invariants, quantities that are the same in different pictures of the same object. Finally, Chapter 12 discusses some of the more important contemporary approaches to the difficult problem of completely analyzing visual scenes.

1.6 BIBLIOGRAPHICAL REMARKS

The published literature on pattern classification and scene analysis has grown to the point where even specialized bibliographies can contain hundreds of references. The references that we give at the end of each chapter hopefully will provide the reader with some historical perspective and a good starting point for further study. Additional guidance can be obtained from other texts and from a number of valuable survey articles.

For a brief overview that treats pattern recognition as one topic in artificial intelligence, the influential article by Minsky (1961) is highly recommended. Nagy (1968) provides an excellent survey of work done using the classification model. The text by Nilsson (1965) provides an exceptionally clear treatment of classification procedures. A lucid and more recent survey of these procedures is given by Ho and Agrawala (1968). Levine (1969) gives a comprehensive survey of the techniques that have been used to extract features from pictures. The general subject of automatic picture processing is well surveyed by Hawkins (1970), and is systematically treated in the scholarly text by Rosenfeld (1969).

There are many interesting subject areas that are related to this book but beyond its scope. Readers interested in image enhancement and picture coding should be aware of the survey by Huang, Schreiber and Tretiak (1971). Those interested in the fascinating area of human and animal perception will find the surveys by Kolers (1968) and Gose (1969) most useful. Those interested in philosophical issues will find the books by Watanabe (1969) and Bongard (1970) thought provoking. Finally, those interested in the practical applications of all of this theory will find a wealth of references in the literature survey by Stevens (1970).

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Chapter 2

BAYES DECISION THEORY

2.1 INTRODUCTION

Bayes decision theory is a fundamental statistical approach to the problem of pattern classification. This approach is based on the assumption that the decision problem is posed in probabilistic terms, and that all of the relevant probability values are known. In this chapter we develop the fundamentals of this theory, and show how it can be viewed as being simply a formalization of common-sense procedures; in subsequent chapters we will consider the problems that arise when the probabilistic structure is not completely known.

While we will give a quite general, abstract development of Bayes decision theory in Section 2.2, we begin our discussion with a specific example. Let us reconsider the hypothetical problem posed in Chapter 1 of designing a classifier to separate two kinds of lumber, ash and birch. Suppose that an observer watching lumber emerge from the mill finds it so hard to predict what type will emerge next that the sequence of types of lumber appears to be random. Using decision-theoretic terminology, we say that as each piece of lumber emerges, nature is in one or the other of the two possible states: either the lumber is ash or the lumber is birch. We let ω denote the *state of nature*, with $\omega = \omega_1$ for ash and $\omega = \omega_2$ for birch. Because the state of nature is so unpredictable, we consider ω to be a random variable.

If the mill produced as much ash as birch, we would say that the next piece of lumber is equally likely to be ash or birch. More generally, we assume that there is some *a priori probability* $P(\omega_1)$ that the next piece is ash, and some a priori probability $P(\omega_2)$ that it is birch. These a priori probabilities reflect our prior knowledge of how likely we are to see ash or birch before

the lumber actually appears. It goes without saying that $P(\omega_1)$ and $P(\omega_2)$ are nonnegative and sum to one.*

Suppose for a moment that we were forced to make a decision about the type of lumber that will appear next without being allowed to see it. The only information we are allowed to use is the value of the a priori probabilities. If a decision must be made with so little information, it seems reasonable to use the following *decision rule:* Decide ω_1 if $P(\omega_1) > P(\omega_2)$; otherwise decide ω_2.

This may seem like a strange procedure, in that we always make the same decision even though we know that both types of lumber will appear. How well it works depends upon the values of the a priori probabilities. If $P(\omega_1)$ is very much greater than $P(\omega_2)$, our decision in favor of ω_1 will be right most of the time. If $P(\omega_1) = P(\omega_2)$, we have only a fifty-fifty chance of being right. In general, the probability of error is the smaller of $P(\omega_1)$ and $P(\omega_2)$, and we shall see later that under these conditions no other decision rule can yield a smaller probability of error.

In most circumstances, one is not asked to make decisions with so little evidence. In our example, we can use the brightness measurement x as evidence. Different samples of lumber will yield different brightness readings, and it is natural to express this variability in probabilistic terms; we consider x to be a continuous random variable whose distribution depends on the state of nature. Let $p(x \mid \omega_j)$ be the *state-conditional probability density* function for x, the probability density function for x given that the state of nature is ω_j. Then the difference between $p(x \mid \omega_1)$ and $p(x \mid \omega_2)$ describes the difference in brightness between ash and birch (see Figure 2.1).

Suppose that we know both the a priori probabilities $P(\omega_j)$ and the conditional densities $p(x \mid \omega_j)$. Suppose further that we measure the brightness of a piece of lumber and discover the value of x. How does this measurement influence our attitude concerning the true state of nature? The answer to this question is provided by *Bayes Rule:*

$$P(\omega_j \mid x) = \frac{p(x \mid \omega_j)P(\omega_j)}{p(x)}, \tag{1}$$

where

$$p(x) = \sum_{j=1}^{2} p(x \mid \omega_j)P(\omega_j). \tag{2}$$

Bayes rule shows how observing the value of x changes the a priori probability $P(\omega_j)$ to the *a posteriori* probability $P(\omega_j \mid x)$. The variation of $P(\omega_j \mid x)$ with x is illustrated in Figure 2.2 for the case $P(\omega_1) = 2/3$ and $P(\omega_2) = 1/3$.

* Regarding notation, we generally use an upper-case P to denote a probability mass function and a lower-case p to denote a probability density function. Probability density functions are nonnegative and integrate to one.

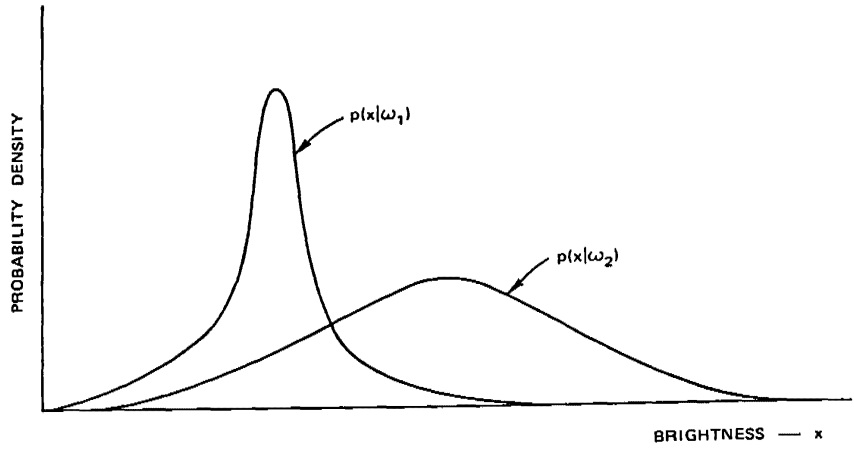


FIGURE 2.1. Hypothetical class-conditional probability density functions.

If we have an observation x for which $P(\omega_1 \mid x)$ is greater than $P(\omega_2 \mid x)$, we would be naturally inclined to decide that the true state of nature is ω_1. Similarly, if $P(\omega_2 \mid x)$ is greater than $P(\omega_1 \mid x)$, we would be inclined to choose ω_2. To justify this procedure, let us calculate the probability of error whenever we make a decision. Whenever we observe a particular x,

$$P(\text{error} \mid x) = \begin{cases} P(\omega_1 \mid x) & \text{if we decide } \omega_2 \\ P(\omega_2 \mid x) & \text{if we decide } \omega_1. \end{cases}$$

Clearly, in every instance in which we observe the same value for x, we can minimize the probability of error by deciding ω_1 if $P(\omega_1 \mid x) > P(\omega_2 \mid x)$, and ω_2 if $P(\omega_2 \mid x) > P(\omega_1 \mid x)$. Of course, we may never observe exactly the same value of x twice. Will this rule minimize the average probability of

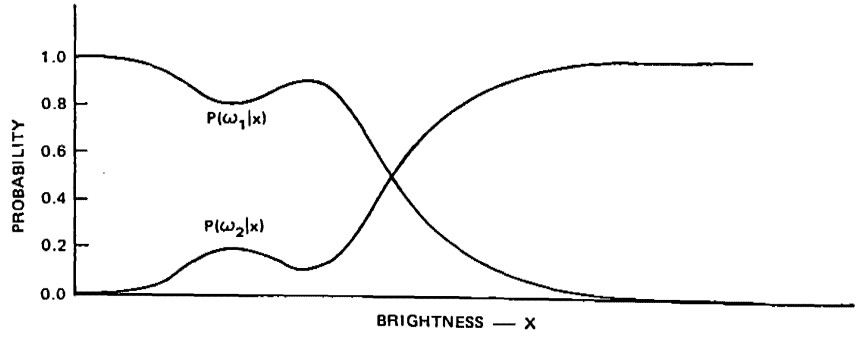


FIGURE 2.2. A posteriori probabilities for $P(\omega_1) = \frac{2}{3}$, $P(\omega_2) = \frac{1}{3}$.

error? Yes, because the average probability of error is given by

$$P(\text{error}) = \int_{-\infty}^{\infty} P(\text{error}, x)\, dx$$

$$= \int_{-\infty}^{\infty} P(\text{error} \mid x) p(x)\, dx,$$

and if for every x, $P(\text{error} \mid x)$ is as small as possible, the integral must be as small as possible. Thus we have justified the following *Bayes decision rule* for minimizing the probability of error:

Decide ω_1 if $P(\omega_1 \mid x) > P(\omega_2 \mid x)$; otherwise decide ω_2.

This form of the decision rule emphasizes the role of the a posteriori probabilities. By using Eq. (1), we can express the rule in terms of the conditional and a priori probabilities. Note that $p(x)$ in Eq. (1) is unimportant as far as making a decision is concerned. It is basically just a scale factor that assures us that $P(\omega_1 \mid x) + P(\omega_2 \mid x) = 1$. By eliminating this scale factor, we obtain the following completely equivalent decision rule:

Decide ω_1 if $p(x \mid \omega_1)P(\omega_1) > p(x \mid \omega_2)P(\omega_2)$; otherwise decide ω_2.

Some additional insight can be obtained by considering a few special cases. If for some x, $p(x \mid \omega_1) = p(x \mid \omega_2)$, then that particular observation gives us no information about the state of nature; in this case, the decision hinges entirely on the a priori probabilities. On the other hand, if $P(\omega_1) = P(\omega_2)$, then the states of nature are equally likely a priori; in this case the decision is based entirely on $p(x \mid \omega_j)$, the *likelihood* of ω_j with respect to x. In general, both of these factors are important in making a decision, and the Bayes decision rule combines them to achieve the minimum probability of error.

2.2 BAYES DECISION THEORY— THE CONTINUOUS CASE

We shall now formalize the ideas just considered, and shall generalize them in four ways:

(1) We shall allow the use of more than one feature.
(2) We shall allow more than two states of nature.
(3) We shall allow actions other than deciding on the state of nature.
(4) We shall introduce a loss function more general than probability of error.

These generalizations and their attendant notational complexities should not be allowed to obscure the fact that things are basically much the same as they were in our simple example. Allowing the use of more than one feature merely requires replacing the scalar x by the *feature vector* $\mathbf{x}$. Allowing more than two states of nature provides us with a useful generalization for a small notational expense. Allowing actions other than classification primarily allows the possibility of rejection, i.e., of refusing to make a decision in close cases; this is a useful option if being indecisive is not too costly. The loss function states exactly how costly each action is. In theory, it also lets us treat situations in which some kinds of mistakes are more costly than others, although most of the nice analytical results are obtained for the case where all errors are equally costly. With this as a preamble, let us begin the formal treatment.

Let $\Omega = \{\omega_1, \ldots, \omega_s\}$ be the finite set of s states of nature and $A = \{\alpha_1, \ldots, \alpha_a\}$ be the finite set of a possible actions. Let $\lambda(\alpha_i \mid \omega_j)$ be the loss incurred for taking action α_i when the state of nature is ω_j. Let the feature vector $\mathbf{x}$ be a d-component vector-valued random variable, and let $p(\mathbf{x} \mid \omega_j)$ be the state-conditional probability density function for $\mathbf{x}$, the probability density function for $\mathbf{x}$ conditioned on ω_j being the state of nature. Finally, let $P(\omega_j)$ be the a priori probability that nature is in state ω_j. Then the a posteriori probability $P(\omega_j \mid \mathbf{x})$ can be computed from $p(\mathbf{x} \mid \omega_j)$ by Bayes rule:

$$P(\omega_j \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid \omega_j)P(\omega_j)}{p(\mathbf{x})}, \tag{3}$$

where

$$p(\mathbf{x}) = \sum_{j=1}^{s} p(\mathbf{x} \mid \omega_j)P(\omega_j). \tag{4}$$

Suppose that we observe a particular $\mathbf{x}$ and that we contemplate taking action α_i. If the true state of nature is ω_j, we will incur the loss $\lambda(\alpha_i \mid \omega_j)$. Since $P(\omega_j \mid \mathbf{x})$ is the probability that the true state of nature is ω_j, the expected loss associated with taking action α_i is merely

$$R(\alpha_i \mid \mathbf{x}) = \sum_{j=1}^{s} \lambda(\alpha_i \mid \omega_j)P(\omega_j \mid \mathbf{x}). \tag{5}$$

In decision-theoretic terminology, an expected loss is called a *risk*, and $R(\alpha_i \mid \mathbf{x})$ is known as the *conditional risk*. Whenever we encounter a particular observation $\mathbf{x}$, we can minimize our expected loss by selecting the action that minimizes the conditional risk. We shall now show that this actually is the optimal Bayes decision procedure.

Stated formally, our problem is to find a Bayes decision rule against $P(\omega_j)$ that minimizes the overall risk. A *decision rule* is a function $\alpha(\mathbf{x})$ that tells us

which action to take for every possible observation.* To be more specific, for every $\mathbf{x}$ the *decision function* $\alpha(\mathbf{x})$ assumes one of the a values $\alpha_1, \ldots, \alpha_a$. The overall risk R is the expected loss associated with a given decision rule. Since $R(\alpha_i \mid \mathbf{x})$ is the conditional risk associated with action α_i, and since the decision rule specifies the action, the overall risk is given by

$$R = \int R(\alpha(\mathbf{x}) \mid \mathbf{x}) p(\mathbf{x})\, d\mathbf{x}, \tag{6}$$

where $d\mathbf{x}$ is our notation for a d-space volume element, and where the integral extends over the entire feature space. Clearly, if $\alpha(\mathbf{x})$ is chosen so that $R(\alpha(\mathbf{x}) \mid \mathbf{x})$ is as small as possible for every $\mathbf{x}$, then the overall risk will be minimized. This justifies the following statement of the *Bayes decision rule:* To minimize the overall risk, compute the conditional risk

$$R(\alpha_i \mid \mathbf{x}) = \sum_{j=1}^{s} \lambda(\alpha_i \mid \omega_j) P(\omega_j \mid \mathbf{x}) \tag{5}$$

for $i = 1, \ldots, a$ and select the action α_i for which $R(\alpha_i \mid \mathbf{x})$ is minimum. (Note that if more than one action minimizes $R(\alpha_i \mid \mathbf{x})$, it does not matter which of these actions is taken, and any convenient tie-breaking rule can be used.) The resulting minimum overall risk is called the *Bayes risk* and is the best performance that can be achieved.

2.3 TWO-CATEGORY CLASSIFICATION

Let us specialize these results by considering the two-category classification problem. Here action α_1 corresponds to deciding that the true state of nature is ω_1, and action α_2 corresponds to deciding that it is ω_2. For notational simplicity, let $\lambda_{ij} = \lambda(\alpha_i \mid \omega_j)$, the loss incurred for deciding ω_i when the true state of nature is ω_j. If we write out the conditional risk given by Eq. (5), we obtain

$$R(\alpha_1 \mid \mathbf{x}) = \lambda_{11} P(\omega_1 \mid \mathbf{x}) + \lambda_{12} P(\omega_2 \mid \mathbf{x})$$
$$R(\alpha_2 \mid \mathbf{x}) = \lambda_{21} P(\omega_1 \mid \mathbf{x}) + \lambda_{22} P(\omega_2 \mid \mathbf{x}).$$

There are a variety of ways of expressing the minimum-risk decision rule each having its own minor advantages. The fundamental rule is to decide ω_1 if $R(\alpha_1 \mid \mathbf{x}) < R(\alpha_2 \mid \mathbf{x})$. In terms of the a posteriori probabilities, we decide, ω_1 if

$$(\lambda_{21} - \lambda_{11}) P(\omega_1 \mid \mathbf{x}) > (\lambda_{12} - \lambda_{22}) P(\omega_2 \mid \mathbf{x}).$$

* The reader familiar with game theory will recognize this as a deterministic decision rule. In game theory, nature is replaced by a malicious opponent who can take advantage of a deterministic strategy, and randomized decision rules are often advantageous. However, randomized decision rules offer no such advantage in our situation. Problem 8 leads the reader through a mathematical demonstration of this fact.

Ordinarily, the loss incurred for making an error is greater than the loss incurred for being correct, and both of the factors $\lambda_{21} - \lambda_{11}$ and $\lambda_{12} - \lambda_{22}$ are positive. Thus, our decision is basically determined by the more likely state of nature, although we must scale the a posteriori probabilities by the appropriate loss differences. By invoking Bayes rule, we can replace the a posteriori probabilities by the a priori probabilities and the conditional densities. This results in the equivalent rule to decide ω_1 if

$$(\lambda_{21} - \lambda_{11})p(\mathbf{x} \mid \omega_1)P(\omega_1) > (\lambda_{12} - \lambda_{22})p(\mathbf{x} \mid \omega_2)P(\omega_2).$$

Another alternative, which follows at once under the reasonable assumption that $\lambda_{21} > \lambda_{11}$, is to decide ω_1 if

$$\frac{p(\mathbf{x} \mid \omega_1)}{p(\mathbf{x} \mid \omega_2)} > \frac{\lambda_{12} - \lambda_{22}}{\lambda_{21} - \lambda_{11}} \frac{P(\omega_2)}{P(\omega_1)}.$$

This form of the decision rule focusses on the x-dependence of the probability densities. Viewed as a function of ω_j, $p(\mathbf{x} \mid \omega_j)$ is called the *likelihood* of ω_j with respect to $\mathbf{x}$, and $p(\mathbf{x} \mid \omega_1)/p(\mathbf{x} \mid \omega_2)$ is called the *likelihood ratio*. Thus, the Bayes decision rule can be interpreted as calling for decision ω_1 if the likelihood ratio exceeds a threshold value that is independent of the observation $\mathbf{x}$.

2.4 MINIMUM-ERROR-RATE CLASSIFICATION

In classification problems, each state of nature is usually associated with a different one of the c classes, and the action α_i is usually interpreted as the decision that the true state of nature is ω_i.* If action α_i is taken and the true state of nature is ω_j, then the decision is correct if $i = j$, and in error if $i \neq j$. If errors are to be avoided, it is natural to seek a decision rule that minimizes the average probability of error, i.e., the *error rate*.

A loss function of particular interest for this case is the so-called *symmetrical* or *zero-one* loss function,

$$\lambda(\alpha_i \mid \omega_j) = \begin{cases} 0 & i = j \\ 1 & i \neq j \end{cases} \qquad i, j = 1, \ldots, c. \tag{7}$$

This loss function assigns no loss to a correct decision, and assigns a unit loss to any error. Thus, all errors are equally costly. The risk corresponding to this loss function is precisely the average probability of error, since the

* In this case $a = s = c$, the number of classes. Sometimes it is useful to define a reject action α_{c+1}; this case is the subject of Problems 6 and 7.

conditional risk is

$$R(\alpha_i \mid \mathbf{x}) = \sum_{j=1}^{c} \lambda(\alpha_i \mid \omega_j) P(\omega_j \mid \mathbf{x})$$

$$= \sum_{j \neq i} P(\omega_j \mid \mathbf{x})$$

$$= 1 - P(\omega_i \mid \mathbf{x}), \tag{8}$$

and $P(\omega_i \mid \mathbf{x})$ is the conditional probability that action α_i is correct. The Bayes decision rule to minimize risk calls for selecting the action that minimizes the conditional risk. Thus, to minimize the average probability of error, we should select the i that *maximizes* the a posteriori probability $P(\omega_i \mid \mathbf{x})$. In other words, for *minimum error rate:*

$$\text{Decide } \omega_i \text{ if } P(\omega_i \mid \mathbf{x}) > P(\omega_j \mid \mathbf{x}) \text{ for all } j \neq i.$$

2.5 CLASSIFIERS, DISCRIMINANT FUNCTIONS, AND DECISION SURFACES

2.5.1 The Multicategory Case

There are many different ways to represent pattern classifiers. One way, which yields something like a canonical form for classifiers, is in terms of a set of *discriminant functions* $g_i(\mathbf{x})$, $i = 1, \ldots, c$. The classifier is said to assign a feature vector $\mathbf{x}$ to class ω_i if

$$g_i(\mathbf{x}) > g_j(\mathbf{x}) \qquad \text{for all } j \neq i. \tag{9}$$

Thus, the classifier is viewed as a machine that computes c discriminant functions and selects the category corresponding to the largest discriminant. This representation of a classifier is illustrated in block-diagram form in Figure 2.3.

A Bayes classifier is easily and naturally represented in this way. For the general case, we can let $g_i(\mathbf{x}) = -R(\alpha_i \mid \mathbf{x})$, since the maximum discriminant function will then correspond to the minimum conditional risk. For the minimum-error-rate case, we can simplify things further by taking $g_i(\mathbf{x}) = P(\omega_i \mid \mathbf{x})$, so that the maximum discriminant function corresponds to the maximum a posteriori probability.

Clearly, the choice of discriminant functions is not unique. We can always multiply the discriminant functions by a positive constant or bias them by an additive constant without influencing the decision. More generally, if we replace every $g_i(\mathbf{x})$ by $f(g_i(\mathbf{x}))$, where f is a monotonically increasing function,

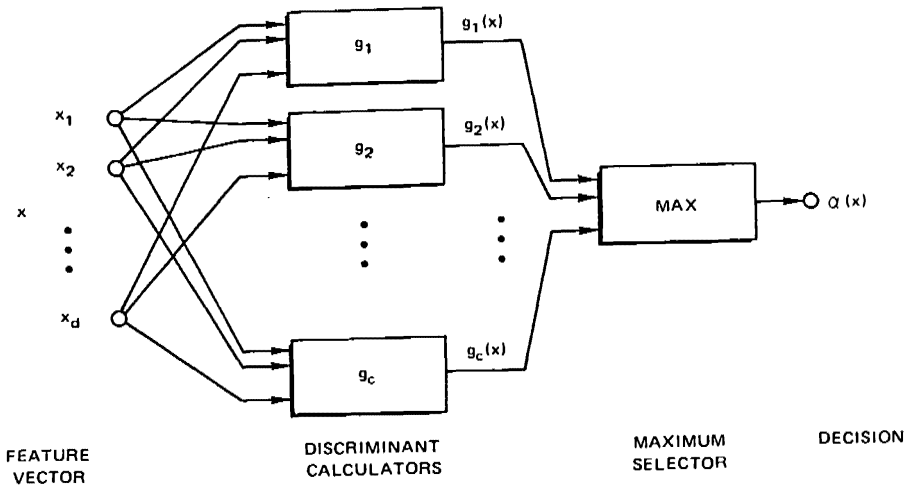


FIGURE 2.3. A pattern classifier.

the resulting classification is unchanged. This observation can lead to significant analytical and computational simplifications. In particular, for minimum-error-rate classification, any of the following choices gives identical classification results, but some can be much simpler to understand or to compute than others:

$$g_i(\mathbf{x}) = P(\omega_i \mid \mathbf{x}) \tag{10}$$

$$g_i(\mathbf{x}) = \frac{p(\mathbf{x} \mid \omega_i)P(\omega_i)}{\sum_{j=1}^{c} p(\mathbf{x} \mid \omega_j)P(\omega_j)} \tag{11}$$

$$g_i(\mathbf{x}) = p(\mathbf{x} \mid \omega_i)P(\omega_i) \tag{12}$$

$$g_i(\mathbf{x}) = \log p(\mathbf{x} \mid \omega_i) + \log P(\omega_i). \tag{13}$$

Even though the discriminant functions can be written in a variety of forms, the decision rules are equivalent. The effect of any decision rule is to divide the feature space into *c decision regions*, $\mathscr{R}_1, \ldots, \mathscr{R}_c$. If $g_i(\mathbf{x}) > g_j(\mathbf{x})$ for all $j \neq i$, then $\mathbf{x}$ is in $\mathscr{R}_i$, and the decision rule calls for us to assign $\mathbf{x}$ to ω_i. The regions are separated by *decision boundaries*, surfaces in feature space where ties occur among the largest discriminant functions (see Figure 2.4). If $\mathscr{R}_i$ and $\mathscr{R}_j$ are contiguous, the equation for the decision boundary separating them is

$$g_i(\mathbf{x}) = g_j(\mathbf{x}). \tag{14}$$

While this equation may appear to take different forms depending on the forms chosen for the discriminant functions, the decision boundaries are, of

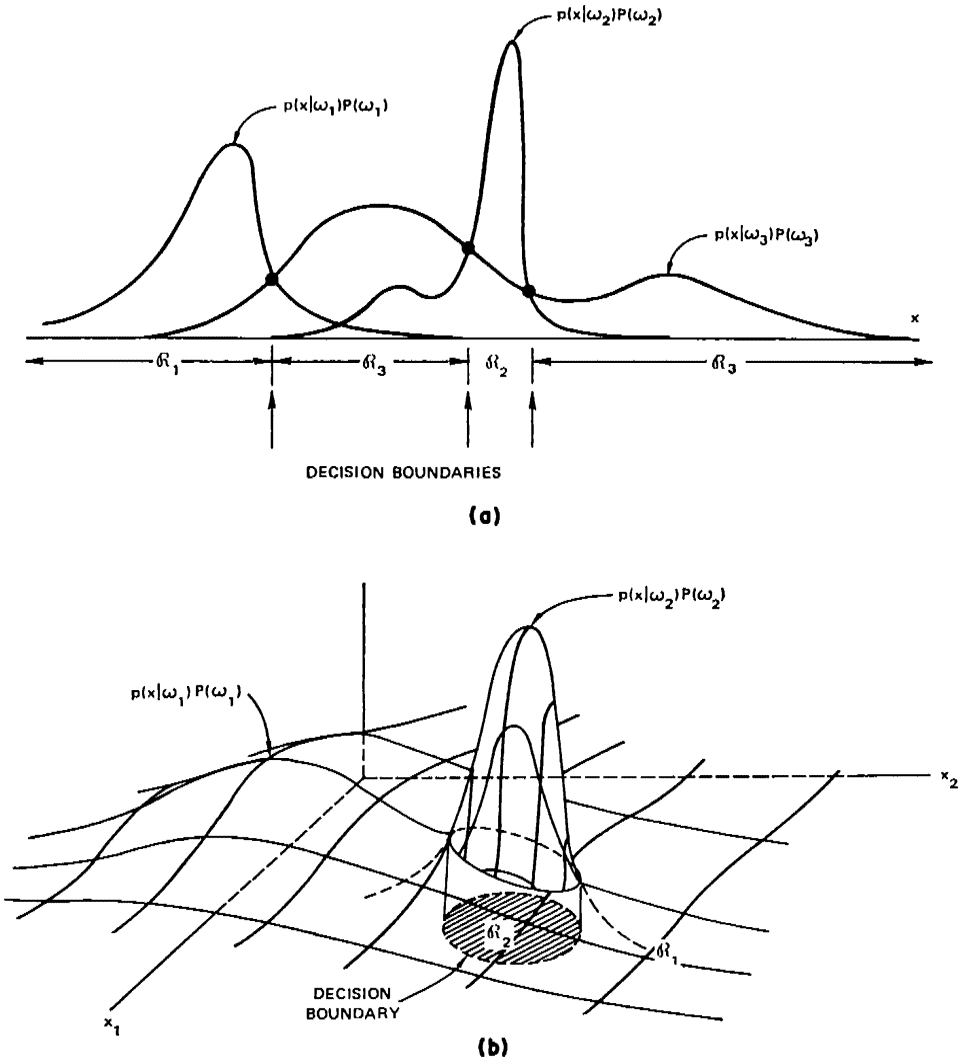


FIGURE 2.4. Examples of decision boundaries and decision regions.

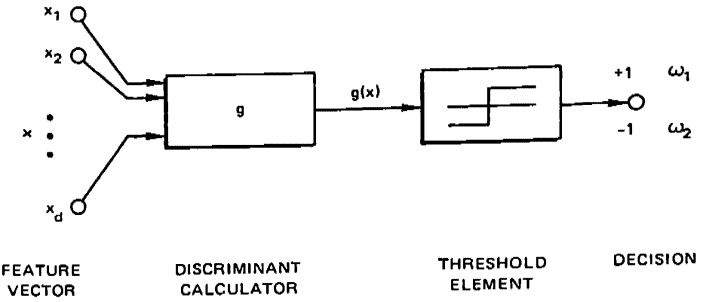


FIGURE 2.5. A two-category pattern classifier.

course, the same. For points on the decision boundary the classification is not uniquely defined. For a Bayes classifier, the conditional risk associated with either decision is the same, and it does not matter how ties are broken. Generally speaking, the problem of breaking ties is an academic question when the conditional density functions are continuous.

2.5.2 The Two-Category Case

While the two-category case is just a special instance of the multicategory case, it has traditionally received separate treatment. Instead of using two discriminant functions g_1 and g_2 and assigning $\mathbf{x}$ to ω_1 if $g_1 > g_2$, it is more common to define one discriminant function

$$g(\mathbf{x}) = g_1(\mathbf{x}) - g_2(\mathbf{x}), \tag{15}$$

and to use the following decision rule: Decide ω_1 if $g(\mathbf{x}) > 0$; otherwise decide ω_2. Thus, a two-category classifier can be viewed as a machine that computes a single discriminant function $g(\mathbf{x})$, and classifies $\mathbf{x}$ according to the algebraic sign of the result (see Figure 2.5). Of the various forms in which the minimum-error-rate discriminant function can be written, the following two are particularly convenient:

$$g(\mathbf{x}) = P(\omega_1 \mid \mathbf{x}) - P(\omega_2 \mid \mathbf{x}) \tag{16}$$

$$g(\mathbf{x}) = \log \frac{p(\mathbf{x} \mid \omega_1)}{p(\mathbf{x} \mid \omega_2)} + \log \frac{P(\omega_1)}{P(\omega_2)}. \tag{17}$$

2.6 ERROR PROBABILITIES AND INTEGRALS

By thinking of a classifier as a device for partitioning feature space into decision regions, we can obtain additional insight into the operation of a Bayes classifier. Consider first the two-category case, and suppose that the

classifier has divided the space into two regions, $\mathscr{R}_1$ and $\mathscr{R}_2$. There are two ways in which a classification error can occur; either an observation $\mathbf{x}$ falls in $\mathscr{R}_2$ and the true state of nature is ω_1, or $\mathbf{x}$ falls in $\mathscr{R}_1$ and the true state of nature is ω_2. Since these events are mutually exclusive and exhaustive,

$$\begin{aligned} P(\text{error}) &= P(\mathbf{x} \in \mathscr{R}_2, \omega_1) + P(\mathbf{x} \in \mathscr{R}_1, \omega_2) \\ &= P(\mathbf{x} \in \mathscr{R}_2 \mid \omega_1)P(\omega_1) + P(\mathbf{x} \in \mathscr{R}_1 \mid \omega_2)P(\omega_2) \\ &= \int_{\mathscr{R}_2} p(\mathbf{x} \mid \omega_1)P(\omega_1)\, d\mathbf{x} + \int_{\mathscr{R}_1} p(\mathbf{x} \mid \omega_2)P(\omega_2)\, d\mathbf{x}. \end{aligned} \tag{18}$$

This result is illustrated in the one-dimensional case in Figure 2.6. The two terms in the sum are merely the areas in the tails of the functions $p(\mathbf{x} \mid \omega_i)P(\omega_i)$. Because the regions $\mathscr{R}_1$ and $\mathscr{R}_2$ were chosen arbitrarily, the probability of error is not as small as it might be. By moving the decision boundary to the left, it is clear that we can eliminate the dark "triangular" area and reduce the probability of error. In general, if $p(\mathbf{x} \mid \omega_1)P(\omega_1) > p(\mathbf{x} \mid \omega_2)P(\omega_2)$, it is advantageous to have $\mathbf{x}$ be in $\mathscr{R}_1$ so that the smaller quantity will contribute to the integral; this is exactly what the Bayes decision rule achieves.

In the multiclass case, there are more ways to be wrong than to be right, and it is simpler to compute the probability of being correct. Clearly

$$\begin{aligned} P(\text{correct}) &= \sum_{i=1}^{c} P(\mathbf{x} \in \mathscr{R}_i, \omega_i) \\ &= \sum_{i=1}^{c} P(\mathbf{x} \in \mathscr{R}_i \mid \omega_i)P(\omega_i) \\ &= \sum_{i=1}^{c} \int_{\mathscr{R}_i} p(\mathbf{x} \mid \omega_i)P(\omega_i)\, d\mathbf{x}. \end{aligned} \tag{19}$$

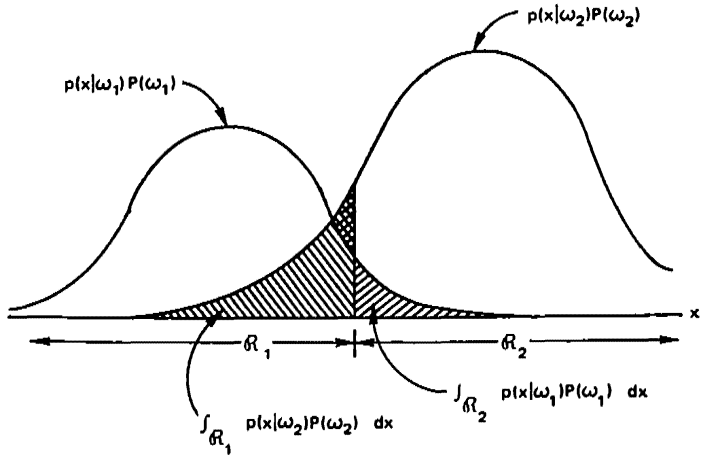


FIGURE 2.6. Components of the probability of error.

This result is valid no matter how the feature space is partitioned into decision regions. The Bayes classifier maximizes this probability by choosing the regions so that the integrands are maximum; no other partitioning can yield a smaller probability of error.

2.7 THE NORMAL DENSITY

The structure of a Bayes classifier is determined primarily by the conditional densities $p(\mathbf{x} \mid \omega_i)$. Of the various density functions that have been investigated, none has received more attention than the multivariate normal density. It must be confessed that this attention is due largely to its analytical tractability. However, the multivariate normal density is also an appropriate model for an important situation, viz., the case where the feature vectors $\mathbf{x}$ for a given class ω_i are continuous valued, mildly corrupted versions of a single typical or prototype vector $\boldsymbol{\mu}_i$. This is what one would expect if the feature extractor were intentionally designed to extract features that were different for patterns in different classes but as similar as possible for patterns in the same class. In this section we provide a brief exposition of the properties of the multivariate normal density, focusing on the properties of greatest interest for classification problems.

2.7.1 The Univariate Normal Density

We begin with the univariate normal density

$$p(x) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] \tag{20}$$

for which

$$E[x] = \int_{-\infty}^{\infty} x p(x)\, dx = \mu \tag{21}$$

and

$$E[(x-\mu)^2] = \int_{-\infty}^{\infty} (x-\mu)^2 p(x)\, dx = \sigma^2. \tag{22}$$

The univariate normal density is completely specified by two parameters, the *mean* μ and the *variance* σ^2. For simplicity, we often abbreviate Eq. (20) by writing $p(x) \sim N(\mu, \sigma^2)$ to say that x is distributed normally with mean μ and variance σ^2. Normally distributed samples tend to cluster about the mean, with a spread proportional to the standard deviation σ; approximately 95% of the samples drawn from a normal population will fall in the interval $|x - \mu| \leq 2\sigma$.

2.7.2 The Multivariate Normal Density

The general multivariate normal density is written as

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp[-\tfrac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^t \Sigma^{-1}(\mathbf{x} - \boldsymbol{\mu})] \tag{23}$$

where $\mathbf{x}$ is a d-component column vector, $\boldsymbol{\mu}$ is the d-component *mean vector*, Σ is the d-by-d *covariance matrix*, $(\mathbf{x} - \boldsymbol{\mu})^t$ is the transpose of $\mathbf{x} - \boldsymbol{\mu}$, Σ^{-1} is the inverse of Σ, and $|\Sigma|$ is the determinant of Σ. For simplicity, we often abbreviate Eq. (23) as $p(\mathbf{x}) \sim N(\boldsymbol{\mu}, \Sigma)$. Formally,

$$\boldsymbol{\mu} = E[\mathbf{x}] \tag{24}$$

and

$$\Sigma = E[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^t], \tag{25}$$

where the expected value of a vector or a matrix is found by taking the expected values of its components. To be more specific, if x_i is the ith component of $\mathbf{x}$, μ_i is the ith component of $\boldsymbol{\mu}$, and σ_{ij} is the i-jth component of Σ, then

$$\mu_i = E[x_i] \tag{26}$$

and

$$\sigma_{ij} = E[(x_i - \mu_i)(x_j - \mu_j)]. \tag{27}$$

The covariance matrix Σ is always symmetric and positive semidefinite. We shall restrict our attention to the case in which Σ is positive definite, so that the determinant of Σ is strictly positive.* The diagonal element σ_{ii} is the variance of x_i, and the off-diagonal element σ_{ij} is the covariance of x_i and x_j. If x_i and x_j are statistically independent, $\sigma_{ij} = 0$. If all of the off-diagonal elements are zero, $p(\mathbf{x})$ reduces to the product of the univariate normal densities for the components of $\mathbf{x}$.

It is not hard to show that the distribution of any linear combination of normally distributed random variables is again normal. In particular, if A is a d-by-n matrix and $\mathbf{y} = A^t\mathbf{x}$ is an n-component vector, then $p(\mathbf{y}) \sim N(A^t\boldsymbol{\mu}, A^t\Sigma A)$. In the special case where A is a unit-length vector $\mathbf{a}$, $y = \mathbf{a}^t\mathbf{x}$ is a scalar that represents the projection of $\mathbf{x}$ onto a line in the direction of $\mathbf{a}$. Thus, $\mathbf{a}^t\Sigma\mathbf{a}$ is the variance of the projection of $\mathbf{x}$ onto $\mathbf{a}$. In general, knowledge of the covariance matrix allows us to calculate the dispersion of the data in any direction.

The multivariate normal density is completely specified by $d + d(d + 1)/2$ parameters, the elements of the mean vector $\boldsymbol{\mu}$ and the independent elements

* If sample vectors drawn from a normal population are confined to a linear subspace, $|\Sigma| = 0$ and $p(\mathbf{x})$ is degenerate. This happens, for example, when one component of $\mathbf{x}$ has zero variance, or when two components are identical. We are specifically excluding such situations.

of the covariance matrix Σ. Samples drawn from a normal population tend to fall in a single cloud or cluster (see Figure 2.7). The center of the cluster is determined by the mean vector, and the shape of the cluster is determined by the covariance matrix. It follows from Eq. (23) that the loci of points of constant density are hyperellipsoids for which the quadratic form $(\mathbf{x} - \boldsymbol{\mu})^t \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu})$ is constant. The principal axes of these hyperellipsoids are given by the eigenvectors of Σ, the eigenvalues determining the lengths of these axes. The quantity

$$r^2 = (\mathbf{x} - \boldsymbol{\mu})^t \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) \tag{28}$$

is sometimes called the squared *Mahalanobis distance* from $\mathbf{x}$ to $\boldsymbol{\mu}$. Thus, the contours of constant density are hyperellipsoids of constant Mahalanobis distance to $\boldsymbol{\mu}$. The volume of these hyperellipsoids measures the scatter of the samples about the mean. It can be shown that the volume of the hyperellipsoid corresponding to a Mahalanobis distance r is given by

$$V = V_d \, |\Sigma|^{1/2} r^d, \tag{29}$$

where V_d is the volume of a d-dimensional unit hypersphere:

$$V_d = \begin{cases} \dfrac{\pi^{d/2}}{\left(\frac{d}{2}\right)!} & d \text{ even} \\ \dfrac{2^d \pi^{(d-1)/2} \left(\frac{d-1}{2}\right)!}{d!} & d \text{ odd.} \end{cases} \tag{30}$$

Thus, for a given dimensionality, the scatter of the samples varies directly with $|\Sigma|^{1/2}$.

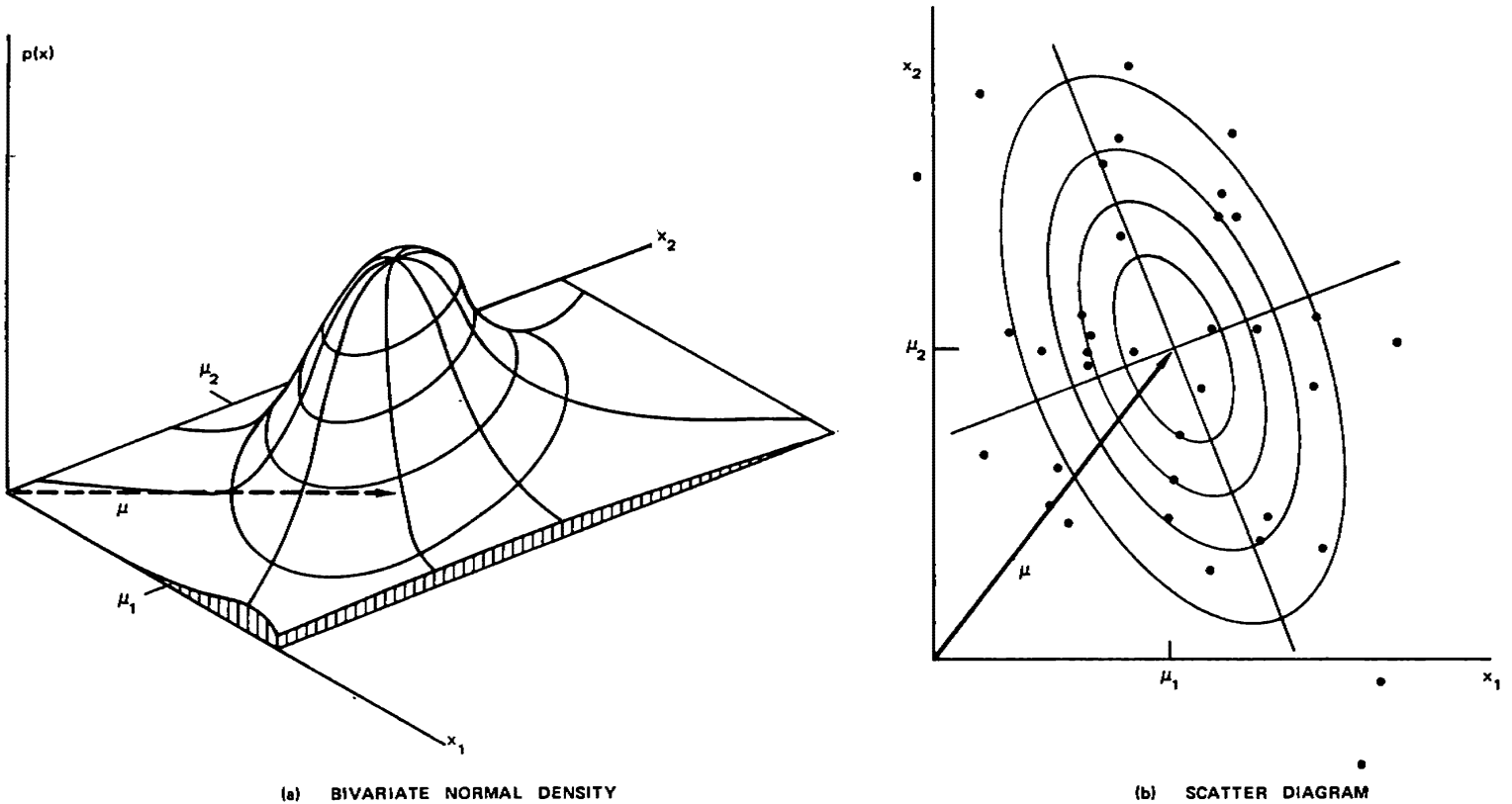
2.8 DISCRIMINANT FUNCTIONS FOR THE NORMAL DENSITY

In Section 2.5 we saw that minimum-error-rate classification can be achieved by use of the discriminant functions

$$g_i(\mathbf{x}) = \log p(\mathbf{x} \mid \omega_i) + \log P(\omega_i). \tag{13}$$

This expression can be readily evaluated if the densities $p(\mathbf{x} \mid \omega_i)$ are multivariate normal. Let $p(\mathbf{x} \mid \omega_i) \sim N(\boldsymbol{\mu}_i, \Sigma_i)$. Then, from Eq. (23),

$$g_i(\mathbf{x}) = -\tfrac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_i)^t \Sigma_i^{-1} (\mathbf{x} - \boldsymbol{\mu}_i) - \frac{d}{2} \log 2\pi - \tfrac{1}{2} \log |\Sigma_i| + \log P(\omega_i). \tag{31}$$



(a) BIVARIATE NORMAL DENSITY

(b) SCATTER DIAGRAM

FIGURE 2.7. Two representations of a normal density.

Let us examine this result for a number of special cases.

2.8.1 Case 1: $\Sigma_i = \sigma^2 I$

The simplest case occurs when the features are statistically independent, and when each feature has the same variance, σ^2. In this case the covariance matrix is diagonal, being merely σ^2 times the identity matrix, I. Geometrically, this corresponds to the situation in which the samples fall in equal-size hyperspherical clusters, the cluster for the ith class being centered about the mean vector $\boldsymbol{\mu}_i$. The computation of the determinant and the inverse of Σ_i is particularly easy: $|\Sigma_i| = \sigma^{2d}$ and $\Sigma_i^{-1} = (1/\sigma^2)I$. Since both $|\Sigma_i|$ and the $(d/2)\log 2\pi$ term in Eq. (31) are independent of i, they are unimportant additive constants that can be ignored. Thus, we obtain the simple discriminant functions

$$g_i(\mathbf{x}) = -\frac{\|\mathbf{x} - \boldsymbol{\mu}_i\|^2}{2\sigma^2} + \log P(\omega_i), \tag{32}$$

where $\|\cdot\|$ is the Euclidean norm, with

$$\|\mathbf{x} - \boldsymbol{\mu}_i\|^2 = (\mathbf{x} - \boldsymbol{\mu}_i)^t(\mathbf{x} - \boldsymbol{\mu}_i). \tag{33}$$

If the a priori probabilities $P(\omega_i)$ are the same for all c classes, then the $\log P(\omega_i)$ term becomes another unimportant additive constant that can be ignored. In this case, the optimum decision rule can be stated very simply: To classify a feature vector $\mathbf{x}$, measure the Euclidean distance $\|\mathbf{x} - \boldsymbol{\mu}_i\|$ from $\mathbf{x}$ to each of the c mean vectors, and assign $\mathbf{x}$ to the category of the nearest mean. Such a classifier is called a *minimum-distance* classifier. If each mean vector is thought of as being an ideal prototype or template for patterns in its class, then this is essentially a *template-matching* procedure. If the a priori probabilities are not equal, then Eq. (32) shows that the squared distance $\|\mathbf{x} - \boldsymbol{\mu}_i\|^2$ must be normalized by the variance σ^2 and biased by subtracting $\log P^2(\omega_i)$; thus, if $\mathbf{x}$ is equally near two different mean vectors, the decision will favor the a priori more likely category.

It is not actually necessary to compute distances in either of these cases. Expansion of the quadratic form $(\mathbf{x} - \boldsymbol{\mu}_i)^t(\mathbf{x} - \boldsymbol{\mu}_i)$ yields

$$g_i(\mathbf{x}) = -\frac{1}{2\sigma^2}[\mathbf{x}^t\mathbf{x} - 2\boldsymbol{\mu}_i^t\mathbf{x} + \boldsymbol{\mu}_i^t\boldsymbol{\mu}_i] + \log P(\omega_i),$$

which appears to be a quadratic function of $\mathbf{x}$. However, the quadratic term $\mathbf{x}^t\mathbf{x}$ is the same for all i, making it an ignorable additive constant. Thus, we obtain the equivalent *linear* discriminant functions

$$g_i(\mathbf{x}) = \mathbf{w}_i^t\mathbf{x} + w_{i0}, \tag{34}$$

where*

$$\mathbf{w}_i = \frac{1}{\sigma^2}\boldsymbol{\mu}_i \tag{35}$$

and

$$w_{i0} = -\frac{1}{2\sigma^2}\boldsymbol{\mu}_i^t\boldsymbol{\mu}_i + \log P(\omega_i). \tag{36}$$

A classifier that uses linear discriminant functions is called a *linear machine*. This kind of classifier has many interesting theoretical properties, some of which will be discussed in detail in Chapter 5. At this point we merely note that the decision surfaces for a linear machine are pieces of hyperplanes defined by the linear equations $g_i(\mathbf{x}) = g_j(\mathbf{x})$. For our particular case, this equation can be written as

$$\mathbf{w}^t(\mathbf{x} - \mathbf{x}_0) = 0, \tag{37}$$

where

$$\mathbf{w} = \boldsymbol{\mu}_i - \boldsymbol{\mu}_j \tag{38}$$

and

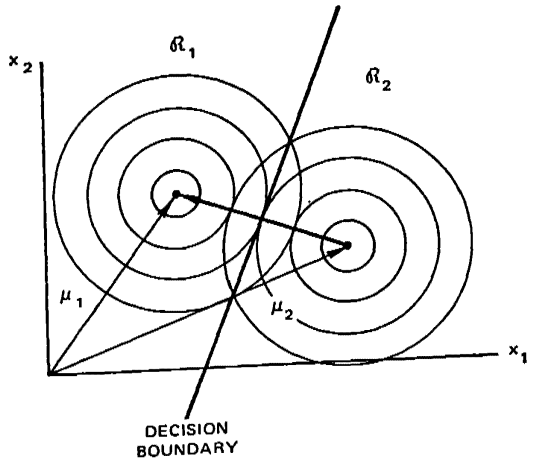
$$\mathbf{x}_0 = \tfrac{1}{2}(\boldsymbol{\mu}_i + \boldsymbol{\mu}_j) - \frac{\sigma^2}{\|\boldsymbol{\mu}_i - \boldsymbol{\mu}_j\|^2}\log\frac{P(\omega_i)}{P(\omega_j)}(\boldsymbol{\mu}_i - \boldsymbol{\mu}_j). \tag{39}$$

This equation defines a hyperplane through the point $\mathbf{x}_0$ and orthogonal to the vector $\mathbf{w}$. Since $\mathbf{w} = \boldsymbol{\mu}_i - \boldsymbol{\mu}_j$, the hyperplane separating $\mathscr{R}_i$ and $\mathscr{R}_j$ is orthogonal to the line between the means. If $P(\omega_i) = P(\omega_j)$, then the point $\mathbf{x}_0$ is halfway between the means, and the hyperplane is the perpendicular bisector of the line between the means (see Figure 2.8). This result could have been anticipated from the fact that the classifier for this case is a minimum-distance classifier. If $P(\omega_i) \neq P(\omega_j)$, the point $\mathbf{x}_0$ shifts away from the more likely mean. Note, however, that if the variance σ^2 is small relative to the squared distance $\|\boldsymbol{\mu}_i - \boldsymbol{\mu}_j\|^2$, then the position of the decision boundary is relatively insensitive to the exact values of the a priori probabilities.

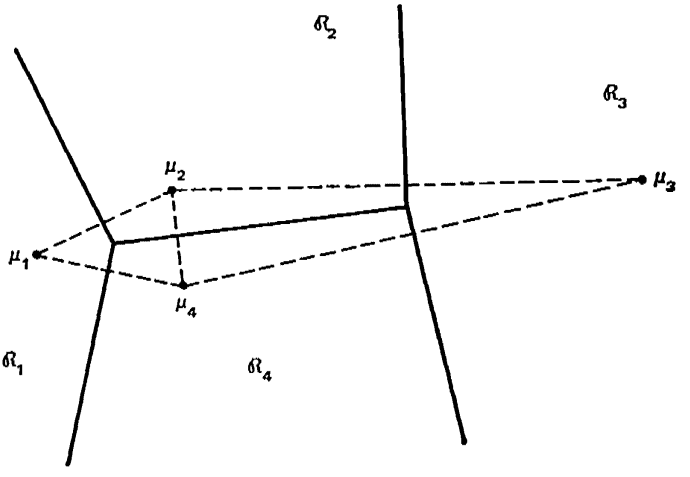
2.8.2 Case 2: $\Sigma_i = \Sigma$

Another simple case arises when the covariance matrices for all of the classes are identical. Geometrically, this corresponds to the situation in which the samples fall in hyperellipsoidal clusters of equal size and shape, the cluster for the ith class being centered about the mean vector $\boldsymbol{\mu}_i$. Since both $|\Sigma_i|$ and the $(d/2)\log 2\pi$ term in Eq. (31) are independent of i, they can be ignored

* Readers familiar with signal detection theory will recognize this as a correlation detector. The discriminant $g_i(\mathbf{x})$ crosscorrelates the input $\mathbf{x}$ with the stored reference signal $\boldsymbol{\mu}_i$. The constant w_{i0} accounts for both the energy in the reference signal and its a priori probability of occurrence.



(a) TWO-CLASS PROBLEM



(b) FOUR-CLASS PROBLEM

FIGURE 2.8. Decision boundaries for a minimum-distance classifier.

as superfluous additive constants. This results in the discriminant functions

$$g_i(\mathbf{x}) = -\tfrac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_i)^t \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}_i) + \log P(\omega_i). \tag{40}$$

If the a priori probabilities $P(\omega_i)$ are the same for all c classes, then the $\log P(\omega_i)$ term can be ignored. In this case, the optimal decision rule can once again be stated very simply: To classify a feature vector $\mathbf{x}$, measure the squared Mahalanobis distance $(\mathbf{x} - \boldsymbol{\mu}_i)^t \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}_i)$ from $\mathbf{x}$ to each of the c

mean vectors, and assign $\mathbf{x}$ to the category of the nearest mean.* As before, unequal a priori probabilities bias the decision in favor of the a priori more likely category.

Expansion of the quadratic form $(\mathbf{x} - \boldsymbol{\mu}_i)^t \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}_i)$ discloses that the quadratic term $\mathbf{x}^t\boldsymbol{\Sigma}^{-1}\mathbf{x}$ is independent of i. If it is deleted, the resulting discriminant functions are again linear:

$$g_i(\mathbf{x}) = \mathbf{w}_i^t\mathbf{x} + w_{i0}, \tag{41}$$

where

$$\mathbf{w}_i = \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_i \tag{42}$$

and

$$w_{i0} = -\tfrac{1}{2}\boldsymbol{\mu}_i^t\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_i + \log P(\omega_i). \tag{43}$$

Since the discriminants are linear, the resulting decision boundaries are again hyperplanes (see Figure 2.9). If $\mathcal{R}_i$ and $\mathcal{R}_j$ are contiguous, the boundary between them has the equation

$$\mathbf{w}^t(\mathbf{x} - \mathbf{x}_0) = 0 \tag{44}$$

where

$$\mathbf{w} = \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_i - \boldsymbol{\mu}_j) \tag{45}$$

and

$$\mathbf{x}_0 = \tfrac{1}{2}(\boldsymbol{\mu}_i + \boldsymbol{\mu}_j) - \frac{\log \dfrac{P(\omega_i)}{P(\omega_j)}}{(\boldsymbol{\mu}_i - \boldsymbol{\mu}_j)^t\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_i - \boldsymbol{\mu}_j)}(\boldsymbol{\mu}_i - \boldsymbol{\mu}_j). \tag{46}$$

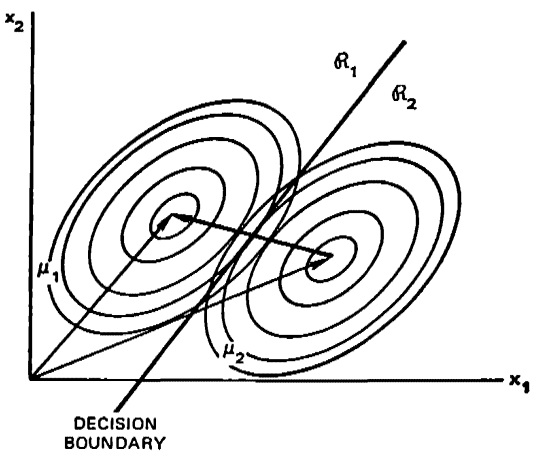


FIGURE 2.9. Decision boundary for a minimum-Mahalanobis-distance classifier.

* An alternative interpretation can be obtained by subjecting the feature coordinates to a linear transformation that rotates and scales the axes so that the hyperellipsoids of constant Mahalanobis distance become hyperspheres. This transformation reduces Case 2 to Case 1, and allows Mahalanobis distance to be interpreted as Euclidean distance in the transformed space.

Since $\mathbf{w} = \Sigma^{-1}(\boldsymbol{\mu}_i - \boldsymbol{\mu}_j)$ is generally not in the direction of $\boldsymbol{\mu}_i - \boldsymbol{\mu}_j$, the hyperplane separating $\mathcal{R}_i$ and $\mathcal{R}_j$ is generally not orthogonal to the line between the means. However, it does intersect that line at the point $\mathbf{x}_0$ which is halfway between the means if the a priori probabilities are equal. If the a priori probabilities are not equal, the boundary hyperplane is translated away from the more likely mean.

2.8.3 Case 3: Σ_i Arbitrary

In the general multivariate normal case, the covariance matrices are different for each category. The only term that can be dropped from Eq. (31) is the $(d/2)\log 2\pi$ term, and the resulting discriminant functions are inherently quadratic:

$$g_i(\mathbf{x}) = \mathbf{x}^t W_i \mathbf{x} + \mathbf{w}_i^t \mathbf{x} + w_{i0}, \tag{47}$$

where

$$W_i = -\tfrac{1}{2}\Sigma_i^{-1} \tag{48}$$

$$\mathbf{w}_i = \Sigma_i^{-1}\boldsymbol{\mu}_i \tag{49}$$

and

$$w_{i0} = -\tfrac{1}{2}\boldsymbol{\mu}_i^t \Sigma_i^{-1}\boldsymbol{\mu}_i - \tfrac{1}{2}\log|\Sigma_i| + \log P(\omega_i). \tag{50}$$

The decision surfaces are *hyperquadrics*, and can assume any of the general forms—pairs of hyperplanes, hyperspheres, hyperellipsoids, hyperparaboloids, and hyperhyperboloids of various types. The two-dimensional examples sketched in Figure 2.10 indicate how these different forms can arise. In all cases the variables x_1 and x_2 are class-conditionally independent, and thus the covariance matrices are diagonal. The different decision surfaces arise solely from differences between the variances. These variances are indicated by the numbered contours of constant probability density. In Figure 2.10*a* $p(\mathbf{x} \mid \omega_2)$ has smaller variances than $p(\mathbf{x} \mid \omega_1)$. Thus, samples from Class 2 are more likely to be found near the mean for that class, and, due to circular symmetry, the decision boundary is a circle enclosing $\boldsymbol{\mu}_2$. By stretching the x_2 axis as shown in Figure 2.10b, the decision boundary is stretched into an ellipse. In Figure 2.10c both densities have the same variance in the x_1 direction, but $p(\mathbf{x} \mid \omega_1)$ has more variance than $p(\mathbf{x} \mid \omega_2)$ in the x_2 direction. Thus, samples with large x_2 values are probably from Class 1, and the decision boundary is a parabola. By increasing the x_1 variance for $p(\mathbf{x} \mid \omega_2)$ as shown in Figure 2.10d, the boundary changes to a hyperbola. Finally, the special symmetry shown in Figure 2.10e causes the hyperbolic boundary to degenerate to a pair of straight lines.

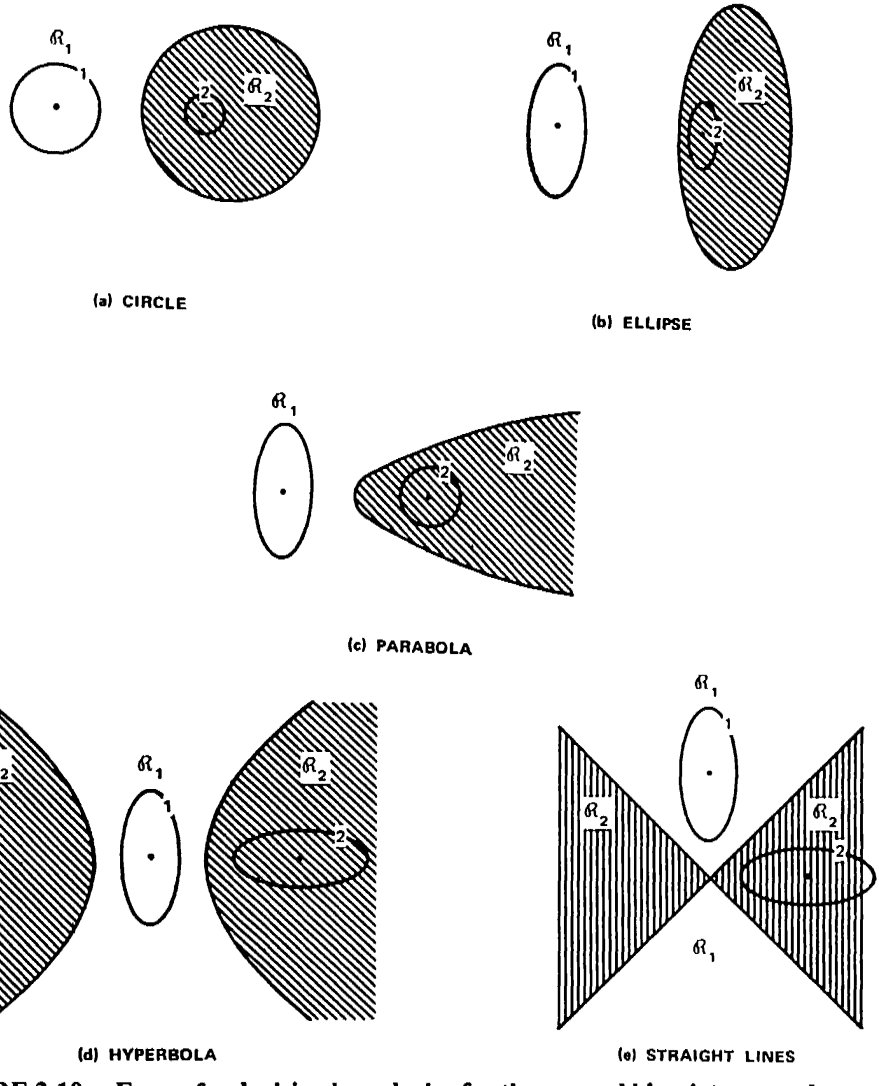


FIGURE 2.10. Forms for decision boundaries for the general bivariate normal case.

2.9 BAYES DECISION THEORY— THE DISCRETE CASE

Until now we have assumed that the feature vector $\mathbf{x}$ could be any point $\mathbf{x}$ in Euclidean d-space. However, in many practical applications the components of $\mathbf{x}$ are binary-valued or ternary-valued variables, so that $\mathbf{x}$ can assume only one of m discrete values $\mathbf{v}_1, \ldots, \mathbf{v}_m$. In such cases, the probability density function $p(\mathbf{x} \mid \omega_j)$ becomes singular; integrals such as

$$\int p(\mathbf{x} \mid \omega_j)\, d\mathbf{x}$$

turn into sums such as

$$\sum_k P(\mathbf{v}_k \mid \omega_j),$$

where $P(\mathbf{v}_k \mid \omega_j)$ is the conditional probability that $\mathbf{x} = \mathbf{v}_k$, given that the state of nature is ω_j. Bayes rule becomes

$$P(\omega_j \mid \mathbf{x}) = \frac{P(\mathbf{x} \mid \omega_j)P(\omega_j)}{P(\mathbf{x})}, \tag{51}$$

where

$$P(\mathbf{x}) = \sum_{j=1}^{s} P(\mathbf{x} \mid \omega_j)P(\omega_j). \tag{52}$$

The definition of the conditional risk $R(\alpha_i \mid \mathbf{x})$ is unchanged, and the fundamental Bayes decision rule remains the same: To minimize the overall risk, select the action α_i for which $R(\alpha_i \mid \mathbf{x})$ is minimum. The basic rule to minimize the error-rate by maximizing the a posteriori probability is also unchanged; by using Bayes rule, we obtain the following equivalent discriminant functions:

$$g_i(\mathbf{x}) = P(\omega_i \mid \mathbf{x}) \tag{53}$$

$$g_i(\mathbf{x}) = P(\mathbf{x} \mid \omega_i)P(\omega_i) \tag{54}$$

$$g_i(\mathbf{x}) = \log P(\mathbf{x} \mid \omega_i) + \log P(\omega_i). \tag{55}$$

In the two-category case, the following discriminant functions are often convenient:

$$g(\mathbf{x}) = P(\omega_1 \mid \mathbf{x}) - P(\omega_2 \mid \mathbf{x}) \tag{56}$$

$$g(\mathbf{x}) = \log \frac{P(\mathbf{x} \mid \omega_1)}{P(\mathbf{x} \mid \omega_2)} + \log \frac{P(\omega_1)}{P(\omega_2)}. \tag{57}$$

2.10 INDEPENDENT BINARY FEATURES

As an example of a specific classification problem involving discrete features, consider the two-class case in which the components of the feature vector are binary valued and conditionally independent. To be more specific, let $\mathbf{x} = (x_1, \ldots, x_d)^t$, where the components x_i are either 1 or 0, with

$$p_i = \text{Prob}(x_i = 1 \mid \omega_1)$$

and

$$q_i = \text{Prob}(x_i = 1 \mid \omega_2).$$

This is a model of a classification problem in which each feature gives us a yes/no answer about the pattern. If $p_i > q_i$, we expect the ith feature to give

a "yes" answer more frequently when the state of nature is ω_1 than when it is ω_2. By assuming conditional independence, we can write $P(\mathbf{x} \mid \omega_i)$ as the product of the probabilities for the components of $\mathbf{x}$. A particularly convenient way of writing this is as follows:

$$P(\mathbf{x} \mid \omega_1) = \prod_{i=1}^{d} p_i^{x_i}(1 - p_i)^{1-x_i}$$

$$P(\mathbf{x} \mid \omega_2) = \prod_{i=1}^{d} q_i^{x_i}(1 - q_i)^{1-x_i}.$$

Then the likelihood ratio is given by

$$\frac{P(\mathbf{x} \mid \omega_1)}{P(\mathbf{x} \mid \omega_2)} = \prod_{i=1}^{d} \left(\frac{p_i}{q_i}\right)^{x_i} \left(\frac{1 - p_i}{1 - q_i}\right)^{1-x_i},$$

and Eq. (57) yields the discriminant function

$$g(\mathbf{x}) = \sum_{i=1}^{d} \left[x_i \log \frac{p_i}{q_i} + (1 - x_i) \log \frac{1 - p_i}{1 - q_i} \right] + \log \frac{P(\omega_1)}{P(\omega_2)}.$$

Inspection of this equation shows that it is linear in the x_i. That is, we can write

$$g(\mathbf{x}) = \sum_{i=1}^{d} w_i x_i + w_0,$$

where

$$w_i = \log \frac{p_i(1 - q_i)}{q_i(1 - p_i)} \qquad i = 1, \ldots, d$$

and

$$w_0 = \sum_{i=1}^{d} \log \frac{1 - p_i}{1 - q_i} + \log \frac{P(\omega_1)}{P(\omega_2)}.$$

Let us examine these results to see what insight they can give. Recall first that we decide ω_1 if $g(\mathbf{x}) > 0$ and ω_2 if $g(\mathbf{x}) \leq 0$. We have seen that $g(\mathbf{x})$ is a weighted combination of the components of $\mathbf{x}$. The magnitude of the weight w_i measures the significance of a "yes" answer for x_i in determining the classification. If $p_i = q_i$, x_i gives us no information about the state of nature, and $w_i = 0$. If $p_i > q_i$, then $1 - p_i < 1 - q_i$ and w_i is positive. Thus, in this case a "yes" answer for x_i contributes w_i votes for ω_1. Furthermore, for any fixed $q_i < 1$, w_i gets larger as p_i gets larger. On the other hand, if $p_i < q_i$, w_i is negative, and a "yes" answer contributes $|w_i|$ votes for ω_2.

The a priori probabilities $P(\omega_i)$ appear in the discriminant only through the so-called threshold weight, w_0. Increasing $P(\omega_1)$ increases w_0 and biases the decision in favor of ω_1, while decreasing $P(\omega_1)$ has the opposite effect. Geometrically, the vectors $\mathbf{v}_k$ appear as the vertices of a d-dimensional hypercube. The decision surface defined by $g(\mathbf{x}) = 0$ is a hyperplane that separates

ω_1 vertices from ω_2 vertices. Clearly, in the discrete case one can perturb this hyperplane in many ways without crossing any vertices and changing the probability of error. Any one of these hyperplanes is an optimal separating surface, and all yield the optimal performance.

2.11 COMPOUND BAYES DECISION THEORY AND CONTEXT

Let us reconsider our introductory example of designing a classifier to sort two types of lumber, ash and birch. Our original assumption was that the sequence of types of lumber was so unpredictable that the state of nature looked like a random variable. Without abandoning this attitude, let us consider the possibility that the consecutive states of nature might not be statistically independent. For example, even though the a priori probabilities for ash and birch might be equal, it is possible that once a piece of lumber of one type emerges, it is much more likely that the next several pieces will be the same type than different types. In this case, the consecutive states of nature are dependent, and we should be able to exploit this dependence to gain improved performance. This is one example of the use of *context* to aid decision making.

The way in which we exploit such information is somewhat different when we can wait for n pieces of lumber to emerge and then make all n decisions jointly than when we must decide as each piece of lumber emerges. The first problem is a *compound decision problem*, and the second is a *sequential compound decision problem*. The former case is conceptually simpler, and is the only case we shall examine.

To state the general problem, let $\boldsymbol{\omega} = (\omega(1), \ldots, \omega(n))^t$ be a vector denoting the n states of nature, with $\omega(i)$ taking on one of the c values $\omega_1, \ldots, \omega_c$. Let $P(\boldsymbol{\omega})$ be the a priori probability for the n states of nature. Let $X = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$ be a matrix giving the n observed feature vectors, with $\mathbf{x}_i$ being the feature vector obtained when the state of nature was $\omega(i)$. Finally, let $p(X \mid \boldsymbol{\omega})$ be the conditional probability density function for X, given the true set of states of nature $\boldsymbol{\omega}$. Then the a posteriori probability of $\boldsymbol{\omega}$ is given by

$$P(\boldsymbol{\omega} \mid X) = \frac{p(X \mid \boldsymbol{\omega})P(\boldsymbol{\omega})}{p(X)}, \tag{58}$$

where

$$p(X) = \sum_{\boldsymbol{\omega}} p(X \mid \boldsymbol{\omega})P(\boldsymbol{\omega}). \tag{59}$$

In general, one can define a loss matrix for the compound decision problem and seek a decision rule that minimizes the compound risk. The development

of this theory parallels our development for the simple decision problem, and concludes that the optimal procedure is to minimize the compound conditional risk. In particular, if there is no loss for being correct, and if all errors are equally costly, then the procedure reduces to computing $P(\boldsymbol{\omega} \mid X)$ for all $\boldsymbol{\omega}$ and selecting the $\boldsymbol{\omega}$ for which this a posteriori probability is maximum.

While this provides the theoretical solution, in practice the computation of $P(\boldsymbol{\omega} \mid X)$ can easily prove to be an enormous task. If each component $\omega(i)$ can have one of c values, there are c^n possible values of $\boldsymbol{\omega}$ to consider. Some simplification can be obtained if the distribution of the feature vector $\mathbf{x}_i$ depends only on the corresponding state of nature $\omega(i)$, not on the values of the other feature vectors or the other states of nature. In this case the joint density $p(X \mid \boldsymbol{\omega})$ is merely the product of the component densities $p(\mathbf{x}_i \mid \omega(i))$:

$$p(X \mid \boldsymbol{\omega}) = \prod_{i=1}^{n} p(\mathbf{x}_i \mid \omega(i)). \tag{60}$$

While this simplifies the problem of computing $p(X \mid \boldsymbol{\omega})$, there is still the problem of computing the a priori probability $P(\boldsymbol{\omega})$. This joint probability is central to the compound Bayes decision problem, since it reflects the interdependence of the states of nature. Thus, it is unacceptable to simplify the problem of calculating $P(\boldsymbol{\omega})$ by assuming that the states of nature are independent. In addition, practical applications usually require some method of avoiding the computation of $P(\boldsymbol{\omega} \mid X)$ for all c^n possible values of $\boldsymbol{\omega}$. We shall leave these problems as topics worth some pondering, and shall refer the interested reader to the literature for further details.

2.12 REMARKS

We have now completed an exposition of Bayes decision theory, with special emphasis on the solution for the multivariate normal case. The basic ideas are very simple. To minimize the overall risk, one should always choose the action that minimizes the conditional risk

$$R(\alpha_i \mid \mathbf{x}) = \sum_{j=1}^{c} \lambda(\alpha_i \mid \omega_j) P(\omega_j \mid \mathbf{x}).$$

In particular, to minimize the probability of error in a classification problem, one should always choose the state of nature that maximizes the a posteriori probability $P(\omega_j \mid \mathbf{x})$. Bayes rule allows us to calculate these probabilities from the a priori probabilities $P(\omega_j)$ and the conditional densities $p(\mathbf{x} \mid \omega_j)$.

For most pattern classification applications, the chief problem in applying these results is that the conditional densities $p(\mathbf{x} \mid \omega_j)$ are not known. In some cases we may know the form these densities assume, but may not know

characterizing parameter values. The classic case occurs when the densities are known to be, or can be assumed to be multivariate normal, but the values of the mean vectors and the covariance matrices are not known. More commonly even less is known about the conditional densities, and procedures that are less sensitive to specific assumptions about the densities must be used. Most of the remainder of Part I of this book will be devoted to various procedures that have been developed to attack this problem.

2.13 BIBLIOGRAPHICAL AND HISTORICAL REMARKS

Decision theory is associated with the names of many well known statisticians, and there is a large body of literature on the topic. Among the standard textbooks on decision theory are those by Wald (1950), Blackwell and Girschick (1954), and the more elementary text by Chernoff and Moses (1959). We are also fond of the text by Ferguson (1967), who presents many topics in statistics from a decision theoretic viewpoint. Decision theory is also closely related to the theory of games, which is developed in the classic work by von Neumann and Morgenstern (1944), and the text by Luce and Raiffa (1957).

The pioneering decision theory work by Neyman and Pearson (1928, 1933) dealt with hypothesis testing, and used the probability of error as a criterion. Wald (1939) generalized this work by introducing the notions of loss and risk. Certain conceptual problems have always attended the use of loss functions and a priori probabilities. In fact, the Bayesian approach is avoided by many statisticians, partly because there are problems for which a decision is made only once (so that average loss is not meaningful), and partly because there may be no reasonable way to determine the a priori probabilities. Neither of these difficulties seems to present a serious problem in typical pattern recognition applications, and for simplicity we have taken a strictly Bayesian approach.

Chow (1957) was one of the first to apply Bayesian decision theory to pattern recognition. His analysis included a provision for rejection, and he later established a fundamental relation between error and reject rates (Chow 1970). The exact calculation of the probability of error is remarkably complicated, and most of the published results concern bounds on the error rate (Albrecht and Werner 1964; Chu and Chueh 1967; Lainiotis and Park 1971). The use of discriminant functions for classification problems was introduced by Fisher (1936), and we shall examine his approach to their use in Chapter 4. Our use of the term follows the pattern set by Nilsson (1965). Anderson (1958) treats the multivariate normal case in great detail, and

derives the quadratic discriminant functions in a slightly different form. Marill and Green (1960) showed how this solution could be applied in a pattern classification context. Cooper (1964) has investigated other continuous distributions for which linear and quadratic discriminant functions are optimal.

Nilsson (1965) attributes the derivation of the linear discriminant functions for the binary independent (or multivariate Bernoulli) case to J. W. Jones, although the first published solution appears to be due to Minsky (1961), with other proofs being given by Winder (1963) and Chow (1965). Kazmierczak and Steinbuch (1963) derived quadratic optimal discriminant functions for the ternary independent case; it is easy to generalize this and derive nth degree polynomial discriminant functions that are optimal for the $(n + 1)$-ary independent case. If the independence assumption is relaxed, higher degree polynomials are needed even in the binary case. This will become more clear when we examine polynomial expansions of joint probabilities in Chapter 4.

Of course, high degree polynomials involving many variables are not computationally desirable. Thus, in those cases where the optimal discriminant function is not linear, it is tempting to seek the optimal linear discriminant. Unfortunately, it turns out to be surprisingly difficult to derive the minimum-risk linear discriminant function. Anderson and Bahadur (1962) have solved the general two-category multivariate normal case, but no other general solutions have been found. However, as we shall see in Chapter 5, many solutions can be found when criteria other than minimum risk are used.

General compound decision theory embraces a greater variety of problems than the simple Bayesian one that we described. Abend (1966) gives a clear introduction to compound decision theory, and a number of significant references to the statistical literature. Raviv (1967) and Abend (1968) derive optimal procedures when there is a Markov dependence between states of nature, and Raviv gives the results of applying such procedures to recognizing English legal text. Abend, Harley and Kanal (1965) show how the Markov dependence approach can be extended from one-dimensional to two-dimensional situations. A computationally efficient method of using context is described by Riseman and Ehrich (1971), who reference other papers on the use of context in character recognition.

Finally, it should be mentioned that throughout Part I we tacitly assume that all d components of the feature vector are measured before we contemplate making a decision. Another alternative is to use a decision tree, evaluating the features sequentially until a decision can be made. The statistical treatment of this approach requires considering the cost of measuring features as well as the cost of making errors, and is the subject of sequential decision theory (Wald 1947; Fu 1968). Slagle and Lee (1971) show

how techniques developed for searching game trees can be applied to such problems.

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PROBLEMS

1. Let the conditional densities for a two-category one-dimensional problem be given by the Cauchy distribution

$$p(x \mid \omega_i) = \frac{1}{\pi b} \cdot \frac{1}{1 + \left(\frac{x - a_i}{b}\right)^2}, \qquad i = 1, 2.$$

If $P(\omega_1) = P(\omega_2)$, show that $P(\omega_1 \mid x) = P(\omega_2 \mid x)$ if $x = (1/2)(a_1 + a_2)$. Sketch

$P(\omega_1 \mid x)$ for the case $a_1 = 3$, $a_2 = 5$, $b = 1$. How does $P(\omega_1 \mid x)$ behave as $x \to -\infty$? $+\infty$?

2. Using the conditional densities given in Problem 1, and assuming equal a priori probabilities, show that the minimum probability of error is given by

$$P(\text{error}) = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \left| \frac{a_2 - a_1}{2b} \right|.$$

Sketch this as a function of $|(a_2 - a_1)/b|$.

3. Consider the following decision rule for a two-category one-dimensional problem: Decide ω_1 if $x > \theta$; otherwise decide ω_2. Show that the probability of error for this rule is given by

$$P(\text{error}) = P(\omega_1) \int_{-\infty}^{\theta} p(x \mid \omega_1)\, dx + P(\omega_2) \int_{\theta}^{\infty} p(x \mid \omega_2)\, dx.$$

By differentiating, show that a necessary condition to minimize $P(\text{error})$ is that θ satisfy

$$p(\theta \mid \omega_1)P(\omega_1) = p(\theta \mid \omega_2)P(\omega_2).$$

Does this define θ uniquely? Give an example where a value of θ satisfying this equation actually maximizes the probability of error.

4. Let $\omega_{\max}(\mathbf{x})$ be the state of nature for which $P(\omega_{\max} \mid \mathbf{x}) \geq P(\omega_i \mid \mathbf{x})$ for all $i, i = 1, \ldots, c$. Show that $P(\omega_{\max} \mid \mathbf{x}) \geq 1/c$. In addition, show that for the minimum-error-rate decision rule the average probability of error is given by

$$P(\text{error}) = 1 - \int P(\omega_{\max} \mid \mathbf{x}) p(\mathbf{x})\, d\mathbf{x}.$$

Use these two results to show that $P(\text{error}) \leq (c - 1)/c$. Describe a situation for which $P(\text{error}) = (c - 1)/c$.

5. If a and b are nonnegative numbers, show that $\min(a, b) \leq \sqrt{ab}$. Use this to show that the error rate for a two-category Bayes classifier must satisfy

$$P(\text{error}) \leq \sqrt{P(\omega_1)P(\omega_2)}\, \rho \leq \tfrac{1}{2}\rho,$$

where ρ is the so-called *Bhattacharyya coefficient*

$$\rho = \int [p(\mathbf{x} \mid \omega_1)p(\mathbf{x} \mid \omega_2)]^{1/2}\, d\mathbf{x}.$$

6. In many pattern classification problems one has the option either to assign the pattern to one of c classes, or to *reject* it as being unrecognizable. If the cost for rejects is not too high, rejection may be a desirable action. Let

$$\lambda(\alpha_i \mid \omega_j) = \begin{cases} 0 & i = j \quad i, j = 1, \ldots, c \\ \lambda_r & i = c + 1 \\ \lambda_s & \text{otherwise,} \end{cases}$$

where λ_r is the loss incurred for choosing the $(c + 1)$th action of rejection, and λ_s is the loss incurred for making a substitution error. Show that the minimum risk

is obtained if we decide ω_i if $P(\omega_i \mid \mathbf{x}) \geq P(\omega_j \mid \mathbf{x})$ for all j and if $P(\omega_i \mid \mathbf{x}) \geq 1 - \lambda_r/\lambda_s$, and reject otherwise. What happens if $\lambda_r = 0$? What happens if $\lambda_r > \lambda_s$?

7. Using the results of Problem 6, show that the following discriminant functions are optimal:

$$g_i(\mathbf{x}) = \begin{cases} p(\mathbf{x} \mid \omega_i)P(\omega_i) & i = 1, \ldots, c \\ \dfrac{\lambda_s - \lambda_r}{\lambda_s} \displaystyle\sum_{j=1}^{c} p(\mathbf{x} \mid \omega_j)P(\omega_j) & i = c + 1. \end{cases}$$

Sketch these discriminant functions and the decision regions for the two-category one-dimensional case with $p(x \mid \omega_1) \sim N(1, 1)$, $p(x \mid \omega_2) \sim N(-1, 1)$, $P(\omega_1) = P(\omega_2) = 1/2$, and $\lambda_r/\lambda_s = 1/4$. Describe qualitatively what happens as λ_r/λ_s is increased from 0 to 1.

8. Suppose that we replace the deterministic decision function $\alpha(\mathbf{x})$ with a *randomized rule*, viz., the probability $P(\alpha_i \mid \mathbf{x})$ of taking action α_i upon observing $\mathbf{x}$. Show that the resulting risk is given by

$$R = \int \left[\sum_{i=1}^{a} R(\alpha_i \mid \mathbf{x})P(\alpha_i \mid \mathbf{x}) \right] p(\mathbf{x})\, d\mathbf{x}.$$

In addition, show that R is minimized by choosing $P(\alpha_i \mid \mathbf{x}) = 1$ for the action α_i associated with the minimum conditional risk $R(\alpha_i \mid \mathbf{x})$, thereby showing that no benefit can be gained from randomizing.

9. Consider the multivariate normal density for which $\sigma_{ij} = 0$ and $\sigma_{ii} = \sigma_i^2$. Show that

$$p(\mathbf{x}) = \frac{1}{\displaystyle\prod_{i=1}^{d} \sqrt{2\pi}\,\sigma_i} \exp\left[-\frac{1}{2} \sum_{i=1}^{d} \left(\frac{x_i - \mu_i}{\sigma_i} \right)^2 \right].$$

Describe the contours of constant density, and write an expression for the Mahalanobis distance from $\mathbf{x}$ to $\boldsymbol{\mu}$.

10. Let $p(x \mid \omega_i) \sim N(\mu_i, \sigma^2)$ for a two-category one-dimensional problem with $P(\omega_1) = P(\omega_2) = 1/2$. Show that the minimum probability of error is given by

$$P_e = \frac{1}{\sqrt{2\pi}} \int_a^\infty e^{-(1/2)u^2}\, du,$$

where $a = |\mu_2 - \mu_1|/2\sigma$. Use the inequality

$$\frac{1}{\sqrt{2\pi}} \int_a^\infty e^{-(1/2)t^2}\, dt \leq \frac{1}{\sqrt{2\pi}\, a} e^{-(1/2)a^2}$$

to show that P_e goes to zero as $|\mu_2 - \mu_1|/\sigma$ goes to infinity.

11. Let $p(\mathbf{x} \mid \omega_i) \sim N(\boldsymbol{\mu}_i, \sigma^2 I)$ for a two-category d-dimensional problem with $P(\omega_1) = P(\omega_2) = 1/2$. Show that the minimum probability of error is given by

$$P_e = \frac{1}{\sqrt{2\pi}} \int_a^\infty e^{-(1/2)u^2}\, du,$$

where $a = \|\mu_2 - \mu_1\|/2\sigma$. Let $\mu_1 = 0$ and $\mu_2 = (\mu, \ldots, \mu)^t$. Use the inequality of Problem 10 to show that P_e approaches zero as d approaches infinity. Express the meaning of this result in words.

12. Let $p(\mathbf{x} \mid \omega_i) \sim N(\mu_i, \Sigma)$ for a two-category d-dimensional problem with arbitrary a priori probabilities, and consider the Mahalanobis distance

$$r_i^2 = (\mathbf{x} - \mu_i)^t \Sigma^{-1} (\mathbf{x} - \mu_i).$$

(a) Show that the gradient of r_i^2 is given by

$$\nabla r_i^2 = 2\Sigma^{-1}(\mathbf{x} - \mu_i).$$

(b) Show that ∇r_i^2 points in the same direction along any line through μ_i.

(c) Show that ∇r_1^2 and ∇r_2^2 point in opposite directions along the line from μ_1 to μ_2.

(d) Show that the optimal separating hyperplane is tangent to the constant probability density hyperellipsoids at the point that the separating hyperplane cuts the line from μ_1 to μ_2.

13. Under the assumption that $\lambda_{21} > \lambda_{11}$ and $\lambda_{12} > \lambda_{22}$, show that the general minimum risk discriminant function for the independent binary case described in Section 2.10 is given by $g(\mathbf{x}) = \mathbf{w}^t\mathbf{x} + w_0$, where $\mathbf{w}$ is unchanged, and

$$w_0 = \sum_{i=1}^{d} \log \frac{1 - p_i}{1 - q_i} + \log \frac{P(\omega_1)}{P(\omega_2)} + \log \frac{\lambda_{21} - \lambda_{11}}{\lambda_{12} - \lambda_{22}}.$$

14. Let the components of the vector $\mathbf{x} = (x_1, \ldots, x_d)^t$ be binary valued (1 or 0). Let $P(\omega_j)$ be the a priori probability for the state of nature ω_j $(j = 1, \ldots, c)$, and let

$$p_{ij} = \text{Prob}(x_i = 1 \mid \omega_j) \qquad \begin{matrix} i = 1, \ldots, d \\ j = 1, \ldots, c \end{matrix}$$

with the components x_i being statistically independent for all $\mathbf{x}$ in ω_j. Show that the minimum probability of error is achieved by the following decision rule:

Decide ω_k if $g_k(\mathbf{x}) \geq g_j(\mathbf{x})$ for all j, where

$$g_j(\mathbf{x}) = \sum_{i=1}^{d} x_i \log \frac{p_{ij}}{1 - p_{ij}} + \sum_{i=1}^{d} \log(1 - p_{ij}) + \log P(\omega_j).$$

15. Let the components of the vector $\mathbf{x} = (x_1, \ldots, x_d)^t$ be ternary valued (1, 0 or -1), with

$$p_{ij} = \text{Prob}(x_i = 1 \mid \omega_j)$$

$$q_{ij} = \text{Prob}(x_i = 0 \mid \omega_j)$$

$$r_{ij} = \text{Prob}(x_i = -1 \mid \omega_j)$$

and with the components x_i being statistically independent for all $\mathbf{x}$ in ω_j. Show that a minimum probability of error decision rule can be derived that involves discriminant functions $g_j(\mathbf{x})$ that are quadratic functions of the components x_i. Suggest a generalization of the results of Problems 14 and 15.

16. Let $\mathbf{x}$ be distributed as in Problem 14 with $c = 2$, d odd, and

$$p_{i1} = p > \tfrac{1}{2} \qquad i = 1, \ldots, d$$
$$p_{i2} = 1 - p \qquad i = 1, \ldots, d$$

and

$$P(\omega_1) = P(\omega_2) = \tfrac{1}{2}.$$

(a) Show that the minimum-error-rate decision rule becomes:

$$\text{Decide } \omega_1 \text{ if } \sum_{i=1}^{d} x_i > \frac{d}{2}.$$

(b) Show that the minimum probability of error is given by

$$P_e(d, p) = \sum_{k=0}^{(d-1)/2} \binom{d}{k} p^k (1-p)^{d-k}.$$

(c) What is the limiting value of $P_e(d, p)$ as $p \to 1/2$?

(d) Show that $P_e(d, p)$ approaches zero as $d \to \infty$. (This is difficult to do without invoking the Law of Large Numbers. It is worthwhile to understand why it is true, however, and those who are curious but short on time should see pp. 139–142 of W. Feller, *An Introduction to Probability Theory and Its Applications* (John Wiley, New York, Volume I, Second Edition, 1959).)

Chapter 3

PARAMETER ESTIMATION AND SUPERVISED LEARNING

3.1 PARAMETER ESTIMATION AND SUPERVISED LEARNING

In Chapter 2 we saw how we could design an optimal classifier if we knew the a priori probabilities $P(\omega_j)$ and the class-conditional densities $p(\mathbf{x} \mid \omega_j)$. Unfortunately, in pattern recognition applications we rarely if ever have this kind of complete knowledge about the probabilistic structure of the problem. In a typical case we merely have some vague, general knowledge about the situation, together with a number of *design samples*—particular representatives of the patterns we want to classify.* The problem, then, is to find some way to use this information to design the classifier.

One approach to this problem is to use the samples to estimate the unknown probabilities and probability densities, and to use the resulting estimates as if they were the true values. In typical pattern classification problems, the estimation of the a priori probabilities presents no serious difficulties. However, estimation of the class-conditional densities is quite another matter. The number of available samples always seems too small, and serious problems arise when the dimensionality of the feature vector $\mathbf{x}$ is large. If our general knowledge about the problem permits us to parameterize the

* In the statistical literature, a sample of size n is a set of n such representatives. In calling each representative a sample, we are following the practice of the engineering literature. Statisticians should consider each of our samples as a sample of size one.

conditional densities, the severity of these problems can be reduced significantly. Suppose, for example, that we can reasonably assume that $p(\mathbf{x} \mid \omega_j)$ is a normal density with mean $\boldsymbol{\mu}_j$ and covariance matrix Σ_j, although we do not know the exact values of these quantities. This simplifies the problem from one of estimating a *function* $p(\mathbf{x} \mid \omega_j)$ to one of estimating the *parameters* $\boldsymbol{\mu}_j$ and Σ_j.

The problem of parameter estimation is a classical problem in statistics, and it can be approached in several ways. We shall consider two common and reasonable procedures, *maximum likelihood* estimation and *Bayesian* estimation. Although the results obtained by these two procedures are frequently nearly identical, the approaches are conceptually quite different. Maximum likelihood methods view the parameters as quantities whose values are fixed but unknown. The best estimate is defined to be the one that maximizes the probability of obtaining the samples actually observed. Bayesian methods view the parameters as random variables having some known a priori distribution. Observation of the samples converts this to an a posteriori density, thereby revising our opinion about the true values of the parameters.

In the Bayesian case, we shall see that a typical effect of observing additional samples is to sharpen the a posteriori density function, causing it to peak near the true values of the parameters. This phenomenon is known as *Bayesian learning*. It is important to distinguish between *supervised learning* and *unsupervised learning*. In both cases, samples $\mathbf{x}$ are assumed to be obtained by selecting a state of nature ω_j with probability $P(\omega_j)$, and then independently selecting $\mathbf{x}$ according to the probability law $p(\mathbf{x} \mid \omega_j)$. The distinction is that with supervised learning we know the state of nature (class label) for each sample, whereas with unsupervised learning we do not. As one would expect, the problem of unsupervised learning is the more difficult one. In this chapter we shall consider only the supervised case, deferring consideration of unsupervised learning to Chapter 6.

3.2 MAXIMUM LIKELIHOOD ESTIMATION

3.2.1 The General Principle

Suppose that we separate a set of samples according to class, so that we have c sets of samples $\mathcal{X}_1, \ldots, \mathcal{X}_c$, with the samples in $\mathcal{X}_j$ having been drawn independently according to the probability law $p(\mathbf{x} \mid \omega_j)$. We assume that $p(\mathbf{x} \mid \omega_j)$ has a known parametric form, and is therefore determined uniquely by the value of a parameter vector $\boldsymbol{\theta}_j$. For example, we might have $p(\mathbf{x} \mid \omega_j) \sim N(\boldsymbol{\mu}_j, \Sigma_j)$, where the components of $\boldsymbol{\theta}_j$ include the components of both $\boldsymbol{\mu}_j$ and Σ_j. To show the dependence of $p(\mathbf{x} \mid \omega_j)$ on $\boldsymbol{\theta}_j$ explicitly, we write

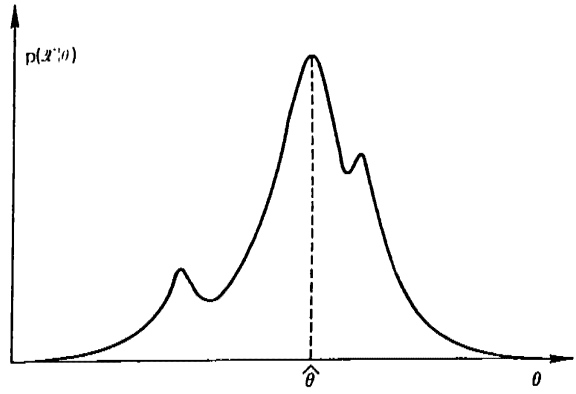

FIGURE 3.1. The maximum likelihood estimate for a parameter $\boldsymbol{\theta}$.

$p(\mathbf{x} \mid \omega_j)$ as* $p(\mathbf{x} \mid \omega_j, \boldsymbol{\theta}_j)$. Our problem is to use the information provided by the samples to obtain good estimates for the unknown parameter vectors $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_c$.

To simplify treatment of this problem, we shall assume that samples in $\mathcal{X}_i$ give no information about $\boldsymbol{\theta}_j$ if $i \neq j$. That is, we shall assume that the parameters for the different classes are functionally independent.† This permits us to work with each class separately, and to simplify our notation by deleting indications of class distinctions. Thus, with this assumption we have c separate problems of the following form: Use a set $\mathcal{X}$ of samples drawn independently according to the probability law $p(\mathbf{x} \mid \boldsymbol{\theta})$ to estimate the unknown parameter vector $\boldsymbol{\theta}$.

Suppose that $\mathcal{X}$ contains n samples, $\mathcal{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$. Then, since the samples were drawn independently,

$$p(\mathcal{X} \mid \boldsymbol{\theta}) = \prod_{k=1}^{n} p(\mathbf{x}_k \mid \boldsymbol{\theta}). \tag{1}$$

Viewed as a function of $\boldsymbol{\theta}$, $p(\mathcal{X} \mid \boldsymbol{\theta})$ is called the *likelihood* of $\boldsymbol{\theta}$ with respect to the set of samples. The *maximum likelihood estimate* of $\boldsymbol{\theta}$ is, by definition, that value $\hat{\boldsymbol{\theta}}$ that maximizes $p(\mathcal{X} \mid \boldsymbol{\theta})$ (see Figure 3.1). Intuitively, it corresponds to the value of $\boldsymbol{\theta}$ that in some sense best agrees with the actually observed samples.

* Some authors prefer to write $p(\mathbf{x} \mid \omega_j; \boldsymbol{\theta}_j)$, since, strictly speaking, the notation $p(\mathbf{x} \mid \omega_j, \boldsymbol{\theta}_j)$ implies that $\boldsymbol{\theta}_j$ is a random variable. We shall forgo this notational distinction, treating $\boldsymbol{\theta}_j$ as an ordinary parameter for maximum likelihood analysis and as a random variable for Bayesian analysis.

† Sometimes this is not the case, as, for example, when all of the samples share the same covariance matrix. The way to treat such cases is indicated in Problem 6.

For analytical purposes, it is usually easier to work with the logarithm of the likelihood than with the likelihood itself. Since the logarithm is monotonically increasing, the $\hat{\boldsymbol{\theta}}$ that maximizes the log-likelihood also maximizes the likelihood. If $p(\mathcal{X} \mid \boldsymbol{\theta})$ is a well behaved, differentiable function of $\boldsymbol{\theta}$, $\hat{\boldsymbol{\theta}}$ can be found by the standard methods of differential calculus. Let $\boldsymbol{\theta}$ be the p-component vector $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_p)^t$, let $\nabla_{\boldsymbol{\theta}}$ be the gradient operator

$$\nabla_{\boldsymbol{\theta}} = \begin{bmatrix} \dfrac{\partial}{\partial \theta_1} \\ \cdot \\ \cdot \\ \cdot \\ \dfrac{\partial}{\partial \theta_p} \end{bmatrix}, \tag{2}$$

and let $l(\boldsymbol{\theta})$ be the log-likelihood function

$$l(\boldsymbol{\theta}) = \log p(\mathcal{X} \mid \boldsymbol{\theta}). \tag{3}$$

Then

$$l(\boldsymbol{\theta}) = \sum_{k=1}^{n} \log p(\mathbf{x}_k \mid \boldsymbol{\theta}) \tag{4}$$

and

$$\nabla_{\boldsymbol{\theta}} l = \sum_{k=1}^{n} \nabla_{\boldsymbol{\theta}} \log p(\mathbf{x}_k \mid \boldsymbol{\theta}). \tag{5}$$

Thus, a set of necessary conditions for the maximum likelihood estimate for $\boldsymbol{\theta}$ can be obtained from the set of p equations $\nabla_{\boldsymbol{\theta}} l = \mathbf{0}$.

3.2.2 The Multivariate Normal Case: Unknown Mean

To see how these results apply to a specific case, suppose that the samples are drawn from a normal population with mean $\boldsymbol{\mu}$ and covariance matrix Σ. For simplicity, consider first the case where only the mean is unknown. Then

$$\log p(\mathbf{x}_k \mid \boldsymbol{\mu}) = -\tfrac{1}{2} \log\{(2\pi)^d \mid \Sigma \mid\} - \tfrac{1}{2}(\mathbf{x}_k - \boldsymbol{\mu})^t \Sigma^{-1} (\mathbf{x}_k - \boldsymbol{\mu})$$

and

$$\nabla_{\boldsymbol{\mu}} \log p(\mathbf{x}_k \mid \boldsymbol{\mu}) = \Sigma^{-1}(\mathbf{x}_k - \boldsymbol{\mu}).$$

Identifying $\boldsymbol{\theta}$ with $\boldsymbol{\mu}$, we see from Eq. (5) that the maximum likelihood estimate for $\boldsymbol{\mu}$ must satisfy

$$\sum_{k=1}^{n} \Sigma^{-1}(\mathbf{x}_k - \hat{\boldsymbol{\mu}}) = \mathbf{0}.$$

Multiplying by Σ and rearranging, we obtain

$$\hat{\boldsymbol{\mu}} = \frac{1}{n}\sum_{k=1}^{n} \mathbf{x}_k. \tag{6}$$

This is a very satisfying result. It says that the maximum likelihood estimate for the unknown population mean is just the arithmetic average of the samples—the *sample mean*. Geometrically, if we think of the n samples as a cloud of points, the sample mean is the centroid of the cloud. The sample mean has a number of desirable statistical properties as well, and one would be inclined to use this rather obvious estimate even without knowing that it is the maximum likelihood solution.

3.2.3 The General Multivariate Normal Case

In the general (and more typical) multivariate normal case, neither the mean $\boldsymbol{\mu}$ nor the covariance matrix Σ is known. Thus, these unknown parameters constitute the components of the parameter vector $\boldsymbol{\theta}$. Consider the univariate case with $\theta_1 = \mu$ and $\theta_2 = \sigma^2$. Here

$$\log p(x_k \mid \boldsymbol{\theta}) = -\tfrac{1}{2}\log 2\pi\theta_2 - \frac{1}{2\theta_2}(x_k - \theta_1)^2$$

and

$$\nabla_{\boldsymbol{\theta}} \log p(x_k \mid \boldsymbol{\theta}) = \begin{bmatrix} \dfrac{1}{\theta_2}(x_k - \theta_1) \\ -\dfrac{1}{2\theta_2} + \dfrac{(x_k - \theta_1)^2}{2\theta_2^2} \end{bmatrix}.$$

Then, Eq. (5) leads to the conditions

$$\sum_{k=1}^{n} \frac{1}{\hat{\theta}_2}(x_k - \hat{\theta}_1) = 0$$

and

$$-\sum_{k=1}^{n} \frac{1}{\hat{\theta}_2} + \sum_{k=1}^{n} \frac{(x_k - \hat{\theta}_1)^2}{\hat{\theta}_2^2} = 0,$$

where $\hat{\theta}_1$ and $\hat{\theta}_2$ are the maximum likelihood estimates for θ_1 and θ_2, respectively. By substituting $\hat{\mu} = \hat{\theta}_1$, $\hat{\sigma}^2 = \hat{\theta}_2$ and doing a little rearranging, we obtain the following maximum likelihood estimates for μ and σ^2:

$$\hat{\mu} = \frac{1}{n}\sum_{k=1}^{n} x_k \tag{7}$$

$$\hat{\sigma}^2 = \frac{1}{n}\sum_{k=1}^{n} (x_k - \hat{\mu})^2. \tag{8}$$

While the analysis of the multivariate case is basically very similar, considerably more manipulation is involved. The well known* result is that the maximum likelihood estimates for μ and Σ are given by

$$\hat{\mu} = \frac{1}{n}\sum_{k=1}^{n} \mathbf{x}_k \tag{9}$$

and

$$\hat{\Sigma} = \frac{1}{n}\sum_{k=1}^{n}(\mathbf{x}_k - \hat{\mu})(\mathbf{x}_k - \hat{\mu})^t. \tag{10}$$

Thus, once again we find that the maximum likelihood estimate for the mean vector is the sample mean. The maximum likelihood estimate for the covariance matrix is the arithmetic average of the n matrices $(\mathbf{x}_k - \hat{\mu}) \times (\mathbf{x}_k - \hat{\mu})^t$. Since the true covariance matrix is the expected value of the matrix $(\mathbf{x} - \mu)(\mathbf{x} - \mu)^t$, this is also a very satisfying result.

3.3 THE BAYES CLASSIFIER

Readers familiar with statistics know that the maximum likelihood estimate for a covariance matrix is biased; that is, the expected value of $\hat{\Sigma}$ is not equal to Σ. An unbiased estimate for Σ is supplied by the *sample covariance matrix*

$$C = \frac{1}{n-1}\sum_{k=1}^{n}(\mathbf{x}_k - \hat{\mu})(\mathbf{x}_k - \hat{\mu})^t. \tag{11}$$

Clearly, $\hat{\Sigma} = [(n-1)/n]C$, and these two estimates are essentially identical when n is large. However, the existence of two similar but nevertheless distinct estimates for the covariance matrix is disconcerting to many students, and it is natural to ask which one is "correct." Of course, the answer is that these estimates are neither right nor wrong, they are just different. What the existence of two different estimates actually shows is that no single estimate possesses all of the properties one might desire. For our purposes, the most desirable property is rather complex—we want the estimate that leads to the best classification performance. While it is usually both reasonable and sound to design a classifier by substituting the maximum likelihood estimates for the unknown parameters, one might well wonder if other estimates might not lead to better performance. In this section we address this question from a Bayesian viewpoint.

* Cf., T. W. Anderson, *An Introduction to Multivariate Statistical Analysis*, Chap. 3 (John Wiley, New York, 1958).

3.3.1 The Class-Conditional Densities

The computation of the a posteriori probabilities $P(\omega_i \mid \mathbf{x})$ lies at the heart of Bayesian classification. Bayes rule allows us to compute these probabilities from the a priori probabilities $P(\omega_i)$ and the class-conditional densities $p(\mathbf{x} \mid \omega_i)$, but how can we proceed when these quantities are unknown? The general answer to this question is that the best we can do is to compute $P(\omega_i \mid \mathbf{x})$ using all of the information at our disposal. Part of this information might be a priori knowledge, such as knowledge of the functional forms for unknown densities and ranges for the values of unknown parameters. Part of this information might reside in a set of samples. If we let $\mathcal{X}$ denote the set of samples, then we can emphasize the role of the samples by saying that our goal is to compute the a posteriori probabilities $P(\omega_i \mid \mathbf{x}, \mathcal{X})$. From these probabilities we can obtain the Bayes classifier.

By Bayes rule,*

$$P(\omega_i \mid \mathbf{x}, \mathcal{X}) = \frac{p(\mathbf{x} \mid \omega_i, \mathcal{X})P(\omega_i \mid \mathcal{X})}{\sum_{j=1}^{c} p(\mathbf{x} \mid \omega_j, \mathcal{X})P(\omega_j \mid \mathcal{X})}. \tag{12}$$

As this equation suggests, we can use the information provided by the samples to help determine both the class-conditional densities and the a priori probabilities.

Although we could maintain this generality, we shall henceforth assume that the true values of the a priori probabilities are known, so that $P(\omega_i \mid \mathcal{X}) = P(\omega_i)$. Furthermore, since we are treating the supervised case, we can separate the samples by class into c subsets $\mathcal{X}_1, \ldots, \mathcal{X}_c$, with the samples in $\mathcal{X}_i$ belonging to ω_i. In many cases of interest, and in all of the cases we shall treat, the samples in $\mathcal{X}_j$ have no influence on $p(\mathbf{x} \mid \omega_i, \mathcal{X})$ if $i \neq j$. This has two simplifying consequences. First, it allows us to work with each class separately, using only the samples in $\mathcal{X}_i$ to determine $p(\mathbf{x} \mid \omega_i, \mathcal{X})$. Used in conjunction with our assumption that the a priori probabilities are known, this allows us to write Eq. (12) as

$$P(\omega_i \mid \mathbf{x}, \mathcal{X}) = \frac{p(\mathbf{x} \mid \omega_i, \mathcal{X}_i)P(\omega_i)}{\sum_{j=1}^{c} p(\mathbf{x} \mid \omega_j, \mathcal{X}_j)P(\omega_j)}. \tag{13}$$

Second, because each class can be treated independently, we can dispense with needless class distinctions and simplify our notation. In essence, we have c

* Note that every probability and probability density function in this equation is conditioned by the set of samples. The fact that this equation is merely Bayes rule becomes more clear when common conditioning quantities are ignored. The reader may find this device helpful in interpreting similar equations elsewhere in this chapter.

separate problems of the following form: Use a set $\mathcal{X}$ of samples drawn independently according to the fixed but unknown probability law $p(\mathbf{x})$ to determine $p(\mathbf{x} \mid \mathcal{X})$. This is the central problem of Bayesian learning.

3.3.2 The Parameter Distribution

Although the desired probability density $p(\mathbf{x})$ is unknown, we assume that it has a known parametric form. The only thing assumed unknown is the value of a parameter vector $\boldsymbol{\theta}$. We shall express the fact that $p(\mathbf{x})$ is unknown but has known parametric form by saying that the function $p(\mathbf{x} \mid \boldsymbol{\theta})$ is completely known. The Bayesian approach assumes that the unknown parameter vector is a random variable. Any information we might have about $\boldsymbol{\theta}$ prior to observing the samples is assumed to be contained in a *known* a priori density $p(\boldsymbol{\theta})$. Observation of the samples converts this to an a posteriori density $p(\boldsymbol{\theta} \mid \mathcal{X})$, which, hopefully, is sharply peaked about the true value of $\boldsymbol{\theta}$.

Our basic goal is to compute $p(\mathbf{x} \mid \mathcal{X})$, which is as close as we can come to obtaining the unknown $p(\mathbf{x})$. We do this by integrating the joint density $p(\mathbf{x}, \boldsymbol{\theta} \mid \mathcal{X})$ over $\boldsymbol{\theta}$. That is,

$$p(\mathbf{x} \mid \mathcal{X}) = \int p(\mathbf{x}, \boldsymbol{\theta} \mid \mathcal{X})\, d\boldsymbol{\theta},$$

where the integration extends over the entire parameter space.* Now we can always write $p(\mathbf{x}, \boldsymbol{\theta} \mid \mathcal{X})$ as the product $p(\mathbf{x} \mid \boldsymbol{\theta}, \mathcal{X})p(\boldsymbol{\theta} \mid \mathcal{X})$. Since the selection of $\mathbf{x}$ and of the samples in $\mathcal{X}$ is done independently, the first factor is merely $p(\mathbf{x} \mid \boldsymbol{\theta})$. That is, the distribution of $\mathbf{x}$ is known completely once we know the value of the parameter vector. Thus,

$$p(\mathbf{x} \mid \mathcal{X}) = \int p(\mathbf{x} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \mathcal{X})\, d\boldsymbol{\theta}. \tag{14}$$

This key equation links the desired "class-conditional" density $p(\mathbf{x} \mid \mathcal{X})$ to the a posteriori density $p(\boldsymbol{\theta} \mid \mathcal{X})$ for the unknown parameter vector. If $p(\boldsymbol{\theta} \mid \mathcal{X})$ peaks very sharply about some value $\hat{\boldsymbol{\theta}}$, we obtain $p(\mathbf{x} \mid \mathcal{X}) \approx p(\mathbf{x} \mid \hat{\boldsymbol{\theta}})$, i.e., the result we would obtain by substituting the estimate $\hat{\boldsymbol{\theta}}$ for the true parameter vector. In general, if we are less certain about the exact value of $\boldsymbol{\theta}$, this equation directs us to average $p(\mathbf{x} \mid \boldsymbol{\theta})$ over the possible values of $\boldsymbol{\theta}$. Thus, when the unknown densities have a known parametric form, the samples exert their influence on $p(\mathbf{x} \mid \mathcal{X})$ through the a posteriori density $p(\boldsymbol{\theta} \mid \mathcal{X})$.

* Throughout this chapter we shall take the domain of integration for all integrals to be the entire space involved.

3.4 LEARNING THE MEAN OF A NORMAL DENSITY

3.4.1 The Univariate Case: $p(\mu \mid \mathcal{X})$

In this section we calculate the a posteriori density $p(\boldsymbol{\theta} \mid \mathcal{X})$ and the desired probability density $p(\mathbf{x} \mid \mathcal{X})$ for the case where $p(\mathbf{x} \mid \boldsymbol{\mu}) \sim N(\boldsymbol{\mu}, \Sigma)$, the mean vector $\boldsymbol{\mu}$ being the unknown parameter vector. For simplicity, we begin with the univariate case, so that

$$p(x \mid \mu) \sim N(\mu, \sigma^2), \tag{15}$$

where the only unknown quantity is the mean μ. We assume that whatever prior knowledge we might have about μ can be expressed by a *known* a priori density $p(\mu)$. In the sequel, we shall make the further assumption that

$$p(\mu) \sim N(\mu_0, \sigma_0^2), \tag{16}$$

where both μ_0 and σ_0^2 are known. Roughly speaking, μ_0 represents our best a priori guess for μ, and σ_0^2 measures our uncertainty about this guess. The assumption that the a priori distribution for μ is normal will simplify the subsequent mathematics. However, the crucial assumption is not so much that the a priori distribution for μ is normal, but that it exists and is known.

Having selected the a priori density for μ, we can view the situation as follows. Imagine that a value is drawn for μ from a population governed by the probability law $p(\mu)$. Once this value is drawn, it becomes the true value of μ and completely determines the density for x. Suppose now that n samples $x_1, \ldots, x_n$ are independently drawn from the resulting population. Letting $\mathcal{X} = \{x_1, \ldots, x_n\}$, we use Bayes rule to obtain

$$p(\mu \mid \mathcal{X}) = \frac{p(\mathcal{X} \mid \mu)p(\mu)}{\int p(\mathcal{X} \mid \mu)p(\mu)\, d\mu}$$

$$= \alpha \prod_{k=1}^{n} p(x_k \mid \mu)p(\mu), \tag{17}$$

where α is a scale factor that depends on $\mathcal{X}$ but is independent of μ. This equation shows how the observation of a set of samples affects our ideas about the true value of μ, changing the a priori density $p(\mu)$ into an a

posteriori density $p(\mu \mid \mathcal{X})$. Since $p(x_k \mid \mu) \sim N(\mu, \sigma^2)$ and $p(\mu) \sim N(\mu_0, \sigma_0^2)$,

$$p(\mu \mid \mathcal{X}) = \alpha \prod_{k=1}^{n} \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left[-\frac{1}{2}\left(\frac{x_k - \mu}{\sigma}\right)^2\right] \frac{1}{\sqrt{2\pi}\,\sigma_0} \exp\left[-\frac{1}{2}\left(\frac{\mu - \mu_0}{\sigma_0}\right)^2\right]$$

$$= \alpha' \exp\left[-\frac{1}{2}\left\{\sum_{k=1}^{n}\left(\frac{\mu - x_k}{\sigma}\right)^2 + \left(\frac{\mu - \mu_0}{\sigma_0}\right)^2\right\}\right]$$

$$= \alpha'' \exp\left[-\frac{1}{2}\left\{\left(\frac{n}{\sigma^2} + \frac{1}{\sigma_0^2}\right)\mu^2 - 2\left(\frac{1}{\sigma^2}\sum_{k=1}^{n} x_k + \frac{\mu_0}{\sigma_0^2}\right)\mu\right\}\right], \tag{18}$$

where factors that do not depend on μ have been absorbed in the constants α' and α''. Thus, $p(\mu \mid \mathcal{X})$ is an exponential function of a quadratic function of μ, i.e., is again a normal density. Since this is true for any number of samples, $p(\mu \mid \mathcal{X})$ remains normal as the number n of samples is increased, and $p(\mu \mid \mathcal{X})$ is said to be a *reproducing density*. If we write $p(\mu \mid \mathcal{X}) \sim N(\mu_n, \sigma_n^2)$, then μ_n and σ_n^2 can be found by equating coefficients in Eq. (18) with corresponding coefficients in

$$p(\mu \mid \mathcal{X}) = \frac{1}{\sqrt{2\pi}\,\sigma_n} \exp\left[-\frac{1}{2}\left(\frac{\mu - \mu_n}{\sigma_n}\right)^2\right]. \tag{19}$$

This yields

$$\frac{1}{\sigma_n^2} = \frac{n}{\sigma^2} + \frac{1}{\sigma_0^2} \tag{20}$$

and

$$\frac{\mu_n}{\sigma_n^2} = \frac{n}{\sigma^2} m_n + \frac{\mu_0}{\sigma_0^2}, \tag{21}$$

where m_n is the *sample mean*

$$m_n = \frac{1}{n}\sum_{k=1}^{n} x_k. \tag{22}$$

Solving explicitly for μ_n and σ_n^2, we obtain

$$\mu_n = \frac{n\sigma_0^2}{n\sigma_0^2 + \sigma^2} m_n + \frac{\sigma^2}{n\sigma_0^2 + \sigma^2}\mu_0 \tag{23}$$

and

$$\sigma_n^2 = \frac{\sigma_0^2\sigma^2}{n\sigma_0^2 + \sigma^2}. \tag{24}$$

These equations show how the a priori information is combined with the empirical information in the samples to obtain the a posteriori density $p(\mu \mid \mathcal{X})$. Roughly speaking, μ_n represents our best guess for μ after observing

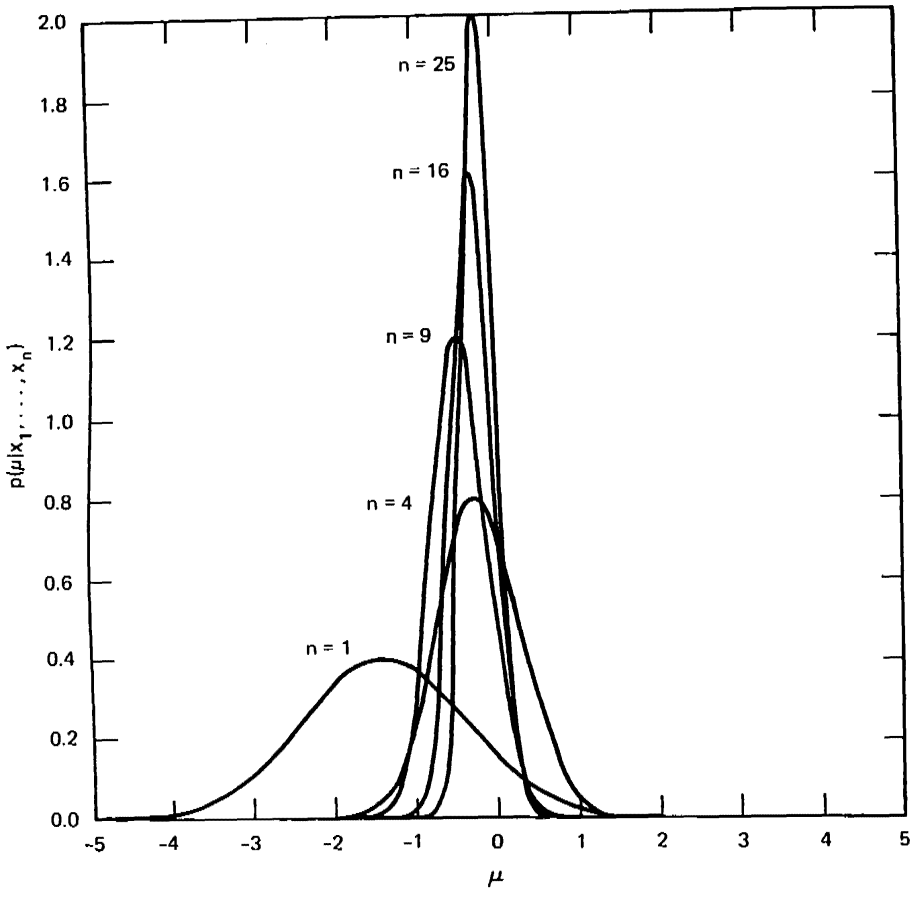

FIGURE 3.2. Learning the mean of a normal density.

n samples, and σ_n^2 measures our uncertainty about this guess. Since σ_n^2 decreases monotonically with n, approaching σ^2/n as n approaches infinity, each additional observation decreases our uncertainty about the true value of μ. As n increases, $p(\mu \mid \mathscr{X})$ becomes more and more sharply peaked, approaching a Dirac delta function as n approaches infinity. This behavior is commonly known as *Bayesian learning* (see Figure 3.2).

In general, μ_n is a linear combination of m_n and μ_0, with coefficients that are nonnegative and sum to one. Thus, μ_n always lies somewhere between m_n and μ_0. If $\sigma_0 \neq 0$, μ_n approaches the sample mean as n approaches infinity. If $\sigma_0 = 0$, we have a degenerate case in which our a priori certainty that $\mu = \mu_0$ is so strong that no number of observations can change our opinion. At the other extreme, if $\sigma_0 \gg \sigma$, we are so uncertain about our a priori guess that we take $\mu_n = m_n$, using only the samples to estimate μ. In

general, the relative balance between prior knowledge and empirical data is set by the ratio of σ^2 to σ_0^2, which is sometimes called the *dogmatism*. If the dogmatism is not infinite, after enough samples are taken the exact values assumed for μ_0 and σ_0^2 will be unimportant, and μ_n will converge to the sample mean.

3.4.2 The Univariate Case: $p(x \mid \mathcal{X})$

Having obtained the a posteriori density $p(\mu \mid \mathcal{X})$, all that remains is to obtain the "class-conditional" density $p(x \mid \mathcal{X})$.* From Eqs. (14), (15), and (19),

$$p(x \mid \mathcal{X}) = \int p(x \mid \mu)p(\mu \mid \mathcal{X})\, d\mu$$

$$= \int \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] \frac{1}{\sqrt{2\pi}\,\sigma_n} \exp\left[-\frac{1}{2}\left(\frac{\mu-\mu_n}{\sigma_n}\right)^2\right] d\mu$$

$$= \frac{1}{2\pi\sigma\sigma_n} \exp\left[-\frac{1}{2}\frac{(x-\mu_n)^2}{\sigma^2+\sigma_n^2}\right] f(\sigma, \sigma_n),$$

where

$$f(\sigma, \sigma_n) = \int \exp\left[-\frac{1}{2}\frac{\sigma^2+\sigma_n^2}{\sigma^2\sigma_n^2}\left(\mu - \frac{\sigma_n^2 x + \sigma^2\mu_n}{\sigma^2+\sigma_n^2}\right)^2\right] d\mu.$$

That is, as a function of x, $p(x \mid \mathcal{X})$ is proportional to $\exp[-(1/2)(x-\mu_n)^2/(\sigma^2+\sigma_n^2)]$, and hence $p(x \mid \mathcal{X})$ is normally distributed with mean μ_n and variance $\sigma^2+\sigma_n^2$:

$$p(x \mid \mathcal{X}) \sim N(\mu_n, \sigma^2+\sigma_n^2). \tag{25}$$

In other words, to obtain the "class-conditional" density $p(x \mid \mathcal{X})$, whose parametric form is known to be $p(x \mid \mu) \sim N(\mu, \sigma^2)$, we merely replace μ by μ_n and σ^2 by $\sigma^2+\sigma_n^2$. In effect, the conditional mean μ_n is treated as if it were the true mean, and the known variance is increased to account for the additional uncertainty in x resulting from our lack of exact knowledge of the mean μ. This, then, is our final result; the density $p(x \mid \mathcal{X})$ is the desired class-conditional density $p(x \mid \omega_j, \mathcal{X}_j)$, and together with the a priori probabilities $P(\omega_j)$ it gives us the probabilistic information needed to design the Bayes classifier.

3.4.3 The Multivariate Case

The treatment of the multivariate case is a direct generalization of the univariate case. Thus, we shall only sketch the proof briefly. As before, we

* Recall that we dropped class distinctions for simplicity, but that all the samples come from the same class, say ω_j, and $p(x \mid \mathcal{X})$ is really $p(x \mid \omega_j, \mathcal{X}_j)$.

assume that

$$p(\mathbf{x} \mid \boldsymbol{\mu}) \sim N(\boldsymbol{\mu}, \Sigma) \tag{26}$$

and

$$p(\boldsymbol{\mu}) \sim N(\boldsymbol{\mu}_0, \Sigma_0), \tag{27}$$

where Σ, Σ_0, and $\boldsymbol{\mu}_0$ are assumed to be known. After observing a set $\mathcal{X}$ of n independent samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$, we use Bayes rule to obtain

$$\begin{aligned} p(\boldsymbol{\mu} \mid \mathcal{X}) &= \alpha \prod_{k=1}^{n} p(\mathbf{x}_k \mid \boldsymbol{\mu}) p(\boldsymbol{\mu}) \\ &= \alpha'' \exp\left[-\tfrac{1}{2}\left\{ \boldsymbol{\mu}^t (n\Sigma^{-1} + \Sigma_0^{-1})\boldsymbol{\mu} - 2\boldsymbol{\mu}^t \left(\Sigma^{-1} \sum_{k=1}^{n} \mathbf{x}_k + \Sigma_0^{-1}\boldsymbol{\mu}_0 \right) \right\} \right], \end{aligned}$$

which has the form

$$p(\boldsymbol{\mu} \mid \mathcal{X}) = \alpha''' \exp[-\tfrac{1}{2}(\boldsymbol{\mu} - \boldsymbol{\mu}_n)^t \Sigma_n^{-1} (\boldsymbol{\mu} - \boldsymbol{\mu}_n)].$$

Thus, $p(\boldsymbol{\mu} \mid \mathcal{X}) \sim N(\boldsymbol{\mu}_n, \Sigma_n)$, and once again we have a reproducing density. Equating coefficients, we obtain the analogs of Eqs. (20) and (21),

$$\Sigma_n^{-1} = n\Sigma^{-1} + \Sigma_0^{-1} \tag{28}$$

and

$$\Sigma_n^{-1}\boldsymbol{\mu}_n = n\Sigma^{-1}\mathbf{m}_n + \Sigma_0^{-1}\boldsymbol{\mu}_0, \tag{29}$$

where $\mathbf{m}_n$ is the sample mean

$$\mathbf{m}_n = \frac{1}{n} \sum_{k=1}^{n} \mathbf{x}_k. \tag{30}$$

The solution of these equations for $\boldsymbol{\mu}_n$ and Σ_n is simplified by knowledge of the matrix identity

$$(A^{-1} + B^{-1})^{-1} = A(A + B)^{-1}B = B(A + B)^{-1}A,$$

which is valid for any pair of nonsingular, d-by-d matrices A and B. After a little manipulation, we obtain the final results

$$\boldsymbol{\mu}_n = \Sigma_0 \left(\Sigma_0 + \frac{1}{n}\Sigma \right)^{-1} \mathbf{m}_n + \frac{1}{n}\Sigma \left(\Sigma_0 + \frac{1}{n}\Sigma \right)^{-1} \boldsymbol{\mu}_0 \tag{31}$$

and

$$\Sigma_n = \Sigma_0 \left(\Sigma_0 + \frac{1}{n}\Sigma \right)^{-1} \frac{1}{n}\Sigma. \tag{32}$$

The proof that $p(\mathbf{x} \mid \mathcal{X}) \sim N(\boldsymbol{\mu}_n, \Sigma + \Sigma_n)$ can be obtained as before by performing the integration

$$p(\mathbf{x} \mid \mathcal{X}) = \int p(\mathbf{x} \mid \boldsymbol{\mu}) p(\boldsymbol{\mu} \mid \mathcal{X})\, d\boldsymbol{\mu}.$$

However, this result can be obtained with less effort by observing that $\mathbf{x}$ can be viewed as the sum of two random variables, a random vector $\boldsymbol{\mu}$ with $p(\boldsymbol{\mu} \mid \mathcal{X}) \sim N(\boldsymbol{\mu}_n, \Sigma_n)$ and an independent random vector $\mathbf{y}$ with $p(\mathbf{y}) \sim N(\mathbf{0}, \Sigma)$. Since the sum of two independent, normally distributed vectors is again a normally distributed vector whose mean is the sum of the means and whose covariance matrix is the sum of the covariance matrices, we have

$$p(\mathbf{x} \mid \mathcal{X}) \sim N(\boldsymbol{\mu}_n, \Sigma + \Sigma_n), \tag{33}$$

and the generalization is complete.

3.5 GENERAL BAYESIAN LEARNING

We have just seen how the Bayesian approach can be used to obtain the desired density $p(\mathbf{x} \mid \mathcal{X})$ in a special, multivariate normal case. This approach can be generalized to apply to any situation in which the unknown density can be parameterized. The basic assumptions are summarized as follows:

(1) The form of the density $p(\mathbf{x} \mid \boldsymbol{\theta})$ is assumed to be known, but the value of the parameter vector $\boldsymbol{\theta}$ is not known exactly.
(2) Our initial knowledge about $\boldsymbol{\theta}$ is assumed to be contained in a known a priori density $p(\boldsymbol{\theta})$.
(3) The rest of our knowledge about $\boldsymbol{\theta}$ is contained in a set $\mathcal{X}$ of n samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$ drawn independently according to the unknown probability law $p(\mathbf{x})$.

The basic problem is to compute the a posteriori density $p(\boldsymbol{\theta} \mid \mathcal{X})$, since from this we can use Eq. (14) to compute $p(\mathbf{x} \mid \mathcal{X})$:

$$p(\mathbf{x} \mid \mathcal{X}) = \int p(\mathbf{x} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \mathcal{X})\, d\boldsymbol{\theta}. \tag{14}$$

By Bayes rule,

$$p(\boldsymbol{\theta} \mid \mathcal{X}) = \frac{p(\mathcal{X} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta})}{\int p(\mathcal{X} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta})\, d\boldsymbol{\theta}}, \tag{34}$$

and by the independence assumption

$$p(\mathcal{X} \mid \boldsymbol{\theta}) = \prod_{k=1}^{n} p(\mathbf{x}_k \mid \boldsymbol{\theta}). \tag{35}$$

This constitutes the formal solution to the problem. Eqs. (14) and (34) illuminate its relation to the maximum likelihood solution. Suppose that $p(\mathcal{X} \mid \boldsymbol{\theta})$ reaches a sharp peak at $\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}$. If the a priori density $p(\boldsymbol{\theta})$ is not zero at $\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}$ and does not change much in the surrounding neighborhood, then

$p(\boldsymbol{\theta} \mid \mathcal{X})$ also peaks at that point. Thus, Eq. (14) shows that $p(\mathbf{x} \mid \mathcal{X})$ will be approximately $p(\mathbf{x} \mid \hat{\boldsymbol{\theta}})$, the result one would obtain by using the maximum likelihood estimate as if it were the true value. If the peak of $p(\mathcal{X} \mid \boldsymbol{\theta})$ is not so sharp that the influence of a priori information on the uncertainty in the true value of $\boldsymbol{\theta}$ can be ignored, then the Bayesian solution tells us how to use the available information to compute the desired density $p(\mathbf{x} \mid \mathcal{X})$.

While we have obtained the formal Bayesian solution to the problem, a number of interesting questions remain. One concerns the difficulty of carrying out these computations. Another concerns the convergence of $p(\mathbf{x} \mid \mathcal{X})$ to $p(\mathbf{x})$. We shall discuss the matter of convergence briefly, and shall then turn to the computational question.

To indicate explicitly the number of samples in a set, we shall write $\mathcal{X}^n = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$. Then from Eq. (35), if $n > 1$

$$p(\mathcal{X}^n \mid \boldsymbol{\theta}) = p(\mathbf{x}_n \mid \boldsymbol{\theta}) p(\mathcal{X}^{n-1} \mid \boldsymbol{\theta}).$$

Substituting this in Eq. (34) and using Bayes rule, we see that the a posteriori density satisfies the recursion relation

$$p(\boldsymbol{\theta} \mid \mathcal{X}^n) = \frac{p(\mathbf{x}_n \mid \boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \mathcal{X}^{n-1})}{\int p(\mathbf{x}_n \mid \boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \mathcal{X}^{n-1})\, d\boldsymbol{\theta}} \tag{36}$$

With the understanding that $p(\boldsymbol{\theta} \mid \mathcal{X}^0) = p(\boldsymbol{\theta})$, repeated use of this equation produces the sequence of densities $p(\boldsymbol{\theta})$, $p(\boldsymbol{\theta} \mid \mathbf{x}_1)$, $p(\boldsymbol{\theta} \mid \mathbf{x}_1, \mathbf{x}_2)$, and so forth. This is called the *recursive Bayes* approach to parameter estimation. When this sequence of densities converges to a Dirac delta function centered about the true parameter value, the resulting behavior is frequently called *Bayesian learning*.

For most of the typically encountered probability densities $p(\mathbf{x} \mid \boldsymbol{\theta})$, the sequence of a posteriori densities does converge to a delta function. Roughly speaking, this implies that with a large number of samples there is only one value for $\boldsymbol{\theta}$ that causes $p(\mathbf{x} \mid \boldsymbol{\theta})$ to fit the data, i.e., that $\boldsymbol{\theta}$ can be determined uniquely from $p(\mathbf{x} \mid \boldsymbol{\theta})$. When this is the case, $p(\mathbf{x} \mid \boldsymbol{\theta})$ is said to be *identifiable*. A rigorous proof of convergence under these conditions requires a precise statement of the properties required of $p(\mathbf{x} \mid \boldsymbol{\theta})$ and $p(\boldsymbol{\theta})$ and considerable care, but presents no serious problems.

There are occasions, however, when more than one value of $\boldsymbol{\theta}$ may yield the same value for $p(\mathbf{x} \mid \boldsymbol{\theta})$. In such cases, $\boldsymbol{\theta}$ can not be determined uniquely from $p(\mathbf{x} \mid \boldsymbol{\theta})$, and $p(\boldsymbol{\theta} \mid \mathcal{X}^n)$ will peak near all of the values of $\boldsymbol{\theta}$ that explain the data. Fortunately, this ambiguity is erased by the integration in Eq. (14), since $p(\mathbf{x} \mid \boldsymbol{\theta})$ is the same for all of these values of $\boldsymbol{\theta}$. Thus, $p(\mathbf{x} \mid \mathcal{X}^n)$ will typically converge to $p(\mathbf{x})$ whether or not $p(\mathbf{x} \mid \boldsymbol{\theta})$ is identifiable. While this might make the problem of identifiability appear to be something of a straw

man, we shall see in Chapter 6 that identifiability presents a genuine problem in the case of unsupervised learning.

3.6 SUFFICIENT STATISTICS

From a practical viewpoint, the formal solution provided by Eqs. (14), (34), and (35) is not computationally attractive. In pattern classification applications it is not unusual to have dozens or hundreds of unknown parameters and thousands of samples, which makes the direct computation and tabulation of $p(\mathcal{X} \mid \boldsymbol{\theta})$ or $p(\boldsymbol{\theta} \mid \mathcal{X})$ quite out of the question. The only hope for a computationally feasible solution lies in being able to find a parametric form for $p(\mathbf{x} \mid \boldsymbol{\theta})$ that on the one hand matches the characteristics of the problem and on the other hand allows a reasonable analytical solution.

Consider the simplification that occurred in the problem of learning the mean of a multivariate normal density. Assuming that the a priori density $p(\boldsymbol{\mu})$ was normal, we found that the a posteriori density $p(\boldsymbol{\mu} \mid \mathcal{X})$ was also normal. Equally important, Eqs. (31) and (32) show that the basic data processing required was merely the computation of the sample mean $\mathbf{m}_n$. This easily computed and easily updated statistic contained all the information in the samples relevant to estimating the unknown population mean. One might suspect that this simplicity is just one more happy property of the normal distribution, and that such good fortune is not likely to occur in other cases. While this is largely true, there is a family of distributions for which computationally feasible solutions can be obtained, and the key to their simplicity lies in the notion of a *sufficient statistic.*

To begin with, any function of the samples is a statistic. Roughly speaking, a sufficient statistic $\mathbf{s}$ is a function* of the samples $\mathcal{X}$ that contains all of the information relevant to estimating some parameter $\boldsymbol{\theta}$. Intuitively, one might expect the definition of a sufficient statistic to involve the requirement that $p(\boldsymbol{\theta} \mid \mathbf{s}, \mathcal{X}) = p(\boldsymbol{\theta} \mid \mathbf{s})$. However, this would require treating $\boldsymbol{\theta}$ as a random variable, limiting the definition to a Bayesian domain. Thus, the conventional definition is as follows: A statistic $\mathbf{s}$ is said to be *sufficient* for $\boldsymbol{\theta}$ if $p(\mathcal{X} \mid \mathbf{s}, \boldsymbol{\theta})$ is independent of $\boldsymbol{\theta}$. If we think of $\boldsymbol{\theta}$ as a random variable, we can write

$$p(\boldsymbol{\theta} \mid \mathbf{s}, \mathcal{X}) = \frac{p(\mathcal{X} \mid \mathbf{s}, \boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \mathbf{s})}{p(\mathcal{X} \mid \mathbf{s})},$$

whereupon it becomes evident that $p(\boldsymbol{\theta} \mid \mathbf{s}, \mathcal{X}) = p(\boldsymbol{\theta} \mid \mathbf{s})$ if $\mathbf{s}$ is sufficient for $\boldsymbol{\theta}$. Conversely, if $\mathbf{s}$ is a statistic for which $p(\boldsymbol{\theta} \mid \mathbf{s}, \mathcal{X}) = p(\boldsymbol{\theta} \mid \mathbf{s})$, and if $p(\boldsymbol{\theta} \mid \mathbf{s}) \neq 0$, it is easy to show that $p(\mathcal{X} \mid \mathbf{s}, \boldsymbol{\theta})$ is independent of $\boldsymbol{\theta}$. Thus, the intuitive and the conventional definitions are basically equivalent.

* When we must distinguish between the function and its value, we shall write $\mathbf{s} = \boldsymbol{\varphi}(\mathcal{X})$.

A fundamental theorem concerning sufficient statistics is the *factorization theorem*, which states that $\mathbf{s}$ is sufficient for $\boldsymbol{\theta}$ if and only if $p(\mathcal{X} \mid \boldsymbol{\theta})$ can be factored into the product of two functions, one depending only on $\mathbf{s}$ and $\boldsymbol{\theta}$, and the other depending only on the samples. The virtue of the factorization theorem is that it allows us to shift our attention from the rather complicated density $p(\mathcal{X} \mid \mathbf{s}, \boldsymbol{\theta})$ used to define a sufficient statistic to the simpler function

$$p(\mathcal{X} \mid \boldsymbol{\theta}) = \prod_{k=1}^{n} p(\mathbf{x}_k \mid \boldsymbol{\theta}).$$

In addition, the factorization theorem makes it clear that the characteristics of a sufficient statistic are completely determined by the density $p(\mathbf{x} \mid \boldsymbol{\theta})$, and have nothing to do with a felicitous choice for an a priori density $p(\boldsymbol{\theta})$. A proof of the factorization theorem in the continuous case is slightly sticky because degenerate situations are involved. Since the proof has some intrinsic interest, however, we include a proof for the simpler discrete case.

The Factorization Theorem: A statistic $\mathbf{s}$ is sufficient for $\boldsymbol{\theta}$ if and only if the probability $P(\mathcal{X} \mid \boldsymbol{\theta})$ can be written as the product

$$P(\mathcal{X} \mid \boldsymbol{\theta}) = g(\mathbf{s}, \boldsymbol{\theta})h(\mathcal{X}). \tag{37}$$

Proof: *(a)* Suppose first that $\mathbf{s}$ is sufficient for $\boldsymbol{\theta}$, so that $P(\mathcal{X} \mid \mathbf{s}, \boldsymbol{\theta})$ is independent of $\boldsymbol{\theta}$. Since we want to show that $P(\mathcal{X} \mid \boldsymbol{\theta})$ can be factored, our attention is directed toward computing $P(\mathcal{X} \mid \boldsymbol{\theta})$ in terms of $P(\mathcal{X} \mid \mathbf{s}, \boldsymbol{\theta})$. We do this by summing the joint probability $P(\mathcal{X}, \mathbf{s} \mid \boldsymbol{\theta})$ over all values of $\mathbf{s}$:

$$\begin{aligned} P(\mathcal{X} \mid \boldsymbol{\theta}) &= \sum_{\mathbf{s}} P(\mathcal{X}, \mathbf{s} \mid \boldsymbol{\theta}) \\ &= \sum_{\mathbf{s}} P(\mathcal{X} \mid \mathbf{s}, \boldsymbol{\theta}) P(\mathbf{s} \mid \boldsymbol{\theta}). \end{aligned}$$

But since $\mathbf{s} = \boldsymbol{\varphi}(\mathcal{X})$, there is only one possible value for $\mathbf{s}$, and thus

$$P(\mathcal{X} \mid \boldsymbol{\theta}) = P(\mathcal{X} \mid \mathbf{s}, \boldsymbol{\theta}) P(\mathbf{s} \mid \boldsymbol{\theta}).$$

Moreover, since by hypothesis $P(\mathcal{X} \mid \mathbf{s}, \boldsymbol{\theta})$ is independent of $\boldsymbol{\theta}$, the first factor depends only on $\mathcal{X}$. Identifying $P(\mathbf{s} \mid \boldsymbol{\theta})$ with $g(\mathbf{s}, \boldsymbol{\theta})$, we see that $P(\mathcal{X} \mid \boldsymbol{\theta})$ factors as desired.

(b) To show that the ability to factor $P(\mathcal{X} \mid \boldsymbol{\theta})$ as the product $g(\mathbf{s}, \boldsymbol{\theta})h(\mathcal{X})$ implies that $\mathbf{s}$ is sufficient for $\boldsymbol{\theta}$, we must show that such a factoring implies that the conditional probability $P(\mathcal{X} \mid \mathbf{s}, \boldsymbol{\theta})$ is independent of $\boldsymbol{\theta}$. Because $\mathbf{s} = \boldsymbol{\varphi}(\mathcal{X})$, specifying a value for $\mathbf{s}$ constrains the possible sets of samples to some set $\overline{\mathcal{X}}$. Formally, $\overline{\mathcal{X}} = \{\mathcal{X} \mid \boldsymbol{\varphi}(\mathcal{X}) = \mathbf{s}\}$. If $\overline{\mathcal{X}}$ is empty, no assignment of values to the samples can yield that value of $\mathbf{s}$, and $P(\mathbf{s} \mid \boldsymbol{\theta}) = 0$. Excluding

such cases, i.e., considering only values of s that can arise, we have

$$P(\mathcal{X} \mid \mathbf{s}, \boldsymbol{\theta}) = \frac{P(\mathcal{X}, \mathbf{s} \mid \boldsymbol{\theta})}{P(\mathbf{s} \mid \boldsymbol{\theta})}.$$

The denominator can be computed by summing the numerator over all values of $\mathcal{X}$. Since the numerator will be zero if $\mathcal{X} \notin \overline{\mathcal{X}}$, we can restrict the summation to $\mathcal{X} \in \overline{\mathcal{X}}$. That is,

$$P(\mathcal{X} \mid \mathbf{s}, \boldsymbol{\theta}) = \frac{P(\mathcal{X}, \mathbf{s} \mid \boldsymbol{\theta})}{\sum_{\mathcal{X} \in \overline{\mathcal{X}}} P(\mathcal{X}, \mathbf{s} \mid \boldsymbol{\theta})}.$$

But by the same argument used before, since $\mathbf{s} = \varphi(\mathcal{X})$, $P(\mathcal{X}, \mathbf{s} \mid \boldsymbol{\theta}) = P(\mathcal{X} \mid \boldsymbol{\theta})$. Furthermore, by hypothesis $P(\mathcal{X} \mid \boldsymbol{\theta}) = g(\mathbf{s}, \boldsymbol{\theta})h(\mathcal{X})$. Thus,

$$P(\mathcal{X} \mid \mathbf{s}, \boldsymbol{\theta}) = \frac{g(\mathbf{s}, \boldsymbol{\theta})h(\mathcal{X})}{\sum_{\mathcal{X} \in \overline{\mathcal{X}}} g(\mathbf{s}, \boldsymbol{\theta})h(\mathcal{X})} = \frac{h(\mathcal{X})}{\sum_{\mathcal{X} \in \overline{\mathcal{X}}} h(\mathcal{X})},$$

which is independent of $\boldsymbol{\theta}$. Thus, by definition, s is sufficient for $\boldsymbol{\theta}$. ∎

It should be pointed out that there are trivial ways of constructing sufficient statistics. For example, one can define s to be a vector whose components are the n samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$, so that $g(\mathbf{s}, \boldsymbol{\theta}) = p(\mathcal{X} \mid \boldsymbol{\theta})$ and $h(\mathcal{X}) = 1$. One can even produce a scalar sufficient statistic by the trick of interleaving the digits in the decimal expansions of the components of the n samples. Sufficient statistics such as these are of little interest, since they do not provide us with simpler results. The ability to factor $p(\mathcal{X} \mid \boldsymbol{\theta})$ into a product $g(\mathbf{s}, \boldsymbol{\theta})h(\mathcal{X})$ is interesting only when the function g and the sufficient statistic s are simple.*

It should also be mentioned that the factoring of $p(\mathcal{X} \mid \boldsymbol{\theta})$ into $g(\mathbf{s}, \boldsymbol{\theta})h(\mathcal{X})$ is obviously not unique. If $f(\mathbf{s})$ is any function of s, then $g'(\mathbf{s}, \boldsymbol{\theta}) = f(\mathbf{s})g(\mathbf{s}, \boldsymbol{\theta})$ and $h'(\mathcal{X}) = h(\mathcal{X})/f(\mathbf{s})$ are equivalent factors. This kind of ambiguity can be eliminated by defining the *kernel density*

$$\bar{g}(\mathbf{s}, \boldsymbol{\theta}) = \frac{g(\mathbf{s}, \boldsymbol{\theta})}{\int g(\mathbf{s}, \boldsymbol{\theta})\, d\boldsymbol{\theta}} \tag{38}$$

which is invariant to this kind of scaling.

What is the importance of sufficient statistics and kernel densities for parameter estimation? The general answer is that the only practical applications of classical parameter estimation to pattern classification involve density

* In statistics, the concept of a minimal sufficient statistic is related to what we want. However, even a minimal sufficient statistic is of little interest if it does not simplify the computational problem.

functions that possess simple sufficient statistics and simple kernel densities. In the case of maximum likelihood estimation, when searching for a value of $\boldsymbol{\theta}$ that maximizes $p(\mathcal{X} \mid \boldsymbol{\theta}) = g(\mathbf{s}, \boldsymbol{\theta})h(\mathcal{X})$, we can restrict our attention to $g(\mathbf{s}, \boldsymbol{\theta})$. In this case, the normalization provided by Eq. (38) is of no particular value unless $\bar{g}(\mathbf{s}, \boldsymbol{\theta})$ is simpler than $g(\mathbf{s}, \boldsymbol{\theta})$. The significance of the kernel density is revealed in the Bayesian case. If we substitute $p(\mathcal{X} \mid \boldsymbol{\theta}) = g(\mathbf{s}, \boldsymbol{\theta})h(\mathcal{X})$ in Eq. (34), we obtain

$$p(\boldsymbol{\theta} \mid \mathcal{X}) = \frac{g(\mathbf{s}, \boldsymbol{\theta})p(\boldsymbol{\theta})}{\int g(\mathbf{s}, \boldsymbol{\theta})p(\boldsymbol{\theta})\, d\boldsymbol{\theta}}. \tag{39}$$

If our a priori knowledge of $\boldsymbol{\theta}$ is very vague, $p(\boldsymbol{\theta})$ will tend to be uniform, changing very slowly with $\boldsymbol{\theta}$. If $p(\boldsymbol{\theta})$ is essentially uniform, $p(\boldsymbol{\theta} \mid \mathcal{X})$ is approximately the same as the kernel density. Roughly speaking, the kernel density is the a posteriori distribution of the parameter vector when the a priori distribution is uniform.* Even when the a priori distribution is far from uniform, the kernel density typically gives the asymptotic distribution of the parameter vector. In particular, when $p(\mathbf{x} \mid \boldsymbol{\theta})$ is indentifiable and when the number of samples is large, $g(\mathbf{s}, \boldsymbol{\theta})$ usually peaks sharply at some value $\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}$. If the a priori density $p(\boldsymbol{\theta})$ is continuous at $\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}$ and if $p(\hat{\boldsymbol{\theta}})$ is not zero, $p(\boldsymbol{\theta} \mid \mathcal{X})$ will approach the kernel density $\bar{g}(\mathbf{s}, \boldsymbol{\theta})$.

3.7 SUFFICIENT STATISTICS AND THE EXPONENTIAL FAMILY

To see how the Factorization Theorem can be used to obtain sufficient statistics, consider once again the familiar multivariate normal case with $p(\mathbf{x} \mid \boldsymbol{\theta}) \sim N(\boldsymbol{\theta}, \Sigma)$. Here

$$\begin{aligned} p(\mathcal{X} \mid \boldsymbol{\theta}) &= \prod_{k=1}^{n} \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp[-\tfrac{1}{2}(\mathbf{x}_k - \boldsymbol{\theta})^t\Sigma^{-1}(\mathbf{x}_k - \boldsymbol{\theta})] \\ &= \frac{1}{(2\pi)^{nd/2}|\Sigma|^{n/2}} \exp\left[-\tfrac{1}{2}\sum_{k=1}^{n}(\boldsymbol{\theta}^t\Sigma^{-1}\boldsymbol{\theta} - 2\boldsymbol{\theta}^t\Sigma^{-1}\mathbf{x}_k + \mathbf{x}_k^t\Sigma^{-1}\mathbf{x}_k)\right] \\ &= \exp\left[-\frac{n}{2}\boldsymbol{\theta}^t\Sigma^{-1}\boldsymbol{\theta} + \boldsymbol{\theta}^t\Sigma^{-1}\left(\sum_{k=1}^{n}\mathbf{x}_k\right)\right] \\ &\quad \times \frac{1}{(2\pi)^{nd/2}|\Sigma|^{n/2}} \exp\left[-\tfrac{1}{2}\sum_{k=1}^{n}\mathbf{x}_k^t\Sigma^{-1}\mathbf{x}_k\right]. \end{aligned}$$

* If the parameter space is finite, we can actually let $p(\boldsymbol{\theta})$ be a uniform distribution. While it is not possible to have a uniform distribution over a parameter space of infinite extent, this situation can often be approximated arbitrarily well.

This factoring isolates the $\boldsymbol{\theta}$ dependence of $p(\mathcal{X} \mid \boldsymbol{\theta})$ in the first factor, and from the factorization theorem we see that $\sum_{k=1}^{n} \mathbf{x}_k$ is sufficient for $\boldsymbol{\theta}$. Of course, any one-to-one function of this statistic is also sufficient for $\boldsymbol{\theta}$; in particular, the sample mean

$$\mathbf{m}_n = \frac{1}{n} \sum_{k=1}^{n} \mathbf{x}_k$$

is also sufficient for $\boldsymbol{\theta}$. Using this statistic, we can write

$$g(\mathbf{m}_n, \boldsymbol{\theta}) = \exp\left[-\frac{n}{2} (\boldsymbol{\theta}^t \Sigma^{-1} \boldsymbol{\theta} - 2\boldsymbol{\theta}^t \Sigma^{-1} \mathbf{m}_n) \right].$$

By using Eq. (38), or by completing the square, we obtain the kernel density

$$\bar{g}(\mathbf{m}_n, \boldsymbol{\theta}) = \frac{1}{(2\pi)^{d/2} \left| \frac{1}{n} \Sigma \right|^{1/2}} \exp\left[-\tfrac{1}{2} (\boldsymbol{\theta} - \mathbf{m}_n)^t \left(\frac{1}{n} \Sigma \right)^{-1} (\boldsymbol{\theta} - \mathbf{m}_n) \right].$$

From this it is immediately clear that $\mathbf{m}_n$ is the maximum likelihood estimate for $\boldsymbol{\theta}$. The Bayesian a posteriori density can be obtained from $\bar{g}(\mathbf{m}_n, \boldsymbol{\theta})$ by performing the integration indicated in Eq. (39). If the a priori density is essentially uniform, $p(\boldsymbol{\theta} \mid \mathcal{X}) = \bar{g}(\mathbf{m}_n, \boldsymbol{\theta})$.

This same general approach can be used to find sufficient statistics for other density functions. In particular, it applies to any member of the *exponential family*, a group of probability and probability density functions that possess simple sufficient statistics. Members of the exponential family include the normal, exponential, Rayleigh, Poisson, and many other familiar distributions. They can all be written in the form

$$p(\mathbf{x} \mid \boldsymbol{\theta}) = \alpha(\mathbf{x}) \exp[\mathbf{a}(\boldsymbol{\theta}) + \mathbf{b}(\boldsymbol{\theta})^t \mathbf{c}(\mathbf{x})]. \tag{40}$$

Thus,

$$p(\mathcal{X} \mid \boldsymbol{\theta}) = \exp\left[n\mathbf{a}(\boldsymbol{\theta}) + \mathbf{b}(\boldsymbol{\theta})^t \sum_{k=1}^{n} \mathbf{c}(\mathbf{x}_k) \right] \prod_{k=1}^{n} \alpha(\mathbf{x}_k) = g(\mathbf{s}, \boldsymbol{\theta}) h(\mathcal{X}), \tag{41}$$

where we can take

$$\mathbf{s} = \frac{1}{n} \sum_{k=1}^{n} \mathbf{c}(\mathbf{x}_k), \tag{42}$$

$$g(\mathbf{s}, \boldsymbol{\theta}) = \exp[n\{\mathbf{a}(\boldsymbol{\theta}) + \mathbf{b}(\boldsymbol{\theta})^t \mathbf{s}\}], \tag{43}$$

and

$$h(\mathcal{X}) = \prod_{k=1}^{n} \alpha(\mathbf{x}_k). \tag{44}$$

The distributions, sufficient statistics, and unnormalized kernels for a number of commonly encountered members of the exponential family are given in Table 3-1. It is a fairly routine matter to derive maximum likelihood

TABLE 3-1. Common Distributions from the Exponential Family

Name	Distribution	Domain	s	$[g(s, \theta)]^{1/n}$
Univariate Normal	$p(x \mid \boldsymbol{\theta}) = \sqrt{\frac{\theta_2}{2\pi}}\, e^{-(1/2)\theta_2(x-\theta_1)^2}$	$\theta_2 > 0$	$\begin{bmatrix} \frac{1}{n}\sum_{k=1}^{n} x_k \\ \frac{1}{n}\sum_{k=1}^{n} x_k^2 \end{bmatrix}$	$\theta_2^{1/2} e^{-(1/2)\theta_2(s_2 - 2\theta_1 s_1 + \theta_1^2)}$
Multivariate Normal	$p(\mathbf{x} \mid \boldsymbol{\theta}) = \frac{\lvert\Theta_2\rvert^{1/2}}{(2\pi)^{d/2}}\, e^{-(1/2)(\mathbf{x}-\boldsymbol{\theta}_1)^t \Theta_2 (\mathbf{x}-\boldsymbol{\theta}_1)}$	Θ_2 positive definite	$\begin{bmatrix} \frac{1}{n}\sum_{k=1}^{n} \mathbf{x}_k \\ \frac{1}{n}\sum_{k=1}^{n} \mathbf{x}_k \mathbf{x}_k^t \end{bmatrix}$	$\lvert\Theta_2\rvert^{1/2} e^{-(1/2)(\mathrm{tr}\,\Theta_2 S_2 - 2\boldsymbol{\theta}_1^t \Theta_2 \mathbf{s}_1 + \boldsymbol{\theta}_1^t \Theta_2 \boldsymbol{\theta}_1)}$
Exponential	$p(x \mid \theta) = \begin{cases} \theta e^{-\theta x} & x \geq 0 \\ 0 & \text{otherwise} \end{cases}$	$\theta > 0$	$\frac{1}{n}\sum_{k=1}^{n} x_k$	$\theta e^{-\theta s}$
Rayleigh	$p(x \mid \theta) = \begin{cases} 2\theta x e^{-\theta x^2} & x \geq 0 \\ 0 & \text{otherwise} \end{cases}$	$\theta > 0$	$\frac{1}{n}\sum_{k=1}^{n} x_k^2$	$\theta e^{-\theta s}$
Maxwell	$p(x \mid \theta) = \begin{cases} \frac{4}{\sqrt{\pi}}\, \theta^{3/2} x^2 e^{-\theta x^2}, & x \geq 0 \\ 0 & \text{otherwise} \end{cases}$	$\theta > 0$	$\frac{1}{n}\sum_{k=1}^{n} x_k^2$	$\theta^{3/2} e^{-\theta s}$

Gamma	$p(x \mid \theta) = \begin{cases} \dfrac{\theta_2^{\theta_1+1}}{\Gamma(\theta_1+1)} x^{\theta_1} e^{-\theta_2 x}, & x \geq 0 \\ 0 & \text{otherwise} \end{cases}$		$\theta_1 > -1$ $\theta_2 > 0$	$\begin{bmatrix} \left(\prod_{k=1}^{n} x_k\right)^{1/n} \\ \frac{1}{n}\sum_{k=1}^{n} x_k \end{bmatrix}$	$\dfrac{\theta_2^{\theta_1+1}}{\Gamma(\theta_1+1)} s_1^{\theta_1} e^{-\theta_2 s_2}$
Beta	$p(x \mid \theta) = \begin{cases} \dfrac{\Gamma(\theta_1+\theta_2+2)}{\Gamma(\theta_1+1)\Gamma(\theta_2+1)} x^{\theta_1}(1-x)^{\theta_2}, & 0 \leq x \leq 1 \\ 0 & \text{otherwise} \end{cases}$		$\theta_1 > -1$ $\theta_2 > -1$	$\begin{bmatrix} \left(\prod_{k=1}^{n} x_k\right)^{1/n} \\ \left(\prod_{k=1}^{n} (1-x_k)\right)^{1/n} \end{bmatrix}$	$\dfrac{\Gamma(\theta_1+\theta_2+2)}{\Gamma(\theta_1+1)\Gamma(\theta_2+1)} s_1^{\theta_1} s_2^{\theta_2}$
Poisson	$P(x \mid \theta) = \dfrac{\theta^x}{x!} e^{-\theta},$	$x = 0, 1, 2, \ldots$	$\theta > 0$	$\frac{1}{n}\sum_{k=1}^{n} x_k$	$\theta^s e^{-\theta}$
Bernoulli	$P(x \mid \theta) = \theta^x (1-\theta)^{1-x},$	$x = 0, 1$	$0 < \theta < 1$	$\frac{1}{n}\sum_{k=1}^{n} x_k$	$\theta^s (1-\theta)^{1-s}$
Binomial	$P(x \mid \theta) = \dfrac{m!}{x!(m-x)!} \theta^x (1-\theta)^{m-x},$	$x = 0, 1, \ldots, m$	$0 < \theta < 1$	$\frac{1}{n}\sum_{k=1}^{n} x_k$	$\theta^s (1-\theta)^{m-s}$
Multinomial	$P(\mathbf{x} \mid \theta) = \dfrac{m!}{\prod_{i=1}^{d} x_i!} \prod_{i=1}^{d} \theta_i^{x_i},$	$x_i = 0, 1, \ldots, m$ $\sum_{i=1}^{d} x_i = m$	$0 < \theta_i < 1$ $\sum_{i=1}^{d} \theta_i = 1$	$\frac{1}{n}\sum_{k=1}^{n} \mathbf{x}_k$	$\prod_{i=1}^{d} \theta_i^{s_i}$

estimates and Bayesian a posteriori distributions from these solutions. With two exceptions, the solutions given are for univariate cases, though they can be used in multivariate situations if statistical independence can be assumed.*

It would be pleasant to conclude that this collection of results solves most problems in pattern classification. Unfortunately this is not the case. In many applications, these members of the exponential family with their smooth variations and unimodal shapes do not give good approximations to the densities actually encountered. The simplifying assumption of statistical independence, though frequently made, is rarely valid. Even when a member of the exponential family gives a good approximation to the unknown density, there are usually many unknown parameters to estimate but only a limited number of available samples. As we shall see, this can cause optimal estimates to give less than satisfactory results, and can even lead to situations where "optimal" systems do not perform as well as "suboptimal" ones.

3.8 PROBLEMS OF DIMENSIONALITY

3.8.1 An Unexpected Problem

In practical multicategory applications, it is not at all unusual to encounter problems involving fifty or a hundred features, particularly if the features are binary valued. The designer usually believes that each feature is useful for at least some of the discriminations. While he may doubt that each feature provides independent information, he has not intentionally included superfluous features.

If the features are statistically independent, there are some theoretical results that suggest the possibility of excellent performance. For example, consider the two-class multivariate normal case where $p(\mathbf{x} \mid \omega_j) \sim N(\boldsymbol{\mu}_j, \Sigma)$, $j = 1, 2$. If the a priori probabilities are equal, then it is not hard to show that the Bayes error rate is given by

$$P(e) = \frac{1}{\sqrt{2\pi}} \int_{r/2}^{\infty} \exp[-\tfrac{1}{2}u^2]\, du, \tag{45}$$

where r^2 is the squared Mahalanobis distance

$$r^2 = (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^t \Sigma^{-1} (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2). \tag{46}$$

* To be more precise, the necessary assumption is that $p(\mathbf{x} \mid \omega_j, \boldsymbol{\theta}_j) = \prod_{i=1}^{d} p(x_i \mid \omega_j, \theta_{ij})$ In the literature, when one encounters the statement that "the features are assumed to be statistically independent," what is almost always meant is that they are assumed class-conditionally independent.

Thus, the probability of error decreases as r increases, approaching zero as r approaches infinity. In the independent case, $\Sigma = \text{diag}(\sigma_1^2, \ldots, \sigma_d^2)$, and

$$r^2 = \sum_{i=1}^{d} \left(\frac{\mu_{i1} - \mu_{i2}}{\sigma_i} \right)^2. \tag{47}$$

This shows how each feature contributes to reducing the probability of error. The most useful features are the ones for which the difference between the means is large relative to the standard deviations. However, no feature is useless if its means for the two classes differ. An obvious way to reduce the error rate further is to introduce new, independent features. Each new feature need not add much, but if r can be increased without limit, the probability of error can be made arbitrarily small.

In general, if the performance obtained with a given set of features is inadequate, it is natural to consider adding new features, particularly ones that will help separate the class pairs most frequently confused. Although increasing the number of features increases the cost and complexity of both the feature extractor and the classifier, it is reasonable to believe that the performance will improve. After all, if the probabilistic structure of the problem were completely known, the Bayes risk could not possibly be increased by adding new features; at worst, the Bayes classifier would ignore the new features, and if the new features provide any additional information, the performance must improve.

Unfortunately, it has frequently been observed in practice that, beyond a certain point, the inclusion of additional features leads to worse rather than better performance. This apparent paradox presents a genuine and serious problem for classifier design. The basic source of the problem can always be traced to the fact that the number of design samples is finite. However, analysis of the problem is both difficult and subtle. Simple cases do not exhibit the experimentally observed phenomena, and more realistic cases are difficult to analyze. In an attempt to provide some insight, we shall discuss several topics related to problems of dimensionality and sample size. While most of the analytical results will be presented without proof, the interested reader will find pertinent references in the Bibliographical and Historical Remarks.

3.8.2 Estimating a Covariance Matrix

We begin by considering the problem of estimating a covariance matrix. This requires the estimation of $d(d + 1)/2$ parameters, the d diagonal elements and $d(d - 1)/2$ independent off-diagonal elements. We observe first that the

appealing maximum likelihood estimate

$$\hat{\Sigma} = \frac{1}{n}\sum_{k=1}^{n}(\mathbf{x}_k - \mathbf{m}_n)(\mathbf{x}_k - \mathbf{m}_n)^t$$

is the sum of $n - 1$ independent d-by-d matrices of rank one, and thus is guaranteed to be singular if $n \leq d$. Since we must invert $\hat{\Sigma}$ to obtain the discriminant functions, we have an algebraic requirement for at least $d + 1$ samples. To smooth out statistical fluctuations and obtain a really good estimate, it would not be surprising if several times that number of samples were needed.

It frequently happens that the number of available samples is inadequate, and the question of how to proceed arises. One possibility is to reduce the dimensionality, either by redesigning the feature extractor, by selecting an appropriate subset of the existing features, or by combining the existing features in some way.* Another possibility is to assume that all c classes share the same covariance matrix, and to pool the available data. Yet another alternative is to look for a better estimate for Σ. If any reasonable a priori estimate Σ_0 is available, a Bayesian or pseudo-Bayesian estimate of the form $\lambda\Sigma_0 + (1 - \lambda)\hat{\Sigma}$ might be employed. If Σ_0 is diagonal, this diminishes the troublesome effects of "accidental" correlations. Alternatively, one can remove chance correlations heuristically by thresholding the sample covariance matrix. For example, one might assume that all covariances for which the magnitude of the correlation coefficient is not near unity are actually zero. An extreme of this approach is to assume statistical independence, thereby making all the off-diagonal elements be zero, regardless of empirical evidence to the contrary. Even though such assumptions are almost surely incorrect, the resulting heuristic estimates often provide better performance than the maximum likelihood estimate.

Here we have another apparent paradox. The classifier that results from assuming independence is almost certainly suboptimal. It is understandable that it will perform better if it happens that the features actually are independent, but how can it provide better performance when this assumption is untrue?

The answer again involves the problem of insufficient data, and some insight into its nature can be gained from considering an analogous problem in curve fitting. Figure 3.3 shows a set of five data points and several candidate curves for fitting them. The data points were obtained by adding zero-mean, independent noise to a parabola. Thus, of all the possible polynomials, a parabola should give the best fit, assuming that we are interested

* We shall have more to say about dimensionality reduction in Chapters 4 and 6.

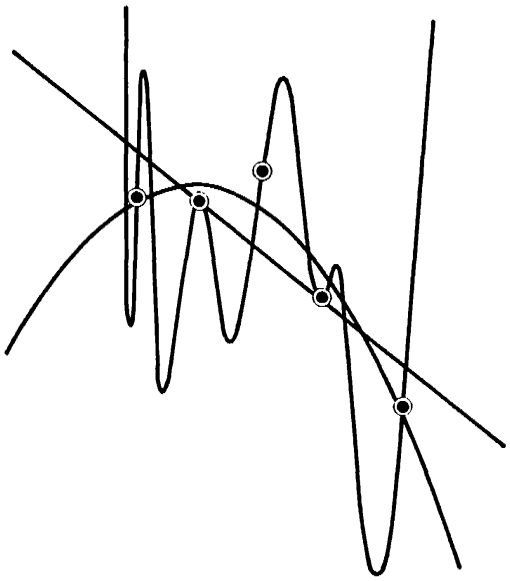

FIGURE 3.3. Fitting curves to a set of data points.

in fitting data obtained in the future as well as the points at hand. The straight line shown fits the given data fairly well. The parabola provides a better fit, but one might wonder whether the data are adequate to fix the curve. The best parabola for a larger data set might be quite different, and over the interval shown the straight line could easily be superior. The tenth-degree polynomial fits the given data perfectly. However, no one would expect such an under-determined solution to fit new data well. Indeed, many more samples would be needed to get a good fit with a tenth-degree polynomial than with a second-degree polynomial, despite the fact that the latter is a special case of the former. In general, reliable interpolation or extrapolation can not be obtained unless the solution is overdetermined.

3.8.3 The Capacity of a Separating Plane

The importance of having an overdetermined solution is as significant for classification as it is for estimation. For a relatively simple example, consider the partitioning of a d-dimensional feature space by a hyperplane $\mathbf{w}^t\mathbf{x} + w_0 = 0$. Suppose that we are given n sample points in general position,* each point being labelled either ω_1 or ω_2. Of the 2^n possible dichotomies of n points in d dimensions, a certain fraction $f(n, d)$ are said to be linear dichotomies. These are the labellings for which there exists a hyperplane

* Points in d-space are in general position if no subset of $d + 1$ points falls in a $(d - 1)$-dimensional subspace.

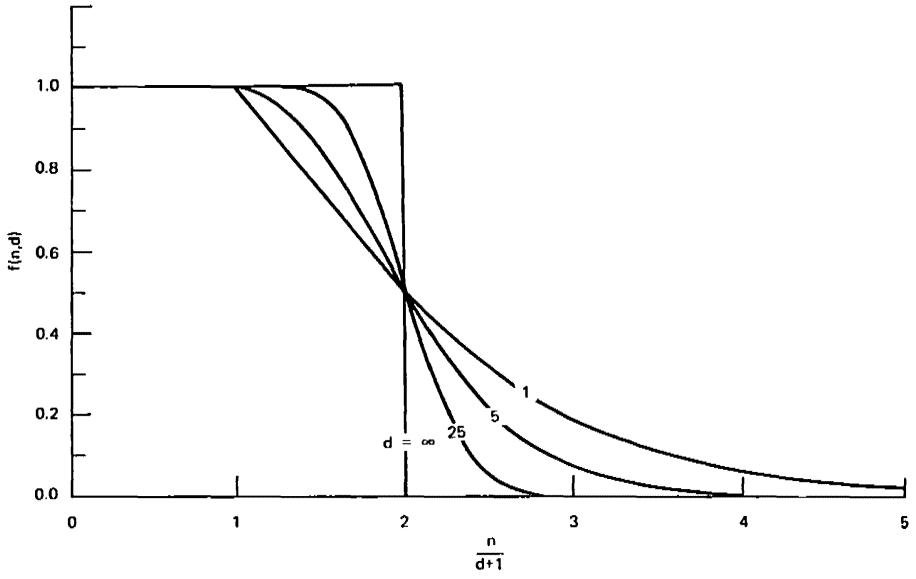

FIGURE 3.4. The fraction of dichotomies of n points in d dimensions that are linear.

separating the points labelled ω_1 from the points labelled ω_2. It can be shown that this fraction is given by

$$f(n, d) = \begin{cases} 1 & n \leq d + 1 \\ \dfrac{2}{2^n} \displaystyle\sum_{i=0}^{d} \binom{n-1}{i} & n > d + 1. \end{cases} \tag{48}$$

This function is plotted in Figure 3.4 for several values of d. Note that all dichotomies of $d + 1$ or fewer points are linear. That means that a hyperplane is not overconstrained by the requirement of correctly classifying $d + 1$ or fewer points. In fact, if d is large it is not until n is a sizeable fraction of $2(d + 1)$ that the problem begins to become difficult. At $n = 2(d + 1)$, which is sometimes called the *capacity* of a hyperplane, half of the possible dichotomies are still linear. Thus, a linear discriminant is not effectively overdetermined until the number of samples is several times as large as the dimensionality.

3.8.4 The Problem-Average Error Rate

The examples we have given thus far suggest that the problem with having only a small number of samples is that the resulting classifier will not perform well on new data. Thus, we expect the error rate to be a function of the number

n of samples, typically decreasing to some minimum value as n approaches infinity. To investigate this analytically, we must carry out the following steps:

(1) Estimate the unknown parameters from samples.
(2) Use these estimates to determine the classifier.
(3) Calculate the error rate for the resulting classifier.

In general, this analysis is very complicated. The answer depends on everything—on the particular samples obtained, on the way they are used to determine the classifier, and on the unknown, underlying probability structure. However, by using histogram approximations to the unknown probability densities and averaging appropriately, it is possible to draw some interesting conclusions.

Consider the two-class case in which the two classes are equally likely a priori. Suppose that we partition the feature space into some number m of disjoint cells $\mathscr{C}_1, \ldots, \mathscr{C}_m$. If the conditional densities $p(\mathbf{x} \mid \omega_1)$ and $p(\mathbf{x} \mid \omega_2)$ do not vary appreciably within any cell, then instead of needing to know the exact value of $\mathbf{x}$, we need only know into which cell $\mathbf{x}$ falls. This reduces the problem to the discrete case. Let $p_i = P(\mathbf{x} \in \mathscr{C}_i \mid \omega_1)$ and $q_i = P(\mathbf{x} \in \mathscr{C}_i \mid \omega_2)$. Then, since we have assumed that $P(\omega_1) = P(\omega_2) = 1/2$, the vectors $\mathbf{p} = (p_1, \ldots, p_m)^t$ and $\mathbf{q} = (q_1, \ldots, q_m)^t$ determine the probability structure of the problem. If $\mathbf{x}$ falls in $\mathscr{C}_i$, the Bayes decision rule is to decide ω_i if $p_i > q_i$. The resulting Bayes error rate is given by

$$P(e \mid \mathbf{p}, \mathbf{q}) = \frac{1}{2} \sum_{i=1}^{m} \min[p_i, q_i].$$

When the parameters $\mathbf{p}$ and $\mathbf{q}$ are unknown and must be estimated from a set of samples, the resulting error rate will be larger than the Bayes rate. The exact answer will depend on the set of samples and the way in which they are used to obtain the classifier. Suppose that half of the samples are labelled ω_1 and half are labelled ω_2, with n_{ij} being the number that fall in $\mathscr{C}_i$ and are labelled ω_j. Suppose further that we design the classifier by using the maximum likelihood estimates $\hat{p}_i = 2n_{i1}/n$ and $\hat{q}_i = 2n_{i2}/n$ as if they were the true values. Then a new feature vector falling in $\mathscr{C}_i$ will be assigned to ω_1 if $n_{i1} > n_{i2}$. With all of these assumptions, it follows that the probability of error for the resulting classifier is given by

$$P(e \mid \mathbf{p}, \mathbf{q}, \mathscr{X}) = \frac{1}{2} \sum_{n_{i1} > n_{i2}} q_i + \frac{1}{2} \sum_{n_{i1} \leq n_{i2}} p_i.$$

To evaluate this probability of error, we need to know the true conditional probabilities $\mathbf{p}$ and $\mathbf{q}$, and the set of samples, or at least the numbers n_{ij}. Different sets of n random samples will yield different values for $P(e \mid \mathbf{p}, \mathbf{q}, \mathscr{X})$. We can use the fact that the numbers n_{ij} have a multinomial distribution to

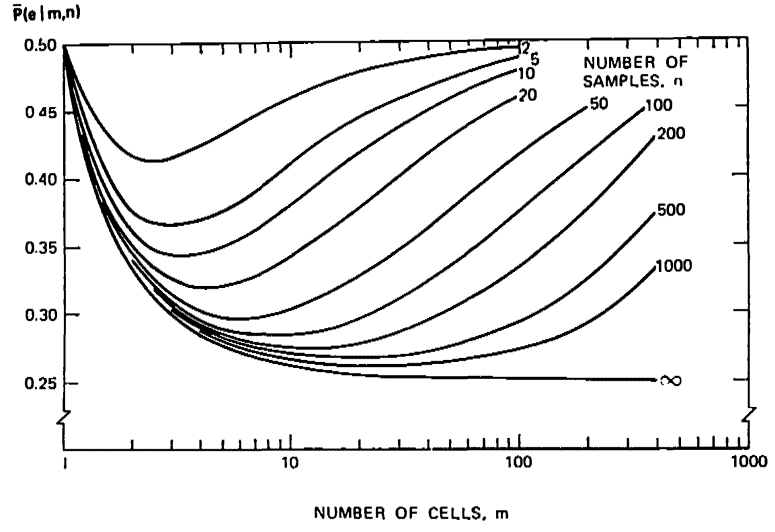

FIGURE 3.5. The problem-average error rate (Adapted from G. F. Hughes, 1968).

average over all of the possible sets of n random samples and obtain an average probability of error $P(e \mid \mathbf{p}, \mathbf{q}, n)$. Roughly speaking, this is the typical error rate one should expect for n samples. However, evaluation of this average error rate still requires knowing the underlying problem, i.e., the values for $\mathbf{p}$ and $\mathbf{q}$. If $\mathbf{p}$ and $\mathbf{q}$ are quite different, the average error rate will be near zero, while if $\mathbf{p}$ and $\mathbf{q}$ are quite similar it will be near one-half.

A sweeping way to eliminate this dependence of the answer on the problem is to average the answer over all possible problems! That is, we assume some a priori distribution for the unknown parameters $\mathbf{p}$ and $\mathbf{q}$, and average $P(e \mid \mathbf{p}, \mathbf{q}, n)$ with respect to $\mathbf{p}$ and $\mathbf{q}$. The resulting *problem-average probability of error* $\bar{P}(e \mid m, n)$ will depend only on the number m of cells, the number n of samples, and the a priori distribution.

Of course, choosing the a priori distribution is a delicate matter. By favoring easy problems, we can make $\bar{P}$ approach zero, and by favoring hard problems we can make $\bar{P}$ approach one-half. We would like to choose an a priori distribution corresponding to the class of problems we typically encounter, but there is no obvious way to do that. A bold approach is merely to assume that problems are "uniformly distributed," i.e., that the vectors $\mathbf{p}$ and $\mathbf{q}$ are distributed uniformly over the simplexes $p_i \geq 0$, $\sum_{i=1}^{m} p_i = 1$, $q_i \geq 0$, $\sum_{i=1}^{m} q_i = 1$. G. F. Hughes, who suggested this approach, actually carried out the required computations and obtained the results shown graphically in Figure 3.5. Let us consider some of the implications of these results.

Note first that the curves show $\bar{P}$ as a function of the number of cells for a

fixed number of samples. With an infinite number of samples, the maximum likelihood estimates are perfect, and $\bar{P}$ is the average of the Bayes error rate over all problems. The corresponding curve for $\bar{P}(e \mid m, \infty)$ decreases rapidly from 0.5 at $m = 1$ to the asymptotic value of 0.25 as m approaches infinity. The fact that $\bar{P} = 0.5$ if $m = 1$ is not surprising, since if there is only one cell the decision must be based solely on the a priori probabilities. The fact that $\bar{P}$ approaches 0.25 as m approaches infinity is aesthetically pleasing, since it it halfway between the extremes of 0.0 and 0.5. The fact that the problem-average error rate is so high merely shows that many hopelessly difficult classification problems are included in this average. Clearly, it would be rash indeed to conclude that the "average" pattern recognition problem will have this error rate.

However, the most interesting feature of these curves is that for every curve involving a finite number of samples there is an optimum number of cells. This is directly related to the fact that with a finite number of samples the performance will worsen if too many features are used. In this case it is clear why this occurs. At first, increasing the number of cells makes it easier to distinguish between $p(\mathbf{x} \mid \omega_1)$ and $p(\mathbf{x} \mid \omega_2)$ (as represented by the vectors $\mathbf{p}$ and $\mathbf{q}$), thereby allowing improved performance. However, if the number of cells becomes too large, there will not be enough samples to fill them. Eventually, the number of samples in most cells will be zero, and we must return to using just the ineffective a priori probabilities for classification. Thus, for any finite n, $\bar{P}(e \mid m, n)$ must approach 0.5 as m approaches infinity.

The value of m for which $\bar{P}(e \mid m, n)$ is minimum is remarkably small. For $n = 500$ samples, it is somewhere around $m = 20$ cells. Suppose that we were to form the cells by dividing each feature axis into l intervals. Then with d features we would have $m = l^d$ cells. If $l = 2$, which is extremely crude quantization, this implies that using more than four or five binary features will lead to worse rather than better performance. This is a very pessimistic result, but then so is the statement that the average error rate is 0.25. These numerical values are a consequence of the a priori distribution chosen for the problems, and are of no significance when one is facing a particular problem. The main thing to be learned from this analysis is that the performance of a classifier certainly does depend on the number of design samples, and that if this number is fixed, increasing the number of features beyond a certain point is likely to be counterproductive.

3.9 ESTIMATING THE ERROR RATE

There are at least two reasons for wanting to know the error rate of a classifier. One is to see if the classifier performs well enough to be useful. Another is to compare its performance with a competing design.

One approach to estimating the error rate is to compute it from the assumed parametric model. For example, in the two-class multivariate normal case, one might compute $P(e)$ from Eqs. (45) and (46), substituting estimates of the means and the covariance matrix for the unknown parameters. However, there are three problems with this approach. First, such an estimate for $P(e)$ is almost always overoptimistic; characteristics that make the design samples peculiar or unrepresentative will not be revealed. Second, one should always suspect the validity of an assumed parametric model; a performance evaluation based on the same model can not be believed unless the evaluation is unfavorable. Finally, in more general situations it is very difficult to compute the error rate exactly, even if the probabilistic structure is completely known.

An empirical approach that avoids these problems is to test the classifier experimentally. In practice, this is frequently done by running the classifier on a set of *test samples*, using the fraction of the samples that are misclassified as an estimate of the error rate. Needless to say, the test samples should be different from the design samples or the estimated error rate will definitely be optimistic.* If the true but unknown error rate of the classifier is p, and if k of the n independent, randomly drawn test samples are misclassified, then k has the binomial distribution†

$$P(k) = \binom{n}{k} p^k (1 - p)^{n-k}. \tag{49}$$

Thus, the fraction of test samples misclassified is exactly the maximum likelihood estimate for p:

$$\hat{p} = \frac{k}{n}. \tag{50}$$

The properties of this estimate for the parameter p of a binomial distribution are well known. In particular, Figure 3.6 shows 95 percent confidence intervals as a function of $\hat{p}$ and n. For a given value of $\hat{p}$, the probability is 0·95 that the true value of p lies in the interval between the lower and upper

* In the early work on pattern recognition, when experiments were often done with very small numbers of samples, the same data were often used for designing and testing the classifier. This mistake is frequently referred to as "testing on the training data." A related but less obvious problem arises when a classifier undergoes a long series of refinements guided by the results of repeated testing on the same test data. This form of "training on the testing data" often escapes attention until new test samples are obtained.

† For this assumption to be satisfied, the selection of the states of nature must be done randomly. In multiclass problems, this can result in some classes not being represented at all. To circumvent this obvious small-sample defect, it is common practice to make the number of test samples in each class correspond, at least roughly, to the a priori probabilities. This improves the estimate of the error rate, but complicates an exact analysis.

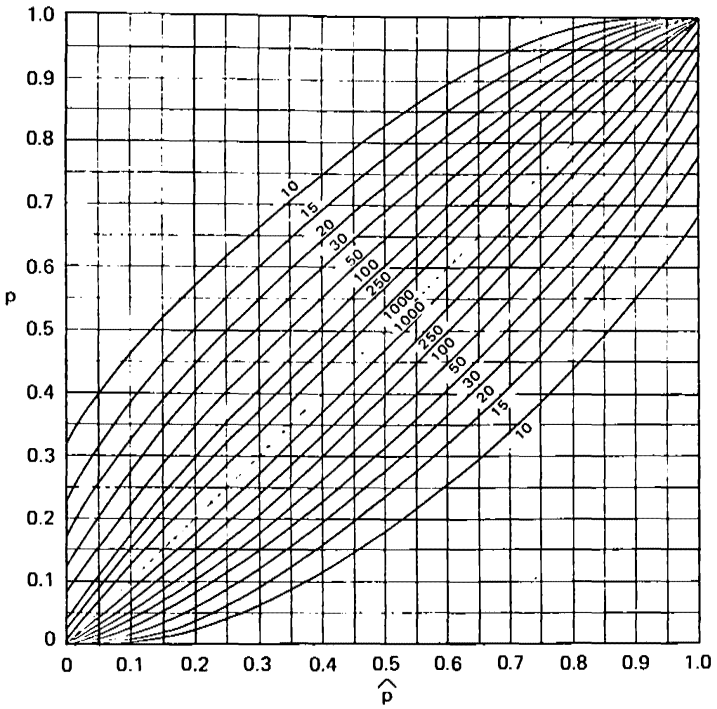

FIGURE 3.6. Confidence intervals for error-rate estimates (From Highleyman, 1962. Copyright 1962, American Telephone and Telegraph Company (reprinted by permission.).)

curves for the number n of test samples. These curves show that unless n is fairly large the maximum likelihood estimate must be interpreted with caution. For example, if no errors are made on 50 test samples, with probability 0.95 the true error rate is between zero and eight percent. The classifier would have to make no errors on more than 250 test samples to be reasonably sure that the true error rate is below two percent.

The need for data to design the classifier and additional data to evaluate it presents the designer with a dilemma. If he reserves most of his data for the design, he can not have confidence in the test. If he reserves most of his data for the test, he will not obtain a good design. The question of how best to partition a set of samples into a design set and a test set has received some analysis, and considerable discussion, but no definitive answer.

In fact, there are more options available than just partitioning the data, designing the classifier once, and testing it. For example, one might repeat this process several times, using a different partition each time, and average the resulting error-rate estimates. If computation costs are of no concern, there are strong arguments in favor of doing this n times, each time using

$n - 1$ samples for design and only one sample for test. The basic advantage of this approach is that virtually all of the samples are used in each design, which should lead to a good design, and all of the samples are ultimately used in the tests. This procedure, which is often referred to as "leaving-one-out," is particularly attractive when the number of available samples is quite small. When the number of samples is very large it is probably sufficient to partition the data into a single design set and a single test set. Although there is no theory to guide the designer in intermediate situations, it is at least pleasant to have a large number of reasonable options.

3.10 BIBLIOGRAPHICAL AND HISTORICAL REMARKS

The subject of parameter estimation is a basic topic in statistics, and is well treated in any of the standard texts, such as Hoel (1971) or Wilks (1962). Both maximum likelihood and Bayesian estimates are frequently used, the latter often being taken to be the mean of the a posteriori distribution $p(\boldsymbol{\theta} \mid \mathscr{X})$. Maximum likelihood estimation was introduced by R. A. Fisher, who pointed out many of its desirable properties. In particular, it avoids the thorny matter of choosing an appropriate a priori density $p(\boldsymbol{\theta})$.

The thoughtless use of Laplace's principle of insufficient reason to justify assuming uniform prior distributions, and the practice of assuming that a parameter is random when it is merely unknown were criticized so severely by Fisher and Neyman that Bayesian estimation fell into a period of philosophical disrepute. In recent years, Bayesian methods have regained some of their lost respectability, due in part to the ease with which they can incorporate known constraints on the unknown parameters. With the introduction of new principles, such as the principle of maximum entropy, some of the old paradoxes have been resolved (Jaynes 1968). More controversial, but nevertheless revitalizing support has come from the "subjectivist" or "personalist" school of statisticians, who view the a priori distributions as a statement of belief about the possible values of the unknown parameters (Savage 1962). Since under ordinary circumstances Bayesian and maximum likelihood estimates yield nearly identical results when the sample size is large enough to be useful, these philosophical differences rarely have serious practical consequences.

The Bayesian approach to learning in pattern recognition was initiated by the suggestion that the proper way to use samples when the conditional densities are unknown is in the calculation of $P(\omega_i \mid \mathbf{x}, \mathscr{X})$ (Braverman 1962). Abramson and Braverman (1962) obtained the recursive Bayes solution for learning the mean of a normal density, and Keehn (1965) extended this to the

case where both the mean vector and the covariance matrix are unknown. Bayesian learning in some nonnormal and nonstationary cases has been investigated by Beisner (1968) and Chen (1969). As part of a very general treatment of Bayesian learning, Lainiotis (1970) related the multivariate normal solution to results well known in two other fields, viz., to Kalman filtering in control theory and to correlator-estimator detection in communications theory. Chien and Fu (1967) investigated convergence of the estimates by relating Bayesian learning to stochastic approximation. A good, brief treatment of convergence questions is given by Aoki (1965).

The derivation of a simple expression for the a posteriori density $p(\boldsymbol{\theta} \mid \mathscr{X})$ usually requires a careful choice for the a priori density $p(\boldsymbol{\theta})$, the so-called "natural conjugate" density. Spragins (1965) pointed out that the essential simplification provided by reproducing densities was due not to any special property of the a priori density, but to the existence of a simple sufficient statistic for $p(\mathbf{x} \mid \boldsymbol{\theta})$. The introduction of sufficient statistics is another of the contributions of R. A. Fisher. A rigorous treatment of the factorization theorem is given by Lehmann (1959), and an analysis of forms of densities admitting simple sufficient statistics is given by Dynkin (1961).

The problems raised by high dimensionality are lucidly treated in an article by Kanal and Chandrasekaran (1968), which influenced our treatment of the topic. These problems are not restricted to parametric methods; if anything, they are more severe for the nonparametric methods we shall present in Chapters 4 and 5. Although these problems plagued many experimental projects, they received little attention in the early published literature, probably because they were so difficult to analyze. However, symptoms of the problems can be discerned in frequent remarks about the possible inadequacy or nonrepresentative character of the available data. Kanal and Randall (1964) described the problem of estimating covariance matrices, and gave an ad hoc estimate suggested by T. J. Harley that they found useful. The capacity results for linear separation and their extention to other separating surfaces were given by Cover (1965), who pointed out their implications for generalizing from design samples. Allais (1966) analyzed an estimation problem in which the variables were normally distributed and maximum likelihood estimates of the unknown parameters were used. His analysis disclosed conditions under which increasing the number of variables would increase the expected squared error, and he suggested that similar mechanisms might be at work in classification problems. Unfortunately, this phenomenon does not arise in simple cases. The results of Chandrasekaran (1971) suggest that if the features are statistically independent this effect will never appear. This relegates the phenomenon to dependent cases that are hard to analyze.

The problem-average results of Hughes (1968) cut this Gordian knot by

mixing together all kinds of classification problems—problems with complete dependence, complete independence, and every intermediate degree of dependence. Since the problem-average error rate decreases to some minimum and then increases as the number of features increases, one can conclude that this is rather typical behavior when the number of samples is limited. We gave results for the case where the two classes are equally likely a priori. Hughes also gave the error rates for arbitrary a priori probabilities, but these results were rather hard to understand, the performance sometimes being worse than that obtained on the basis of the a priori probabilities alone. Abend and Harley (1969) traced this behavior to the fact that maximum likelihood rather than Bayesian estimates were used, and Chandrasekaran and Harley (1969) derived and investigated the problem-average error rate for the Bayesian case. In the case of equal a priori probabilities and equal numbers of samples in each class, the maximum likelihood and Bayesian answers turn out to be the same.

The matter of estimating performance and comparing different classifiers was another source of controversy in the early pattern recognition literature. Some of this can be appreciated from the exchange of letters on hand-printed character recognition that appeared in the June 1960 and March 1961 *IRE Transactions on Electronic Computers*. The common procedure of using some of the samples for design and reserving the rest for test is frequently called the *holdout* or *H* method. An analysis by Highleyman (1962) indicated the need for a surprisingly large number of test samples, but Kanal and Chandrasekaran (1968) pointed out that this analysis was essentially for the large-sample case. A Monte Carlo study by Lachenbruch and Mickey (1968) gave evidence for the superiority of the method of leaving one out, which they called the *U* method. Although this method requires the classifier to be designed n times, they point out that in the normal case, at least, the labor of repeatedly inverting covariance matrices can be greatly reduced through the use of Bartlett's identity (see Problem 10). Simple, explicit formulas derived by Fukunaga and Kessell (1971) show that very little extra computation is needed in this case.

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PROBLEMS

1. Let x have an exponential distribution

$$p(x \mid \theta) = \begin{cases} \theta e^{-\theta x} & x \geq 0 \\ 0 & \text{otherwise.} \end{cases}$$

(a) Sketch $p(x \mid \theta)$ versus x for a fixed value of the parameter θ.
(b) Sketch $p(x \mid \theta)$ versus θ, $\theta > 0$, for a fixed value of x.
(c) Suppose that n samples $x_1, \ldots, x_n$ are drawn independently according to $p(x \mid \theta)$. Show that the maximum likelihood estimate for θ is given by

$$\hat{\theta} = \frac{1}{\frac{1}{n}\sum_{k=1}^{n} x_k}.$$

2. Let x have a uniform distribution

$$p(x \mid \theta) = \begin{cases} \frac{1}{\theta} & 0 \leq x \leq \theta \\ 0 & \text{otherwise.} \end{cases}$$

(a) Sketch $p(x_1 \mid \theta)$ versus θ for some arbitrary value of x_1.
(b) Suppose that n samples $x_1, \ldots, x_n$ are drawn independently according to $p(x \mid \theta)$. Show that the maximum likelihood estimate for θ is $\max_k x_k$.

3. Let samples be drawn by successive, independent selections of a state of nature ω_i with unknown probability $P(\omega_i)$. Let $z_{ik} = 1$ if the state of nature for the kth sample is ω_i and $z_{ik} = 0$ otherwise. Show that

$$P(z_{i1}, \ldots, z_{in} \mid P(\omega_i)) = \prod_{k=1}^{n} P(\omega_i)^{z_{ik}}(1 - P(\omega_i))^{1-z_{ik}}$$

and that the maximum likelihood estimate for $P(\omega_i)$ is

$$\hat{P}(\omega_i) = \frac{1}{n}\sum_{k=1}^{n} z_{ik}.$$

4. Let $\mathbf{x}$ be a binary (0, 1) vector with a multivariate Bernoulli distribution

$$P(\mathbf{x} \mid \boldsymbol{\theta}) = \prod_{i=1}^{d} \theta_i^{x_i}(1 - \theta_i)^{1-x_i},$$

where $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_d)^t$ is an unknown parameter vector, θ_i being the probability that $x_i = 1$. Show that the maximum likelihood estimate for $\boldsymbol{\theta}$ is

$$\hat{\boldsymbol{\theta}} = \frac{1}{n} \sum_{k=1}^{n} \mathbf{x}_k.$$

5. Let $p(\mathbf{x} \mid \Sigma) \sim N(\boldsymbol{\mu}, \Sigma)$ where $\boldsymbol{\mu}$ is known and Σ is unknown. Show that the maximum likelihood estimate for Σ is given by

$$\hat{\Sigma} = \frac{1}{n} \sum_{k=1}^{n} (\mathbf{x}_k - \boldsymbol{\mu})(\mathbf{x}_k - \boldsymbol{\mu})^t$$

by carrying out the steps in the following argument:

(a) Prove the matrix identity $\mathbf{a}^t A \mathbf{a} = \text{tr}\{A\mathbf{a}\mathbf{a}^t\}$, where the trace, tr A, is the sum of the diagonal elements of A.

(b) Show that the likelihood function can be written in the form

$$p(\mathbf{x}_1, \ldots, \mathbf{x}_n \mid \Sigma) = \frac{1}{(2\pi)^{nd/2}} |\Sigma^{-1}|^{n/2} \exp\left[-\tfrac{1}{2} \text{tr}\, \Sigma^{-1} \sum_{k=1}^{n} (\mathbf{x}_k - \boldsymbol{\mu})(\mathbf{x}_k - \boldsymbol{\mu})^t \right].$$

(c) Letting $A = \Sigma^{-1}\hat{\Sigma}$ and $\lambda_1, \ldots, \lambda_d$ be the eigenvalues of A, show that this leads to

$$p(\mathbf{x}_1, \ldots, \mathbf{x}_n \mid \Sigma) = \frac{1}{(2\pi)^{nd/2} |\hat{\Sigma}|^{n/2}} (\lambda_1 \cdots \lambda_d)^{n/2} \exp\left[-\frac{n}{2} (\lambda_1 + \cdots + \lambda_d) \right].$$

(d) Complete the proof by showing that the likelihood is maximized by the choice $\lambda_1 = \cdots = \lambda_d = 1$.

6. Suppose that $p(\mathbf{x} \mid \boldsymbol{\mu}_i, \Sigma, \omega_i) \sim N(\boldsymbol{\mu}_i, \Sigma)$, where Σ is a common covariance matrix for all c classes. Let n samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$ be drawn as usual, and let $l_1, \ldots, l_n$ be their labels, so that $l_k = i$ if the state of nature for $\mathbf{x}_k$ was ω_i.

(a) Show that

$$p(\mathbf{x}_1, \ldots, \mathbf{x}_n, l_1, \ldots, l_n \mid \boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_c, \Sigma) = \frac{\prod_{k=1}^{n} P(\omega_{l_k})}{(2\pi)^{nd/2} |\Sigma|^{n/2}} \times \exp\left[-\tfrac{1}{2} \sum_{k=1}^{n} (\mathbf{x}_k - \boldsymbol{\mu}_{l_k})^t \Sigma^{-1} (\mathbf{x}_k - \boldsymbol{\mu}_{l_k}) \right].$$

(b) Using the results for samples drawn from a single normal population, show that the maximum likelihood estimates for $\boldsymbol{\mu}_i$ and Σ are given by

$$\hat{\boldsymbol{\mu}}_i = \frac{\sum_{l_k = i} \mathbf{x}_k}{\sum_{l_k = i} 1}$$

and

$$\hat{\Sigma} = \frac{1}{n}\sum_{k=1}^{n} (\mathbf{x}_k - \hat{\boldsymbol{\mu}}_{l_k})(\mathbf{x}_k - \hat{\boldsymbol{\mu}}_{l_k})^t.$$

7. Consider the problem of learning the mean of a univariate normal distribution. Let $n_0 = \sigma^2/\sigma_0^2$ be the dogmatism, and imagine that μ_0 is formed by averaging n_0 fictitious samples x_k, $k = -n_0 + 1, \ldots, 0$. Show that Eqs. (23) and (24) for μ_n and σ_n^2 yield

$$\mu_n = \frac{1}{n + n_0}\sum_{k=-n_0+1}^{n} x_k$$

and

$$\sigma_n^2 = \frac{\sigma^2}{n + n_0}.$$

Use this result to give an interpretation of the a priori density $p(\mu) \sim N(\mu_0, \sigma_0^2)$.

8. Prove the matrix identity

$$(A^{-1} + B^{-1})^{-1} = A(A + B)^{-1}B = B(A + B)^{-1}A,$$

where A and B are nonsingular matrices of the same order. Use this result in showing that Eqs. (31) and (32) do indeed follow from Eqs. (28) and (29).

9. Let the sample mean $\mathbf{m}_n$ and the sample covariance matrix C_n for a set of n samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$ be defined by

$$\mathbf{m}_n = \frac{1}{n}\sum_{k=1}^{n} \mathbf{x}_k$$

and

$$C_n = \frac{1}{n-1}\sum_{k=1}^{n} (\mathbf{x}_k - \mathbf{m}_n)(\mathbf{x}_k - \mathbf{m}_n)^t.$$

Show that the effect of adding a new sample $\mathbf{x}_{n+1}$ can be computed by the recursion relations

$$\mathbf{m}_{n+1} = \mathbf{m}_n + \frac{1}{n+1}(\mathbf{x}_{n+1} - \mathbf{m}_n)$$

and

$$C_{n+1} = \frac{n-1}{n} C_n + \frac{1}{n+1}(\mathbf{x}_{n+1} - \mathbf{m}_n)(\mathbf{x}_{n+1} - \mathbf{m}_n)^t.$$

10. The relations given in Problem 9 make it easy to update estimates for the covariance matrix. However, one is often interested in the inverse covariance matrix, and matrix inversion is time consuming. By proving the matrix identity

$$(A + \mathbf{x}\mathbf{x}^t)^{-1} = A^{-1} - \frac{A^{-1}\mathbf{x}\mathbf{x}^t A^{-1}}{1 + \mathbf{x}^t A^{-1}\mathbf{x}}$$

and using the results of Problem 9, show that

$$C_{n+1}^{-1} = \frac{n}{n-1}\left[C_n^{-1} - \frac{C_n^{-1}(\mathbf{x}_{n+1} - \mathbf{m}_n)(\mathbf{x}_{n+1} - \mathbf{m}_n)^t C_n^{-1}}{\frac{n^2-1}{n} + (\mathbf{x}_{n+1} - \mathbf{m}_n)^t C_n^{-1}(\mathbf{x}_{n+1} - \mathbf{m}_n)}\right].$$

11. The purpose of this problem is to derive the Bayesian classifier for the multivariate Bernoulli case. As usual, we work with each class separately, interpreting $P(\mathbf{x} \mid \mathcal{X})$ to mean $P(\mathbf{x} \mid \mathcal{X}_i, \omega_i)$. Let the conditional probability for a given class be given by

$$P(\mathbf{x} \mid \boldsymbol{\theta}) = \prod_{i=1}^{d} \theta_i^{x_i}(1 - \theta_i)^{1-x_i},$$

and let $\mathcal{X}$ be a set of n samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$ independently drawn according to this probability law.

(a) If $\mathbf{s} = (s_1, \ldots, s_d)^t$ is the sum of the n samples, show that

$$P(\mathcal{X} \mid \boldsymbol{\theta}) = \prod_{i=1}^{d} \theta_i^{s_i}(1 - \theta_i)^{1-s_i}.$$

(b) Assuming a uniform a priori distribution for $\boldsymbol{\theta}$ and using the identity

$$\int_0^1 \theta^m(1 - \theta)^n \, d\theta = \frac{m!\, n!}{(m + n + 1)!},$$

show that

$$p(\boldsymbol{\theta} \mid \mathcal{X}) = \prod_{i=1}^{d} \frac{(n + 1)!}{s_i!\,(n - s_i)!} \theta_i^{s_i}(1 - \theta_i)^{n-s_i}.$$

Sketch this density for the case $d = 1$, $n = 1$, and for the two resulting possibilities for s_1.

(c) Integrate the product $P(\mathbf{x} \mid \boldsymbol{\theta})p(\boldsymbol{\theta} \mid \mathcal{X})$ over $\boldsymbol{\theta}$ to obtain the desired conditional probability

$$P(\mathbf{x} \mid \mathcal{X}) = \prod_{i=1}^{d} \left(\frac{s_i + 1}{n + 2}\right)^{x_i} \left(1 - \frac{s_i + 1}{n + 2}\right)^{1-x_i}.$$

If we think of obtaining $P(\mathbf{x} \mid \mathcal{X})$ by substituting an estimate $\hat{\boldsymbol{\theta}}$ for $\boldsymbol{\theta}$ in $P(\mathbf{x} \mid \boldsymbol{\theta})$, what is the effective Bayesian estimate for $\boldsymbol{\theta}$?

12. Using the results given in Table 3-1, show that the maximum likelihood estimate for the parameter θ of a Rayleigh distribution is given by

$$\hat{\theta} = \frac{1}{\frac{1}{n}\sum_{k=1}^{n} x_k^2}.$$

13. Using the results given in Table 3-1, show that the maximum likelihood estimate for the parameter θ of a Maxwell distribution is given by

$$\hat{\theta} = \frac{3/2}{\frac{1}{n}\sum_{k=1}^{n} x_k^2}.$$

14. Using the results given in Table 3-1, show that the maximum likelihood estimate for the parameter θ of a multinomial distribution is given by

$$\theta_i = \frac{s_i}{\sum_{j=1}^{d} s_j},$$

where the vector $\mathbf{s} = (s_1, \ldots, s_d)^t$ is the average of the n samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$.

15. Consider the two-class problem described in Problem 16 of Chapter 2, in which the probability of error is known to approach zero as the dimensionality d approaches infinity.

(a) Suppose that a single sample $\mathbf{x} = (x_1, \ldots, x_d)^t$ is drawn from Class 1. Show that the maximum likelihood estimate for p is given by

$$\hat{p} = \frac{1}{d}\sum_{i=1}^{d} x_i.$$

(b) Describe the behavior of $\hat{p}$ as d approaches infinity. Indicate why this means that by letting the number of features increase without limit we can obtain an error-free classifier even though we have only one sample from only one class.

Chapter 4

NONPARAMETRIC TECHNIQUES

4.1 INTRODUCTION

In the last chapter we treated supervised learning under the assumption that the forms for the underlying density functions were known. In most pattern recognition applications this assumption is suspect. The common parametric forms rarely fit the densities actually encountered in practice. In particular, all of the classical parametric densities are unimodal (have a single local maximum), whereas many practical problems involve multimodal densities. In this chapter we shall examine *nonparametric* procedures that can be used without assuming that the forms of the underlying densities are known.

There are several different types of nonparametric methods of interest to pattern recognition. One consists of procedures for estimating the density functions $p(\mathbf{x} \mid \omega_j)$ from sample patterns. If these estimates are satisfactory, they can be substituted for the true densities in designing the optimal classifier. Another consists of procedures for directly estimating the a posteriori probabilities $P(\omega_j \mid \mathbf{x})$. This is closely related to nonparametric decision procedures, such as the nearest-neighbor rule, which bypass probability estimation and go directly to decision functions. Finally, there are nonparametric procedures for transforming the feature space in the hope that it may be possible to employ parametric methods in the transformed space. These discriminant analysis techniques include the well-known Fisher linear discriminant method, which provides an important link between the parametric techniques of Chapter 3 and the adaptive techniques of Chapter 5.

4.2 DENSITY ESTIMATION

The basic ideas behind many of the methods of estimating an unknown probability density function are very simple, although rigorous demonstrations that the estimates converge require considerable care. The most

fundamental techniques rely on the fact that the probability P that a vector $\mathbf{x}$ will fall in a region $\mathscr{R}$ is given by

$$P = \int_{\mathscr{R}} p(\mathbf{x}')\, d\mathbf{x}'. \tag{1}$$

Thus P is a smoothed or averaged version of the density function $p(\mathbf{x})$, and we can estimate this smoothed value of p by estimating the probability P. Suppose that n samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$ are independently drawn according to the probability law $p(\mathbf{x})$. Clearly, the probability that k of these n fall in $\mathscr{R}$ is given by the binomial law

$$P_k = \binom{n}{k} P^k (1 - P)^{n-k},$$

and the expected value for k is

$$E[k] = nP. \tag{2}$$

Moreover, this binomial distribution for k peaks very sharply about the mean, so that we expect that the ratio k/n will be a very good estimate for the probability P, and hence for the smoothed density function. If we now assume that $p(\mathbf{x})$ is continuous and that the region $\mathscr{R}$ is so small that p does not vary appreciably within it, we can write

$$\int_{\mathscr{R}} p(\mathbf{x}')\, d\mathbf{x}' \approx p(\mathbf{x})V, \tag{3}$$

where $\mathbf{x}$ is a point within $\mathscr{R}$ and V is the volume enclosed by $\mathscr{R}$. Combining (1), (2), and (3), we arrive at the following obvious estimate for $p(\mathbf{x})$:

$$p(\mathbf{x}) \approx \frac{k/n}{V}. \tag{4}$$

There are several problems that remain, some practical and some theoretical. If we fix the volume V and take more and more samples, the ratio k/n will converge (in probability) as desired, but we have only obtained an estimate of the space-average value of $p(\mathbf{x})$,

$$\frac{P}{V} = \frac{\int_{\mathscr{R}} p(\mathbf{x}')\, d\mathbf{x}'}{\int_{\mathscr{R}} d\mathbf{x}'}.$$

If we want to obtain $p(\mathbf{x})$ rather than an averaged version of $p(\mathbf{x})$, we must be prepared to let V approach zero. However, if we fix the number n of samples and let V approach zero, the region will eventually become so small that it will enclose no samples, and our estimate $p(\mathbf{x}) \approx 0$ will be useless.*

* If by chance one or more samples coincide at $\mathbf{x}$, the estimate diverges to infinity, which is equally useless.

From a practical standpoint, the number of samples is always limited. Thus, the volume V can not be allowed to become arbitrarily small. If this kind of estimate is to be used, one will have to accept a certain amount of variance in the ratio k/n and a certain amount of averaging of the density $p(\mathbf{x})$.

From a theoretical standpoint, it is interesting to ask how these limitations can be circumvented if an unlimited number of samples is available. Suppose we use the following procedure. To estimate the density at $\mathbf{x}$, we form a sequence of regions $\mathscr{R}_1, \mathscr{R}_2, \ldots$, containing $\mathbf{x}$, the first region to be used with one sample, the second with two, and so on. Let V_n be the volume of $\mathscr{R}_n$, k_n be the number of samples falling in $\mathscr{R}_n$, and $p_n(\mathbf{x})$ be the nth estimate for $p(\mathbf{x})$:

$$p_n(\mathbf{x}) = \frac{k_n/n}{V_n}. \tag{5}$$

If $p_n(\mathbf{x})$ is to converge to $p(\mathbf{x})$, three conditions appear to be required:

(1) $\lim_{n \to \infty} V_n = 0$

(2) $\lim_{n \to \infty} k_n = \infty$

(3) $\lim_{n \to \infty} k_n/n = 0.$

The first condition assures us that the space average P/V will converge to $p(\mathbf{x})$, provided that the regions shrink uniformly and that p is continuous at $\mathbf{x}$. The second condition, which only makes sense if $p(\mathbf{x}) \neq 0$, assures us that the frequency ratio will converge (in probability) to the probability P. The third condition is clearly necessary if $p_n(\mathbf{x})$ given by Eq. (5) is to converge at all. It also says that although a huge number of samples will eventually fall within the small region $\mathscr{R}_n$, they will form a negligibly small fraction of the total number of samples.

There are two common ways of obtaining sequences of regions that satisfy these conditions. One is to shrink an initial region by specifying the volume V_n as some function of n, such as $V_n = 1/\sqrt{n}$. It then must be shown that the random variables k_n and k_n/n behave properly, or, more to the point, that $p_n(\mathbf{x})$ converges to $p(\mathbf{x})$. This is basically the Parzen-window method that will be examined in the next section. The second method is to specify k_n as some function of n, such as $k_n = \sqrt{n}$. Here the volume V_n is grown until it encloses k_n neighbors of $\mathbf{x}$. This is the k_n-nearest-neighbor estimation method. Both of these methods do in fact converge, although it is difficult to make meaningful statements about their finite-sample behavior.

4.3 PARZEN WINDOWS

4.3.1 General Discussion

The Parzen-window approach to estimating densities can be introduced by temporarily assuming that the region $\mathcal{R}_n$ is a d-dimensional hypercube. If h_n is the length of an edge of that hypercube, then its volume is given by

$$V_n = h_n^d. \tag{6}$$

We can obtain an analytic expression for k_n, the number of samples falling in the hypercube, by defining the following *window function:*

$$\varphi(\mathbf{u}) = \begin{cases} 1 & |u_j| \leq 1/2 \qquad j = 1, \ldots, d \\ 0 & \text{otherwise.} \end{cases} \tag{7}$$

Thus, $\varphi(\mathbf{u})$ defines a unit hypercube centered at the origin. It follows that $\varphi((\mathbf{x} - \mathbf{x}_i)/h_n)$ is equal to unity if $\mathbf{x}_i$ falls within the hypercube of volume V_n centered at $\mathbf{x}$, and is zero otherwise. Hence the number of samples in this hypercube is given by

$$k_n = \sum_{i=1}^{n} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h_n}\right),$$

and when we substitute this in Eq. (5) we obtain the estimate

$$p_n(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{V_n} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h_n}\right). \tag{8}$$

This equation suggests a more general approach to estimating density functions. Rather than limiting ourselves to the hypercube window function of Eq. (7), suppose we allow a more general class of window functions. Then Eq. (8) expresses our estimate for $p(\mathbf{x})$ as an average of functions of $\mathbf{x}$ and the samples $\mathbf{x}_i$. In essence, the window function is being used for *interpolation*, each sample contributing to the estimate in accordance with its distance from $\mathbf{x}$.

It is natural to ask that the estimate $p_n(\mathbf{x})$ be a legitimate density function, i.e., that it be nonnegative and integrate to one. This can be assured by requiring the window function to be a legitimate density function. To be more precise, if we require that

$$\varphi(\mathbf{u}) \geq 0 \tag{9}$$

and

$$\int \varphi(\mathbf{u})\, d\mathbf{u} = 1, \tag{10}$$

and if we maintain the relation $V_n = h_n^d$, then it follows at once that $p_n(\mathbf{x})$ also satisfies these conditions.

Let us examine the effect that the *window width* h_n has on $p_n(\mathbf{x})$. If we define the function $\delta_n(\mathbf{x})$ by

$$\delta_n(\mathbf{x}) = \frac{1}{V_n}\varphi\left(\frac{\mathbf{x}}{h_n}\right), \tag{11}$$

then we can write $p_n(\mathbf{x})$ as the average

$$p_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n}\delta_n(\mathbf{x} - \mathbf{x}_i). \tag{12}$$

Since $V_n = h_n^d$, h_n affects both the amplitude and the width of $\delta_n(\mathbf{x})$. If h_n is very large, the amplitude of δ_n is small, and $\mathbf{x}$ must be far from $\mathbf{x}_i$ before $\delta_n(\mathbf{x} - \mathbf{x}_i)$ changes much from $\delta_n(\mathbf{0})$. In this case, $p_n(\mathbf{x})$ is the superposition of n broad, slowly changing functions, and is a very smooth, "out-of-focus" estimate for $p(\mathbf{x})$. On the other hand, if h_n is very small, the peak value of $\delta_n(\mathbf{x} - \mathbf{x}_i)$ is large and occurs near $\mathbf{x} = \mathbf{x}_i$. In this case, $p_n(\mathbf{x})$ is the superposition of n sharp pulses centered at the samples, and is an erratic, "noisy" estimate of $p(\mathbf{x})$. For any value of h_n

$$\int \delta_n(\mathbf{x} - \mathbf{x}_i)\,d\mathbf{x} = \int \frac{1}{V_n}\varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h_n}\right)d\mathbf{x} = \int \varphi(\mathbf{u})\,d\mathbf{u} = 1. \tag{13}$$

Thus, as h_n approaches zero, $\delta_n(\mathbf{x} - \mathbf{x}_i)$ approaches a Dirac delta function centered at $\mathbf{x}_i$, and $p_n(\mathbf{x})$ approaches a superposition of delta functions centered at the samples.

Clearly, the choice of h_n (or V_n) has a major effect on $p_n(\mathbf{x})$. If V_n is too large, the estimate will suffer from too little resolution. If V_n is too small, the estimate will suffer from too much statistical variability. With a limited number of samples, the best one can do is to seek some acceptable compromise. However, with an unlimited number of samples, it is possible to let V_n slowly approach zero as n increases and have $p_n(\mathbf{x})$ converge to the unknown density $p(\mathbf{x})$.

In talking about convergence, we must recognize that we are talking about the convergence of a sequence of random variables, since for any fixed $\mathbf{x}$ the value of $p_n(\mathbf{x})$ depends on the values of the random samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$. Thus, $p_n(\mathbf{x})$ has some mean $\bar{p}_n(\mathbf{x})$ and some variance $\sigma_n^2(\mathbf{x})$. We shall say that the estimate $p_n(\mathbf{x})$ converges to $p(\mathbf{x})$ if*

$$\lim_{n\to\infty}\bar{p}_n(\mathbf{x}) = p(\mathbf{x}) \tag{14}$$

* This type of convergence is called *convergence in mean square*. For a discussion of the modes of convergence of a sequence of random variables, see E. Parzen, *Modern Probability Theory and its Applications*, Chapter 10 (John Wiley, New York, 1960).

and

$$\lim_{n\to\infty} \sigma_n^2(\mathbf{x}) = 0. \tag{15}$$

To prove convergence we must place conditions on the unknown density $p(\mathbf{x})$, on the window function $\varphi(\mathbf{u})$, and on the window width h_n. In general, continuity of p at $\mathbf{x}$ is required, and the conditions imposed by Eqs. (9) and (10) are customarily invoked. With care, it can be shown that the following additional conditions assure convergence:

$$\sup_{\mathbf{u}} \varphi(\mathbf{u}) < \infty \tag{16}$$

$$\lim_{\|\mathbf{u}\|\to\infty} \varphi(\mathbf{u}) \prod_{i=1}^{d} u_i = 0 \tag{17}$$

$$\lim_{n\to\infty} V_n = 0 \tag{18}$$

and

$$\lim_{n\to\infty} nV_n = \infty. \tag{19}$$

Equations (16) and (17) keep φ well behaved, and are satisfied by most density functions that one might think of using for window functions. Equations (18) and (19) state that the volume V_n must approach zero, but at a rate slower than $1/n$. We shall now see why these are the basic conditions for convergence.

4.3.2 Convergence of the Mean

Consider first $\bar{p}_n(\mathbf{x})$, the mean of $p_n(\mathbf{x})$. Since the samples $\mathbf{x}_i$ are identically distributed according to the (unknown) density $p(\mathbf{x})$,

$$\begin{aligned}
\bar{p}_n(\mathbf{x}) &= E[p_n(\mathbf{x})] \\
&= \frac{1}{n}\sum_{i=1}^{n} E\left[\frac{1}{V_n}\varphi\left(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\right)\right] \\
&= \int \frac{1}{V_n}\varphi\left(\frac{\mathbf{x}-\mathbf{v}}{h_n}\right) p(\mathbf{v})\, d\mathbf{v} \\
&= \int \delta_n(\mathbf{x}-\mathbf{v}) p(\mathbf{v})\, d\mathbf{v}.
\end{aligned} \tag{20}$$

This equation shows that the expected value of the estimate is an averaged value of the unknown density, a *convolution* of the unknown density and the window function. Thus, $\bar{p}_n(\mathbf{x})$ is a blurred version of $p(\mathbf{x})$ as seen through the averaging window. But as V_n approaches zero, $\delta_n(\mathbf{x}-\mathbf{v})$ approaches a

delta function centered at $\mathbf{x}$. Thus, if p is continuous at $\mathbf{x}$, Eq. (18) ensures that $\bar{p}_n(\mathbf{x})$ will approach $p(\mathbf{x})$ as n approaches infinity.*

4.3.3 Convergence of the Variance

Equation (20) shows that there is no need for an infinite number of samples to make $\bar{p}_n(\mathbf{x})$ approach $p(\mathbf{x})$; one can achieve this for any n merely by letting V_n approach zero. Of course, for a particular set of n samples, the resulting "spiky" estimate is useless, and this observation emphasizes the need for considering the variance of the estimate. Since $p_n(\mathbf{x})$ is the sum of functions of statistically independent random variables, its variance is the sum of the variances of the separate terms, and hence

$$\begin{aligned}\sigma_n^2(\mathbf{x}) &= \sum_{i=1}^{n} E\left[\left\{\frac{1}{nV_n}\varphi\left(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\right) - \frac{1}{n}\bar{p}_n(\mathbf{x})\right\}^2\right] \\ &= nE\left[\frac{1}{n^2V_n^2}\varphi^2\left(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\right)\right] - \frac{1}{n}\bar{p}_n^2(\mathbf{x}) \\ &= \frac{1}{nV_n}\int \frac{1}{V_n}\varphi^2\left(\frac{\mathbf{x}-\mathbf{v}}{h_n}\right)p(\mathbf{v})\,d\mathbf{v} - \frac{1}{n}\bar{p}_n^2(\mathbf{x}). \end{aligned} \tag{21}$$

By dropping the second term, bounding φ, and using Eq. (20), we obtain

$$\sigma_n^2(\mathbf{x}) \leq \frac{\sup(\varphi)\bar{p}_n(\mathbf{x})}{nV_n}. \tag{22}$$

Clearly, to obtain a small variance we want a large value for V_n, not a small one. However, since the numerator stays finite as n approaches infinity, we can let V_n approach zero and still obtain zero variance, provided that nV_n approaches infinity. For example, we can let $V_n = V_1/\sqrt{n}$ or $V_1/\log n$ or any other function satisfying Eqs. (18) and (19).

This is the principal theoretical result. Unfortunately, it does not tell us how to choose φ and V_n to obtain good results in the finite sample case. Indeed, unless we have more knowledge about $p(\mathbf{x})$ than the mere fact that it is continuous, we have no basis for optimizing finite sample results.

4.3.4 Two Examples

It is interesting to see how the Parzen window method behaves on some simple examples. Consider first the case where $p(\mathbf{x})$ is a zero-mean, unit-variance, univariate normal density. Let the window function be of the same

* This argument is not rigorous but is intuitively clear and basically sound. More careful analysis discloses a problem if the unknown density is not bounded, as happens when $p(\mathbf{x})$ contains delta functions. The added condition of Eq. (17) eliminates this problem.

form:

$$\varphi(u) = \frac{1}{\sqrt{2\pi}} \exp[-\tfrac{1}{2}u^2].$$

Finally, let $h_n = h_1/\sqrt{n}$, where h_1 is a parameter at our disposal. Thus $p_n(x)$ is an average of normal densities centered at the samples:

$$p_n(x) = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{h_n}\varphi\left(\frac{x - x_i}{h_n}\right).$$

While it is not hard to evaluate Eqs. (20) and (21) to find the mean and variance of $p_n(x)$, it is even more interesting to see numerical results. When a particular set of normally distributed random samples was generated and used to compute $p_n(x)$, the results shown in Figure 4.1 were obtained. These results depend both on n and h_1. For $n = 1$, $p_n(x)$ is merely a single gaussian hill centered about the first sample. For $n = 16$ and $h_1 = 1/4$ the contributions of the individual samples are clearly discernible; this is not the case for $h_1 = 1$ and $h_1 = 4$. As n gets larger, the ability of p_n to resolve variations in p increases. Concomitantly, p_n appears to be more sensitive to local sampling irregularities when n is large, although we are assured that p_n will converge to the smooth normal curve as n goes to infinity. While one should not judge on visual appearance alone, it is clear that many samples are required to obtain an accurate estimate.

For the second example, we let $\varphi(u)$ and h_n be the same as before, but let the unknown density be a mixture of two uniform densities:

$$p(x) = \begin{cases} 1 & -2.5 < x < -2 \\ 0.25 & 0 < x < 2 \\ 0 & \text{elsewhere.} \end{cases}$$

Figure 4.2 shows the behavior of Parzen window estimates for this density. As before, the case $n = 1$ tells more about the window function than it tells about the unknown density. For $n = 16$, none of the estimates is particularly good, but the results for $n = 256$ and $h_1 = 1$ are beginning to appear acceptable.

These examples illustrate some of the power and some of the limitations of nonparametric methods. Their power resides in their generality. Exactly the same procedure was used for the unimodal normal case and the bimodal mixture case. With enough samples, we are essentially assured of convergence to an arbitrarily complicated unknown density. On the other hand, the number of samples needed may be very large indeed, much greater than the number that would be required if we knew the form of the unknown density. Little or nothing in the way of data reduction is provided, which leads to severe

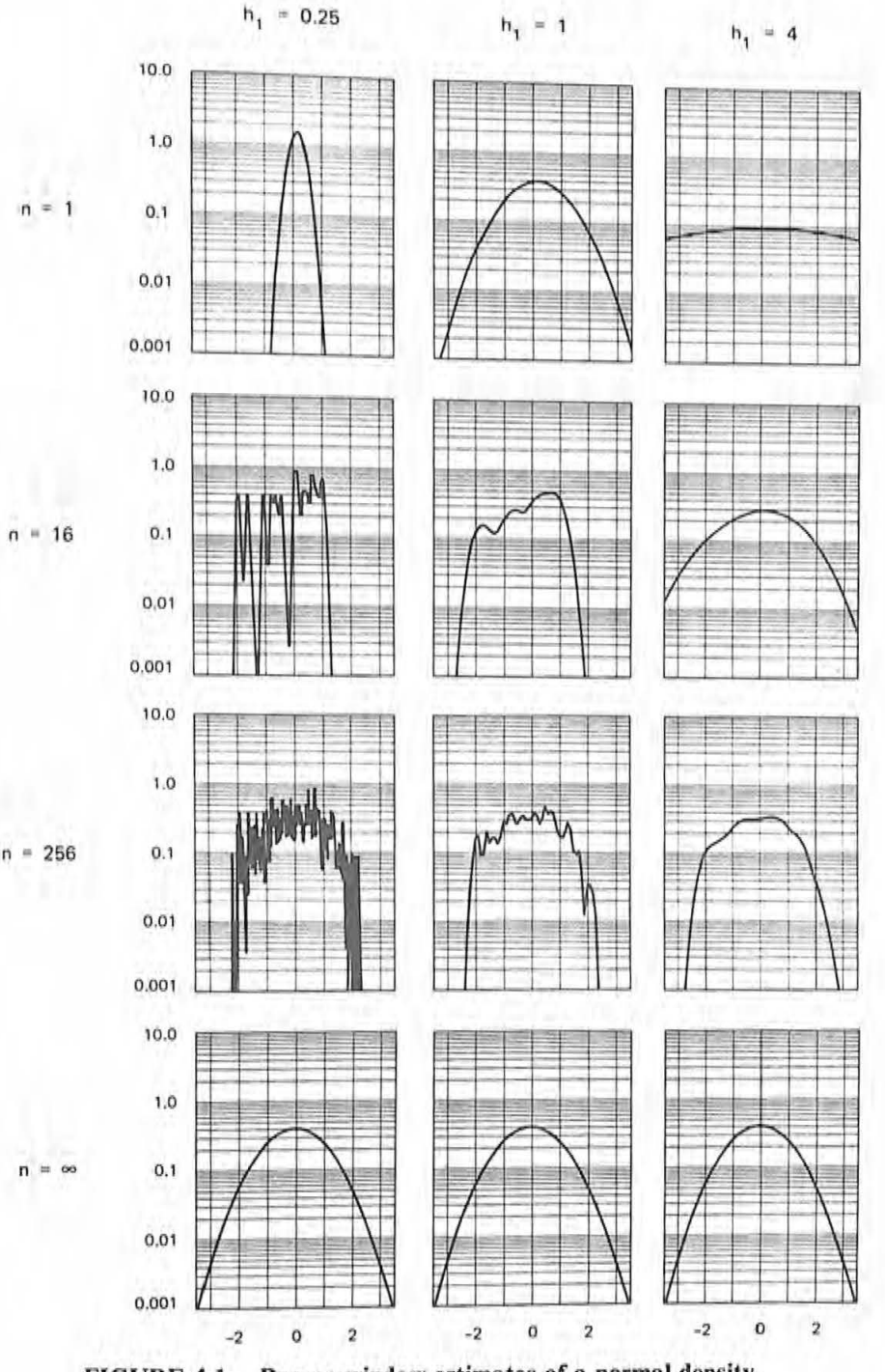

FIGURE 4.1. Parzen-window estimates of a normal density.

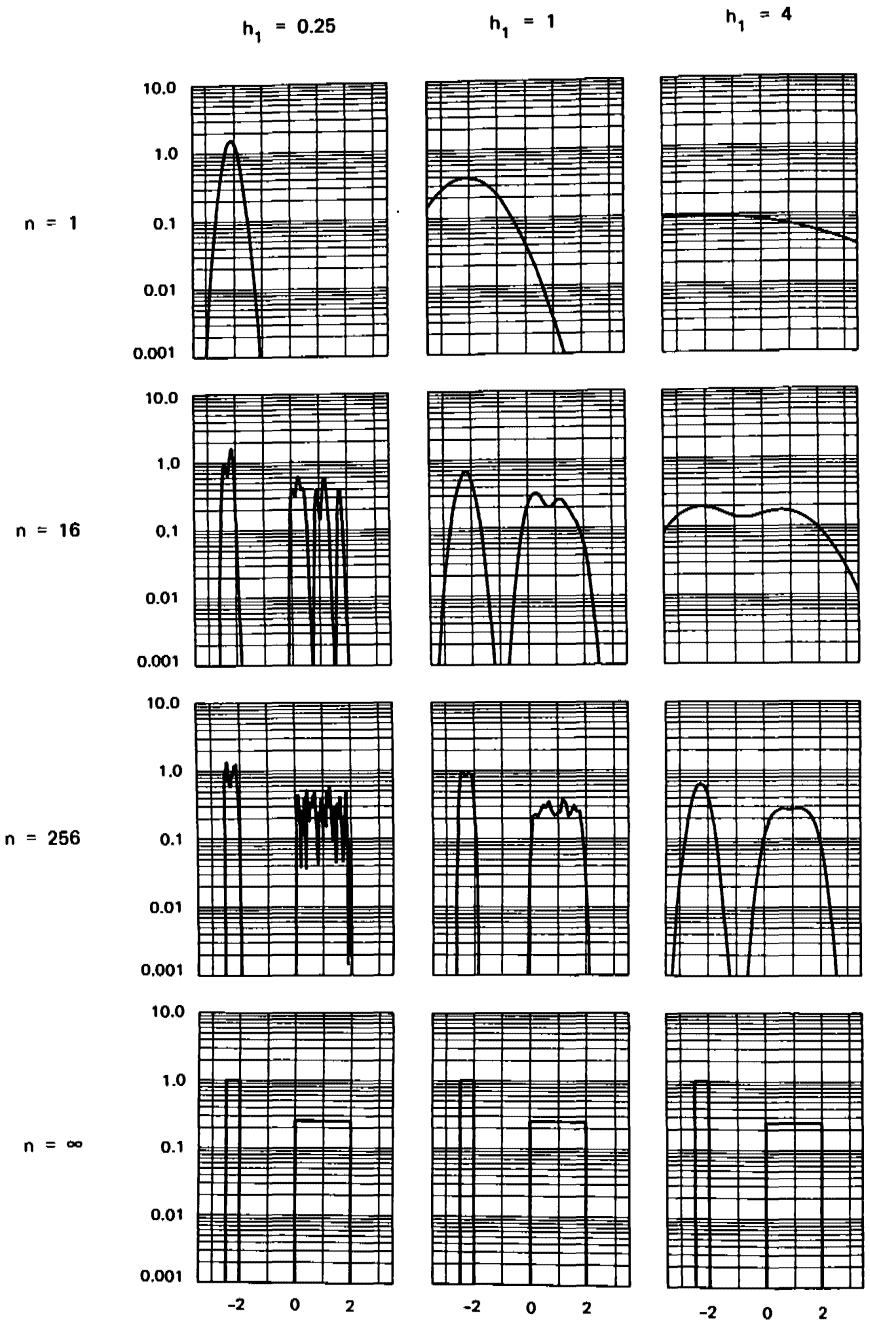

FIGURE 4.2. Parzen-window estimates of a bimodal density.

requirements for computation time and storage. Moreover, the demand for a large number of samples grows exponentially with the dimensionality of the feature space. This limitation is related to what Bellman calls "the curse of dimensionality," and severely restricts the practical application of such nonparametric procedures.

4.4 k_n-NEAREST-NEIGHBOR ESTIMATION

One of the problems encountered in the Parzen-window approach concerns the choice of the sequence of cell volumes $V_1, V_2, \ldots$. For example, if we take $V_n = V_1/\sqrt{n}$, the results for any finite n will be very sensitive to the choice for the initial volume V_1. If V_1 is too small, most of the volumes will be empty, and the estimate $p_n(\mathbf{x})$ will be very erratic. On the other hand, if V_1 is too large, important spatial variations in $p(\mathbf{x})$ may be lost due to averaging over the cell volume. Furthermore, it may well be the case that a cell volume appropriate for one value of $\mathbf{x}$ might be entirely unsuitable elsewhere.

One potential remedy for these problems is to let the cell volume be a function of the data, rather than some arbitrary function of the number of samples. For example, to estimate $p(\mathbf{x})$ from n samples, one can center a cell about $\mathbf{x}$ and let it grow until it captures k_n samples, where k_n is some specified function of n. These samples are the k_n nearest neighbors of $\mathbf{x}$. If the density is high near $\mathbf{x}$, the cell will be relatively small, which leads to good resolution. If the density is low, it is true that the cell will grow large, but it will stop soon after it enters regions of higher density. In either case, if we take

$$p_n(\mathbf{x}) = \frac{k_n/n}{V_n} \tag{5}$$

we want k_n to go to infinity as n goes to infinity, since this assures us that k_n/n will be a good estimate of the probability that a point will fall in the cell of volume V_n. However, we also want k_n to grow sufficiently slowly that the size of the cell needed to capture k_n samples will shrink to zero. Thus, it is clear from Eq. (5) that the ratio k_n/n must go to zero. Although we shall not supply a proof, it can be shown that the conditions $\lim_{n\to\infty} k_n = \infty$ and $\lim_{n\to\infty} k_n/n = 0$ are necessary and sufficient for $p_n(\mathbf{x})$ to converge to $p(\mathbf{x})$ in probability at all points where p is continuous. If we take $k_n = \sqrt{n}$ and assume that $p_n(\mathbf{x})$ is a reasonably good approximation to $p(\mathbf{x})$, we see from Eq. (5) that $V_n \approx 1/(\sqrt{n}p(\mathbf{x}))$. Thus, V_n again has the form $V_1/\sqrt{n}$, but the initial volume V_1 is determined by the nature of the data rather than by some arbitrary choice on our part.

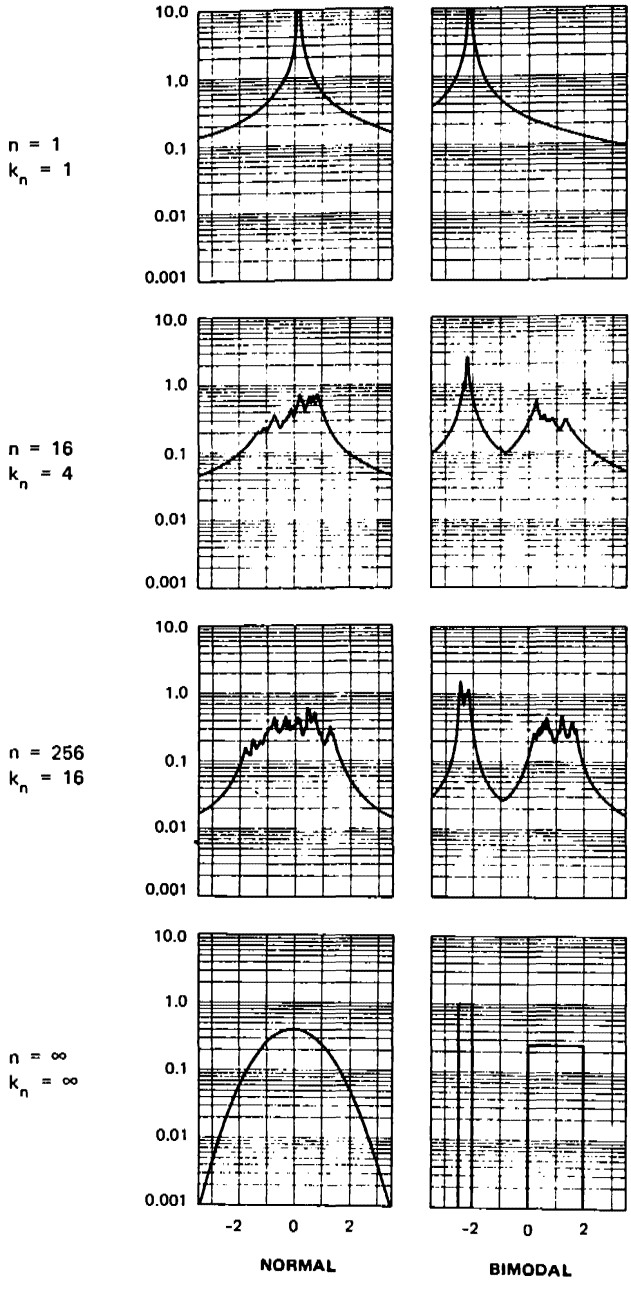

FIGURE 4.3. k_n-nearest neighbor estimates of two densities.

It is instructive to compare the performance of this method with that of the Parzen-window method on the data used in the previous examples. With $n = 1$ and $k_n = \sqrt{n} = 1$, the estimate becomes

$$p_n(x) = \frac{1}{2\,|x - x_1|}.$$

This is clearly a poor estimate of $p(x)$, with its integral embarrassing us by diverging to infinity. As shown in Figure 4.3, the estimate becomes considerably better as n gets larger, even though the integral of the estimate always remains infinite. This unfortunate fact is compensated by the fact that $p_n(x)$ never plunges to zero just because no samples fall within some arbitrary cell or window. While this might seem to be a meager compensation, it can be of considerable value in higher-dimensional spaces.

As with the Parzen-window approach, we could obtain a family of estimates by taking $k_n = k_1\sqrt{n}$ and choosing different values for k_1. However, in the absence of any additional information, one choice is as good as another, and we can be confident only that the results will be asymptotically correct.

4.5 ESTIMATION OF A POSTERIORI PROBABILITIES

The techniques discussed in the previous sections can be used to estimate the a posteriori probabilities $P(\omega_i \mid \mathbf{x})$ from a set of n labelled samples by using the samples to estimate the densities involved. Suppose that we place a cell of volume V around x and capture k samples, k_i of which turn out to be labelled ω_i. Then the obvious estimate for the joint probability $p(\mathbf{x}, \omega_i)$ is

$$p_n(\mathbf{x}, \omega_i) = \frac{k_i/n}{V}.$$

Thus, a reasonable estimate for $P(\omega_i \mid \mathbf{x})$ is

$$P_n(\omega_i \mid \mathbf{x}) = \frac{p_n(\mathbf{x}, \omega_i)}{\sum_{j=1}^{c} p_n(\mathbf{x}, \omega_j)} = \frac{k_i}{k}.$$

That is, the estimate of the a posteriori probability that ω_i is the state of nature is merely the fraction of the samples within the cell that are labelled ω_i. For minimum error rate, we select the category most frequently represented within the cell. If there are enough samples and if the cell is sufficiently small, it can be shown that this will yield performance approaching the best possible.

When it comes to choosing the size of the cell, it is clear that we can use either the Parzen-window approach or the k_n-nearest-neighbor approach. In the first case, V_n would be some specified function of n, such as $V_n = 1/\sqrt{n}$. In the second case, V_n would be expanded until some specified number of samples were captured, such as $k = \sqrt{n}$. In either case, as n goes to infinity an infinite number of samples will fall within the infinitely small cell. The fact that the cell volume can become arbitrarily small and yet contain an arbitrarily large number of samples allows us to learn the unknown probabilities with virtual certainty and thus eventually obtain optimum performance. Interestingly enough, we shall now see that we can obtain comparable performance if we base our decision solely on the label of the single nearest neighbor of $\mathbf{x}$.

4.6 THE NEAREST-NEIGHBOR RULE

4.6.1 General Considerations

Let $\mathscr{X}^n = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ be a set of n labelled samples, and let $\mathbf{x}'_n \in \mathscr{X}^n$ be the sample nearest to $\mathbf{x}$. Then the *nearest-neighbor rule* for classifying $\mathbf{x}$ is to assign it the label associated with $\mathbf{x}'_n$. The nearest-neighbor rule is a suboptimal procedure; its use will usually lead to an error rate greater than the minimum possible, the Bayes rate. We shall see, however, that with an unlimited number of samples the error rate is never worse than twice the Bayes rate.

Before we get immersed in details, let us try to gain a heuristic understanding of why the nearest-neighbor rule should work so well. To begin with, note that the label θ'_n associated with the nearest neighbor is a random variable, and the probability that $\theta'_n = \omega_i$ is merely the a posteriori probability $P(\omega_i \mid \mathbf{x}'_n)$. When the number of samples is very large, it is reasonable to assume that $\mathbf{x}'_n$ is sufficiently close to $\mathbf{x}$ that $P(\omega_i \mid \mathbf{x}'_n) \approx P(\omega_i \mid \mathbf{x})$. In that case, we can view the nearest-neighbor rule as a randomized decision rule that classifies $\mathbf{x}$ by selecting the category ω_i with probability $P(\omega_i \mid \mathbf{x})$. Since this is exactly the probability that nature will be in state ω_i, the nearest-neighbor rule is effectively matching probabilities with nature.

If we define $\omega_m(\mathbf{x})$ by

$$P(\omega_m \mid \mathbf{x}) = \max_i P(\omega_i \mid \mathbf{x}), \tag{23}$$

then the Bayes decision rule always selects ω_m. When $P(\omega_m \mid \mathbf{x})$ is close to unity, the nearest-neighbor selection is almost always the same as the Bayes selection. That is, when the minimum probability of error is small, the nearest-neighbor probability of error is also small. When $P(\omega_m \mid \mathbf{x})$ is close to $1/c$, so

that all classes are essentially equally likely, the selections made by the nearest-neighbor rule and the Bayes decision rule are rarely the same, but the probability of error is approximately $1 - 1/c$ for both. While more careful analysis is clearly necessary, these observations should make the good performance of the nearest-neighbor rule less surprising.

Our analysis of the behavior of the nearest-neighbor rule will be directed at obtaining the large-sample conditional average probability of error $P(e \mid \mathbf{x})$, where the averaging is with respect to the samples. The unconditional average probability of error will then be found by averaging $P(e \mid \mathbf{x})$ over all $\mathbf{x}$:

$$P(e) = \int P(e \mid \mathbf{x})p(\mathbf{x})\, d\mathbf{x}. \tag{24}$$

We note in passing that the Bayes decision rule minimizes $P(e)$ by minimizing $P(e \mid \mathbf{x})$ for every $\mathbf{x}$. If we let $P^*(e \mid \mathbf{x})$ be the minimum possible value of $P(e \mid \mathbf{x})$, and P^* be the minimum possible value of $P(e)$, then

$$P^*(e \mid \mathbf{x}) = 1 - P(\omega_m \mid \mathbf{x}) \tag{25}$$

and

$$P^* = \int P^*(e \mid \mathbf{x})p(\mathbf{x})\, d\mathbf{x}. \tag{26}$$

4.6.2 Convergence of the Nearest Neighbor

We now wish to evaluate the average probability of error for the nearest-neighbor rule. In particular, if $P_n(e)$ is the n-sample error rate, and if

$$P = \lim_{n \to \infty} P_n(e), \tag{27}$$

then we want to show that

$$P^* \leq P \leq P^*\left(2 - \frac{c}{c-1} P^*\right). \tag{28}$$

We begin by observing that when the nearest-neighbor rule is used with a particular set of n samples, the resulting error rate will depend on the accidental characteristics of the samples. In particular, if different sets of n samples are used to classify $\mathbf{x}$, different vectors $\mathbf{x}'_n$ will be obtained for the nearest neighbor of $\mathbf{x}$. Since the decision rule depends on this nearest neighbor, we have a conditional probability of error $P_n(e \mid \mathbf{x}, \mathbf{x}'_n)$ that depends on both $\mathbf{x}$ and $\mathbf{x}'_n$. By averaging over $\mathbf{x}'_n$, we obtain

$$P_n(e \mid \mathbf{x}) = \int P_n(e \mid \mathbf{x}, \mathbf{x}'_n)p(\mathbf{x}'_n \mid \mathbf{x})\, d\mathbf{x}'_n. \tag{29}$$

It is usually very difficult to obtain an exact expression for the conditional density $p(\mathbf{x}'_n \mid \mathbf{x})$. However, since $\mathbf{x}'_n$ is by definition the nearest neighbor of

$\mathbf{x}$, we expect this density to be very peaked in the immediate vicinity of $\mathbf{x}$, and very small elsewhere. Furthermore, as n goes to infinity we expect $p(\mathbf{x}'_n \mid \mathbf{x})$ to approach a delta function centered at $\mathbf{x}$, making the evaluation of Eq. (29) trivial. To show that this is indeed the case, we must assume that at the given $\mathbf{x}$, p is continuous and not equal to zero. Under these conditions, the probability that any sample falls within a hypersphere S centered about $\mathbf{x}$ is some positive number P_s:

$$P_s = \int_{\mathbf{x}' \in S} p(\mathbf{x}')\, d\mathbf{x}'.$$

Thus, the probability that all n of the independently drawn samples fall outside this hypersphere is $(1 - P_s)^n$, which approaches zero as n goes to infinity. Thus $\mathbf{x}'_n$ converges to $\mathbf{x}$ in probability, and $p(\mathbf{x}'_n \mid \mathbf{x})$ approaches a delta function, as expected. In fact, by using measure theoretic methods one can make even stronger (as well as more rigorous) statements about the convergence of $\mathbf{x}'_n$ to $\mathbf{x}$, but this result is sufficient for our purposes.

4.6.3 Error Rate for the Nearest Neighbor Rule

We now turn to the calculation of the conditional probability of error $P_n(e \mid \mathbf{x}, \mathbf{x}'_n)$. To avoid a potential source of confusion, we must state the problem with somewhat greater care than has been exercised so far. When we say that we have n independently drawn labelled samples, we are talking about n pairs of random variables $(\mathbf{x}_1, \theta_1), (\mathbf{x}_2, \theta_2), \ldots, (\mathbf{x}_n, \theta_n)$, where θ_i may be any of the c states of nature $\omega_1, \ldots, \omega_c$. We assume that these pairs were generated by selecting a state of nature ω_j for θ_i with probability $P(\omega_j)$ and then selecting an $\mathbf{x}_i$ according to the probability law $p(\mathbf{x} \mid \omega_j)$, with each pair being selected independently. Suppose now that nature selects a pair $(\mathbf{x}, \theta)$, and that $\mathbf{x}'_n$, labelled θ'_n, is the sample nearest $\mathbf{x}$. Since the state of nature when $\mathbf{x}'_n$ was drawn is independent of the state of nature when $\mathbf{x}$ is drawn,

$$P(\theta, \theta'_n \mid \mathbf{x}, \mathbf{x}'_n) = P(\theta \mid \mathbf{x})P(\theta'_n \mid \mathbf{x}'_n). \tag{30}$$

Now if we use the nearest-neighbor decision rule, we commit an error whenever $\theta \neq \theta'_n$. Thus, the conditional probability of error $P_n(e \mid \mathbf{x}, \mathbf{x}'_n)$ is given by

$$\begin{aligned} P_n(e \mid \mathbf{x}, \mathbf{x}'_n) &= 1 - \sum_{i=1}^{c} P(\theta = \omega_i, \theta'_n = \omega_i \mid \mathbf{x}, \mathbf{x}'_n) \\ &= 1 - \sum_{i=1}^{c} P(\omega_i \mid \mathbf{x})P(\omega_i \mid \mathbf{x}'_n). \end{aligned} \tag{31}$$

To obtain $P_n(e)$ we must substitute this expression in Eq. (29) for $P_n(e \mid \mathbf{x})$ and then average the result over $\mathbf{x}$. This is very difficult in general, but, as we

remarked earlier, the integration called for in Eq. (29) becomes trivial as n goes to infinity and $p(\mathbf{x}'_n \mid \mathbf{x})$ approaches a delta function. If $P(\omega_i \mid \mathbf{x})$ is continuous at $\mathbf{x}$, we obtain

$$\lim_{n\to\infty} P_n(e \mid \mathbf{x}) = \int \left[1 - \sum_{i=1}^{c} P(\omega_i \mid \mathbf{x}) P(\omega_i \mid \mathbf{x}'_n)\right] \delta(\mathbf{x}'_n - \mathbf{x})\, d\mathbf{x}'_n$$

$$= 1 - \sum_{i=1}^{c} P^2(\omega_i \mid \mathbf{x}). \tag{32}$$

Thus, provided we can exchange some limits and integrals,† the asymptotic nearest-neighbor error rate is given by

$$P = \lim_{n\to\infty} P_n(e)$$

$$= \lim_{n\to\infty} \int P_n(e \mid \mathbf{x}) p(\mathbf{x})\, d\mathbf{x}$$

$$= \int \left[1 - \sum_{i=1}^{c} P^2(\omega_i \mid \mathbf{x})\right] p(\mathbf{x})\, d\mathbf{x}. \tag{33}$$

4.6.4 Error Bounds

While Eq. (33) presents an exact result, it is more illuminating to obtain bounds on P in terms of the Bayes rate P^*. An obvious lower bound on P is P^* itself. Furthermore, it can be shown that for any P^* there is a set of conditional and prior probabilities for which the bound is achieved, so that in this sense it is a tight lower bound.

The problem of establishing a tight upper bound is more interesting. The basis for hoping for a low upper bound comes from observing that if the Bayes rate is low, $P(\omega_i \mid \mathbf{x})$ is near one for some i, say $i = m$. Thus the integrand in Eq. (33) is approximately $1 - P^2(\omega_m \mid \mathbf{x}) \approx 2(1 - P(\omega_m \mid \mathbf{x}))$, and since

$$P^*(e \mid \mathbf{x}) = 1 - P(\omega_m \mid \mathbf{x}), \tag{34}$$

integration over $\mathbf{x}$ might yield about twice the Bayes rate, which is still low. To obtain an exact upper bound, we must find out how large the nearest-neighbor error rate P can become for a given Bayes rate P^*. Thus, Eq. (33) leads us to ask how small $\sum_{i=1}^{c} P^2(\omega_i \mid \mathbf{x})$ can be for a given $P(\omega_m \mid \mathbf{x})$. Writing

$$\sum_{i=1}^{c} P^2(\omega_i \mid \mathbf{x}) = P^2(\omega_m \mid \mathbf{x}) + \sum_{i \neq m} P^2(\omega_i \mid \mathbf{x})$$

† Readers familiar with measure theory will recognize that the dominated convergence theorem permits us to make this interchange. If there are regions where $p(\mathbf{x})$ is identically zero, Eq. (32) is not valid for those values of $\mathbf{x}$. (Why?) However, such regions can be excluded from the integration in Eq. (33).

we can bound this sum by minimizing the second term subject to the following constraints:

(1) $P(\omega_i \mid \mathbf{x}) \geq 0$

(2) $\sum_{i \neq m} P(\omega_i \mid \mathbf{x}) = 1 - P(\omega_m \mid \mathbf{x}) = P^*(e \mid \mathbf{x})$.

With a little thought we see that $\sum_{i=1}^{c} P^2(\omega_i \mid \mathbf{x})$ is minimized if all of the a posteriori probabilities except the mth are equal, and the second constraint yields

$$P(\omega_i \mid \mathbf{x}) = \begin{cases} \dfrac{P^*(e \mid \mathbf{x})}{c-1} & i \neq m \\ 1 - P^*(e \mid \mathbf{x}) & i = m. \end{cases} \tag{35}$$

Thus

$$\sum_{i=1}^{c} P^2(\omega_i \mid \mathbf{x}) \geq (1 - P^*(e \mid \mathbf{x}))^2 + \frac{P^{*2}(e \mid \mathbf{x})}{c-1}$$

and

$$1 - \sum_{i=1}^{c} P^2(\omega_i \mid \mathbf{x}) \leq 2P^*(e \mid \mathbf{x}) - \frac{c}{c-1} P^{*2}(e \mid \mathbf{x}). \tag{36}$$

This immediately shows that $P \leq 2P^*$, since we can substitute this result in Eq. (33) and merely drop the second term. However, a tighter bound can be obtained by observing that

$$\begin{aligned} \mathrm{Var}[P^*(e \mid \mathbf{x})] &= \int [P^*(e \mid \mathbf{x}) - P^*]^2 p(\mathbf{x})\, d\mathbf{x} \\ &= \int P^{*2}(e \mid \mathbf{x}) p(\mathbf{x})\, d\mathbf{x} - P^{*2} \geq 0, \end{aligned}$$

so that

$$\int P^{*2}(e \mid \mathbf{x}) p(\mathbf{x})\, d\mathbf{x} \geq P^{*2},$$

with equality holding if and only if the variance of $P^*(e \mid \mathbf{x})$ is zero. Using this result and substituting Eq. (36) in Eq. (33), we obtain the desired bounds

$$P^* \leq P \leq P^*\left(2 - \frac{c}{c-1} P^*\right). \tag{28}$$

It is easy to show that this upper bound is achieved in the so-called zero-information case in which the densities $p(\mathbf{x} \mid \omega_i)$ are identical, so that $P(\omega_i \mid \mathbf{x}) = P(\omega_i)$ and $P^*(e \mid \mathbf{x})$ is independent of $\mathbf{x}$. Thus the bounds given by Eq. (28) are as tight as possible, in the sense that for any P^* there exist conditional and a priori probabilities for which they are achieved. Figure 4.4 illustrates the nature of the bounds graphically. The Bayes rate P^* can be

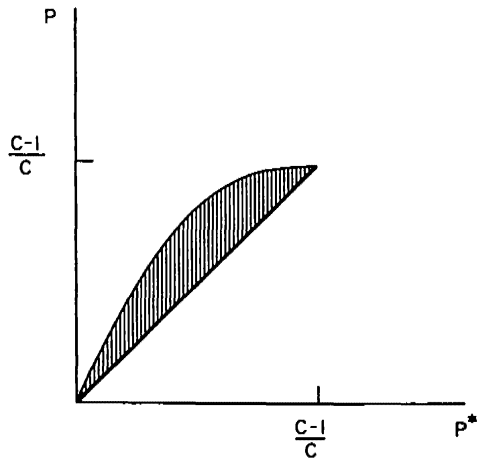

FIGURE 4.4. Bounds on the nearest-neighbor error rate.

anywhere between 0 and $(c - 1)/c$. The bounds meet at these two extreme points. When the Bayes rate is small, the upper bound is approximately twice the Bayes rate. In general, the nearest-neighbor error rate must fall in the shaded area shown.

Since P is always less than or equal to $2P^*$, if one had an infinite collection of data and used an arbitrarily complicated decision rule, one could at most cut the error rate in half. In this sense, at least half of the classification information in an infinite data set resides in the nearest neighbor.

It is natural to ask how well the nearest-neighbor rule works in the finite-sample case, and how rapidly the performance converges to the asymptotic value. Unfortunately, the only statements that can be made in the general case are negative. It can be shown that convergence can be arbitrarily slow, and the error rate $P_n(e)$ need not even decrease monotonically with n. As with other nonparametric methods, it is difficult to obtain anything other than asymptotic results without making further assumptions about the underlying probability structure.

4.7 THE k-NEAREST-NEIGHBOR RULE

An obvious extension of the nearest-neighbor rule is the *k-nearest-neighbor rule*. As one would expect from the name, this rule classifies $\mathbf{x}$ by assigning it the label most frequently represented among the k nearest samples; in other words, a decision is made by examining the labels on the k nearest neighbors and taking a vote. We shall not go into a thorough analysis of the k-nearest-neighbor rule. However, by considering the two-class case with k

odd (to avoid ties), we can gain some additional insight into these procedures.

The basic motivation for considering the k-nearest-neighbor rule rests on our earlier observation about matching probabilities with nature. We notice first that if k is fixed and the number n of samples is allowed to approach infinity, then all of the k nearest neighbors will converge to $\mathbf{x}$. Hence, as in the single-nearest-neighbor case, the labels on each of the k-nearest-neighbors are random variables, independently assuming the value ω_i with probability $P(\omega_i \mid \mathbf{x})$, $i = 1, 2$. If $P(\omega_m \mid \mathbf{x})$ is the larger a posteriori probability, then the Bayes decision rule always selects ω_m. The single-nearest-neighbor rule selects ω_m with probability $P(\omega_m \mid \mathbf{x})$. The k-nearest-neighbor rule selects ω_m if a majority of the k nearest neighbors are labeled ω_m, an event of probability

$$\sum_{i=(k+1)/2}^{k} \binom{k}{i} P(\omega_m \mid \mathbf{x})^i [1 - P(\omega_m \mid \mathbf{x})]^{k-i}.$$

In general, the larger the value of k, the greater the probability that ω_m will be selected.

We could analyze the k-nearest-neighbor rule in much the same way that we analyzed the single-nearest-neighbor rule. However, since the arguments become more involved and supply little additional insight, we shall content ourselves with stating the results. It can be shown that if k is odd, the large-sample two-class error rate for the k-nearest-neighbor rule is bounded above by the function $C_k(P^*)$, where C_k is defined to be the smallest concave function of P^* greater than

$$\sum_{i=0}^{(k-1)/2} \binom{k}{i} [(P^*)^{i+1}(1 - P^*)^{k-i} + (P^*)^{k-i}(1 - P^*)^{i+1}].$$

Now it is perfectly clear that very little insight can be gained by staring at the above function, except perhaps to note the family resemblance to the binomial distribution. Fortunately, it is easy to compute $C_k(P^*)$ and inspect the results. Figure 4.5 shows the bounds on the k-nearest-neighbor error rates for several values of k. The case $k = 1$ corresponds to the two-class instance of Figure 4.4. As k increases, the upper bounds get progressively closer to the lower bound, the Bayes rate. In the limit as k goes to infinity, the two bounds meet and the k-nearest-neighbor rule becomes optimal.

At the risk of sounding repetitive, we conclude by commenting once again on the finite-sample situation encountered in practice. The k-nearest-neighbor rule can be viewed as another attempt to estimate the a posteriori probabilities $P(\omega_i \mid \mathbf{x})$ from samples. We want to use a large value of k to obtain a reliable estimate. On the other hand, we want all of the k nearest neighbors $\mathbf{x}'$ to be very near $\mathbf{x}$ to be sure that $P(\omega_i \mid \mathbf{x}')$ is approximately the same as $P(\omega_i \mid \mathbf{x})$. This forces us to choose a compromise k that is a small

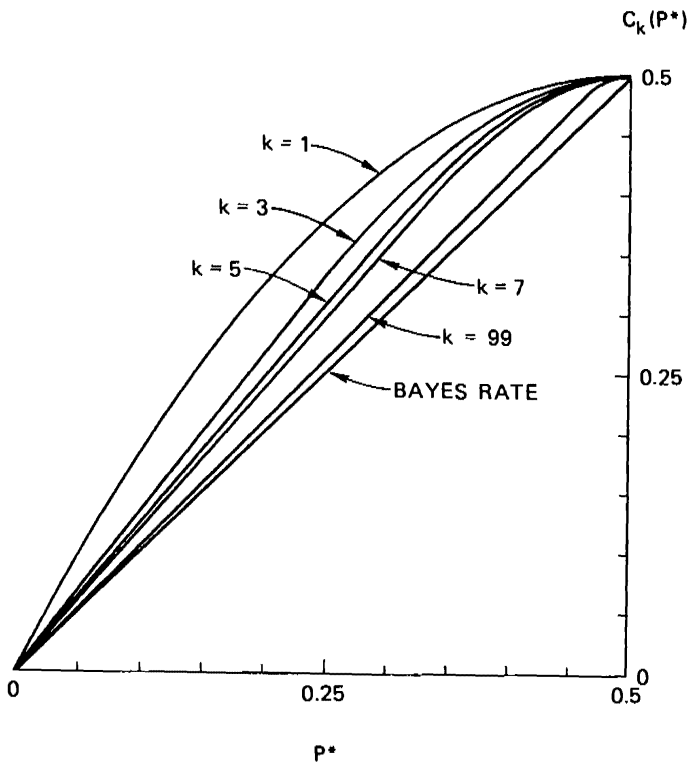

FIGURE 4.5. Bounds on the error-rate for the *k*-nearest-neighbor rule.

fraction of the number of samples. It is only in the limit as n goes to infinity that we can be assured of the nearly optimal behavior of the k-nearest-neighbor rule.

4.8 APPROXIMATIONS BY SERIES EXPANSIONS

All of the nonparametric methods described thus far suffer from the requirement that all of the samples must be stored. Since a large number of samples is needed to obtain good estimates, the memory requirements can be severe. In addition, considerable computation time may be required each time one of the methods is used to estimate $p(\mathbf{x})$ or classify a new $\mathbf{x}$. In certain circumstances the Parzen-window procedure can be modified to reduce these problems considerably. The basic idea is to approximate the window function by a finite series expansion that is acceptably accurate in the region of interest. If we are fortunate and can find two sets of functions $\psi_j(\mathbf{x})$ and $\chi_j(\mathbf{x})$ that

allow the expansion

$$\varphi\left(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\right) = \sum_{j=1}^{m} a_j \psi_j(\mathbf{x}) \chi_j(\mathbf{x}_i), \tag{37}$$

then

$$\sum_{i=1}^{n} \varphi\left(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\right) = \sum_{j=1}^{m} a_j \psi_j(\mathbf{x}) \sum_{i=1}^{n} \chi_j(\mathbf{x}_i)$$

and, from Eq. (8),

$$p_n(\mathbf{x}) = \sum_{j=1}^{m} b_j \psi_j(\mathbf{x}), \tag{38}$$

where

$$b_j = \frac{a_j}{nV_n} \sum_{i=1}^{n} \chi_j(\mathbf{x}_i). \tag{39}$$

If a sufficiently accurate expansion can be obtained with a reasonable value for m, this approach has some obvious advantages. The information in the n samples is reduced to the m coefficients b_j. If additional samples are obtained, Eq. (39) for b_j can be updated easily, and the number of coefficients remains unchanged.* If the functions ψ_j and χ_j are polynomial functions of the components of $\mathbf{x}$ and $\mathbf{x}_i$, the expression for the estimate $p_n(\mathbf{x})$ is also a polynomial, which can be computed relatively efficiently. Furthermore, use of this estimate to obtain discriminant functions $p(\mathbf{x} \mid \omega_i)P(\omega_i)$ leads to a simple way of obtaining *polynomial discriminant functions*.

Before becoming too enthusiastic, however, we should note one of the problems with this approach. A key property of a useful window function is its tendency to peak at the origin and fade away elsewhere. Thus $\varphi((\mathbf{x} - \mathbf{x}_i)/h_n)$ should peak sharply at $\mathbf{x} = \mathbf{x}_i$, and contribute little to the approximation of $p_n(\mathbf{x})$ for $\mathbf{x}$ far from $\mathbf{x}_i$. Unfortunately, polynomials have the annoying property of becoming unbounded. Thus, a polynomial expansion might find the terms associated with an $\mathbf{x}_i$ far from $\mathbf{x}$ contributing most rather than least to the expansion. Hence, it is quite important to be sure that the expansion of each window function is in fact accurate in the region of interest, and this may well require a large number of terms.

There are many types of series expansions one might consider. Readers familiar with integral equations will naturally interpret Eq. (37) as an expansion of the kernel $\varphi(\mathbf{x}, \mathbf{x}_i)$ in a series of eigenfunctions. Rather than computing eigenfunctions, one might choose any reasonable set of functions orthogonal over the region of interest and obtain a least-squares fit to the window function. We shall take an even more straightforward approach and

* It should be pointed out, however, that if h_n is reduced when new samples are added, φ will more nearly approach an impulse, and more terms may in fact be required for an accurate approximation.

expand the window function in a Taylor's series. For simplicity, we confine our attention to a one-dimensional example using a gaussian window function:

$$\sqrt{\pi}\,\varphi(u) = e^{-u^2} \approx \sum_{j=0}^{m-1} (-1)^j \frac{u^{2j}}{j!}.$$

This expansion is most accurate near $u = 0$, and is in error by less than $u^{2m}/m!$. If we substitute

$$u = \frac{x - x_i}{h}$$

we obtain a polynomial of degree $2(m-1)$ in x and x_i. For example, if $m = 2$

$$\sqrt{\pi}\,\varphi\left(\frac{x - x_i}{h}\right) \approx 1 - \left(\frac{x - x_i}{h}\right)^2 \approx 1 + \frac{2}{h^2} x x_i - \frac{1}{h^2} x^2 - \frac{1}{h^2} x_i^2$$

and thus

$$\sqrt{\pi}\,p_n(x) = \frac{1}{nh} \sum_{i=1}^{n} \sqrt{\pi}\,\varphi\left(\frac{x - x_i}{h}\right) \approx b_0 + b_1 x + b_2 x^2$$

where

$$b_0 = \frac{1}{h} - \frac{1}{h^3} \frac{1}{n} \sum_{i=1}^{n} x_i^2$$

$$b_1 = \frac{2}{h^3} \frac{1}{n} \sum_{i=1}^{n} x_i$$

$$b_2 = -\frac{1}{h^3}.$$

This simple expansion condenses the information in n samples into 3 coefficients, b_0, b_1, and b_2. It is accurate if the largest value of $|x - x_i|$ is not greater than h. Unfortunately, this restricts us to a very wide window that is not capable of much resolution. By taking more terms we can use a narrower window. If we let r be the largest value of $|x - x_i|$, use the fact that the error in the m-term expansion of $\sqrt{\pi}\,\varphi[(x - x_i)/h]$ is less than $(r/h)^{2m} m!$, and use Stirling's approximation for $m!$, we find that the error in approximating $p_n(x)$ is less than

$$\frac{1}{\sqrt{\pi}\,h} \frac{\left(\frac{r}{h}\right)^{2m}}{m!} \approx \frac{1}{\sqrt{\pi}\,h\sqrt{2\pi m}} \left[\left(\frac{e}{m}\right)\left(\frac{r}{h}\right)^2\right]^m.$$

Thus, the error becomes small only when $m > e(r/h)^2$. This implies the need for many terms if the window size h is small relative to the distance r from x to the most distant sample. Although this example is rudimentary, similar considerations arise in the multidimensional case even when more sophisticated expansions are used, and the procedure is most attractive when the window size is relatively large.

4.9 APPROXIMATIONS FOR THE BINARY CASE

4.9.1 The Rademacher-Walsh Expansion

When the components of the vector $\mathbf{x}$ are discrete, the problem of estimating a density becomes the problem of estimating the probability $P(\mathbf{x} = \mathbf{v}_k)$. Conceptually, the problem is even simpler—one need only count the number of times that $\mathbf{x}$ is observed to have the value $\mathbf{v}_k$ and rely on the law of large numbers. However, consider the case in which the d components of $\mathbf{x}$ are binary valued (0 or 1). Since there are 2^d possible vectors $\mathbf{v}_k$, we must estimate 2^d probabilities, which is an enormous task for the large values of d frequently encountered in pattern recognition work.

If the components of $\mathbf{x}$ are statistically independent, the problem is greatly simplified. In this case we can write

$$P(\mathbf{x}) = \prod_{i=1}^{d} P(x_i) = \prod_{i=1}^{d} p_i^{x_i}(1 - p_i)^{1-x_i} \tag{40}$$

where

$$p_i = P(x_i = 1) \tag{41}$$

and

$$1 - p_i = P(x_i = 0). \tag{42}$$

Thus, in this special case the estimation of $P(\mathbf{x})$ reduces to the estimation of d probabilities p_i. Moreover, if we consider the logarithm of $P(\mathbf{x})$ we see that it is a linear function of $\mathbf{x}$, which simplifies both its storage and its computation:

$$\log P(\mathbf{x}) = \sum_{i=1}^{d} w_i x_i + w_0 \tag{43}$$

where

$$w_i = \begin{cases} \log \dfrac{p_i}{1 - p_i} & i = 1, \ldots, d \\ \displaystyle\sum_{i=1}^{d} \log(1 - p_i) & i = 0. \end{cases} \tag{44}$$

It is natural to ask whether or not there are any compromise positions between being completely accurate, which requires estimating 2^d probabilities,

and being forced to assume statistical independence, which reduces the problem to one of estimating only d probabilities. One answer is provided by finding an expansion for $P(\mathbf{x})$ and approximating $P(\mathbf{x})$ by a partial sum. When binary variables are involved, it is natural to use the *Rademacher-Walsh polynomials* as basis functions. This set of 2^d polynomials can be obtained by systematically forming products of the distinct factors $2x_i - 1$ taken none at a time, one at a time, two at a time, etc. Thus

$$\varphi_i(\mathbf{x}) = \begin{cases} 1 & i = 0 \\ 2x_1 - 1 & i = 1 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ 2x_d - 1 & i = d \\ (2x_1 - 1)(2x_2 - 1) & i = d + 1 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ (2x_{d-1} - 1)(2x_d - 1) & i = d + 1 + d(d-1)/2 \\ (2x_1 - 1)(2x_2 - 1)(2x_3 - 1) & i = d + 2 + d(d-1)/2 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ (2x_1 - 1) \cdots (2x_d - 1) & i = 2^d - 1. \end{cases} \tag{45}$$

It is not hard to see that these polynomials satisfy the orthogonality relation

$$\sum_{\mathbf{x}} \varphi_i(\mathbf{x})\varphi_j(\mathbf{x}) = \begin{cases} 2^d & i = j \\ 0 & i \neq j, \end{cases} \tag{46}$$

where the summation extends over the 2^d possible values of $\mathbf{x}$. Thus, any function $P(\mathbf{x})$ defined on the unit d-cube can be expanded as

$$P(\mathbf{x}) = \sum_{i=0}^{2^d-1} a_i \varphi_i(\mathbf{x}), \tag{47}$$

where

$$a_i = \frac{1}{2^d} \sum_{\mathbf{x}} \varphi_i(\mathbf{x}) P(\mathbf{x}). \tag{48}$$

Viewing $P(\mathbf{x})$ as a probability function, we see that

$$a_i = \frac{1}{2^d} E[\varphi_i(\mathbf{x})]. \tag{49}$$

Since the Rademacher-Walsh functions $\varphi_i(\mathbf{x})$ are polynomials, we see that the coefficients a_i are essentially moments. Thus, if $P(\mathbf{x})$ is unknown, but if n

samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$ are available, the coefficients a_i can be estimated by computing sample moments $\hat{a}_i$:

$$\hat{a}_i = \frac{1}{n} \sum_{j=1}^{n} \frac{1}{2^d} \varphi_i(\mathbf{x}_j). \tag{50}$$

In the limit as n goes to infinity, the law of large numbers assures us that this estimate will converge (in probability) to the true value for a_i.

Now Eq. (47) gives us an exact expansion of $P(\mathbf{x})$, and, as such, it does not reduce our computational problem. Instead of estimating 2^d joint probabilities, we must estimate 2^d moments, the coefficients a_i. However, we can approximate $P(\mathbf{x})$ by truncating the expansion and computing just the lower order moments. A first-order approximation obtained by taking the first $1 + d$ terms is linear in $\mathbf{x}$. A second-order approximation containing the first $1 + d + d(d-1)/2$ terms is quadratic in $\mathbf{x}$.* In general, Eq. (47) shows that an approximation involving kth degree Rademacher-Walsh polynomials requires the evaluation of moments of order k and lower. These moments can be estimated from data or computed directly from $P(\mathbf{x})$. In this latter case, the fact that one can sum first over variables not involved in the polynomial shows that one need only know marginal probabilities of order k. For example, a first-order expansion is determined by the probabilities $p_i = P(x_i = 1)$:

$$P_1(\mathbf{x}) = a_0 + \sum_{i=1}^{d} a_i(2x_i - 1)$$

where

$$a_i = \begin{cases} 2^{-d} & i = 0 \\ 2^{-d}(2p_i - 1) & i = 1, \ldots, d. \end{cases}$$

It is natural to ask how well such a truncated expansion approximates the actual probability $P(\mathbf{x})$. In general, if we approximate $P(\mathbf{x})$ by a series involving a subset of the Rademacher-Walsh polynomials, such as

$$\tilde{P}(\mathbf{x}) = \sum_{i \in I} b_i \varphi_i(\mathbf{x}),$$

then the orthogonality relations can be used to show that the sum of squared error $\sum (P(\mathbf{x}) - \tilde{P}(\mathbf{x}))^2$ is minimized by the choice $b_i = a_i$. Thus, a truncated expansion is optimal in this mean-squared sense. Furthermore, as long as the constant polynomial φ_0 is included in the approximation, it is easy to show that $\sum \tilde{P}(\mathbf{x}) = 1$, as desired. However, nothing prevents $\tilde{P}(\mathbf{x})$ from becoming negative for some $\mathbf{x}$. Indeed, if φ_0 is not included, $\sum \tilde{P}(\mathbf{x}) = 0$, and

* Because the components of $\mathbf{x}$ are binary, products such as $x_i x_j$ are especially easy to compute and can be implemented in hardware by AND gates.

at least one of the probabilities must be negative. This annoying result can be avoided by expanding $\log P(\mathbf{x})$ rather than $P(\mathbf{x})$, although then we are no longer assured that the resulting approximation for $P(\mathbf{x})$ will sum to one.

4.9.2 The Bahadur-Lazarsfeld Expansion

An interesting alternative expansion is obtained by introducing the normalized variables

$$y_i = \frac{x_i - p_i}{\sqrt{p_i(1 - p_i)}}, \tag{51}$$

assuming of course that p_i is neither zero nor one. These normalized variables have zero mean and unit variance. A set of polynomials much like the Rademacher-Walsh polynomials can be obtained by systematically forming distinct products of the y_i taken none at a time, one at a time, two at a time, etc. Thus

$$\psi_i(\mathbf{x}) = \begin{cases} 1 & i = 0 \\ y_1 & i = 1 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ y_d & i = d \\ y_1 y_2 & i = d + 1 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ y_{d-1} y_d & i = d + 1 + d(d-1)/2 \\ y_1 y_2 y_3 & i = d + 2 + d(d-1)/2 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ y_1 y_2 \cdots y_d & i = 2^d - 1 \end{cases} \tag{52}$$

These polynomials are not orthogonal in themselves, but they are orthogonal with respect to the weighting function

$$P_1(\mathbf{x}) = \prod_{i=1}^{d} p_i^{x_i}(1 - p_i)^{1-x_i}. \tag{53}$$

That is,

$$\sum_{\mathbf{x}} \psi_i(\mathbf{x})\psi_j(\mathbf{x})P_1(\mathbf{x}) = \begin{cases} 1 & i = j \\ 0 & i \neq j. \end{cases} \tag{54}$$

This should be clear from the observation that $P_1(\mathbf{x})$ is the distribution for the independent case, and that in this case the moments $E[\psi_i(\mathbf{x})\psi_j(\mathbf{x})]$ are

either zero or one. It follows that any function defined on the unit d-cube can be expanded as

$$F(\mathbf{x}) = \sum_{i=0}^{2^d-1} a_i \psi_i(\mathbf{x}),$$

where

$$a_i = \sum_{\mathbf{x}} \psi_i(\mathbf{x}) P_1(\mathbf{x}) F(\mathbf{x}).$$

In particular, the function $P(\mathbf{x})/P_1(\mathbf{x})$ has the expansion

$$P(\mathbf{x}) = P_1(\mathbf{x}) \sum_{i=0}^{2^d-1} a_i \psi_i(\mathbf{x}) \tag{55}$$

where

$$a_i = \sum_{\mathbf{x}} \psi_i(\mathbf{x}) P(\mathbf{x}) = E[\psi_i(\mathbf{x})]. \tag{56}$$

Recalling that $\psi_i(\mathbf{x})$ is a product of the normalized variables $y_i = (x_i - p_i)/\sqrt{p_i(1-p_i)}$, we see that the a_i are correlation coefficients. Clearly, $a_0 = 1$ and $a_1 = \cdots = a_d = 0$. If we define

$$\left.\begin{aligned} \rho_{ij} &= \sum_{\mathbf{x}} y_i y_j P(\mathbf{x}) \\ \rho_{ijk} &= \sum_{\mathbf{x}} y_i y_j y_k P(\mathbf{x}) \\ &\vdots \\ \rho_{12\ldots d} &= \sum_{\mathbf{x}} y_1 y_2 \cdots y_d P(\mathbf{x}), \end{aligned}\right\} \tag{57}$$

then we can write the expansion of Eq. (55) as

$$P(\mathbf{x}) = P_1(\mathbf{x})\left[1 + \sum_{i<j} \rho_{ij} y_i y_j + \sum_{i<j<k} \rho_{ijk} y_i y_j y_k + \cdots + \rho_{12\cdots d} y_1 y_2 \cdots y_d\right]. \tag{58}$$

This is known as the *Badahur-Lazarsfeld expansion* of $P(\mathbf{x})$. It contains $2^d - 1$ coefficients, the d first order probabilities p_i, the $\binom{d}{2}$ second-order correlation coefficients ρ_{ij}, the $\binom{d}{3}$ third-order correlation coefficients ρ_{ijk}, and so on. A natural way to approximate $P(\mathbf{x})$ is to ignore all correlations above a certain order. Thus,

$$P_1(\mathbf{x}) = \prod_{i=1}^{d} p_i^{x_i}(1 - p_i)^{1-x_i}$$

is a first-order approximation to $P(\mathbf{x})$,

$$P_2(\mathbf{x}) = P_1(\mathbf{x})\left[1 + \sum_{i<j} \rho_{ij} y_i y_j\right]$$

is a second-order approximation, and so on. If the higher-order correlation coefficients are small and we use the approximation $\log(1 + x) \approx x$, we see that $\log P_1(\mathbf{x})$ is linear in x, $\log P_2(\mathbf{x})$ adds a quadratic correction term, and so on. Thus the logarithm of the Bahadur-Lazarsfeld expansion provides an interesting sequence of approximations. The first is equivalent to assuming independence, and is linear in $\mathbf{x}$. The second accounts for second-order correlations, and is approximately quadratic in $\mathbf{x}$. Each successive approximation accounts for correlations of one higher order, but of course requires the computation of more terms.

4.9.3 The Chow Expansion

Another interesting class of approximations to a joint probability distribution $P(\mathbf{x})$ is based on the identity

$$P(\mathbf{x}) = P(x_1, \ldots, x_d) = P(x_1)P(x_2 \mid x_1)P(x_3 \mid x_2, x_1) \cdots P(x_d \mid x_{d-1}, \ldots, x_1). \tag{59}$$

If the variables are statistically independent, this reduces to the product of the individual probabilities $P(x_i)$. Suppose that the variables are not independent, but that $P(x_i \mid x_{i-1}, \ldots, x_1)$ depends only on the immediately preceding variable x_{i-1}. Then we have a first-order Markov chain, and

$$P(\mathbf{x}) = P(x_1)P(x_2 \mid x_1)P(x_3 \mid x_2) \cdots P(x_d \mid x_{d-1}). \tag{60}$$

We shall see that each factor $P(x_i \mid x_{i-1})$ can be determined by two coefficients; thus, $P(\mathbf{x})$ can be determined by $2d - 1$ coefficients, which is less of an increase in complexity than if we had allowed for all $\binom{d}{2}$ second-order correlations. Similar higher-order Markov approximations can be obtained if we assume that x_i depends only on the k immediately preceding variables.

While an assumption that a given variable x_i depends only upon certain preceding variables is reasonable if we are dealing with a temporal process, it is a rather strange assumption in more general circumstances. However, it is reasonable to expect that a given variable x_i may be primarily dependent upon only a few other variables. Suppose that we can number the variables so that $P(x_i \mid x_{i-1}, \ldots, x_1)$ is solely dependent on some preceding variable, $x_{j(i)}$. For example, suppose that

$$P(x_4 \mid x_3, x_2, x_1) = P(x_4 \mid x_2) \qquad \text{and} \qquad P(x_3 \mid x_2, x_1) = P(x_3 \mid x_1).$$

Then it follows from Eq. (59) that $P(x_1, x_2, x_3, x_4)$ can be written as $P(x_1)P(x_2 \mid x_1)P(x_3 \mid x_1)P(x_4 \mid x_2)$. In general, we obtain the product expansion

$$P(\mathbf{x}) = P(x_1)P(x_2 \mid x_{j(2)}) \cdots P(x_d \mid x_{j(d)}). \tag{61}$$

By substituting 0 or 1 for x_i and $x_{j(i)}$, the reader can verify that

$$P(x_i \mid x_{j(i)}) = [p_i^{x_i}(1 - p_i)^{1-x_i}]^{x_{j(i)}}[q_i^{x_i}(1 - q_i)^{1-x_i}]^{1-x_{j(i)}} \tag{62}$$

where

$$p_i = P(x_i = 1 \mid x_{j(i)} = 1) \tag{63}$$

and

$$q_i = P(x_i = 1 \mid x_{j(i)} = 0). \tag{64}$$

By letting $q_1 = P(x_1 = 1)$, substituting Eq. (62) in Eq. (61), taking the logarithm, and collecting terms, we obtain the *Chow expansion:*

$$\log P(x) = \sum_{i=1}^{d} \log(1 - q_i) + \sum_{i=1}^{d} x_i \log \frac{q_i}{1 - q_i} + \sum_{i=2}^{d} x_{j(i)} \log \frac{1 - p_i}{1 - q_i} + \sum_{i=2}^{d} x_i x_{j(i)} \log \frac{p_i(1 - q_i)}{(1 - p_i)q_i}. \tag{65}$$

Similar results for higher-order dependence can be obtained in an obvious way.

A few observations about these results are in order. First, we note that if the variables are indeed independent, $p_i = q_i$ and the last two sums in the expansion disappear, leaving the familiar expansion for the independent case. When dependence exists, we obtain additional linear and quadratic terms. Of course, the linear terms can be combined, so that the expansion effectively contains a constant, d linear terms, and $d - 1$ quadratic terms.

Comparing this with the second-order Rademacher-Walsh or Bahadur-Lazarsfeld expansions, either of which requires $d(d - 1)/2$ quadratic terms, we see that the savings can be appreciable. Of course, the savings can only be realized if we know the *dependence tree*, the function $j(i)$ which exhibits the limited dependence of one variable on preceding variables. If the dependence tree cannot be inferred from the physical significance of the variables, it may be necessary to compute all of the correlation coefficients merely to find the significant ones. However, even in this case it should be pointed out that one might prefer to use the Chow expansion because the resulting approximate probabilities are always nonnegative and sum to one.

4.10 FISHER'S LINEAR DISCRIMINANT

One of the recurring problems encountered in applying statistical techniques to pattern recognition problems is what Bellman calls the curse of dimensionality. Procedures that are analytically or computationally manageable in low-dimensional spaces can become completely impractical in a space of 50 or 100 dimensions. Thus, various techniques have been developed for

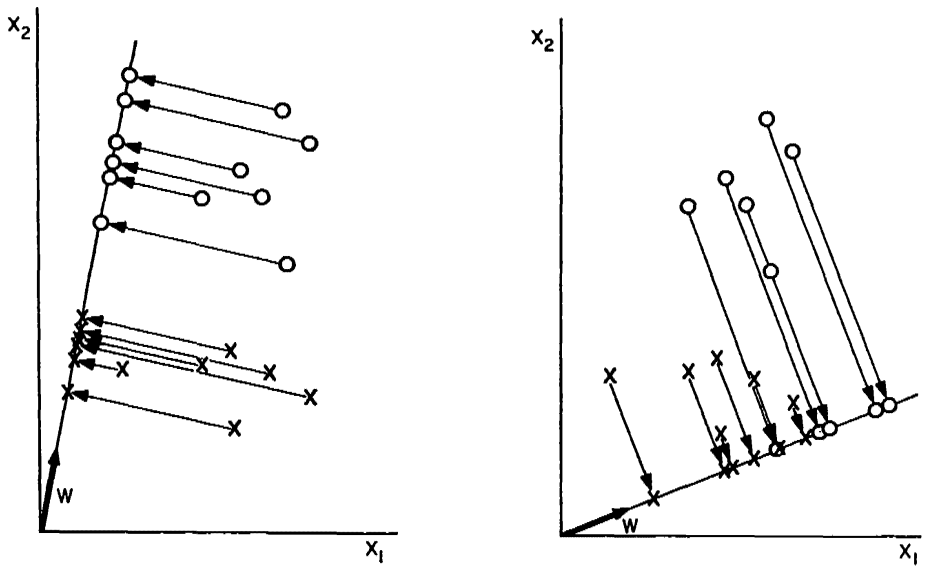

FIGURE 4.6. Projection of samples onto a line.

reducing the dimensionality of the feature space in the hope of obtaining a more manageable problem.

We can reduce the dimensionality from d dimensions to one dimension if we merely project the d-dimensional data onto a line. Of course, even if the samples formed well-separated, compact clusters in d-space, projection on an arbitrary line will usually produce a confused mixture of samples from all of the classes. However, by moving the line around, we might be able to find an orientation for which the projected samples are well separated. This is exactly the goal of classical discriminant analysis.

Suppose that we have a set of n d-dimensional samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$, n_1 in the subset $\mathscr{X}_1$ labelled ω_1 and n_2 in the subset $\mathscr{X}_2$ labelled ω_2. If we form a linear combination of the components of $\mathbf{x}$, we obtain the scalar

$$y = \mathbf{w}^t\mathbf{x} \tag{66}$$

and a corresponding set of n samples $y_1, \ldots, y_n$ divided into the subsets $\mathscr{Y}_1$ and $\mathscr{Y}_2$. Geometrically, if $\|\mathbf{w}\| = 1$, each y_i is the projection of the corresponding $\mathbf{x}_i$ onto a line in the direction of $\mathbf{w}$. Actually, the magnitude of $\mathbf{w}$ is of no real significance, since it merely scales y. The direction of $\mathbf{w}$ is important, however. If we imagine that the samples labelled ω_1 fall more or less in one cluster while those labelled ω_2 fall in another, we want the projections falling on the line to be well separated, not thoroughly intermingled. Figure 4.6 illustrates the effect of choosing two different values for $\mathbf{w}$ for a two-dimensional example.

A measure of the separation between the projected points is the difference of the sample means. If $\mathbf{m}_i$ is the d-dimensional sample mean given by

$$\mathbf{m}_i = \frac{1}{n_i} \sum_{\mathbf{x} \in \mathcal{X}_i} \mathbf{x}, \tag{67}$$

then the sample mean for the projected points is given by

$$\begin{aligned} \tilde{m}_i &= \frac{1}{n_i} \sum_{y \in \mathcal{Y}_i} y \\ &= \frac{1}{n_i} \sum_{\mathbf{x} \in \mathcal{X}_i} \mathbf{w}^t \mathbf{x} = \mathbf{w}^t \mathbf{m}_i. \end{aligned} \tag{68}$$

It follows that $|\tilde{m}_1 - \tilde{m}_2| = |\mathbf{w}^t(\mathbf{m}_1 - \mathbf{m}_2)|$, and that we can make this difference as large as we wish merely by scaling $\mathbf{w}$. Of course, to obtain good separation of the projected data we really want the difference between the means to be large relative to some measure of the standard deviations for each class. Rather than forming sample variances, we define the *scatter* for projected samples labelled ω_i by

$$\tilde{s}_i^2 = \sum_{y \in \mathcal{Y}_i} (y - \tilde{m}_i)^2. \tag{69}$$

Thus, $(1/n)(\tilde{s}_1^2 + \tilde{s}_2^2)$ is an estimate of the variance of the pooled data, and $\tilde{s}_1^2 + \tilde{s}_2^2$ is called the total *within-class scatter* of the projected samples. The *Fisher linear discriminant* is then defined as that linear function* $\mathbf{w}^t\mathbf{x}$ for which the *criterion function*

$$J(\mathbf{w}) = \frac{|\tilde{m}_1 - \tilde{m}_2|^2}{\tilde{s}_1^2 + \tilde{s}_2^2} \tag{70}$$

is maximum.

To obtain J as an explicit function of $\mathbf{w}$, we define the *scatter matrices* S_i and S_W by

$$S_i = \sum_{\mathbf{x} \in \mathcal{X}_i} (\mathbf{x} - \mathbf{m}_i)(\mathbf{x} - \mathbf{m}_i)^t \tag{71}$$

and

$$S_W = S_1 + S_2. \tag{72}$$

Then

$$\begin{aligned} \tilde{s}_i^2 &= \sum_{\mathbf{x} \in \mathcal{X}_i} (\mathbf{w}^t\mathbf{x} - \mathbf{w}^t\mathbf{m}_i)^2 \\ &= \sum_{\mathbf{x} \in \mathcal{X}_i} \mathbf{w}^t(\mathbf{x} - \mathbf{m}_i)(\mathbf{x} - \mathbf{m}_i)^t\mathbf{w} \\ &= \mathbf{w}^t S_i \mathbf{w}, \end{aligned} \tag{73}$$

* It should be noted that we are now using the term "discriminant function" to mean any function of $\mathbf{x}$ that is helpful in solving the decision problem; we do not insist that the resulting discriminant function be used directly to define the classifier. Because $y = \mathbf{w}^t\mathbf{x}$ is a sum of random variables, it is common to make reference to the central limit theorem and to assume that $p(y \mid \omega_i)$ is a normal density, thereby simplifying the problem of obtaining a classifier. When this assumption is not justified, one can still afford to use fairly elaborate methods to estimate $p(y \mid \omega_i)$ and derive an "optimal" classifier.

so that

$$\tilde{s}_1^2 + \tilde{s}_2^2 = \mathbf{w}^t S_W \mathbf{w}. \tag{74}$$

Similarly,

$$\begin{aligned}(\tilde{m}_1 - \tilde{m}_2)^2 &= (\mathbf{w}^t\mathbf{m}_1 - \mathbf{w}^t\mathbf{m}_2)^2 \\ &= \mathbf{w}^t(\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^t\mathbf{w} \\ &= \mathbf{w}^t S_B \mathbf{w}, \end{aligned} \tag{75}$$

where

$$S_B = (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^t. \tag{76}$$

The matrix S_W is called the *within-class scatter matrix*. It is proportional to the sample covariance matrix for the pooled d-dimensional data. It is symmetric and positive semidefinite, and is usually nonsingular if $n > d$. S_B is called the *between-class scatter matrix*. It is also symmetric and positive semidefinite, but because it is the outer product of two vectors, its rank is at most one. In particular, for any $\mathbf{w}$, $S_B\mathbf{w}$ is in the direction of $\mathbf{m}_1 - \mathbf{m}_2$, and S_B is quite singular.

In terms of S_B and S_W, the criterion function J can be written as

$$J(\mathbf{w}) = \frac{\mathbf{w}^t S_B \mathbf{w}}{\mathbf{w}^t S_W \mathbf{w}}. \tag{77}$$

This expression is well known in mathematical physics as the generalized Rayleigh quotient. It is easy to show that a vector $\mathbf{w}$ that maximizes J must satisfy

$$S_B\mathbf{w} = \lambda S_W \mathbf{w} \tag{78}$$

which is a generalized eigenvalue problem. If S_W is nonsingular we can obtain a conventional eigenvalue problem by writing

$$S_W^{-1} S_B \mathbf{w} = \lambda \mathbf{w}. \tag{79}$$

In our particular case, it is unnecessary to solve for the eigenvalues and eigenvectors of $S_W^{-1}S_B$ due to the fact that $S_B\mathbf{w}$ is always in the direction of $\mathbf{m}_1 - \mathbf{m}_2$. Since the scale factor for $\mathbf{w}$ is immaterial, we can immediately write the solution

$$\mathbf{w} = S_W^{-1}(\mathbf{m}_1 - \mathbf{m}_2). \tag{80}$$

Thus, we have obtained Fisher's linear discriminant, the linear function with the maximum ratio of between-class scatter to within-class scatter. The problem has been converted from a d-dimensional problem to a hopefully more manageable one-dimensional problem. This mapping is many-to-one, and in theory can not possibly reduce the minimum achievable error rate. In

general, one is willing to sacrifice some of the theoretically attainable performance for the advantages of working in one dimension. When the conditional densities $p(\mathbf{x} \mid \omega_i)$ are multivariate normal with equal covariance matrices Σ, one need not even sacrifice any performance. In that case we recall that the optimal decision boundary has the equation

$$\mathbf{w}^t\mathbf{x} + w_0 = 0$$

where

$$\mathbf{w} = \Sigma^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2),$$

and where w_0 is a constant involving $\mathbf{w}$ and the prior probabilities. If we use sample means and the sample covariance matrix to estimate $\boldsymbol{\mu}_i$ and Σ, we obtain a vector in the same direction as the $\mathbf{w}$ of Eq. (80) that maximizes J. Thus, for the normal, equal-covariance case, the optimal decision rule is merely to decide ω_1 if Fisher's linear discriminant exceeds some threshold, and to decide ω_2 otherwise.

4.11 MULTIPLE DISCRIMINANT ANALYSIS

For the c-class problem, the natural generalization of Fisher's linear discriminant involves $c - 1$ discriminant functions. Thus, the projection is from a d-dimensional space to a $(c - 1)$-dimensional space, and it is tacitly assumed that $d \geq c$. The generalization for the within-class scatter matrix is obvious:

$$S_W = \sum_{i=1}^{c} S_i \tag{81}$$

where, as before,

$$S_i = \sum_{\mathbf{x} \in \mathcal{X}_i} (\mathbf{x} - \mathbf{m}_i)(\mathbf{x} - \mathbf{m}_i)^t \tag{82}$$

and

$$\mathbf{m}_i = \frac{1}{n_i} \sum_{\mathbf{x} \in \mathcal{X}_i} \mathbf{x}. \tag{83}$$

The proper generalization for S_B is not quite so obvious. Suppose that we define a *total mean vector* $\mathbf{m}$ and a *total scatter matrix* S_T by

$$\mathbf{m} = \frac{1}{n} \sum_{\mathbf{x}} \mathbf{x} = \frac{1}{n} \sum_{i=1}^{c} n_i \mathbf{m}_i \tag{84}$$

and

$$S_T = \sum_{\mathbf{x}} (\mathbf{x} - \mathbf{m})(\mathbf{x} - \mathbf{m})^t. \tag{85}$$

Then it follows that

$$S_T = \sum_{i=1}^{c} \sum_{\mathbf{x}\in\mathcal{X}_i} (\mathbf{x} - \mathbf{m}_i + \mathbf{m}_i - \mathbf{m})(\mathbf{x} - \mathbf{m}_i + \mathbf{m}_i - \mathbf{m})^t,$$

$$= \sum_{i=1}^{c} \sum_{\mathbf{x}\in\mathcal{X}_i} (\mathbf{x} - \mathbf{m}_i)(\mathbf{x} - \mathbf{m}_i)^t + \sum_{i=1}^{c} \sum_{\mathbf{x}\in\mathcal{X}_i} (\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^t$$

$$= S_W + \sum_{i=1}^{c} n_i(\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^t.$$

It is natural to define this second term as the between-class scatter matrix, so that the total scatter is the sum of the within-class scatter and the between-class scatter:

$$S_B = \sum_{i=1}^{c} n_i(\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^t \tag{86}$$

and

$$S_T = S_W + S_B. \tag{87}$$

If we check the two-class case, we find that the resulting between-class scatter matrix is n_1n_2/n times our previous definition. We could redefine S_B for the two-class case to obtain complete consistency, but we shall recall Emerson's remark that a foolish consistency is the hobgoblin of little minds and proceed.

The projection from a d-dimensional space to a $(c - 1)$-dimensional space is accomplished by $c - 1$ discriminant functions

$$y_i = \mathbf{w}_i^t\mathbf{x} \qquad i = 1, \ldots, c - 1. \tag{88}$$

If the y_i are viewed as components of a vector $\mathbf{y}$ and the weight vectors $\mathbf{w}_i$ are viewed as the columns of a d-by-$(c - 1)$ matrix W, then the projection can be written as a single matrix equation

$$\mathbf{y} = W^t\mathbf{x}. \tag{89}$$

The samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$ project to a corresponding set of samples $\mathbf{y}_1, \ldots, \mathbf{y}_n$ which can be described by their own mean vectors and scatter matrices. Thus, if we define

$$\tilde{\mathbf{m}}_i = \frac{1}{n_i} \sum_{\mathbf{y}\in\mathcal{Y}_i} \mathbf{y} \tag{90}$$

$$\tilde{\mathbf{m}} = \frac{1}{n} \sum_{i=1}^{c} n_i\tilde{\mathbf{m}}_i \tag{91}$$

$$\tilde{S}_W = \sum_{i=1}^{c} \sum_{\mathbf{y}\in\mathcal{Y}_i} (\mathbf{y} - \tilde{\mathbf{m}}_i)(\mathbf{y} - \tilde{\mathbf{m}}_i)^t \tag{92}$$

and

$$\tilde{S}_B = \sum_{i=1}^{c} n_i(\tilde{\mathbf{m}}_i - \tilde{\mathbf{m}})(\tilde{\mathbf{m}}_i - \tilde{\mathbf{m}})^t \tag{93}$$

it is a straightforward matter to show that

$$\tilde{S}_W = W^t S_W W \tag{94}$$

and

$$\tilde{S}_B = W^t S_B W. \tag{95}$$

These equations show how the within-class and between-class scatter matrices are transformed by the projection to the lower dimensional space. What we seek is a transformation matrix W that in some sense maximizes the ratio of the between-class scatter to the within-class scatter. A simple scalar measure of scatter is the determinant of the scatter matrix. The determinant is the product of the eigenvalues, and hence is the product of the "variances" in the principal directions, thereby measuring the square of the hyperellipsoidal scattering volume. Using this measure, we obtain the criterion function

$$J(W) = \frac{|\tilde{S}_B|}{|\tilde{S}_W|} = \frac{|W^t S_B W|}{|W^t S_W W|}. \tag{96}$$

The problem of finding a rectangular matrix W that maximizes J is not an easy one. Fortunately, it turns out that the solution is relatively simple.* The columns of an optimal W are the generalized eigenvectors that correspond to the largest eigenvalues in

$$S_B \mathbf{w}_i = \lambda_i S_W \mathbf{w}_i. \tag{97}$$

A few observations about this solution are in order. First, if S_W is nonsingular, this can be converted to a conventional eigenvalue problem as before. However, this is actually undesirable, since it requires an unnecessary computation of the inverse of S_W. Instead, one can find the eigenvalues as the roots of the characteristic polynomial

$$|S_B - \lambda_i S_W| = 0$$

and then solve

$$(S_B - \lambda_i S_W)\mathbf{w}_i = 0$$

directly for the eigenvectors $\mathbf{w}_i$. Because S_B is the sum of c matrices of rank one or less, and because only $c - 1$ of these are independent, S_B is of rank $c - 1$ or less. Thus, no more than $c - 1$ of the eigenvalues are nonzero, and the desired weight vectors correspond to these nonzero eigenvalues. If the within-class scatter is isotropic, the eigenvectors are merely the eigenvectors of S_B, and the eigenvectors with nonzero eigenvalues span the space spanned by the vectors $\mathbf{m}_i - \mathbf{m}$. In this special case the columns of W can be found simply by applying the Gram-Schmidt orthonormalization procedure to the

* A derivation of the solution can be found in S. Wilks, *Mathematical Statistics*, pp. 577–578 (John Wiley, New York, 1962).

$c - 1$ vectors $\mathbf{m}_i - \mathbf{m}$, $i = 1, \ldots, c - 1$. Finally, we observe that in general the solution for W is not unique. The allowable transformations include rotating and scaling the axes in various ways. These are all linear transformations from a $(c - 1)$-dimensional space to a $(c - 1)$-dimensional space, however, and do not change things in any significant way. In particular, they leave the criterion function $J(W)$ invariant.

As in the two-class case, multiple discriminant analysis primarily provides a reasonable way of reducing the dimensionality of the problem. Parametric or nonparametric techniques that might not have been feasible in the original space may work well in the lower-dimensional space. In particular, it may be possible to estimate separate covariance matrices for each class and use the general multivariate normal assumption after the transformation where this could not be done with the original data. In general, the transformation causes some unnecessary overlapping of the data and increases the theoretically achievable error rate, and the problem of classifying the data still remains. There are other ways to reduce the dimensionality of data, and we shall encounter this subject again in Chapter 6. There are also other methods of discriminant analysis, some of which are given in the references for this chapter. Of all of these, Fisher's method remains one of the most fundamental and most widely used techniques.

4.12 BIBLIOGRAPHICAL AND HISTORICAL REMARKS

In this chapter we have examined some fundamental nonparametric techniques that have played a significant role in statistical pattern classification. Many other topics in nonparametric statistics have gone unmentioned, and the interested reader may want to consult Gibbons (1971) or Thomas (1970) for an introduction to this literature. The classical tradition in statistics is to derive estimates of density functions from empirical distribution functions (Fisz, 1963), but this is clumsy in the multivariate case. A frequently referenced but rather inaccessible report by Fix and Hodges (1951) developed the implications of density estimation for classification theory and set the stage for most of the subsequent work on density estimation.

Our treatment of the Parzen-window method is a slight generalization of the univariate formulation by M. Rosenblatt (1956). Rosenblatt's work actually preceded that of Parzen (1962), but Parzen had previously employed similar methods for the estimation of spectra, and the phrase "Parzen-window" is now well established. In addition to demonstrating pointwise convergence, Parzen showed that the estimate of the density is asymptotically normal, and established conditions under which the resulting sample mode

converges to the true mode. The relation between the estimation of densities and the estimation of spectra suggests that by working with characteristic functions one can obtain interesting results in the frequency domain. Watson and Leadbetter (1963) took this approach and showed how the window functions could be optimized in the finite-sample case if constraints could be placed on the spectrum of the unknown density. Undoubtedly, this approach could be used to transfer many of the results in filtering theory to the problem of estimating densities. Except for Fix and Hodges, all of these results were stated for the univariate case. The basic generalizations to the multivariate case were given by Murthy (1965, 1966) and Cacoullos (1966).

A rigorous demonstration that the k_n-nearest-neighbor method yields a consistent estimate of a multivariate density was given by Loftsgaarden and Quesenberry (1965). The surprising nearest-neighbor classification results are due to Cover and Hart (1967), who also found bounds on the performance of the k-nearest-neighbor rule. Wagner (1971) extended these results by showing that the probability of error conditioned on the n samples converges to the average probability of error $P_n(e)$ with probability one. Hellman (1970) showed how the nearest-neighbor rule can be extended to allow rejects. The important topic of rates of convergence is examined by Cover (1968). Since the nearest-neighbor error rate bounds the Bayes rate, it can be used to measure the inherent difficulty of a pattern classification problem. Cover (1969) conjectures that even in the small-sample case the results will tell how well any nonparametric procedure using the same samples will perform. Fralick and Scott (1971) give an experimental comparison of Parzen-window and nearest-neighbor rules used to estimate the Bayes rate.

One problem with all of these methods is that the complete set of samples must be stored, and must be searched each time a new feature vector is to be classified. Many suggestions have been offered for reducing this problem, but few possess any known statistical properties. Barus (1966) gave an interesting approximation to the Fix and Hodges procedure, and Hart (1968) proposed a condensed nearest-neighbor rule. The problem of finding an effective, small reference set is essentially a problem in clustering. Moreover, certain clustering procedures, such as those by Sebestyen (1962) and Sebestyen and Edie (1966), can be interpreted as heuristic methods for approximating probability density functions. Tarter, Holcomb and Kronmal (1967) suggested the use of orthogonal series expansions for density estimation. The idea of obtaining polynomial discriminant functions by approximating the Parzen-window estimate by a Taylor's series was introduced by Specht (1967). Meisel (1969) pointed out that such expansions can require many terms for convergence, and related the Parzen-window approach to the method of potential functions (Arkedev and Braverman, 1966). The method of potential functions is in turn related to the adaptive techniques and the

stochastic approximation techniques discussed in Chapter 5. Most of these techniques are concerned with obtaining a posteriori probabilities. However, Tsypkin (1966) and Kashyap and Blaydon (1968) have shown that in theory they can also be used to estimate density functions.

The prevalence of binary measurements in many practical pattern recognition systems makes the estimation of the joint probability of binary variables of more than academic significance. The Rademacher-Walsh expansion occurs frequently in switching theory, and is closely related to the Bahadur-Lazarsfeld expansion. Bahadur (1961) gives an extension of this latter expansion from the binary case to the general discrete case. Where orthogonal-function expansions minimize mean-square error, Brown (1959) and Lewis (1959) have shown that under certain conditions product approximations maximize entropy. Ito (1969) presents bounds on the error rate that results from truncating series expansions. The idea of simplifying the approximations by limiting the nature of the dependence has been explored by Chow (1962) and by Abend, Harley and Kanal (1965), who were particularly interested in the natural spatial dependencies in binary pictures. The interesting idea of tree dependence was introduced by Chow (1966), and methods for finding the dependence tree were reported by Chow and Liu (1966, 1968). A significant extension of this concept to the multivariate normal case was reported by Chow in 1970.

The subject of discriminant analysis has its origins in the classic paper by R. A. Fisher (1936). The literature on this subject is fairly extensive, and is well surveyed in the paper by Tatsuoka and Tiedeman (1954). The generalization of Fisher's linear discriminant to the multiclass case is due to Bryan (1951). By using criteria other than the ratio of between-class scatter to within-class scatter, other types of linear discriminant functions can be obtained. Kullback (1959) suggests other criteria and investigates their properties, and Peterson and Mattson (1966) develop a general procedure for finding the optimal discriminant function for a fairly broad class of criterion functions. As we remarked before, the goal of all of these techniques is the reduction of the dimensionality of the feature space, and the resulting discriminant functions do not in themselves solve the classification problem. The discriminant functions discussed in the next chapter are designed to solve the classification problem directly.

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PROBLEMS

1. Let $p(x) \sim N(\mu, \sigma^2)$ and $\varphi(x) \sim N(0, 1)$. Show that the Parzen-window estimate

$$p_n(x) = \frac{1}{nh_n} \sum_{i=1}^{n} \varphi\left(\frac{x - x_i}{h_n}\right)$$

has the following properties:

(a) $\bar{p}_n(x) \sim N(\mu, \sigma^2 + h_n^2)$

(b) $\text{Var}[p_n(x)] \approx \dfrac{1}{nh_n 2\sqrt{\pi}} p(x)$

(c) $p(x) - \bar{p}_n(x) \approx \dfrac{1}{2}\left(\dfrac{h_n}{\sigma}\right)^2 \left[1 - \left(\dfrac{x - \mu}{\sigma}\right)^2\right] p(x)$

for small h_n. (Note: if $h_n = h_1/\sqrt{n}$, this shows that the error due to bias goes to zero as $1/n$, whereas the standard deviation of the noise only goes to zero as $1/n^{0.25}$.)

2. Let $p(x)$ be uniform from 0 to a, and let $\varphi(x) = e^{-x}$ for $x > 0$ and 0 for $x \leq 0$. Show that the mean of the Parzen-window estimate is given by

$$\bar{p}_n(x) = \begin{cases} 0 & x < 0 \\ \dfrac{1}{a}(1 - e^{-x/h_n}) & 0 \leq x \leq a \\ \dfrac{1}{a}(e^{a/h_n} - 1)e^{-x/h_n} & a < x \end{cases}$$

Sketch $\bar{p}_n(x)$ versus x for $h_n = a$, $a/4$, and $a/16$. How small does h_n have to be to have less than one percent bias over 99 percent of the range $0 < x < a$?

3. Let $\mathcal{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ be a set of n independent labelled samples and let $\mathcal{X}_k(\mathbf{x}) = \{\mathbf{x}'_1, \ldots, \mathbf{x}'_k\}$ be the k nearest neighbors of $\mathbf{x}$. The k-nearest neighbor rule for classifying $\mathbf{x}$ is to give $\mathbf{x}$ the label most frequently represented in $\mathcal{X}_k(\mathbf{x})$. Consider a two-category problem with $P(\omega_1) = P(\omega_2) = 1/2$. Assume further that the conditional densities $p(\mathbf{x} \mid \omega_i)$ are uniform within unit hyperspheres a distance of ten units apart.

(a) Show that if k is odd the average probability of error is given by

$$P_n(e) = \frac{1}{2^n} \sum_{j=0}^{(k-1)/2} \binom{n}{j}.$$

(b) Show that for this case the single-nearest-neighbor rule has a lower error rate than the k-nearest-neighbor error rate, $k > 1$.

(c) (Optional) If k is allowed to increase with n but is restricted by $k < a\sqrt{n}$, show that $P_n(e) \to 0$ as $n \to \infty$.

4. It is easy to see that the nearest-neighbor error rate P can equal the Bayes rate P^* if $P^* = 0$ (the best possibility) or if $P^* = (c-1)/c$ (the worst possibility). One might ask whether or not there are problems for which $P = P^*$ when P^* is between these extremes.

(a) Show that the Bayes rate for the one-dimensional case where $P(\omega_i) = 1/c$ and

$$p(x \mid \omega_i) = \begin{cases} 1 & 0 \le x \le \dfrac{cr}{c-1} \\ 1 & i \le x \le i + 1 - \dfrac{cr}{c-1} \\ 0 & \text{elsewhere} \end{cases}$$

is $P^* = r$.

(b) Show that for this case $P = P^*$.

5. Consider the following set of seven two-dimensional vectors: $\mathbf{x}_1^t = (1\ 0)$, $\mathbf{x}_2^t = (0\ 1)$, $\mathbf{x}_3^t = (0\ -1)$, $\mathbf{x}_4^t = (0\ 0)$, $\mathbf{x}_5^t = (0\ 2)$, $\mathbf{x}_6^t = (0\ -2)$, $\mathbf{x}_7^t = (-2\ 0)$. Suppose that the first three are labelled ω_1 and the other four are labelled ω_2

(a) Sketch the decision boundary resulting from the nearest-neighbor rule. (It should be composed of nine straight line segments.)

(b) Find the sample means $\mathbf{m}_1$ and $\mathbf{m}_2$ and sketch the decision boundary corresponding to classifying $\mathbf{x}$ by assigning it to the category of the nearest sample mean.

6. Let $\varphi(x) \sim N(0, 1)$ and let

$$p_n(x) = \frac{1}{nh_n} \sum_{i=1}^{n} \varphi\left(\frac{x - x_1}{h_n}\right).$$

Approximate this estimate by factoring the window function and expanding the factor e^{xx_i/h_n^2} in a Taylor's series about the origin.

(a) Show that in terms of the normalized variable $u = x/h_n$ the m-term approximation is given by

$$p_{nm}(x) = \frac{1}{\sqrt{2\pi}\, h_n} e^{-(1/2)u^2} \sum_{j=0}^{m-1} b_j u^j$$

where

$$b_j = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{j!} u_i^j e^{-(1/2)u_i^2}.$$

(b) Suppose that the n samples happen to be extremely tightly clustered about $u = u_0$. Show that the two-term approximation peaks at the two points where $u^2 + u/u_0 - 1 = 0$. Show that one peak occurs approximately at $u = u_0$, as desired, if $u_0 \ll 1$, but that it moves only to $u = 1$ for $u_0 \gg 1$. Sketch p_{n2} versus u for $u_0 = 0.1$, 1, and 10.

7. Let $p_x(\mathbf{x} \mid \omega_i)$ be an arbitrary density with mean $\boldsymbol{\mu}_i$ and covariance matrix $\boldsymbol{\Sigma}_i$, $i = 1, 2$. Let $y = \mathbf{w}^t\mathbf{x}$, and let the induced density $p_y(y \mid \omega_i)$ have mean μ_i and variance σ_i^2.

(a) Show that the criterion function

$$J_1(\mathbf{w}) = \frac{(\mu_1 - \mu_2)^2}{\sigma_1^2 + \sigma_2^2}$$

is minimized by

$$\mathbf{w} = (\boldsymbol{\Sigma}_1 + \boldsymbol{\Sigma}_2)^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2).$$

(b) If $P(\omega_i)$ is the prior probability for ω_i, show that

$$J_2(\mathbf{w}) = \frac{(\mu_1 - \mu_2)^2}{P(\omega_1)\sigma_1^2 + P(\omega_2)\sigma_2^2}$$

is minimized by

$$\mathbf{w} = (P(\omega_1)\boldsymbol{\Sigma}_1 + P(\omega_2)\boldsymbol{\Sigma}_2)^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2).$$

(c) To which of these criterion functions is the $J(\mathbf{w})$ of Eq. (70) more closely related?

8. The expression

$$J_1 = \frac{1}{n_1 n_2} \sum_{y_i \in \mathcal{Y}_1} \sum_{y_j \in \mathcal{Y}_2} (y_i - y_j)^2$$

clearly measures the between-group scatter of two sets of samples, one containing n_1 samples labelled ω_1 and the other containing n_2 labelled ω_2. Similarly,

$$J_2 = \frac{1}{n_1^2} \sum_{y_i \in \mathcal{Y}_1} \sum_{y_j \in \mathcal{Y}_1} (y_i - y_j)^2 + \frac{1}{n_2^2} \sum_{y_i \in \mathcal{Y}_2} \sum_{y_j \in \mathcal{Y}_2} (y_i - y_j)^2$$

clearly measures the total within-group scatter.

(a) Show that

$$J_1 = (m_1 - m_2)^2 + \frac{1}{n_1} s_1^2 + \frac{1}{n_2} s_2^2$$

and

$$J_2 = \frac{1}{n_1} s_1^2 + \frac{1}{n_2} s_2^2.$$

(b) If $y = \mathbf{w}^t\mathbf{x}$, show that the $\mathbf{w}$ minimizing J_1 subject to the constraint that $J_2 = 1$ is given by

$$\mathbf{w} = \lambda\left(\frac{1}{n_1} S_1 + \frac{1}{n_2} S_2\right)^{-1} (\mathbf{m}_1 - \mathbf{m}_2)$$

where

$$\lambda = (\mathbf{m}_1 - \mathbf{m}_2)^t \left(\frac{1}{n_1} S_1 + \frac{1}{n_2} S_2 \right)^{-1} (\mathbf{m}_1 - \mathbf{m}_2)$$

$$\mathbf{m}_i = \frac{1}{n_i} \sum_{\mathbf{x} \in \mathcal{X}_i} \mathbf{x}$$

and

$$S_i = \sum_{\mathbf{x} \in \mathcal{X}_i} (\mathbf{x} - \mathbf{m}_i)(\mathbf{x} - \mathbf{m}_i)^t.$$

9. Using the multiclass definition of the between-group scatter matrix

$$S_B = \sum_{i=1}^{c} n_i (\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^t,$$

show that $S_B = [(n_1 n_2)/n](\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^t$ if $c = 2$.

10. If S_B and S_W are any two real, symmetric, d-by-d matrices, it is well known that there exists a set of n eigenvalues $\lambda_1, \ldots, \lambda_n$ satisfying $|S_B - \lambda_i S_W| = 0$, and a corresponding set of n eigenvectors $\mathbf{e}_1, \ldots, \mathbf{e}_n$ satisfying $S_B \mathbf{e}_i = \lambda_i S_W \mathbf{e}_i$. Furthermore, if S_W is positive definite, the eigenvectors can always be normalized so that

$$\mathbf{e}_i^t S_W \mathbf{e}_j = \delta_{ij}$$

and

$$\mathbf{e}_i^t S_B \mathbf{e}_j = \lambda_i \delta_{ij}.$$

Let $\tilde{S}_W = W^t S_W W$ and $\tilde{S}_B = W^t S_B W$, where W is a d-by-n matrix whose columns correspond to n distinct eignvectors.

(a) Show that $\tilde{S}_W$ is the n-by-n identity matrix, and that $\tilde{S}_B$ is a diagonal matrix whose elements are the corresponding eigenvalues.*

(b) What is the value of $J = |\tilde{S}_B| / |\tilde{S}_W|$?

(c) Let $\mathbf{y} = W^t \mathbf{x}$ be transformed by scaling the axes with a nonsingular n-by-n diagonal matrix D and by rotating this result with an orthogonal matrix Q: $\mathbf{y}' = QD\mathbf{y}$. Show that J is invariant to this transformation.

* This shows that the discriminant functions in multiple discriminant analysis are uncorrelated.

Chapter 5

LINEAR DISCRIMINANT FUNCTIONS

5.1 INTRODUCTION

In Chapter 3 we assumed that the forms for the underlying probability distributions were known, and used the samples to estimate the values of their parameters. In this chapter we shall assume that the forms for the *discriminant functions* are known, and shall use the samples to estimate the values of parameters of the classifier. We shall examine various procedures for determining discriminant functions, some of which are statistical and some of which are not. However, none of them requires knowledge of the forms of underlying probability distributions, and in this sense all of them can be said to be nonparametric.

Throughout this chapter we shall be concerned with discriminant functions that are either linear in the components of $\mathbf{x}$ or linear in some given set of functions of $\mathbf{x}$. Linear discriminant functions have a variety of pleasant properties from an analytical point of view. As we have seen in Chapter 2, they can be optimal if the underlying distributions are cooperative. Even when they are not optimal, one might be willing to sacrifice some performance to gain the advantage of simplicity. Linear discriminant functions are relatively easy to compute, and a classifier of fixed structure is an attractive candidate for implementation as a special-purpose computer.

The Fisher linear discriminant provides a model for the approach we shall adopt. The problem of finding a linear discriminant function will be formulated as a problem of minimizing a criterion function. The obvious criterion function for classification purposes is the *sample risk*, the average loss incurred in classifying the set of design samples. However, because it is so difficult to derive the minimum-risk linear discriminant, we shall investigate several related criterion functions that are analytically more tractable. Most of our attention will be devoted to studying the convergence properties

of various gradient descent procedures for minimizing these criterion functions. The similarities between many of the procedures sometimes makes it difficult to keep the differences between them clear. For this reason we have included a summary of the principal results at the end of Section 5.10 in Table 5-1, which can be consulted as needed.

5.2 LINEAR DISCRIMINANT FUNCTIONS AND DECISION SURFACES

5.2.1 The Two-Category Case

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

$$g(\mathbf{x}) = \mathbf{w}^t\mathbf{x} + w_0, \tag{1}$$

where $\mathbf{w}$ is called the *weight vector* and w_0 the *threshold weight*. A two-category linear classifier implements the following decision rule: Decide ω_1 if $g(\mathbf{x}) > 0$ and ω_2 if $g(\mathbf{x}) < 0$. Thus, $\mathbf{x}$ is assigned to ω_1 if the inner product $\mathbf{w}^t\mathbf{x}$ exceeds the threshold $-w_0$. If $g(\mathbf{x}) = 0$, $\mathbf{x}$ can ordinarily be assigned to either class, but in this chapter we shall leave the assignment undefined.

The equation $g(\mathbf{x}) = 0$ defines the decision surface that separates points assigned to ω_1 from points assigned to ω_2. When $g(\mathbf{x})$ is linear, this decision surface is a *hyperplane*. If $\mathbf{x}_1$ and $\mathbf{x}_2$ are both on the decision surface, then

$$\mathbf{w}^t\mathbf{x}_1 + w_0 = \mathbf{w}^t\mathbf{x}_2 + w_0$$

or

$$\mathbf{w}^t(\mathbf{x}_1 - \mathbf{x}_2) = 0,$$

so that $\mathbf{w}$ is normal to any vector lying in the hyperplane. In general, the hyperplane H divides the feature space into two halfspaces, the decision region $\mathcal{R}_1$ for ω_1 and the decision region $\mathcal{R}_2$ for ω_2. Since $g(\mathbf{x}) > 0$ if $\mathbf{x}$ is in $\mathcal{R}_1$, it follows that the normal vector $\mathbf{w}$ points into $\mathcal{R}_1$. It is sometimes said that any $\mathbf{x}$ in $\mathcal{R}_1$ is on the positive side of H, and any $\mathbf{x}$ in $\mathcal{R}_2$ is on the negative side.

The discriminant function $g(\mathbf{x})$ gives an algebraic measure of the distance from $\mathbf{x}$ to the hyperplane. Perhaps the easiest way to see this is to express $\mathbf{x}$ as

$$\mathbf{x} = \mathbf{x}_p + r\frac{\mathbf{w}}{\|\mathbf{w}\|},$$

where $\mathbf{x}_p$ is the normal projection of $\mathbf{x}$ onto H, and r is the desired algebraic distance, positive if $\mathbf{x}$ is on the positive side and negative if $\mathbf{x}$ is on the negative side. Then, since $g(\mathbf{x}_p) = 0$,

$$g(\mathbf{x}) = \mathbf{w}^t\mathbf{x} + w_0 = r\,\|\mathbf{w}\|,$$

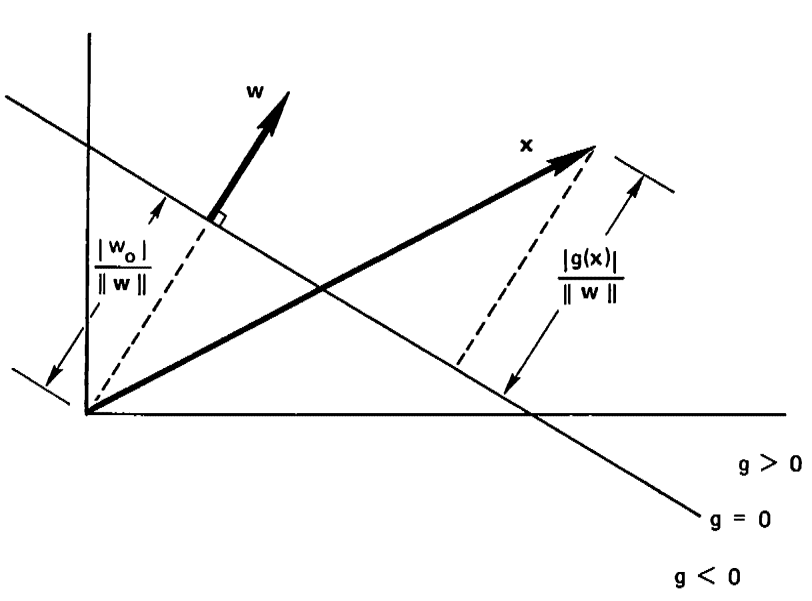

FIGURE 5.1. The linear decision boundary $g(x) = w^t x + w_0 = 0$.

or

$$r = \frac{g(\mathbf{x})}{\|\mathbf{w}\|}.$$

In particular, the distance from the origin to H is given by $w_0/\|\mathbf{w}\|$. If $w_0 > 0$ the origin is on the positive side of H, and if $w_0 < 0$ it is on the negative side. If $w_0 = 0$, then $g(\mathbf{x})$ has the homogeneous form $\mathbf{w}^t\mathbf{x}$, and the hyperplane passes through the origin. A geometric illustration of these algebraic results is given in Figure 5.1.

To summarize, a linear discriminant function divides the feature space by a hyperplane decision surface. The orientation of the surface is determined by the normal vector $\mathbf{w}$, and the location of the surface is determined by the threshold weight w_0. The discriminant function $g(\mathbf{x})$ is proportional to the signed distance from $\mathbf{x}$ to the hyperplane, with $g(\mathbf{x}) > 0$ when $\mathbf{x}$ is on the positive side, and $g(\mathbf{x}) < 0$ when $\mathbf{x}$ is on the negative side.

5.2.2 The Multicategory Case

There is more than one way to devise multicategory classifiers employing linear discriminant functions. For example, one might reduce the problem to $c - 1$ two-class problems, where the ith problem is solved by a linear discriminant function that separates points assigned to ω_i from those not assigned to ω_i. A more extravagant approach would be to use $c(c - 1)/2$

linear discriminants, one for every pair of classes. As illustrated in Figure 5.2, both of these approaches can lead to regions such as the shaded areas in which the classification is undefined. We shall avoid this problem by adopting the approach taken in Chapter 2, defining c linear discriminant functions

$$g_i(\mathbf{x}) = \mathbf{w}_i^t\mathbf{x} + w_{i0} \qquad i = 1, \ldots, c, \tag{2}$$

and assigning $\mathbf{x}$ to ω_i if $g_i(\mathbf{x}) > g_j(\mathbf{x})$ for all $j \neq i$; in case of ties, the classification is left undefined. The resulting classifier is called a *linear machine*. A linear machine divides the feature space into c decision regions, with $g_i(\mathbf{x})$ being the largest discriminant if $\mathbf{x}$ is in region $\mathscr{R}_i$. If $\mathscr{R}_i$ and $\mathscr{R}_j$ are contiguous, the boundary between them is a portion of the hyperplane H_{ij} defined by

$$g_i(\mathbf{x}) = g_j(\mathbf{x})$$

or

$$(\mathbf{w}_i - \mathbf{w}_j)^t\mathbf{x} + (w_{i0} - w_{j0}) = 0.$$

It follows at once that $\mathbf{w}_i - \mathbf{w}_j$ is normal to H_{ij}, and the signed distance from $\mathbf{x}$ to H_{ij} is given by $(g_i - g_j)/\|\mathbf{w}_i - \mathbf{w}_j\|$. Thus, with the linear machine it is not the weight vectors themselves but their *differences* that are important. While there are $c(c-1)/2$ pairs of regions, they need not all be contiguous, and the total number of hyperplane segments appearing in the decision surfaces is often fewer than $c(c-1)/2$. Two-dimensional examples of these surfaces are shown in Figure 5.3.

It is easy to show that the decision regions for a linear machine are convex. This restriction definitely limits the flexibility of the classifier. In particular, every decision region must be singly connected, which tends to make the

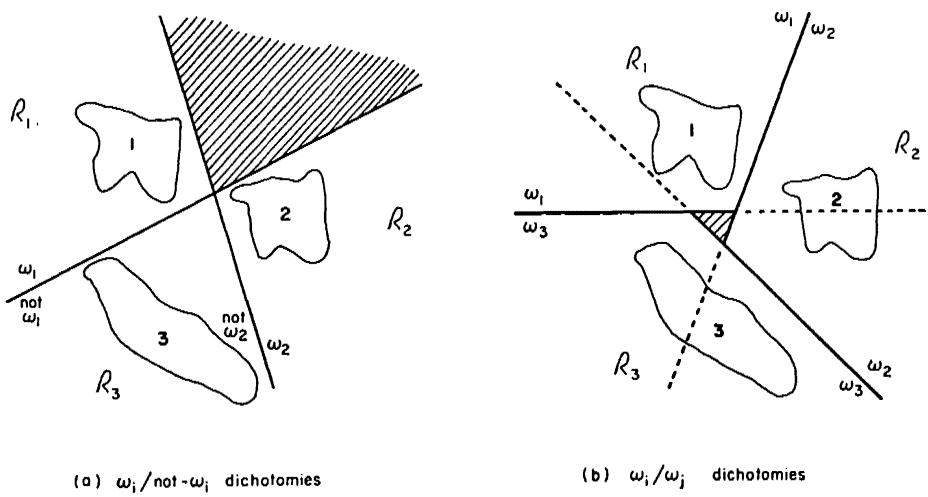

FIGURE 5.2. Linear decision boundaries for a three-class problem.

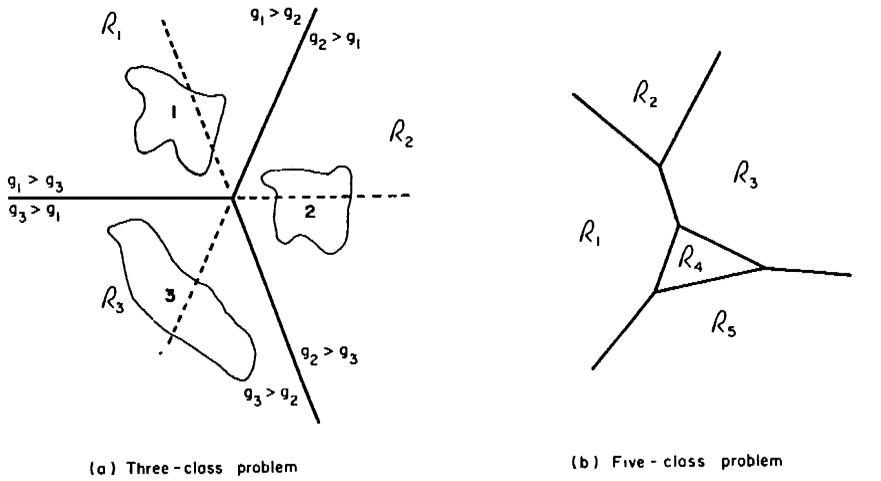

FIGURE 5.3. Decision boundaries produced by a linear machine.

linear machine most suitable for problems for which the conditional densities $p(\mathbf{x} \mid \omega_i)$ are unimodal. Within these limitations, the linear machine offers a fair amount of flexibility and the virtue of analytical simplicity.

5.3 GENERALIZED LINEAR DISCRIMINANT FUNCTIONS

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

$$g(\mathbf{x}) = w_0 + \sum_{i=1}^{d} w_i x_i, \tag{3}$$

where the coefficients w_i are the components of the weight vector $\mathbf{w}$. By adding additional terms involving the products of pairs of components of $\mathbf{x}$, we obtain the *quadratic discriminant function*

$$g(\mathbf{x}) = w_0 + \sum_{i=1}^{d} w_i x_i + \sum_{i=1}^{d} \sum_{j=1}^{d} w_{ij} x_i x_j.$$

Since $x_i x_j = x_j x_i$, we can assume that $w_{ij} = w_{ji}$ with no loss in generality. Thus, the quadratic discriminant function has an additional $d(d + 1)/2$ coefficients at its disposal with which to produce more complicated separating surfaces. The separating surface defined by $g(\mathbf{x}) = 0$ is a second-degree or *hyperquadric* surface. If the symmetric matrix $W = [w_{ij}]$ is nonsingular, then the linear terms in $g(\mathbf{x})$ can be eliminated by translating the axes, and the basic character of the separating surface can be described in terms of the

scaled matrix $\overline{W} = W/(\mathbf{w}^t W^{-1}\mathbf{w} - 4w_0)$. If $\overline{W}$ is a positive multiple of the identity matrix, the separating surface is a *hypersphere*. If $\overline{W}$ is positive definite, the separating surface is a *hyperellipsoid*. If some of the eigenvalues of $\overline{W}$ are positive and others are negative, the surface is one of a variety of types of *hyperhyperboloids*. As we observed in Chapter 2, these are the kinds of separating surfaces that arise in the general multivariate normal case.

By continuing to add terms such as $w_{ijk}x_ix_jx_k$ we can obtain the class of *polynomial discriminant functions*. These can be thought of as truncated series expansions of some arbitrary $g(\mathbf{x})$, and this in turn suggests the *generalized linear discriminant function*

$$g(\mathbf{x}) = \sum_{i=1}^{\hat{d}} a_i y_i(\mathbf{x}) \tag{4}$$

or

$$g(\mathbf{x}) = \mathbf{a}^t\mathbf{y}, \tag{5}$$

where $\mathbf{a}$ is a $\hat{d}$-dimensional weight vector, and where the $\hat{d}$ functions $y_i(\mathbf{x})$ (sometimes called φ functions) can be arbitrary functions of $\mathbf{x}$. By selecting these functions judiciously and letting $\hat{d}$ be sufficiently large, one can approximate any desired discriminant function by such a series expansion. The resulting discriminant function is not linear in $\mathbf{x}$, but it is linear in $\mathbf{y}$. The $\hat{d}$ functions $y_i(\mathbf{x})$ merely map points in d-dimensional $\mathbf{x}$-space to points in $\hat{d}$-dimensional $\mathbf{y}$-space. The homogeneous discriminant $\mathbf{a}^t\mathbf{y}$ separates points in this transformed space by a hyperplane passing through the origin. Thus, the mapping from $\mathbf{x}$ to $\mathbf{y}$ reduces the problem to one of finding a homogeneous linear discriminant function.

Some of the advantages and disadvantages of this approach can be clarified by considering a simple example. Let $g(x)$ be the quadratic discriminant function

$$g(x) = a_1 + a_2x + a_3x^2,$$

so that the three-dimensional vector $\mathbf{y}$ is given by

$$\mathbf{y} = \begin{bmatrix} 1 \\ x \\ x^2 \end{bmatrix}.$$

The mapping from x to $\mathbf{y}$ is illustrated in Figure 5.4. The data remain inherently one dimensional, since varying x causes $\mathbf{y}$ to trace out a curve in three-space. Thus, one thing to notice immediately is that if x is governed by a probability law $p(x)$, the induced density $\hat{p}(\mathbf{y})$ will be degenerate, being zero everywhere except on the curve, where it is infinite. This is a common problem whenever $\hat{d} > d$, and the mapping takes points from a lower-dimensional space to a higher-dimensional space.

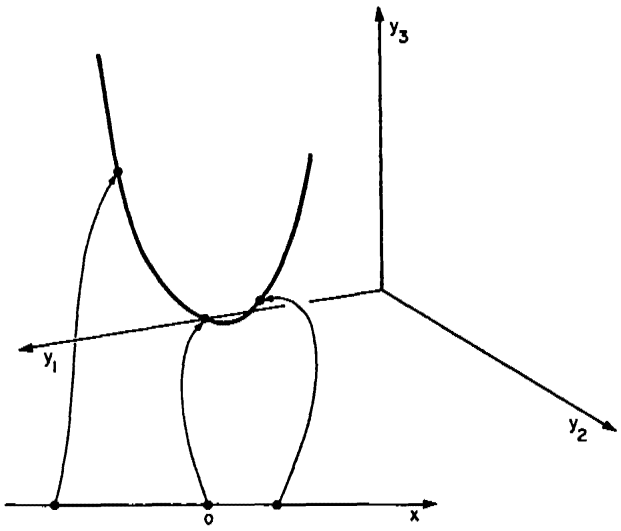

FIGURE 5.4. The mapping $y = (1\ x\ x^2)^t$.

The plane $\hat{H}$ defined by $\mathbf{a}^t\mathbf{y} = 0$ divides the y-space into two decision regions $\hat{\mathscr{R}}_1$ and $\hat{\mathscr{R}}_2$. Figure 5.5 shows the separating plane corresponding to $\mathbf{a} = (-1\ 1\ 2)^t$, and the corresponding decision regions $\mathscr{R}_1$ and $\mathscr{R}_2$ in x-space. The quadratic discriminant function $g(x) = -1 + x + 2x^2$ is positive if $x < -1$ or if $x > 0.5$, so that $\mathscr{R}_1$ is multiply connected. Thus, although the decision regions in y-space are convex, this is by no means the case in x-space. Even with relatively simple functions $y_i(\mathbf{x})$, the decision surfaces induced in x-space can be fairly complex.

Unfortunately, the curse of dimensionality makes it hard to capitalize on this flexibility in practice. A complete quadratic discriminant function involves $\hat{d} = (d + 1)(d + 2)/2$ terms. If d is modestly large, say $d = 50$, this requires the computation of a great many terms. Inclusion of cubic and higher order terms leads to even larger values for $\hat{d}$. Furthermore, the $\hat{d}$ components of the weight vector $\mathbf{a}$ must be determined from samples. If we think of $\hat{d}$ as specifying the number of degrees of freedom for the discriminant function, it is natural to require that the number of samples be not less than the number of degrees of freedom. Clearly, a general series expansion of $g(\mathbf{x})$ can easily lead to completely unrealistic requirements for computation and data.

While it may be hard to realize the potential benefits of a generalized linear discriminant function, we can at least exploit the convenience of being able to write $g(\mathbf{x})$ in the homogeneous form $\mathbf{a}^t\mathbf{y}$. In the particular case of the linear discriminant function

$$g(\mathbf{x}) = w_0 + \sum_{i=1}^{d} w_i x_i \tag{3}$$

we can write

$$\mathbf{y} = \begin{bmatrix} 1 \\ x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_d \end{bmatrix} = \begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix} \tag{6}$$

and

$$\mathbf{a} = \begin{bmatrix} w_0 \\ w_1 \\ \cdot \\ \cdot \\ \cdot \\ w_d \end{bmatrix} = \begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix}. \tag{7}$$

This mapping from d-dimensional x-space to $(d + 1)$-dimensional y-space is mathematically trivial but nonetheless convenient. The addition of a constant component to x preserves all distance relationships among samples. The resulting y vectors all lie in a d-dimensional subspace, which is the x-space itself. The hyperplane decision surface $\hat{H}$ defined by $\mathbf{a}^t\mathbf{y} = 0$ always passes through the origin in y-space, even though the corresponding hyperplane H can be in any position in x-space. The distance from y to $\hat{H}$ is given by $|\mathbf{a}^t\mathbf{y}|/\|\mathbf{a}\|$, or $|g(\mathbf{x})|/\|\mathbf{a}\|$. Since $\|\mathbf{a}\| > \|\mathbf{w}\|$, this distance is less than, or at

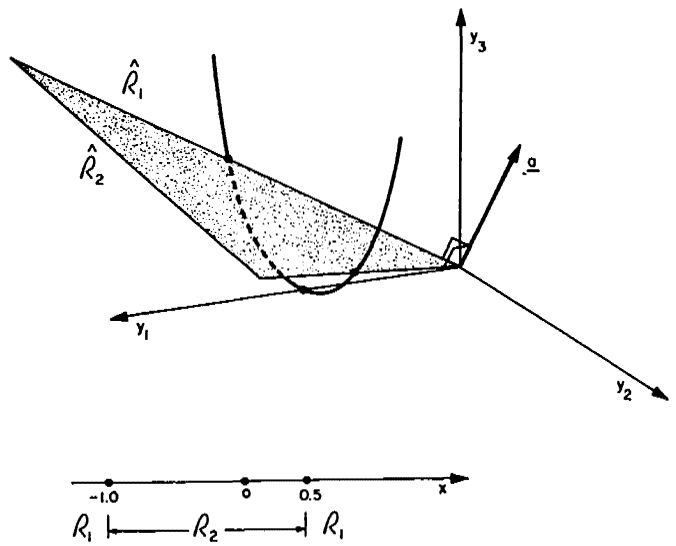

FIGURE 5.5. Decision regions in x-space and y-space.

most equal to the distance from $\mathbf{x}$ to H. By using this mapping we reduce the problem of finding a weight vector $\mathbf{w}$ and a threshold weight w_0 to the problem of finding a single weight vector $\mathbf{a}$.

5.4 THE TWO-CATEGORY LINEARLY-SEPARABLE CASE

5.4.1 Geometry and Terminology

Suppose now that we have a set of n samples $\mathbf{y}_1, \ldots, \mathbf{y}_n$, some labelled ω_1 and some labelled ω_2. We want to use these samples to determine the weights in a linear discriminant function $g(\mathbf{x}) = \mathbf{a}^t\mathbf{y}$. Suppose we have reason to believe that there exists a solution for which the probability of error is very, very low. Then a reasonable approach is to look for a weight vector that classifies all of the samples correctly. If such a weight vector exists, the samples are said to be *linearly separable.*

A sample $\mathbf{y}_i$ is classified correctly if $\mathbf{a}^t\mathbf{y}_i > 0$ and $\mathbf{y}_i$ is labelled ω_1, or if $\mathbf{a}^t\mathbf{y}_i < 0$ and $\mathbf{y}_i$ is labelled ω_2. In the latter case, we observe that $\mathbf{y}_i$ is classified correctly if $\mathbf{a}^t(-\mathbf{y}_i) > 0$. This suggests a normalization that simplifies the treatment of the two-category case, viz., the replacement of all samples labelled ω_2 by their negatives. With this normalization we can forget the labels and look for a weight vector $\mathbf{a}$ such that $\mathbf{a}^t\mathbf{y}_i > 0$ for all of the samples. Such a weight vector is called a *separating vector* or a *solution vector.*

The weight vector $\mathbf{a}$ can be thought of as specifying a point in *weight space.* Each sample $\mathbf{y}_i$ places a constraint on the possible location of a solution vector. The equation $\mathbf{a}^t\mathbf{y}_i = 0$ defines a hyperplane through the origin of weight space having $\mathbf{y}_i$ as a normal vector. The solution vector, if it exists, must be on the positive side of every hyperplane. Thus, the solution vector must lie in the intersection of n half-spaces, and any vector in this region is a solution vector. The corresponding region is called the *solution region.* A two-dimensional example illustrating the solution region for both the normalized and the unnormalized case is shown in Figure 5.6.

From this discussion, it should be clear that the solution vector, if it exists, is not unique. There are several ways to impose additional requirements to constrain the solution vector further. One possibility is to seek a unit-length weight vector that maximizes the minimum distance from the samples to the separating plane. Another possibility is to seek the minimum-length weight vector satisfying $\mathbf{a}^t\mathbf{y}_i \geq b$ for all i, where b is a positive constant called the *margin.* Sometimes it is convenient to require merely that $\mathbf{a}^t\mathbf{y}_i \geq b$. As shown in Figure 5.7, the solution region resulting from the intersections of the halfspaces for which $\mathbf{a}^t\mathbf{y}_i \geq b > 0$ lies within the previous solution region, being insulated from the old boundaries by the distance $b/\|\mathbf{y}_i\|$.

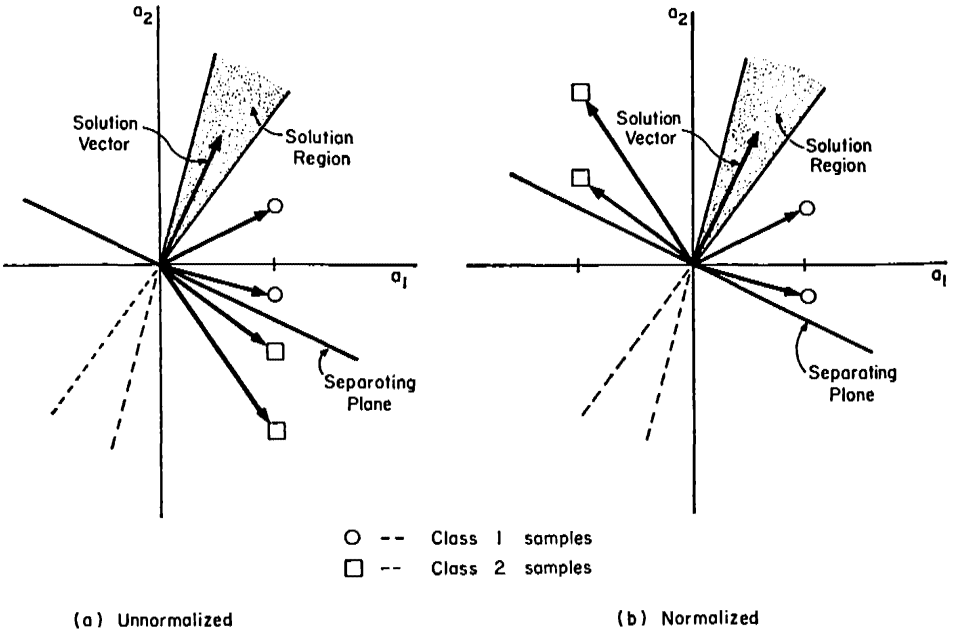

FIGURE 5.6. Linearly separable samples and the solution region in weight space.

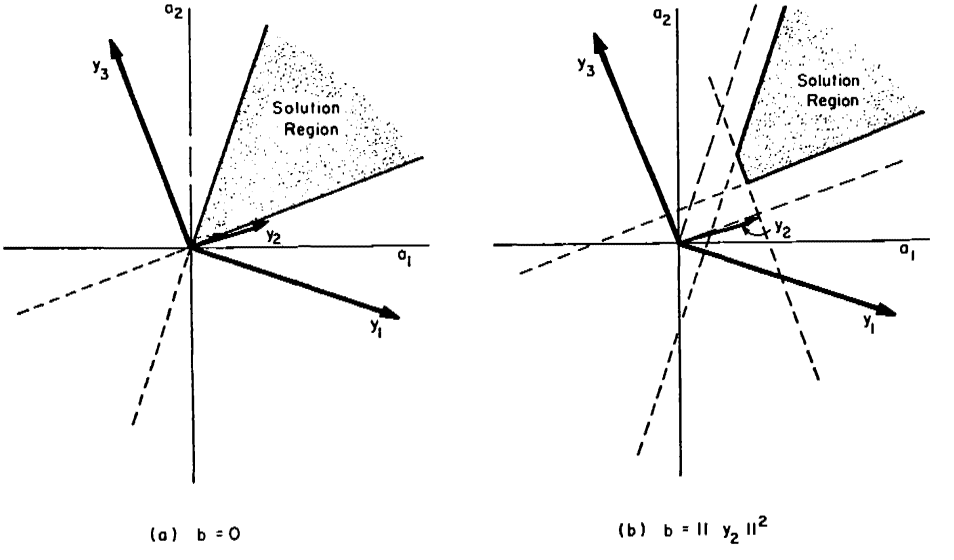

FIGURE 5.7. Effect of the margin on the solution region.

The motivation behind these attempts to find a solution vector closer to the "middle" of the solution region is the intuitive belief that the resulting solution is more likely to classify new samples correctly. In the cases we shall treat, however, we shall be satisfied with any solution strictly within the solution region. Our chief concern will be to see that any iterative procedure used does not converge to a limit point on the boundary. This problem can always be avoided by the introduction of a margin, i.e., by requiring that $\mathbf{a}^t\mathbf{y}_i \geq b > 0$ for all i.

5.4.2 Gradient Descent Procedures

The approach we shall take to finding a solution to the set of linear inequalities $\mathbf{a}^t\mathbf{y}_i > 0$ will be to define a criterion function $J(\mathbf{a})$ that is minimized if $\mathbf{a}$ is a solution vector. This reduces our problem to one of minimizing a scalar function, a problem that can often be solved by a gradient descent procedure. The basic descent procedure is very simple. We start with some arbitrarily chosen weight vector $\mathbf{a}_1$ and compute the gradient vector $\nabla J(\mathbf{a}_1)$. The next value $\mathbf{a}_2$ is obtained by moving some distance from $\mathbf{a}_1$ in the direction of steepest descent, i.e., along the negative of the gradient. In general, $\mathbf{a}_{k+1}$ is obtained from $\mathbf{a}_k$ by the algorithm

$$\mathbf{a}_{k+1} = \mathbf{a}_k - \rho_k \nabla J(\mathbf{a}_k), \tag{8}$$

where ρ_k is a positive scale factor that sets the step size. Hopefully, such a sequence of weight vectors will converge to a solution minimizing $J(\mathbf{a})$.

The many problems associated with gradient descent procedures are well known. Fortunately, we shall be constructing the functions we want to minimize, and shall be able to avoid the most serious of these problems. One that will confront us repeatedly, however, is the choice of the scale factor ρ_k. If ρ_k is too small, convergence is needlessly slow, whereas if ρ_k is too large, the correction process will overshoot and can even diverge. Suppose that the criterion function can be well approximated by the second-order expansion

$$J(\mathbf{a}) \approx J(\mathbf{a}_k) + \nabla J^t(\mathbf{a} - \mathbf{a}_k) + \tfrac{1}{2}(\mathbf{a} - \mathbf{a}_k)^t D(\mathbf{a} - \mathbf{a}_k), \tag{9}$$

where D is the matrix of second partial derivatives $\partial^2 J/\partial a_i\, \partial a_j$ evaluated at $\mathbf{a} = \mathbf{a}_k$. Then, using $\mathbf{a}_{k+1}$ from Eq. (8) in Eq. (9),

$$J(\mathbf{a}_{k+1}) \approx J(\mathbf{a}_k) - \rho_k \|\nabla J\|^2 + \tfrac{1}{2}\rho_k^2 \nabla J^t D\, \nabla J,$$

and it follows that $J(\mathbf{a}_{k+1})$ can be minimized by the choice

$$\rho_k = \frac{\|\nabla J\|^2}{\nabla J^t D\, \nabla J}. \tag{10}$$

An alternative descent procedure can be obtained by ignoring Eq. (8) and by choosing $\mathbf{a}_{k+1}$ to minimize the second-order expansion. This leads to *Newton's algorithm*,

$$\mathbf{a}_{k+1} = \mathbf{a}_k - D^{-1}\nabla J. \tag{11}$$

Generally speaking, Newton's algorithm will usually give a greater improvement *per step* than the simple gradient descent algorithm, even with the optimal value of ρ_k. However, Newton's algorithm is not applicable if the matrix D is singular. Furthermore, even when D is nonsingular, the time required for matrix inversion can easily offset this advantage. In fact, it often takes less time to set ρ_k to a constant ρ that is smaller than necessary and make a few more corrections than to compute the optimal ρ_k at each step. At different times we shall have recourse to all of these solutions.

5.5 MINIMIZING THE PERCEPTRON CRITERION FUNCTION

5.5.1 The Perceptron Criterion Function

Consider now the problem of constructing a criterion function for solving the linear inequalities $\mathbf{a}^t\mathbf{y}_i > 0$. The most obvious choice is to let $J(\mathbf{a}; \mathbf{y}_1, \ldots, \mathbf{y}_n)$ be the number of samples misclassified by $\mathbf{a}$. However, because this function is piecewise constant, it is obviously a poor candidate for a gradient search. A better choice is the *perceptron criterion function*

$$J_p(\mathbf{a}) = \sum_{\mathbf{y}\in\mathcal{Y}} (-\mathbf{a}^t\mathbf{y}), \tag{12}$$

where $\mathcal{Y}(\mathbf{a})$ is the set of samples *misclassified* by $\mathbf{a}$. (If no samples are misclassified, we define J_p to be zero.) Since $\mathbf{a}^t\mathbf{y} \leq 0$ if $\mathbf{y}$ is misclassified, $J_p(\mathbf{a})$ is never negative, being zero only if $\mathbf{a}$ is a solution vector, or if $\mathbf{a}$ is on the decision boundary. Geometrically, $J_p(\mathbf{a})$ is proportional to the sum of the distances from the misclassified samples to the decision boundary. Figure 5.8 illustrates J_p for a simple two-dimensional example.

Since the jth component of the gradient of J_p is $\partial J_p/\partial a_j$, we see from Eq. (12) that

$$\nabla J_p = \sum_{\mathbf{y}\in\mathcal{Y}} (-\mathbf{y}),$$

and hence the basic gradient descent algorithm (8) becomes

$$\mathbf{a}_{k+1} = \mathbf{a}_k + \rho_k \sum_{\mathbf{y}\in\mathcal{Y}_k} \mathbf{y}, \tag{13}$$

where $\mathcal{Y}_k$ is the set of samples misclassified by $\mathbf{a}_k$. Thus, the descent procedure for finding a solution vector can be stated very simply: the next

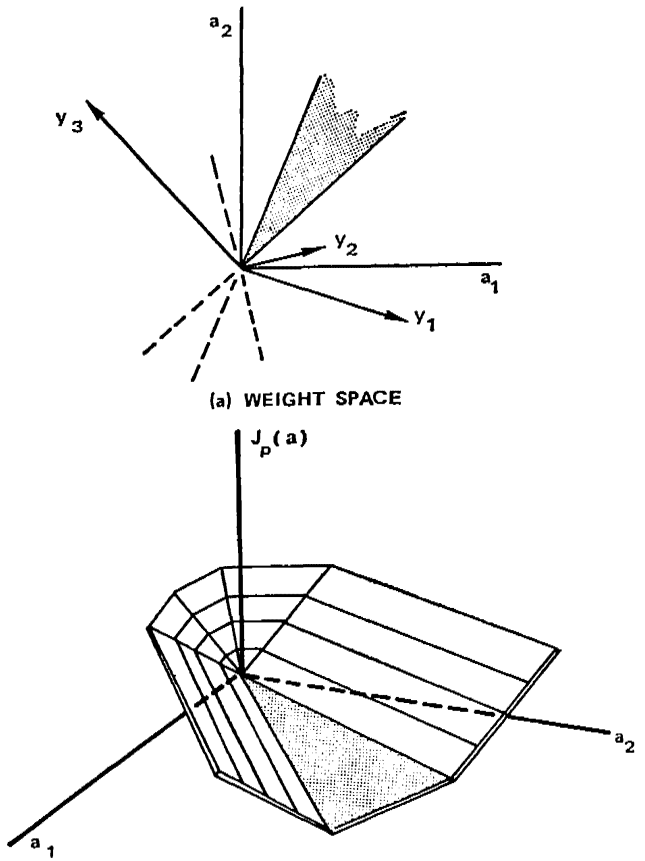

FIGURE 5.8. The perceptron criterion function.

weight vector is obtained by adding some multiple of the sum of the misclassified samples to the present weight vector. Figure 5.9 shows how this algorithm yields a solution vector for a simple two-dimensional example with $\mathbf{a}_1 = \mathbf{0}$, and $\rho_k = 1$. We shall now show that it will yield a solution for any linearly separable problem.

5.5.2 Convergence Proof for Single-Sample Correction

We shall begin our examination of convergence properties of the descent algorithm with a variant that is easier to analyze. Rather than testing $\mathbf{a}_k$ on all of the samples and basing our correction of the set $\mathcal{Y}_k$ of misclassified samples, we shall consider the samples in a sequence and shall modify the weight vector whenever it misclassifies a sample. For the purposes of the convergence proof, the detailed nature of the sequence is unimportant as long

as every sample appears in the sequence infinitely often. The simplest way to assure this is to repeat the samples cyclically.

Two further simplifications help to clarify the exposition. First, we shall temporarily restrict our attention to the case in which ρ_k is constant. This is the so-called *fixed-increment* case. It is clear from Eq. (13) that if ρ_k is constant it merely serves to scale the samples. Thus, in the fixed-increment case we can take $\rho_k = 1$ with no loss in generality. The second simplification merely involves notation. When the samples are considered sequentially, some will be misclassified. Since we shall only change the weight vector when there is an error, we really need only pay attention to the misclassified samples. Thus, we shall denote the sequence of samples by $\mathbf{y}^1, \mathbf{y}^2, \ldots, \mathbf{y}^k, \ldots$, where each $\mathbf{y}^k$ is one of the n samples $\mathbf{y}_1, \ldots, \mathbf{y}_n$, and where each $\mathbf{y}^k$ is misclassified. For example, if the samples $\mathbf{y}_1$, $\mathbf{y}_2$, and $\mathbf{y}_3$ are considered cyclically, and if the marked samples

$$\overset{\checkmark}{\mathbf{y}_1}, \mathbf{y}_2, \overset{\checkmark}{\mathbf{y}_3}, \overset{\checkmark}{\mathbf{y}_1}, \overset{\checkmark}{\mathbf{y}_2}, \mathbf{y}_3, \mathbf{y}_1, \overset{\checkmark}{\mathbf{y}_2}, \ldots$$

are misclassified, then the sequence $\mathbf{y}^1, \mathbf{y}^2, \mathbf{y}^3, \mathbf{y}^4, \mathbf{y}^5, \ldots$ denotes the sequence $\mathbf{y}_1, \mathbf{y}_3, \mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_2, \ldots$. With this understanding, the *fixed-increment rule* for generating a sequence of weight vectors can be written as

$$\left.\begin{aligned} &\mathbf{a}_1 && \text{arbitrary} \\ &\mathbf{a}_{k+1} = \mathbf{a}_k + \mathbf{y}^k && k \geq 1, \end{aligned}\right\} \tag{14}$$

where $\mathbf{a}_k^t \mathbf{y}^k \leq 0$ for all k.

The fixed-increment rule is the simplest of many algorithms that have been proposed for solving systems of linear inequalities. Historically, it first

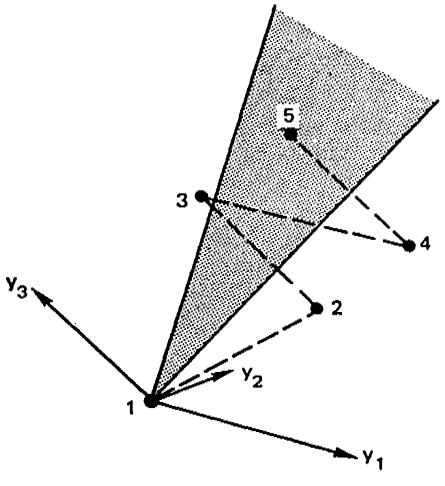

FIGURE 5.9. Finding a solution region by a gradient search.

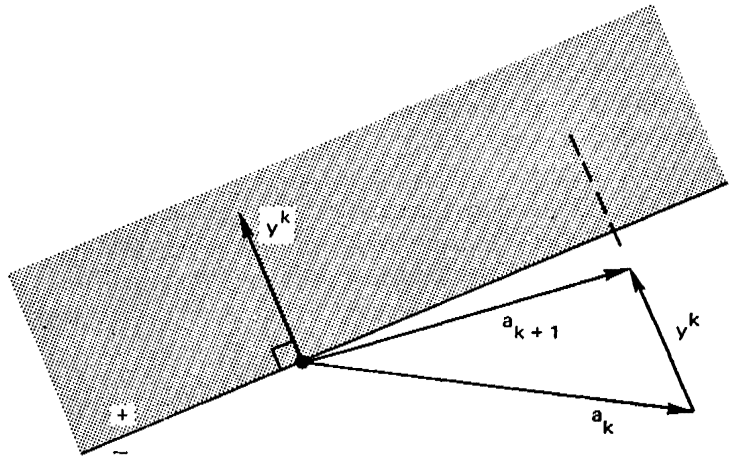

FIGURE 5.10. A step following the fixed-increment rule.

appeared in a reinforcement learning scheme proposed by Frank Rosenblatt for his *perceptron* brain model, and the proof of its convergence is known as the *Perceptron Convergence Theorem*. Geometrically, its interpretation in weight space is particularly clear. Since $\mathbf{a}_k$ misclassifies $\mathbf{y}^k$, $\mathbf{a}_k$ is not on the positive side of the $\mathbf{y}^k$ hyperplane $\mathbf{a}^t\mathbf{y}^k = 0$. The addition of $\mathbf{y}^k$ to $\mathbf{a}_k$ moves the weight vector directly toward and perhaps across this hyperplane (see Figure 5.10). Whether the hyperplane is crossed or not, the new inner product $\mathbf{a}_{k+1}^t\mathbf{y}^k$ is larger than the old inner product $\mathbf{a}_k^t\mathbf{y}^k$ by the amount $\|\mathbf{y}^k\|^2$, and the correction is clearly moving the weight vector in a good direction.

We shall now show that if the samples are linearly separable the sequence of weight vectors will terminate at a solution vector. In seeking a proof, it is natural to try to show that each correction brings the weight vector closer to the solution region. That is, one might try to show that if $\hat{\mathbf{a}}$ is any solution vector, then $\|\mathbf{a}_{k+1} - \hat{\mathbf{a}}\|$ is smaller than $\|\mathbf{a}_k - \hat{\mathbf{a}}\|$. While this turns out not to be true in general, we shall see that it is true for solution vectors that are sufficient long.

Let $\hat{\mathbf{a}}$ be any solution vector, so that $\hat{\mathbf{a}}^t\mathbf{y}_i$ is strictly positive for all i, and let α be a positive scale factor. From Eq. (14),

$$(\mathbf{a}_{k+1} - \alpha\hat{\mathbf{a}}) = (\mathbf{a}_k - \alpha\hat{\mathbf{a}}) + \mathbf{y}^k$$

and hence

$$\|\mathbf{a}_{k+1} - \alpha\hat{\mathbf{a}}\|^2 = \|\mathbf{a}_k - \alpha\hat{\mathbf{a}}\|^2 + 2(\mathbf{a}_k - \alpha\hat{\mathbf{a}})^t\mathbf{y}^k + \|\mathbf{y}^k\|^2.$$

Since $\mathbf{y}^k$ was misclassified, $\mathbf{a}_k^t\mathbf{y}^k \leq 0$, and thus

$$\|\mathbf{a}_{k+1} - \alpha\hat{\mathbf{a}}\|^2 \leq \|\mathbf{a}_k - \alpha\hat{\mathbf{a}}\|^2 - 2\alpha\hat{\mathbf{a}}^t\mathbf{y}^k + \|\mathbf{y}^k\|^2.$$

Since $\hat{\mathbf{a}}^t\mathbf{y}^k$ is strictly positive, the second term will dominate the third if α is sufficiently large. In particular, if we let

$$\beta^2 = \max_i \|\mathbf{y}_i\|^2 \tag{15}$$

and

$$\gamma = \min_i \hat{\mathbf{a}}^t\mathbf{y}_i > 0, \tag{16}$$

then

$$\|\mathbf{a}_{k+1} - \alpha\hat{\mathbf{a}}\|^2 \leq \|\mathbf{a}_k - \alpha\hat{\mathbf{a}}\|^2 - 2\alpha\gamma + \beta^2,$$

and with the choice

$$\alpha = \frac{\beta^2}{\gamma} \tag{17}$$

we obtain

$$\|\mathbf{a}_{k+1} - \alpha\hat{\mathbf{a}}\|^2 \leq \|\mathbf{a}_k - \alpha\hat{\mathbf{a}}\|^2 - \beta^2.$$

Thus, the squared distance from $\mathbf{a}_k$ to $\alpha\hat{\mathbf{a}}$ is reduced by at least β^2 at each correction, and after k corrections

$$\|\mathbf{a}_{k+1} - \alpha\hat{\mathbf{a}}\|^2 \leq \|\mathbf{a}_1 - \alpha\hat{\mathbf{a}}\|^2 - k\beta^2.$$

Since the squared distance can not become negative, it follows that the sequence of corrections must terminate after no more than k_0 corrections, where

$$k_0 = \frac{\|\mathbf{a}_1 - \alpha\hat{\mathbf{a}}\|^2}{\beta^2}. \tag{18}$$

Since a correction occurs whenever a sample is misclassified, and since each sample appears infinitely often in the sequence, it follows that when corrections cease the resulting weight vector must classify all of the samples correctly.

∎

The number k_0 gives us a bound on the number of corrections. If $\mathbf{a}_1 = \mathbf{0}$, we get the following particularly simple expression for k_0:

$$k_0 = \frac{\alpha^2\|\hat{\mathbf{a}}\|^2}{\beta^2} = \frac{\beta^2\|\hat{\mathbf{a}}\|^2}{\gamma^2} = \frac{\max_i\|\mathbf{y}_i\|^2\,\|\hat{\mathbf{a}}\|^2}{\min_i[\mathbf{y}_i^t\hat{\mathbf{a}}]^2}. \tag{19}$$

This shows that the difficulty of the problem is essentially determined by the samples most nearly orthogonal to the solution vector. Unfortunately, it provides no help when we face an unsolved problem, since the bound is expressed in terms of an unknown solution vector. In general, it is clear that linearly-separable problems can be made arbitrarily difficult to solve by making the samples be almost coplanar. Nevertheless, if the samples are linearly separable, the fixed-increment rule will yield a solution after a finite number of corrections.

5.5.3 Some Direct Generalizations

The fixed increment rule can be generalized to provide a variety of related algorithms. We shall briefly consider two variants of particular interest. The first variant introduces a *variable increment* ρ_k and a margin b, and calls for a correction whenever $\mathbf{a}_k^t\mathbf{y}^k$ fails to exceed the margin. The algorithm is given by

$$\left.\begin{aligned} \mathbf{a}_1 &\quad \text{arbitrary} \\ \mathbf{a}_{k+1} &= \mathbf{a}_k + \rho_k\mathbf{y}^k \quad k \geq 1 \end{aligned}\right\}, \tag{20}$$

where now $\mathbf{a}_k^t\mathbf{y}^k \leq b$ for all k. It can be shown that if the samples are linearly separable and if

$$\rho_k \geq 0, \tag{21}$$

$$\lim_{m\to\infty} \sum_{k=1}^{m} \rho_k = \infty \tag{22}$$

and

$$\lim_{m\to\infty} \frac{\sum_{k=1}^{m} \rho_k^2}{\left(\sum_{k=1}^{m} \rho_k\right)^2} = 0, \tag{23}$$

then $\mathbf{a}_k$ converges to a solution vector $\mathbf{a}$ satisfying $\mathbf{a}^t\mathbf{y}_i > b$ for all i. In particular, these conditions on ρ_k are satisfied if ρ_k is a positive constant, or if it decreases like $1/k$.

Another variant of interest is our original gradient descent algorithm for J_p,

$$\left.\begin{aligned} \mathbf{a}_1 &\quad \text{arbitrary} \\ \mathbf{a}_{k+1} &= \mathbf{a}_k + \rho_k \sum_{\mathbf{y}\in\mathscr{Y}_k} \mathbf{y}, \end{aligned}\right\} \tag{24}$$

where $\mathscr{Y}_k$ is the set of samples misclassified by $\mathbf{a}_k$. It is easy to see that this algorithm will also yield a solution once one recognizes that if $\hat{\mathbf{a}}$ is a solution vector for $\mathbf{y}_1, \ldots, \mathbf{y}_n$, then it correctly classifies the correction vector

$$\mathbf{y}^k = \sum_{\mathbf{y}\in\mathscr{Y}_k} \mathbf{y}.$$

Thus, if the samples are linearly separable, all of the possible correction vectors form a linearly separable set, and if ρ_k satisfies Eqs. (21)–(23), the sequence of weight vectors produced by the gradient descent algorithm for J_p will always converge to a solution vector.

It is interesting to note that the conditions on ρ_k are satisfied if ρ_k is a positive constant, if it decreases like $1/k$, or even if it increases like k. Generally speaking, one would prefer to have ρ_k become smaller as time goes on. This is particularly true if there is reason to believe that the set of samples is not linearly separable, since it reduces the disruptive effects of a few "bad"

samples. However, in the separable case it is a curious fact that one can allow ρ_k to become larger and still obtain a solution.

This observation brings out one of the differences between theoretical and practical attitudes. From a theoretical viewpoint, it is interesting that we can obtain a solution in a finite number of steps for any finite set of separable samples, for any initial weight vector $\mathbf{a}_1$, for any nonnegative margin b, and for any scale factor ρ_k satisfying Eqs. (21)–(23). From a practical viewpoint, we want to make wise choices for these quantities. Consider the margin b, for example. If b is much smaller than $\rho_k \|\mathbf{y}^k\|^2$, the amount by which a correction increases $\mathbf{a}_k^t\mathbf{y}^k$, it is clear that it will have little effect at all. If it is much larger than $\rho_k \|\mathbf{y}^k\|^2$, many corrections will be needed to satisfy the condition $\mathbf{a}_k^t\mathbf{y}^k > b$. A value close to $\rho_k \|\mathbf{y}^k\|^2$ is often a useful compromise. In addition to these choices for ρ_k and b, the scaling of the components of $\mathbf{y}^k$ can also have a great effect on the results. The possession of a convergence theorem does not remove the need for thought in applying these techniques.

5.6 RELAXATION PROCEDURES

5.6.1 The Descent Algorithm

The criterion function $J_p(\mathbf{a})$ is by no means the only function we can construct that is minimized when $\mathbf{a}$ is a solution vector. A close but distinct relative is

$$J_q(\mathbf{a}) = \sum_{\mathbf{y}\in\mathcal{Y}} (\mathbf{a}^t\mathbf{y})^2, \tag{25}$$

where $\mathcal{Y}(\mathbf{a})$ again denotes the set of samples misclassified by $\mathbf{a}$. Like J_p, J_q focuses attention on the misclassified samples. Its chief difference is that its gradient is continuous, whereas the gradient of J_p is not. Thus, J_q presents a smoother surface to search. Unfortunately, J_q is so smooth near the boundary of the solution region that the sequence of weight vectors can converge to a point on the boundary. It is particularly embarrassing to spend some time following the gradient merely to reach the boundary point $\mathbf{a} = \mathbf{0}$. Another problem with J_q is that its value can be dominated by the longest sample vectors. Both of these problems are avoided by the criterion function*

$$J_r(\mathbf{a}) = \tfrac{1}{2} \sum_{\mathbf{y}\in\mathcal{Y}} \frac{(\mathbf{a}^t\mathbf{y} - b)^2}{\|\mathbf{y}\|^2}, \tag{26}$$

where now $\mathcal{Y}(\mathbf{a})$ is the set of samples for which $\mathbf{a}^t\mathbf{y} \leq b$. (If $\mathcal{Y}(\mathbf{a})$ is empty, we define J_r to be zero.) Thus, $J_r(\mathbf{a})$ is never negative, and is zero if and only

* The normalization by $\|\mathbf{y}\|^2$ simplifies the choice for ρ_k. In effect, it makes the choice $\rho_k = 1$ correspond to the optimal choice of Eq. (10). This matter is explored further in Problem 13.

if $\mathbf{a}^t\mathbf{y} \geq b$ for all of the samples. The gradient of J_r is given by

$$\nabla J_r = \sum_{\mathbf{y} \in \mathscr{Y}} \frac{\mathbf{a}^t\mathbf{y} - b}{\|\mathbf{y}\|^2}\,\mathbf{y},$$

so that the basic descent algorithm becomes

$$\left.\begin{aligned} &\mathbf{a}_1 \quad \text{arbitrary} \\ &\mathbf{a}_{k+1} = \mathbf{a}_k + \rho_k \sum_{\mathbf{y} \in \mathscr{Y}_k} \frac{b - \mathbf{a}^t\mathbf{y}}{\|\mathbf{y}\|^2}\,\mathbf{y} \end{aligned}\right\}. \tag{27}$$

As before, we find it easier to prove convergence when the samples are considered one at a time rather than jointly. We also limit our attention to the case $\rho_k = \rho$. Thus, we are again led to consider a sequence $\mathbf{y}^1, \mathbf{y}^2, \ldots$ formed from those samples that call for the weight vector to be corrected. The single-sample correction rule analogous to Eq. (27) is

$$\left.\begin{aligned} &\mathbf{a}_1 \quad \text{arbitrary} \\ &\mathbf{a}_{k+1} = \mathbf{a}_k + \rho \frac{b - \mathbf{a}_k^t\mathbf{y}^k}{\|\mathbf{y}^k\|^2}\,\mathbf{y}^k \end{aligned}\right\}, \tag{28}$$

where $\mathbf{a}_k^t\mathbf{y}^k \leq b$ for all k.

This algorithm is known as the *relaxation rule*, and it has a simple geometrical interpretation. The quantity

$$r_k = \frac{b - \mathbf{a}_k^t\mathbf{y}^k}{\|\mathbf{y}^k\|}$$

is the distance from $\mathbf{a}_k$ to the hyperplane $\mathbf{a}^t\mathbf{y}^k = b$. Since $\mathbf{y}^k/\|\mathbf{y}^k\|$ is the unit normal vector for that hyperplane, Eq. (28) calls for $\mathbf{a}_k$ to be moved a certain fraction ρ of the distance from $\mathbf{a}_k$ to the hyperplane. If $\rho = 1$, $\mathbf{a}_k$ is moved exactly to the hyperplane, so that the "tension" created by the inequality $\mathbf{a}_k^t\mathbf{y}^k \leq b$, is "relaxed." From Eq. (28), after a correction,

$$(\mathbf{a}_{k+1}^t\mathbf{y}^k - b) = (1 - \rho)(\mathbf{a}_k^t\mathbf{y}^k - b).$$

If $\rho < 1$, $\mathbf{a}_{k+1}^t\mathbf{y}^k$ is still less than b, while if $\rho > 1$, $\mathbf{a}_{k+1}^t\mathbf{y}^k$ is greater than b. These conditions are referred to as *underrelaxation* and *overrelaxation*, respectively. In general, we shall restrict ρ to the range $0 < \rho < 2$.

5.6.2 Convergence Proof

When the relaxation rule is applied to a set of linearly separable samples, the number of corrections may or may not be finite. If it is finite, then of course we have obtained a solution vector. If it is not finite, we shall see that $\mathbf{a}_k$ converges to a limit vector on the boundary of the solution region. Since the

region in which $\mathbf{a}^t\mathbf{y} \geq b$ is contained in a larger region where $\mathbf{a}^t\mathbf{y} > 0$ if $b > 0$, this implies that $\mathbf{a}_k$ will enter this larger region at least once, eventually remaining there for all k greater than some finite k_0.

The proof depends upon the fact that if $\hat{\mathbf{a}}$ is *any* vector in the solution region, i.e., any vector satisfying $\hat{\mathbf{a}}^t\mathbf{y}_i > b$ for all i, then at each step $\mathbf{a}_k$ gets closer to $\hat{\mathbf{a}}$. This fact follows at once from Eq. (28), since

$$\|\mathbf{a}_{k+1} - \hat{\mathbf{a}}\|^2 = \|\mathbf{a}_k - \hat{\mathbf{a}}\|^2 - 2\rho \frac{(b - \mathbf{a}_k^t\mathbf{y}^k)}{\|\mathbf{y}^k\|^2}(\hat{\mathbf{a}} - \mathbf{a}_k)^t\mathbf{y}^k + \rho^2 \frac{(b - \mathbf{a}_k^t\mathbf{y}^k)^2}{\|\mathbf{y}^k\|^2}$$

and

$$(\hat{\mathbf{a}} - \mathbf{a}_k)^t\mathbf{y}^k > b - \mathbf{a}_k^t\mathbf{y}^k \geq 0,$$

so that

$$\|\mathbf{a}_{k+1} - \hat{\mathbf{a}}\|^2 \leq \|\mathbf{a}_k - \hat{\mathbf{a}}\|^2 - \rho(2 - \rho)\frac{(b - \mathbf{a}_k^t\mathbf{y}^k)^2}{\|\mathbf{y}^k\|^2}.$$

Since we restrict ρ to the range $0 < \rho < 2$, it follows that $\|\mathbf{a}_{k+1} - \hat{\mathbf{a}}\| \leq \|\mathbf{a}_k - \hat{\mathbf{a}}\|$. Thus, the vectors in the sequence $\mathbf{a}_1, \mathbf{a}_2, \ldots$ get closer and closer to $\hat{\mathbf{a}}$, and in the limit as k goes to infinity the distance $\|\mathbf{a}_k - \hat{\mathbf{a}}\|$ approaches some limiting distance $r(\hat{\mathbf{a}})$. This means that as k goes to infinity $\mathbf{a}_k$ is confined to the surface of a hypersphere with center $\hat{\mathbf{a}}$ and radius $r(\hat{\mathbf{a}})$. Since this is true for any $\hat{\mathbf{a}}$ in the solution region, the limiting $\mathbf{a}_k$ is confined to the intersection of the hyperspheres centered about all of the possible solution vectors.

Let us show that the common intersection of these hyperspheres is a single point on the boundary of the solution region. Suppose first that there are at least two points $\mathbf{a}'$ and $\mathbf{a}''$ on the common intersection. Then $\|\mathbf{a}' - \hat{\mathbf{a}}\| = \|\mathbf{a}'' - \hat{\mathbf{a}}\|$ for every $\hat{\mathbf{a}}$ in the solution region. But this implies that the solution region is contained in the $(\hat{d} - 1)$-dimensional hyperplane of points equidistant from $\mathbf{a}'$ to $\mathbf{a}''$, whereas we know that the solution region is $\hat{d}$-dimensional. (Stated formally, if $\hat{\mathbf{a}}^t\mathbf{y}_i > 0$ for $i = 1, \ldots, n$, then for any $\hat{d}$-dimensional vector $\mathbf{v}$, $(\hat{\mathbf{a}} + \epsilon\mathbf{v})^t\mathbf{y}_i > 0$ for $i = 1, \ldots, n$ if ϵ is sufficiently small.) Thus, $\mathbf{a}_k$ converges to a single point $\mathbf{a}$. This point is certainly not inside the solution region, for then the sequence would be finite. It is not outside either, since each correction causes the weight vector to move ρ times its distance from the boundary plane, thereby preventing the vector from being bounded away from the boundary forever. Hence the limit point must be on the boundary.

5.7 NONSEPARABLE BEHAVIOR

The fixed-increment and relaxation procedures give us a number of simple methods for finding a separating vector when the samples are linearly

separable. All of these methods are called *error-correction procedures*, because they call for a modification of the weight vector when and only when an error is encountered. Their success on separable problems is largely due to this relentless search for an error-free solution. In practice, one would only consider the use of these methods if there was reason to believe that the error rate for the optimal linear discriminant function is low.

Of course, even if a separating vector is found for the design samples, it does not follow that the resulting classifier will perform well on independent test data. In Chapter 3 we pointed out that *any* set of fewer than $2\hat{d}$ samples is likely to be linearly separable. Thus, one should use several times that many design samples to overdetermine the classifier, thereby ensuring that the performance on design and test data will be similar. Unfortunately, sufficiently large design sets are almost certainly not linearly separable. This makes it important to know how the error-correction procedures will behave when the samples are nonseparable.

Since no weight vector can correctly classify every sample in a nonseparable set, it is clear that the corrections in an error-correction procedure can never cease. Each algorithm produces an infinite sequence of weight vectors, any member of which may or may not yield a useful solution. The exact nonseparable behavior of these rules has been studied thoroughly in only a few special cases. It is known, for example, that the length of the weight vectors produced by the fixed-increment rule is bounded. Empirical rules for terminating the correction procedure are often based on this tendency for the length of the weight vector to fluctuate near some limiting value. From a theoretical viewpoint, if the components of the samples are integer-valued, the fixed-increment procedure produces a finite-state process. If the correction process is terminated at some arbitrary point, the weight vector may or may not be in a good state. By averaging the weight vectors produced by the correction rule, one can reduce the risk of obtaining a bad solution by accidentally choosing an unfortunate termination time.

A number of similar heuristic modifications to the error-correction rules have been suggested and studied empirically. The goal of these modifications is to obtain acceptable performance on nonseparable problems while preserving the ability to find a separating vector on separable problems. A common suggestion is the use of a variable increment ρ_k, with ρ_k approaching zero as k approaches infinity. The rate at which ρ_k approaches zero is quite important. If it is too slow, the results will still be sensitive to those samples that render the set nonseparable. If it is too fast, the weight vector may converge prematurely with less than optimal results. One way to choose ρ_k is to make it a function of recent performance, decreasing it as performance improves. Another way is to program ρ_k by a choice such as $\rho_k = \rho_1/k$. When we examine stochastic approximation techniques, we shall see that

this latter choice is the theoretical solution to an analogous problem. Before we take up this topic, however, we shall consider an approach that sacrifices the ability to obtain a separating vector for good compromise performance on both separable and nonseparable problems.

5.8 MINIMUM SQUARED ERROR PROCEDURES

5.8.1 Minimum Squared Error and the Pseudoinverse

The criterion functions we have considered thus far have focussed their attention on the misclassified samples. We shall now consider a criterion function that involves all of the samples. Where previously we have sought a weight vector $\mathbf{a}$ making all of the inner products $\mathbf{a}^t\mathbf{y}_i$ positive, now we shall try to make $\mathbf{a}^t\mathbf{y}_i = b_i$, where the b_i are some arbitrarily specified positive constants. Thus, we have replaced the problem of finding the solution to a set of linear inequalities with the more stringent but better understood problem of finding the solution to a set of linear equations.

The treatment of simultaneous linear equations is simplified by introducing matrix notation. Let Y be the n-by-$\hat{d}$ matrix whose ith row is the vector $\mathbf{y}_i^t$, and let $\mathbf{b}$ be the column vector $\mathbf{b} = (b_1, \ldots, b_n)^t$. Then our problem is to find a weight vector $\mathbf{a}$ satisfying

$$Y\mathbf{a} = \mathbf{b}. \tag{29}$$

If Y were nonsingular, we could write $\mathbf{a} = Y^{-1}\mathbf{b}$ and obtain a formal solution at once. However, Y is rectangular, usually with more rows than columns. When there are more equations than unknowns, $\mathbf{a}$ is overdetermined, and ordinarily no exact solution exists. However, we can seek a weight vector $\mathbf{a}$ that minimizes some function of the error between $Y\mathbf{a}$ and $\mathbf{b}$. If we define the error vector $\mathbf{e}$ by

$$\mathbf{e} = Y\mathbf{a} - \mathbf{b}, \tag{30}$$

then one approach is to try to minimize the squared length of the error vector. This is equivalent to minimizing the sum-of-squared-error criterion function

$$J_s(\mathbf{a}) = \|Y\mathbf{a} - \mathbf{b}\|^2 = \sum_{i=1}^{n} (\mathbf{a}^t\mathbf{y}_i - b_i)^2. \tag{31}$$

The problem of minimizing the sum of squared errors is a classical one. It can be solved by a gradient search procedure, as we shall see in Section 5.8.4. A simple closed-form solution can also be found by forming the gradient

$$\nabla J_s = \sum_{i=1}^{n} 2(\mathbf{a}^t\mathbf{y}_i - b_i)\mathbf{y}_i = 2Y^t(Y\mathbf{a} - \mathbf{b})$$

and setting it equal to zero. This yields the necessary condition

$$Y^t Y\mathbf{a} = Y^t\mathbf{b}, \tag{32}$$

and we have converted the problem of solving $Y\mathbf{a} = \mathbf{b}$ to that of solving $Y^tY\mathbf{a} = Y^t\mathbf{b}$. This celebrated equation has the great advantage that the $\hat{d}$-by-$\hat{d}$ matrix Y^tY is square and often nonsingular. If it is nonsingular, we can solve for $\mathbf{a}$ uniquely as

$$\begin{aligned}\mathbf{a} &= (Y^tY)^{-1}Y^t\mathbf{b} \\ &= Y^\dagger\mathbf{b},\end{aligned} \tag{33}$$

where the $\hat{d}$-by-n matrix

$$Y^\dagger = (Y^tY)^{-1}Y^t \tag{34}$$

is called the *pseudoinverse* of Y. Note that if Y is square and nonsingular, the pseudoinverse coincides with the regular inverse. Note also that $Y^\dagger Y = I$, but $YY^\dagger \neq I$ in general. If Y^tY is singular, the solution to Eq. (32) is not unique. However, a minimum-squared-error (MSE) solution always exists. In particular, if $Y^\dagger$ is defined more generally by

$$Y^\dagger = \lim_{\epsilon \to 0} (Y^tY + \epsilon I)^{-1}Y^t, \tag{35}$$

it can be shown that this limit always exists, and that $\mathbf{a} = Y^\dagger\mathbf{b}$ is a MSE solution to $Y\mathbf{a} = \mathbf{b}$. These and other interesting properties of the pseudoinverse are well treated in the literature.

The MSE solution depends on the margin vector $\mathbf{b}$, and we shall see that different choices for $\mathbf{b}$ give the solution different properties. If $\mathbf{b}$ is fixed arbitrarily, there is no reason to believe that the MSE solution yields a separating vector in the linearly separable case. However, it is reasonable to hope that by minimizing the squared-error criterion function we might obtain a useful discriminant function in both the separable and the nonseparable cases. We shall now examine two properties of the solution that support this hope.

5.8.2 Relation to Fisher's Linear Discriminant

In this section we shall show that with the proper choice of the vector $\mathbf{b}$, the MSE discriminant function $\mathbf{a}^t\mathbf{y}$ is directly related to Fisher's linear discriminant. To do this, we must return to the use of linear rather than generalized linear discriminant functions. We assume that we have a set of n d-dimensional samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$, n_1 of which are in the subset $\mathcal{X}_1$ labelled ω_1, and n_2 of which are in the subset $\mathcal{X}_2$ labelled ω_2. Further, we assume that a sample $\mathbf{y}_i$ is formed from $\mathbf{x}_i$ by adding a threshold component of unity, and by multiplying the resulting vector by -1 if the sample is labelled ω_2. With no loss in generality, we can assume that the first n_1 samples are

labelled ω_1 and the second n_2 are labelled ω_2. Then the matrix Y can be partitioned as follows:

$$Y = \begin{bmatrix} \mathbf{u}_1 & X_1 \\ -\mathbf{u}_2 & -X_2 \end{bmatrix},$$

where $\mathbf{u}_i$ is a column vector of n_i ones, and X_i is a n_i-by-d matrix whose rows are the samples labelled ω_i. We partition $\mathbf{a}$ and $\mathbf{b}$ correspondingly, with

$$\mathbf{a} = \begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix}$$

and with

$$\mathbf{b} = \begin{bmatrix} \frac{n}{n_1}\mathbf{u}_1 \\ \frac{n}{n_2}\mathbf{u}_2 \end{bmatrix}.$$

We shall see that this special choice for $\mathbf{b}$ links the MSE solution to Fisher's linear discriminant.

We begin by writing Eq. (32) for $\mathbf{a}$ in terms of the partitioned matrices:

$$\begin{bmatrix} \mathbf{u}_1^t & -\mathbf{u}_2^t \\ X_1^t & -X_2^t \end{bmatrix} \begin{bmatrix} \mathbf{u}_1 & X_1 \\ -\mathbf{u}_2 & -X_2 \end{bmatrix} \begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix} = \begin{bmatrix} \mathbf{u}_1^t & -\mathbf{u}_2^t \\ X_1^t & -X_2^t \end{bmatrix} \begin{bmatrix} \frac{n}{n_1}\mathbf{u}_1 \\ \frac{n}{n_2}\mathbf{u}_2 \end{bmatrix}. \tag{36}$$

By defining the sample means $\mathbf{m}_i$ and the pooled sample scatter matrix S_W as

$$\mathbf{m}_i = \frac{1}{n_i} \sum_{\mathbf{x} \in \mathcal{X}_i} \mathbf{x} \qquad i = 1, 2 \tag{37}$$

and

$$S_W = \sum_{i=1}^{2} \sum_{\mathbf{x} \in \mathcal{X}_i} (\mathbf{x} - \mathbf{m}_i)(\mathbf{x} - \mathbf{m}_i)^t, \tag{38}$$

we can multiply the matrices in Eq. (36) and obtain

$$\begin{bmatrix} n & (n_1\mathbf{m}_1 + n_2\mathbf{m}_2)^t \\ (n_1\mathbf{m}_1 + n_2\mathbf{m}_2) & S_W + n_1\mathbf{m}_1\mathbf{m}_1^t + n_2\mathbf{m}_2\mathbf{m}_2^t \end{bmatrix} \begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix} = \begin{bmatrix} 0 \\ n(\mathbf{m}_1 - \mathbf{m}_2) \end{bmatrix}.$$

This can be viewed as a pair of equations, the first of which can be solved for w_0 in terms of $\mathbf{w}$:

$$w_0 = -\mathbf{m}^t\mathbf{w}, \tag{39}$$

where $\mathbf{m}$ is the mean of all of the samples. Substituting this in the second equation and performing a few algebraic manipulations, we obtain

$$\left[\frac{1}{n} S_W + \frac{n_1 n_2}{n^2} (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^t\right]\mathbf{w} = \mathbf{m}_1 - \mathbf{m}_2. \tag{40}$$

Since the vector $(\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^t\mathbf{w}$ is in the direction of $\mathbf{m}_1 - \mathbf{m}_2$ for any value of $\mathbf{w}$, we can write

$$\frac{n_1 n_2}{n^2} (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^t\mathbf{w} = (1 - \alpha)(\mathbf{m}_1 - \mathbf{m}_2),$$

where α is some scalar. Then Eq. (40) yields

$$\mathbf{w} = \alpha n S_W^{-1}(\mathbf{m}_1 - \mathbf{m}_2), \tag{41}$$

which, except for an unimportant scale factor, is identical to the solution for Fisher's linear discriminant. In addition, we obtain the threshold weight w_0 and the following decision rule: Decide ω_1 if $\mathbf{w}^t(\mathbf{x} - \mathbf{m}) > 0$; otherwise decide ω_2.

5.8.3 Asymptotic Approximation to an Optimal Discriminant

Another property of the MSE solution that recommends its use is that if $\mathbf{b} = \mathbf{u}_n$ it approaches a minimum mean-squared-error approximation to the Bayes discriminant function

$$g_0(\mathbf{x}) = P(\omega_1 \mid \mathbf{x}) - P(\omega_2 \mid \mathbf{x}) \tag{42}$$

in the limit as the number of samples approaches infinity. To demonstrate this fact, we must assume that the samples are drawn independently according to the probability law

$$p(\mathbf{x}) = p(\mathbf{x} \mid \omega_1)P(\omega_1) + p(\mathbf{x} \mid \omega_2)P(\omega_2). \tag{43}$$

In terms of the augmented vector $\mathbf{y}$, the MSE solution yields the series expansion $g(\mathbf{x}) = \mathbf{a}^t\mathbf{y}$, where $\mathbf{y} = \mathbf{y}(\mathbf{x})$. If we define the mean-squared approximation error by

$$\epsilon^2 = \int [\mathbf{a}^t\mathbf{y} - g_0(\mathbf{x})]^2 p(\mathbf{x})\, d\mathbf{x}, \tag{44}$$

then our goal is to show that ϵ^2 is minimized by the solution $\mathbf{a} = Y^\dagger\mathbf{u}_n$.

The proof is simplified if we preserve the distinction between Class 1 and Class 2 samples. In terms of the unnormalized data, the criterion function J_s becomes

$$\begin{aligned} J_s(\mathbf{a}) &= \sum_{\mathbf{y}\in\mathscr{Y}_1} (\mathbf{a}^t\mathbf{y} - 1)^2 + \sum_{\mathbf{y}\in\mathscr{Y}_2} (\mathbf{a}^t\mathbf{y} + 1)^2 \\ &= n\left[\frac{n_1}{n} \cdot \frac{1}{n_1} \sum_{\mathbf{y}\in\mathscr{Y}_1} (\mathbf{a}^t\mathbf{y} - 1)^2 + \frac{n_2}{n} \cdot \frac{1}{n_2} \sum_{\mathbf{y}\in\mathscr{Y}_2} (\mathbf{a}^t\mathbf{y} + 1)^2\right]. \end{aligned}$$

Thus, by the law of large numbers, as n approaches infinity $(1/n)J_s(\mathbf{a})$ approaches

$$\bar{J}(\mathbf{a}) = P(\omega_1)E_1[(\mathbf{a}^t\mathbf{y} - 1)^2] + P(\omega_2)E_2[(\mathbf{a}^t\mathbf{y} + 1)^2], \tag{45}$$

with probability one, where

$$E_1[(\mathbf{a}^t\mathbf{y} - 1)^2] = \int (\mathbf{a}^t\mathbf{y} - 1)^2 p(\mathbf{x} \mid \omega_1)\, d\mathbf{x}$$

and

$$E_2[(\mathbf{a}^t\mathbf{y} + 1)^2] = \int (\mathbf{a}^t\mathbf{y} + 1)^2 p(\mathbf{x} \mid \omega_2)\, d\mathbf{x}.$$

Now, if we recognize from Eq. (42) that

$$g_0(\mathbf{x}) = \frac{p(\mathbf{x}, \omega_1) - p(\mathbf{x}, \omega_2)}{p(\mathbf{x})}$$

we see that

$$\begin{aligned}
\bar{J}(\mathbf{a}) &= \int (\mathbf{a}^t\mathbf{y} - 1)^2 p(\mathbf{x}, \omega_1)\, d\mathbf{x} + \int (\mathbf{a}^t\mathbf{y} + 1)^2 p(\mathbf{x}, \omega_2) d\mathbf{x} \\
&= \int (\mathbf{a}^t\mathbf{y})^2 p(\mathbf{x})\, d\mathbf{x} - 2\int \mathbf{a}^t\mathbf{y} g_0(\mathbf{x}) p(\mathbf{x})\, d\mathbf{x} + 1 \\
&= \int [\mathbf{a}^t\mathbf{y} - g_0(\mathbf{x})]^2 p(\mathbf{x})\, d\mathbf{x} + \left[1 - \int g_0^2(\mathbf{x}) p(\mathbf{x})\, d\mathbf{x}\right].
\end{aligned} \tag{46}$$

The second term in this sum is independent of the weight vector $\mathbf{a}$. Hence, the $\mathbf{a}$ that minimizes J_s also minimizes ϵ^2, the mean-squared-error between $\mathbf{a}^t\mathbf{y}$ and $g_0(\mathbf{x})$.

This result gives considerable insight into the MSE procedure. By approximating $g_0(\mathbf{x})$, the discriminant function $\mathbf{a}^t\mathbf{y}$ gives direct information about the a posteriori probabilities $P(\omega_1 \mid \mathbf{x}) = (1 + g_0)/2$ and $P(\omega_2 \mid \mathbf{x}) = (1 - g_0)/2$. The quality of the approximation depends on the functions $y_i(\mathbf{x})$ and the number of terms in the expansion $\mathbf{a}^t\mathbf{y}$. Unfortunately, the mean-square-error criterion places emphasis on points where $p(\mathbf{x})$ is large, rather than on points near the decision surface $g_0(\mathbf{x}) = 0$. Thus, the discriminant function that "best" approximates the Bayes discriminant does not necessarily minimize the probability of error. Despite this defect, the MSE solution has interesting properties, and has received considerable attention in the literature. We shall encounter the mean-square approximation of $g_0(\mathbf{x})$ again when we consider stochastic approximation methods.

5.8.4 The Widrow-Hoff Procedure

We remarked earlier that $J_s(\mathbf{a}) = \| Y\mathbf{a} - \mathbf{b}\|^2$ could be minimized by a gradient descent procedure. Such an approach has two advantages over merely computing the pseudoinverse: (1) it avoids the problems that arise when Y^tY is

singular, and (2) it avoids the need for working with large matrices. In addition, the computation involved is effectively a feedback scheme which automatically copes with some of the computational problems due to roundoff or truncation. Since $\nabla J_s = 2Y^t(Y\mathbf{a} - \mathbf{b})$, the obvious descent algorithm is

$$\left.\begin{aligned} &\mathbf{a}_1 \quad \text{arbitrary} \\ &\mathbf{a}_{k+1} = \mathbf{a}_k - \rho_k Y^t(Y\mathbf{a}_k - \mathbf{b}) \end{aligned}\right\}.$$

It is a good exercise to show that if

$$\rho_k = \rho_1/k,$$

where ρ_1 is any positive constant, then this rule generates a sequence of weight vectors that converges to a limiting vector $\mathbf{a}$ satisfying

$$Y^t(Y\mathbf{a} - \mathbf{b}) = 0.$$

Thus, the descent algorithm always yields a solution regardless of whether or not Y^tY is singular.

While the $\hat{d}$-by-$\hat{d}$ matrix Y^tY is usually smaller than the $\hat{d}$-by-n matrix $Y^\dagger$, the storage requirements can be reduced still further by considering the samples sequentially and using the *Widrow-Hoff* or *LMS rule*

$$\left.\begin{aligned} &\mathbf{a}_1 \quad \text{arbitrary} \\ &\mathbf{a}_{k+1} = \mathbf{a}_k + \rho_k(b_k - \mathbf{a}_k^t\mathbf{y}^k)\mathbf{y}^k \end{aligned}\right\}. \tag{47}$$

At first glance this descent algorithm appears to be essentially the same as the relaxation rule. The primary difference is that the relaxation rule is an error-correction rule, so that $\mathbf{a}_k^t\mathbf{y}^k$ is always less than b_k, whereas the Widrow-Hoff rule "corrects" $\mathbf{a}_k$ whenever $\mathbf{a}_k^t\mathbf{y}^k$ does not equal b_k. In most cases of interest, it is impossible to satisfy all of the equations $\mathbf{a}^t\mathbf{y}^k = b_k$, so that corrections never cease. Thus, ρ_k must decrease with k to obtain convergence, the choice $\rho_k = \rho_1/k$ being common. Exact analysis of the behavior of the Widrow-Hoff rule in the deterministic case is rather complicated, and merely indicates that the sequence of weight vectors tends to converge to the desired solution. Instead of pursuing this topic further, we shall turn to a very similar rule that arises from a stochastic descent procedure.

5.8.5 Stochastic Approximation Methods

All of the iterative descent procedures we have considered thus far have been described in deterministic terms. We are given a particular set of samples, and we generate a particular sequence of weight vectors. In this section we digress briefly to consider a MSE procedure in which the samples are drawn randomly, resulting in a random sequence of weight vectors. A complete

analysis would require use of the theory of stochastic approximation, and will not be attempted. However, the main ideas, which will be presented without proof, are simple.

Suppose that samples are drawn independently by selecting a state of nature with probability $P(\omega_i)$ and then selecting an $\mathbf{x}$ according to the probability law $p(\mathbf{x} \mid \omega_i)$. For each $\mathbf{x}$ we let z be its *label*, with $z = +1$ if $\mathbf{x}$ is labelled ω_1 and $z = -1$ if $\mathbf{x}$ is labelled ω_2. Then the data consist of an infinite sequence of independent pairs $(\mathbf{x}_1, z_1), (\mathbf{x}_2, z_2), \ldots, (\mathbf{x}_k, z_k), \ldots$.

Even though the label variable z is binary-valued, it can be thought of as a noisy version of the Bayes discriminant function $g_0(\mathbf{x})$. This follows from the observation that

$$P(z = 1 \mid \mathbf{x}) = P(\omega_1 \mid \mathbf{x}),$$

and

$$P(z = -1 \mid \mathbf{x}) = P(\omega_2 \mid \mathbf{x}),$$

so that the conditional mean of z is given by

$$E_{z|x}[z] = \sum_z zP(z \mid \mathbf{x}) = P(\omega_1 \mid \mathbf{x}) - P(\omega_2 \mid \mathbf{x}) = g_0(\mathbf{x}). \tag{48}$$

Suppose that we wish to approximate $g_0(\mathbf{x})$ by the finite series expansion

$$g(\mathbf{x}) = \mathbf{a}^t\mathbf{y} = \sum_{i=1}^{\hat{d}} a_i y_i(\mathbf{x}),$$

where both the basis functions $y_i(\mathbf{x})$ and the number of terms $\hat{d}$ are known. Then we can seek a weight vector $\hat{\mathbf{a}}$ that minimizes the mean-squared approximation error

$$\epsilon^2 = E[(\mathbf{a}^t\mathbf{y} - g_0(\mathbf{x}))^2]. \tag{49}$$

Minimization of ϵ^2 would appear to require knowledge of the Bayes discriminant $g_0(\mathbf{x})$. However, as one might have guessed from the analogous situation in Section 5.8.3, it can be shown that the weight vector $\hat{\mathbf{a}}$ that minimizes ϵ^2 also minimizes the criterion function

$$J_m(\mathbf{a}) = E[(\mathbf{a}^t\mathbf{y} - z)^2]. \tag{50}$$

This should also be plausible from the fact that z is essentially a noisy version of $g_0(\mathbf{x})$ (see Figure 5.11). Since

$$\nabla J_m = 2E[(\mathbf{a}^t\mathbf{y} - z)\mathbf{y}],$$

we can obtain the closed-form solution

$$\hat{\mathbf{a}} = E[\mathbf{y}\mathbf{y}^t]^{-1}E[z\mathbf{y}]. \tag{51}$$

Thus, one way to use the samples is to estimate $E[\mathbf{y}\mathbf{y}^t]$ and $E[z\mathbf{y}]$, and use Eq. (51) to obtain the MSE optimum linear discriminant. An alternative is to

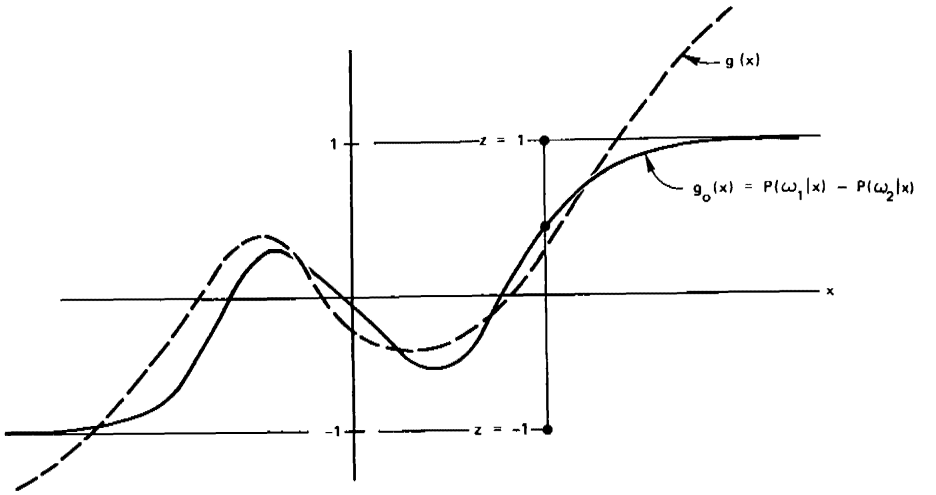

FIGURE 5.11. Approximating the Bayes discriminant function.

minimize $J_m(\mathbf{a})$ by a gradient descent procedure. Suppose that in place of the true gradient we substitute the noisy version $2(\mathbf{a}^t\mathbf{y}_k - z_k)\mathbf{y}_k$. This leads to the descent algorithm

$$\mathbf{a}_{k+1} = \mathbf{a}_k + \rho_k(z_k - \mathbf{a}_k^t\mathbf{y}_k)\mathbf{y}_k, \tag{52}$$

which is basically just the Widrow-Hoff rule. It can be shown that if $E[\mathbf{y}\mathbf{y}^t]$ is nonsingular and if the coefficients ρ_k satisfy

$$\lim_{m\to\infty} \sum_{k=1}^{m} \rho_k = +\infty \tag{53}$$

and

$$\lim_{m\to\infty} \sum_{k=1}^{m} \rho_k^2 < \infty, \tag{54}$$

then $\mathbf{a}_k$ converges to $\hat{\mathbf{a}}$ in mean square:

$$\lim_{k\to\infty} E[\|\mathbf{a}_k - \hat{\mathbf{a}}\|^2] = 0. \tag{55}$$

The reasons we need these conditions on ρ_k are simple. The first condition keeps the weight vector from converging so fast that a systematic error will remain forever uncorrected. The second condition ensures that random fluctuations are eventually suppressed. Both conditions are satisfied by the conventional choice $\rho_k = 1/k$. Unfortunately, this kind of programmed decrease of ρ_k, independent of the problem at hand, often leads to very slow convergence.

Of course, this is neither the only nor the best descent algorithm for minimizing J_m. For example, if we note that the matrix of second partial derivatives for J_m is given by

$$D = 2E[\mathbf{y}\mathbf{y}^t],$$

we see that Newton's algorithm for minimizing J_m (Eq. (11)) is

$$\mathbf{a}_{k+1} = \mathbf{a}_k + E[\mathbf{y}\mathbf{y}^t]^{-1}E[(z - \mathbf{a}^t\mathbf{y})\mathbf{y}].$$

A stochastic analog of this algorithm is

$$\mathbf{a}_{k+1} = \mathbf{a}_k + R_{k+1}(z_k - \mathbf{a}_k^t\mathbf{y}_k)\mathbf{y}_k \tag{56}$$

with

$$R_{k+1}^{-1} = R_k^{-1} + \mathbf{y}_k\mathbf{y}_k^t, \tag{57}$$

or, equivalently,*

$$R_{k+1} = R_k - \frac{R_k\mathbf{y}_k(R_k\mathbf{y}_k)^t}{1 + \mathbf{y}_k^tR_k\mathbf{y}_k}. \tag{58}$$

This algorithm also produces a sequence of weight vectors that converges to the optimal solution in mean square. Its convergence is faster, but it requires more computation per step.

These gradient procedures can be viewed as methods for minimizing a criterion function, or finding the zero of its gradient, in the presence of noise. In the statistical literature, functions such as J_m and ∇J_m that have the form $E[f(\mathbf{a}, \mathbf{x})]$ are called *regression functions*, and the iterative algorithms are called *stochastic approximation procedures*. The best known of these are the Kiefer-Wolfowitz procedure for minimizing a regression function, and the Robbins-Monro procedure for finding a root of a regression function. Often the easiest way to obtain a convergence proof for a particular descent or approximation procedure is to show that it satisfies the convergence conditions for these more general procedures. Unfortunately, an exposition of these methods in their full generality would lead us rather far afield, and we must close this digression by referring the interested reader to the literature.

5.9 THE HO-KASHYAP PROCEDURES

5.9.1 The Descent Procedure

The procedures we have considered thus far differ in several ways. The perceptron and relaxation procedures find separating vectors if the samples are linearly separable, but do not converge on nonseparable problems. The MSE procedures yield a weight vector whether the samples are linearly separable or not, but there is no guarantee that this vector is a separating vector in the separable case. If the margin vector $\mathbf{b}$ is chosen arbitrarily, all we can say is that the MSE procedures minimize $\|Y\mathbf{a} - \mathbf{b}\|^2$. Now if the

* This recursive formula for computing R_k, which is roughly $(1/k)E[\mathbf{y}\mathbf{y}^t]^{-1}$, can not be used if R_k is singular. The equivalence of Eq. (57) and Eq. (58) follows from Problem 10 of Chapter 3.

samples happen to be linearly separable, then there exists an $\hat{\mathbf{a}}$ and a $\hat{\mathbf{b}}$ such that

$$Y\hat{\mathbf{a}} = \hat{\mathbf{b}} > 0,$$

where by $\hat{\mathbf{b}} > 0$, we mean that every component of $\hat{\mathbf{b}}$ is positive. Clearly, were we to take $\mathbf{b} = \hat{\mathbf{b}}$ and apply the MSE procedure, we would obtain a separating vector. Of course, we usually do not know $\hat{\mathbf{b}}$ beforehand. However, we shall now see how the MSE procedure can be modified to obtain both a separating vector $\mathbf{a}$ and a margin vector $\mathbf{b}$. The underlying idea comes from the observation that if the samples are separable, and if both $\mathbf{a}$ and $\mathbf{b}$ in the criterion function

$$J_s(\mathbf{a}, \mathbf{b}) = \|Y\mathbf{a} - \mathbf{b}\|^2$$

are allowed to vary (subject to the constraint $\mathbf{b} > 0$), then the minimum value of J_s is zero, and the $\mathbf{a}$ that achieves that minimum is a separating vector.

To minimize J_s, we shall use a modified gradient descent procedure. The gradient of J_s with respect to $\mathbf{a}$ is given by

$$\nabla_{\mathbf{a}} J_s = 2Y^t(Y\mathbf{a} - \mathbf{b}), \tag{59}$$

and the gradient of J_s with respect to $\mathbf{b}$ is given by

$$\nabla_{\mathbf{b}} J_s = -2(Y\mathbf{a} - \mathbf{b}). \tag{60}$$

For any value of $\mathbf{b}$, we can always take

$$\mathbf{a} = Y^{\dagger}\mathbf{b}, \tag{61}$$

thereby obtaining $\nabla_{\mathbf{a}} J_s = 0$ and minimizing J_s with respect to $\mathbf{a}$ in one step. We are not so free to modify $\mathbf{b}$, however, since we must respect the constraint $\mathbf{b} > 0$, and we must avoid a descent procedure that converges to $\mathbf{b} = 0$. One way to prevent $\mathbf{b}$ from converging to zero is to start with $\mathbf{b} > 0$ and to refuse to reduce any of its components. We can do this and still try to follow the negative gradient if we first set all positive components of $\nabla_{\mathbf{b}} J_s$ to zero. Thus, if we let $|\mathbf{v}|$ denote the vector whose components are the magnitudes of the corresponding components of $\mathbf{v}$, we are led to consider a descent procedure of the form

$$\mathbf{b}_{k+1} = \mathbf{b}_k - \rho_k^{\frac{1}{2}}[\nabla_{\mathbf{b}} J_s - |\nabla_{\mathbf{b}} J_s|].$$

Using Eqs. (60) and (61), and being a bit more specific, we obtain the *Ho-Kashyap algorithm* for minimizing $J_s(\mathbf{a}, \mathbf{b})$:

$$\left.\begin{aligned} &\mathbf{b}_1 > 0 \text{ but otherwise arbitrary} \\ &\mathbf{b}_{k+1} = \mathbf{b}_k + 2\rho\mathbf{e}_k^+ \end{aligned}\right\} \tag{62}$$

where $\mathbf{e}_k$ is the error vector

$$\mathbf{e}_k = Y\mathbf{a}_k - \mathbf{b}_k, \tag{63}$$

$\mathbf{e}_k^+$ is the positive part of the error vector

$$\mathbf{e}_k^+ = \tfrac{1}{2}(\mathbf{e}_k + |\mathbf{e}_k|), \tag{64}$$

and

$$\mathbf{a}_k = Y^\dagger \mathbf{b}_k, \qquad k = 1, 2, \ldots . \tag{65}$$

Since the weight vector $\mathbf{a}_k$ is completely determined by the margin vector $\mathbf{b}_k$, this is basically an algorithm for producing a sequence of margin vectors. The initial vector $\mathbf{b}_1$ is positive to begin with, and if $\rho > 0$, all subsequent vectors $\mathbf{b}_k$ are positive. We might worry that if none of the components of $\mathbf{e}_k$ is positive, so that $\mathbf{b}_k$ stops changing, we might fail to find a solution. However, we shall see that in that case either $\mathbf{e}_k = 0$ and we have a solution, or $\mathbf{e}_k \leq 0$ and we have proof that the samples are not linearly separable.

5.9.2 Convergence Proof

We shall now show that if the samples are linearly separable, and if $0 < \rho < 1$, then the Ho–Kashyap procedure will yield a solution vector in a finite number of steps. To make the algorithm terminate, we should add a terminating condition stating that corrections cease once a solution vector is obtained. However, it is mathematically more convenient to let the corrections continue and show that the error vector $\mathbf{e}_k$ either becomes zero for some finite k, or converges to zero as k goes to infinity.

It is clear that either $\mathbf{e}_k = 0$ for some k, say k_0, or there are no zero vectors in the sequence $\mathbf{e}_1, \mathbf{e}_2, \ldots$. In the first case, once a zero vector is obtained, no further changes occur to $\mathbf{a}_k$, $\mathbf{b}_k$, or $\mathbf{e}_k$, and $Y\mathbf{a}_k = \mathbf{b}_k > 0$ for all $k \geq k_0$. Thus, if we happen to obtain a zero error vector, the algorithm automatically terminates with a solution vector.

Suppose now that $\mathbf{e}_k$ is never zero for finite k. To see that $\mathbf{e}_k$ must nevertheless converge to zero, we begin by asking whether or not we might possibly obtain an $\mathbf{e}_k$ with no positive components. This would be most unfortunate, since we would have $Y\mathbf{a}_k \leq \mathbf{b}_k$, and since $\mathbf{e}_k^+$ would be zero, we would obtain no further changes in $\mathbf{a}_k$, $\mathbf{b}_k$, or $\mathbf{e}_k$. Fortunately, this can never happen if the samples are linearly separable. A proof is simple, and is based on the fact that if $Y^t Y\mathbf{a}_k = Y^t\mathbf{b}_k$, then $Y^t\mathbf{e}_k = 0$. But if the samples are linearly separable, there exists an $\hat{\mathbf{a}}$ and a $\hat{\mathbf{b}} > 0$ such that

$$Y\hat{\mathbf{a}} = \hat{\mathbf{b}}.$$

Thus,

$$\mathbf{e}_k^t Y\hat{\mathbf{a}} = 0 = \mathbf{e}_k^t\hat{\mathbf{b}},$$

and since all the components of $\hat{\mathbf{b}}$ are positive, either $\mathbf{e}_k = 0$ or at least one of the components of $\mathbf{e}_k$ must be positive. Since we have excluded the case $\mathbf{e}_k = 0$, it follows that $\mathbf{e}_k^+$ can not be zero for finite k.

The proof that the error vector always converges to zero exploits the fact that the matrix $YY^\dagger$ is symmetric, positive semidefinite, and satisfies

$$(YY^\dagger)^t(YY^\dagger) = YY^\dagger. \tag{66}$$

Although these results are true in general, for simplicity we demonstrate them only for the case where Y^tY is nonsingular. In this case $YY^\dagger = Y(Y^tY)^{-1}Y^t$, and the symmetry is evident. Since Y^tY is positive definite, so is $(Y^tY)^{-1}$; thus, $\mathbf{b}^tY(Y^tY)^{-1}Y^t\mathbf{b} \geq 0$ for any $\mathbf{b}$, and $YY^\dagger$ is at least positive semidefinite. Finally, Eq. (66) follows from

$$(YY^\dagger)^t(YY^\dagger) = [Y(Y^tY)^{-1}Y^t][Y(Y^tY)^{-1}Y^t].$$

To see that $\mathbf{e}_k$ must converge to zero, we eliminate $\mathbf{a}_k$ between Eqs. (63) and (65) and obtain

$$\mathbf{e}_k = (YY^\dagger - I)\mathbf{b}_k.$$

Then, using Eq. (62), we obtain the recursion relation

$$\begin{aligned}\mathbf{e}_{k+1} &= (YY^\dagger - I)(\mathbf{b}_k + 2\rho\mathbf{e}_k^+) \\ &= \mathbf{e}_k + 2\rho(YY^\dagger - I)\mathbf{e}_k^+,\end{aligned} \tag{67}$$

so that

$$\tfrac{1}{4}\|\mathbf{e}_{k+1}\|^2 = \tfrac{1}{4}\|\mathbf{e}_k\|^2 + \rho\mathbf{e}_k^t(YY^\dagger - I)\mathbf{e}_k^+ + \|\rho(YY^\dagger - I)\mathbf{e}_k^+\|^2.$$

Both the second and the third terms simplify considerably. Since $\mathbf{e}_k^tY = 0$, the second term becomes

$$\rho\mathbf{e}_k^t(YY^\dagger - I)\mathbf{e}_k^+ = -\rho\mathbf{e}_k^t\mathbf{e}_k^+ = -\rho\|\mathbf{e}_k^+\|^2,$$

the nonzero components of $\mathbf{e}_k^+$ being the positive components of $\mathbf{e}_k$. Since $YY^\dagger$ is symmetric and is equal to $(YY^\dagger)^t(YY^\dagger)$, the third term simplifies to

$$\begin{aligned}\|\rho(YY^\dagger - I)\mathbf{e}_k^+\|^2 &= \rho^2\mathbf{e}_k^{+t}(YY^\dagger - I)^t(YY^\dagger - I)\mathbf{e}_k^+ \\ &= \rho^2\|\mathbf{e}_k^+\|^2 - \rho^2\mathbf{e}_k^{+t}YY^\dagger\mathbf{e}_k^+.\end{aligned}$$

Thus

$$\tfrac{1}{4}(\|\mathbf{e}_k\|^2 - \|\mathbf{e}_{k+1}\|^2) = \rho(1-\rho)\|\mathbf{e}_k^+\|^2 + \rho^2\mathbf{e}_k^{+t}YY^\dagger\mathbf{e}_k^+. \tag{68}$$

Since $\mathbf{e}_k^+$ is nonzero by assumption, and since $YY^\dagger$ is positive semidefinite, $\|\mathbf{e}_k\|^2 > \|\mathbf{e}_{k+1}\|^2$ if $0 < \rho < 1$. Thus, the sequence $\|\mathbf{e}_1\|^2, \|\mathbf{e}_2\|^2, \ldots$ is monotonically decreasing and must converge to some limiting value $\|\mathbf{e}\|^2$. But for convergence to take place, $\mathbf{e}_k^+$ must converge to zero, so that all of the positive components of $\mathbf{e}_k$ must converge to zero. And since $\mathbf{e}_k^t\hat{\mathbf{b}} = 0$ for all k, it follows that all of the components of $\mathbf{e}_k$ must converge to zero. Thus, if $0 < \rho < 1$ and if the samples are linearly separable, $\mathbf{a}_k$ will converge to a solution vector as k goes to infinity.

If we test the signs of the components of $Y\mathbf{a}_k$ at each step and terminate the algorithm when they are all positive, we will in fact obtain a separating

vector in a finite number of steps. This follows from the fact that $Y\mathbf{a}_k = \mathbf{b}_k + \mathbf{e}_k$, and that the components of $\mathbf{b}_k$ never decrease. Thus, if $b_{\min}$ is the smallest component of $\mathbf{b}_1$ and if $\mathbf{e}_k$ converges to zero, $\mathbf{e}_k$ must enter the hypersphere $\|\mathbf{e}_k\| = b_{\min}$ after a finite number of steps, at which point $Y\mathbf{a}_k > 0$. Although we ignored terminating conditions to simplify the proof, such a terminating condition would always be used in practice.

5.9.3 Nonseparable Behavior

If the convergence proof just given is examined to see how the assumption of separability was employed, it will be seen that it was needed twice. First, the fact that $\mathbf{e}_k^t\hat{\mathbf{b}} = 0$ was used to show that either $\mathbf{e}_k = 0$ for some finite k, or $\mathbf{e}_k^+$ is never zero and corrections go on forever. Second, this same constraint was used to show that if $\mathbf{e}_k^+$ converges to zero, $\mathbf{e}_k$ must converge to zero.

If the samples are not linearly separable, it no longer follows that if $\mathbf{e}_k^+$ is zero then $\mathbf{e}_k$ must be zero. Indeed, on a nonseparable problem one may well obtain a nonzero error vector having no positive components. If this occurs, the algorithm automatically terminates and we have proof that the samples are not separable.

What happens if the patterns are not separable, but $\mathbf{e}_k^+$ is never zero? In this case it still follows that

$$\mathbf{e}_{k+1} = \mathbf{e}_k + 2\rho(YY^\dagger - I)\mathbf{e}_k^+ \tag{67}$$

and

$$\tfrac{1}{4}(\|\mathbf{e}_k\|^2 - \|\mathbf{e}_{k+1}\|^2) = \rho(1 - \rho)\,\|\mathbf{e}_k^+\|^2 + \rho^2\mathbf{e}_k^{+t}YY^\dagger\mathbf{e}_k^+. \tag{68}$$

Thus, the sequence $\|\mathbf{e}_1\|^2, \|\mathbf{e}_2\|^2, \ldots$ must still converge, though the limiting value $\|\mathbf{e}\|^2$ can not be zero. Since convergence requires that $\mathbf{e}_k^+$ converge to zero, in the nonseparable case we conclude that either $\mathbf{e}_k^+ = 0$ for some finite k, or $\mathbf{e}_k^+$ converges to zero while $\|\mathbf{e}_k\|$ is bounded away from zero. Thus, the Ho–Kashyap algorithm provides us with a separating vector in the separable case, and with evidence of nonseparability in the nonseparable case. However, there is no bound on the number of steps needed to disclose nonseparability.

5.9.4 Some Related Procedures

If we write $Y^\dagger = (Y^tY)^{-1}Y^t$ and make use of the fact that $Y^t\mathbf{e}_k = 0$, we can rewrite the Ho–Kashyap algorithm as

$$\left.\begin{aligned} &\mathbf{b}_1 > 0 \text{ but otherwise arbitrary} \\ &\mathbf{a}_1 = Y^\dagger\mathbf{b}_1 \\ &\mathbf{b}_{k+1} = \mathbf{b}_k + \rho(\mathbf{e}_k + |\mathbf{e}_k|) \\ &\mathbf{a}_{k+1} = \mathbf{a}_k + \rho Y^\dagger|\mathbf{e}_k| \end{aligned}\right\}, \tag{69}$$

where, as usual,

$$\mathbf{e}_k = Y\mathbf{a}_k - \mathbf{b}_k. \tag{70}$$

This algorithm differs from the perceptron and relaxation algorithms for solving linear inequalities in at least three ways: (1) it varies both the weight vector $\mathbf{a}$ and the margin vector $\mathbf{b}$, (2) it provides evidence of nonseparability, but (3) it requires the computation of the pseudoinverse of Y. Even though this last computation need be done only once, it can be time consuming, and it requires special treatment if Y^tY is singular. An interesting alternative algorithm that resembles Eq. (69) but avoids the need for computing $Y^\dagger$ is

$$\left.\begin{aligned} &\mathbf{b}_1 > 0 \qquad \text{but otherwise arbitrary} \\ &\mathbf{a}_1 \qquad\quad \text{arbitrary} \\ &\mathbf{b}_{k+1} = \mathbf{b}_k + (\mathbf{e}_k + |\mathbf{e}_k|) \\ &\mathbf{a}_{k+1} = \mathbf{a}_k + \rho R Y^t |\mathbf{e}_k| \end{aligned}\right\}, \tag{71}$$

where R is an arbitrary, constant, positive-definite $\hat{d}$-by-$\hat{d}$ matrix. We shall show that if ρ is properly chosen, this algorithm also yields a solution vector in a finite number of steps, provided that a solution exists. Furthermore, if no solution exists the vector $Y^t|\mathbf{e}_k|$ either vanishes, exposing the nonseparability, or converges to zero.

The proof is fairly straightforward. Whether the samples are linearly separable or not, Eqs. (70) and (71) show that

$$\begin{aligned} \mathbf{e}_{k+1} &= Y\mathbf{a}_{k+1} - \mathbf{b}_{k+1} \\ &= (\rho YRY^t - I)|\mathbf{e}_k|. \end{aligned}$$

Thus,

$$\|\mathbf{e}_{k+1}\|^2 = |\mathbf{e}_k|^t (\rho^2 YRY^tYRY - 2\rho YRY^t + I)|\mathbf{e}_k|$$

and

$$\|\mathbf{e}_k\|^2 - \|\mathbf{e}_{k+1}\|^2 = (Y^t|\mathbf{e}_k|)^t A(Y^t|\mathbf{e}_k|), \tag{72}$$

where

$$A = 2\rho R - \rho^2 RY^tR. \tag{73}$$

Clearly, if ρ is positive but sufficiently small, A will be approximately $2\rho R$ and hence positive definite. Thus, if $Y^t|\mathbf{e}_k| \neq 0$ we will have $\|\mathbf{e}_k\|^2 > \|\mathbf{e}_{k+1}\|^2$.

At this point we must distinguish between the separable and the nonseparable case. In the separable case there exists an $\hat{\mathbf{a}}$ and a $\hat{\mathbf{b}} > 0$ satisfying $Y\hat{\mathbf{a}} = \hat{\mathbf{b}}$. Thus, if $|\mathbf{e}_k| \neq 0$,

$$|\mathbf{e}_k|^t Y\hat{\mathbf{a}} = |\mathbf{e}_k|^t\hat{\mathbf{b}} > 0,$$

so that $Y^t|\mathbf{e}_k|$ can not be zero unless $\mathbf{e}_k$ is zero. Thus, the sequence $\|\mathbf{e}_1\|^2$, $\|\mathbf{e}_2\|^2, \ldots$ is monotonically decreasing and must converge* to some limiting value $\|\mathbf{e}\|^2$. But for convergence to take place, $Y^t|\mathbf{e}_k|$ must converge to zero, which implies that $|\mathbf{e}_k|$ and hence $\mathbf{e}_k$ must converge to zero. Since $\mathbf{e}_k$ starts out positive and never decreases, it follows that $\mathbf{a}_k$ must converge to a separating vector. Moreover, by the same argument used before, a solution must actually be obtained after a finite number of steps.

In the nonseparable case, $\mathbf{e}_k$ can neither be zero nor converge to zero. It may happen that $Y^t|\mathbf{e}_k| = 0$ at some step, which would provide proof of nonseparability. However, it is also possible for the sequence of corrections to go on forever. In this case, it again follows that the sequence $\|\mathbf{e}_1\|^2$, $\|\mathbf{e}_2\|^2, \ldots$ must converge to a limiting value $\|\mathbf{e}\|^2 \neq 0$, and that $Y^t|\mathbf{e}_k|$ must converge to zero. Thus, we again obtain evidence of nonseparability in the nonseparable case.

Before closing this discussion, let us look briefly at the question of choosing ρ and R. The simplest choice for R is the identity matrix, in which case $A = 2\rho I - \rho^2 Y^t Y$. This matrix will be positive definite, thereby assuring convergence, if $0 < \rho < 2/\lambda_{\max}$, where $\lambda_{\max}$ is the largest eigenvalue of $Y^t Y$. Since the trace of $Y^t Y$ is both the sum of the eigenvalues of $Y^t Y$ and the sum of the squares of the elements of Y, one can use the pessimistic bound $\hat{d}\lambda_{\max} \leq \sum \|\mathbf{y}_i\|^2$ in selecting a value for ρ.

A more interesting approach is to change ρ at each step, selecting that value that maximizes $\|\mathbf{e}_k\|^2 - \|\mathbf{e}_{k+1}\|^2$. Eqs. (72) and (73) give

$$\|\mathbf{e}_k\|^2 - \|\mathbf{e}_{k+1}\|^2 = |\mathbf{e}_k|^t\, Y(2\rho R - \rho^2 R Y^t Y R) Y^t |\mathbf{e}_k|. \tag{74}$$

By differentiating with respect to ρ, we obtain the optimal value

$$\rho_k = \frac{|\mathbf{e}_k|^t\, YRY^t\, |\mathbf{e}_k|}{|\mathbf{e}_k|^t\, YRY^tYRY^t\, |\mathbf{e}_k|}, \tag{75}$$

which, for $R = I$, simplifies to

$$\rho_k = \frac{\|\, Y^t\, |\mathbf{e}_k|\, \|^2}{\|\, YY^t\, |\mathbf{e}_k|\, \|^2}. \tag{76}$$

This same approach can also be used to select the matrix R. By replacing R in Eq. (74) by the symmetric matrix $R + \delta R$ and neglecting second-order terms, we obtain

$$\delta(\|\mathbf{e}_k\|^2 - \|\mathbf{e}_{k+1}\|^2) = |\mathbf{e}_k|\, Y[\delta R^t(I - \rho Y^t YR) + (I - \rho R Y^t Y)\, \delta R] Y^t |\mathbf{e}_k|.$$

* It is possible, of course, that at some step we obtain $\mathbf{e}_k = 0$, in which case convergence occurs at that point.

Thus, the decrease in the squared error vector is maximized by the choice

$$R = \frac{1}{\rho}(Y^t Y)^{-1} \tag{77}$$

and since $\rho R Y^t = Y^\dagger$, the descent algorithm becomes virtually identical with the original Ho–Kashyap algorithm.

5.10 LINEAR PROGRAMMING PROCEDURES

5.10.1 Linear Programming

The perceptron, relaxation, and Ho–Kashyap procedures are basically gradient descent procedures for solving simultaneous linear inequalities. Linear programming techniques are procedures for maximizing or minimizing linear functions subject to linear equality or inequality constraints. This at once suggests that one might be able to solve linear inequalities by using them as the constraints in a suitable linear programming problem. In this section we shall consider two of several ways that this can be done. The reader need have no knowledge of linear programming to understand these formulations, though such knowledge would certainly be useful in applying the techniques.

A classical linear programming problem can be stated as follows: Find a vector $\mathbf{u} = (u_1, \ldots, u_m)^t$ that minimizes the linear *objective function*

$$z = \boldsymbol{\alpha}^t \mathbf{u} \tag{78}$$

subject to the constraint

$$A\mathbf{u} \geq \boldsymbol{\beta}, \tag{79}$$

where $\boldsymbol{\alpha}$ is an m-by-1 *cost vector*, $\boldsymbol{\beta}$ is an l-by-1 vector, and A is an l-by-m matrix. The *simplex algorithm*, described in any text on linear programming, is the classical iterative procedure for solving this problem. For technical reasons, it requires the imposition of one more constraint, viz.,

$$\mathbf{u} \geq 0. \tag{80}$$

If we think of $\mathbf{u}$ as being the weight vector $\mathbf{a}$, this constraint is unacceptable, since in most cases the solution vector will have both positive and negative components. However, suppose that we write

$$\mathbf{a} = \mathbf{a}^+ - \mathbf{a}^-, \tag{81}$$

where

$$\mathbf{a}^+ = \tfrac{1}{2}(|\mathbf{a}| + \mathbf{a}) \tag{82}$$

and

$$\mathbf{a}^- = \tfrac{1}{2}(|\mathbf{a}| - \mathbf{a}). \tag{83}$$

Then both $\mathbf{a}^+$ and $\mathbf{a}^-$ are nonnegative, and by identifying the components of $\mathbf{u}$ with the components of $\mathbf{a}^+$ and $\mathbf{a}^-$, for example, we can accept the constraint $\mathbf{u} \geq 0$.

5.10.2 The Linearly Separable Case

Suppose that we have a set of n samples $\mathbf{y}_1, \ldots, \mathbf{y}_n$ and we want a weight vector $\mathbf{a}$ that satisfies $\mathbf{a}^t\mathbf{y}_i \geq b_i > 0$ for all i. How can we formulate this as a linear programming problem? One approach is to introduce what is called an *artificial variable* t by writing

$$\mathbf{a}^t\mathbf{y}_i + t \geq b_i$$

and

$$t \geq 0.$$

If t is sufficiently large, there is no problem in satisfying these constraints; for example, they are satisfied if $\mathbf{a} = 0$ and $t = \max_i b_i$.* However, this hardly solves our original problem. What we want is a solution with $t = 0$, which is the smallest value t can have and still satisfy $t \geq 0$. Thus, we are led to consider the following problem: Minimize t over all values of t and $\mathbf{a}$ that satisfy the conditions $\mathbf{a}^t\mathbf{y}_i + t \geq b_i$ and $t \geq 0$. If the answer is zero, the samples are linearly separable, and we have a solution. If the answer is positive, there is no separating vector, but we have proof that the samples are nonseparable.

Formally, our problem is to find a vector $\mathbf{u}$ that minimizes the objective function $z = \boldsymbol{\alpha}^t\mathbf{u}$ subject to the constraints $A\mathbf{u} \geq \boldsymbol{\beta}$ and $\mathbf{u} \geq 0$, where

$$A = \begin{bmatrix} \mathbf{y}_1^t & -\mathbf{y}_1^t & 1 \\ \mathbf{y}_2^t & -\mathbf{y}_2^t & 1 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \mathbf{y}_n^t & -\mathbf{y}_n^t & 1 \end{bmatrix}, \quad \mathbf{u} = \begin{bmatrix} \mathbf{a}^+ \\ \mathbf{a}^- \\ t \end{bmatrix}, \quad \boldsymbol{\alpha} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{bmatrix}.$$

Thus, the linear programming problem involves $m = 2\hat{d} + 1$ variables and $l = n$ constraints, plus the simplex algorithm constraints $\mathbf{u} \geq 0$. The simplex

* In linear programming terminology, any solution satisfying the constraints is called a *feasible solution*. A feasible solution for which the number of nonzero variables does not exceed the number of constraints (not counting the simplex requirement for nonnegative variables) is called a *basic feasible solution*. Thus, the solution $\mathbf{a} = 0$ and $t = \max_i b_i$ is a basic feasible solution. Possession of such a solution simplifies the application of the simplex algorithm.

algorithm will find the minimum value of the objective function $z = \alpha^t \mathbf{u} = t$ in a finite number of steps, and will exhibit a vector $\hat{\mathbf{u}}$ yielding that value. If the samples are linearly separable, the minimum value of t will be zero, and a solution vector $\hat{\mathbf{a}}$ can be obtained from $\hat{\mathbf{u}}$. If the samples are not separable, the minimum value of t will be positive. The resulting $\hat{\mathbf{u}}$ is usually not very useful as an approximate solution, but at least one obtains proof of non-separability.

5.10.3 Minimizing the Perceptron Criterion Function

In most pattern classification applications one cannot assume that the samples are linearly separable. In particular, when the patterns are not separable, one still wants to obtain a weight vector that classifies as many samples correctly as possible. Unfortunately, the number of errors is not a linear function of the components of the weight vector, and its minimization is not a linear programming problem. However, it turns out that the problem of minimizing the perceptron criterion function can be posed as a problem in linear programming. Since minimization of this criterion function yields a separating vector in the separable case and a reasonable solution in the non-separable case, this approach is quite attractive.

The basic perceptron criterion function is given by

$$J_p(\mathbf{a}) = \sum_{\mathbf{y} \in \mathcal{Y}} (-\mathbf{a}^t \mathbf{y}), \tag{12}$$

where $\mathcal{Y}(\mathbf{a})$ is the set of samples misclassified by $\mathbf{a}$. To avoid the useless solution $\mathbf{a} = 0$, we introduce a positive margin vector $\mathbf{b}$ and write

$$J_p'(\mathbf{a}) = \sum_{\mathbf{y}_i \in \mathcal{Y}'} (b_i - \mathbf{a}^t \mathbf{y}_i), \tag{84}$$

where $\mathbf{y}_i \in \mathcal{Y}'$ if $\mathbf{a}^t \mathbf{y}_i \leq b_i$. Clearly, J_p' is a piecewise-linear function of $\mathbf{a}$, not a linear function, and linear programming techniques are not immediately applicable. However, by introducing n artificial variables and their constraints we can construct an equivalent linear objective function. Consider the problem of finding vectors $\mathbf{a}$ and $\mathbf{t}$ that minimize the linear function

$$z = \sum_{i=1}^{n} t_i$$

subject to the constraints

$$t_i \geq 0$$

and

$$t_i \geq b_i - \mathbf{a}^t \mathbf{y}_i.$$

Clearly, for any fixed value of $\mathbf{a}$, the minimum value of z is exactly equal to $J_p'(\mathbf{a})$, since under these constraints the best we can do is to take $t_i = \max(0, b_i - \mathbf{a}^t\mathbf{y}_i)$. If we minimize z over $\mathbf{t}$ *and* $\mathbf{a}$, we shall obtain the minimum possible value of $J_p'(\mathbf{a})$. Thus, we have converted the problem of minimizing $J_p'(\mathbf{a})$ to one of minimizing a linear function z subject to linear inequality constraints. Letting $\mathbf{u}_n$ denote an n-dimensional unit vector, we obtain the following problem with $m = 2\hat{d} + n$ variables and $l = n$ constraints: Minimize $\boldsymbol{\alpha}^t\mathbf{u}$ subject to $A\mathbf{u} \geq \boldsymbol{\beta}$ and $\mathbf{u} \geq 0$, where

$$A = \begin{bmatrix} \mathbf{y}_1^t & -\mathbf{y}_1^t & 1 & 0 & \cdots & 0 \\ \mathbf{y}_2^t & -\mathbf{y}_2^t & 0 & 1 & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & \cdot & & \cdot \\ \mathbf{y}_n^t & -\mathbf{y}_n^t & 0 & 0 & \cdots & 1 \end{bmatrix}, \quad \mathbf{u} = \begin{bmatrix} \mathbf{a}^+ \\ \mathbf{a}^- \\ \mathbf{t} \end{bmatrix}, \quad \boldsymbol{\alpha} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{u}_n \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ b_n \end{bmatrix}.$$

The choice $\mathbf{a} = \mathbf{0}$ and $t_i = b_i$ provides a basic feasible solution to start the simplex algorithm, and the simplex algorithm will provide an $\hat{\mathbf{a}}$ minimizing $J_p'(\mathbf{a})$ in a finite number of steps.

5.10.4 Remarks

We have shown two ways to formulate the problem of finding a linear discriminant function as a problem in linear programming. There are other possible formulations, the ones involving the so-called *dual problem* being of particular interest from a computational standpoint. Generally speaking, methods such as the simplex method are merely sophisticated gradient descent methods for extremizing linear functions subject to linear constraints. The coding of a linear programming algorithm is usually more complicated than the coding of the simpler descent procedures we described earlier. However, general purpose linear programming packages can often be used directly or modified appropriately with relatively little effort. When this can be done, one can secure the advantage of guaranteed convergence on both separable and nonseparable problems.

The various algorithms for finding linear discriminant functions presented in this chapter are summarized in Table 5-1. It is natural to ask which one is best, but none uniformly dominates or is uniformly dominated by all others. The choice depends upon such considerations as desired characteristics, ease of programming, the number of samples, and the dimensionality of the samples. If a linear discriminant function can yield a low error rate, any of these procedures, intelligently applied, can provide good performance.

TABLE 5-1. Summary of Descent Procedures for Obtaining Linear Discriminant Functions

Name	Criterion Function	Descent Algorithm	Conditions	Remarks
Fixed Increment	$J_p = \sum_{\mathbf{a}^t\mathbf{y} \le 0} (-\mathbf{a}^t\mathbf{y})$	$\mathbf{a}_{k+1} = \mathbf{a}_k + \mathbf{y}^k \qquad (\mathbf{a}_k^t\mathbf{y}^k \le 0)$	—	Finite convergence if linearly separable to solution with $\mathbf{a}^t\mathbf{y} > 0$; $\mathbf{a}_k$ always bounded.
Variable Increment	$J_p' = \sum_{\mathbf{a}^t\mathbf{y} \le b} -(\mathbf{a}^t\mathbf{y} - b)$	$\mathbf{a}_{k+1} = \mathbf{a}_k + \rho_k\mathbf{y}^k \qquad (\mathbf{a}_k^t\mathbf{y}^k \le b)$	$\rho_k \ge 0, \Sigma\rho_k \to \infty, \frac{\Sigma\rho_k^2}{(\Sigma\rho_k)^2} \to 0$	Convergence if linearly separable to solution with $\mathbf{a}^t\mathbf{y} > b$. Finite convergence if $0 < \alpha \le \rho_k \le \beta < \infty$.
Relaxation	$J_r = \frac{1}{2} \sum_{\mathbf{a}^t\mathbf{y} \le b} \frac{(\mathbf{a}^t\mathbf{y} - b)^2}{\|\mathbf{y}\|^2}$	$\mathbf{a}_{k+1} = \mathbf{a}_k + \rho \frac{b - \mathbf{a}_k^t\mathbf{y}^k}{\|\mathbf{y}^k\|^2}\mathbf{y}^k \qquad (\mathbf{a}_k^t\mathbf{y}^k \le b)$	$0 < \rho < 2$	Convergence if linearly separable to solution with $\mathbf{a}^t\mathbf{y} \ge b$. If $b > 0$, finite convergence to solution with $\mathbf{a}^t\mathbf{y} > 0$.
Widrow-Hoff	$\frac{1}{2}J_s = \frac{1}{2}\sum(\mathbf{a}^t\mathbf{y}_i - b_i)^2$	$\mathbf{a}_{k+1} = \mathbf{a}_k + \rho_k(b_k - \mathbf{a}_k^t\mathbf{y}^k)\mathbf{y}^k$	$\rho_k > 0, \rho_k \to 0$	Tends toward solution minimizing J_s.
Stochastic Approximation	$J_m = E[(\mathbf{a}^t\mathbf{y} - z)^2]$	$\mathbf{a}_{k+1} = \mathbf{a}_k + \rho_k(z_k - \mathbf{a}_k^t\mathbf{y}_k)\mathbf{y}_k$	$\Sigma\rho_k \to \infty, \Sigma\rho_k^2 \to L < \infty$	Involves an infinite number of randomly drawn samples; converges in mean square to a solution minimizing J_m; also provides a MSE approximation to Bayes discriminant.
		$\mathbf{a}_{k+1} = \mathbf{a}_k + R_k(z_k - \mathbf{a}_k^t\mathbf{y}_k)\mathbf{y}_k$	$R_{k+1}^{-1} = R_k^{-1} + \mathbf{y}_k\mathbf{y}_k^t$	

Pseudoinverse	$J_s = \|Y\mathbf{a} - \mathbf{b}\|^2$	$\mathbf{a} = Y\dagger\mathbf{b}$	—	Classical MSE solution; special choices for $\mathbf{b}$ yield Fisher's linear discriminant and MSE approximation to Bayes discriminant.
Ho-Kashyap	$J_s = \|Y\mathbf{a} - \mathbf{b}\|^2$	$\mathbf{b}_{k+1} = \mathbf{b}_k + \rho(\mathbf{e}_k + \|\mathbf{e}_k\|)$ $\mathbf{e}_k = Y\mathbf{a}_k - \mathbf{b}_k$ $\mathbf{a}_k = Y\dagger\mathbf{b}_k$	$0 < \rho < 1$, $\mathbf{b}_1 > 0$	$\mathbf{a}_k$ is MSE solution for each $\mathbf{b}_k$; finite convergence if linearly separable; if $\mathbf{e}_k \leq 0$ but $\mathbf{e}_k \neq 0$, the samples are nonseparable.
		$\mathbf{b}_{k+1} = \mathbf{b}_k + (\mathbf{e}_k + \|\mathbf{e}_k\|)$ $\mathbf{a}_{k+1} = \mathbf{a}_k + \rho_k R Y^t \|\mathbf{e}_k\|$	$\rho_k = \dfrac{\|\mathbf{e}_k\|^t YRY^t \|\mathbf{e}_k\|}{\|\mathbf{e}_k\|^t YRY^t YRY^t \|\mathbf{e}_k\|}$ is optimum R symmetric, positive definite; $\mathbf{b}_1 > 0$	Finite convergence if linearly separable; if $Y^t\|\mathbf{e}_k\| = 0$ but $\mathbf{e}_k \neq 0$, the samples are nonseparable.
Linear Programming	$t = \max_{\mathbf{a}^t\mathbf{y}_i \leq b_i} [-(\mathbf{a}^t\mathbf{y}_i - b_i)]$	Simplex algorithm	$\mathbf{a}^t\mathbf{y}_i + t \geq b_i$, $t \geq 0$	Finite convergence in both separable and nonseparable cases; useful solution only if separable.
	$J_p' = \sum_{i=1}^{n} t_i$ $= \sum_{\mathbf{a}^t\mathbf{y}_i \leq b_i} -(\mathbf{a}^t\mathbf{y}_i - b_i)$	Simplex algorithm	$\mathbf{a}^t\mathbf{y}_i + t_i \geq b_i$, $t_i \geq 0$	Finite convergence to solution minimizing perceptron criterion function whether separable or not.

5.11 THE METHOD OF POTENTIAL FUNCTIONS

A discussion of methods for determining linear discriminant functions would not be complete without mentioning the method of potential functions. This approach is related to several of the techniques we have discussed, including Parzen-window estimates, the perceptron procedure, and stochastic approximation. The method originally developed from the idea that if the samples $\mathbf{x}_i$ were thought of as points in space, and if electrical charges q_i were placed at these points, positive if $\mathbf{x}_i$ were labelled ω_1 and negative if $\mathbf{x}_i$ were labelled ω_2, then perhaps the resulting electrostatic potential would serve as a useful discriminant function (see Figure 5.12). If the potential at a point $\mathbf{x}$ due to a unit charge at a point $\mathbf{x}_i$ is $K(\mathbf{x}, \mathbf{x}_i)$, then the potential due to n charges is given by

$$g(\mathbf{x}) = \sum_{i=1}^{n} q_i K(\mathbf{x}, \mathbf{x}_i). \tag{85}$$

The *potential function* $K(\mathbf{x}, \mathbf{x}_i)$ of classical physics varies inversely with $\|\mathbf{x} - \mathbf{x}_i\|$, but many other functions are equally suitable. There is a clear analogy between $K(\mathbf{x}, \mathbf{x}_i)$ and the Parzen-window function $\varphi[(\mathbf{x} - \mathbf{x}_i)/h]$, and the behavior of the discriminant function $g(\mathbf{x})$ is generally similar to the behavior of the difference of the Parzen-window estimates of two densities. However, since we are interested only in constructing a useful discriminant function, we are much less constrained in choosing a potential function than

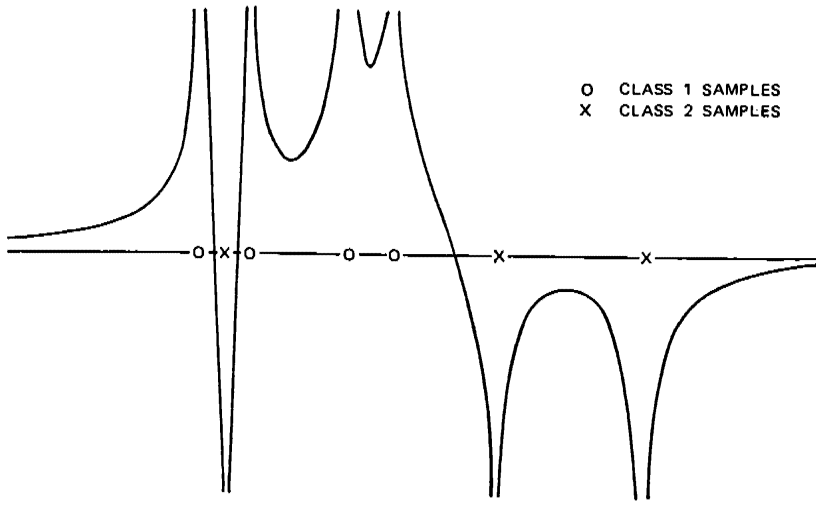

FIGURE 5.12. The potential field as a discriminant function.

we are in choosing a window function. The most frequently suggested potential functions are maximum when $\mathbf{x} = \mathbf{x}_i$ and decrease monotonically to zero as $\|\mathbf{x} - \mathbf{x}_i\|$ approaches infinity. However, even these constraints can be ignored if it is convenient to do so.

Suppose that we have a set of n samples and we construct a discriminant function according to Eq. (85). Suppose further that we check one of the samples, say $\mathbf{x}_k$, and discover that it is misclassified by $g(\mathbf{x})$. Then it is natural to think of changing q_k slightly in an attempt to correct the error.* Suppose that we either add a unit charge to q_k if $\mathbf{x}_k$ is labelled ω_1 or subtract a unit charge if $\mathbf{x}_k$ is labelled ω_2. If we let $g'(\mathbf{x})$ denote the discriminant function after the correction, we see that this leads to the following algorithm for constructing a discriminant function:

$$g'(\mathbf{x}) = \begin{cases} g(\mathbf{x}) + K(\mathbf{x}, \mathbf{x}_k) & \text{if } \mathbf{x}_k \text{ is labelled } \omega_1 \quad \text{and } g(\mathbf{x}_k) \leq 0 \\ g(\mathbf{x}) - K(\mathbf{x}, \mathbf{x}_k) & \text{if } \mathbf{x}_k \text{ is labelled } \omega_2 \quad \text{and } g(\mathbf{x}_k) \geq 0 \\ g(\mathbf{x}) & \text{otherwise.} \end{cases} \tag{86}$$

This error-correction rule bears a close resemblance to the fixed-increment rule. The exact nature of this relation becomes clear if it is possible to represent $K(\mathbf{x}, \mathbf{x}_k)$ by the symmetric, finite expansion

$$K(\mathbf{x}, \mathbf{x}_k) = \sum_{j=1}^{\hat{d}} y_j(\mathbf{x}) y_j(\mathbf{x}_k) = \mathbf{y}_k^t \mathbf{y}. \tag{87}$$

where $\mathbf{y} = \mathbf{y}(\mathbf{x})$ and $\mathbf{y}_k = \mathbf{y}(\mathbf{x}_k)$. Substituting this in Eq. (85), we obtain

$$g(\mathbf{x}) = \mathbf{a}^t \mathbf{y},$$

where

$$\mathbf{a} = \sum_{i=1}^{n} q_i \mathbf{y}_i.$$

Furthermore, the algorithm for changing $g(\mathbf{x})$ to $g'(\mathbf{x})$ is merely the unnormalized fixed-increment rule,

$$\mathbf{a}' = \begin{cases} \mathbf{a} + \mathbf{y}_k & \text{if } \mathbf{y}_k \text{ is labelled } \omega_1 \quad \text{and } \mathbf{a}^t \mathbf{y}_k \leq 0 \\ \mathbf{a} - \mathbf{y}_k & \text{if } \mathbf{y}_k \text{ is labelled } \omega_2 \quad \text{and } \mathbf{a}^t \mathbf{y}_k \geq 0 \\ \mathbf{a} & \text{otherwise.} \end{cases}$$

Thus, when $K(\mathbf{x}, \mathbf{x}_k)$ has the form of Eq. (87), we can prove convergence by the same techniques we used for the fixed-increment rule. Moreover, it is

* If the potential function peaks sufficiently sharply relative to the distance between samples, it is clear that we can always adjust the charges so that all of the samples are correctly classified. However, if the potential function is relatively spread out, this may not be the case.

clear that we can take the other procedures, such as the relaxation, MSE, and stochastic approximation procedures, and immediately obtain parallel procedures and convergence proofs involving potential functions.

The method of potential functions is not restricted to potential functions having finite expansions, however. Any convenient function, such as

$$K(\mathbf{x}, \mathbf{x}_k) = \frac{\sigma^2}{\sigma^2 + \|\mathbf{x} - \mathbf{x}_k\|^2}$$

or

$$K(\mathbf{x}, \mathbf{x}_k) = \exp\left[-\frac{1}{2\sigma^2}\|\mathbf{x} - \mathbf{x}_k\|^2\right],$$

can be selected for a potential function,* and a discriminant function can be obtained by considering the samples in a sequence $\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^k, \ldots$, and using iterative rules such as

$$g_{k+1}(\mathbf{x}) = g_k(\mathbf{x}) + r_k(\mathbf{x}, \mathbf{x}^k)K(\mathbf{x}, \mathbf{x}^k),$$

where r_k is some function of the error.

From a practical standpoint, this use of the method of potential functions encounters many of the same problems encountered with the use of Parzen-window estimates. The potential function must be carefully chosen to obtain good interpolation between sample points. If the number of samples is large, the computational problems are severe. This procedure is most attractive when either the number of samples is small, or the dimensionality of $\mathbf{x}$ is sufficiently small to allow $g(\mathbf{x})$ to be stored as a table for discrete values of $\mathbf{x}$.

5.12 MULTICATEGORY GENERALIZATIONS

5.12.1 Kesler's Construction

There is no uniform way to extend all of the two-category procedures we have discussed to the multicategory case. In Section 5.2.2 we defined a multicategory classifier called a linear machine which classifies a pattern by computing c linear discriminant functions

$$g_i(\mathbf{x}) = \mathbf{w}_i^t\mathbf{x} + w_{i0} \qquad i = 1, \ldots, c,$$

* Those familiar with integral equations will see the similarity between $K(\mathbf{x}, \mathbf{x}_k)$ and the kernel $K(s, t)$. Under certain conditions, symmetric kernels possess infinite series expansions of the form $\sum \varphi_i(s)\varphi_i(t)/\lambda_i$, where the φ_i and λ_i are the eigenfunctions and eigenvalues of K, respectively (see Courant and Hilbert, Chapter Three, 1953). The familiar orthogonal functions of mathematical physics are eigenfunctions of symmetric kernels, and their use is often suggested for the construction of potential functions. However, these suggestions are more appealing for their mathematical beauty than their practical usefulness.

and assigning $\mathbf{x}$ to the category corresponding to the largest discriminant. This is a natural generalization for the multiclass case, particularly in view of the results of Chapter 2 for the multivariate normal problem. It can obviously be extended to generalized linear discriminant functions by letting $\mathbf{y}(\mathbf{x})$ be a $\hat{d}$-dimensional vector of functions of $\mathbf{x}$, and by writing

$$g_i(\mathbf{x}) = \mathbf{a}_i^t\mathbf{y} \qquad i = 1, \ldots, c, \tag{88}$$

where again $\mathbf{x}$ is assigned to ω_i if $g_i(\mathbf{x}) > g_j(\mathbf{x})$ for all $j \neq i$.

The generalization of our procedures from a two-category linear classifier to a multicategory linear machine is simplest in the linearly-separable case. Suppose that we have a set of labelled samples $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n$, with n_1 in the subset $\mathscr{Y}_1$ labelled ω_1, n_2 in the subset $\mathscr{Y}_2$ labelled $\omega_2, \ldots$, and n_c in the subset $\mathscr{Y}_c$ labelled ω_c. We say that this set is linearly separable if there exists a linear machine that classifies all of them correctly. That is, if these samples are linearly separable, then there exists a set of weight vectors $\hat{\mathbf{a}}_1, \ldots, \hat{\mathbf{a}}_c$ such that if $\mathbf{y}_k \in \mathscr{Y}_i$, then

$$\hat{\mathbf{a}}_i^t\mathbf{y}_k > \hat{\mathbf{a}}_j^t\mathbf{y}_k \tag{89}$$

for all $j \neq i$.

One of the pleasant things about this definition is that it is possible to manipulate these inequalities and reduce the multicategory problem to the two-category case. Suppose for the moment that $\mathbf{y} \in \mathscr{Y}_1$, so that Eq. (89) becomes

$$\hat{\mathbf{a}}_1^t\mathbf{y} - \hat{\mathbf{a}}_j^t\mathbf{y} > 0, \qquad j = 2, \ldots, c. \tag{90}$$

This set of $c - 1$ inequalities can be thought of as requiring that the $c\hat{d}$-dimensional weight vector

$$\hat{\boldsymbol{\alpha}} = \begin{bmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{a}_c \end{bmatrix}$$

correctly classifies all $c - 1$ of the $c\hat{d}$-dimensional samples

$$\boldsymbol{\eta}_{12} = \begin{bmatrix} \mathbf{y} \\ -\mathbf{y} \\ \mathbf{0} \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{0} \end{bmatrix} \quad \boldsymbol{\eta}_{13} = \begin{bmatrix} \mathbf{y} \\ \mathbf{0} \\ -\mathbf{y} \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{0} \end{bmatrix} \quad \cdots \quad \boldsymbol{\eta}_{1c} = \begin{bmatrix} \mathbf{y} \\ \mathbf{0} \\ \mathbf{0} \\ \cdot \\ \cdot \\ \cdot \\ -\mathbf{y} \end{bmatrix}.$$

More generally, if $\mathbf{y} \in \mathcal{Y}_i$, we construct $(c-1)\,\hat{cd}$-dimensional samples $\boldsymbol{\eta}_{ij}$ by partitioning $\boldsymbol{\eta}_{ij}$ into $\hat{cd}$-dimensional subvectors, with the ith subvector being $\mathbf{y}$, the jth being $-\mathbf{y}$, and all others being zero. Clearly, if $\hat{\boldsymbol{\alpha}}^t\boldsymbol{\eta}_{ij} > 0$ for all $j \neq i$, then the linear machine corresponding to the components of $\hat{\boldsymbol{\alpha}}$ classifies $\mathbf{y}$ correctly.

This construction, due to Carl Kesler, multiplies the dimensionality of the data by c and the number of samples by $c-1$, which does not make its direct use attractive. Its importance resides in the fact that it allows us to convert many multicategory error-correction procedures to two-category procedures for the purpose of obtaining a convergence proof.

5.12.2 The Fixed-Increment Rule

In this section we shall use Kesler's construction to obtain a convergence proof for a generalization of the fixed-increment rule for a linear machine. Suppose that we have a set of n linearly-separable samples $\mathbf{y}_1, \ldots, \mathbf{y}_n$, and we use them to form an infinite sequence in which every sample appears infinitely often. Let L_k denote the linear machine whose weight vectors are $\mathbf{a}_1(k), \ldots, \mathbf{a}_c(k)$. Starting with an arbitrary initial linear machine L_1, we want to use the sequence of samples to construct a sequence of linear machines that converges to a solution machine, one that classifies all of the samples correctly. We shall propose an error-correction rule, in which weight changes are made if and only if the present linear machine misclassifies a sample. Let $\mathbf{y}^k$ denote the kth sample requiring correction, and suppose that $\mathbf{y}^k \in \mathcal{Y}_i$. Since $\mathbf{y}^k$ requires correction, there must be at least one $j \neq i$ for which

$$\mathbf{a}_i(k)^t\mathbf{y}^k \leq \mathbf{a}_j(k)^t\mathbf{y}^k. \tag{91}$$

Then, the fixed-increment rule for correcting L_k is

$$\left.\begin{aligned} \mathbf{a}_i(k+1) &= \mathbf{a}_i(k) + \mathbf{y}^k \\ \mathbf{a}_j(k+1) &= \mathbf{a}_j(k) - \mathbf{y}^k \\ \mathbf{a}_l(k+1) &= \mathbf{a}_l(k), \quad l \neq i \quad \text{and} \quad l \neq j. \end{aligned}\right\} \tag{92}$$

We shall now show that this rule must lead to a solution machine after a finite number of corrections. The proof is simple. For each linear machine L_k there corresponds a weight vector

$$\boldsymbol{\alpha}_k = \begin{bmatrix} \mathbf{a}_1(k) \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{a}_c(k) \end{bmatrix}. \tag{93}$$

For each sample $\mathbf{y} \in \mathcal{Y}_i$ there are $c - 1$ samples η_{ij} formed as described in the previous section. In particular, corresponding to the vector $\mathbf{y}^k$ satisfying Eq. (91) there is a vector

$$\eta_{ij}^k = \begin{bmatrix} \cdot \\ \cdot \\ \cdot \\ \mathbf{y}^k \\ \cdot \\ \cdot \\ \cdot \\ -\mathbf{y}^k \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \begin{matrix} \\ \\ \\ \leftarrow i \\ \\ \\ \\ \leftarrow j \\ \\ \\ \\ \end{matrix}$$

satisfying

$$\alpha_k^t \eta_{ij}^k \leq 0.$$

Furthermore, the fixed-increment rule for correcting L_k is exactly the same as the fixed-increment rule for correcting α_k, viz.,

$$\alpha_{k+1} = \alpha_k + \eta_{ij}^k.$$

Thus, we have obtained a complete correspondence between the multicategory case and the two-category case, in which the multicategory procedure produces a sequence of samples $\eta^1, \eta^2, \ldots, \eta^k, \ldots$ and a sequence of weight vectors $\alpha_1, \alpha_2, \ldots, \alpha_k, \ldots$. By our results for the two-category case, this latter sequence can not be infinite, but must terminate in a solution vector. Hence, the sequence $L_1, L_2, \ldots, L_k, \ldots$ must terminate in a solution machine after a finite number of corrections.

This use of Kesler's construction to establish equivalences between multicategory and two-category procedures is a powerful theoretical tool. It can be used to extend all of our results for the perceptron and relaxation procedures to the multicategory case, and applies as well to the error-correction rules for the method of potential functions. Unfortunately, it is not as directly useful in generalizing the MSE or the linear programming approaches.

5.12.3 Generalizations for MSE Procedures

Perhaps the simplest way to obtain a natural generalization of the MSE procedures to the multiclass case is to consider the problem as a set of c two-class problems. The ith problem is to obtain a weight vector $\mathbf{a}_i$ that is a

minimum-squared-error solution to the equations

$$\left.\begin{aligned} \mathbf{a}_i^t\mathbf{y} &= 1 \qquad \text{for all } \mathbf{y} \in \mathcal{Y}_i \\ \mathbf{a}_i^t\mathbf{y} &= -1 \qquad \text{for all } \mathbf{y} \notin \mathcal{Y}_i. \end{aligned}\right\}$$

In view of the results of Section 5.8.3, we can say that when the number of samples is very large we will obtain a minimum mean-squared-error approximation to the Bayes discriminant function

$$P(\omega_i \mid \mathbf{x}) - P(\text{not } \omega_i \mid \mathbf{x}) = 2P(\omega_i \mid \mathbf{x}) - 1.$$

This observation has two immediate consequences. First, it suggests a modification in which we seek a weight vector $\mathbf{a}_i$ that is a minimum-squared-error solution to the equations

$$\left.\begin{aligned} \mathbf{a}_i^t\mathbf{y} &= 1 \qquad \text{for all } \mathbf{y} \in \mathcal{Y}_i \\ \mathbf{a}_i^t\mathbf{y} &= 0 \qquad \text{for all } \mathbf{y} \notin \mathcal{Y}_i, \end{aligned}\right\} \tag{94}$$

so that $\mathbf{a}^t\mathbf{y}$ will be a minimum mean-squared-error approximation to $P(\omega_i \mid \mathbf{x})$. Second, it justifies the use of the resulting discriminant functions in a linear machine, in which we assign $\mathbf{y}$ to ω_i if $\mathbf{a}_i^t\mathbf{y} > \mathbf{a}_j^t\mathbf{y}$ for all $j \neq i$.

The pseudoinverse solution to the multiclass MSE problem can be written in a form analogous to the form for the two-class case. Let Y be the n-by-$\hat{d}$ matrix of samples, which we assume to be partitioned as

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \cdot \\ \cdot \\ \cdot \\ Y_c \end{bmatrix}, \tag{95}$$

with the samples labelled ω_i comprising the rows of Y_i. Similarly, let A be the $\hat{d}$-by-c matrix of weight vectors

$$A = [\mathbf{a}_1\mathbf{a}_2 \cdots \mathbf{a}_c], \tag{96}$$

and let B be the n-by-c matrix

$$B = \begin{bmatrix} B_1 \\ B_2 \\ \cdot \\ \cdot \\ \cdot \\ B_c \end{bmatrix}, \tag{97}$$

where all of the elements of B_i are zero except for those in the ith column, which are unity. Then the trace of the "squared" error matrix $(YA - B)^t \times (YA - B)$ is minimized by the solution*

$$A = Y^{\dagger}B, \tag{98}$$

where, as usual, $Y^{\dagger}$ is the pseudoinverse of Y.

This result can be generalized in a theoretically interesting fashion. Let λ_{ij} be the loss incurred for deciding ω_i when the true state of nature is ω_j, and let the jth submatrix of B be given by

$$B_j = -\begin{bmatrix} \lambda_{1j} & \lambda_{2j} & \cdots & \lambda_{cj} \\ \lambda_{1j} & \lambda_{2j} & \cdots & \lambda_{cj} \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ \lambda_{1j} & \lambda_{2j} & \cdots & \lambda_{cj} \end{bmatrix} \begin{matrix} \uparrow \\ \\ \\ n_j \\ \\ \\ \downarrow \end{matrix} \qquad j = 1, \ldots, c. \tag{99}$$

Then, as the number of samples approaches infinity, the solution $A = Y^{\dagger}B$ yields discriminant functions $\mathbf{a}_i^t\mathbf{y}$ which provide a minimum-mean-square-error approximation to the Bayes discriminant function

$$g_{0i}(\mathbf{x}) = -\sum_{j=1}^{c} \lambda_{ij} P(\omega_j \mid \mathbf{x}). \tag{100}$$

The proof of this result is a direct extension of the proof given in Section 5.8.3, and, following time-honored tradition, we leave it as an exercise for the reader.

5.13 BIBLIOGRAPHICAL AND HISTORICAL REMARKS

Because linear discriminant functions are so amenable to analysis, far more papers have been written about them than the subject deserves. Thus, the following list of references, long as it is, is by no means exhaustive. Historically, all of this work begins with the classic paper by R. A. Fisher (1936). The application of linear discriminant functions to pattern classification was well described by Highleyman (1962), who posed the problem of finding the

* If we let $\mathbf{b}_i$ denote the ith column of B, the trace of $(YA - B)^t(YA - B)$ is equal to the sum of the squared lengths of the error vectors $Y\mathbf{a}_i - \mathbf{b}_i$. The solution $A = Y^{\dagger}B$ not only minimizes this sum, but it also minimizes each term in the sum.

optimal (minimum-risk) linear discriminant, and proposed plausible gradient descent procedures* to determine a solution from samples. Unfortunately, little can be said about such procedures without knowing the underlying distributions, and even then the situation is analytically complex (cf., Anderson and Bahadur, 1962).

While this work was statistically oriented, many of the pattern recognition papers that appeared in the late 1950's and early 1960's adopted other viewpoints. One viewpoint was that of neural-net brain models, in which individual neurons were modelled as threshold elements, two-category linear machines. This work had its origins in a famous paper by McCulloch and Pitts (1943), and tended to emphasize the goal of error-free performance and the feature of adaptivity or learning. Rosenblatt's perceptron (Rosenblatt, 1957, 1962; Block, 1962) employed various reinforcement rules for changing the neural weight values to improve performance. The best known of these was the fixed-increment rule, which guaranteed error-free performance whenever it could be achieved. Nilsson (1965) presents two proofs of the Perceptron Convergence Theorem and references several others, including the elegant and generalizable proof by Novikoff (1962). Our proof is based on the one given by Ridgway (1962). The behavior of the fixed-increment rule on nonseparable problems was analyzed by Efron (1964); Minsky and Papert (1969) and Block and Levin (1970) provide more accessible analyses. Simple modifications designed to improve performance on nonseparable problems were suggested by Duda and Singleton (1964) and Butz (1967).

A frequently proposed alternative for nonseparable problems was the use of more complicated discriminant functions, or the use of more complicated, sometimes random networks of threshold elements. The more general class of perceptrons as well as various piecewise linear classifiers (Nilsson, 1965; Duda and Fossum, 1966; Mangasarian, 1968) can be described in these terms. Unfortunately, the analysis of such networks is very difficult. Hawkins (1961) gives a good summary of various approaches to learning in threshold element networks, and Minsky and Selfridge (1961) give a critique of this work.

Another viewpoint for much of the early pattern recognition work was that of switching theory. Here again the basic emphasis was on obtaining error-free performance. The switching circuit most frequently proposed for pattern recognition applications was a single threshold element, which has also been called a threshold logic unit, a linear-input element, a majority gate, and, when adaptive, an adaline. Winder (1963) provides a good survey of pertinent work in this area. The standard procedures for realizing threshold functions are basically methods for solving simultaneous linear inequalities. Many of these are algebraic, however, and are not suitable for pattern

* Our presentation of iterative procedures as gradient-descent methods for minimizing criterion functions was inspired by a report by Blaydon (1967).

recognition applications. The relaxation procedure for solving linear inequalities was developed by Agmon (1954) and Motzkin and Schoenberg (1954); the use of a margin to obtain a solution in a finite number of steps was suggested by Mays (1964).

The fact that systems of linear inequalities could be solved by linear programming* was noted by Charnes (1953). Minnick showed how linear programming could be used to determine the weights for a threshold element (Minnick, 1961), and Mangasarian suggested its use in pattern classification (Mangasarian, 1965). All of these methods provided either a solution, or proof of nonseparability without a useful solution. In an important paper, Smith (1968) showed that the perceptron error criterion could be minimized by linear programming. Grinold (1969) pointed out that the computational advantages of the dual formulation could be extended to Smith's approach by using the revised simplex method with upper-bounded variables.

Not all of the papers with a switching theory orientation were concerned solely with error-free performance. In fact, one of the first papers to suggest the use of an adaptive threshold element for pattern classification posed the problem and its solution in statistical terms (Mattson, 1959). Similarly, the Widrow-Hoff procedure for minimizing the mean-square error was originally described as a stochastic descent procedure (Widrow and Hoff, 1960), and had its origins in Wiener filtering problems in communication and control theory. Koford and Groner (1966) pointed out the relation between the MSE solution and Fisher's linear discriminant, and Patterson and Womack (1966) showed that the MSE solution also gave a minimum-squared-error approximation to the Bayes discriminant. The fact that the pseudoinverse provided a closed-form solution was noted by Ho and Kashyap (1965), who linked the MSE solution to classical switching theory with their iterative procedures (Ho and Kashyap, 1965, 1966). The theory of the pseudoinverse (also known as the general reciprocal, generalized inverse, or Moore-Penrose inverse) is treated thoroughly by Rao and Mitra (1971).

The pattern recognition applications of stochastic approximation and the method of potential functions have an intertwined history. The method of potential functions was originally proposed by Bashkirov, Braverman, and Muchnik (1964), and its theoretical properties were developed in a series of papers by Aizerman, Braverman, and Rozonoer. The first of these linked the potential function correction rule to the fixed-increment rule (Aizerman, et al., 1964a), and shortly thereafter the method was modified to provide a minimum-squared-error approximation to the Bayes discriminant function (Aizerman, et al., 1964b). The relation of the method of potential functions to stochastic

* There are many fine books on linear programming, including the standard texts by Dantzig (1963) and Gass (1969). An exceptionally clear, elementary treatment is given by Glicksman (1963).

approximation was pointed out by Tsypkin and by Aizerman, et al., (1965), and independently by Blaydon (1966). As Aizerman points out, the method of potential functions is a rather general approach to pattern classification that can be specialized in a variety of ways (Aizerman 1969), although the specialization that has received most attention is the one involving stochastic approximation. The subject of stochastic approximation is treated thoroughly by Wasan (1969); a briefer treatment by Wilde (1964) is also highly recommended. Pattern classification applications can be found in Blaydon and Ho (1966), Fu (1968), Yau and Schumpert (1968), and in the many references they cite.

The problem of handling multiclass problems has been more vexing for some procedures than for others. The linear-machine structure is naturally suggested by the multivariate-normal solution, or by even simpler classifiers that use the nearest-mean or maximum-correlation criteria. This type of classifier was used in the early magnetic-ink character readers (Eldredge, Kamphoefner, and Wendt, 1956), and adaptive versions were investigated long before convergence proofs were known (e.g., Roberts, 1960, and the well known lernmatrix of Steinbuch, 1963). Kesler's construction and the convergence proof for the fixed-increment rule are attributed to Carl Kesler by Nilsson (1965). Chaplin and Levadi (1967) suggested a multiclass version of the MSE procedure in which the goal was to map vectors y in a given class into one of the vertices of a $(c - 1)$-dimensional simplex. Our treatment of multicategory MSE procedures is based on the generalized inverse approach of Wee (1968). Yau and Shumpert (1968) give multiclass versions of the stochastic approximation approach, and Smith (1969) suggests a procedure for extending the linear programming approach to the multiclass case.

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PROBLEMS

1. (a) Show that the distance from the hyperplane $g(\mathbf{x}) = \mathbf{w}^t\mathbf{x} + w_0 = 0$ to the point $\mathbf{x}$ is $|g(\mathbf{x})|/\|\mathbf{w}\|$ by minimizing $\|\mathbf{x} - \mathbf{x}_q\|^2$ subject to the constraint $g(\mathbf{x}_q) = 0$.

(b) Show that the projection of $\mathbf{x}$ onto the hyperlane is given by

$$\mathbf{x}_p = \mathbf{x} - \frac{g(\mathbf{x})}{\|\mathbf{w}\|^2}\,\mathbf{w}.$$

2. Consider the three-category linear machine with discriminant functions $g_i(\mathbf{x}) = \mathbf{w}_i\mathbf{x} + w_{i0}$, $i = 1, 2, 3$. For the special case where $\mathbf{x}$ is two dimensional and the threshold weights w_{i0} are zero, sketch the weight vectors with their tails at the origin, the three lines joining their heads, and the decision boundaries. How does this sketch change when a constant vector is added to the three weight vectors?

3. In the multicategory case, a set of samples is said to be linearly separable if there exists a linear machine that can classify them all correctly. If for any ω_i samples labelled ω_i can be separated from all others by a single hyperplane, we shall say the samples are *totally linearly separable*. Show that totally linearly separable samples must be linearly separable, but that the converse need not be true. (Hint: for the converse, consider a case in which a linear machine like the one in Problem 2 separates the samples.)

4. A set of samples is said to be *pairwise linearly separable* if there exist $c(c - 1)/2$ hyperplanes H_{ij} such that H_{ij} separates samples labelled ω_i from samples ω_j. Show that a pairwise-linearly-separable set of patterns may not be linearly separable. (Hint: find a configuration of samples that requires decision boundaries like those shown in Figure 5-2b.)

5. Consider a linear machine with discriminant functions $g_i(\mathbf{x}) = \mathbf{w}_i^t\mathbf{x} + w_{i0}$, $i = 1, \ldots, c$. Show that the decision regions are convex by showing that if $\mathbf{x}_1 \in \mathscr{R}_i$ and $\mathbf{x}_2 \in \mathscr{R}_i$ then $\lambda\mathbf{x}_1 + (1 - \lambda)\mathbf{x}_2 \in \mathscr{R}_i$ if $0 \leq \lambda \leq 1$.

6. Let $\{\mathbf{y}_1, \ldots, \mathbf{y}_n\}$ be a finite set of linearly separable samples, and let $\mathbf{a}$ be called a solution vector if $\mathbf{a}^t\mathbf{y}_i \geq b$ for all i. Show that the minimum-length solution vector is unique. (Hint: consider the effect of averaging two solution vectors.)

7. The *convex hull* of a set of vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n$ is the set of all vectors of the form

$$\mathbf{x} = \sum_{i=1}^{n} \alpha_i\mathbf{x}_i$$

where the coefficients α_i are nonnegative and sum to one. Given two sets of vectors, show that either they are linearly separable or their convex hulls intersect. (Hint: suppose that both statements are true, and consider the classification of a point in the intersection of the convex hulls.)

8. A classifier is said to be a *piecewise linear machine* if its discriminant functions have the form

$$g_i(\mathbf{x}) = \max_{j=1,\ldots,n_i} g_{ij}(\mathbf{x}),$$

where

$$g_{ij}(\mathbf{x}) = \mathbf{w}_{ij}^t\mathbf{x} + w_{ij0}, \qquad \begin{matrix} i = 1, \ldots, c \\ j = 1, \ldots, n_i. \end{matrix}$$

(a) Indicate how a piecewise linear machine can be viewed in terms of a linear machine for classifying subclasses of patterns.
(b) Show that the decision regions of a piecewise linear machine can be nonconvex; multiply connected.

9. Let the d components of $\mathbf{x}$ be either 0 or 1. Suppose we assign $\mathbf{x}$ to ω_1 if the number of nonzero components of $\mathbf{x}$ is odd, and to ω_2 otherwise. (In switching theory, this is called the *parity* function.)
(a) Show that this dichotomy is not linearly separable if $d > 1$.
(b) Show that this problem can be solved by a piecewise linear machine with $d + 1$ weight vectors $\mathbf{w}_{ij}$ (see Problem 8). (Hint: consider vectors of the form $\mathbf{w}_{ij} = \alpha_{ij}(1, 1, \ldots, 1)^t$.)

10. In the convergence proof for the perceptron procedure the scale factor α was taken to be β^2/γ. Using the notation in Section 5.5.2, show that if α is greater than $\beta^2/2\gamma$ the maximum number of corrections is given by

$$k_0 = \frac{\|\mathbf{a}_1 - \alpha\mathbf{a}\|^2}{2\alpha\gamma - \beta^2}.$$

If $\mathbf{a}_1 = \mathbf{0}$, what value of α minimizes k_0?

11. Modify the convergence proof given in Section 5.5.2 to prove the convergence of the following correction procedure: starting with an arbitrary initial weight vector $\mathbf{a}_1$, correct $\mathbf{a}_k$ according to

$$\mathbf{a}_{k+1} = \mathbf{a}_k + \rho_k\mathbf{y}^k$$

if and only if $\mathbf{a}_k^t\mathbf{y}^k$ fails to exceed the margin b, where ρ_k is bounded by $0 < \rho_a \leq \rho_k \leq \rho_b < \infty$. What happens if b is negative?

12. Let $\{\mathbf{y}_1, \ldots, \mathbf{y}_n\}$ be a finite set of linearly separable samples. Suggest an exhaustive procedure that will find a separating vector in a finite number of steps. (Hint: consider weight vectors whose components are integer valued.)

13. Consider the criterion function

$$J_q(\mathbf{a}) = \sum_{\mathbf{y}\in\mathcal{Y}} (\mathbf{a}^t\mathbf{y} - b)^2$$

where $\mathcal{Y}(\mathbf{a})$ is the set of samples for which $\mathbf{a}^t\mathbf{y} \leq b$. Suppose that $\mathbf{y}_1$ is the only sample in $\mathcal{Y}(\mathbf{a}_k)$. Show that $\nabla J_q(\mathbf{a}_k) = 2(\mathbf{a}_k^t\mathbf{y}_1 - b)\mathbf{y}_1$ and that the matrix of second partial derivatives is given by $D = 2\mathbf{y}_1\mathbf{y}_1^t$. Use this to show that when the optimal

ρ_k is used in Eq. (8) the gradient descent algorithm yields

$$\mathbf{a}_{k+1} = \mathbf{a}_k + \frac{b - \mathbf{a}^t\mathbf{y}_1}{\|\mathbf{y}_1\|^2}\,\mathbf{y}_1.$$

14. Show that the scale factor α in the MSE solution corresponding to Fisher's linear discriminant (Section 5.8.2) is given by

$$\alpha = \frac{1}{1 + \dfrac{n_1 n_2}{n}(\mathbf{m}_1 - \mathbf{m}_2)^t S_W^{-1}(\mathbf{m}_1 - \mathbf{m}_2)}$$

15. Generalize the results of Section 5.8.3 to show that the vector $\mathbf{a}$ that minimizes the criterion function

$$J_s'(\mathbf{a}) = \sum_{\mathbf{y}\in\mathscr{Y}_1} (\mathbf{a}^t\mathbf{y} - (\lambda_{21} - \lambda_{11}))^2 + \sum_{\mathbf{y}\in\mathscr{Y}_2} (\mathbf{a}^t\mathbf{y} - (\lambda_{12} - \lambda_{22}))^2$$

provides asymptotically a minimum-mean-squared-error approximation to the Bayes discriminant function $(\lambda_{21} - \lambda_{11})P(\omega_1 \mid \mathbf{x}) - (\lambda_{12} - \lambda_{22})P(\omega_2 \mid \mathbf{x})$.

16. Consider the criterion function $J_m(\mathbf{a}) = E[(\mathbf{a}^t\mathbf{y}(\mathbf{x}) - z)^2]$ and the Bayes discriminant function $g_0(\mathbf{x})$.

(a) Show that

$$J_m = E[(\mathbf{a}^t\mathbf{y} - g_0)^2] - 2E[(\mathbf{a}^t\mathbf{y} - g_0)(z - g_0)] + E[(z - g_0)^2]$$

(b) Use the fact that the conditional mean of z is $g_0(\mathbf{x})$ in showing that the $\hat{\mathbf{a}}$ that minimizes J_m also minimizes $E[(\mathbf{a}^t\mathbf{y} - g_0)^2]$

17. A scalar analog of the relation $R_{k+1}^{-1} = R_k^{-1} + \mathbf{y}_k\mathbf{y}_k^t$ used in stochastic approximation is $\rho_{k+1}^{-1} = \rho_k^{-1} + y_k^2$. Show that this has the closed-form solution

$$\rho_k = \frac{\rho_1}{1 + \rho_1 \sum_{i=1}^{k-1} y_i^2}.$$

Assuming that $\rho_1 > 0$ and $0 < a \le y_i^2 \le b < \infty$, indicate why this sequence of coefficients will satisfy $\sum \rho_k \to +\infty$ and $\sum \rho_k^2 \to L < \infty$.

18. The linear programming problem formulated in Section 5.10.2 involved minimizing a single artificial variable t under the constraints $\mathbf{a}^t\mathbf{y}_i + t > b_i$ and $t \ge 0$. Show that the resulting weight vector minimizes the criterion function

$$J_t(\mathbf{a}) = \max_{\mathbf{a}^t\mathbf{y}_i \le b_i} [b_i - \mathbf{a}^t\mathbf{y}_i].$$

19. Suggest a multiclass generalization of the method of potential functions involving c discriminant functions, and suggest an error-correction procedure for determining the discriminant functions iteratively.

Chapter 6

UNSUPERVISED LEARNING AND CLUSTERING

6.1 INTRODUCTION

Until now we have assumed that the training samples used to design a classifier were labelled to show their category membership. Procedures that use labelled samples are said to be supervised. Now we shall investigate a number of *unsupervised* procedures that use unlabelled samples. That is, we shall see what can be done when all one has is a collection of samples without being told their classification.

One might wonder why anyone is interested in such an unpromising problem, and whether or not it is even possible in principle to learn anything of value from unlabelled samples. There are three basic reasons for interest in unsupervised procedures. First, the collection and labelling of a large set of sample patterns can be surprisingly costly and time consuming. If a classifier can be crudely designed on a small, labelled set of samples, and then "tuned up" by allowing it to run without supervision on a large, unlabelled set, much time and trouble can be saved. Second, in many applications the characteristics of the patterns can change slowly with time. If these changes can be tracked by a classifier running in an unsupervised mode, improved performance can be achieved. Finally, in the early stages of an investigation it may be valuable to gain some insight into the nature or structure of the data. The discovery of distinct subclasses or major departures from expected characteristics may significantly alter the approach taken to designing the classifier.

The answer to the question of whether or not it is possible in principle to learn anything from unlabelled data depends upon the assumptions one is

willing to accept—theorems can not be proved without premises. We shall begin with the very restrictive assumption that the functional forms for the underlying probability densities are known, and that the only thing that must be learned is the value of an unknown parameter vector. Interestingly enough, the formal solution to this problem will turn out to be almost identical to the solution for the problem of supervised learning given in Chapter 3. Unfortunately, in the unsupervised case the solution suffers from the usual problems associated with parametric assumptions without providing any of the benefits of computational simplicity. This will lead us to various attempts to reformulate the problem as one of partitioning the data into subgroups or clusters. While some of the resulting clustering procedures have no known significant theoretical properties, they are still among the more useful tools for pattern recognition problems.

6.2 MIXTURE DENSITIES AND IDENTIFIABILITY

We begin by assuming that we know the complete probability structure for the problem with the sole exception of the values of some parameters. To be more specific, we make the following assumptions:

(1) The samples come from a known number c of classes.
(2) The a priori probabilities $P(\omega_j)$ for each class are known, $j = 1, \ldots, c$.
(3) The forms for the class-conditional probability densities $p(\mathbf{x} \mid \omega_j, \boldsymbol{\theta}_j)$ are known, $j = 1, \ldots, c$.
(4) All that is unknown are the values for the c parameter vectors $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_c$.

Samples are assumed to be obtained by selecting a state of nature ω_j with probability $P(\omega_j)$ and then selecting an $\mathbf{x}$ according to the probability law $p(\mathbf{x} \mid \omega_j, \boldsymbol{\theta}_j)$. Thus, the probability density function for the samples is given by

$$p(\mathbf{x} \mid \boldsymbol{\theta}) = \sum_{j=1}^{c} p(\mathbf{x} \mid \omega_j, \boldsymbol{\theta}_j) P(\omega_j), \tag{1}$$

where $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_c)$. A density function of this form is called a *mixture density*. The conditional densities $p(\mathbf{x} \mid \omega_j, \boldsymbol{\theta}_j)$ are called the *component densities*, and the a priori probabilities $P(\omega_j)$ are called the *mixing parameters*. The mixing parameters can also be included among the unknown parameters, but for the moment we shall assume that only $\boldsymbol{\theta}$ is unknown.

Our basic goal will be to use samples drawn from this mixture density to estimate the unknown parameter vector $\boldsymbol{\theta}$. Once we know $\boldsymbol{\theta}$ we can decompose the mixture into its components, and the problem is solved. Before

seeking explicit solutions to this problem, however, let us ask whether or not it is possible in principle to recover $\boldsymbol{\theta}$ from the mixture. Suppose that we had an unlimited number of samples, and that we used one of the nonparametric methods of Chapter 4 to determine the value of $p(\mathbf{x} \mid \boldsymbol{\theta})$ for every $\mathbf{x}$. If there is only one value of $\boldsymbol{\theta}$ that will produce the observed values for $p(\mathbf{x} \mid \boldsymbol{\theta})$, then a solution is at least possible in principle. However, if several different values of $\boldsymbol{\theta}$ can produce the same values for $p(\mathbf{x} \mid \boldsymbol{\theta})$, then there is no hope of obtaining a unique solution.

These considerations lead us to the following definition: a density $p(\mathbf{x} \mid \boldsymbol{\theta})$ is said to be *identifiable* if $\boldsymbol{\theta} \neq \boldsymbol{\theta}'$ implies that there exists an $\mathbf{x}$ such that $p(\mathbf{x} \mid \boldsymbol{\theta}) \neq p(\mathbf{x} \mid \boldsymbol{\theta}')$. As one might expect, the study of unsupervised learning is greatly simplified if we restrict ourselves to identifiable mixtures. Fortunately, most mixtures of commonly encountered density functions are identifiable. Mixtures of discrete distributions are not always so obliging. For a simple example, consider the case where x is binary and $P(x \mid \boldsymbol{\theta})$ is the mixture

$$\begin{aligned} P(x \mid \boldsymbol{\theta}) &= \tfrac{1}{2}\theta_1^x(1-\theta_1)^{1-x} + \tfrac{1}{2}\theta_2^x(1-\theta_2)^{1-x} \\ &= \begin{cases} \tfrac{1}{2}(\theta_1 + \theta_2) & \text{if } x = 1 \\ 1 - \tfrac{1}{2}(\theta_1 + \theta_2) & \text{if } x = 0. \end{cases} \end{aligned}$$

If we know, for example, that $P(x = 1 \mid \boldsymbol{\theta}) = 0.6$, and hence that $P(x = 0 \mid \boldsymbol{\theta}) = 0.4$, then we know the function $P(x \mid \boldsymbol{\theta})$, but we cannot determine $\boldsymbol{\theta}$, and hence cannot extract the component distributions. The most we can say is that $\theta_1 + \theta_2 = 1.2$. Thus, here we have a case in which the mixture distribution is not identifiable, and hence a case for which unsupervised learning is impossible in principle.

This kind of problem commonly occurs with discrete distributions. If there are too many components in the mixture, there may be more unknowns than independent equations, and identifiability can be a real problem. For the continuous case, the problems are less severe, although certain minor difficulties can arise due to the possibility of special cases. Thus, while it can be shown that mixtures of normal densities are usually identifiable, the parameters in the simple mixture density

$$p(x \mid \boldsymbol{\theta}) = \frac{P(\omega_1)}{\sqrt{2\pi}} \exp[-\tfrac{1}{2}(x-\theta_1)^2] + \frac{P(\omega_2)}{\sqrt{2\pi}} \exp[-\tfrac{1}{2}(x-\theta_2)^2]$$

can not be uniquely identified if $P(\omega_1) = P(\omega_2)$, for then θ_1 and θ_2 can be interchanged without affecting $p(x \mid \boldsymbol{\theta})$. To avoid such irritations, we shall acknowledge that identifiability can be a problem, but shall henceforth assume that the mixture densities we are working with are identifiable.

6.3 MAXIMUM LIKELIHOOD ESTIMATES

Suppose now that we are given a set $\mathscr{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ of n unlabelled samples drawn independently from the mixture density

$$p(\mathbf{x} \mid \boldsymbol{\theta}) = \sum_{j=1}^{c} p(\mathbf{x} \mid \omega_j, \boldsymbol{\theta}_j) P(\omega_j), \tag{1}$$

where the parameter vector $\boldsymbol{\theta}$ is fixed but unknown. The likelihood of the observed samples is by definition the joint density

$$p(\mathscr{X} \mid \boldsymbol{\theta}) = \prod_{k=1}^{n} p(\mathbf{x}_k \mid \boldsymbol{\theta}). \tag{2}$$

The maximum likelihood estimate $\hat{\boldsymbol{\theta}}$ is that value of $\boldsymbol{\theta}$ that maximizes $p(\mathscr{X} \mid \boldsymbol{\theta})$.

If we assume that $p(\mathscr{X} \mid \boldsymbol{\theta})$ is a differentiable function of $\boldsymbol{\theta}$, then we can derive some interesting necessary conditions for $\hat{\boldsymbol{\theta}}$. Let l be the logarithm of the likelihood, and let $\nabla_{\boldsymbol{\theta}_i} l$ be the gradient of l with respect to $\boldsymbol{\theta}_i$. Then

$$l = \sum_{k=1}^{n} \log p(\mathbf{x}_k \mid \boldsymbol{\theta}) \tag{3}$$

and

$$\nabla_{\boldsymbol{\theta}_i} l = \sum_{k=1}^{n} \frac{1}{p(\mathbf{x}_k \mid \boldsymbol{\theta})} \nabla_{\boldsymbol{\theta}_i} \left[\sum_{j=1}^{c} p(\mathbf{x}_k \mid \omega_j, \boldsymbol{\theta}_j) P(\omega_j) \right].$$

If we assume that the elements of $\boldsymbol{\theta}_i$ and $\boldsymbol{\theta}_j$ are functionally independent if $i \neq j$, and if we introduce the a posteriori probability

$$P(\omega_i \mid \mathbf{x}_k, \boldsymbol{\theta}) = \frac{p(\mathbf{x}_k \mid \omega_i, \boldsymbol{\theta}_i) P(\omega_i)}{p(\mathbf{x}_k \mid \boldsymbol{\theta})} \tag{4}$$

we see that the gradient of the log-likelihood can be written in the interesting form

$$\nabla_{\boldsymbol{\theta}_i} l = \sum_{k=1}^{n} P(\omega_i \mid \mathbf{x}_k, \boldsymbol{\theta}) \nabla_{\boldsymbol{\theta}_i} \log p(\mathbf{x}_k \mid \omega_i, \boldsymbol{\theta}_i). \tag{5}$$

Since the gradient must vanish at the $\boldsymbol{\theta}_i$ that maximizes l, the maximum-likelihood estimate $\hat{\boldsymbol{\theta}}_i$ must satisfy the conditions

$$\sum_{k=1}^{n} P(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}}) \nabla_{\boldsymbol{\theta}_i} \log p(\mathbf{x}_k \mid \omega_i, \hat{\boldsymbol{\theta}}_i) = 0, \qquad i = 1, \ldots, c. \tag{6}$$

Conversely, among the solutions to these equations for $\hat{\boldsymbol{\theta}}_i$ we will find the maximum-likelihood solution.

It is not hard to generalize these results to include the a priori probabilities $P(\omega_i)$ among the unknown quantities. In this case the search for the maximum value of $p(\mathcal{X} \mid \boldsymbol{\theta})$ extends over $\boldsymbol{\theta}$ and $P(\omega_i)$, subject to the constraints

$$P(\omega_i) \geq 0 \qquad i = 1, \ldots, c \tag{7}$$

and

$$\sum_{i=1}^{c} P(\omega_i) = 1. \tag{8}$$

Let $\hat{P}(\omega_i)$ be the maximum likelihood estimate for $P(\omega_i)$, and let $\hat{\boldsymbol{\theta}}_i$ be the maximum likelihood estimate for $\boldsymbol{\theta}_i$. The diligent reader will be able to show that if the likelihood function is differentiable and if $\hat{P}(\omega_i) \neq 0$ for any i, then $\hat{P}(\omega_i)$ and $\hat{\boldsymbol{\theta}}_i$ must satisfy

$$\hat{P}(\omega_i) = \frac{1}{n} \sum_{k=1}^{n} \hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}}) \tag{9}$$

and

$$\sum_{k=1}^{n} \hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}}) \nabla_{\boldsymbol{\theta}_i} \log p(\mathbf{x}_k \mid \omega_i, \hat{\boldsymbol{\theta}}_i) = 0, \tag{10}$$

where

$$\hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}}) = \frac{p(\mathbf{x}_k \mid \omega_i, \hat{\boldsymbol{\theta}}_i)\hat{P}(\omega_i)}{\sum_{j=1}^{c} p(\mathbf{x}_k \mid \omega_j, \hat{\boldsymbol{\theta}}_j)\hat{P}(\omega_j)}. \tag{11}$$

6.4 APPLICATION TO NORMAL MIXTURES

It is enlightening to see how these general results apply to the case where the component densities are multivariate normal, $p(\mathbf{x} \mid \omega_i, \boldsymbol{\theta}_i) \sim N(\boldsymbol{\mu}_i, \Sigma_i)$. The following table illustrates a few of the different cases that can arise depending upon which parameters are known ($\surd$) and which are unknown (?):

Case	$\boldsymbol{\mu}_i$	Σ_i	$P(\omega_i)$	c
1	?	$\surd$	$\surd$	$\surd$
2	?	?	?	$\surd$
3	?	?	?	?

Case 1 is the simplest, and will be considered in detail because of its pedagogic value. Case 2 is more realistic, though somewhat more involved.

Case 3 represents the problem we face on encountering a completely unknown set of data. Unfortunately, it can not be solved by maximum-likelihood methods. We shall postpone discussion of what can be done when the number of classes is unknown until later in this chapter.

6.4.1 Case 1: Unknown Mean Vectors

If the only unknown quantities are the mean vectors μ_i, then θ_i can be identified with μ_i and Eq. (6) can be used to obtain necessary conditions on the maximum likelihood estimate for μ_i. Since

$$\log p(\mathbf{x} \mid \omega_i, \mu_i) = -\log[(2\pi)^{d/2}|\Sigma_i|^{1/2}] - \tfrac{1}{2}(\mathbf{x} - \mu_i)^t\Sigma_i^{-1}(\mathbf{x} - \mu_i),$$

$$\nabla_{\mu_i} \log p(\mathbf{x} \mid \omega_i, \mu_i) = \Sigma_i^{-1}(\mathbf{x} - \mu_i).$$

Thus, Eq. (6) for the maximum-likelihood estimate $\hat{\mu}_i$ yields

$$\sum_{k=1}^{n} P(\omega_i \mid \mathbf{x}_k, \hat{\mu})\Sigma_i^{-1}(\mathbf{x}_k - \hat{\mu}_i) = 0, \text{ where } \hat{\mu} = (\hat{\mu}_1, \ldots, \hat{\mu}_c).$$

After multiplying by Σ_i and rearranging terms, we obtain

$$\hat{\mu}_i = \frac{\sum_{k=1}^{n} P(\omega_i \mid \mathbf{x}_k, \hat{\mu})\mathbf{x}_k}{\sum_{k=1}^{n} P(\omega_i \mid \mathbf{x}_k, \hat{\mu})}. \tag{12}$$

This equation is intuitively very satisfying. It shows that the estimate for μ_i is merely a weighted average of the samples. The weight for the kth sample is an estimate of how likely it is that $\mathbf{x}_k$ belongs to the ith class. If $P(\omega_i \mid \mathbf{x}_k, \hat{\mu})$ happened to be one for some of the samples and zero for the rest, then $\hat{\mu}_i$ would be the mean of those samples estimated to belong to the ith class. More generally, suppose that $\hat{\mu}_i$ is sufficiently close to the true value of μ_i that $P(\omega_i \mid \mathbf{x}_k, \hat{\mu})$ is essentially the true a posteriori probability for ω_i. If we think of $P(\omega_i \mid \mathbf{x}_k, \hat{\mu})$ as the fraction of those samples having value $\mathbf{x}_k$ that come from the ith class, then we see that Eq. (12) essentially gives $\hat{\mu}_i$ as the average of the samples coming from the ith class.

Unfortunately, Eq. (12) does not give $\hat{\mu}_i$ explicitly, and if we substitute

$$P(\omega_i \mid \mathbf{x}_k, \hat{\mu}) = \frac{p(\mathbf{x}_k \mid \omega_i, \hat{\mu}_i)P(\omega_i)}{\sum_{j=1}^{c} p(\mathbf{x}_k \mid \omega_j, \hat{\mu}_j)P(\omega_j)}$$

with $p(\mathbf{x} \mid \omega_i, \hat{\mu}_i) \sim N(\hat{\mu}_i, \Sigma_i)$, we obtain a tangled snarl of coupled simultaneous nonlinear equations. These equations usually do not have a unique

solution, and we must test the solutions we get to find the one that actually maximizes the likelihood.

If we have some way of obtaining fairly good initial estimates $\hat{\boldsymbol{\mu}}_i(0)$ for the unknown means, Eq. (12) suggests the following iterative scheme for improving the estimates:

$$\hat{\boldsymbol{\mu}}_i(j+1) = \frac{\sum_{k=1}^{n} P(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\mu}}(j))\mathbf{x}_k}{\sum_{k=1}^{n} P(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\mu}}(j))}. \tag{13}$$

This is basically a gradient ascent or hill-climbing procedure for maximizing the log-likelihood function. If the overlap between component densities is small, then the coupling between classes will be small and convergence will be fast. However, when convergence does occur, all that we can be sure of is that the gradient is zero. Like all hill-climbing procedures, this one carries no guarantee of yielding the global maximum.

6.4.2 An Example

To illustrate the kind of behavior that can occur, consider the simple one-dimensional, two-component normal mixture

$$p(x \mid \mu_1, \mu_2) = \frac{1}{3\sqrt{2\pi}} \exp[-\tfrac{1}{2}(x-\mu_1)^2] + \frac{2}{3\sqrt{2\pi}} \exp[-\tfrac{1}{2}(x-\mu_2)^2].$$

The 25 samples shown in Table 6-1 were drawn from this mixture with

TABLE 6-1. Twenty-five Samples from a Normal Mixture

k	x_k	(Class)	k	x_k	(Class)
1	0.608	2	13	3.240	2
2	−1.590	1	14	2.400	2
3	0.235	2	15	−2.499	1
4	3.949	2	16	2.608	2
5	−2.249	1	17	−3.458	1
6	2.704	2	18	0.257	2
7	−2.473	1	19	2.569	2
8	0.672	2	20	1.415	2
9	0.262	2	21	1.410	2
10	1.072	2	22	−2.653	1
11	−1.773	1	23	1.396	2
12	0.537	2	24	3.286	2
			25	−0.712	1

$\mu_1 = -2$ and $\mu_2 = 2$. Let us use these samples to compute the log-likelihood function

$$l(\mu_1, \mu_2) = \sum_{k=1}^{n} \log p(x_k \mid \mu_1, \mu_2)$$

for various values of μ_1 and μ_2. Figure 6.1 is a contour plot that shows how l varies with μ_1 and μ_2. The maximum value of l occurs at $\hat{\mu}_1 = -2.130$ and $\hat{\mu}_2 = 1.668$, which is in the rough vicinity of the true values $\mu_1 = -2$ and $\mu_2 = 2$.* However, l reaches another peak of comparable height at $\hat{\mu}_1 = 2.085$ and $\hat{\mu}_2 = -1.257$. Roughly speaking, this solution corresponds to interchanging μ_1 and μ_2. Note that had the a priori probabilities been equal,

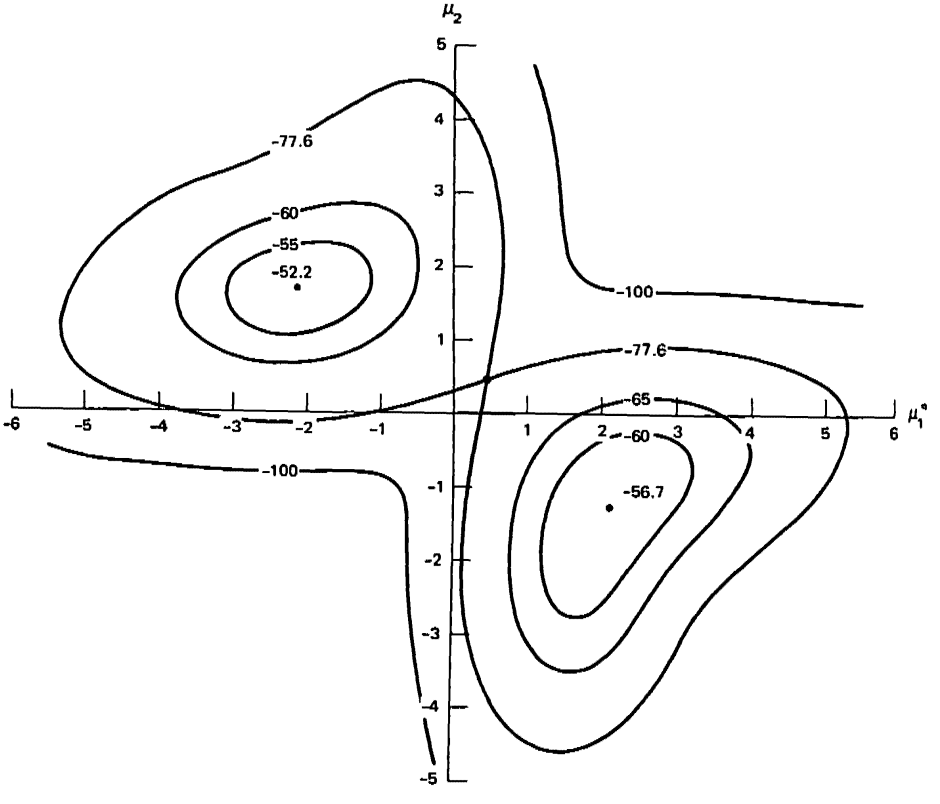


FIGURE 6.1. Contours of a log-likelihood function.

* If the data in Table 6-1 are separated by class, the resulting sample means are $m_1 = -2.176$ and $m_2 = 1.684$. Thus, the maximum likelihood estimates for the unsupervised case are close to the maximum likelihood estimates for the supervised case.

interchanging μ_1 and μ_2 would have produced no change in the log-likelihood function. Thus, when the mixture density is not identifiable, the maximum likelihood solution is not unique.

Additional insight into the nature of these multiple solutions can be obtained by examining the resulting estimates for the mixture density. Figure 6.2 shows the true mixture density and the estimates obtained by using the maximum likelihood estimates as if they were the true parameter

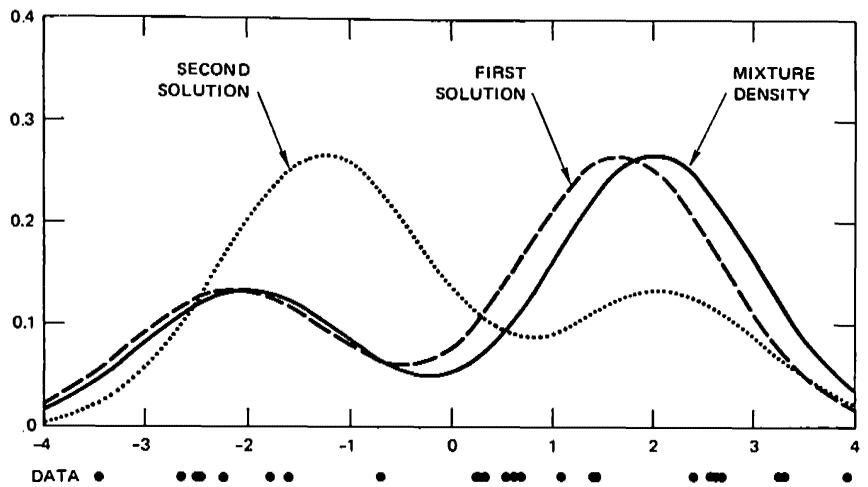


FIGURE 6.2. Estimates of the mixture density.

values. The 25 sample values are shown as a scatter of points along the abscissa. Note that the peaks of both the true mixture density and the maximum likelihood solution are located so as to encompass two major groups of data points. The estimate corresponding to the smaller local maximum of the log-likelihood function has a mirror-image shape, but its peaks also encompass reasonable groups of data points. To the eye, neither of these solutions is clearly superior, and both are interesting.

If Eq. (13) is used to determine solutions to Eq. (12) iteratively, the results depend on the starting values $\hat{\mu}_1(0)$ and $\hat{\mu}_2(0)$. Figure 6.3 shows how different starting points lead to different solutions, and gives some indication of rates of convergence. Note that if $\hat{\mu}_1(0) = \hat{\mu}_2(0)$, convergence to a saddle point occurs in one step. This is not a coincidence. It happens for the simple reason that for this starting point $P(\omega_i \mid x_k, \hat{\mu}_1(0), \hat{\mu}_2(0)) = P(\omega_i)$. Thus, Eq. (13) yields the mean of all of the samples for $\hat{\mu}_1$ and $\hat{\mu}_2$ for all successive iterations. Clearly, this is a general phenomenon, and such saddle-point solutions can

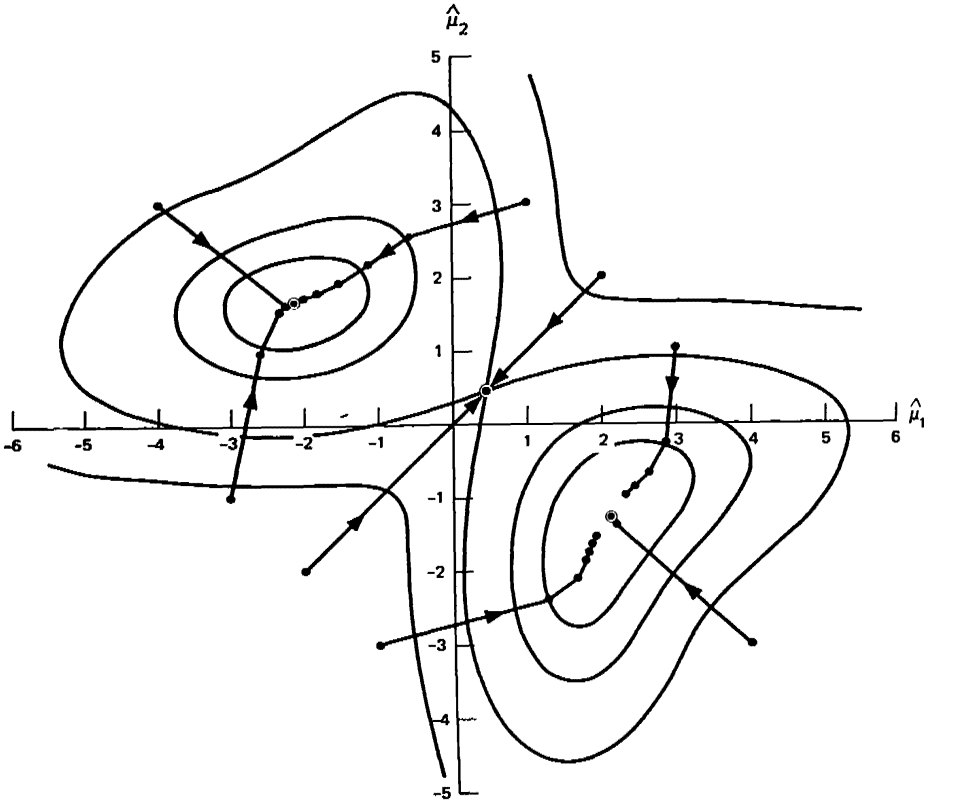


FIGURE 6.3. Trajectories for the iterative procedure.

be expected if the starting point does not bias the search away from a symmetric answer.

6.4.3 Case 2: All Parameters Unknown

If μ_i, Σ_i, and $P(\omega_i)$ are all unknown, and if no constraints are placed on the covariance matrix, then the maximum likelihood principle yields useless singular solutions. The reason for this can be appreciated from the following simple example. Let $p(x \mid \mu, \sigma^2)$ be the two-component normal mixture

$$p(x \mid \mu, \sigma^2) = \frac{1}{2\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] + \frac{1}{2\sqrt{2\pi}} \exp[-\tfrac{1}{2}x^2].$$

The likelihood function for n samples drawn according to this probability law is merely the product of the n densities $p(x_k \mid \mu, \sigma^2)$. Suppose that we

let $\mu = x_1$, so that

$$p(x_1 \mid \mu, \sigma^2) = \frac{1}{2\sqrt{2\pi}\sigma} + \frac{1}{2\sqrt{2\pi}} \exp[-\tfrac{1}{2}x_1^2].$$

Clearly, for the rest of the samples

$$p(x_k \mid \mu, \sigma^2) \geq \frac{1}{2\sqrt{2\pi}} \exp[-\tfrac{1}{2}x_k^2],$$

so that

$$p(x_1, \ldots, x_n \mid \mu, \sigma^2) \geq \left\{\frac{1}{\sigma} + \exp[-\tfrac{1}{2}x_1^2]\right\} \frac{1}{(2\sqrt{2\pi})^n} \exp\left[-\tfrac{1}{2}\sum_{k=2}^{n} x_k^2\right].$$

Thus, by letting σ approach zero we can make the likelihood arbitrarily large, and the maximum likelihood solution is singular.

Ordinarily, singular solutions are of no interest, and we are forced to conclude that the maximum likelihood principle fails for this class of normal mixtures. However, it is an empirical fact that meaningful solutions can still be obtained if we restrict our attention to the largest of the finite local maxima of the likelihood function. Assuming that the likelihood function is well behaved at such maxima, we can use Eqs. (9)–(11) to obtain estimates for μ_i, Σ_i, and $P(\omega_i)$. When we include the elements of Σ_i in the elements of the parameter vector θ_i, we must remember that only half of the off-diagonal elements are independent. In addition, it turns out to be much more convenient to let the independent elements of Σ_i^{-1} rather than Σ_i be the unknown parameters. With these observations, the actual differentiation of

$$\log p(\mathbf{x}_k \mid \omega_i, \theta_i) = \log \frac{|\Sigma_i^{-1}|^{1/2}}{(2\pi)^{d/2}} - \tfrac{1}{2}(\mathbf{x}_k - \mu_i)^t \Sigma_i^{-1}(\mathbf{x}_k - \mu_i)$$

with respect to the elements of μ_i and Σ_i^{-1} is relatively routine. Let $x_p(k)$ be the pth element of $\mathbf{x}_k$, $\mu_p(i)$ be the pth element of μ_i, $\sigma_{pq}(i)$ be the pqth element of Σ_i, and $\sigma^{pq}(i)$ be the pqth element of Σ_i^{-1}. Then

$$\nabla_{\mu_i} \log p(\mathbf{x}_k \mid \omega_i, \theta_i) = \Sigma_i^{-1}(\mathbf{x}_k - \mu_i)$$

and

$$\frac{\partial \log p(\mathbf{x}_k \mid \omega_i, \theta_i)}{\partial \sigma^{pq}(i)} = \left(1 - \frac{\delta_{pq}}{2}\right)[\sigma_{pq}(i) - (x_p(k) - \mu_p(i))(x_q(k) - \mu_q(i))],$$

where δ_{pq} is the Kronecker delta. Substituting these results in Eq. (10) and doing a small amount of algebraic manipulation, we obtain the following

equations for the local-maximum-likelihood estimates $\hat{\mu}_i$, $\hat{\Sigma}_i$, and $\hat{P}(\omega_i)$:

$$\hat{P}(\omega_i) = \frac{1}{n}\sum_{k=1}^{n}\hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}}) \tag{14}$$

$$\hat{\mu}_i = \frac{\sum_{k=1}^{n}\hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}})\mathbf{x}_k}{\sum_{k=1}^{n}\hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}})} \tag{15}$$

$$\Sigma_i = \frac{\sum_{k=1}^{n}\hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}})(\mathbf{x}_k - \hat{\mu}_i)(\mathbf{x}_k - \hat{\mu}_i)^t}{\sum_{k=1}^{n}\hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}}_i)} \tag{16}$$

where

$$\begin{aligned}\hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}}) &= \frac{p(\mathbf{x}_k \mid \omega_i, \hat{\boldsymbol{\theta}}_i)\hat{P}(\omega_i)}{\sum_{j=1}^{c} p(\mathbf{x}_k \mid \omega_j, \hat{\boldsymbol{\theta}}_j)\hat{P}(\omega_j)} \\ &= \frac{|\hat{\Sigma}_i|^{-1/2}\exp[-\frac{1}{2}(\mathbf{x}_k - \hat{\mu}_i)^t\hat{\Sigma}_i^{-1}(\mathbf{x}_k - \hat{\mu}_i)]\hat{P}(\omega_i)}{\sum_{j=1}^{c}|\hat{\Sigma}_j|^{-1/2}\exp[-\frac{1}{2}(\mathbf{x}_k - \hat{\mu}_j)^t\hat{\Sigma}_j^{-1}(\mathbf{x}_k - \hat{\mu}_j)]\hat{P}(\omega_j)}.\end{aligned} \tag{17}$$

While the notation may make these equations appear to be rather formidable, their interpretation is actually quite simple. In the extreme case where $\hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}})$ is one when $\mathbf{x}_k$ is from Class ω_i and zero otherwise, $\hat{P}(\omega_i)$ is the fraction of samples from ω_i, $\hat{\mu}_i$ is the mean of those samples, and $\hat{\Sigma}_i$ is the corresponding sample covariance matrix. More generally, $\hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}})$ is between zero and one, and all of the samples play some role in the estimates. However, the estimates are basically still frequency ratios, sample means, and sample covariance matrices.

The problems involved in solving these implicit equations are similar to the problems discussed in Section 6.4.1, with the additional complication of having to avoid singular solutions. Of the various techniques that can be used to obtain a solution, the most obvious approach is to use initial estimates to evaluate Eq. (17) for $\hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}})$ and then to use Eqs. (14)–(16) to update these estimates. If the initial estimates are very good, having perhaps been obtained from a fairly large set of labelled samples, convergence can be quite rapid. However, the results do depend upon the starting point, and the problem of multiple solutions is always present. Furthermore, the repeated computation and inversion of the sample covariance matrices can be quite time consuming.

Considerable simplification can be obtained it it is possible to assume that the covariance matrices are diagonal. This has the added virtue of reducing the number of unknown parameters, which is very important when the number of samples is not large. If this assumption is too strong, it still may be possible to obtain some simplification by assuming that the c covariance matrices are equal, which also eliminates the problem of singular solutions. The derivation of the appropriate maximum likelihood equations for this case is treated in Problems 5 and 6.

6.4.4 A Simple Approximate Procedure

Of the various techniques that can be used to simplify the computation and accelerate convergence, we shall briefly consider one elementary, approximate method. From Eq. (17), it is clear that the probability $\hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}})$ is large when the squared Mahalanobis distance $(\mathbf{x}_k - \hat{\boldsymbol{\mu}}_i)^t \hat{\boldsymbol{\Sigma}}_i^{-1}(\mathbf{x}_k - \hat{\boldsymbol{\mu}}_i)$ is small. Suppose that we merely compute the squared Euclidean distance $\|\mathbf{x}_k - \hat{\boldsymbol{\mu}}_i\|^2$, find the mean $\hat{\boldsymbol{\mu}}_m$ nearest to $\mathbf{x}_k$, and approximate $\hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}})$ as

$$\hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}}) \approx \begin{cases} 1 & i = m \\ 0 & \text{otherwise.} \end{cases}$$

Then the iterative application of Eq. (15) leads to the following procedure* for finding $\hat{\boldsymbol{\mu}}_1, \ldots, \hat{\boldsymbol{\mu}}_c$:

Procedure: Basic Isodata

1. Choose some initial values for the means $\hat{\boldsymbol{\mu}}_1, \ldots, \hat{\boldsymbol{\mu}}_c$.

Loop: 2. Classify the n samples by assigning them to the class of the closest mean.

3. Recompute the means as the average of the samples in their class.

4. If any mean changed value, go to Loop; otherwise, stop.

This is typical of a class of procedures that are known as *clustering* procedures. Later on we shall place it in the class of iterative optimization procedures, since the means tend to move so as to minimize a squared-error

* Throughout this chapter we shall name and describe various iterative procedures as if they were computer programs. All of these procedures have in fact been programmed, often with much more elaborate provisions for doing such things as breaking ties, avoiding trap states, and allowing more sophisticated terminating conditions. Thus, we occasionally include the word "basic" in their names to emphasize the fact that our interest is limited to explaining essential concepts.

criterion function. At the moment we view it merely as an approximate way to obtain maximum likelihood estimates for the means. The values obtained can be accepted as the answer, or can be used as starting points for the more exact computations.

It is interesting to see how this procedure behaves on the example data in Table 6-1. Figure 6.4 shows the sequence of values for $\hat{\mu}_1$ and $\hat{\mu}_2$ obtained

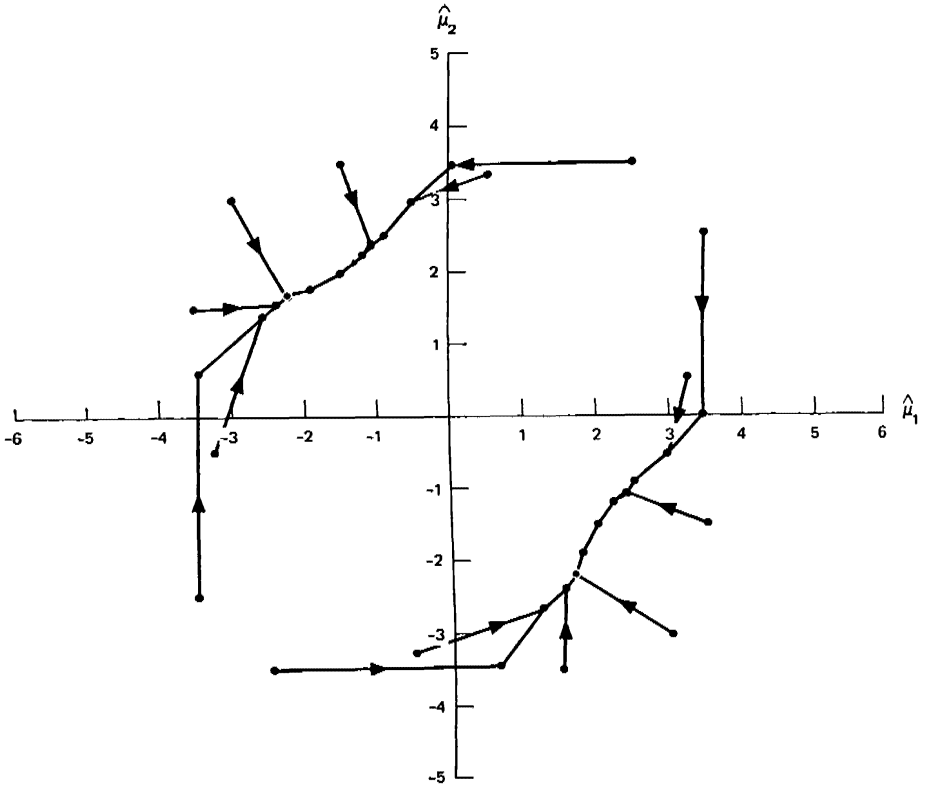


FIGURE 6.4. Trajectories for the Basic Isodata Procedure.

for several different starting points. Since interchanging $\hat{\mu}_1$ and $\hat{\mu}_2$ merely interchanges the labels assigned to the data, the trajectories are symmetric about the line $\hat{\mu}_1 = \hat{\mu}_2$. The trajectories lead either to the point $\hat{\mu}_1 = -2.176$, $\hat{\mu}_2 = 1.684$ or to its image. This is close to the solution found by the maximum likelihood method (viz., $\hat{\mu}_1 = -2.130$ and $\hat{\mu}_2 = 1.668$), and the trajectories show a general resemblance to those shown in Figure 6.3 In general, when the overlap between the component densities is small the maximum likelihood approach and the Isodata procedure can be expected to give similar results.

6.5 UNSUPERVISED BAYESIAN LEARNING

6.5.1 The Bayes Classifier

Maximum likelihood methods do not consider the parameter vector $\boldsymbol{\theta}$ to be random—it is just unknown. Prior knowledge about likely values for $\boldsymbol{\theta}$ is irrelevant, although in practice such knowledge may be used in choosing good starting points for hill-climbing procedures. In this section we shall take a Bayesian approach to unsupervised learning. We shall assume that $\boldsymbol{\theta}$ is a random variable with a known a priori distribution $p(\boldsymbol{\theta})$, and we shall use the samples to compute the a posteriori density $p(\boldsymbol{\theta} \mid \mathcal{X})$. Interestingly enough, the analysis will virtually parallel the analysis of supervised Bayesian learning, showing that the two problems are formally very similar.

We begin with an explicit statement of our basic assumptions. We assume that:

1. The number of classes is known.
2. The a priori probabilities $P(\omega_j)$ for each class are known, $j = 1, \ldots, c$.
3. The forms for the class-conditional probability densities $p(\mathbf{x} \mid \omega_j, \boldsymbol{\theta}_j)$ are known, $j = 1, \ldots, c$, but the parameter vector $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_c)$ is not known.
4. Part of our knowledge about $\boldsymbol{\theta}$ is contained in a known a priori density $p(\boldsymbol{\theta})$.
5. The rest of our knowledge about $\boldsymbol{\theta}$ is contained in a set $\mathcal{X}$ of n samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$ drawn independently from the mixture density

$$p(\mathbf{x} \mid \boldsymbol{\theta}) = \sum_{j=1}^{c} p(\mathbf{x} \mid \omega_j, \boldsymbol{\theta}_j) P(\omega_j). \tag{1}$$

At this point we could go directly to the calculation of $p(\boldsymbol{\theta} \mid \mathcal{X})$. However, let us first see how this density is used to determine the Bayes classifier. Suppose that a state of nature is selected with probability $P(\omega_i)$ and a feature vector $\mathbf{x}$ is selected according to the probability law $p(\mathbf{x} \mid \omega_i, \boldsymbol{\theta}_i)$. To derive the Bayes classifier we must use all of the information at our disposal to compute the a posteriori probability $P(\omega_i \mid \mathbf{x})$. We exhibit the role of the samples explicitly by writing this as $P(\omega_i \mid \mathbf{x}, \mathcal{X})$. By Bayes rule,

$$P(\omega_i \mid \mathbf{x}, \mathcal{X}) = \frac{p(\mathbf{x} \mid \omega_i, \mathcal{X}) P(\omega_i \mid \mathcal{X})}{\sum_{j=1}^{c} p(\mathbf{x} \mid \omega_j, \mathcal{X}) P(\omega_j \mid \mathcal{X})}.$$

Since the selection of the state of nature ω_i was done independently of the previously drawn samples, $P(\omega_i \mid \mathcal{X}) = P(\omega_i)$, and we obtain

$$P(\omega_i \mid \mathbf{x}, \mathcal{X}) = \frac{p(\mathbf{x} \mid \omega_i, \mathcal{X})P(\omega_i)}{\sum_{j=1}^{c} p(\mathbf{x} \mid \omega_j, \mathcal{X})P(\omega_j)}. \tag{18}$$

We introduce the unknown parameter vector by writing

$$\begin{aligned} p(\mathbf{x} \mid \omega_i, \mathcal{X}) &= \int p(\mathbf{x}, \boldsymbol{\theta} \mid \omega_i, \mathcal{X})\, d\boldsymbol{\theta} \\ &= \int p(\mathbf{x} \mid \boldsymbol{\theta}, \omega_i, \mathcal{X}) p(\boldsymbol{\theta} \mid \omega_i, \mathcal{X})\, d\boldsymbol{\theta}. \end{aligned}$$

Since the selection of $\mathbf{x}$ is independent of the samples, $p(\mathbf{x} \mid \boldsymbol{\theta}, \omega_i, \mathcal{X}) = p(\mathbf{x} \mid \omega_i, \boldsymbol{\theta}_i)$. Similarly, since knowledge of the state of nature when $\mathbf{x}$ is selected tells us nothing about the distribution of $\boldsymbol{\theta}$, $p(\boldsymbol{\theta} \mid \omega_i, \mathcal{X}) = p(\boldsymbol{\theta} \mid \mathcal{X})$. Thus we obtain

$$p(\mathbf{x} \mid \omega_i, \mathcal{X}) = \int p(\mathbf{x} \mid \omega_i, \boldsymbol{\theta}_i) p(\boldsymbol{\theta} \mid \mathcal{X})\, d\boldsymbol{\theta}. \tag{19}$$

That is, our best estimate of $p(\mathbf{x} \mid \omega_i)$ is obtained by averaging $p(\mathbf{x} \mid \omega_i, \boldsymbol{\theta}_i)$ over $\boldsymbol{\theta}_i$. Whether or not this is a good estimate depends on the nature of $p(\boldsymbol{\theta} \mid \mathcal{X})$, and thus our attention turns at last to that density.

6.5.2 Learning the Parameter Vector

Using Bayes rule, we can write

$$p(\boldsymbol{\theta} \mid \mathcal{X}) = \frac{p(\mathcal{X} \mid \boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(\mathcal{X} \mid \boldsymbol{\theta})p(\boldsymbol{\theta})\, d\boldsymbol{\theta}} \tag{20}$$

where the independence of the samples yields

$$p(\mathcal{X} \mid \boldsymbol{\theta}) = \prod_{k=1}^{n} p(\mathbf{x}_k \mid \boldsymbol{\theta}). \tag{21}$$

Alternatively, letting $\mathcal{X}^n$ denote the set of n samples, we can write Eq. (20) in the recursive form

$$p(\boldsymbol{\theta} \mid \mathcal{X}^n) = \frac{p(\mathbf{x}_n \mid \boldsymbol{\theta})p(\boldsymbol{\theta} \mid \mathcal{X}^{n-1})}{\int p(\mathbf{x}_n \mid \boldsymbol{\theta})p(\boldsymbol{\theta} \mid \mathcal{X}^{n-1})\, d\boldsymbol{\theta}}. \tag{22}$$

These are the basic equations for unsupervised Bayesian learning. Eq. (20) emphasizes the relation between the Bayesian and the maximum likelihood

solutions. If $p(\boldsymbol{\theta})$ is essentially uniform over the region where $p(\mathscr{X} \mid \boldsymbol{\theta})$ peaks, then $p(\boldsymbol{\theta} \mid \mathscr{X})$ peaks at the same place. If the only significant peak occurs at $\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}$ and if the peak is very sharp, then Eqs. (19) and (18) yield

$$p(\mathbf{x} \mid \omega_i, \mathscr{X}) \approx p(\mathbf{x} \mid \omega_i, \hat{\boldsymbol{\theta}}_i)$$

and

$$P(\omega_i \mid \mathbf{x}, \mathscr{X}) \approx \frac{p(\mathbf{x} \mid \omega_i, \hat{\boldsymbol{\theta}}_i)P(\omega_i)}{\sum_{j=1}^{c} p(\mathbf{x} \mid \omega_j, \hat{\boldsymbol{\theta}}_j)P(\omega_j)}.$$

That is, these conditions justify the use of the maximum likelihood estimate as if it were the true value of $\boldsymbol{\theta}$ in designing the Bayes classifier.

Of course, if $p(\boldsymbol{\theta})$ has been obtained by supervised learning using a large set of labelled samples, it will be far from uniform, and it will have a dominant influence on $p(\boldsymbol{\theta} \mid \mathscr{X}^n)$, when n is small. Eq. (22) shows how the observation of an additional unlabelled sample modifies our opinion about the true value of $\boldsymbol{\theta}$, and emphasizes the ideas of updating and learning. If the mixture density $p(\mathbf{x} \mid \boldsymbol{\theta})$ is identifiable, then each additional sample tends to sharpen $p(\boldsymbol{\theta} \mid \mathscr{X}^n)$, and under fairly general conditions $p(\boldsymbol{\theta} \mid \mathscr{X}^n)$ can be shown to converge (in probability) to a Dirac delta function centered at the true value of $\boldsymbol{\theta}$. Thus, even though we do not know the categories of the samples, identifiability assures us that we can learn the unknown parameter vector $\boldsymbol{\theta}$, and thereby learn the component densities $p(\mathbf{x} \mid \omega_i, \boldsymbol{\theta})$.

This, then, is the formal Bayesian solution to the problem of unsupervised learning. In retrospect, the fact that unsupervised learning of the parameters of a mixture density is so similar to supervised learning of the parameters of a component density is not at all surprising. Indeed, if the component density is itself a mixture, there would appear to be no essential difference between the two problems.

However, there are some significant differences between supervised and unsupervised learning. One of the major differences concerns the problem of identifiability. With supervised learning, lack of identifiability merely means that instead of obtaining a unique parameter vector we obtain an equivalence class of parameter vectors. However, since all of these yield the same component density, lack of identifiability presents no theoretical difficulty. With unsupervised learning, lack of identifiability is much more serious. When $\boldsymbol{\theta}$ can not be determined uniquely, the mixture can not be decomposed into its true components. Thus, while $p(\mathbf{x} \mid \mathscr{X}^n)$ may still converge to $p(\mathbf{x})$, $p(\mathbf{x} \mid \omega_i, \mathscr{X}^n)$ given by Eq. (19) will not in general converge to $p(\mathbf{x} \mid \omega_i)$, and a theoretical barrier to learning exists.

Another serious problem for unsupervised learning is computational complexity. With supervised learning, the possibility of finding sufficient

statistics allows solutions that are analytically pleasing and computationally feasible. With unsupervised learning, there is no way to avoid the fact that the samples are obtained from a mixture density,

$$p(\mathbf{x} \mid \boldsymbol{\theta}) = \sum_{j=1}^{c} p(\mathbf{x} \mid \omega_j, \boldsymbol{\theta}_j) P(\omega_j), \tag{1}$$

and this gives us little hope of ever finding simple exact solutions for $p(\boldsymbol{\theta} \mid \mathcal{X})$. Such solutions are tied to the existence of a simple sufficient statistic, and the factorization theorem requires the ability to factor $p(\mathcal{X} \mid \boldsymbol{\theta})$ as

$$p(\mathcal{X} \mid \boldsymbol{\theta}) = g(\mathbf{s}, \boldsymbol{\theta}) h(\mathcal{X}).$$

But from Eqs. (21) and (1),

$$p(\mathcal{X} \mid \boldsymbol{\theta}) = \prod_{k=1}^{n} \left[\sum_{j=1}^{c} p(\mathbf{x}_k \mid \omega_j, \boldsymbol{\theta}_j) P(\omega_j) \right].$$

Thus, $p(\mathcal{X} \mid \boldsymbol{\theta})$ is the sum of c^n products of component densities. Each term in this sum can be interpreted as the joint probability of obtaining the samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$ bearing a particular labelling, with the sum extending over all of the ways that the samples could be labelled. Clearly, this results in a thorough mixture of $\boldsymbol{\theta}$ and the x's, and no simple factoring should be expected. An exception to this statement arises if the component densities do not overlap, so that as $\boldsymbol{\theta}$ varies only one term the mixture density is non-zero. In that case, $p(\mathcal{X} \mid \boldsymbol{\theta})$ is the product of the n nonzero terms, and may possess a simple sufficient statistic. However, since that case allows the class of any sample to be determined, it actually reduces the problem to one of supervised learning, and thus is not a significant exception.

Another way to compare supervised and unsupervised learning is to substitute the mixture density for $p(\mathbf{x}_n \mid \boldsymbol{\theta})$ in Eq. (22) and obtain

$$p(\boldsymbol{\theta} \mid \mathcal{X}^n) = \frac{\sum_{j=1}^{c} p(\mathbf{x}_n \mid \omega_j, \boldsymbol{\theta}_j) P(\omega_j)}{\sum_{j=1}^{c} \int p(\mathbf{x}_n \mid \omega_j, \boldsymbol{\theta}_j) P(\omega_j) p(\boldsymbol{\theta} \mid \mathcal{X}^{n-1})\, d\boldsymbol{\theta}} p(\boldsymbol{\theta} \mid \mathcal{X}^{n-1}). \tag{23}$$

If we consider the special case where $P(\omega_1) = 1$ and all the other a priori probabilities are zero, corresponding to the supervised case in which all samples come from Class 1, then Eq. (23) simplifies to

$$p(\boldsymbol{\theta} \mid \mathcal{X}^n) = \frac{p(\mathbf{x}_n \mid \omega_1, \boldsymbol{\theta}_1)}{\int p(\mathbf{x}_n \mid \omega_1, \boldsymbol{\theta}_1) p(\boldsymbol{\theta} \mid \mathcal{X}^{n-1})\, d\boldsymbol{\theta}} p(\boldsymbol{\theta} \mid \mathcal{X}^{n-1}). \tag{24}$$

Let us compare Eqs. (23) and (24) to see how observing an additional sample changes our estimate of $\boldsymbol{\theta}$. In each case we can ignore the denominator, which is independent of $\boldsymbol{\theta}$. Thus, the only significant difference is that in the supervised case we multiply the "a priori" density for $\boldsymbol{\theta}$ by the component density $p(\mathbf{x}_n \mid \omega_1, \boldsymbol{\theta}_1)$, while in the unsupervised case we multiply it by the mixture density $\sum_{j=1}^{c} p(\mathbf{x}_n \mid \omega_j, \boldsymbol{\theta}_j)P(\omega_j)$. Assuming that the sample really did come from Class 1, we see that the effect of not knowing this category membership in the unsupervised case is to diminish the influence of $\mathbf{x}_n$ on changing $\boldsymbol{\theta}$. Since $\mathbf{x}_n$ could have come from any of the c classes, we cannot use it with full effectiveness in changing the component(s) of $\boldsymbol{\theta}$ associated with any one category. Rather, we must distribute its effect over the various categories in accordance with the probability that it arose from each category.

6.5.3 An Example

Consider the one-dimensional, two-component mixture with $p(x \mid \omega_1) \sim N(\mu, 1)$, $p(x \mid \omega_2, \theta) \sim N(\theta, 1)$, where μ, $P(\omega_1)$ and $P(\omega_2)$ are known. Here

$$p(x \mid \theta) = \frac{P(\omega_1)}{\sqrt{2\pi}} \exp[-\tfrac{1}{2}(x-\mu)^2] + \frac{P(\omega_2)}{\sqrt{2\pi}} \exp[-\tfrac{1}{2}(x-\theta)^2].$$

Viewed as a function of x, this mixture density is a superposition of two normal densities, one peaking at $x = \mu$ and the other peaking at $x = \theta$. Viewed as a function of θ, $p(x \mid \theta)$ has a single peak at $\theta = x$. Suppose that the a priori density $p(\theta)$ is uniform from a to b. Then after one observation

$$p(\theta \mid x_1) = \alpha p(x_1 \mid \theta)p(\theta)$$

$$= \begin{cases} \alpha'[P(\omega_1)\exp[-\tfrac{1}{2}(x_1-\mu)^2] \\ \qquad + P(\omega_2)\exp[-\tfrac{1}{2}(x_1-\theta)^2]] & a \le \theta \le b \\ 0 & \text{otherwise,} \end{cases}$$

where α and α' are normalizing constants, independent of θ. If the sample x_1 is in the range $a \le x_1 \le b$, then $p(\theta \mid x_1)$ peaks at $\theta = x_1$. Otherwise it peaks either at $\theta = a$ if $x_1 < a$ or at $\theta = b$ if $x_1 > b$. Note that the additive constant $\exp[-(1/2)(x_1-\mu)^2]$ is large if x_1 is near μ, and thus the peak of $p(\theta \mid x_1)$ is less pronounced if x_1 is near μ. This corresponds to the fact that if x_1 is near μ, it is more likely to have come from the $p(x \mid \omega_1)$ component, and hence its influence on our estimate for θ is diminished.

With the addition of a second sample x_2, $p(\theta \mid x_1)$ changes to

$$p(\theta \mid x_1, x_2) = \beta p(x_2 \mid \theta) p(\theta \mid x_1)$$

$$= \begin{cases} \beta' [P(\omega_1)P(\omega_1) \exp[-\frac{1}{2}(x_1 - \mu)^2 - \frac{1}{2}(x_2 - \mu)^2] \\ + P(\omega_1)P(\omega_2) \exp[-\frac{1}{2}(x_1 - \mu)^2 - \frac{1}{2}(x_2 - \theta)^2] \\ + P(\omega_2)P(\omega_1) \exp[-\frac{1}{2}(x_1 - \theta)^2 - \frac{1}{2}(x_2 - \mu)^2] \\ + P(\omega_2)P(\omega_2) \exp[-\frac{1}{2}(x_1 - \theta)^2 - \frac{1}{2}(x_2 - \theta)^2]] \\ \qquad\qquad a \leq \theta \leq b \\ 0 \qquad\qquad \text{otherwise.} \end{cases}$$

Unfortunately, the primary thing we learn from this expression is that $p(\theta \mid \mathcal{X}^n)$ is already complicated when $n = 2$. The four terms in the sum correspond to the four ways in which the samples could have been drawn from the two component populations. With n samples there will be 2^n terms,

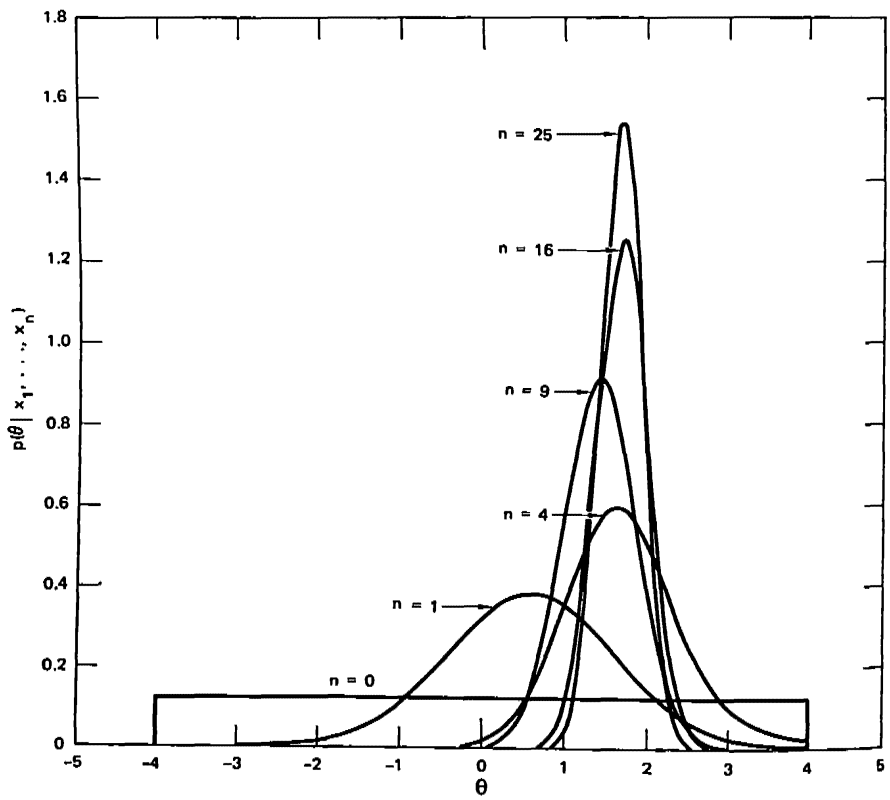


FIGURE 6.5. Unsupervised Bayesian learning.

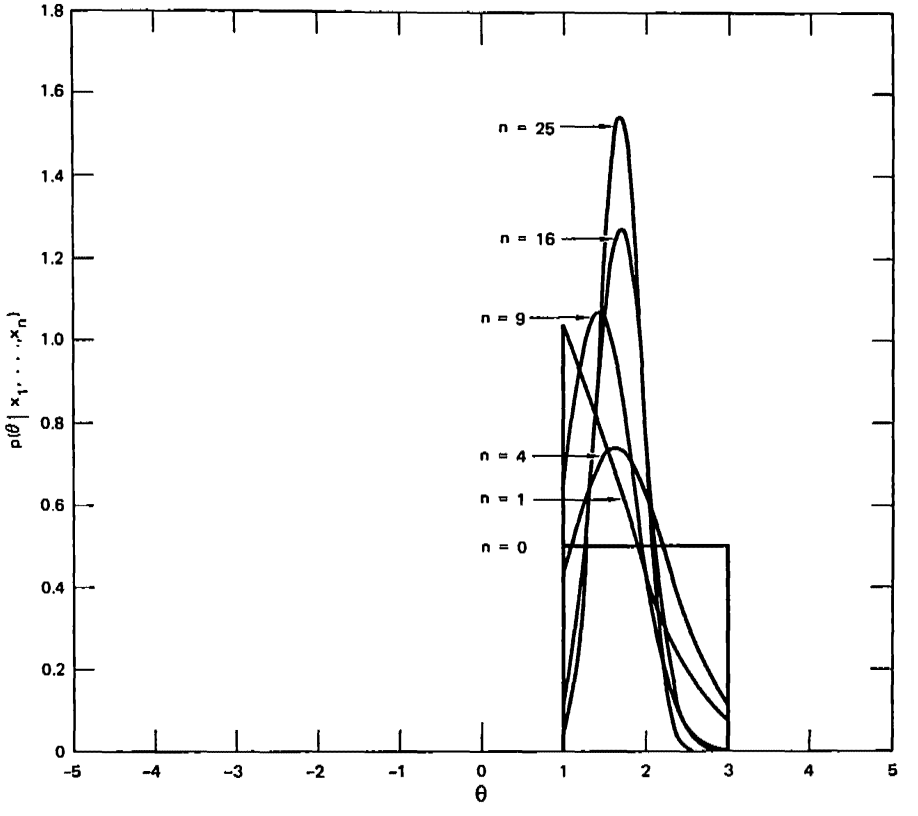


FIGURE 6.6. The effect of narrowing the a priori density.

and no simple sufficient statistics can be found to facilitate understanding or to simplify computations.

It is possible to use the relation

$$p(\theta \mid \mathcal{X}^n) = \frac{p(x_n \mid \theta)p(\theta \mid \mathcal{X}^{n-1})}{\int p(x_n \mid \theta)p(\theta \mid \mathcal{X}^{n-1})\, d\theta}$$

and numerical integration to obtain an approximate numerical solution for $p(\theta \mid \mathcal{X}^n)$. This was done for the data in Table 6-1 using the values $\mu = 2$, $P(\omega_1) = 1/3$, and $P(\omega_2) = 2/3$. An a priori density $p(\theta)$ uniform from -4 to 4 encompasses the data in that table. When this was used to start the recursive computation of $p(\theta \mid \mathcal{X}^n)$, the results shown in Figure 6.5 were obtained. As n goes to infinity we can confidently expect $p(\theta \mid \mathcal{X}^n)$ to approach an impulse centered at $\theta = 2$. This graph gives some idea of the rate of convergence.

One of the main differences between the Bayesian and the maximum likelihood approaches to unsupervised learning appears in the presence of the a priori density $p(\theta)$. Figure 6.6 shows how $p(\theta \mid \mathcal{X}^n)$ changes when $p(\theta)$

is assumed to be uniform from 1 to 3, corresponding to more certain initial knowledge about θ. The results of this change are most pronounced when n is small. It is here also that the differences between the Bayesian and the maximum likelihood solutions are most significant. As n increases, the importance of prior knowledge diminishes, and in this particular case the curves for $n = 25$ are virtually identical. In general, one would expect the difference to be small when the number of unlabelled samples is several times the effective number of labelled samples used to determine $p(\theta)$.

6.5.4 Decision-Directed Approximations

Although the problem of unsupervised learning can be stated as merely the problem of estimating parameters of a mixture density, neither the maximum likelihood nor the Bayesian approach yields analytically simple results. Exact solutions for even the simplest nontrivial examples lead to computational requirements that grow exponentially with the number of samples. The problem of unsupervised learning is too important to abandon just because exact solutions are hard to find, however, and numerous procedures for obtaining approximate solutions have been suggested.

Since the basic difference between supervised and unsupervised learning is the presence or absence of labels for the samples, an obvious approach to unsupervised learning is to use the a priori information to design a classifier and to use the decisions of this classifier to label the samples. This is called the *decision-directed* approach to unsupervised learning, and it is subject to many variations. It can be applied sequentially by updating the classifier each time an unlabelled sample is classified. Alternatively, it can be applied in parallel by waiting until all n samples are classified before updating the classifier. If desired, this process can be repeated until no changes occur in the way the samples are labelled.* Various heuristics can be introduced to make the extent of any corrections depend upon the confidence of the classification decision.

There are some obvious dangers associated with the decision-directed approach. If the initial classifier is not reasonably good, or if an unfortunate sequence of samples is encountered, the errors in classifying the unlabelled samples can drive the classifier the wrong way, resulting in a solution corresponding roughly to one of the lesser peaks of the likelihood function. Even if the initial classifier is optimal, the resulting labelling will not in general be the same as the true class membership; the act of classification will exclude samples from the tails of the desired distribution, and will include samples from the tails of the other distributions. Thus, if there is significant

* The Basic Isodata procedure described in Section 6.4.4 is essentially a decision-directed procedure of this type.

overlap between the component densities, one can expect biased estimates and less than optimal results.

Despite these drawbacks, the simplicity of decision-directed procedures makes the Bayesian approach computationally feasible, and a flawed solution is often better than none. If conditions are favorable, performance that is nearly optimal can be achieved at far less computational expense. The literature contains a few rather complicated analyses of particular decision-directed procedures, and numerous reports of experimental results. The basic conclusions are that most of these procedures work well if the parametric assumptions are valid, if there is little overlap between the component densities, and if the initial classifier design is at least roughly correct.

6.6 DATA DESCRIPTION AND CLUSTERING

Let us reconsider our original problem of learning something of use from a set of unlabelled samples. Viewed geometrically, these samples form clouds of points in a d-dimensional space. Suppose that we knew that these points came from a single normal distribution. Then the most we could learn from the data would be contained in the sufficient statistics—the sample mean and the sample covariance matrix. In essence, these statistics constitute a compact description of the data. The sample mean locates the center of gravity of the cloud. It can be thought of as the single point $\mathbf{x}$ that best represents all of the data in the sense of minimizing the sum of squared distances from $\mathbf{x}$ to the samples. The sample covariance matrix tells us how well the sample mean describes the data in terms of the amount of scatter that exists in various directions. If the data points are actually normally distributed, then the cloud has a simple hyperellipsoidal shape, and the sample mean tends to fall in the region where the samples are most densely concentrated.

Of course, if the samples are not normally distributed, these statistics can give a very misleading description of the data. Figure 6.7 shows four different data sets that all have the same mean and covariance matrix. Obviously, second-order statistics are incapable of revealing all of the structure in an arbitrary set of data.

By assuming that the samples come from a mixture of c normal distributions, we can approximate a greater variety of situations. In essence, this corresponds to assuming that the samples fall in hyperellipsoidally-shaped clouds of various sizes and orientations. If the number of component densities is not limited, we can approximate virtually any density function in this way, and use the parameters of the mixture to describe the data. Unfortunately, we have seen that the problem of estimating the parameters of a mixture

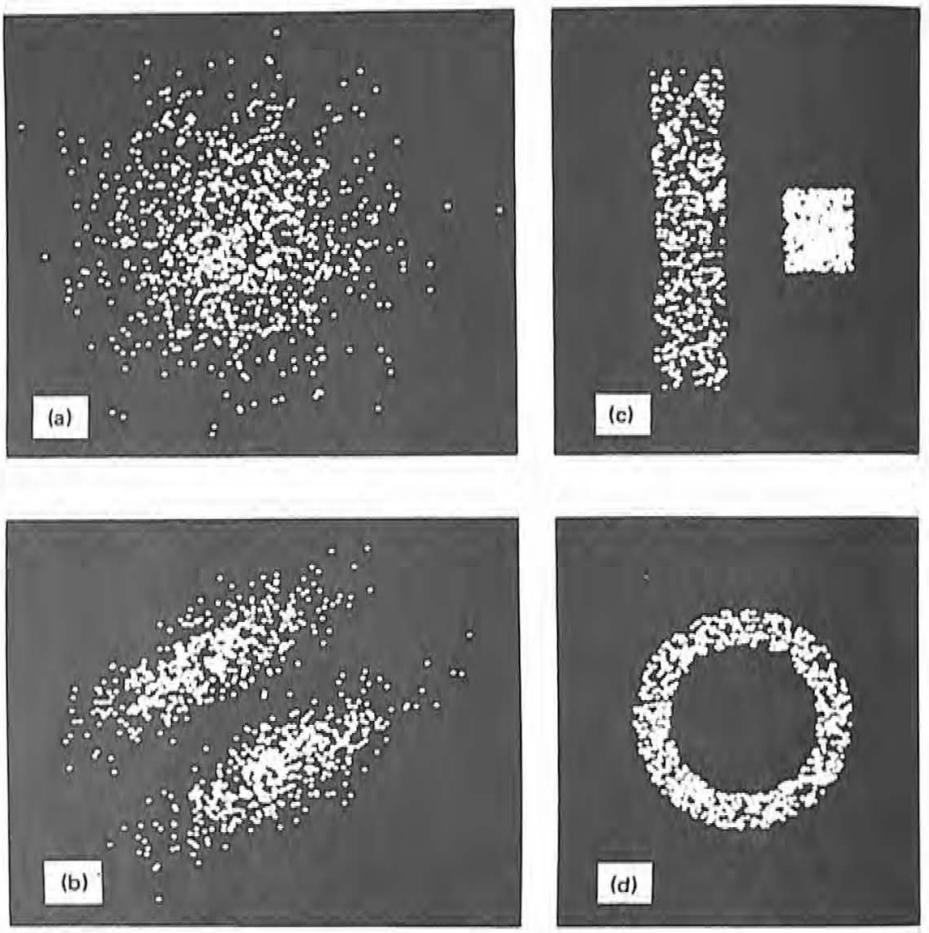


FIGURE 6.7. Data sets having identical second-order statistics.

density is not trivial. Furthermore, in situations where we have relatively little a priori knowledge about the nature of the data, the assumption of particular parametric forms may lead to poor or meaningless results. Instead of finding structure in the data, we would be imposing structure on it.

One alternative is to use one of the nonparametric methods described in Chapter 4 to estimate the unknown mixture density. If accurate, the resulting estimate is certainly a complete description of what we can learn from the data. Regions of high local density, which might correspond to significant subclasses in the population, can be found from the peaks or modes of the estimated density.

If the goal is to find subclasses, a more direct alternative is to use a *clustering procedure*. Roughly speaking, clustering procedures yield a data description in terms of clusters or groups of data points that possess strong internal similarities. The more formal procedures use a criterion function, such as the sum of the squared distances from the cluster centers, and seek the grouping that extremizes the criterion function. Because even this can lead to unmanageable computational problems, other procedures have been proposed that are intuitively appealing but that lead to solutions having no established properties. Their use is usually justified on the ground that they are easy to apply and often yield interesting results that may guide the application of more rigorous procedures.

6.7 SIMILARITY MEASURES

Once we describe the clustering problem as one of finding natural groupings in a set of data, we are obliged to define what we mean by a natural grouping. In what sense are we to say that the samples in one cluster are more like one another than like samples in other clusters? This question actually involves two separate issues—how should one measure the similarity between samples, and how should one evaluate a partitioning of a set of samples into clusters? In this section we address the first of these issues.

The most obvious measure of the similarity (or dissimilarity) between two samples is the distance between them. One way to begin a clustering investigation is to define a suitable distance function and compute the matrix of distances between all pairs of samples. If distance is a good measure of dissimilarity, then one would expect the distance between samples in the same cluster to be significantly less than the distance between samples in different clusters.

Suppose for the moment that we say that two samples belong to the same cluster if the Euclidean distance between them is less than some threshold distance d_0. It is immediately obvious that the choice of d_0 is very important. If d_0 is very large, all of the samples will be assigned to one cluster. If d_0 is very small, each sample will form an isolated cluster. To obtain "natural" clusters, d_0 will have to be greater than typical within-cluster distances and less than typical between-cluster distances (see Figure 6.8).

Less obvious perhaps is the fact that the results of clustering depend on the choice of Euclidean distance as a measure of dissimilarity. This choice implies that the feature space is isotropic. Consequently, clusters defined by Euclidean distance will be invariant to translations or rotations—rigid-body motions of the data points. However, they will not be invariant to linear transformations in general, or to other transformations that distort the

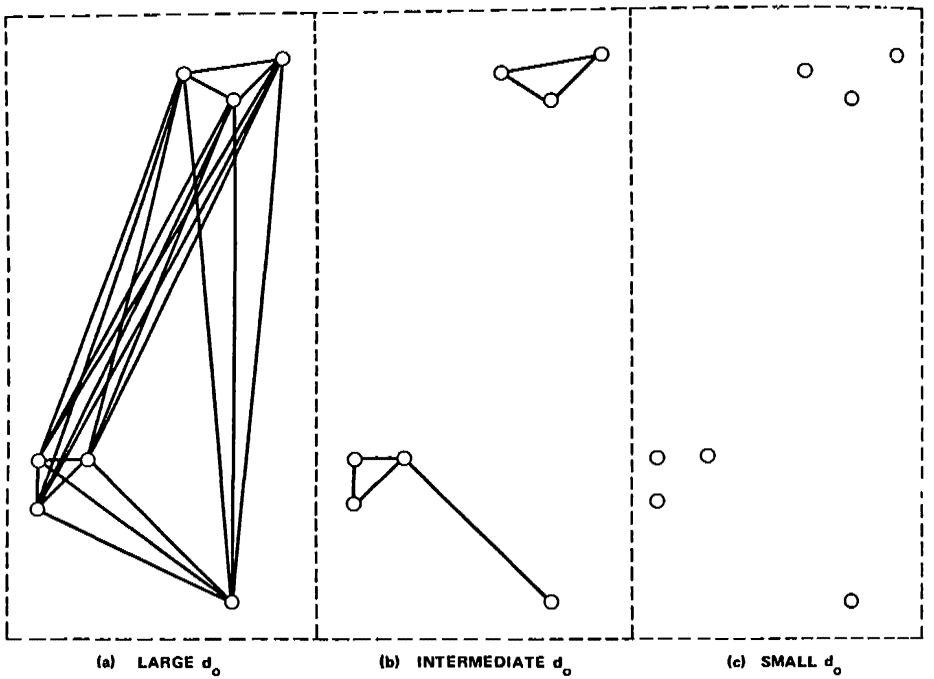


FIGURE 6.8. The effect of a distance threshold on clustering (Lines are drawn between points closer than a distance d_0 apart).

distance relationships. Thus, as Figure 6.9 illustrates, a simple scaling of the coordinate axes can result in a different grouping of the data into clusters. Of course, this is of no concern for problems in which arbitrary rescaling is an unnatural or meaningless transformation. However, if clusters are to mean anything, they should be invariant to transformations natural to the problem.

One way to achieve invariance is to normalize the data prior to clustering. For example, to obtain invariance to displacement and scale changes, one might translate and scale the axes so that all of the features have zero mean and unit variance. To obtain invariance to rotation, one might rotate the axes so that they coincide with the eigenvectors of the sample covariance matrix. This transformation to *principal components* can be preceded and/or followed by normalization for scale.

However, the reader should not conclude that this kind of normalization is necessarily desirable. Consider, for example, the matter of translating and scaling the axes so that each feature has zero mean and unit variance. The rationale usually given for this normalization is that it prevents certain features from dominating distance calculations merely because they have

large numerical values. Subtracting the mean and dividing by the standard deviation is an appropriate normalization if this spread of values is due to normal random variation; however, it can be quite inappropriate if the spread is due to the presence of subclasses (see Figure 6.10). Thus, this routine normalization may be less than helpful in the cases of greatest interest. Section 6.8.3 describes some better ways to obtain invariance to scaling.

An alternative to normalizing the data and using Euclidean distance is to use some kind of normalized distance, such as the Mahalanobis distance. More generally, one can abandon the use of distance altogether and introduce a nonmetric *similarity function* $s(\mathbf{x}, \mathbf{x}')$ to compare two vectors $\mathbf{x}$ and $\mathbf{x}'$. Conventionally, this is a symmetric function whose value is large when $\mathbf{x}$ and $\mathbf{x}'$ are similar. For example, when the angle between two vectors is a

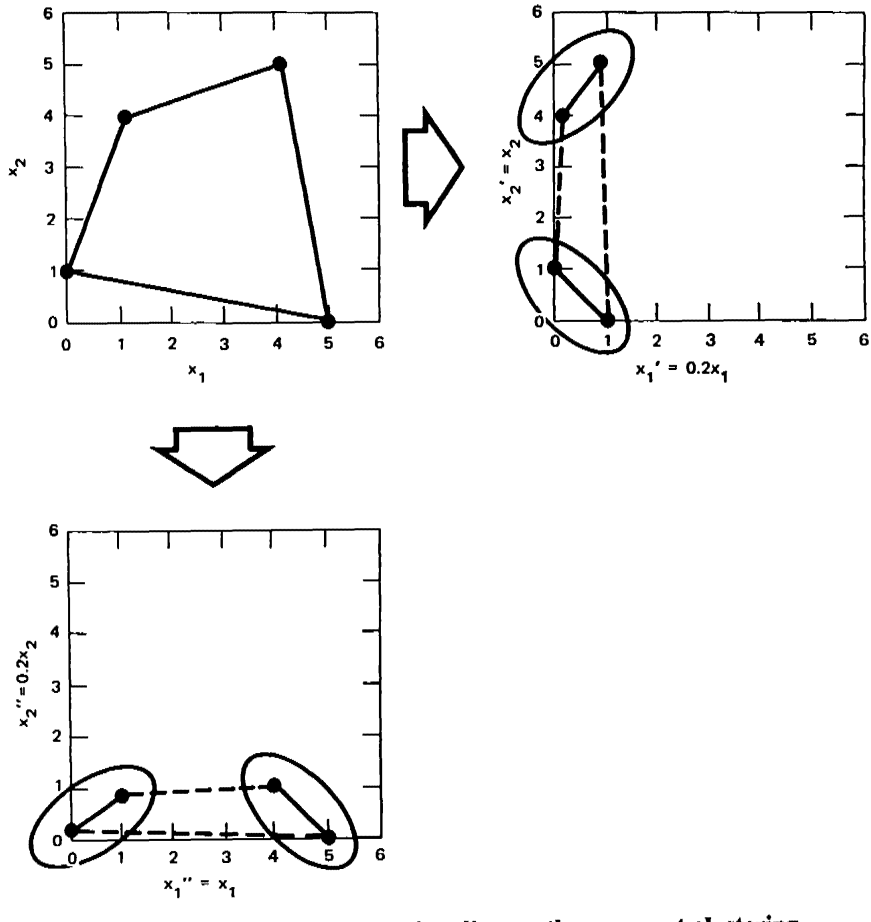


FIGURE 6.9. The effect of scaling on the apparent clustering.

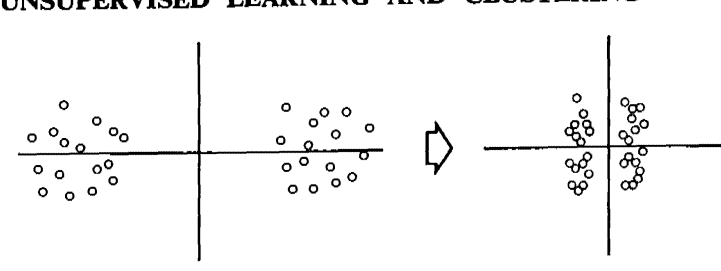


FIGURE 6.10. Undesirable effects of normalization.

meaningful measure of their similarity, then the normalized inner product

$$s(\mathbf{x}, \mathbf{x}') = \frac{\mathbf{x}^t\mathbf{x}'}{\|\mathbf{x}\| \, \|\mathbf{x}'\|}$$

may be an appropriate similarity function. This measure, which is the cosine of the angle between $\mathbf{x}$ and $\mathbf{x}'$, is invariant to rotation and dilation, though it is not invariant to translation and general linear transformations.

When the features are binary valued (0 or 1), this similarity function has a simple nongeometrical interpretation in terms of measuring shared features or shared attributes. Let us say that a sample $\mathbf{x}$ *possesses* the ith attribute if $x_i = 1$. Then $\mathbf{x}^t\mathbf{x}'$ is merely the number of attributes possessed by $\mathbf{x}$ and $\mathbf{x}'$, and $\|\mathbf{x}\| \, \|\mathbf{x}'\| = (\mathbf{x}^t\mathbf{x}\mathbf{x}'^t\mathbf{x}')^{1/2}$ is the geometric mean of the number of attributes possessed by $\mathbf{x}$ and the number possessed by $\mathbf{x}'$. Thus, $s(\mathbf{x}, \mathbf{x}')$ is a measure of the relative possession of common attributes. Some simple variations are

$$s(\mathbf{x}, \mathbf{x}') = \frac{\mathbf{x}^t\mathbf{x}'}{d},$$

the fraction of attributes shared, and

$$s(\mathbf{x}, \mathbf{x}') = \frac{\mathbf{x}^t\mathbf{x}'}{\mathbf{x}^t\mathbf{x} + \mathbf{x}'^t\mathbf{x}' - \mathbf{x}^t\mathbf{x}'},$$

the ratio of the number of shared attributes to the number possessed by $\mathbf{x}$ or $\mathbf{x}'$. This latter measure (sometimes known as the Tanimoto coefficient) is frequently encountered in the fields of information retrieval and biological taxonomy. Other measures of similarity arise in other applications, the variety of measures testifying to the diversity of problem domains.

We feel obliged to mention that fundamental issues in measurement theory are involved in the use of any distance or similarity function. The calculation of the similarity between two vectors always involves combining the values of their components. Yet, in many pattern recognition applications the components of the feature vector measure seemingly noncomparable

quantities. Using our early example of classifying lumber, how can one compare the brightness to the straightness-of-grain? Should the comparison depend on whether the brightness is measured in candles/m^2 or in foot-lamberts? How does one treat vectors whose components have a mixture of nominal, ordinal, interval, and ratio scales?* Ultimately, there is no methodological answer to these questions. When a user selects a particular similarity function or normalizes his data in a particular way, he introduces information that gives the procedure meaning. We have given examples of some alternatives that have proved to be useful. Beyond that we can do little more than alert the unwary to these pitfalls of clustering.

6.8 CRITERION FUNCTIONS FOR CLUSTERING

Suppose that we have a set $\mathcal{X}$ of n samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$ that we want to partition into exactly c disjoint subsets $\mathcal{X}_1, \ldots, \mathcal{X}_c$. Each subset is to represent a cluster, with samples in the same cluster being somehow more similar than samples in different clusters. One way to make this into a well-defined problem is to define a criterion function that measures the clustering quality of any partition of the data. Then the problem is one of finding the partition that extremizes the criterion function. In this section we examine the characteristics of several basically similar criterion functions, postponing until later the question of how to find an optimal partition.

6.8.1 The Sum-of-Squared-Error Criterion

The simplest and most widely used criterion function for clustering is the sum-of-squared-error criterion. Let n_i be the number of samples in $\mathcal{X}_i$ and let $\mathbf{m}_i$ be the mean of those samples,

$$\mathbf{m}_i = \frac{1}{n_i} \sum_{\mathbf{x} \in \mathcal{X}_i} \mathbf{x}. \tag{25}$$

Then the sum of squared errors is defined by

$$J_e = \sum_{i=1}^{c} \sum_{\mathbf{x} \in \mathcal{X}_i} \|\mathbf{x} - \mathbf{m}_i\|^2. \tag{26}$$

This criterion function has a simple interpretation. For a given cluster $\mathcal{X}_i$, the mean vector $\mathbf{m}_i$ is the best representative of the samples in $\mathcal{X}_i$ in the sense that it minimizes the sum of the squared lengths of the "error" vectors $\mathbf{x} - \mathbf{m}_i$. Thus, J_e measures the total squared error incurred in representing the n samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$ by the c cluster centers $\mathbf{m}_1, \ldots, \mathbf{m}_c$. The value of

* These fundamental considerations are by no means unique to clustering. They appear, for example, whenever one chooses a parametric form for an unknown probability density function, a metric for nonparametric density estimation, or scale factors for linear discriminant functions. Clustering problems merely expose them more clearly.

J_e depends on how the samples are grouped into clusters, and an optimal partitioning is defined as one that minimizes J_e. Clusterings of this type are often called *minimum variance* partitions.

What kind of clustering problems are well suited to a sum-of-squared-error criterion? Basically, J_e is an appropriate criterion when the clusters form essentially compact clouds that are rather well separated from one another. It should work well for the two or three clusters in Figure 6.11, but one would not expect reasonable results for the data in Figure 6.12.* A less obvious problem arises when there are great differences in the number of samples in

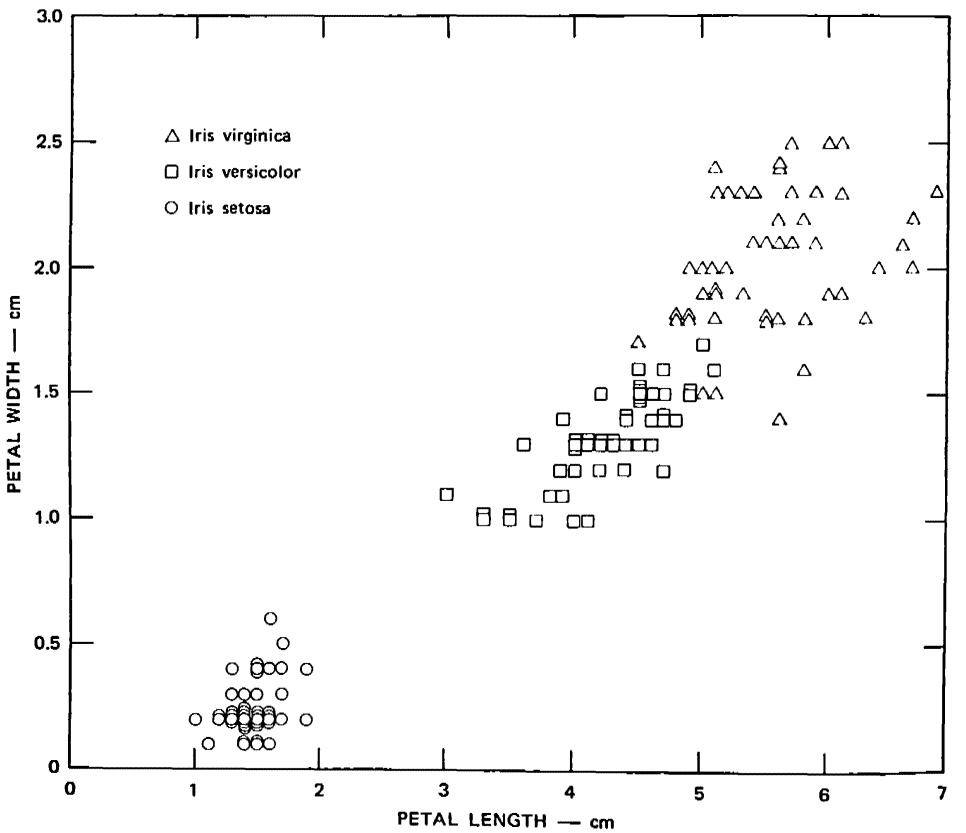


FIGURE 6.11. A two-dimensional section of the Anderson iris data.

* These two data sets are well known for quite different reasons. Figure 6.11 shows two of four measurements made by E. Anderson on 150 samples of three species of iris. These data were listed and used by R. A. Fisher in his classic paper on discriminant analysis (Fisher 1936), and have since become a favorite example for illustrating clustering procedures. Figure 6.12 is well known in astronomy as the Hertzsprung and Russell (or spectrum-luminosity) diagram, which led to the subdivision of stars into such categories as giants, supergiants, main sequence stars, and dwarfs. It was used by E. W. Forgey and again by D. Wishart (1969) to illustrate the limitations of simple clustering procedures.

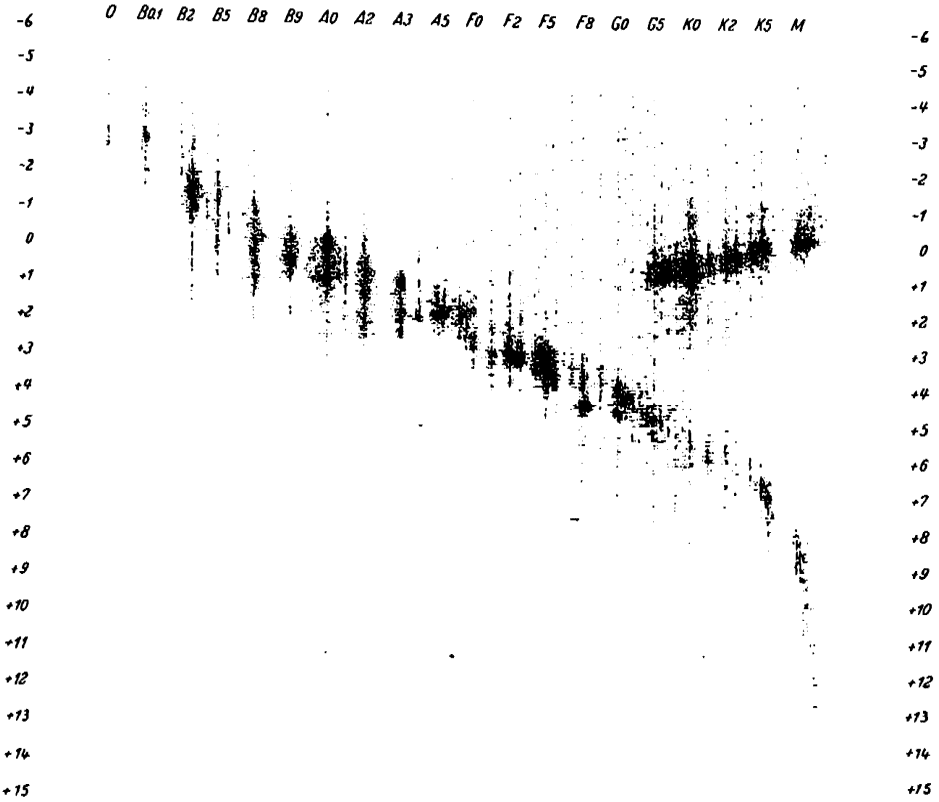


FIGURE 6.12. The Herzsprung-Russell Diagram (Courtesy Lunds Universitet Institutionen für Astronomi).

different clusters. In that case it can happen that a partition that splits a large cluster is favored over one that maintains the integrity of the clusters merely because the slight reduction in squared error achieved is multiplied by many terms in the sum (see Figure 6.13). This situation frequently arises because of the presence of "outliers" or "wild shots," and brings up the problem of interpreting and evaluating the results of clustering. Since little can be said about that problem, we shall merely observe that if additional considerations render the results of minimizing J_e unsatisfactory, then these considerations should be used, if possible, in formulating a better criterion function.

6.8.2 Related Minimum Variance Criteria

By some simple algebraic manipulation we can eliminate the mean vectors from the expression for J_e and obtain the equivalent expression

$$J_e = \tfrac{1}{2} \sum_{i=1}^{c} n_i \bar{s}_i, \tag{27}$$

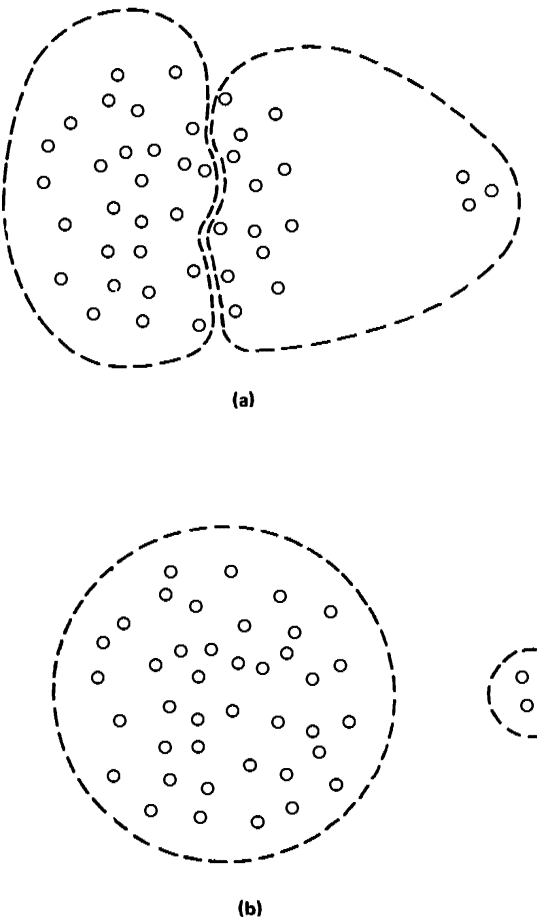


FIGURE 6.13. The problem of splitting large clusters: the sum of squared error is smaller for (a) than for (b).

where

$$\bar{s}_i = \frac{1}{n_i^2} \sum_{\mathbf{x} \in \mathcal{X}_i} \sum_{\mathbf{x}' \in \mathcal{X}_i} \|\mathbf{x} - \mathbf{x}'\|^2. \tag{28}$$

Eq. (28) leads us to interpret $\bar{s}_i$ as the average squared distance between points in the ith cluster, and emphasizes the fact that the sum-of-squared-error criterion uses Euclidean distance as the measure of similarity. It also suggests an obvious way of obtaining other criterion functions. For example, one can replace $\bar{s}_i$ by the average, the median, or perhaps the maximum distance between points in a cluster. More generally, one can introduce an appropriate

similarity function $s(\mathbf{x}, \mathbf{x}')$ and replace $\bar{s}_i$ by functions such as

$$\bar{s}_i = \frac{1}{n_i^2} \sum_{\mathbf{x} \in \mathcal{X}_i} \sum_{\mathbf{x}' \in \mathcal{X}_i} s(\mathbf{x}, \mathbf{x}') \tag{29}$$

or

$$\bar{s}_i = \min_{\mathbf{x}, \mathbf{x}' \in \mathcal{X}_i} s(\mathbf{x}, \mathbf{x}'). \tag{30}$$

As before, we define an optimal partitioning as one that extremizes the criterion function. This creates a well-defined problem, and the hope is that its solution discloses the intrinsic structure of the data.

6.8.3 Scattering Criteria

6.8.3.1 THE SCATTER MATRICES

Another interesting class of criterion functions can be derived from the scatter matrices used in multiple discriminant analysis. The following definitions directly parallel the definitions given in Section 4.11.

Mean vector for ith cluster:

$$\mathbf{m}_i = \frac{1}{n_i} \sum_{\mathbf{x} \in \mathcal{X}_i} \mathbf{x}. \tag{31}$$

Total mean vector:

$$\mathbf{m} = \frac{1}{n} \sum_{\mathcal{X}} \mathbf{x} = \frac{1}{n} \sum_{i=1}^{c} n_i \mathbf{m}_i. \tag{32}$$

Scatter matrix for ith cluster:

$$S_i = \sum_{\mathbf{x} \in \mathcal{X}_i} (\mathbf{x} - \mathbf{m}_i)(\mathbf{x} - \mathbf{m}_i)^t. \tag{33}$$

Within-cluster scatter matrix:

$$S_W = \sum_{i=1}^{c} S_i. \tag{34}$$

Between-cluster scatter matrix:

$$S_B = \sum_{i=1}^{c} n_i (\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^t. \tag{35}$$

Total scatter matrix:

$$S_T = \sum_{\mathbf{x} \in \mathcal{X}} (\mathbf{x} - \mathbf{m})(\mathbf{x} - \mathbf{m})^t. \tag{36}$$

As before, it follows from these definitions that the total scatter matrix is the sum of the within-cluster scatter matrix and the between-cluster scatter matrix:

$$S_T = S_W + S_B. \tag{37}$$

Note that the total scatter matrix does not depend on how the set of samples is partitioned into clusters. It depends only on the total set of samples. The within-cluster and between-cluster scatter matrices do depend on the partitioning, however. Roughly speaking, there is an exchange between these two matrices, the between-cluster scatter going up as the within-cluster scatter goes down. This is fortunate, since by trying to minimize the within-cluster scatter we will also tend to maximize the between-cluster scatter.

To be more precise in talking about the amount of within-cluster or between-cluster scatter, we need a scalar measure of the "size" of a scatter matrix. The two measures that we shall consider are the *trace* and the *determinant*. In the univariate case, these two measures are equivalent, and we can define an optimal partition as one that minimizes S_W or maximizes S_B. In the multivariate case things are somewhat more complicated, and a number of related but distinct optimality criteria have been suggested.

6.8.3.2 THE TRACE CRITERION

Perhaps the simplest scalar measure of a scatter matrix is its trace, the sum of its diagonal elements. Roughly speaking, the trace measures the square of the scattering radius, since it is proportional to the sum of the variances in the coordinate directions. Thus, an obvious criterion function to minimize is the trace of S_W. In fact, this criterion is nothing more or less than the sum-of-squared-error criterion, since Eqs. (33) and (34) yield

$$\operatorname{tr} S_W = \sum_{i=1}^{c} \operatorname{tr} S_i = \sum_{i=1}^{c} \sum_{\mathbf{x} \in \mathcal{X}_i} \|\mathbf{x} - \mathbf{m}_i\|^2 = J_e. \tag{38}$$

Since $\operatorname{tr} S_T = \operatorname{tr} S_W + \operatorname{tr} S_B$ and $\operatorname{tr} S_T$ is independent of how the samples are partitioned, we see that no new results are obtained by trying to maximize $\operatorname{tr} S_B$. However, it is comforting to know that in trying to minimize the within-cluster criterion $J_e = \operatorname{tr} S_W$ we are also maximizing the between-cluster criterion

$$\operatorname{tr} S_B = \sum_{i=1}^{c} n_i \|\mathbf{m}_i - \mathbf{m}\|^2. \tag{39}$$

6.8.3.3 THE DETERMINANT CRITERION

In Section 4.11 we used the determinant of the scatter matrix to obtain a scalar measure of scatter. Roughly speaking, this measures the square of the scattering volume, since it is proportional to the product of the variances in the directions of the principal axes. Since S_B will be singular if the number of clusters is less than or equal to the dimensionality, $|S_B|$ is obviously a poor choice for a criterion function. S_W can also become singular, and will

certainly be so if $n - c$ is less than the dimensionality d.* However, if we assume that S_W is nonsingular, we are led to consider the criterion function

$$J_d = |S_W| = \left| \sum_{i=1}^{c} S_i \right|. \tag{40}$$

The partition that minimizes J_d is often similar to the one that minimizes J_e, but the two need not be the same. We observed before that the minimum-squared-error partition might change if the axes are scaled. This does not happen with J_d. To see why, let T be a nonsingular matrix and consider the change of variables $\mathbf{x}' = T\mathbf{x}$. Keeping the partitioning fixed, we obtain new mean vectors $\mathbf{m}_i' = T\mathbf{m}_i$ and new scatter matrices $S_i' = TS_iT^t$. Thus, J_d changes to

$$J_d' = |S_W'| = |TS_WT^t| = |T|^2 J_d.$$

Since the scale factor $|T|^2$ is the same for all partitions, it follows that J_d and J_d' rank the partitions in the same way, and hence that the optimal clustering based on J_d is invariant to nonsingular linear transformations of the data.

6.8.3.4 INVARIANT CRITERIA

It is not hard to show that the eigenvalues $\lambda_1, \ldots, \lambda_d$ of $S_W^{-1}S_B$ are invariant under nonsingular linear transformations of the data. Indeed, these eigenvalues are the basic linear invariants of the scatter matrices. Their numerical values measure the ratio of between-cluster to within-cluster scatter in the direction of the eigenvectors, and partitions that yield large values are usually desirable. Of course, as we pointed out in Section 4.11, the fact that the rank of S_B can not exceed $c - 1$ means that no more than $c - 1$ of these eigenvalues can be nonzero. Nevertheless, good partitions are ones for which the nonzero eigenvalues are large.

One can invent a great variety of invariant clustering criteria by composing appropriate functions of these eigenvalues. Some of these follow naturally from standard matrix operations. For example, since the trace of a matrix is the sum of its eigenvalues, one might elect to maximize the criterion function†

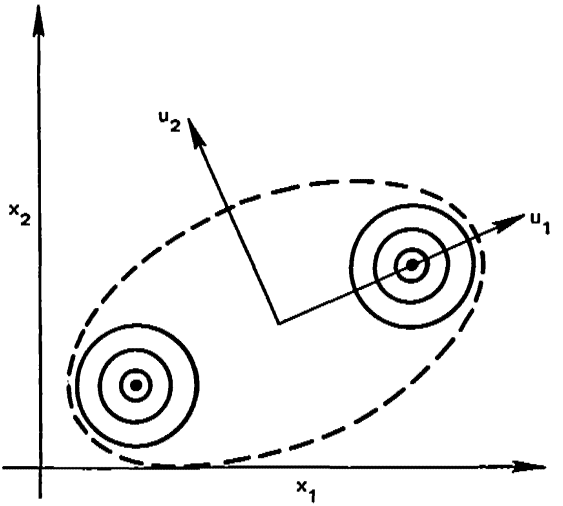
$$\text{tr } S_W^{-1}S_B = \sum_{i=1}^{d} \lambda_i. \tag{41}$$

* This follows from the fact that the rank of S_i can not exceed $n_i - 1$, and thus the rank of S_W can not exceed $\Sigma(n_i - 1) = n - c$. Of course, if the samples are confined to a lower dimensional subspace it is possible to have S_W be singular even though $n - c \geq d$. In such cases, some kind of dimensionality-reduction procedure must be used before the determinant criterion can be applied (see Section 6.14).

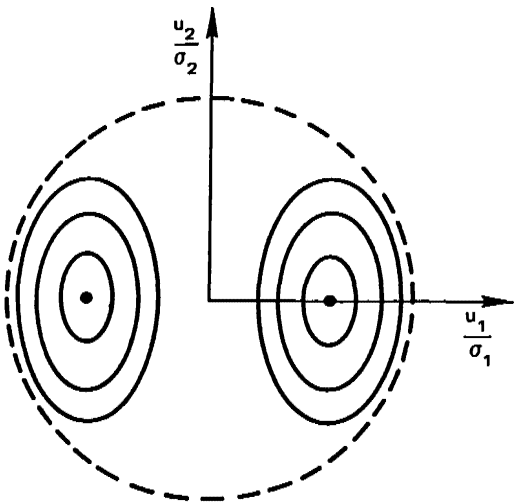
† Another invariant criterion is

$$|S_W^{-1}S_B| = \prod_{i=1}^{d} \lambda_i.$$

However, since its value is usually zero it is not very useful.



(a) UNNORMALIZED



(b) NORMALIZED

FIGURE 6.14. The effect of transforming to normalized principal components (Note: the partition that minimizes $S_T^{-1}S_W$ in (a) minimizes the sum of squared errors in (b).).

By using the relation $S_T = S_W + S_B$, one can derive the following invariant relatives of tr S_W and $|S_W|$:

$$\text{tr } S_T^{-1} S_W = \sum_{i=1}^{d} \frac{1}{1 + \lambda_i} \tag{42}$$

$$\frac{|S_W|}{|S_T|} = \prod_{i=1}^{d} \frac{1}{1 + \lambda_i}. \tag{43}$$

Since all of these criterion functions are invariant to linear transformations, the same is true of the partitions that extremize them. In the special case of two clusters, only one eigenvalue is nonzero, and all of these criteria yield the same clustering. However, when the samples are partitioned into more than two clusters, the optimal partitions, though often similar, need not be the same.

With regard to the criterion functions involving S_T, note that S_T does not depend on how the samples are partitioned into clusters. Thus, the clusterings that minimize $|S_W|/|S_T|$ are exactly the same as the ones that minimize $|S_W|$. If we rotate and scale the axes so that S_T becomes the identity matrix, we see that minimizing tr $S_T^{-1} S_W$ is equivalent to minimizing the sum-of-squared-error criterion tr S_W after performing this normalization. Figure 6.14 illustrates the effects of this transformation graphically. Clearly, this criterion suffers from the very defects that we warned about in Section 6.7, and it is probably the least desirable of these criteria.

One final warning about invariant criteria is in order. If different apparent groupings can be obtained by scaling the axes or by applying any other linear transformation, then all of these groupings will be exposed by invariant procedures. Thus, invariant criterion functions are more likely to possess multiple local extrema, and are correspondingly more difficult to extremize.

The variety of the criterion functions we have discussed and the somewhat subtle differences between them should not be allowed to obscure their essential similarity. In every case the underlying model is that the samples form c fairly well separated clouds of points. The within-cluster scatter matrix S_W is used to measure the compactness of these clouds, and the basic goal is to find the most compact grouping. While this approach has proved useful for many problems, it is not universally applicable. For example, it will not extract a very dense cluster embedded in the center of a diffuse cluster, or separate intertwined line-like clusters. For such cases one must devise other criterion functions that are better matched to the structure present or being sought.

6.9 ITERATIVE OPTIMIZATION

Once a criterion function has been selected, clustering becomes a well-defined problem in discrete optimization: find those partitions of the set of samples

that extremize the criterion function. Since the sample set is finite, there are only a finite number of possible partitions. Thus, in theory the clustering problem can always be solved by exhaustive enumeration. However, in practice such an approach is unthinkable for all but the simplest problems. There are approximately $c^n/c!$ ways of partitioning a set of n elements into c subsets,† and this exponential growth with n is overwhelming. For example, an exhaustive search for the best set of 5 clusters in 100 samples would require considering more than 10^{67} partitionings. Thus, in most applications an exhaustive search is completely infeasible.

The approach most frequently used in seeking optimal partitions is iterative optimization. The basic idea is to find some reasonable initial partition and to "move" samples from one group to another if such a move will improve the value of the criterion function. Like hill-climbing procedures in general, these approaches guarantee local but not global optimization. Different starting points can lead to different solutions, and one never knows whether or not the best solution has been found. Despite these limitations, the fact that the computational requirements are bearable makes this approach significant.

Let us consider the use of iterative improvement to minimize the sum-of-squared-error criterion J_e, written as

$$J_e = \sum_{i=1}^{c} J_i,$$

where

$$J_i = \sum_{\mathbf{x} \in \mathcal{X}_i} \|\mathbf{x} - \mathbf{m}_i\|^2$$

and

$$\mathbf{m}_i = \frac{1}{n_i} \sum_{\mathbf{x} \in \mathcal{X}_i} \mathbf{x}.$$

Suppose that a sample $\hat{\mathbf{x}}$ currently in cluster $\mathcal{X}_i$ is tentatively moved to $\mathcal{X}_j$. Then $\mathbf{m}_j$ changes to

$$\mathbf{m}_j^* = \mathbf{m}_j + \frac{\hat{\mathbf{x}} - \mathbf{m}_j}{n_j + 1}$$

† The reader who likes combinatorial problems will enjoy showing that there are exactly

$$\frac{1}{c!} \sum_{i=1}^{c} \binom{c}{i} (-1)^{c-i} i^n$$

partitions of n items into c nonempty subsets. (see W. Feller, *An Introduction to Probability Theory and Its Applications*, Vol. I, p. 58 (John Wiley, New York, Second Edition, 1959)). If $n \gg c$, the last term is the most significant.

and J_j increases to

$$J_j^* = \sum_{\mathbf{x}\in\mathscr{X}_j} \|\mathbf{x} - \mathbf{m}_j^*\|^2 + \|\hat{\mathbf{x}} - \mathbf{m}_j^*\|^2$$

$$= \sum_{\mathbf{x}\in\mathscr{X}_j} \left\| \mathbf{x} - \mathbf{m}_j - \frac{\hat{\mathbf{x}} - \mathbf{m}_j}{n_j + 1} \right\|^2 + \left\| \frac{n_j}{n_j + 1} (\hat{\mathbf{x}} - \mathbf{m}_j) \right\|^2$$

$$= J_j + \frac{n_j}{n_j + 1} \|\hat{\mathbf{x}} - \mathbf{m}_j\|^2.$$

Under the assumption that $n_i \neq 1$ (singleton clusters should not be destroyed), a similar calculation shows that $\mathbf{m}_i$ changes to

$$\mathbf{m}_i^* = \mathbf{m}_i - \frac{\hat{\mathbf{x}} - \mathbf{m}_i}{n_i - 1}$$

and J_i decreases to

$$J_i^* = J_i - \frac{n_i}{n_i - 1} \|\hat{\mathbf{x}} - \mathbf{m}_i\|^2.$$

These equations greatly simplify the computation of the change in the criterion function. The transfer of $\hat{\mathbf{x}}$ from $\mathscr{X}_i$ to $\mathscr{X}_j$ is advantageous if the decrease in J_i is greater than the increase in J_j. This is the case if

$$n_i/(n_i - 1) \|\hat{\mathbf{x}} - \mathbf{m}_i\|^2 > n_j/(n_j + 1) \|\hat{\mathbf{x}} - \mathbf{m}_j\|^2,$$

which typically happens whenever $\hat{\mathbf{x}}$ is closer to $\mathbf{m}_j$ than $\mathbf{m}_i$. If reassignment is profitable, the greatest decrease in sum of squared error is obtained by selecting the cluster for which $n_j/(n_j + 1) \|\hat{\mathbf{x}} - \mathbf{m}_j\|^2$ is minimum. This leads to the following clustering procedure:

Procedure: Basic Minimum Squared Error

1. Select an initial partition of the n samples into clusters and compute J_e and the means $\mathbf{m}_1, \ldots, \mathbf{m}_c$.

Loop: 2. Select the next candidate sample $\hat{\mathbf{x}}$. Suppose that $\hat{\mathbf{x}}$ is currently in $\mathscr{X}_i$.

3. If $n_i = 1$ go to Next; otherwise compute

$$\rho_j = \begin{cases} \dfrac{n_j}{n_j + 1} \|\hat{\mathbf{x}} - \mathbf{m}_j\|^2 & j \neq i \\ \dfrac{n_i}{n_i - 1} \|\hat{\mathbf{x}} - \mathbf{m}_i\|^2 & j = i. \end{cases}$$

4. Transfer $\hat{\mathbf{x}}$ to $\mathscr{X}_k$ if $\rho_k \leq \rho_j$ for all j.
5. Update J_e, $\mathbf{m}_i$, and $\mathbf{m}_k$.

Next: 6. If J_e has not changed in n attempts, stop; otherwise go to Loop.

If this procedure is compared to the Basic Isodata procedure described in Section 6.4.4, it is clear that the former is essentially a sequential version of the latter. Where the Basic Isodata procedure waits until all n samples have been reclassified before updating, the Basic Minimum Squared Error procedure updates after each sample is reclassified. It has been experimentally observed that this procedure is more susceptible to being trapped at a local minimum, and it has the further disadvantage of making the results depend on the order in which the candidates are selected. However, it is at least a stepwise optimal procedure, and it can be easily modified to apply to problems in which samples are acquired sequentially and clustering must be done in real time.

One question that plagues all hill-climbing procedures is the choice of the starting point. Unfortunately, there is no simple, universally good solution to this problem. One approach is to select c samples randomly for the initial cluster centers, using them to partition the data on a minimum-distance basis. Repetition with different random selections can give some indication of the sensitivity of the solution to the starting point. Another approach is to find the c-cluster starting point from the solution to the $(c-1)$-cluster problem. The solution for the one-cluster problem is the total sample mean; the starting point for the c-cluster problem can be the final means for the $(c-1)$-cluster problem plus the sample that is furthest from the nearest cluster center. This approach leads us directly to the so-called hierarchical clustering procedures, which are simple methods that can provide very good starting points for iterative optimization.

6.10 HIERARCHICAL CLUSTERING

6.10.1 Definitions

Let us consider a sequence of partitions of the n samples into c clusters. The first of these is a partition into n clusters, each cluster containing exactly one sample. The next is a partition into $n-1$ clusters, the next a partition into $n-2$, and so on until the nth, in which all the samples form one cluster. We shall say that we are at level k in the sequence when $c = n - k + 1$. Thus, level one corresponds to n clusters and level n to one. Given any two samples $\mathbf{x}$ and $\mathbf{x}'$, at some level they will be grouped together in the same cluster. If the sequence has the property that whenever two samples are in the same cluster at level k they remain together at all higher levels, then the sequence is said to be a *hierarchical clustering*. The classical examples of hierarchical clustering appear in biological taxonomy, where individuals are grouped into species, species into genera, genera into families, and so on.

In fact, this kind of clustering permeates classificatory activities in the sciences.

For every hierarchical clustering there is a corresponding tree, called a *dendrogram*, that shows how the samples are grouped. Figure 6.15 shows a dendrogram for a hypothetical problem involving six samples. Level 1 shows the six samples as singleton clusters. At level 2, samples x_3 and x_5 have been grouped to form a cluster, and they stay together at all subsequent levels. If it is possible to measure the similarity between clusters, then the dendrogram is usually drawn to scale to show the similarity between the clusters that are grouped. In Figure 6.15, for example, the similarity between the two groups of samples that are merged at level 6 has a value of 30. The similarity values are often used to help determine whether the groupings are natural or forced. For our hypothetical example, one would be inclined to say that the groupings at levels 4 or 5 are natural, but that the large reduction in similarity needed to go to level 6 makes that grouping forced. We shall see shortly how such similarity values can be obtained.

Because of their conceptual simplicity, hierarchical clustering procedures are among the best-known methods. The procedures themselves can be divided into two distinct classes, agglomerative and divisive. *Agglomerative* (bottom-up, clumping) procedures start with n singleton clusters and form

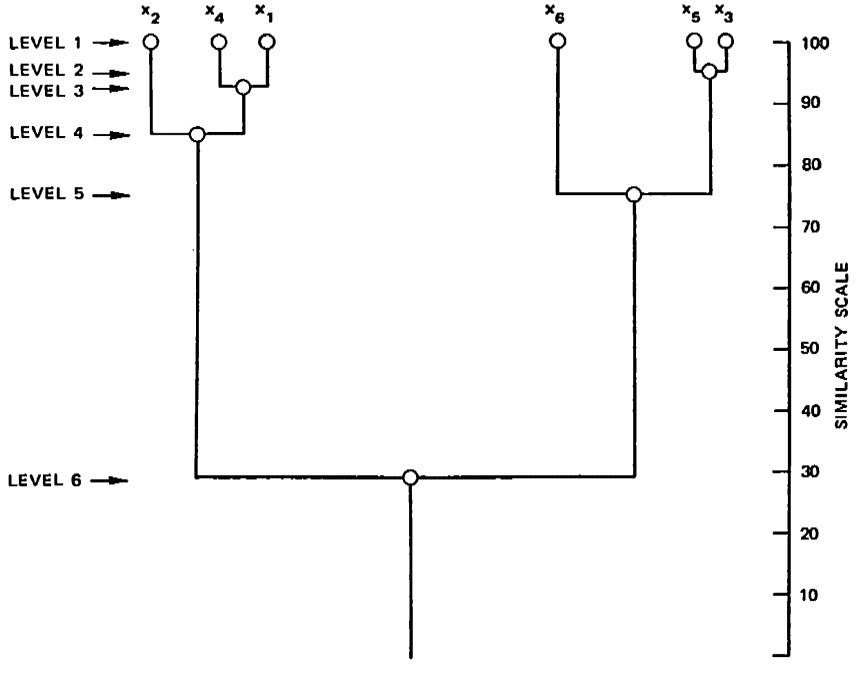


FIGURE 6.15. A dendrogram for hierarchical clustering.

the sequence by successively merging clusters. *Divisive* (top-down, splitting) procedures start with all of the samples in one cluster and form the sequence by successively splitting clusters. The computation needed to go from one level to another is usually simpler for the agglomerative procedures. However, when there are many samples and one is interested in only a small number of clusters, this computation will have to be repeated many times. For simplicity, we shall limit our attention to the agglomerative procedures, referring the reader to the literature for divisive methods.

6.10.2 Agglomerative Hierarchical Clustering

The major steps in agglomerative clustering are contained in the following procedure:

Procedure: Basic Agglomerative Clustering

1. Let $\hat{c} = n$ and $\mathscr{X}_i = \{\mathbf{x}_i\}$, $i = 1, \ldots, n$.

Loop: 2. If $\hat{c} \leq c$, stop.

3. Find the nearest pair of distinct clusters, say $\mathscr{X}_i$ and $\mathscr{X}_j$.

4. Merge $\mathscr{X}_i$ and $\mathscr{X}_j$, delete $\mathscr{X}_j$, and decrement $\hat{c}$ by one.

5. Go to Loop.

As described, this procedure terminates when the specified number of clusters has been obtained. However, if we continue until $c = 1$ we can produce a dendrogram like that shown in Figure 6.15. At any level the distance between nearest clusters can provide the dissimilarity value for that level. The reader will note that we have not said how to measure the distance between two clusters. The considerations here are much like those involved in selecting a criterion function. For simplicity, we shall restrict our attention to the following distance measures, leaving extensions to other similarity measures to the reader's imagination:

$$d_{\min}(\mathscr{X}_i, \mathscr{X}_j) = \min_{\mathbf{x} \in \mathscr{X}_i, \mathbf{x}' \in \mathscr{X}_j} \|\mathbf{x} - \mathbf{x}'\|$$

$$d_{\max}(\mathscr{X}_i, \mathscr{X}_j) = \max_{\mathbf{x} \in \mathscr{X}_i, \mathbf{x}' \in \mathscr{X}_j} \|\mathbf{x} - \mathbf{x}'\|$$

$$d_{\text{avg}}(\mathscr{X}_i, \mathscr{X}_j) = \frac{1}{n_i n_j} \sum_{\mathbf{x} \in \mathscr{X}_i} \sum_{\mathbf{x}' \in \mathscr{X}_j} \|\mathbf{x} - \mathbf{x}'\|$$

$$d_{\text{mean}}(\mathscr{X}_i, \mathscr{X}_j) = \|\mathbf{m}_i - \mathbf{m}_j\|.$$

All of these measures have a minimum-variance flavor, and they usually yield the same results if the clusters are compact and well separated. However, if the clusters are close to one another, or if their shapes are not basically hyperspherical, quite different results can be obtained. We shall use the two-dimensional point sets shown in Figure 6.16 to illustrate some of the differences.

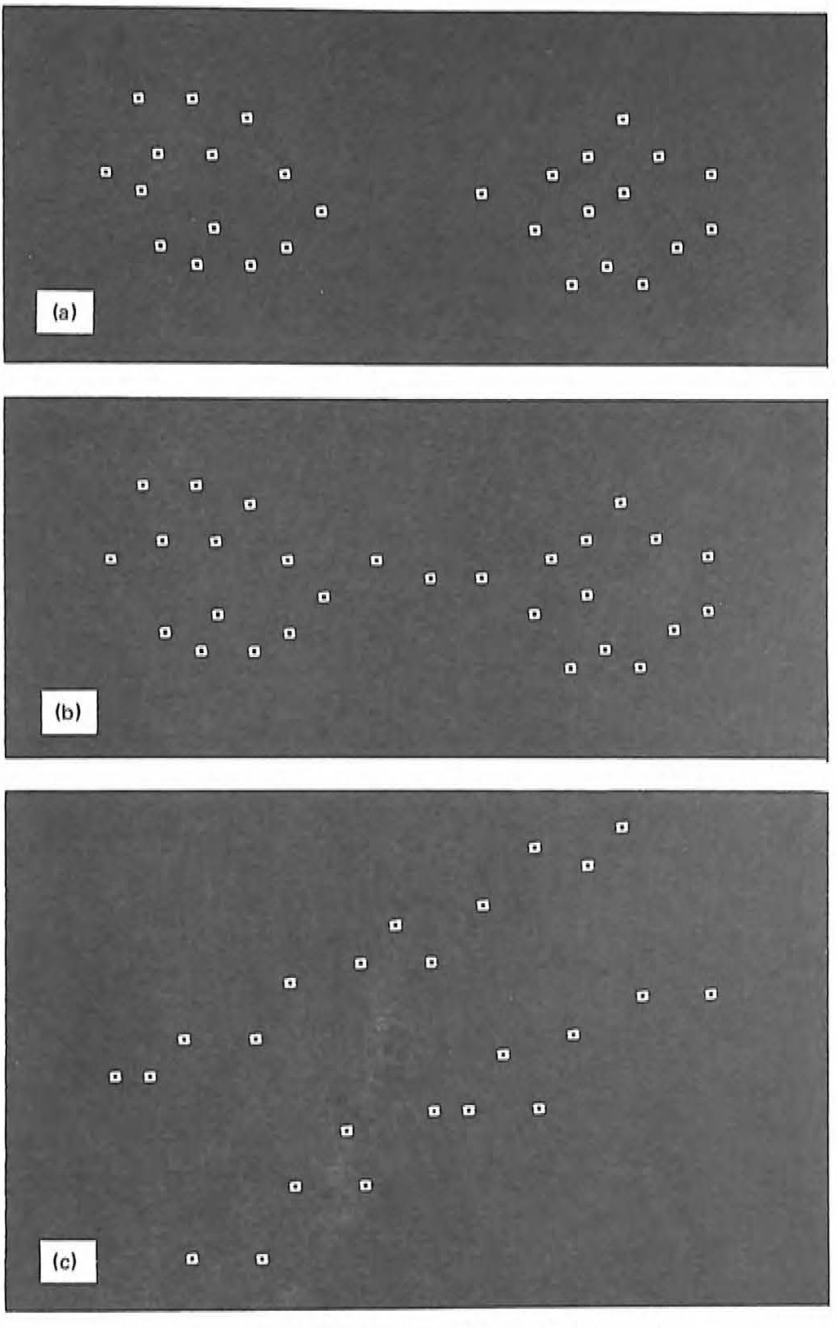


FIGURE 6.16. Three illustrative examples.

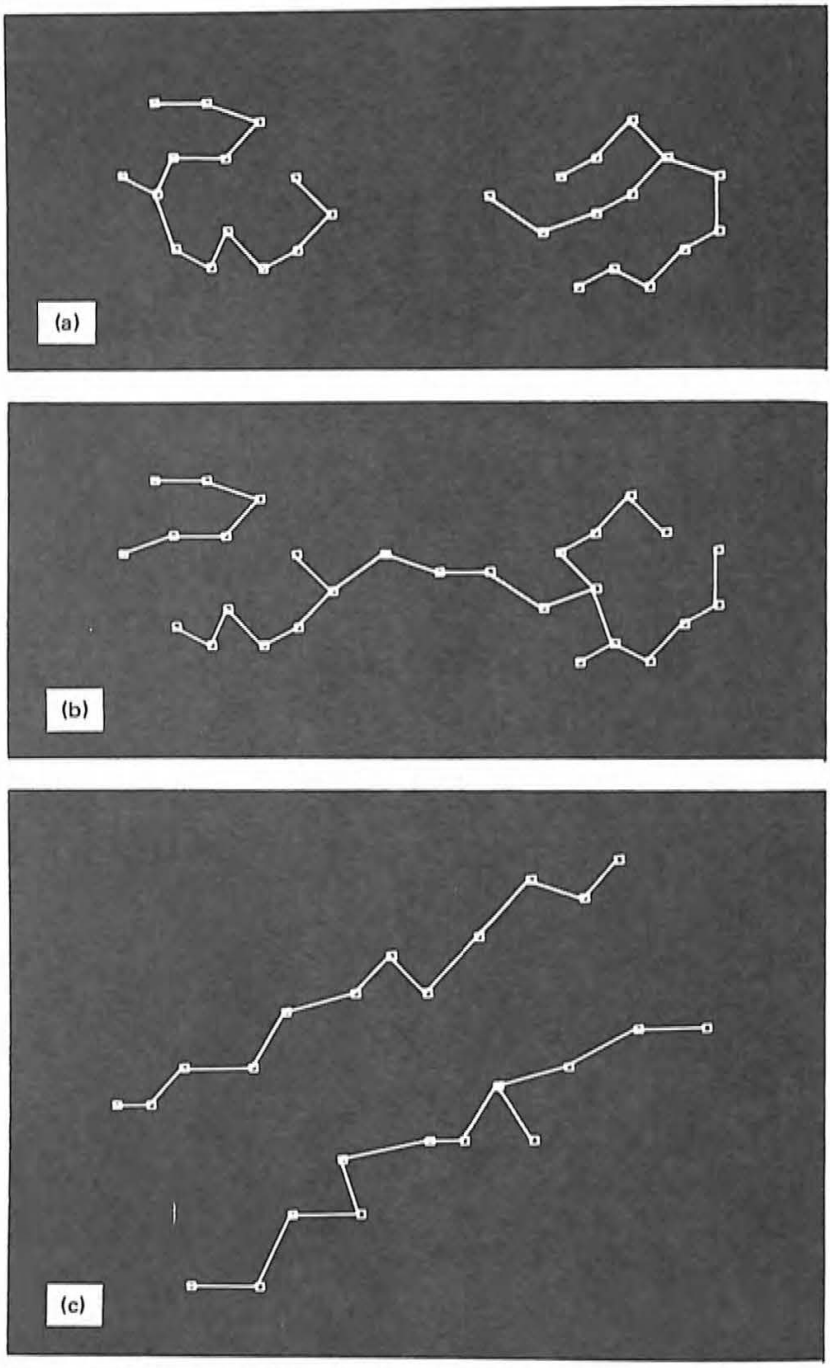


FIGURE 6.17. Results of the nearest-neighbor algorithm.

6.10.2.1 THE NEAREST-NEIGHBOR ALGORITHM

Consider first the behavior when $d_{\min}$ is used.* Suppose that we think of the data points as being nodes of a graph, with edges forming a path between nodes in the same subset $\mathcal{X}_i$.† When $d_{\min}$ is used to measure the distance between subsets, the nearest neighbors determine the nearest subsets. The merging of $\mathcal{X}_i$ and $\mathcal{X}_j$ corresponds to adding an edge between the nearest pair of nodes in $\mathcal{X}_i$ and $\mathcal{X}_j$. Since edges linking clusters always go between distinct clusters, the resulting graph never has any closed loops or circuits; in the terminology of graph theory, this procedure generates a *tree*. If it is allowed to continue until all of the subsets are linked, the result is a *spanning tree*, a tree with a path from any node to any other node. Moreover, it can be shown that the sum of the edge lengths of the resulting tree will not exceed the sum of the edge lengths for any other spanning tree for that set of samples. Thus, with the use of $d_{\min}$ as the distance measure, the agglomerative clustering procedure becomes an algorithm for generating a *minimal spanning tree*.

Figure 6.17 shows the results of applying this procedure to the data of Figure 6.16. In all cases the procedure was stopped at $c = 2$; a minimal spanning tree can be obtained by adding the shortest possible edge between the two clusters. In the first case where the clusters are compact and well separated, the obvious clusters are found. In the second case, the presence of a few points located so as to produce a bridge between the clusters results in a rather unexpected grouping into one large, elongated cluster, and one small, compact cluster. This behavior is often called the "chaining effect," and is sometimes considered to be a defect of this distance measure. To the extent that the results are very sensitive to noise or to slight changes in position of the data points, this is certainly a valid criticism. However, as the third case illustrates, this very tendency to form chains can be advantageous if the clusters are elongated or possess elongated limbs.

6.10.2.2 THE FURTHEST-NEIGHBOR ALGORITHM

When $d_{\max}$ is used to measure the distance between subsets, the growth of elongated clusters is discouraged.‡ Application of the procedure can be thought of as producing a graph in which edges connect all of the nodes in

* In the literature, the resulting procedure is often called the *nearest-neighbor* or the *minimum* algorithm. If it is terminated when the distance between nearest clusters exceeds an arbitrary threshold, it is called the *single-linkage* algorithm.

† Although we will not make deep use of graph theory, we assume that the reader has a general familiarity with the subject. A clear, rigorous treatment is given by O. Ore, *Theory of Graphs* (American Math. Soc. Colloquium Publ., Vol. 38, 1962).

‡ In the literature, the resulting procedure is often called the *furthest neighbor* or the *maximum* algorithm. If it is terminated when the distance between nearest clusters exceeds an arbitrary threshold, it is called the *complete-linkage* algorithm.

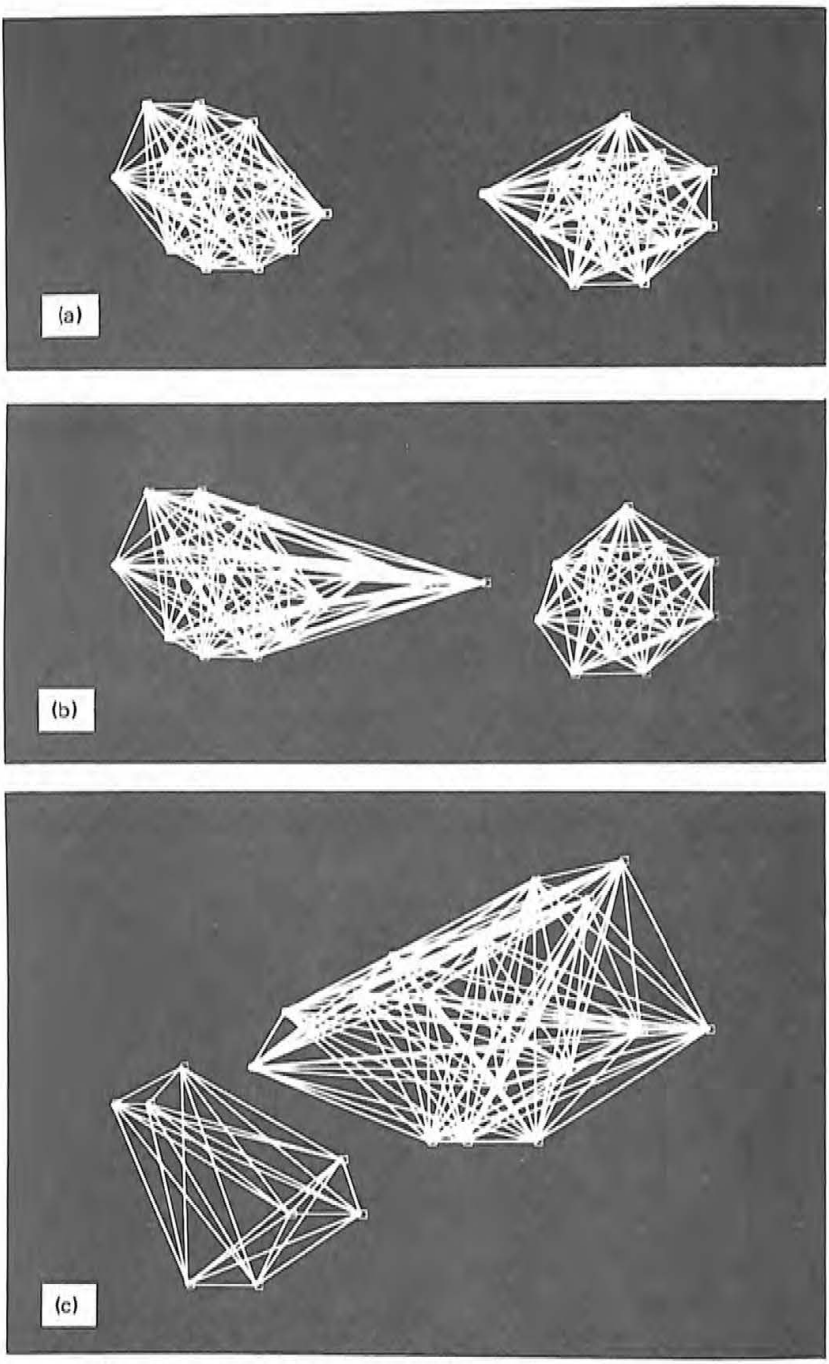


FIGURE 6.18. Results of the furthest-neighbor algorithm.

a cluster. In the terminology of graph theory, every cluster constitutes a *complete* subgraph. The distance between two clusters is determined by the most distant nodes in the two clusters. When the nearest clusters are merged, the graph is changed by adding edges between every pair of nodes in the two clusters. If we define the *diameter* of a cluster as the largest distance between points in the cluster, then the distance between two clusters is merely the diameter of their union. If we define the diameter of a partition as the largest diameter for clusters in the partition, then each iteration increases the diameter of the partition as little as possible. As Figure 6.18 illustrates, this is advantageous when the true clusters are compact and roughly equal in size. However, when this is not the case, as happens with the two elongated clusters, the resulting groupings can be meaningless. This is another example of imposing structure on data rather than finding structure in it.

6.10.2.3 COMPROMISES

The minimum and maximum measures represent two extremes in measuring the distance between clusters. Like all procedures that involve minima or maxima, they tend to be overly sensitive to "mavericks" or "sports" or "outliers" or "wildshots." The use of averaging is an obvious way to ameliorate these problems, and d_{avg} and d_{mean} are natural compromises between $d_{\min}$ and $d_{\max}$. Computationally, d_{mean} is the simplest of all of these measures, since the others require computing all $n_i n_j$ pairs of distances $\|\mathbf{x} - \mathbf{x}'\|$. However, a measure such as d_{avg} can be used when the distances $\|\mathbf{x} - \mathbf{x}'\|$ are replaced by similarity measures, where the similarity between mean vectors may be difficult or impossible to define. We leave it to the reader to decide how the use of d_{avg} or d_{mean} might change the way that the points in Figure 6.16 are grouped.

6.10.3 Stepwise-Optimal Hierarchical Clustering

We observed earlier that if clusters are grown by merging the nearest pair of clusters, then the results have a minimum variance flavor. However, when the measure of distance between clusters is chosen arbitrarily, one can rarely assert that the resulting partition extremizes any particular criterion function. In effect, hierarchical clustering defines a cluster as whatever results from applying the clustering procedure. However, with a simple modification it is possible to obtain a stepwise-optimal procedure for extremizing a criterion function. This is done merely by replacing Step 3 of the Basic Agglomerative Clustering Procedure (Section 6.10.2) by

3′. Find the pair of distinct clusters $\mathcal{X}_i$ and $\mathcal{X}_j$ whose merger would increase (or decrease) the criterion function as little as possible.

This assures us that at each iteration we have done the best possible thing, even if it does not guarantee that the final partition is optimal.

We saw earlier that the use of $d_{\max}$ causes the smallest possible stepwise increase in the diameter of the partition. Another simple example is provided by the sum-of-squared-error criterion function J_e. By an analysis very similar to that used in Section 6.9, we find that the pair of clusters whose merger increases J_e as little as possible is the pair for which the "distance"

$$d_e(\mathcal{X}_i, \mathcal{X}_j) = \sqrt{\frac{n_i n_j}{n_i + n_j}} \|\mathbf{m}_i - \mathbf{m}_j\|$$

is minimum. Thus, in selecting clusters to be merged, this criterion takes into account the number of samples in each cluster as well as the distance between clusters. In general, the use of d_e tends to favor growth by adding singletons or small clusters to large clusters over merging medium-sized clusters. While the final partition may not minimize J_e, it usually provides a very good starting point for further iterative optimization.

6.10.4 Hierarchical Clustering and Induced Metrics

Suppose that we are unable to supply a metric for our data, but that we can measure a *dissimilarity* value $\delta(\mathbf{x}, \mathbf{x}')$ for every pair of samples, where $\delta(\mathbf{x}, \mathbf{x}') \geq 0$, equality holding if and only if $\mathbf{x} = \mathbf{x}'$. Then agglomerative clustering can still be used, with the understanding that the nearest pair of clusters is the least dissimilar pair. Interestingly enough, if we define the dissimilarity between two clusters by

$$\delta_{\min}(\mathcal{X}_i, \mathcal{X}_j) = \min_{\mathbf{x} \in \mathcal{X}_i, \mathbf{x}' \in \mathcal{X}_j} \delta(\mathbf{x}, \mathbf{x}')$$

or

$$\delta_{\max}(\mathcal{X}_i, \mathcal{X}_j) = \max_{\mathbf{x} \in \mathcal{X}_i, \mathbf{x}' \in \mathcal{X}_j} \delta(\mathbf{x}, \mathbf{x}'),$$

then the hierarchical clustering procedure will induce a distance function for the given set of n samples. Furthermore, the ranking of the distances between samples will be invariant to any monotonic transformation of the dissimilarity values.

To see how this comes about, we begin by defining the *value* v_k for the clustering at level k. For level 1, $v_1 = 0$. For all higher levels, v_k is the minimum dissimilarity between pairs of distinct clusters at level $k - 1$. A moment's reflection will make it clear that with both $\delta_{\min}$ and $\delta_{\max}$ the value v_k either stays the same or increases as k increases. Moreover, we shall assume that no two of the n samples are identical, so that $v_2 > 0$. Thus, $0 = v_1 < v_2 \leq v_3 \leq \cdots \leq v_n$.

We can now define the *distance* $d(\mathbf{x}, \mathbf{x}')$ between $\mathbf{x}$ and $\mathbf{x}'$ as the value of the lowest level clustering for which $\mathbf{x}$ and $\mathbf{x}'$ are in the same cluster. To show that this is a legitimate distance function, or *metric*, we need to show three things:

(1) $d(\mathbf{x}, \mathbf{x}') = 0 \Leftrightarrow \mathbf{x} = \mathbf{x}'$
(2) $d(\mathbf{x}, \mathbf{x}') = d(\mathbf{x}', \mathbf{x})$
(3) $d(\mathbf{x}, \mathbf{x}'') \leq d(\mathbf{x}, \mathbf{x}') + d(\mathbf{x}', \mathbf{x}'')$.

It is easy to see that the first requirement is satisfied. The lowest level for which $\mathbf{x}$ and $\mathbf{x}$ are in the same cluster is level 1, so that $d(\mathbf{x}, \mathbf{x}) = v_1 = 0$. Conversely, if $d(\mathbf{x}, \mathbf{x}') = 0$, the fact that $v_2 > 0$ implies that $\mathbf{x}$ and $\mathbf{x}'$ must be in the same cluster at level 1, and hence that $\mathbf{x} = \mathbf{x}'$. The truth of the second requirement follows immediately from the definition of $d(\mathbf{x}, \mathbf{x}')$. This leaves the third requirement, the triangle inequality. Let $d(\mathbf{x}, \mathbf{x}') = v_i$ and $d(\mathbf{x}', \mathbf{x}'') = v_j$, so that $\mathbf{x}$ and $\mathbf{x}'$ are in the same cluster at level i and $\mathbf{x}'$ and $\mathbf{x}''$ are in the same cluster at level j. Because of the hierarchical nesting of clusters, one of these clusters includes the other. If $k = \max(i, j)$, it is clear that at level k $\mathbf{x}$, $\mathbf{x}'$, and $\mathbf{x}''$ are all in the same cluster, and hence that

$$d(\mathbf{x}, \mathbf{x}'') \leq v_k.$$

But since the values v_k are monotonically nondecreasing, it follows that $v_k = \max(v_i, v_j)$ and hence that

$$d(\mathbf{x}, \mathbf{x}'') \leq \max(d(\mathbf{x}, \mathbf{x}'), d(\mathbf{x}', \mathbf{x}'')).$$

This is known as the *ultrametric inequality*. It is even stronger than the triangle inequality, since $\max(d(\mathbf{x}, \mathbf{x}'), d(\mathbf{x}', \mathbf{x}'')) \leq d(\mathbf{x}, \mathbf{x}') + d(\mathbf{x}', \mathbf{x}'')$. Thus, all the conditions are satisfied, and we have created a bona fide metric for comparing the n samples.

6.11 GRAPH THEORETIC METHODS

In two or three instances we have used linear graphs to add insight into the nature of certain clustering procedures. Where the mathematics of normal mixtures and minimum-variance partitions seems to keep returning us to the picture of clusters as isolated clumps of points, the language and concepts of graph theory lead us to consider much more intricate structures. Unfortunately, few of these possibilities have been systematically explored, and there is no uniform way of posing clustering problems as problems in graph theory. Thus, the effective use of these ideas is still largely an art, and the reader who wants to explore the possibilities should be prepared to be creative.

We begin our brief look into graph-theoretic methods by reconsidering the simple procedure that produced the graphs shown in Figure 6.8. Here a

threshold distance d_0 was selected, and two points were said to be in the same cluster if the distance between them was less than d_0. This procedure can easily be generalized to apply to arbitrary similarity measures. Suppose that we pick a threshold value s_0 and say that $\mathbf{x}$ is similar to $\mathbf{x}'$ if $s(\mathbf{x}, \mathbf{x}') > s_0$. This defines an n-by-n *similarity matrix* $S = [s_{ij}]$, where

$$s_{ij} = \begin{cases} 1 & \text{if } s(\mathbf{x}_i, \mathbf{x}_j) > s_0 \\ 0 & \text{otherwise} \end{cases} \qquad i, j = 1, \ldots, n$$

This matrix defines a *similarity graph* in which nodes correspond to points and an edge joins node i and node j if and only if $s_{ij} = 1$.

The clusterings produced by the single-linkage algorithm and by a modified version of the complete-linkage algorithm are readily described in terms of this graph. With the single-linkage algorithm, two samples $\mathbf{x}$ and $\mathbf{x}'$ are in the same cluster if and only if there exists a chain $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k$ such that $\mathbf{x}$ is similar to $\mathbf{x}_1$, $\mathbf{x}_1$ is similar to $\mathbf{x}_2$, and so on for the whole chain. Thus, this clustering corresponds to the *connected components* of the similarity graph. With the complete-linkage algorithm, all samples in a given cluster must be similar to one another, and no sample can be in more than one cluster. If we drop this second requirement, then this clustering corresponds to the *maximal complete subgraphs* of the similarity graph, the "largest" subgraphs with edges joining all pairs of nodes. (In general, the clusters of the complete-linkage algorithm will be found among the maximal complete subgraphs, but they cannot be determined without knowing the unquantized similarity values.)

In the preceding section we noted that the nearest-neighbor algorithm could be viewed as an algorithm for finding a minimal spanning tree. Conversely, given a minimal spanning tree we can find the clusterings produced by the nearest-neighbor algorithm. Removal of the longest edge produces the two-cluster grouping, removal of the next longest edge produces the three-cluster grouping, and so on. This amounts to an inverted way of obtaining a divisive hierarchical procedure, and suggests other ways of dividing the graph into subgraphs. For example, in selecting an edge to remove, we can compare its length to the lengths of other edges incident upon its nodes. Let us say that an edge is *inconsistent* if its length l is significantly larger than $\bar{l}$, the average length of all other edges incident on its nodes. Figure 6.19 shows a minimal spanning tree for a two-dimensional point set and the clusters obtained by systematically removing all edges for which $l > 2\bar{l}$. Note how the sensitivity of this criterion to local conditions gives results that are quite different from merely removing the two longest edges.

When the data points are strung out into long chains, a minimal spanning tree forms a natural skeleton for the chain. If we define the *diameter path* as

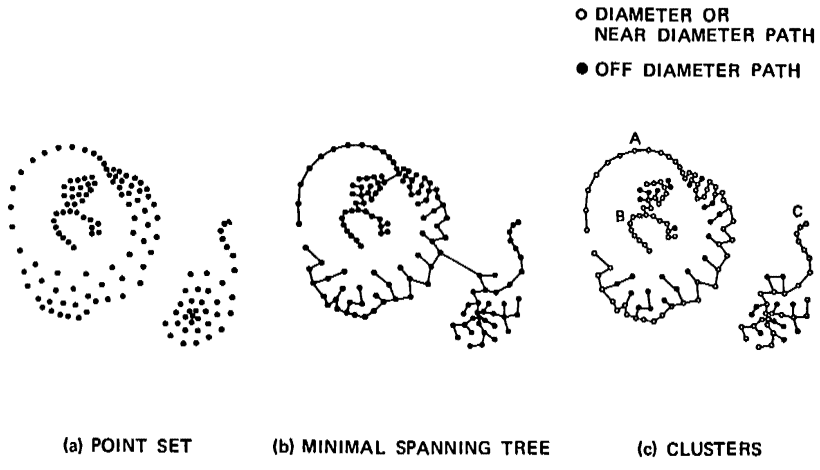


FIGURE 6.19. Clusters formed by removing inconsistent edges (From C. T. Zahn, 1971. Copyright 1971, Institute of Electrical and Electronics Engineers, reprinted by permission.)

the longest path through the tree, then a chain will be characterized by the shallow depth of branching off the diameter path. In contrast, for a large, uniform cloud of data points, the tree will usually not have an obvious diameter path, but rather several distinct, near-diameter paths. For any of these, an appreciable number of nodes will be off the path. While slight changes in the locations of the data points can cause major rerouting of a minimal spanning tree, they typically have little effect on such statistics.

One of the useful statistics that can be obtained from a minimal spanning tree is the edge length distribution. Figure 6.20 shows a situation in which a dense cluster is embedded in a sparse one. The lengths of the edges of the minimal spanning tree exhibit two distinct clusters which would easily be detected by a minimum-variance procedure. By deleting all edges longer than some intermediate value, we can extract the dense cluster as the largest connected component of the remaining graph. While more complicated configurations can not be disposed of this easily, the flexibility of the graph-theoretic approach suggests that it is applicable to a wide variety of clustering problems.

6.12 THE PROBLEM OF VALIDITY

With almost all of the procedures we have considered thus far we have assumed that the number of clusters is known. That is a reasonable assumption if we are upgrading a classifier that has been designed on a small sample set, or if we are tracking slowly time-varying patterns. However, it is a very

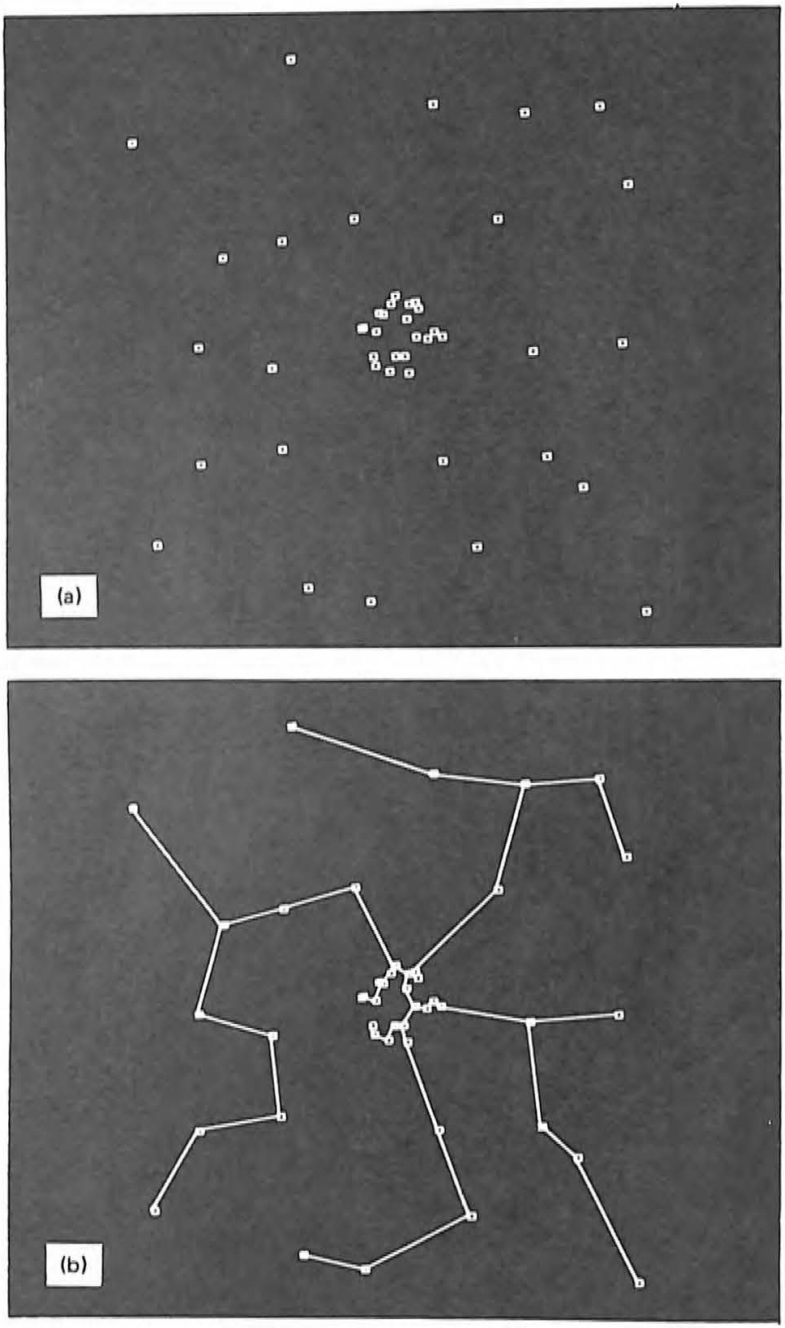


FIGURE 6.20. A minimal spanning tree with a bimodal edge length distribution.

unnatural assumption if we are exploring an essentially unknown set of data. Thus, a constantly recurring problem in cluster analysis is that of deciding just how many clusters are present.

When clustering is done by extremizing a criterion function, a common approach is to repeat the clustering procedure for $c = 1$, $c = 2$, $c = 3$, etc., and to see how the criterion function changes with c. For example, it is clear that the sum-of-squared-error criterion J_e must decrease monotonically with c, since the squared error can be reduced each time c is increased merely by transferring a single sample to the new cluster. If the n samples are really grouped into $\hat{c}$ compact, well separated clusters, one would expect to see J_e decrease rapidly until $c = \hat{c}$, decreasing much more slowly thereafter until it reaches zero at $c = n$. Similar arguments have been advanced for hierarchical clustering procedures, the usual assumption being that large disparities in the levels at which clusters merge indicate the presence of natural groupings.

A more formal approach to this problem is to devise some measure of goodness of fit that expresses how well a given c-cluster description matches the data. The chi-square and Kolmogorov-Smirnov statistics are the traditional measures of goodness of fit, but the curse of dimensionality usually demands the use of simpler measures, such as a criterion function $J(c)$. Since we expect a description in terms of $c + 1$ clusters to give a better fit than a description in terms of c clusters, we would like to know what constitutes a statistically significant improvement in $J(c)$.

A formal way to proceed is to advance the *null hypothesis* that there are exactly c clusters present, and to compute the sampling distribution for $J(c + 1)$ under this hypothesis. This distribution tells us what kind of apparent improvement to expect when a c-cluster description is actually correct. The decision procedure would be to accept the null hypothesis if the observed value of $J(c + 1)$ falls within limits corresponding to an acceptable probability of false rejection.

Unfortunately, it is usually very difficult to do anything more than crudely estimate the sampling distribution of $J(c + 1)$. The resulting solutions are not above suspicion, and the statistical problem of testing cluster validity is still essentially unsolved. However, under the assumption that a suspicious test is better than none, we include the following approximate analysis for the simple sum-of-squared-error criterion.

Suppose that we have a set $\mathscr{X}$ of n samples and we want to decide whether or not there is any justification for assuming that they form more than one cluster. Let us advance the null hypothesis that all n samples come from a normal population with mean μ and covariance matrix $\sigma^2 I$. If this hypothesis were true, any clusters found would have to have been formed by chance, and any observed decrease in the sum of squared error obtained by clustering would have no significance.

The sum of squared error $J_e(1)$ is a random variable, since it depends on the particular set of samples:

$$J_e(1) = \sum_{\mathbf{x}\in\mathscr{X}} \|\mathbf{x} - \mathbf{m}\|^2,$$

where $\mathbf{m}$ is the mean of the n samples. Under the null hypothesis, the distribution for $J_e(1)$ is approximately normal with mean $nd\sigma^2$ and variance $2nd\sigma^4$.

Suppose now that we partition the set of samples into two subsets $\mathscr{X}_1$ and $\mathscr{X}_2$ so as to minimize $J_e(2)$, where

$$J_e(2) = \sum_{i=1}^{2} \sum_{\mathbf{x}\in\mathscr{X}_i} \|\mathbf{x} - \mathbf{m}_i\|^2,$$

$\mathbf{m}_i$ being the mean of the samples in $\mathscr{X}_i$. Under the null hypothesis, this partitioning is spurious, but it nevertheless results in a value for $J_e(2)$ that is smaller than $J_e(1)$. If we knew the sampling distribution for $J_e(2)$, we could determine how small $J_e(2)$ would have to be before we were forced to abandon a one-cluster null hypothesis. Lacking an analytical solution for the optimal partitioning, we cannot derive an exact solution for the sampling distribution. However, we can obtain a rough estimate by considering the suboptimal partition provided by a hyperplane through the sample mean. For large n, it can be shown that the sum of squared error for this partition is approximately normal with mean $n(d - 2/\pi)\sigma^2$ and variance $2n(d - 8/\pi^2)\sigma^4$.

This result agrees with our statement that $J_e(2)$ is smaller than $J_e(1)$, since the mean of $J_e(2)$ for the suboptimal partition—$n(d - 2/\pi)\sigma^2$—is less than the mean for $J_e(1)$—$nd\sigma^2$. To be considered significant, the reduction in the sum of squared error must certainly be greater than this. We can obtain an approximate critical value for $J_e(2)$ by assuming that the suboptimal partition is nearly optimal, by using the normal approximation for the sampling distribution, and by estimating σ^2 by

$$\hat{\sigma}^2 = \frac{1}{nd} \sum_{\mathbf{x}\in\mathscr{X}} \|\mathbf{x} - \mathbf{m}\|^2 = \frac{1}{nd} J_e(1).$$

The final result can be stated as follows: Reject the null hypothesis at the p-percent significance level if

$$\frac{J_e(2)}{J_e(1)} < 1 - \frac{2}{\pi d} - \alpha\sqrt{\frac{2(1 - 8/\pi^2 d)}{nd}}, \tag{44}$$

where α is determined by

$$p = 100 \int_{\alpha}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-1/2u^2}\, du.$$

Thus, this provides us with a test for deciding whether or not the splitting of a cluster is justified. Clearly, the c-cluster problem can be treated by applying the same test to all clusters found.

6.13 LOW-DIMENSIONAL REPRESENTATIONS AND MULTIDIMENSIONAL SCALING

Part of the problem of deciding whether or not a given clustering means anything stems from our inability to visualize the structure of multidimensional data. This problem is further aggravated when similarity or dissimilarity measures are used that lack the familiar properties of distance. One way to attack this problem is to try to represent the data points as points in some lower-dimensional space in such a way that the distances between points in the lower-dimensional space correspond to the dissimilarities between points in the original space. If acceptably accurate representations can be found in two or perhaps three dimensions, this can be an extremely valuable way to gain insight into the structure of the data. The general process of finding a configuration of points whose interpoint distances correspond to dissimilarities is often called *multidimensional scaling*.

Let us begin with the simpler case where it is meaningful to talk about the distances between the n samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$. Let $\mathbf{y}_i$ be the lower-dimensional *image* of $\mathbf{x}_i$, δ_{ij} be the distance between $\mathbf{x}_i$ and $\mathbf{x}_j$, and d_{ij} be the distance between $\mathbf{y}_i$ and $\mathbf{y}_j$. Then we are looking for a *configuration* of image points $\mathbf{y}_1, \ldots, \mathbf{y}_n$ for which the $n(n-1)/2$ distances d_{ij} between image points are as close as possible to the corresponding original distances δ_{ij}. Since it will usually not be possible to find a configuration for which $d_{ij} = \delta_{ij}$ for all i and j, we need some criterion for deciding whether or not one configuration is better than another. The following sum-of-squared-error functions are all reasonable candidates:

$$J_{ee} = \frac{1}{\sum_{i<j} \delta_{ij}^2} \sum_{i<j} (d_{ij} - \delta_{ij})^2 \tag{45}$$

$$J_{ff} = \sum_{i<j} \left(\frac{d_{ij} - \delta_{ij}}{\delta_{ij}} \right)^2 \tag{46}$$

$$J_{ef} = \frac{1}{\sum_{i<j} \delta_{ij}} \sum_{i<j} \frac{(d_{ij} - \delta_{ij})^2}{\delta_{ij}} . \tag{47}$$

Since these criterion functions involve only the distances between points, they are invariant to rigid-body motions of the configurations. Moreover,

they have all been normalized so that their minimum values are invariant to dilations of the sample points. J_{ee} emphasizes the largest errors, regardless whether the distances δ_{ij} are large or small. J_{ff} emphasizes the largest fractional errors, regardless whether the errors $|d_{ij} - \delta_{ij}|$ are large or small. J_{ef} is a useful compromise, emphasizing the largest product of error and fractional error.

Once a criterion function has been selected, an optimal configuration $\mathbf{y}_1, \ldots, \mathbf{y}_n$ is defined as one that minimizes that criterion function. An optimal configuration can be sought by a standard gradient-descent procedure, starting with some initial configuration and changing the $\mathbf{y}_i$'s in the direction of greatest rate of decrease in the criterion function. Since

$$d_{ij} = \|\mathbf{y}_i - \mathbf{y}_j\|,$$

the gradient of d_{ij} with respect to $\mathbf{y}_i$ is merely a unit vector in the direction of $\mathbf{y}_i - \mathbf{y}_j$. Thus, the gradients of the criterion functions are easy to compute:*

$$\nabla_{\mathbf{y}_k} J_{ee} = \frac{2}{\sum_{i<j} \delta_{ij}^2} \sum_{j \neq k} (d_{kj} - \delta_{kj}) \frac{\mathbf{y}_k - \mathbf{y}_j}{d_{kj}}$$

$$\nabla_{\mathbf{y}_k} J_{ff} = 2 \sum_{j \neq k} \frac{d_{kj} - \delta_{kj}}{\delta_{kj}^2} \frac{\mathbf{y}_k - \mathbf{y}_j}{d_{kj}}$$

$$\nabla_{\mathbf{y}_k} J_{ef} = \frac{2}{\sum_{i<j} \delta_{ij}} \sum_{j \neq k} \frac{d_{kj} - \delta_{kj}}{\delta_{kj}} \frac{\mathbf{y}_k - \mathbf{y}_j}{d_{kj}}.$$

The starting configuration can be chosen randomly, or in any convenient way that spreads the image points about. If the image points lie in a $\hat{d}$-dimensional space, then a simple and effective starting configuration can be found by selecting those $\hat{d}$ coordinates of the samples that have the largest variance.

The following example illustrates the kind of results than can be obtained by these techniques.† The data consist of thirty points spaced at unit intervals along a three-dimensional helix:

$$x_1(k) = \cos x_3$$
$$x_2(k) = \sin x_3$$
$$x_3(k) = k/\sqrt{2}, \qquad k = 0, 1, \ldots, 29.$$

* Second partial derivatives can also be computed easily, so that Newton's algorithm can be used. Note that if $\mathbf{y}_i = \mathbf{y}_j$, the unit vector from $\mathbf{y}_i$ to $\mathbf{y}_j$ is undefined. Should that situation arise, $(\mathbf{y}_i - \mathbf{y}_j)/d_{ij}$ can be replaced by an arbitrary unit vector.

† This example was taken from J. W. Sammon, Jr., "A nonlinear mapping for data structure analysis," *IEEE Trans. Comp.*, C-18, 401–409 (May 1969).

Figure 6.21(a) shows a perspective representation of the three-dimensional data. When the J_{ef} criterion was used, twenty iterations of a gradient descent procedure produced the two-dimensional configuration shown in Figure 6.21(b). Of course, translations, rotations, and reflections of this configuration would be equally good solutions.

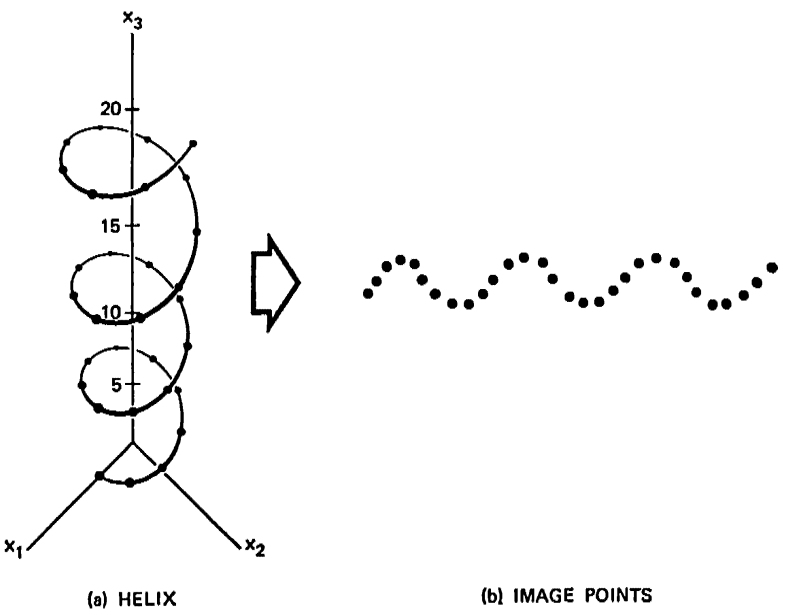
In nonmetric multidimensional scaling problems, the quantities δ_{ij} are dissimilarities whose numerical values are not as important as their rank order. An ideal configuration would be one for which the rank order of the distances d_{ij} is the same as the rank order of the dissimilarities δ_{ij}. Let us order the $m = n(n-1)/2$ dissimilarities so that $\delta_{i_1 j_1} \leq \cdots \leq \delta_{i_m j_m}$, and let $\hat{d}_{ij}$ be *any* m numbers satisfying the *monotonicity constraint*

$$\hat{d}_{i_1 j_1} \leq \hat{d}_{i_2 j_2} \leq \cdots \leq \hat{d}_{i_m j_m}.$$

In general, the distances d_{ij} will not satisfy this constraint, and the numbers $\hat{d}_{ij}$ will not be distances. However, the degree to which the d_{ij} satisfy this constraint is measured by

$$J_{\text{mon}} = \min_{\hat{d}_{ij}} \sum_{i<j} (d_{ij} - \hat{d}_{ij})^2,$$

where it is always to be understood that the $\hat{d}_{ij}$ must satisfy the monotonicity constraint. Thus, J_{mon} measures the degree to which the configuration of



(a) HELIX (b) IMAGE POINTS

FIGURE 6.21. A two-dimensional representation of data points in three dimensions (Adapted from J. W. Sammon, 1969).

points $\mathbf{y}_1, \ldots, \mathbf{y}_n$ represents the original data. Unfortunately, $\hat{J}_{\text{mon}}$ can not be used to define an optimal configuration because it can be made to vanish by collapsing the configuration to a single point. However, this defect is easily removed by a normalization such as the following:

$$J_{\text{mon}} = \frac{\hat{J}_{\text{mon}}}{\sum_{i<j} d_{ij}^2} . \tag{48}$$

Thus, J_{mon} is invariant to translations, rotations, and dilations of the configuration, and an optimal configuration can be defined as one that minimizes this criterion function. It has been observed experimentally that when the number of points is larger than dimensionality of the image space, the monotonicity constraint is actually quite confining. This might be expected from the fact that the number of constraints grows as the square of the number of points, and it is the basis for the frequently encountered statement that this procedure allows the recovery of metric information from nonmetric data. The quality of the representation generally improves as the dimensionality of the image space is increased, and it may be necessary to go beyond three dimensions to obtain an acceptably small value of J_{mon}. However, this may be a small price to pay to allow the use of the many clustering procedures available for data points in metric spaces.

6.14 CLUSTERING AND DIMENSIONALITY REDUCTION

Because the curse of dimensionality plagues so many pattern recognition procedures, a variety of methods for dimensionality reduction have been proposed. Unlike the procedures that we have just examined, most of these methods provide a functional mapping, so that one can determine the image of an arbitrary feature vector. The classical procedures of statistics are *principal components analysis* and *factor analysis*, both of which reduce dimensionality by forming linear combinations of the features.* If we think of the problem as one of removing or combining (i.e., grouping) highly correlated features, then it becomes clear that the techniques of clustering

* The object of principal components analysis (known in the communication theory literature as the Karhunen-Loéve expansion) is to find a lower-dimensional representation that accounts for the variance of the features. The object of factor analysis is to find a lower-dimensional representation that accounts for the correlations among the features. For more information, see M. G. Kendall and A. Stuart, *The Advanced Theory of Statistics, Vol. 3*, Chapter 43 (Hafner, New York, 1966) or H. H. Harman, *Modern Factor Analysis* (University of Chicago Press, Chicago and London, Second Edition, 1967).

are applicable to this problem. In terms of the *data matrix*, whose n rows are the d-dimensional samples, ordinary clustering can be thought of as a grouping of the rows, with a smaller number of cluster centers being used to represent the data, whereas dimensionality reduction can be though of as a grouping the columns, with combined features being used to represent the data.

Let us consider a simple modification of hierarchical clustering to reduce dimensionality. In place of an n-by-n matrix of distances between samples, we consider a d-by-d *correlation matrix* $R = [\rho_{ij}]$, where the correlation coefficient ρ_{ij} is related to the covariances (or sample covariances) by

$$\rho_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}\sigma_{jj}}}.$$

Since $0 \leq \rho_{ij}^2 \leq 1$, with $\rho_{ij}^2 = 0$ for uncorrelated features and $\rho_{ij}^2 = 1$ for completely correlated features, ρ_{ij}^2 plays the role of a similarity function for features. Two features for which ρ_{ij}^2 is large are clearly good candidates to be merged into one feature, thereby reducing the dimensionality by one. Repetition of this process leads to the following hierarchical procedure:

Procedure: Hierarchical Dimensionality Reduction

1. Let $\hat{d} = d$ and $\mathscr{F}_i = \{x_i\}$, $i = 1, \ldots, d$.

Loop:

2. If $\hat{d} = d'$, stop.
3. Compute the correlation matrix and find the most correlated pair of distinct clusters of features, say $\mathscr{F}_i$ and $\mathscr{F}_j$.
4. Merge $\mathscr{F}_i$ and $\mathscr{F}_j$, delete $\mathscr{F}_j$, and decrement $\hat{d}$ by one.
5. Go to Loop.

Probably the simplest way to merge two groups of features is just to average them. (This tacitly assumes that the features have been scaled so that their numerical ranges are comparable.) With this definition of a new feature, there is no problem in defining the correlation matrix for groups of features. It is not hard to think of variations on this general theme, but we shall not pursue this topic further.

For the purposes of pattern *classification*, the most serious criticism of all of the approaches to dimensionality reduction that we have mentioned is that they are overly concerned with faithful *representation* of the data. Greatest emphasis is usually placed on those features or groups of features that have the greatest variability. But for classification, we are interested in *discrimination*, not representation. Roughly speaking, the most interesting features are the ones for which the difference in the class means is large relative to the standard deviations, not the ones for which the standard deviations are large. In short, we are interested in something more like the method of multiple discriminant analysis described in Chapter 4.

There is a growing body of theory on methods of dimensionality reduction for pattern classification. Some of these methods seek to form new features out of linear combinations of old ones. Others seek merely a smaller subset of the original features. A major problem confronting this theory is that the division of pattern recognition into feature extraction followed by classification is theoretically artificial. A completely optimal feature extractor can never be anything but an optimal classifier. It is only when constraints are placed on the classifier or limitations are placed on the size of the set of samples that one can formulate nontrivial (and very complicated) problems. Various ways of circumventing this problem that may be useful under the proper circumstances can be found in the literature, and we have included a few entry points to this literature. When it is possible to exploit knowledge of the problem domain to obtain more informative features, that is usually a more profitable course of action. In the second half of this book we shall devote ourselves to a systematic examination of ways of extracting features from visual data, and with the larger problem of visual scene analysis.

6.15 BIBLIOGRAPHICAL AND HISTORICAL REMARKS

The literature on unsupervised learning and clustering is so large and is scattered across so many disciplines that the following references must be viewed as little more than a selective random sampling. Fortunately, several of the references we cite contain extensive bibliographies, relieving us of many scholarly burdens. Historically, the literature dates back at least to 1894 when Karl Pearson used sample moments to determine the parameters in a mixture of two univariate normal densities. Assuming exact knowledge of values of the mixture density, Doetsch (1936) used Fourier transforms to decompose univariate normal mixtures. Medgyessy (1961) extended this approach to other classes of mixtures, in the process exposing the problem of identifiability. Teicher (1961, 1963) and later Yakowitz and Spragins (1968) demonstrated the identifiability of several families of mixtures, the latter authors showing the equivalence of identifiability and linear independence of the component densities.

The phrases "unsupervised learning" or "learning without a teacher" usually refer to estimation of parameters of the component densities from samples drawn from the mixture density. Spragins (1966) and Cooper (1969) give valuable surveys of this work, and its relation to compound sequential Bayes learning is clarified by Cover (1969). Some of this work is quite general, being primarily concerned with theoretical possibilities. Thus, Stanat (1968) shows how Doetsch's method can be applied to learn multivariate normal

and multivariate Bernoulli mixtures, and Yakowitz (1970) demonstrates the possibility of learning virtually any identifiable mixture.

Surprisingly few papers treat maximum-likelihood estimates. Hasselblad (1966) derived maximum-likelihood formulas for estimating the parameters of univariate normal mixtures. Day (1969) derived the formulas for the multivariate, equal covariance matrix case, and pointed out the existence of singular solutions with general normal mixtures. Our treatment of the multivariate case is based directly on the exceptionally clear paper by Wolfe (1970), who also derived formulas for multivariate Bernoulli mixtures. The formulation of the Bayesian approach to unsupervised learning is usually attributed to Daly (1962); more general formulations have since been given by several authors (cf., Hilborn and Lainiotis 1968). Daly pointed out the exponential growth of the optimum system and the need for approximate solutions. Spragins' survey provides references to the literature on decision-directed approximations prior to 1966, with subsequent work being referenced by Patrick, Costello, and Monds (1970). Approximate solutions have also been obtained by the use of histograms (Patrick and Hancock 1966), quantized parameters (Fralick 1967), and randomized decisions (Agrawala 1970).

We have not mentioned all the ways that one might use to estimate unknown parameters. In particular, we have neglected the time-honored and robust method of sample moments, primarily because the situation becomes very complicated when there are more than two components in the mixture. However, some interesting solutions for special cases have been derived by David and Paul Cooper (1964) and elaborated further by Paul Cooper (1967). Because of its slow convergence, we have also omitted mention of the use of stochastic approximation; for the interested reader, the article by Young and Coraluppi (1970) can be recommended.

Much of the early work in clustering was done in the biological sciences, where it appears in studies of numerical taxonomy. Here the major concern is with hierarchical clustering. The influential book by Sokal and Sneath (1963) is an excellent source of references to this literature. Psychologists and sociologists have also contributed to clustering, although they are usually more concerned with clustering features than with clustering samples (Tryon 1939; Tryon and Bailey 1970). The advent of the digital computer made cluster analysis practical, and caused the literature on clustering to spread over many disciplines. The well known survey by Ball (1965) gives a comprehensive overview of this work and is highly recommended; Ball's insights have had a major influence on our treatment of the subject. We have also benefited from the dissertation by Ling (1971), which includes a list of 140 references. The surveys by Bolshev (1969) and Dorofeyuk (1971) give extensive references to the Russian literature on clustering.

Sokal and Sneath (1963) and Ball (1965) list many of the similarity measures and criterion functions that have seen use. The matters of measurement scales, invariance criteria, and appropriate statistical operations are illuminated by Stevens (1968), and related fundamental philosophical issues concerning clustering are treated by Watanabe (1969). The critique of clustering given by Fleiss and Zubin (1969) points out the unhappy consequences of being careless about such matters.

Jones (1968) credits Thorndike (1953) with being the first to use the sum-of-squared-error criterion, which appears so frequently in the literature. The invariant criteria we presented were derived from Friedman and Rubin (1967), who pointed out that these criteria are related to Hotelling's Trace Criterion and the F-ratio of classical statistics. The observation that all these criteria give the same optimal partitions in the two-cluster case is due to Fukunaga and Koontz (1970). Of the various criteria we did not mention, the "cohesion" criterion of Watanabe (1969, Chapter 8) is of particular interest since it involves more than pairwise similarity.

In the text we outlined the basic steps in a number of standard optimization and clustering programs. These descriptions were intentionally simplified, and even the more complete descriptions found in the literature do not always mention such matters as how ties are broken or how "wild shots" are rejected. The Isodata algorithm of Ball and Hall (1967) differs from our simplified description in several ways, most notably in the splitting of clusters that have too much within-cluster variability, and the merging of clusters that have too little between-cluster variability. Our description of the basic minimum-squared-error procedure is derived from an unpublished computer program developed by R. C. Singleton and W. H. Kautz at Stanford Research Institute in 1965. This procedure is also closely related to the adaptive sequential procedure of Sebestyen (1962), and to the so-called k-means procedure, whose convergence properties were studied by MacQueen (1967). Interesting applications of such procedures to character recognition are described by Andrews, Atrubin, and Hu (1968) and by Casey and Nagy (1968).

Sokal and Sneath (1963) reference much of the early work on hierarchical clustering, and Wishart (1969) gives explicit references to the original sources for the single-linkage, nearest-neighbor, complete-linkage, furthest-neighbor, minimum-squared-error, and several other procedures. Lance and Williams (1967) show how most of these procedures can be obtained by specializing a general distance function in different ways; in addition, they reference the major papers on divisive hierarchical clustering. The relation between single-linkage procedures and minimal spanning trees was shown by Gower and Ross (1969), who recommended a simple, efficient algorithm for finding minimal spanning trees given by Prim (1957). The equivalence between

hierarchical clustering and a distance function satisfying the ultrametric inequality was shown by Johnson (1967).

The great majority of papers on clustering have either explicitly or implicitly accepted some form of minimum-variance criterion. Wishart (1969) pointed out the serious limitations inherent in this approach, and as an alternative suggested a procedure resembling k_n-nearest-neighbor estimation of modes of the mixture density. Critiques of minimum-variance methods have also been given by Ling (1971) and Zahn (1971), both of whom favored graph-theoretic approaches to clustering. Zahn's work, though intended for data of any dimensionality, was motivated by a desire to find mathematical procedures that group sets of points in two dimensions in a way that seems visually natural. (Haralick and Kelly (1969) and Haralick and Dinstein (1971) also treat certain picture processing operations as clustering procedures, a viewpoint that applies to many of the procedures described in Part II of this book.)

Most of the early work on graph-theoretic methods was done for information retrieval purposes. Auguston and Minker (1970) credit Kuhns (1959) with the first application of graph theory to clustering. They give an experimental comparison of several graph-theoretic techniques intended for information retrieval applications, and give many references to work in this domain. It is interesting that among papers with a graph-theoretic orientation we find three that are concerned with statistical tests for cluster validity, viz., those by Bonner (1964), Hartigan (1967), and Ling (1971). Hall, Tepping, and Ball (1971) computed how the sum of squared error varies with the dimensionality of the data and the assumed number of clusters for both uniform and simplex data, and suggested these distributions as useful standards for comparison. Wolfe (1970) suggests a test for cluster validity based on an assumed chi-square distribution for the log-likelihood function.

Green and Carmone (1970), whose valuable monograph on multidimensional scaling contains an extensive bibliography, trace the origins of multidimensional scaling to a paper by Richardson (1938). Recent interest in the topic was stimulated by two developments, nonmetric multidimensional scaling and computer graphics applications. The nonmetric approach originated by Shepard (1962) and extended by Kruskal (1964a) is well suited to many problems in psychology and sociology. The computational aspects of minimizing the criterion J_{mon} subject to a monotonicity constraint are described in detail by Kruskal (1964b). Calvert (1968) used a variation of Shepard's criterion to provide a two-dimensional computer display of multivariate data. The computationally simpler J_{ef} criterion was proposed and used by Sammon (1969) to display data for interactive analysis.

The interest in man-machine systems stems partly from the difficulty of specifying criterion functions and clustering procedures that do what we

really want them to do. Mattson and Dammann (1965) were one of the first to suggest a man-machine solution to this problem. The great potential of interactive systems is well described by Ball and Hall (1970) in a paper on their PROMENADE system. Other well-known systems include BC TRY (Tryon and Bailey 1966; 1970), SARF (Stanley, Lendaris, and Nienow 1967), INTERSPACE (Patrick 1969), and OLPARS (Sammon 1970).

Neither automatic nor man-machine systems for pattern recognition can escape the fundamental problems of high-dimensional data. Various procedures have been proposed for reducing the dimensionality, either by selecting the best subset of the available features or by combining the features, usually in a linear fashion. To avoid enormous computational problems, most of these procedures use some criterion other than probability of error in making the selection. For example, Miller (1962) used a $\text{tr } S_W^{-1}S_B$ criterion, Lewis (1962) used an entropy criterion, and Marill and Green (1963) used a divergence criterion. In some cases one can bound the probability of error by more easily computed criterion functions, but the final test is always one of actual performance. In the text we restricted our attention to a simple procedure due to King (1967), selecting it primarily because of its close relation to clustering. An excellent presentation of mathematical methods for dimensionality reduction is given by Meisel (1972).

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PROBLEMS

1. Suppose that x can assume the values $0, 1, \ldots, m$ and that $P(x \mid \theta)$ is a mixture of c binomial distributions

$$P(x \mid \theta) = \sum_{j=1}^{c} \binom{m}{x} \theta_j^m (1 - \theta_j)^{m-x} P(\omega_j).$$

Assuming that the a priori probabilities are known, explain why this mixture is not identifiable if $m < c$. How does this answer change if the a priori probabilities are also unknown?

2. Let $\mathbf{x}$ be a binary vector and $P(\mathbf{x} \mid \theta)$ be a mixture of c multivariate Bernoulli distributions,

$$P(\mathbf{x} \mid \theta) = \sum_{i=1}^{c} P(\mathbf{x} \mid \omega_i, \theta_i) P(\omega_i)$$

where

$$P(\mathbf{x} \mid \omega_i, \theta_i) = \prod_{j=1}^{d} \theta_{ij}^{x_j} (1 - \theta_{ij})^{1-x_j}.$$

(a) Show that

$$\frac{\partial \log P(\mathbf{x} \mid \omega_i, \boldsymbol{\theta}_i)}{\partial \theta_{ij}} = \frac{\mathbf{x}_i - \theta_{ij}}{\theta_{ij}(1 - \theta_{ij})}.$$

(b) Using the general equations for maximum likelihood estimates, show that the maximum likelihood estimate $\hat{\boldsymbol{\theta}}_i$ for $\boldsymbol{\theta}_i$ must satisfy

$$\hat{\boldsymbol{\theta}}_i = \frac{\sum_{k=1}^{n} \hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}}_i)\mathbf{x}_k}{\sum_{k=1}^{n} \hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}}_i)}.$$

3. Consider the univariate normal mixture

$$p(\mathbf{x} \mid \boldsymbol{\theta}) = \frac{P(\omega_1)}{\sqrt{2\pi}\,\sigma_1} \exp\left[-\frac{1}{2}\left(\frac{x - \mu_1}{\sigma_1}\right)^2\right] + \frac{P(\omega_2)}{\sqrt{2\pi}\,\sigma_2} \exp\left[-\frac{1}{2}\left(\frac{x - \mu_2}{\sigma_2}\right)^2\right].$$

Write a computer program that uses the general maximum likelihood equations of Section 6.4.3 iteratively to estimate the unknown means, variances, and a priori probabilities. Use this program to find maximum likelihood estimates of these parameters for the data in Table 6-1. (Answer: $\hat{\mu}_1 = -2.404$, $\hat{\mu}_2 = 1.491$, $\hat{\sigma}_1 = 0.577$, $\hat{\sigma}_2 = 1.338$, $\hat{P}(\omega_1) = 0.268$, $\hat{P}(\omega_2) = 0.732$.)

4. Let $p(\mathbf{x} \mid \boldsymbol{\theta})$ be a c-component normal mixture with $p(\mathbf{x} \mid \omega_i, \boldsymbol{\theta}_i) \sim N(\boldsymbol{\mu}_i, \sigma_i^2 I)$. Using the results of Section 6.3, show that the maximum likelihood estimate for σ_i^2 must satisfy

$$\hat{\sigma}_i^2 = \frac{\frac{1}{d}\sum_{k=1}^{n} \hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}}_i)\, \|\mathbf{x}_k - \hat{\boldsymbol{\mu}}_i\|^2}{\sum_{k=1}^{m} \hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}}_i)}$$

where $\hat{\boldsymbol{\mu}}_i$ and $\hat{P}(\omega_i \mid \mathbf{x}_k, \hat{\boldsymbol{\theta}}_i)$ are given by Eqs. (15) and (17), respectively.

5. The derivation of the equations for maximum likelihood estimation of parameters of a mixture density was made under the assumption that the parameters in each component density are functionally independent. Suppose instead that

$$p(\mathbf{x} \mid \alpha) = \sum_{j=1}^{c} p(\mathbf{x} \mid \omega_j, \alpha)P(\omega_j),$$

where α is a parameter that appears in a number of the component densities. Let l be the n-sample log-likelihood function, and show that

$$\frac{\partial l}{\partial \alpha} = \sum_{k=1}^{n} \sum_{j=1}^{c} P(\omega_j \mid \mathbf{x}_k, \alpha) \frac{\partial \log p(\mathbf{x}_k \mid \omega_j, \alpha)}{\partial \alpha}$$

where

$$P(\omega_j \mid \mathbf{x}_k, \alpha) = \frac{p(\mathbf{x}_k \mid \omega_j, \alpha)P(\omega_j)}{p(\mathbf{x}_k \mid \alpha)}.$$

6. Let $p(\mathbf{x} \mid \omega_i, \boldsymbol{\theta}_i) \sim N(\boldsymbol{\mu}_i, \Sigma)$, where Σ is a common covariance matrix for the c component densities. Let σ_{pq} be the pqth element of Σ, σ^{pq} be the pqth element of Σ^{-1}, $x_p(k)$ be the pth element of $\mathbf{x}_k$, and $\mu_p(i)$ be the pth element of $\boldsymbol{\mu}_i$.

(a) Show that

$$\frac{\partial \log p(\mathbf{x}_k \mid \omega_i, \boldsymbol{\theta}_i)}{\partial \sigma^{pq}} = \left(1 - \frac{\delta_{pq}}{2}\right)[\sigma_{pq} - (x_p(k) - \mu_p(i))(x_q(k) - \mu_q(i))].$$

(b) Use this result and the results of Problem 5 to show that the maximum likelihood estimate for Σ must satisfy

$$\hat{\Sigma} = \frac{1}{n}\sum_{k=1}^{n} \mathbf{x}_k\mathbf{x}_k^t - \sum_{i=1}^{c} \hat{P}(\omega_i)\hat{\boldsymbol{\mu}}_i\hat{\boldsymbol{\mu}}_i^t,$$

where $\hat{P}(\omega_i)$ and $\hat{\boldsymbol{\mu}}_i$ are the maximum likelihood estimates given by Eqs. (14) and (15) in the text.

7. Show that the maximum likelihood estimate of an a priori probability can be zero by considering the following special case. Let $p(x \mid \omega_1) \sim N(0, 1)$ and $p(x \mid \omega_2) \sim N(0, (1/2))$, so that $P(\omega_1)$ is the only unknown parameter in the mixture

$$p(x) = \frac{P(\omega_1)}{\sqrt{2\pi}} e^{-(1/2)x^2} + \frac{(1 - P(\omega_1))}{\sqrt{\pi}} e^{-x^2}.$$

Show that the maximum likelihood estimate $\hat{P}(\omega_1)$ of $P(\omega_1)$ is zero if one sample x_1 is observed and if $x_1^2 < \log 2$. What is the value of $\hat{P}(\omega_1)$ if $x_1^2 > \log 2$?

8. Consider the univariate normal mixture

$$p(x \mid \mu_1, \ldots, \mu_c) = \sum_{j=1}^{c} \frac{P(\omega_j)}{\sqrt{2\pi}\,\sigma} \exp\left[-\frac{1}{2}\left(\frac{x - \mu_j}{\sigma}\right)^2\right]$$

in which all the components have the same, known variance, σ^2. Suppose that the means are so far apart compared to σ that for any observed x all but one of the terms in this sum are negligible. Use a heuristic argument to show that the value of

$$\max_{\mu_1,\ldots,\mu_c} \left\{\frac{1}{n} \log p(x_1, \ldots, x_n \mid \mu_1, \ldots, \mu_c)\right\}$$

ought to be approximately

$$\sum_{j=1}^{c} P(\omega_j) \log P(\omega_j) - \tfrac{1}{2} \log 2\pi\sigma e$$

when the number n of independently drawn samples is large. Compare this with the value shown on Figure 6.1.

9. Let θ_1 and θ_2 be unknown parameters for the component densities $p(x \mid \omega_1, \theta_1)$ and $p(x \mid \omega_2, \theta_2)$, respectively. Assume that θ_1 and θ_2 are initially statistically independent, so that $p(\theta_1, \theta_2) = p_1(\theta_1)p_2(\theta_2)$. Show that after one sample x_1 from the mixture density is observed, $p(\theta_1, \theta_2 \mid x_1)$ can no longer be factored as

$$p(\theta_1 \mid x_1)p_2(\theta_2 \mid x_1)$$

if

$$\frac{\partial p(x \mid \omega_i, \theta_i)}{\partial \theta_i} \neq 0, \qquad i = 1, 2.$$

What does this imply in general about the statistical dependence of parameters in unsupervised learning?

10. Let $\mathbf{x}_1, \ldots, \mathbf{x}_n$ be n d-dimensional samples and Σ be any nonsingular d-by-d matrix. Show that the vector $\mathbf{x}$ that minimizes

$$\sum_{k=1}^{m} (\mathbf{x}_k - \mathbf{x})^t \Sigma^{-1} (\mathbf{x}_k - \mathbf{x})$$

is the sample mean, $\frac{1}{n} \sum_{k=1}^{n} \mathbf{x}_k$.

11. Let $s(\mathbf{x}, \mathbf{x}') = \mathbf{x}^t\mathbf{x}'/(\|\mathbf{x}\| \cdot \|\mathbf{x}'\|)$. Interpret this similarity measure if the d features have binary values, where $x_i = 1$ if $\mathbf{x}$ possesses the ith feature and $x_i = -1$ if it does not. Show that for this case

$$\|\mathbf{x} - \mathbf{x}'\|^2 = 2d(1 - s(\mathbf{x}, \mathbf{x}')).$$

12. If a set of n samples $\mathcal{X}$ is partitioned into c disjoint subsets $\mathcal{X}_1, \ldots, \mathcal{X}_c$, the sample mean $\mathbf{m}_i$ for samples in $\mathcal{X}_i$ is undefined if $\mathcal{X}_i$ is empty. In such a case, the sum of squared errors involves only the nonempty subsets:

$$J_e = \sum_{\substack{\text{nonempty} \\ \mathcal{X}_i}} \sum_{\mathbf{x} \in \mathcal{X}_i} \|\mathbf{x} - \mathbf{m}_i\|^2.$$

Assuming that $n \geq c$, show that there are no empty subsets in a partition that minimizes J_e.

13. Consider a set of $n = 2k + 1$ samples, k of which coincide at $x = -2$, k at $x = 0$, and one at $x = a > 0$. Show that the two-cluster partitioning that minimizes J_e groups the k samples at $x = 0$ with the one at $x = a$ if $a^2 < 2(k + 1)$. What is the optimal grouping if $a^2 > 2(k + 1)$?

14. Let $\mathbf{x}_1 = (4\ 5)^t$, $\mathbf{x}_2 = (1\ 4)^t$, $\mathbf{x}_3 = (0\ 1)^t$ and $\mathbf{x}_4 = (5\ 0)^t$, and consider the following three partitions:

1. $\mathcal{X}_1 = \{\mathbf{x}_1, \mathbf{x}_2\}$, $\mathcal{X}_2 = \{\mathbf{x}_3, \mathbf{x}_4\}$
2. $\mathcal{X}_1 = \{\mathbf{x}_1, \mathbf{x}_4\}$, $\mathcal{X}_2 = \{\mathbf{x}_2, \mathbf{x}_3\}$
3. $\mathcal{X}_1 = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$, $\mathcal{X}_2 = \{\mathbf{x}_4\}$.

Show that by the sum-of-squared error (or tr S_W) criterion, the third partition is favored, whereas by the invariant $|S_W|$ criterion the first two partitions are favored. (Numerical answers for the three partitions: (1) and (2), tr $S_W = 18$, $|S_W| = 16$; (3), tr $S_W = 52/3$, $|S_W| = 64/3$.)

15. Show the eigenvalues $\lambda_1, \ldots, \lambda_d$ of $S_W^{-1}S_B$ are invariant to nonsingular linear transformations of the data. Show that the eigenvalues $\nu_1, \ldots, \nu_d$ of $S_T^{-1}S_W$ are related to those of $S_W^{-1}S_B$ by $\nu_i = 1/(1 + \lambda_i)$. How does this show that $J_d = |S_W|/|S_T|$ is invariant to nonsingular linear transformations of the data?

16. One way to generalize the basic-minimum-squared-error procedure is to define the criterion function

$$J_T = \sum_{i=1}^{c} \sum_{\mathbf{x} \in \mathcal{X}_i} (\mathbf{x} - \mathbf{m}_i)^t S_T^{-1} (\mathbf{x} - \mathbf{m}_i),$$

where $\mathbf{m}_i$ is the mean of the n_i samples in $\mathcal{X}_i$ and S_T is the total scatter matrix.

(a) Show that J_T is invariant to nonsingular linear transformations of the data.

(b) Show that the transfer of a sample $\hat{\mathbf{x}}$ from $\mathcal{X}_i$ to $\mathcal{X}_j$ causes J_T to change to

$$J_T^* = J_T - \left[\frac{n_j}{n_j + 1}(\hat{\mathbf{x}} - \mathbf{m}_j)^t S_T^{-1}(\hat{\mathbf{x}} - \mathbf{m}_j) - \frac{n_i}{n_i - 1}(\hat{\mathbf{x}} - \mathbf{m}_i)^t S_T^{-1}(\hat{\mathbf{x}} - \mathbf{m}_i)\right].$$

(c) Suggest an iterative procedure for minimizing J_T.

17. Use the facts that $S_T = S_W + S_B$, $J_e = \text{tr } S_W$, and $\text{tr } S_B = \sum n_i \|\mathbf{m}_i - \mathbf{m}\|^2$ to derive the equations given in Section 6.9 for the change in J_e resulting from transferring a sample $\hat{\mathbf{x}}$ from cluster $\mathcal{X}_i$ to cluster $\mathcal{X}_j$.

18. Let cluster $\mathcal{X}_i$ contain n_i samples, and let d_{ij} be some measure of the distance between two clusters $\mathcal{X}_i$ and $\mathcal{X}_j$. In general, one might expect that if $\mathcal{X}_i$ and $\mathcal{X}_j$ are merged to form a new cluster $\mathcal{X}_k$, then the distance from $\mathcal{X}_k$ to some other cluster $\mathcal{X}_h$ is not simply related to d_{hi} and d_{hj}. However, consider the equation

$$d_{hk} = \alpha d_{hi} + \alpha_j d_{hj} + \beta d_{ij} + \gamma |d_{hi} - d_{hj}|.$$

Show that the following choices for the coefficients α_i, α_j, β, and γ lead to the distance functions indicated. (For other cases, see Lance and Williams, 1967.)

(a) $d_{\min}$: $\alpha_i = \alpha_j = 0.5$, $\beta = 0$, $\gamma = -0.5$.

(b) $d_{\max}$: $\alpha_i = \alpha_j = 0.5$, $\beta = 0$, $\gamma = 0.5$.

(c) d_{avg}: $\alpha_i = \dfrac{n_i}{n_i + n_j}$, $\alpha_j = \dfrac{n_j}{n_i + n_j}$, $\beta = \gamma = 0$.

(d) d_{mean}^2: $\alpha_i = \dfrac{n_i}{n_i + n_j}$, $\alpha_j = \dfrac{n_j}{n_i + n_j}$, $\beta = -\alpha_i\alpha_j$, $\gamma = 0$.

19. Consider a hierarchical clustering procedure in which clusters are merged so as to produce the smallest increase in the sum-of-squared error at each step. If the ith cluster contains n_i samples with sample mean $\mathbf{m}_i$, show that the smallest increase results from merging the pair of clusters for which

$$\frac{n_i n_j}{n_i + n_j}\|\mathbf{m}_i - \mathbf{m}_j\|^2$$

is minimum.

20. Consider the representation of the points $\mathbf{x}_1 = (1\ 0)^t$, $\mathbf{x}_2 = (0\ 0)^t$ and $\mathbf{x}_3 = (0\ 1)^t$ by a one-dimensional configuration. To obtain a unique solution, assume that the image points satisfy $0 = y_1 < y_2 < y_3$.

(a) Show that the criterion function J_{ee} is minimized by the configuration with $y_2 = (1 + \sqrt{2})/3$ and $y_3 = 2y_2$.

(b) Show that the criterion function J_{ff} is minimized by the configuration with $y_2 = (2 + \sqrt{2})/4$ and $y_3 = 2y_2$.