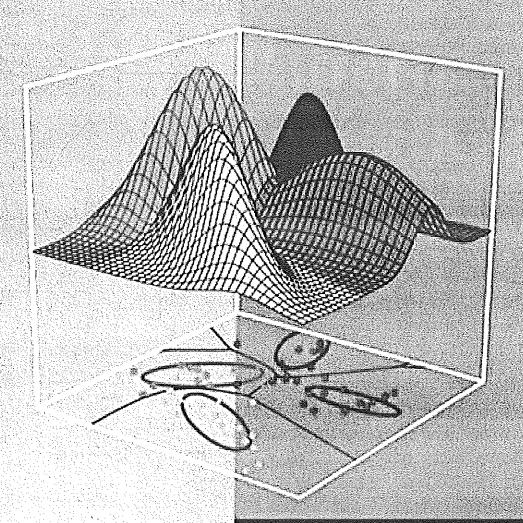


Richard O. Duda Peter E. Hart David G. Stork

Patitienn Classification



Second Edition

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2 CONTENTS

Chapter 1

Introduction

The ease with which we recognize a face, understand spoken words, read handwritten characters, identify our car keys in our pocket by feel, and decide whether an apple is ripe by its smell belies the astoundingly complex processes that underlie these acts of pattern recognition. Pattern recognition — the act of taking in raw data and taking an action based on the "category" of the pattern — has been crucial for our survival, and over the past tens of millions of years we have evolved highly sophisticated neural and cognitive systems for such tasks.

1.1 Machine Perception

It is natural that we should seek to design and build machines that can recognize patterns. From automated speech recognition, fingerprint identification, optical character recognition, DNA sequence identification and much more, it is clear that reliable, accurate pattern recognition by machine would be immensely useful. Moreover, in solving the myriad problems required to build such systems, we gain deeper understanding and appreciation for pattern recognition systems in the natural world — most particularly in humans. For some applications, such as speech and visual recognition, our design efforts may in fact be influenced by knowledge of how these are solved in nature, both in the algorithms we employ and the design of special purpose hardware.

1.2 An Example

To illustrate the complexity of some of the types of problems involved, let us consider the following imaginary and somewhat fanciful example. Suppose that a fish packing plant wants to automate the process of sorting incoming fish on a conveyor belt according to species. As a pilot project it is decided to try to separate sea bass from salmon using optical sensing. We set up a camera, take some sample images and begin to note some physical differences between the two types of fish — length, lightness, width, number and shape of fins, position of the mouth, and so on — and these suggest features to explore for use in our classifier. We also notice noise or variations in the

images — variations in lighting, position of the fish on the conveyor, even "static" due to the electronics of the camera itself.

MODEL

Given that there truly are differences between the population of sea bass and that of salmon, we view them as having different models — different descriptions, which are typically mathematical in form. The overarching goal and approach in pattern classification is to hypothesize the class of these models, process the sensed data to eliminate noise (not due to the models), and for any sensed pattern choose the model that corresponds best. Any techniques that further this aim should be in the conceptual toolbox of the designer of pattern recognition systems.

PRE-PROCESSING

FEATURE EXTRACTION

Our prototype system to perform this very specific task might well have the form shown in Fig. 1.1. First the camera captures an image of the fish. Next, the camera's signals are preprocessed to simplify subsequent operations without loosing relevant information. In particular, we might use a segmentation operation in which the images of different fish are somehow isolated from one another and from the background. The SEGMENTATION information from a single fish is then sent to a feature extractor, whose purpose is to reduce the data by measuring certain "features" or "properties." 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 as to the species.

The preprocessor might automatically adjust for average light level, or threshold the image to remove the background of the conveyor belt, and so forth. For the moment let us pass over how the images of the fish might be segmented and consider how the feature extractor and classifier might be designed. Suppose somebody at the fish plant tells us that a sea bass is generally longer than a salmon. These, then, give us our tentative models for the fish: sea bass have some typical length, and this is greater than that for salmon. Then length becomes an obvious feature, and we might attempt to classify the fish merely by seeing whether or not the length l of a fish exceeds some critical value l^* . To choose l^* we could obtain some design or training samples of the different types of fish, (somehow) make length measurements, and inspect the results.

TRAINING SAMPLES

> Suppose that we do this, and obtain the histograms shown in Fig. 1.2. These disappointing histograms bear out the statement that sea bass are somewhat longer than salmon, on average, but it is clear that this single criterion is quite poor; no matter how we choose l^* , we cannot reliably separate sea bass from salmon by length

> Discouraged, but undeterred by these unpromising results, we try another feature — the average lightness of the fish scales. Now we are very careful to eliminate variations in illumination, since they can only obscure the models and corrupt our new classifier. The resulting histograms, shown in Fig. 1.3, are much more satisfactory — the classes are much better separated.

> So far we have tacitly assumed that the consequences of our actions are equally costly: deciding the fish was a sea bass when in fact it was a salmon was just as undesirable as the converse. Such a symmetry in the cost is often, but not invariably the case. For instance, as a fish packing company we may know that our customers easily accept occasional pieces of tasty salmon in their cans labeled "sea bass," but they object vigorously if a piece of sea bass appears in their cans labeled "salmon." If we want to stay in business, we should adjust our decision boundary to avoid antagonizing our customers, even if it means that more salmon makes its way into the cans of sea bass. In this case, then, we should move our decision boundary x^* to smaller values of lightness, thereby reducing the number of sea bass that are classified as salmon (Fig. 1.3). The more our customers object to getting sea bass with their

COST

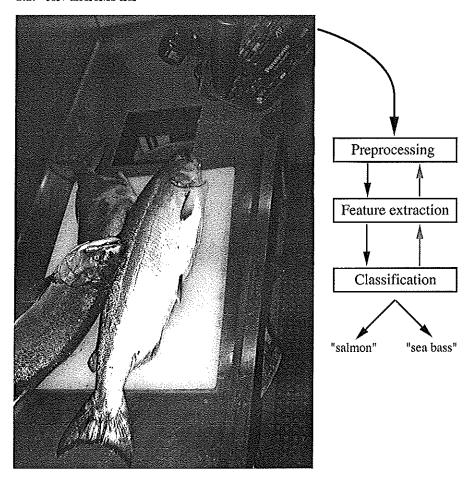


Figure 1.1: The objects to be classified are first sensed by a transducer (camera), whose signals are preprocessed, then the features extracted and finally the classification emitted (here either "salmon" or "sea bass"). Although the information flow is often chosen to be from the source to the classifier ("bottom-up"), some systems employ "top-down" flow as well, in which earlier levels of processing can be altered based on the tentative or preliminary response in later levels (gray arrows). Yet others combine two or more stages into a unified step, such as simultaneous segmentation and feature extraction.

salmon — i.e., the more costly this type of error — the lower we should set the decision threshold x^* in Fig. 1.3.

Such considerations suggest that there is an overall single cost associated with our decision, and our true task is to make a decision rule (i.e., set a decision boundary) so as to minimize such a cost. This is the central task of *decision theory* of which pattern classification is perhaps the most important subfield.

Even if we know the costs associated with our decisions and choose the optimal decision boundary x^* , we may be dissatisfied with the resulting performance. Our first impulse might be to seek yet a different feature on which to separate the fish. Let us assume, though, that no other single visual feature yields better performance than that based on lightness. To improve recognition, then, we must resort to the use

DECISION THEORY

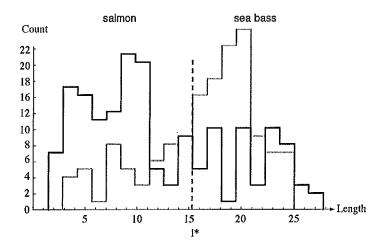


Figure 1.2: Histograms for the length feature for the two categories. No single threshold value l^* (decision boundary) will serve to unambiguously discriminate between the two categories; using length alone, we will have some errors. The value l^* marked will lead to the smallest number of errors, on average.

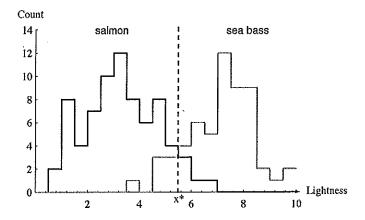


Figure 1.3: Histograms for the lightness feature for the two categories. No single threshold value x^* (decision boundary) will serve to unambiguously discriminate between the two categories; using lightness alone, we will have some errors. The value x^* marked will lead to the smallest number of errors, on average.

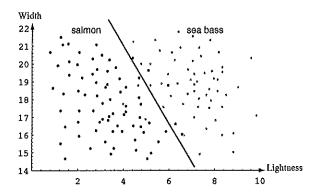


Figure 1.4: The two features of lightness and width for sea bass and salmon. The dark line might serve as a decision boundary of our classifier. Overall classification error on the data shown is lower than if we use only one feature as in Fig. 1.3, but there will still be some errors.

of more than one feature at a time.

In our search for other features, we might try to capitalize on the observation that sea bass are typically wider than salmon. Now we have two features for classifying fish — the lightness x_1 and the width x_2 . If we ignore how these features might be measured in practice, we realize that the feature extractor has thus reduced the image of each fish to a point or feature vector \mathbf{x} in a two-dimensional feature space, where

$$\mathbf{x} = \left[\begin{array}{c} x_1 \\ x_2 \end{array} \right].$$

Our problem now is to partition the feature space into two regions, where for all patterns in one region we will call the fish a sea bass, and all points in the other we call it a salmon. Suppose that we measure the feature vectors for our samples and obtain the scattering of points shown in Fig. 1.4. This plot suggests the following rule for separating the fish: Classify the fish as sea bass if its feature vector falls above the decision boundary shown, and as salmon otherwise.

This rule appears to do a good job of separating our samples and suggests that perhaps incorporating yet more features would be desirable. Besides the lightness and width of the fish, we might include some shape parameter, such as the vertex angle of the dorsal fin, or the placement of the eyes (as expressed as a proportion of the mouth-to-tail distance), and so on. How do we know beforehand which of these features will work best? Some features might be redundant: for instance if the eye color of all fish correlated perfectly with width, then classification performance need not be improved if we also include eye color as a feature. Even if the difficulty or computational cost in attaining more features is of no concern, might we ever have too many features?

Suppose that other features are too expensive or expensive to measure, or provide little improvement (or possibly even degrade the performance) in the approach described above, and that we are forced to make our decision based on the two features in Fig. 1.4. If our models were extremely complicated, our classifier would have a decision boundary more complex than the simple straight line. In that case all the

DECISION BOUNDARY

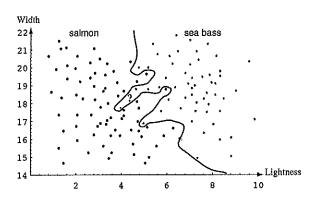


Figure 1.5: Overly complex models for the fish will lead to decision boundaries that are complicated. While such a decision may lead to perfect classification of our training samples, it would lead to poor performance on future patterns. The novel test point marked? is evidently most likely a salmon, whereas the complex decision boundary shown leads it to be misclassified as a sea bass.

GENERAL-IZATION training patterns would be separated perfectly, as shown in Fig. 1.5. With such a "solution," though, our satisfaction would be premature because the central aim of designing a classifier is to suggest actions when presented with *novel* patterns, i.e., fish not yet seen. This is the issue of *generalization*. It is unlikely that the complex decision boundary in Fig. 1.5 would provide good generalization, since it seems to be "tuned" to the particular training samples, rather than some underlying characteristics or true model of all the sea bass and salmon that will have to be separated.

Naturally, one approach would be to get more training samples for obtaining a better estimate of the true underlying characteristics, for instance the probability distributions of the categories. In most pattern recognition problems, however, the amount of such data we can obtain easily is often quite limited. Even with a vast amount of training data in a continuous feature space though, if we followed the approach in Fig. 1.5 our classifier would give a horrendously complicated decision boundary — one that would be unlikely to do well on novel patterns.

Rather, then, we might seek to "simplify" the recognizer, motivated by a belief that the underlying models will not require a decision boundary that is as complex as that in Fig. 1.5. Indeed, we might be satisfied with the slightly poorer performance on the training samples if it means that our classifier will have better performance on novel patterns.* But if designing a very complex recognizer is unlikely to give good generalization, precisely how should we quantify and favor simpler classifiers? How would our system automatically determine that the simple curve in Fig. 1.6 is preferable to the manifestly simpler straight line in Fig. 1.4 or the complicated boundary in Fig. 1.5? Assuming that we somehow manage to optimize this tradeoff, can we then predict how well our system will generalize to new patterns? These are some of the central problems in statistical pattern recognition.

For the same incoming patterns, we might need to use a drastically different cost

^{*} The philosophical underpinnings of this approach derive from William of Occam (1284-1347?), who advocated favoring simpler explanations over those that are needlessly complicated — Entia non sunt multiplicanda practer necessitatem ("Entities are not to be multiplied without necessity"). Decisions based on overly complex models often lead to lower accuracy of the classifier.

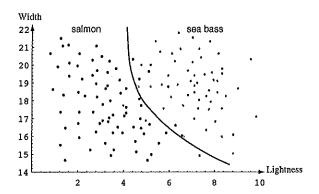


Figure 1.6: The decision boundary shown might represent the optimal tradeoff between performance on the training set and simplicity of classifier.

function, and this will lead to different actions altogether. We might, for instance, wish instead to separate the fish based on their sex — all females (of either species) from all males if we wish to sell roe. Alternatively, we might wish to cull the damaged fish (to prepare separately for cat food), and so on. Different decision tasks may require features and yield boundaries quite different from those useful for our original categorization problem.

This makes it quite clear that our decisions are fundamentally task or cost specific, and that creating a single *general purpose* artificial pattern recognition device — i.e., one capable of acting accurately based on a wide variety of tasks — is a profoundly difficult challenge. This, too, should give us added appreciation of the ability of humans to switch rapidly and fluidly between pattern recognition tasks.

Since classification is, at base, the task of recovering the model that generated the patterns, different classification techniques are useful depending on the type of candidate models themselves. In statistical pattern recognition we focus on the statistical properties of the patterns (generally expressed in probability densities), and this will command most of our attention in this book. Here the model for a pattern may be a single specific set of features, though the actual pattern sensed has been corrupted by some form of random noise. Occasionally it is claimed that neural pattern recognition (or neural network pattern classification) should be considered its own discipline, but despite its somewhat different intellectual pedigree, we will consider it a close descendant of statistical pattern recognition, for reasons that will become clear. If instead the model consists of some set of crisp logical rules, then we employ the methods of syntactic pattern recognition, where rules or grammars describe our decision. For example we might wish to classify an English sentence as grammatical or not, and here statistical descriptions (word frequencies, word correlations, etc.) are inapapropriate.

It was necessary in our fish example to choose our features carefully, and hence achieve a representation (as in Fig. 1.6) that enabled reasonably successful pattern classification. A central aspect in virtually every pattern recognition problem is that of achieving such a "good" representation, one in which the structural relationships among the components is simply and naturally revealed, and one in which the true (unknown) model of the patterns can be expressed. In some cases patterns should be represented as vectors of real-valued numbers, in others ordered lists of attributes, in yet others descriptions of parts and their relations, and so forth. We seek a represen-

tation in which the patterns that lead to the same action are somehow "close" to one another, yet "far" from those that demand a different action. The extent to which we create or learn a proper representation and how we quantify near and far apart will determine the success of our pattern classifier. A number of additional characteristics are desirable for the representation. We might wish to favor a small number of features, which might lead to simpler decision regions, and a classifier easier to train. We might also wish to have features that are robust, i.e., relatively insensitive to noise or other errors. In practical applications we may need the classifier to act quickly, or use few electronic components, memory or processing steps.

ANALYSIS BY SYNTHESIS

A central technique, when we have insufficient training data, is to incorporate knowledge of the problem domain. Indeed the less the training data the more important is such knowledge, for instance how the patterns themselves were produced. One method that takes this notion to its logical extreme is that of analysis by synthesis, where in the ideal case one has a model of how each pattern is generated. Consider speech recognition. Amidst the manifest acoustic variability among the possible "dee"s that might be uttered by different people, one thing they have in common is that they were all produced by lowering the jaw slightly, opening the mouth, placing the tongue tip against the roof of the mouth after a certain delay, and so on. We might assume that "all" the acoustic variation is due to the happenstance of whether the talker is male or female, old or young, with different overall pitches, and so forth. At some deep level, such a "physiological" model (or so-called "motor" model) for production of the utterances is appropriate, and different (say) from that for "doo" and indeed all other utterances. If this underlying model of production can be determined from the sound (and that is a very big if), then we can classify the utterance by how it was produced. That is to say, the production representation may be the "best" representation for classification. Our pattern recognition systems should then analyze (and hence classify) the input pattern based on how one would have to synthesize that pattern. The trick is, of course, to recover the generating parameters from the sensed pattern.

Consider the difficulty in making a recognizer of all types of chairs — standard office chair, contemporary living room chair, beanbag chair, and so forth — based on an image. Given the astounding variety in the number of legs, material, shape, and so on, we might despair of ever finding a representation that reveals the unity within the class of chair. Perhaps the only such unifying aspect of chairs is functional: a chair is a stable artifact that supports a human sitter, including back support. Thus we might try to deduce such functional properties from the image, and the property "can support a human sitter" is very indirectly related to the orientation of the larger surfaces, and would need to be answered in the affirmative even for a beanbag chair. Of course, this requires some reasoning about the properties and naturally touches upon computer vision rather than pattern recognition proper.

Without going to such extremes, many real world pattern recognition systems seek to incorporate at least *some* knowledge about the method of production of the patterns or their functional use in order to insure a good representation, though of course the goal of the representation is classification, not reproduction. For instance, in optical character recognition (OCR) one might confidently assume that handwritten characters are written as a sequence of strokes, and first try to recover a stroke representation from the sensed image, and then deduce the character from the identified strokes.

1.2.1 Related fields

Pattern classification differs from classical statistical hypothesis testing, wherein the sensed data are used to decide whether or not to reject a null hypothesis in favor of some alternative hypothesis. Roughly speaking, if the probability of obtaining the data given some null hypothesis falls below a "significance" threshold, we reject the null hypothesis in favor of the alternative. For typical values of this criterion, there is a strong bias or predilection in favor of the null hypothesis; even though the alternate hypothesis may be more probable, we might not be able to reject the null hypothesis. Hypothesis testing is often used to determine whether a drug is effective, where the null hypothesis is that it has no effect. Hypothesis testing might be used to determine whether the fish on the conveyor belt belong to a single class (the null hypothesis) or from two classes (the alternative). In contrast, given some data, pattern classification seeks to find the most probable hypothesis from a set of hypotheses — "this fish is probably a salmon."

Pattern classification differs, too, from *image processing*. In image processing, the input is an image and the output is an image. Image processing steps often include rotation, contrast enhancement, and other transformations which preserve all the original information. Feature extraction, such as finding the peaks and valleys of the intensity, lose information (but hopefully preserve everything relevant to the task at hand.)

IMAGE PROCESSING

As just described, feature extraction takes in a pattern and produces feature values. The number of features is virtually always chosen to be fewer than the total necessary to describe the complete target of interest, and this leads to a loss in information. In acts of associative memory, the system takes in a pattern and emits another pattern which is representative of a general group of patterns. It thus reduces the information somewhat, but rarely to the extent that pattern classification does. In short, because of the crucial role of a decision in pattern recognition information, it is fundamentally an information reduction process. The classification step represents an even more radical loss of information, reducing the original several thousand bits representing all the color of each of several thousand pixels down to just a few bits representing the chosen category (a single bit in our fish example.)

ASSOCIATIVE MEMORY

1.3 The Sub-problems of Pattern Classification

We have alluded to some of the issues in pattern classification and we now turn to a more explicit list of them. In practice, these typically require the bulk of the research and development effort. Many are domain or problem specific, and their solution will depend upon the knowledge and insights of the designer. Nevertheless, a few are of sufficient generality, difficulty, and interest that they warrant explicit consideration.

1.3.1 Feature Extraction

The conceptual boundary between feature extraction and classification proper is somewhat arbitrary: an ideal feature extractor would yield a representation that makes the job of the classifier trivial; conversely, an omnipotent classifier would not need the help of a sophisticated feature extractor. The distinction is forced upon us for practical, rather than theoretical reasons. Generally speaking, the task of feature extraction is much more problem and domain dependent than is classification proper, and thus requires knowledge of the domain. A good feature extractor for sorting fish would

surely be of little use for identifying fingerprints, or classifying photomicrographs of blood cells. How do we know which features are most promising? Are there ways to automatically learn which features are best for the classifier? How many shall we use?

1.3.2 Noise

The lighting of the fish may vary, there could be shadows cast by neighboring equipment, the conveyor belt might shake — all reducing the reliability of the feature values actually measured. We define *noise* very general terms: any property of the sensed pattern due not to the true underlying model but instead to randomness in the world or the sensors. All non-trivial decision and pattern recognition problems involve noise in some form. In some cases it is due to the transduction in the signal and we may consign to our preprocessor the role of cleaning up the signal, as for instance visual noise in our video camera viewing the fish. An important problem is knowing somehow whether the variation in some signal is noise or instead to complex underlying models of the fish. How then can we use this information to improve our classifier?

1.3.3 Overfitting

In going from Fig 1.4 to Fig. 1.5 in our fish classification problem, we were, implicitly, using a more complex model of sea bass and of salmon. That is, we were adjusting the complexity of our classifier. While an overly complex model may allow perfect classification of the training samples, it is unlikely to give good classification of novel patterns — a situation known as overfitting. One of the most important areas of research in statistical pattern classification is determining how to adjust the complexity of the model — not so simple that it cannot explain the differences between the categories, yet not so complex as to give poor classification on novel patterns. Are there principled methods for finding the best (intermediate) complexity for a classifier?

1.3.4 Model Selection

We might have been unsatisfied with the performance of our fish classifier in Figs. 1.4 & 1.5, and thus jumped to an entirely different class of model, for instance one based on some function of the number and position of the fins, the color of the eyes, the weight, shape of the mouth, and so on. How do we know when a hypothesized model differs significantly from the true model underlying our patterns, and thus a new model is needed? In short, how are we to know to reject a class of models and try another one? Are we as designers reduced to random and tedious trial and error in model selection, never really knowing whether we can expect improved performance? Or might there be principled methods for knowing when to jettison one class of models and invoke another? Can we automate the process?

1.3.5 Prior Knowledge

In one limited sense, we have already seen how prior knowledge — about the lightness of the different fish categories helped in the design of a classifier by suggesting a promising feature. Incorporating prior knowledge can be far more subtle and difficult. In some applications the knowledge ultimately derives from information about the production of the patterns, as we saw in analysis-by-synthesis. In others the knowledge may be about the *form* of the underlying categories, or specific attributes of the patterns, such as the fact that a face has two eyes, one nose, and so on.

1.3.6 Missing Features

Suppose that during classification, the value of one of the features cannot be determined, for example the width of the fish because of occlusion by another fish (i.e., the other fish is in the way). How should the categorizer compensate? Since our two-feature recognizer never had a single-variable threshold value x^* determined in anticipation of the possible absence of a feature (cf., Fig. 1.3), how shall it make the best decision using only the feature present? The naive method, of merely assuming that the value of the missing feature is zero or the average of the values for the training patterns, is provably non-optimal. Likewise we occasionally have missing features during the creation or learning in our recognizer. How should we train a classifier or use one when some features are missing?

OCCLUSION

1.3.7 Mereology

We effortlessly read a simple word such as BEATS. But consider this: Why didn't we read instead other words that are perfectly good subsets of the full pattern, such as BE, BEAT, EAT, AT, and EATS? Why don't they enter our minds, unless explicitly brought to our attention? Or when we saw the B why didn't we read a P or an I, which are "there" within the B? Conversely, how is it that we can read the two unsegmented words in POLOPONY — without placing the entire input into a single word category?

This is the problem of *subsets and supersets* — formally part of mereology, the study of part/whole relationships. It is closely related to that of prior knowledge and segmentation. In short, how do we recognize or group together the "proper" number of elements — neither too few nor too many? It appears as though the best classifiers try to incorporate as much of the input into the categorization as "makes sense," but not too much. How can this be done?

1.3.8 Segmentation

In our fish example, we have tacitly assumed that the fish were isolated, separate on the conveyor belt. In practice, they would often be abutting or overlapping, and our system would have to determine where one fish ends and the next begins — the individual patterns have to be *segmented*. If we have already recognized the fish then it would be easier to segment them. But how can we segment the images before they have been categorized or categorize them before they have been segmented? It seems we need a way to know when we have switched from one model to another, or to know when we just have background or "no category." How can this be done?

Segmentation is one of the deepest problems in automated speech recognition. We might seek to recognize the individual sounds (e.g., phonemes, such as "ss," "k," ...), and then put them together to determine the word. But consider two nonsense words, "sklee" and "skloo." Speak them aloud and notice that for "skloo" you push your lips forward (so-called "rounding" in anticipation of the upcoming "oo") before you utter the "ss." Such rounding influences the sound of the "ss," lowering the frequency spectrum compared to the "ss" sound in "sklee" — a phenomenon known as anticipatory coarticulation. Thus, the "oo" phoneme reveals its presence in the "ss" earlier than the "k" and "l" which nominally occur before the "oo" itself! How do we segment the "oo" phoneme from the others when they are so manifestly intermingled? Or should we even try? Perhaps we are focusing on groupings of the wrong size, and that the most useful unit for recognition is somewhat larger, as we saw in subsets and

supersets (Sect. 1.3.7). A related problem occurs in connected cursive handwritten character recognition: How do we know where one character "ends" and the next one "begins"?

1.3.9 Context

We might be able to use *context* — input-dependent information other than from the target pattern itself — to improve our recognizer. For instance, it might be known for our fish packing plant that if we are getting a sequence of salmon, that it is highly likely that the next fish will be a salmon (since it probably comes from a boat that just returned from a fishing area rich in salmon). Thus, if after a long series of salmon our recognizer detects an ambiguous pattern (i.e., one very close to the nominal decision boundary), it may nevertheless be best to categorize it too as a salmon. We shall see how such a simple correlation among patterns — the most elementary form of context — might be used to improve recognition. But how, precisely, should we incorporate such information?

Context can be highly complex and abstract. The utterance "jeetyet?" may seem nonsensical, unless you hear it spoken by a friend in the context of the cafeteria at lunchtime — "did you eat yet?" How can such a visual and temporal context influence your speech recognition?

1.3.10 Invariances

In seeking to achieve an optimal representation for a particular pattern classification task, we confront the problem of *invariances*. In our fish example, the absolute position on the conveyor belt is irrelevant to the category and thus our representation should also be insensitive to absolute position of the fish. Here we seek a representation that is invariant to the transformation of *translation* (in either horizontal or vertical directions). Likewise, in a speech recognition problem, it might be required only that we be able to distinguish between utterances regardless of the particular moment they were uttered; here the "translation" invariance we must ensure is in *time*.

The "model parameters" describing the orientation of our fish on the conveyor belt are horrendously complicated — due as they are to the sloshing of water, the bumping of neighboring fish, the shape of the fish net, etc. — and thus we give up hope of ever trying to use them. These parameters are irrelevant to the model parameters that interest us anyway, i.e., the ones associated with the differences between the fish categories. Thus here we try to build a classifier that is invariant to transformations such as rotation.

ORIENTATION

The orientation of the fish on the conveyor belt is irrelevant to its category. Here the transformation of concern is a two-dimensional rotation about the camera's line of sight. A more general invariance would be for rotations about an arbitrary line in three dimensions. The image of even such a "simple" object as a coffee cup undergoes radical variation as the cup is rotated to an arbitrary angle — the handle may become hidden, the bottom of the inside volume come into view, the circular lip appear oval or a straight line or even obscured, and so forth. How might we insure that our pattern recognizer is invariant to such complex changes?

The overall size of an image may be irrelevant for categorization. Such differences might be due to variation in the range to the object; alternatively we may be genuinely unconcerned with differences between sizes — a young, small salmon is still a salmon.

SIZE

For patterns that have inherent temporal variation, we may want our recognizer to be insensitive to the *rate* at which the pattern evolves. Thus a slow hand wave and a fast hand wave may be considered as equivalent. Rate variation is a deep problem in speech recognition, of course; not only do different individuals talk at different rates, but even a single talker may vary in rate, causing the speech signal to change in complex ways. Likewise, cursive handwriting varies in complex ways as the writer speeds up — the placement of dots on the i's, and cross bars on the t's and f's, are the first casualties of rate increase, while the appearance of l's and e's are relatively inviolate. How can we make a recognizer that changes its representations for some categories differently from that for others under such rate variation?

A large number of highly complex transformations arise in pattern recognition, and many are domain specific. We might wish to make our handwritten optical character recognizer insensitive to the overall thickness of the pen line, for instance. Far more severe are transformations such as non-rigid deformations that arise in three-dimensional object recognition, such as the radical variation in the image of your hand as you grasp an object or snap your fingers. Similarly, variations in illumination or the complex effects of cast shadows may need to be taken into account.

The symmetries just described are continuous — the pattern can be translated, rotated, sped up, or deformed by an arbitrary amount. In some pattern recognition applications other — discrete — symmetries are relevant, such as flips left-to-right, or top-to-bottom.

In all of these invariances the problem arises: How do we determine whether an invariance is present? How do we efficiently incorporate such knowledge into our recognizer?

1.3.11 Evidence Pooling

In our fish example we saw how using *multiple* features could lead to improved recognition. We might imagine that we could do better if we had several component *classifiers*. If these categorizers agree on a particular pattern, there is no difficulty. But suppose they disagree. How should a "super" classifier *pool the evidence* from the component recognizers to achieve the best decision?

Imagine calling in ten experts for determining if a particular fish is diseased or not. While nine agree that the fish is healthy, one expert does not. Who is right? It may be that the lone dissenter is the only one familiar with the particular very rare symptoms in the fish, and is in fact correct. How would the "super" categorizer know when to base a decision on a minority opinion, even from an expert in one small domain who is not well qualified to judge throughout a broad range of problems?

1.3.12 Costs and Risks

We should realize that a classifier rarely exists in a vacuum. Instead, it is generally to be used to recommend actions (put this fish in this bucket, put that fish in that bucket), each action having an associated cost or risk. Conceptually, the simplest such risk is the classification error: what percentage of new patterns are called the wrong category. However the notion of risk is far more general, as we shall see. We often design our classifier to recommend actions that minimize some total expected cost or risk. Thus, in some sense, the notion of category itself derives from the cost or task. How do we incorporate knowledge about such risks and how will they affect our classification decision?

RATE

DEFORMATION

DISCRETE SYMMETRY Finally, can we estimate the total risk and thus tell whether our classifier is acceptable even before we field it? Can we estimate the lowest possible risk of *any* classifier, to see how close ours meets this ideal, or whether the problem is simply too hard overall?

1.3.13 Computational Complexity

Some pattern recognition problems can be solved using algorithms that are highly impractical. For instance, we might try to hand label all possible 20×20 binary pixel images with a category label for optical character recognition, and use table lookup to classify incoming patterns. Although we might achieve error-free recognition, the labeling time and storage requirements would be quite prohibitive since it would require a labeling each of $2^{20\times 20}\approx 10^{120}$ patterns. Thus the computational complexity of different algorithms is of importance, especially for practical applications.

In more general terms, we may ask how an algorithm scales as a function of the number of feature dimensions, or the number of patterns or the number of categories. What is the tradeoff between computational ease and performance? In some problems we know we can design an excellent recognizer, but not within the engineering constraints. How can we optimize within such constraints? We are typically less concerned with the complexity of learning, which is done in the laboratory, than the complexity of making a decision, which is done with the fielded application. While computational complexity generally correlates with the complexity of the hypothesized model of the patterns, these two notions are conceptually different.

This section has catalogued some of the central problems in classification. It has been found that the most effective methods for developing classifiers involve learning from examples, i.e., from a set of patterns whose category is known. Throughout this book, we shall see again and again how methods of learning relate to these central problems, and are essential in the building of classifiers.

1.4 Learning and Adaptation

In the broadest sense, any method that incorporates information from training samples in the design of a classifier employs learning. Because nearly all practical or interesting pattern recognition problems are so hard that we cannot guess classification decision ahead of time, we shall spend the great majority of our time here considering learning. Creating classifiers then involves posit some general form of model, or form of the classifier, and using training patterns to learn or estimate the unknown parameters of the model. Learning refers to some form of algorithm for reducing the error on a set of training data. A range of gradient descent algorithms that alter a classifier's parameters in order to reduce an error measure now permeate the field of statistical pattern recognition, and these will demand a great deal of our attention. Learning comes in several general forms.

1.4.1 Supervised Learning

In supervised learning, a teacher provides a category label or cost for each pattern in a training set, and we seek to reduce the sum of the costs for these patterns. How can we be sure that a particular learning algorithm is powerful enough to learn the solution to a given problem and that it will be stable to parameter variations?

1.5. CONCLUSION 17

How can we determine if it will converge in finite time, or scale reasonably with the number of training patterns, the number of input features or with the perplexity of the problem? How can we insure that the learning algorithm appropriately favors "simple" solutions (as in Fig. 1.6) rather than complicated ones (as in Fig. 1.5)?

1.4.2 Unsupervised Learning

In unsupervised learning or clustering there is no explicit teacher, and the system forms clusters or "natural groupings" of the input patterns. "Natural" is always defined explicitly or implicitly in the clustering system itself, and given a particular set of patterns or cost function, different clustering algorithms lead to different clusters. Often the user will set the hypothesized number of different clusters ahead of time, but how should this be done? How do we avoid inappropriate representations?

1.4.3 Reinforcement Learning

The most typical way to train a classifier is to present an input, compute its tentative category label, and use the known target category label to improve the classifier. For instance, in optical character recognition, the input might be an image of a character, the actual output of the classifier the category label "R," and the desired output a "B." In reinforcement learning or learning with a critic, no desired category signal is given; instead, the only teaching feedback is that the tentative category is right or wrong. This is analogous to a critic who merely states that something is right or wrong, but does not say specifically how it is wrong. (Thus only binary feedback is given to the classifier; reinforcement learning also describes the case where a single scalar signal, say some number between 0 and 1, is given by the teacher.) In pattern classification, it is most common that such reinforcement is binary — either the tentative decision is correct or it is not. (Of course, if our problem involves just two categories and equal costs for errors, then learning with a critic is equivalent to standard supervised learning.) How can the system learn which are important from such non-specific feedback?

CRITIC

1.5 Conclusion

At this point the reader may be overwhelmed by the number, complexity and magnitude of these sub-problems. Further, these sub-problems are rarely addressed in isolation and they are invariably interrelated. Thus for instance in seeking to reduce the complexity of our classifier, we might affect its ability to deal with invariance. We point out, though, that the good news is at least three-fold: 1) there is an "existence proof" that many of these problems can indeed be solved — as demonstrated by humans and other biological systems, 2) mathematical theories solving some of these problems have in fact been discovered, and finally 3) there remain many fascinating unsolved problems providing opportunities for progress.

Summary by Chapters

The overall organization of this book is to address first those cases where a great deal of information about the models is known (such as the probability densities, category labels, ...) and to move, chapter by chapter, toward problems where the form of the

distributions are unknown and even the category membership of training patterns is unknown. We begin in Chap. ?? (Bayes decision theory) by considering the ideal case in which the probability structure underlying the categories is known perfectly. While this sort of situation rarely occurs in practice, it permits us to determine the optimal (Bayes) classifier against which we can compare all other methods. Moreover in some problems it enables us to predict the error we will get when we generalize to novel patterns. In Chap. ?? (Maximum Likelihood and Bayesian Parameter Estimation) we address the case when the full probability structure underlying the categories is not known, but the general forms of their distributions are — i.e., the models. Thus the uncertainty about a probability distribution is represented by the values of some unknown parameters, and we seek to determine these parameters to attain the best categorization. In Chap. ?? (Nonparametric techniques) we move yet further from the Bayesian ideal, and assume that we have no prior parameterized knowledge about the underlying probability structure; in essence our classification will be based on information provided by training samples alone. Classic techniques such as the nearest-neighbor algorithm and potential functions play an important role here.

We then in Chap. ?? (Linear Discriminant Functions) return somewhat toward the general approach of parameter estimation. We shall assume that the so-called "discriminant functions" are of a very particular form — viz., linear — in order to derive a class of incremental training rules. Next, in Chap. ?? (Nonlinear Discriminants and Neural Networks) we see how some of the ideas from such linear discriminants can be extended to a class of very powerful algorithms such as backpropagation and others for multilayer neural networks; these neural techniques have a range of useful properties that have made them a mainstay in contemporary pattern recognition research. In Chap. ?? (Stochastic Methods) we discuss simulated annealing by the Boltzmann learning algorithm and other stochastic methods. We explore the behavior of such algorithms with regard to the matter of local minima that can plague other neural methods. Chapter ?? (Non-metric Methods) moves beyond models that are statistical in nature to ones that can be best described by (logical) rules. Here we discuss tree-based algorithms such as CART (which can also be applied to statistical data) and syntactic based methods, such as grammar based, which are based on crisp rules.

Chapter ?? (Theory of Learning) is both the most important chapter and the most difficult one in the book. Some of the results described there, such as the notion of capacity, degrees of freedom, the relationship between expected error and training set size, and computational complexity are subtle but nevertheless crucial both theoretically and practically. In some sense, the other chapters can only be fully understood (or used) in light of the results presented here; you cannot expect to solve important pattern classification problems without using the material from this chapter.

We conclude in Chap. ?? (Unsupervised Learning and Clustering), by addressing the case when input training patterns are not labeled, and that our recognizer must determine the cluster structure. We also treat a related problem, that of learning with a critic, in which the teacher provides only a single bit of information during the presentation of a training pattern — "yes," that the classification provided by the recognizer is correct, or "no," it isn't. Here algorithms for reinforcement learning will be presented.

Bibliographical and Historical Remarks

Classification is among the first crucial steps in making sense of the blooming buzzing confusion of sensory data that intelligent systems confront. In the western world, the foundations of pattern recognition can be traced to Plato [2], later extended by Aristotle [1], who distinguished between an "essential property" (which would be shared by all members in a class or "natural kind" as he put it) from an "accidental property" (which could differ among members in the class). Pattern recognition can be cast as the problem of finding such essential properties of a category. It has been a central theme in the discipline of philosophical epistemology, the study of the nature of knowledge. A more modern treatment of some philosophical problems of pattern recognition, relating to the technical matter in the current book can be found in [22, 4, 18]. In the eastern world, the first Zen patriarch, Bodhidharma, would point at things and demand students to answer "What is that?" as a way of confronting the deepest issues in mind, the identity of objects, and the nature of classification and decision. A delightful and particularly insightful book on the foundations of artificial intelligence, including pattern recognition, is [9].

Early technical treatments by Minsky [14] and Rosenfeld [16] are still valuable, as are a number of overviews and reference books [5]. The modern literature on decision theory and pattern recognition is now overwhelming, and comprises dozens of journals, thousands of books and conference proceedings and innumerable articles; it continues to grow rapidly. While some disciplines such as statistics [7], machine learning [17] and neural networks [8], expand the foundations of pattern recognition, others, such as computer vision [6, 19] and speech recognition [15] rely on it heavily. Perceptual Psychology, Cognitive Science [12], Psychobiology [21] and Neuroscience [10] analyze how pattern recognition is achieved in humans and other animals. The extreme view that everything in human cognition — including rule-following and logic — can be reduced to pattern recognition is presented in [13]. Pattern recognition techniques have been applied in virtually every scientific and technical discipline.

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