Pattern Recognition: Introduction and Terminology

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37 Steps

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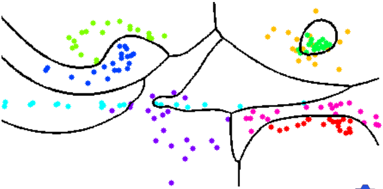

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About this ebook

This ebook gives the starting student an introduction into the field of pattern recognition. It may serve as reference to others by giving intuitive descriptions of the terminology. The book is the first in a series of ebooks on topics and examples in the field.

Our goal is an informal explanation of the concepts. For thorough mathematical descriptions we refer to the textbooks and lectures. In ten chapters the topics of pattern recognition are summarized and its terminology is introduced. In the glossary about 200 terms are described. All glossary terms are linked, forward and backward by hypertext. In the glossary chapter external links are provided to internet pages, papers tutorials, Wikipedia entries, examples, etcetera. Internal links are in dark blue in order to preserve the readability. External links are in blue.

This ebook is offered by the authors of a website on pattern recognition tools, `http://37steps.com/`. Here more information, software, data and examples can be found. The book itself does not assume the use of specific software. The code for generating the examples, however, is written in Matlab using PRTools. It can be inspected by clicking on the figures or example links.

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The medium size version of the book has been formatted such that it is suitable for a computer screen. The small size version is suitable for an e-reader like the Kindle. Here external links may not work. Reading and browsing through the ebook may still be of interest to get acquainted to the pattern recognition terminology.

About 37Steps

The website `http://37steps.com` has been created by the authors after they left university. They have been engaged with pattern recognition for decades and put together their insights, experiences and software. All material is for free. However, donations are appreciated: http://37steps.com/donations.

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Chapter 1

Introduction

1.1 Recognition and consciousness

For a very small child a walk into the world is a walk into the wild: all is new and exciting. Every object, every sound, every shape provides a new experience. Consequently, it does not know how to interpret what is happening, nor is it able to walk or to grasp objects properly. It does not know how to hold an item or how to walk. That is beneficial, as it also does not know about danger and, as a result, can freely explore the world around. Such an exploration cannot continue forever. If the child has to become independent of its protecting environment, it will have to know and to understand, it will have to act and to deal with the world in a sensible way.

The miracle of memory helps to overcome the state of ignorance. It converts the chaos of the wild into a world where we can organize the information and find our way. Thanks to the memory we find our way back to a safe place or to a place where the food has been stored. Thanks to the memory we learn to avoid the danger.

We recognize the past in the present. Thanks to successes and disappointments we learn how to deal with them. Memory yields **consciousness**. And consciousness is the basis for **recognition** and understanding.

How is this possible? The human abilities of consciousness and recognition are miracles as large as the physical basis of gravity and light. They are there. We can build some models, but we are still far from understanding how the light that enters the eye generates the word or the idea 'tree' in the mind. At the bottom there is the first principle: we may say that we understand, but what do we mean by that? Do we understand understanding? The entire field of pattern recognition is an effort to come somewhat closer to this understanding. This can be done in a scientific way, or by attempts to create artificial devices that mimic the human ability. Here we will give an introduction how results of the first are used for the second.

The present is never equal to the past. There are always differences. Every street, every tree or every person that we meet is different from all streets, trees and persons we have seen before. How do we know that the new place where we find ourselves is a street anyway? How do we know that the figure on the quilt is a tree?

Or, how do we know that we know the person who is standing at the door? Even if she is our partner and we have lived with her for 37 years the question how we recognize her is intriguing.

There may be just minor differences between what we see in the very moment and what we have left behind this morning and that is still in our memory. But, why are some differences minor while others are major? How do we judge that? How do we know which differences are essential? In one way or the other we are able to judge that different observations refer to the same object we have seen before. Even, in the case we have never seen a particular object, we are able to recognize to which class of similar objects it belongs.

The ability to judge the **similarity** between objects or events is called **generalization**. Given a few examples, sometimes even a single one, we are able to tell whether a new, unseen object belongs to the same group. Its similarity to previously observed objects is sufficiently large. Human beings are pattern recognizers, not just because of this **recognition** ability, but especially because we are aware of it. We can handle it, we can teach the patterns to others and discuss with them our observations.

The generalization skill develops our consciousness further. It constitutes the basis of any science, in particular, the natural sciences. The question how we do this, how we come from observations to memory and to generalization is thereby the basic scientific question of pattern recognition.

1.2 Creating artificial PR systems

From the early development of computers, scientists and engineers tried to imitate the human recognition ability by mechanical means, either partially or in its entirety. Two types of main results have been obtained from these efforts so far.

First, scientific results have been gained: a better understanding of the human perception, reasoning and the ability to gain new knowledge which may be applied in a changing environment. This resulted in more insight in the human senses and the neural system. To some extent, this understanding can be expressed in mental, psychological and philosophical terms. Herewith **observations**, facts and existing knowledge are combined by reasoning yielding some new conclusions.

Attempts to design sensors, computers and programs that imitate such processes bring an additional prospect to the investigation of possible biological models. An ever returning difficulty, however, is the relation of low level phenomena occurring in the senses and the nerves with high level understanding and conceptual thinking. How do externally measurable, physical and biological processes generate the internal observation of recognition and understanding? This problem is related to the so-called **semantic gap** and is one of the main unsolved scientific questions.

Second, many contributions to the engineering practise have been created. Various **pattern recognition** systems have been developed that are of practical use, as for the assistance in medical diagnosis, industrial inspection, personal identification and man-machine interaction. Very often, they are not based on a detailed simulation of the human processes, but on specific approaches to the problem at hand.

It is striking and interesting to observe that artificial recognition devices, especially the ones that **learn from examples**, are almost not, or just superficially based on a modeling of the human perception and learning abilities. This can be compared with other biological studies. We know a lot of how birds fly, but airplanes are constructed differently. One of the reasons is that the artificial systems may serve different purposes: they need to be more stable and should sometimes be faster and larger, at the cost of a reduced flexibility.

In this book, we will focus on the pattern recognition research aiming at the development of automatic systems. We will especially deal with the possibilities of these systems to learn from sets of examples. A general, global description of such systems will be presented, resulting in a intuitive characterization of the various steps and procedures that can be distinguished in their design and operation. This will be illustrated by simple examples.

The main goal of the book is to give the student a first introduction into the terminology used in the field of pattern recognition. In the final chapter a glossary is presented in which short characterizations of the main terms are given with backward references to the places where they have been introduced or used for the first time. A few non-standard terms are added for completeness. For most other ones holds that they used in the literature in various different ways. Therefore, strict definitions are not presented here. It is expected that readers have some implicit pattern recognition ability and are able to learn from the examples as they have been made available.

Chapter 2

A small example

After all these introductory words it is more than time to discuss a simple example. Let us take a small dataset, the so-called Kimia images. This is a set of silhouettes of 2D figures. Figure 1 shows two of the classes, elephants and camels, each given by 12 examples. Suppose we take out one elephant and show it to somebody who has no knowledge about these animals, e.g. a 3-year old boy. Would he be able to name it if we would show him the other 23 figures and name for each of them the class? It is probable that he wouldn't have any problem with that.

Let us now try to do the same with a computer. We need to compare figures in a numeric way: compute some type of distances or similarities. To that end a comparable **representation** has to be established. As the images have all different sizes, counting pixel differences is not straightforward. We will try something very elementary and compute the sizes (blob areas in pixels) and perimeter lengths (in pixels). They are graphically represented in the **scatter plot** of Figure 2. This is a picture of what is called a **feature space**.

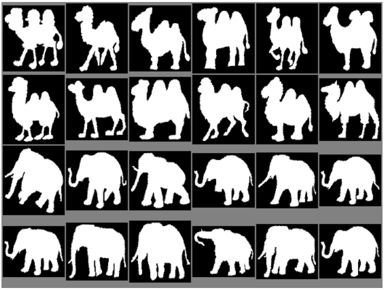

Figure 1: Two classes in the Kimia dataset

This is a vector space in which **objects**, here the animal blobs, are represented by characteristic properties, here area and perimeter length.

If the features really correspond to characteristic properties, then similar objects are close in feature space. Similar objects are expected to belong to the same class. In the plot the objects are encircled that have nearest neighbors of a different class. The fraction of encircled objects gives an indication of the usefulness of this feature space for recognizing new, similar objects of the same classes.

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A problem with this feature space is that the area is dominating over the perimeter as the spread of its values is much larger. If features are considered to be equally important, feature spaces should be created in which they are equally scaled. This is done in the next scatter plot, Figure 3, by dividing all feature values by

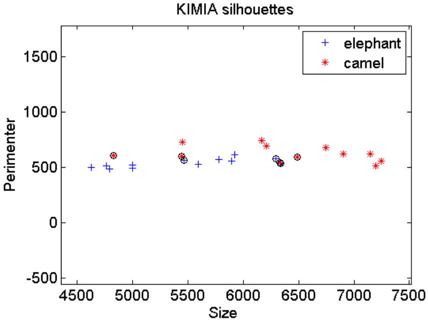

Figure 2: Scatter plots of two classes in the Kimia dataset based on perimeter and area. Objects are encircled for which the nearest neighbor is of a different class. Two erroneously classified objects are almost on top of each other. Note that the perimeter is hardly of significance as the values of the area feature are much larger.

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their corresponding standard deviation.

In this case the result of the scaling is that less objects are assigned to the wrong class, indicating that the scaled feature space is better for classification. The improvement (5 instead of 7 errors), however, is in this case not significant. It is certainly not true that rescaling is always better. In some cases it known that the features as they are measured are informative. This should not be spoiled. Anyway, whether scaling is appropriate or not should always be considered.

Once a feature space is found that is appropriate for classifying new objects with unknown **class memberships**, it can be used for computing a definite **classifier**. Several procedures are possible. In Figure 4 the result of the same classifier as used above is shown using the entire available **training set**. For new objects the same features, area and perimeter should be measured and the same scaling factor as found for the training set should be applied.

In order to have a reliable estimate of the classification accuracy of this classifier, an additional test set is needed, representative for the application and independent of the training set. If the entire design set (the union of training set and test set) is used for training the classifier, it is expected to be better, i.e. to have a lower classification error. Using this design set or one of its subsets (training set or test set), however, it will be optimistically biased as they are used for training this classifier. Strategies for dealing with this dilemma, computing the best classifier or estimating a reliable

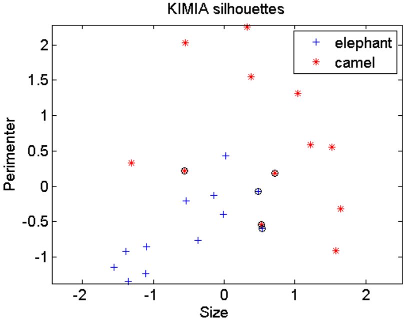

Figure 3: Scatter plots of two classes in the Kimia dataset based on perimeter and area. The values of perimeter and area are rescaled using their standard deviation. Objects are encircled for which the nearest neighbor is of a different class.

classification error, are discussed in section 8.1.

To end this chapter we summarize the steps that have been taken in the design of the pattern classifier and the main concepts used.

Representation If we want to build automatic recognition system for real world objects they should be represented in a way they can be compared

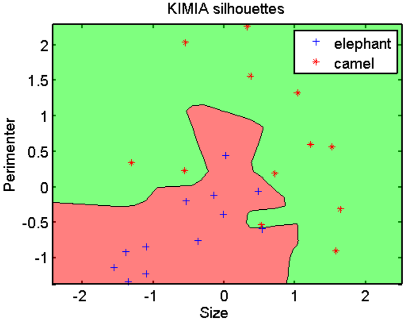

Figure 4: The classifier computed for the entire available dataset.

by a computer. Here we used a camera to obtain black-and-white images in which the objects are blobs. The areas and perimeters of the blobs are used to construct 2D vectors in a feature space.

Adaptation By studying the representation is was found that the area dominated as it showed much larger values and thereby much larger differences between the objects. The variations were normalized by dividing by the standard deviation to give features an equal spread. Consequently, distances between objects are now equally influenced by the two features.

Evaluation We need to find how good a particular representation is. This is useful for finding better representations and for optimizing an adaptation. See also chapter 6 and chapter 8.

Generalization The final system should be such that it is possible to apply it to new, unseen objects, that have not been used in the design. In the above example we used the computation of a classifier as a particular kind of generalization. Seel also chapter 7

In addition the following concepts have been used:

Object Used for real world physical objects and events as well as for their representations, e.g. in a feature space.

Feature A characteristic, measurable property of objects useful for representation and generalization. Characteristic is meant here as contributing to the distinction of objects of different classes. Features are sometimes called **attributes**.

Class A set of objects that, as such, has to be distinguished from other objects in the problem.

Label Often used as the name of the class to which a particular object belongs. Sometimes it is just a number, being an index in the list of names of classes to be distinguished.

Training set The set of objects with known class labels used for computing a classifier.

Test set The set of objects with known class labels used for estimating the classification error of a trained classifier.

Design set The total set of objects that is used in designing a recognition system. Subsets are used

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training, evaluation or special steps in the adaptation.

Classifier The final function that distinguishes the classes of interest.

The entire technology of the creation of a recognition system based on given objects is sometimes referred to as **learning from examples**.

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Chapter 3

Review of PR problems

Here some examples will be given of Pattern Recognition (PR) applications and the types of data that the analyst in this field may encounter.

3.1 Pattern recognition applications

By its nature PR can be applied in any field in which observations are studied that can be represented in a numeric way. It is only worthwhile to use a PR approach if the problems can be formulated as **classification** problems: it should be of interest to assign new objects to some class. Moreover, this problem should not be easily solvable by other means, e.g. a threshold on a sensor, or a perfectly fitting physical model. Applications areas of PR are often fields that recently became of interest, or in which new sensors have been introduced, or that are very complicated. In such situations a sufficiently useful physical may not be available or is infeasible. PR may be of help to start an analysis.

In almost all the natural sciences PR techniques are used in one way or the other. In some of them, e.g.

astronomy, chemometrics and taxonomy, very similar techniques are used under different names. Classification procedures have here been studied independently and sometimes even before PR was established as an area of research. In some way the field of PR as a separate technology became of interest after it was found that in various disciplines similar problems arose. Various fields with many researchers continued independently. This might be regretted, but it has definite its positive sides as thereby different paths are followed and different solutions are found.

Important application areas to which many PR researchers contribute are biology, health, medical imaging, psychology, human behavior, ecology, seismics, space engineering, aeronautics, oceanology, navigation, transport, computer vision and speech. In all these areas new sensors or new measurement technologies are introduced. Often the possibilities that arise grow much faster than the possibilities to process, analyze and interpret the generated data.

In addition to these areas of science and engineering, there are various applications of societal interest, e.g. security, forensics, mail delivery, personal identification by biometrics, signature verification, fraud detection and computer crimes. Sometimes similar sensors as in scientific research are used like photo sensors and microphones, but also entirely different types of measurements may be used. Examples are text and computer events.

The common ground between many of these application areas is the much smaller set of different data types. As far as they are similar, general procedures can be developed. A review of the main data types is presented in the next section.

3.2 Data types

Here some common data types are discussed as they are encountered by an analyst in the PR field studying **observations** on real world **objects**.

Independently observed features Features measured by separate sensors, e.g. the weight and size of cars in an application of car type recognition. It should be emphasized that such features are independently measured, but the obtained feature values are not statistically independent as they involve the same object.

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Time signals Sensor outputs observed as a function of time, e.g. speech. Such data may run continuously with out a clear start or end. If the signals are properly segmented, e.g. into words, objects can be aligned: at the same time sample the same phoneme is expected. Objects can thereby be compared as a function of time.

Spectra Unsegmented time signals can be transformed into spectra by a Fourier analysis. Time signals of different length may be compared by spectra over the same frequency interval. Examples are the recognition of types of earthquakes in seismics and speaker recognition from audio signals.

Images This is a very common data type. There are various subtypes. The pixel values can be binary, gray, RGB and even multi-band (more than three colors) and hyperspectral. In the latter case an entire spectrum per pixel is measured, like in remote sensing. As for the time signals, objects in images may be positioned on arbitrary places, or might be aligned after segmentation. In addition objects may have different sizes and may be really 2D or just 2D views of 3D objects.

Text For instance newspaper articles to be classified on topic, or letters to be classified on author.

Symbolic sequences Sequences of symbols, e.g. representing DNA structures or a series of events in an internet stream.

Graphs Complicated objects like an image of a building can be represented by a graph: connections between elements and their properties are used as attributes of nodes and edges.

In advanced applications combinations of such datatypes may arise, e.g. videos (images as a function of time, combined with sound). Sometimes one datatype is transformed into another, e.g. a time signal may be represented as a series of spectra over short time periods, a so-called spectrogram. This looks like an image, but **segmentation** might be needed to locate a specific event. Such an event may be represented by a some features like time length and the power of some specific features.

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Chapter 4

The PR system in operation

A completed pattern recognition system, as we want to design it, may look like shown in Figure 5. We will discuss the separate elements.

Object to be recognized This object, possibly an event is a part of the world outside the recognition system. It has an unknown class and it is the task of the system to derive this class from its observations. An example is the heart beat of patient that should be classified as normal/abnormal.

Sensor This can be a single sensor or a set of sensors. In our example it may consist of a few electrodes measuring the ECG (electrocardiogram) adjusted to the breast of the patient.

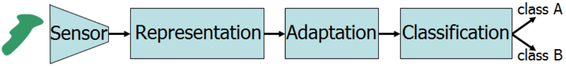

Figure 5: Pattern recognition system.

Representation The time signals retrieved from the electrodes cannot be directly used. By segmentation separate heart beats have to be isolated. Next they should be sampled in a standard way, e.g. every heart beat should be represented by 256 samples. In this way an object representation is realized suitable for the classification of heart beats.

Adaptation The 256 time samples should be adapted to the classifier found in designing the system. As such they might not yet characterize the differences between normal and abnormal heart beats sufficiently. Moreover, for some classifiers the number of 256 is too large. So in this step the initial representation is adapted to a final one that suits the final step. This may result into a few features.

Classification Finally, the classifier found during design, takes the features as an input and an optimized function maps the features found for a single heart beat to normal/abnormal. Sometimes a score between 0 and 1 is returned. They may also be combined over a series of heart beats.

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The two steps called here representation and adaptation are often combined into a single representation step. Often this step is called **feature extraction**. We split it here into two, to emphasize that there is a part that is entirely defined by the designer of the system, independent of the design set, and a part that is optimized by training the classifier. We will return on that later in chapter 6

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Chapter 5

PR system design

The design of a system as described in the previous chapter is based on two sources of knowledge. The expertise of the analyst as well as the application expert (often not the same person) is needed for various choices like the sensors and the initial signal processing. Also a gross list of possible useful and measurable features has to be created by these two persons.

The second source of knowledge is the **design set**: a set of objects, preferably drawn at random from the same source as the future objects to be classified. All or many of these objects should have a known **class label**: their true class memberships should be known. They are used for optimizing the representation (the adaptation of an initial representation to the demands of the classifier) and for classifier **training**. Training a classifier is also an optimization step, but often with a different criterion than the adaptation.

Usually the design set is stored for an initial representation, chosen on the basis of the background knowledge of the application. It may be randomly split into two

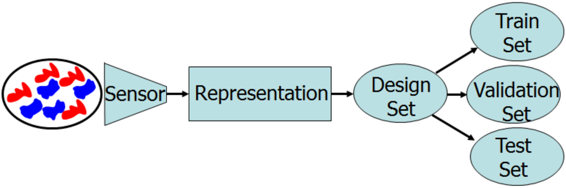

Figure 6: The design set is split at random into different subsets.

or three different sets:

Training set This is the set used for adapting the representation (if needed) and training the classifier. See Figure 6.

Validation set This set is only used for designing advanced systems or when one wants to validate the choice of an algorithm or classifier. See Figure 7.

Test set After optimizing the recognition system, its performance is estimated by a test set. See Figure 8.

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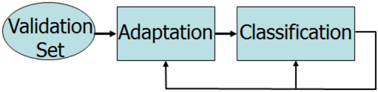

Figure 7: The validation set is used for optimizing choices for algorithms and classifiers.

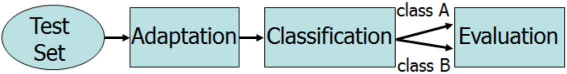

Figure 8: The test set is used for an evaluation of the final system.

Sometimes the training set is used for **validation** as well. These sets serve a similar task: optimizing the recognition system. It should be taken into account, however, that after training a classifier with a particular dataset, the performance measured on the basis of this set might be treacherously good. Using the training set for evaluation is in general a bad idea.

More often the test set is used for validation. Consequently the test set is used multiple times, e.g. for choosing an algorithm for adapting the representation to the classifier, for choosing a good classifier on the basis of their performances after training, and finally for reporting the performance of the entire system to the costumer or supervisor. This usage is very common, but formally wrong. Whenever a dataset has been used for performance estimation, followed by a change of the system in an attempt to improve it, this dataset has in fact been used for training. The resulting system is (somewhat) adapted to that dataset and consequently this dataset cannot be used anymore for an independent evaluation, see chapter 8.

The ultimate consequence of this reasoning is that a test set can only be used once. In practise this is usually prohibitive as the available dataset will be limited in size. System designers usually prefer to use all available data for optimizing the system and take it for granted that their final performance estimate is biased.

Chapter 6

Representation

6.1 Object representation

The task of the representation step is to make objects numerically comparable. If x and y are the representations of two objects then it should be possible to compute $d_{xy} = D(x, y)$ in which D is some distance measure and d_{xy} is a scalar reflecting the difference between x and y. For simple sensors or for an advanced definition of D no additional representation is needed. Otherwise, the sensor outputs have to be transformed into a representation for which distance functions are available. Some examples:

Graphs, a **structural representation** build by nodes and edges. An example is the graph representation of images by segments (nodes) with connections (the graph edges) to neighboring segments. The computation of graph distances is not trivial, especially not if the nodes or edges have attributes.

Symbolic sequence, a structural representation by a sequence of symbols, like text or a DNA sequence.

Sampled domain, like images and time signals. In order to compute distances between images or between time signals is it advantageous if they all have the same size.

Features, a set of relevant object properties. The same features have to be measured for all objects in order to make the comparable.

The structural representation will not be further discussed here. On the basis of computed distances between structures a so-called **dissimilarity representation** can be built, see below.

Objects given as images or time signals may need further processing before they can constitute a proper initial representation. Here are some possibilities:

Segmentation This is of interest for images and time signals. All pixels or time samples outside the domain of interest should be removed. After that the object representations have different sizes and

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cannot easily be compared directly. So segmentation is often followed by the computation of features of the segments.

Scaling For objects observed under possible different circumstances (e.g. light conditions) it is necessary to adjust the amplitudes properly. The best way to do this is application dependent. Possibilities are to multiply the entire signal such that their means or maxima are equal (e.g. divide by such a number by which it becomes one). Time signals like speech may be better normalized on their standard deviation (or mean amplitudes). For some sensors it is needed that minima (zero level) become equal.

Centering In case objects have some samples around them that do not belong to the objects themselves, they should be positioned such that they can be compared pixel wise (sample by sample). The best way to do this is by centering as the object borders are not always well defined.

Resampling Depending on the next steps it may be needed that objects are represented by the same numbers of samples.

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Rotation For many objects in images their rotation is not important for recognition. In order to make an efficient comparison a standard rotated view may be used. Sometimes it is needed to put restrictions to such a rotation, e.g. to avoid that de digits '6' and '9' become equal.

Normalization All the above and possible others are sometimes referred to as object normalization.

Object properties that are not relevant for class differences are named **invariants**. Examples may be position in an image or size. In the design of a pattern recognition system they should be removed if possible. During training of a recognition system the insignificance of such properties may be discovered automatically, but this requires a training set that is sufficiently large. It is thereby more efficient to remove them. The above normalization steps may take care of some of them.

6.2 Vector representations

A very common, almost 'standard' representation is the vector space. All objects are represented by vectors having the same length and using the same set of properties as their elements. The scatter plot in Figure 3 is an example of a 2-dimensional vector representation. Usually vector spaces have higher dimensionality, from tens to possibly over 1000.

The popularity of the **vector representation** is caused by the availability of many tools for analyzing sets of vectors. Classes may be studied by computing their densities, estimated from the training set. Classifiers in a k-dimensional vector space are (k-1)-dimensional linear or nonlinear surfaces separating class regions in the space. The data (sets of objects) may be found to lie (which sufficient accuracy) in a linear or nonlinear subspace of possibly much lower dimensionality, from which it can be concluded that the relevant features describing the object variability are a (non)linear function of the used object properties.

Multi-variate statistics, linear vector algebra and matrix manipulation are important tools to study vector representations. We will summarize three ways to arrive at such a representation.

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Feature representation The space built by the possibly relevant object properties is called the feature space. They may be derived from images or time signals according to some preprocessing, but they may also be measured directly by a dedicated sensor, e.g. a temperature. As features can be based on entirely different physical phenomena, their scaling may be different as well. Normalizing their variabilities as discussed in section 6.1 may be needed to avoid not-intended build-in preferences for some features.

It should be emphasized that the feature representation is reducing: some object differences are not taken into account. Consequently different objects can have the same representations in the feature space. If this happens for objects of different classes, the classes overlap. Classifiers may then be built on the basis of class density estimators.

Pixel representation In case it is not clear what features should be defined, one may try to sample the images or time signals by which the objects are given. The normalization steps discussed in section 6.1 are now relevant. In particular it is necessary that all object representations have the same size in pixels or samples. Moreover, alignment by shifting and rotation may be needed as well.

If the images of all objects have the same number of pixels, an image, and thereby the objects, can be represented in a vector space. It has as many dimensions as the image has pixels. An example is the MNIST dataset, a heavily used benchmark consisting of 70000 images of 28x28 pixels. These are gray value images. The pixel representation is thereby 784. If color (RGB) images are used like this, the dimensionality would be three times larger.

Instead of images, samplings of time signals or spectra may be used in the same fashion. In these cases time samples or frequency amplitudes are used instead of pixel intensities to build the vector space. Spectra are usually already automatically aligned (same frequencies have the same meaning). They thereby constitute a more simple example of a pixel representation than images. (Although time samples and frequencies are not pixels, still 'pixel representation' is sometimes used for lack of something better).

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In case objects are entirely defined by their image (e.g. 2D objects) or time signal (e.g. speech), an automatic recognition system gets the same information as a human observer. It may thereby reach the same or even a better performance. If human recognition is error free, or class labels are assigned in a consistent way by the human expert, classes will not overlap in a **pixel space**.

Dissimilarity representation The good aspect of the pixel representation is that any, by the sensors observed object change, is reflected in the representation. A severe drawback is that neighboring pixels are expected to be highly correlated. In the representation, however, their relation is similar to the relation of two remote pixels. The entire object is teared into pieces, which are used independently for representation. Neighborhood relations are lost.

The **dissimilarity representation** tries to do both, be sensitive for all object differences, but treat neighboring pixels different than remote pixels. The application expert is asked to design a **dissimilarity** measure $d_{xy} = D(x, y)$ between objects such that this is realized. Examples are the Hausdorff distance between shapes and the

Earthmover distance between spectra. Next a set of prototype objects $P = p_i, i = 1, \ldots, k$ has to be defined, called the **representation set**. Any object x is now represented by a vector of distances $\mathbf{d}$ to the representation set: $\mathbf{d} = (D(x, p_1), \ldots, D(x, p$ This constitutes the **dissimilarity space**.

Any distance measure between objects can be used for this representation. Preferably they should have the above discussed properties. Other choices appear sometimes to perform surprisingly well, including the Euclidean distance in feature spaces and pixel spaces. An explanation for this is that such a dissimilarity space is a nonlinear transformation of the original space. Consequently, simple linear classifiers in the dissimilarity space correspond to non-linear classifiers in the original representation space. The non-linearity used for this is not arbitrary, but is in some way natural for the given original representation.

There is another way than the dissimilarity space to arrive at a vector space from dissimilarities. That is **embedding**: finding a vector space in which the distances are equal to the given dissimilarities. In general such a space is non-Euclidean as it cannot always be based on an **Euclidean**

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geometry. In such cases it cannot easily be used for generalization.

The **feature space** is traditionally the main representation. The vector spaces resulting from the pixel representation and the dissimilarity representation are formally not feature spaces as their bases are just indirectly constituted by object properties. It is very common, however, to use "feature space" in referring to a pixel space or a dissimilarity space.

6.3 Dimension reduction

Generalization procedures like classifiers sometimes heavily focus on their performance on the training set. If this set is small in relation to the dimensionality of the feature space they may **overtrain**, i.e. they adapt more to the local noise than to the global class differences as a result of the **curse of dimensionality**. To avoid this, separate **dimension reduction** procedures are used. There are two different approaches:

Feature extraction finds combinations (often linear) of the given features such that the **class separa-**

bility is maintained as good as possible. Criteria are usually not classification performance (as this will introduce overtraining again), but general measures of the preserved information content.

Feature selection is more restrictive as it selects features instead of searching for good combinations. Selection may be preferred over extraction as the final feature representation is here in terms of a reduced set of original features. This may give more insight in what is important for recognition. Moreover, sensors related to not-selected features may be removed.

Note that by both approaches a subspace of the original feature space is found. Class separability will reduce or, at best, remain equal. It is impossible that it will increase. However, classifiers may have a more easy job by which the final performance increases.

The most important algorithms for reduction and selection are:

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Principal Component Analysis (PCA) is an unsupervised approach (not using class labels of the training set) for linear feature extraction. It maximizes the explained variance.

Linear Discriminant Analysis (LDA), also named Fisher Mapping, is a **supervised approach** (using class labels of the training set) for linear feature extraction. It maximizes the **between scatter** (differences in class means) over the **within scatter** (object differences within a class, averaged over the classes).

Individual selection takes the best features according to their individual performance.

Forward selection starts with the best single feature and extends the selection iteratively with the feature that maximizes the performance of the selected set.

Backward selection starts with all features and reduces the selection iteratively with the feature that least reduces the performance of the selected set.

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There are more advanced selection algorithms like **branch and bound** and **floating search**. They only make sense for large training sets as extended searches bear the danger of overtraining. Moreover, they are very time consuming. Also the backward selection, mentioned above, has to be treated with care as it starts with measuring the performance of all features. This is already tricky when feature selection is done because of a too large dimensionality of the space.

If one has a much too large feature set w.r.t. the training set size, e.g. 1000 to be reduced to 10, a feasible approach might be:

1. Select by individual selection 50 features.
2. Select by forward selection 20 out of these 50.
3. Select by backward selection 10 out of 20.

Several criteria are possible in feature selection. They can be divided in filter and wrapper approaches. In **filter** approaches a global separability criterion is used like the Mahalanobis distance. This is comparable to LDA in feature extraction.

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In the **wrapper** approach a classifier is used and its performance used as a criterion. As training has to be repeated for all steps this can be very time consuming. Moreover, it is needed to have a separate test set for measuring the performance. Even more advanced and time consuming is to do cross-validation, see section 8.1. Although wrapper approaches are popular in the literature, there is again the danger of overtraining caused by the repeated use of a test set. It may be used thousands of times and starts thereby to become a training set.

For the selection and optimization of representations various criteria are used, but there is no such thing as a 'ground truth'. However, at the end a representation is as good as the generalization that can be based on it. We discuss here no specific procedures for the evaluation of representations and just refer to the evaluation chapter 8.

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Chapter 7

Generalization

7.1 Class models or decision functions

Once we have a proper representation, it can be used for **learning from examples** procedures. Such procedure estimates an unknown property of an object given a set of example objects for which the property is known. This is also called **generalization**. It is based on the assumption that some properties are heavily dependent on others. Thereby it is not needed to observe them directly. They can be indirectly determined from other observations.

In PR generalization is mainly used to find the class of an object. This is particulary of interest when there is no measurement possible that reveals the class and only a human expert is able to name it. For example, there is no *single* measurable property that determines that a chair is a chair. It can only be established in an automatic way from a *set* of measurable properties. A set of examples of known chairs, collected by a human expert, in this context often called the **teacher**, has to be used for **training** a generalization algorithm, e.g. a **classifier**. This results into a **trained classifier** which is a function of measurable properties. Depending on the outcome of this function a new object may be classified as a chair.

Here some ways will be discussed to find classifiers for objects represented in a vector space. Such a classifier determines from the set of labeled object examples, the **training set**, for every other point in the vector space what its label might be. (A **labeled object** is an object with known class membership). The output of a classifier might be a unique **crisp label**, a set of possible labels, or for all or the main classes a confidence.

A classification **confidence** is a number between 0 and 1. The larger the more likely the related class. As an extreme objects are sometimes **rejected**. This implies that for the supplied representation vector of the object to be classified not sufficient information is available to make any sensible decision. Most classifiers don't have an explicit reject option, but from thresholds on confidences rejects may be decided.

There are two opposite approaches from which classifiers can be built.

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Class models For each class a model is build using objects of that class only, usually a probability density function. The procedures for the **estimation of density functions** can be distinguished in parametric and non-parametric approaches. By **parametric estimation** the parameters of some standard function are estimated, e.g. the mean and **covariance matrix** a **normal distribution**(also called **Gaussian distribution**). **Non-parametric estimators**, like the **Parzen** density estimator, replace every sample by elementary function, also called kernel, and average them.

As a result of the density estimation for every point in the vector space a distance or a confidence for that class will be found, independent of possible other classes. So this is a class-by-class approach. The advantage of this approach is that if classes have known **prior probabilities** (class frequencies of objects to be classified), these can be used to weight the models.

Decision functions In this case objects of different classes are used simultaneously for a direct estimate of the decision function between the classes. Decision functions often act between two classes or between groups of classes (so called **binary**

classification problems). In case of more than two classes (**multi-class classification problems**) they can be used in two fashions: **one-against-one** and **one-against-rest**. In the first case classifiers are found for all pairs of classes. In the second each classifier tries to separate a single class form all other. In both cases a second level of decision making has to be defined for a final classification.

Some decision functions, e.g. the ones based on neural networks, directly implement a multi-class classifier.

The advantage of the decision function approach is that just is estimated what is needed. Directly training a decision function is more efficient than the detour over estimating full class models. A disadvantage is that the use of class prior probabilities is for this approach difficult, tricky or impossible.

7.2 Classifiers

Here the most important classifiers are shortly summarized.

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Template matching A few representative objects (**prototypes**) are selected by the teacher, at least one per class. Classification is done by assigning the class of the nearest to the object to be classified.

Nearest mean This is like template matching. There is now a single prototype per class which is defined as the mean of all training objects available for that class.

1-Nearest neighbor This is also like template matching, but now all available training objects are used as prototypes.

Fisher classifier This is a two-class classifier (discriminant). It is defined as the plane perpendicular to the direction in feature space that maximizes the between scatter over the within scatter, see LDA. It is also known as **Fisher's Linear Discriminant** (FLD). In case of equal class priors it is almost identical to the Bayes normal classifier assuming equal covariances.

Bayes classifier This classifier selects the class with the highest **posterior probability**, determined by the class densities and the class priors. This is the minimum error classifier (the error it realizes

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is sometimes called **Bayes error**). Usually densities are unknown and should be estimated. See Bayes normal and Parzen below.

Bayes normal The **Bayes classifier** assuming normal distributions for all classes. If the class covariance matrices are assumed to be equal the classifier is linear (almost identical to **LDA**), otherwise quadratic (**QDA**).

Parzen classifier The **Parzen classifier** is a Bayes classifier using a **kernel** density estimator for the class distributions. Depending on the implementation the same or different kernels are used for the classes. The choice of the kernel function is usually a spherical normal distribution. Its width should be optimized or chosen by the teacher.

k-Nearest neighbor (*k*NN) The *k*-Nearest neighbor classifier selects the majority class of the *k*-nearest neighbors in the training set.

Naive Bayes This is another Bayes classifier based on estimated densities, now assuming independent features. Thereby class densities are estimated by multiplying feature density estimates. The latter can be based on histograms, Parzen densities, normal distributions, etcetera.

Decision tree Usually a binary decision tree is used in which the nodes are single featurethresholds. During training for every node the next best featureis selected for the part of the training set that arrives in the given node. There are various criteria and stopping strategies.

Neural network Originally neural networks are studied as a simulation of the human nervous system. Later they are used as well for building artificial recognition systems. This resulted in a large set of architectures with very different properties. Consequently, the performance of a neural network classifier heavily depends on the choices made by the analyst, and thereby on his skills. The main properties of neural network classifiers are that they can be trained by very large datasets, training is computationally demanding, the classification function is usually nonlinear and results can be reasonably good.

Support vector machine (SVM) The SVM is in the research communities of machine learning and pattern recognition a very frequently applied and studied classifier. It is based on a solid theoretical foundation called Empirical Risk Minimization (ERM) which aims to maximize the distances of the training objects to the classifier. Originally it is designed for linear decision functions, but by the use of **kernels** and the so-called **kernel trick** also non-linear functions can be computed.

Adaboost This classifier is based on combining a large set of simple, usually linear, **weak classifiers**, resulting in a complex, nonlinear architecture. Iteratively additional base classifiers are added emphasizing difficult (often erroneously classified) objects in the training set. (A **base classifier** is one of the constituting classifiers in a combined classifier)

Random decision forest Also this classifier combines many simple base base classifiers, in this case decision trees with just a few nodes based on randomly selected features.

The bottom five classifiers in the above list have many adjustable parameters to be set by the user. Finding the best values is challenging. A well known approach is a so-called **grid search**: systematically a large set of parameter combinations is evaluated, often by cross-validation. There is a high risk of overtraining.

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Chapter 8

Evaluation

Evaluation is an essential aspect of the design of pattern recognition systems. Every choice, every training step, as well as the overall set-up are guided by expectations resulting from past experience or estimates of the realized **accuracy**. Without evaluation there is no learning. It is thereby crucial to have proper procedures, but also to be aware of the general behavior of the performance as a function of training set size and dimensionality.

In the next sections short reviews are given of **error estimation** procedures, section 8.1, the error as a function of the size of the training set (learning curves), section 8.2, and the dimensionality (feature curves), section 8.3. Finally some general considerations and guidelines for the accuracy are presented, section 8.4.

8.1 Error estimation

The **classification error** can be estimated by counting the number of erroneous classifications made in a set of objects with known true class labels (a **test set**). This set should be representative for the future objects to be classified. Usually this is realized by random sampling. The objects are thereby i.i.d. (independent and identically distributed) random variables. The fraction of errors, the **test error**, is in that case an unbiased estimate of the expected classification error.

This error estimation procedure (**testing**) can be performed over the set of classes or class-by-class and weighted with the probabilities of encountering objects of a particular class, the **class priors**. This should be done when the **class frequencies** in the available set of objects are different from the known, true class prior probabilities.

The objects in the **training set** are not independent from the classifier to be tested. Formally they should not be used. It is expected the they will result in an optimistically biased error estimate. However, the training set error, also called **apparent error** or **resubstitution error**, can be informative in comparison with the **true error** (the error for an infinite independent test set), estimated by the available test set. The difference is a measure for the bias, and thereby for **overtraining**. The larger, the more the classifier has been adapted to the noise in the training set, instead of the class differences.

An independent **test set** is needed for an unbiased estimate of the true classification error. To get its variance as small as possible the size of the test set should be as large as possible. Larger test sets, however, will result in smaller **training sets**, as they are subsets of the same design set. This results in worse classifiers. Thereby, there is a trade-off between very accurate estimates of the performance of a bad classifier (large test sets, small training sets), and inaccurate estimates of the performance of a good classifier (small test sets, large training sets).

A common compromise for the above dilemma is a 50-50 split of the **design set** in equal parts for training sets and for testing. The final classifier, delivered to the customer, will be trained on the entire design set. The performance of a classifier trained by a dataset half of this size will not be very much worse. This is the **hold-out error**, which is slightly pessimistic.

The roles of test set and training set in a 50-50 split may be reversed and the results averaged. This is called 2-fold **cross-validation**. The entire design set participates in testing by which the variance in the resulting estimate in comparison with the hold-out procedure is reduced. It is, however, equally pessimistic as it estimates an error of a classifier that is trained by just 50% of the data used for the final classifier.

Instead of 2-fold cross-validation also **n-fold cross-validation** can be used by a rotation procedure. In this approach n classifiers are trained by a fraction of $(n-1)/n$ of the design set and tested by the remaining objects, a fraction of $1/n$ of the design set. Again, all objects are used for testing, but they test classifiers that are very close to the final classifier. They are more similar to each other as well as to the final classifier for larger values of n. The variance is thereby smaller (classifiers are more equal) and the estimate is even less pessimistic. The cost of this procedure is that training times are increased by a factor of n. Common choices for n are $n = 5$ and $n = 10$.

The n classifiers, based on random subsets of a $(n-1)/n$ fraction of the design set, are all somewhat different. A repetition of the cross-validation will generate another set of n classifiers. Averaging the performances of a number (e.g. 10) of **repeated n-fold cross-validations** will yield a somewhat more accurate estimate the classification error. The variance in the performance results can be used to test whether differences between classifiers are significant.

A special case is the **leave-one-out cross-validation** (**LOO**). It uses as many folds as the size of the design set. Every classifier is trained by all-but-one objects in the design set and is tested by just the single object that was left out. In this case makes no sense as it would generate the same result. The tested classifiers are all almost equal to the final one. Consequently the estimated error, usually called the **LOO-error** has a minimum pessimistic bias.

8.2 Learning curves

Here we discuss why plotting and analyzing learning curves may reveal some interesting characteristics of classifiers. A **learning curve** shows the performance or classification error of a classifier as a function of the size of the training set. As the error has to be estimated from an independent test set it can not be studied up to the size of the design set.

In Figure 9 on example is given based on the Iris dataset, a 3-class dataset (different types of the Iris flower) with 50 objects per class, given by 4 features. Random sub-

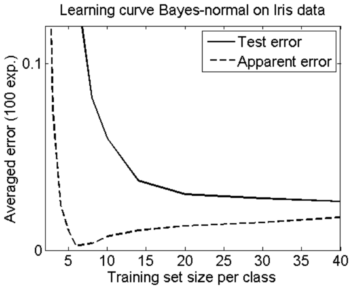

Figure 9: Learning curve of Bayes Normal for the Iris dataset. The error curve for the test set is shown as well (apparent error).

sets of 2-40 objects per class are used for training, the remaining ones for testing. This is repeated 100 times to get smooth results.

The plot shows the averaged estimates of the error on the test set as well as on the training set, the so called apparent error. The test error approaches some asymptotic value. It can be observed that this value has not been reached yet as the curve still goes down. Enlarging the dataset is thereby expected to yield better results.

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The apparent error reaches a minimum for 6 training objects per class. For less objects no proper normal distributionscan be estimated. For increasing sample sizes after 6 objects per class the classifier better and better generalizes as the estimated distributions approach the real distributions. It is expected that the two curves approach the same asymptotic value. The test error from above, the apparent error from below.. The difference between the two errors can be understood as the amount of overtraining. It is caused by the adaptationadaptation of the classifier to the noise in the data (caused by small datasets) instead of to the true class

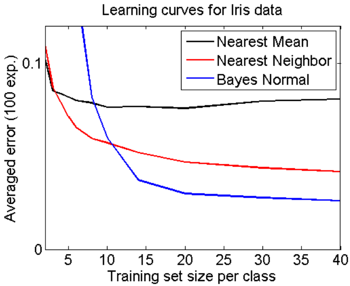

Figure 10: Learning curves for the Iris dataset.

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distributions.

In Figure 10 the learning curves for three classifiers are shown. The differ in complexity. A general tendency of such curves is that low-complexity classifiers do relatively well for small training sets, while that high-complexity classifiers need large training sets. It can be seen that the most simple classifier, the nearest mean, shows a reasonable performance for just a few training objects, while the most complex classifier, Bayes Normal, at moment suffers from the noise in the data. Because of its complexity it is sensitive for noise, but for large training sets its sensitivity can well be used to shape a good decision function.

This scissor phenomenon is very characteristic for classifiers with a different complexity. It shows that there is no unique best classifier for some problems, but that it depends on the size of the training set.

8.3 Feature curves

The behavior of the classifier performance as a function of the dimensionality is significant for selecting features and their number. **Feature curves** show an estimate of the true classification error as a function of the number of features. In Figure 11 and Figure 12 some example are given based on the Bayes normal classifier.

For classifiers trained by a small training set, feature curves may show a minimum for a low number of features. This shows **overtraining** for larger dimensionalities, see the sections on dimension reduction 6.3 and error estimations 8.1. The larger the training set, the more features can be used.

The result depends on the order of the features. In Figure 11 the features are ranked according to a forward selection procedure based on the **Mahalanobis distance**. In Figure 12 features are randomly ordered. The dataset has 36 features of which most are uninformative. Consequently, in a random order many uninformative features may be used in the beginning. After 8 features it is almost sure that the most significant features (or very similar copies) are included.

8.4 Accuracy guidelines

8.4.1 The number of features.

From the discussions on the evaluation in chapter 8 it is clear that there is a relation between training set size and feature size: the more features are added, the larger the training set should be to obtain a similar accuracy for the trained result. This holds for the increasing number of parameters involved in the classifier. The added features, however, might be informative, so in spite of the increasing noise in the parameter estimates, the classifier error may still decrease. The optimal number of features for a given size of the training set thereby depends on the separability added by the new features. The sensitivity for the noise in the data also depends on the characteristics of the chosen classifier.

Consequently, there is no general rule for the number of features, unless their distribution, the size of the training set and the chosen classifier are specified.

8.4.2 The size of the training set

By studying the learning curves it can be concluded that in expectation the more training objects the better, but that at some moment this will hardly help for the given representation and classifier. When the apparent error is close the test error the asymptotic value is reached. As the asymptotic behavior is exponential a very rough rule of thumb is that by doubling the training set size not more will be gained in accuracy than the difference with the error at half the present size.

Classifiers that are based on covariances need at least more objects than features for estimating a non-singular matrix that can be inverted, otherwise a proper **regularization** is needed. Classifiers that are based on density estimation need to fill the space. As a rule of thumb it is sometimes stated that training sets of 5-10 times the dimensionality are needed. This holds per class as the densities are computed class-wise. However, it appears that with some some regularization for much less samples reasonable results may be obtained.

8.4.3 The size of the test set

Here clear answers are possible. If one estimates an error with true value ϵ, based on an independent randomly selected (i.i.d) test set of size n, then the standard deviation of the estimate is $\sqrt{\epsilon \times (1-\epsilon)/n}$. If one likes to have this smaller than (e.g.) 0.1ϵ it directly follows for small ϵ that $n > 100/\epsilon$.

This result is for some problems shocking. In case $\epsilon = 0.1$ a test set of size $n = 1000$ is needed to estimate the error with a standard deviation of 0.01. This result in a 95% confidence interval of about $0.08 < \epsilon < 0.12$, which is not very accurate. A test set of 1000 objects, however, is for many applications very large.

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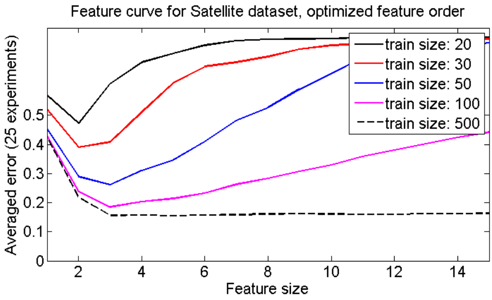

Figure 11: Satellite dataset feature curves, optimized order.

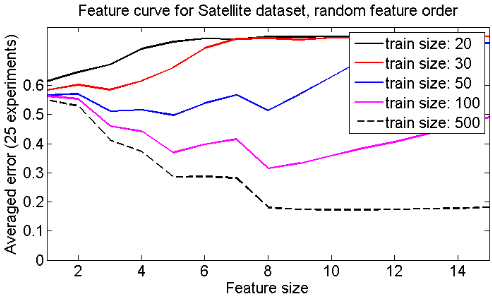

Figure 12: Satellite dataset feature curves, random order.

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Chapter 9

Exploratory data analysis

The final target of pattern recognition is to design a system that, by the two steps of representation and generalization, is able to correctly classify new objects with a sufficient accuracy. There are well defined evaluation tools to predict or measure the obtained performance. In its design, however, some additional knowledge of the data characteristics may be helpful to select and adjust the appropriate procedure. In this chapter some approaches are discussed that may be helpful for this.

9.1 Cluster analysis

In **cluster analysis** a grouping of the objects is studied without using class information supplied by the teacher. It is thereby an **unsupervised learning** technique (like PCA). The target is to find **clusters**: subgroups of similar objects in a given set of objects. We consider two types of representations, vector spaces and dissimilarities.

Generalization is not necessarily the target of cluster analysis. However, it may be followed by the computation of a classifier to assign new objects to one of the detected clusters. Here we will restrain to possible **clustering** procedures.

Like for classification, distances and densities play an important role in the design of clustering procedures. There are three kinds of approaches. For each of them the main algorithms will be shortly characterized.

9.1.1 Hierarchical techniques

These are characterized by the construction of a hierarchy of clusters. On the lowest level every object is defined as a separate cluster. On every level above that the two nearest clusters are merged, until in the top level all objects are collected into a single cluster. The various techniques differ in the way the distance between two clusters is defined. The three main distance definitions are:

Single linkage: the distance between two clusters is the minimum distance between any two objects of the two clusters.

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Complete linkage: the distance between two clusters is the maximum distance between any two objects of the two clusters.

Average linkage: the distance between two clusters is the average distance of all distances between two objects of the two clusters. This is different but might be similar as the distance between the cluster means of the objects are given by a vector representation.

These approaches can be used for objects given by a dissimilarity representation as well as by a vector representation. In the latter case object distances are usually defined by the Euclidean metric.

The entire hierarchy can be represented by a **dendrogram**: a graph tree in which every node represents the merge of two clusters and the size of the edges is determined by the distance between the corresponding clusters. The dendrogram is used to determine an appropriate cluster level and to find outlier objects that do not belong to any cluster. This post-analysis determines the number of clusters that is found.

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9.1.2 Partitional techniques

These techniques are based on a desired number of clusters. They start from some initial clustering, which might be random. In an iterative procedure the clustering is implicitly or explicitly optimized according to some procedure. Some well known algorithms are:

k-Means: In every iteration a new clustering is defined by assigning all objects to the nearest cluster mean derived from the previous clustering.

k-Centers: This is also called k-Medians. In every iteration a new clustering is defined by assigning all objects to the nearest cluster center derived from the previous clustering. The centra of a cluster is the object in the cluster for which the distance to the most remote object in the cluster is minimum.

EM clustering: Expectation-Maximization clustering. This is in fact a generalization of the above procedures. In every iteration a new clustering is defined by assigning all objects to the cluster to which it fits best according to a model describing the clusters. These models are derived from the previous clustering. A well known option

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for these models is the normal distributions. In PRTools an arbitrary classifier can be used.

9.1.3 Mode seeking

In the mode seeking strategy clusters correspond to the modes (local maxima) of the density function. Objects are assigned to the cluster of the mode that is found by following the density gradient upwards. The two main procedures are based on the non-parametric density estimates based on kernels and nearest neighbors. In both cases there is width parameter that influences the smoothness of the density estimate and thereby the number of modes and the number of clusters.

Mean shift: This procedure is based on Parzen density estimates. The modes are found by following the gradient from a number of start points (objects). This is time consuming and mainly feasible in for lower dimensional vector spaces.

k-NN mode seeking: In the k-NN approach densities are related to the distance to the k-th neighbor. Pointers are set from all objects to the object with the highest density in their neighborhood.

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Following pointers is fast and modes are uniquely defined (objects that point to themselves).

The mean shift algorithm requires less objects than k-NN mode seeking and is frequently used for color image segmentation. k-NN mode seeking has no restrictions for the dimensionality and can be applied to very large datasets by two steps in which the distances of all objects to all other objects have to be computed.

9.2 Visualization

Visualization tools may give the analyst some insight into the set of objects under study. This can be helpful to select an appropriate strategy for representation or generalization. Here three types of tools are shortly summarizes,

9.2.1 Scatterplots

Multi-dimensional data can be visualized by 2D or pseudo-3D projections. It has to be realized that if the intrinsic dimension is high many objects may be shown close to each other in the projection, but that have very large

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distances. Three well-known techniques for linear projection are:

PCA: Principal component analysis finds, by an **eigenvalue decomposition** of the covariance matrix, the linear subspace that shows the largest variances.

LDA: Linear discriminant analysis or Fisher mapping shows the subspace in which the between scatter (the variances of the class means) is optimized with respect to the within scatter (the variances within the classes).

KLT: Karhunen-Loeve transform is sometimes used as an alternative name for PCA. Sometimes it is distinguished from that by computing an eigenvalue decomposition of the average of the class covariance matrices. It thereby computes the linear subspace that shows the largest within scatter.

It is likely that in high-dimensional datasets objects are in a lower-dimensional non-linear subspace. Three popular techniques for finding nonlinear mappings are:

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MDS: Multi-dimensional scaling is a general, classical procedure that aims to create a low-dimensional vector subspace in which the objects are positioned such that some measure for the difference between the original and realized distances (called the stress) is minimized.

KPCA Kernel PCA. This is a kernelized version of PCA. The non-linearity is determined by the choice of the kernel.

tSNE A recent procedure called t-distributed stochastic neighbor embedding. Like the other procedures similar objects are modeled by nearby points and dissimilar objects are modeled by distant points in the scatter plot. In this case there is, however, a high emphasis on the first. The criterion used here is to minimize the Kullback-Leibler divergence between the original and realized distributions of objects distances.

9.2.2 Graph trees

Somewhat more general than a scatter plot of a (non-linear) subspace is to show relations between objects is a **graph**. The nodes are the objects and the edges show something of their relations. A **graph tree** is an undirected graph in which any two nodes are connected by exactly one path. Some examples:

Decision tree: This is a visual representation of the **Decision Tree classifier** mentioned in section 7.2. Every node is based on a subset of the original training set. The top node contains the entire set. At every node the subset is split (using some simple classifier, often a threshold on a feature) into some subsets. When the subsets are (sufficiently) homogeneous the node is not split further and a class label is assigned to such an end node. An original vector representation is hereby implicitly split into a number of cells containing (almost entirely) training objects of the same class.

Dendrogram: A **dendrogram** shows by a graph tree the result of a hierarchical clustering. The structure is similar to the decision tree. A top node contains all objects. The end nodes are the basic clusters or the individual objects. The edges combine the nodes hierarchically.

MST In a Minimum Spanning Tree all objects are a node and the edges represent their distances. The spanning of such a graph tree is the sum of all distances that are represented by an edge. The MST is the tree with the minimum spanning. It is the result of the single linkage hierarchical clustering is by that procedure sequentially the clusters of the two most neighboring objects in different clusters are connected.

9.2.3 Curves

Various function can be plotted to characterize some properties of a (labeled) dataset. Here are some of the main ones.

Eigenspectra: The spectrum of a covariance matrix is the set of its eigenvalues. With the not so often used word **eigenspectrum** we point to the curve that plots the ranked eigenvalues. It shows graphically how many eigenvectors are significant, which is the dimensionality of the linear subspace in which most of the variability is concentrated. The cumulative eigenspectrum may show this even more clearly, e.g. for what dimensionality 95% of the total variance (the sum of all eigenvalues) is reached.

Density plots: Plots of a two-dimensional probability density distribution can be shown by equal-density curves in a scatter plot. The density plot of a single feature is usually shown as a function (the density) along a feature axis. Multiple curves in the same plot may be used to study densities of different classes, showing the class separability of that feature.

Learning curves: These show some performance measure (e.g. the classification error) as a function of the size of the training set, see section 8.2.

Feature curves: These show some performance measure (e.g. the classification error) as a function of the dimensionality, see section 8.3.

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Chapter 10

Glossary

This chapter summarizes the terminology as it is used in the previous chapters. Some additional terms are included as well. Almost all occurrences of the terms in the book, including the ones in this chapter, are linked to the corresponding glossary entry. The headings of the glossary entry are linked backward to the most significant place in the main text.

At the end the description of every glossary entry backward links are provided to pages, chapters and sections. In addition, external links are given to papers, Wikipedia entries, tutorials, video's and other internet locations. A browser is needed to support this. For a number of entries, also links are supplied to Matlab examples written by PRTools.

Adaboost An advanced combined classifier based on sequentially generating a large set of weak classifiers emphasizing training objects that are often incorrectly classified by one of these (boosting). page-54 wiki tutorial paper video example

Adaptation This is not a specific pattern recognition term. It is used here for the step by which the representation is optimized for the generalization, e.g. for classification. page-18 page-27

Apparent error Also called resubstitution error or training error. It is the fraction of objects used for designing (training) a classifier that is incorrectly classified by that classifier. It is usually a positively biased estimator of the true classification error. page-56 example

Attribute A symbolic or numeric property of an object that might be useful to determine its class. The word feature is used for this as well. Different objects however may have different numbers of attributes. Usually, the same set of features is measured for all objects in a single problem. Thereby, objects can be represented by a feature vector, or by a set of attributes. page-19

Backward search See backward selection.

Backward selection The selection of features or prototypes on the basis of the performance decrease after removal from an already selected set. The selection is usually started with a large set of best performing individuals, or with the entire available set. See also feature selection. page-44 example example

Base classifier One of the constituting classifiers in a combined classifier like adaboost or a random forest. See also ensemble classifier. example

Bayes classifier This is a classifier based on the Bayes rule. It combines given class prior probabilities $P(\omega)$ with class probability densities $P(x|\omega)$ for the object vector representation x such that the classification error ϵ is minimum under the assumption that these probabilities and densities hold for the objects to be classified. If this assumption is violated (e.g. by using bad density estimates) the classifier may be far from optimal.

For a two-class problem with $\omega \in A, B$ this classifier can be written as:

$$S(x) = P(x|A)P(A) - P(x|B)P(B),$$
$$\text{if } S(x) > 0 \text{ then } A \text{ else } B$$

For a multi-class problem with classes $\omega \in \Omega$ the classifier a more general formulation is:

$$\hat{\omega}(x) = \text{argmax}_{\omega \in \Omega}\{P(x|\omega)P(\omega)P(x)\}$$

.

As the denominator $P(x)$ does not depend on ω, it can be omitted. The rule thereby simplifies to:

$$\hat{\omega}(x) = \text{argmax}_{\omega \in \Omega}\{P(x|\omega)P(\omega)\}$$

page-51 wiki example

Bayes normal classifier The Bayes classifier using density estimates based on the training set assuming normal distributions. The result is either a quadratic classifier (different covariance matrices), also named QDA, or a linear classifier (equal covariance matrices), also named LDA. page-52 tutorial example

Bayes error The classification error made by the Bayes classifier for the case its assumptions are correct. By definition this is the lowest classification error that can be achieved for the given problem.page-51 tutorial wiki example

Bayes rule For a class ω and an object representation vector x, this rule relates the class posterior probability $P(\omega|x)$ with the class probability density $P(\omega|x)$, the class prior probability $P(\omega)$ and the joint probability density function $P(x)$ over the

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set of classes:

$$P(\omega|x) = \frac{P(x|\omega)P(\omega)}{P(x)} = \frac{P(x|\omega)P(\omega)}{\sum_{\omega \in \Omega} P(x,\omega)}$$

tutorial video wiki wiki

Between scatter The estimated variance or covariance of the means of a collection of sets of data points. It is thereby the scatter of the set means. The averaged scatter of the sets is called the the within scatter. The two scatters constitute together the scatter of the combined sets. page-44 paper paper wiki

Binary classification A classification problem in which a discriminant between two classes has to be found. page-49

Boosting Training classifiers by emphasizing the objects that are likely to be misclassified. It is specifically used in training ensemble classifiers, e.g. by the adaboost algorithm. video wiki

Branch and bound The optimization of some selection (e.g of features or prototypes) on the basis of a monotonic criterion, based on backward selection. The branch and bound algorithm minimizes the search tree by using the monotonicity. See also feature selection. page-45 paper wiki

Class A class is a set of objects that within a given context is recognized as similar. Such a class has usually a unique name, the class name. The individual objects within a class have a label that refers to this name. If the class is human defined it is sometimes also called a concept. page-19

Class frequency The frequency of which objects of a particular class in a dataset. It can be used as an estimate for the class prior in case the dataset is representative for the classification problem. page-56

Class label A pointer assigned to an object that refers to its class or class name. Note the inconsistency in terminology: an object label is the same pointer, from an object to a class. page-19

Class membership The class to which a class label points, in case of crisp labels, or the value(s) of the soft labels. page-15

Class name A name assigned to a class of objects. Sometimes very symbolic like A or B, sometimes

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with a very practical meaning like 'healthy' or 'diseased'.

Class separability Some general measure related to the possible classification performance given an object representation and a training set. page-42 tutorial

Class posterior The probability $P(\omega|x)$ of a particular class ω for a given object x. The difference with the class prior is that the posterior probability depends on the observed object. See also confidence. page-51 paper

Class prior The probability $P(\omega)$ that an arbitrary object belongs to class ω. The difference with the class posterior is that the prior is independent of an observed object. page-56

Classification The assignment of a class (in fact a class name) to an object by evaluating a trained classifier for that object. page-21 page-27 paper tutorial wiki

Classification accuracy This is one minus the classification error. Sometimes, the accuracy is also multiplied by 100 and presented as a percentage. See also classification performance. page-55

Classification error The probability that an arbitrarily selected object from a set of classes is incorrectly classified by a given trained classifiers. Alternatively it is used for the fraction of objects of a given finite set of objects that is incorrectly classified. See also apparent error (or training error), test error and true error. Sometimes, this error is also multiplied by 100 and presented in percentage. page-55 section 8.1 paper example

Classification performance A general expression referring to how well a classifier classifies unseen objects. There is no sharp mathematical definition of the performance. In general, the higher the performance, the higher the classification accuracy and thereby the lower the classification error. paper paper tutorial

Classification problem The problem for which a classifier has to be found. Usually it is defined for a given representation and design set. See also recognition problem. Some specific problems are the one-class classification problem (finding a boundary around a single class), the binary classification problem (finding a discriminant between two classes) and the multi-class classification problem

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(finding a classifier between a number of classes, possibly two). page-49 wiki

Classifier A classifier is a rule that assigns a class label to any object in a particular object representation.

Some classifiers may reject some objects. Some classifiers may assign multiple class labels. Instead of or in addition to class labels classifiers may output class posteriors, confidence, distances or densities for a all possible classes. In the additional step, the most likely class or classes have to be determined.

The word classifier is used for both, untrained as well as trained classifiers. The first refers to the rule, the way the classifier is trained. Sometimes this is also called a learner. The second refers to the realized version, the function that assigns labels or confidences. In section 7.2 a set of classifiers is listed. page-15 page-20 page-47 section 7.2 paper wiki example

Cluster A set of objects that are similar in their representation. It depends on the problem and the representation whether classes and clusters coincide. In a single class sometimes several clusters can be distinguished. page-68

Cluster analysis The study of a dataset by comparing the results of various clusterings. page-68 section 9.1 paper paper tutorial video wiki example

Clustering The process of finding clusters. It is a way of unsupervised learning. Three different approaches are the hierarchical techniques, the partitional clustering and mode seeking. page-68 paper video example

Combined classifier An advanced classifier constituted by a set of more simple classifiers (called base classifiers). They are combined by the combining classifier according to some combining rule. If the base classifiers are of the same type, the combined classifier is called an ensemble classifier. Well known examples are adaboost and the random forest classifier. A neural network classifier may also be considered as a combined classifier. paper example

Combining rule The way a set of classifiers is combined into a single one. The combining rule can be a fixed rule like majority voting, the average

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or the product of posterior probabilities. It can also be a trained combiner. paper paper tutorial example

Concept A concept is a general idea, or something conceived in the mind. In pattern recognition it is sometimes used for a class or a cluster for which the underlying set of objects is the complete set of specific examples for which the concept is applicable (occasionally a single representative or typical object is also called a concept). The concept is the step that consciousness makes after recognizing patterns in observations and before a name (a word) has been a assigned to it. wiki

Confidence A value between 0 and 1 that indicates the likelihood that a particular outcome (e.g. class membership) is correct. This term is used instead of posterior probability when probabilities in the strict sense are not well defined. Class confidences may, like class posteriors, be interpreted as soft labels. page-48 paper example

Consciousness The ability of a thinker, observer or actor to observe his own state of mind. page-6

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Covariance A statistical measure for the linear dependence of two stochastic variables:

$$\mathrm{cov}(x, y) = \mathrm{E}[(x - \mathrm{E}[x])(y - \mathrm{E}[y])]$$

The covariance of a variable with itself is called variance. In pattern recognition the covariance is often used to study the relation of two features. See also covariance matrix. page-48

Covariance matrix This symmetric matrix encodes all covariances of a set stochastic variables, e.g. the features used for representation. Multi-dimension Gaussian distributions are fully described by their mean vector and the covariance matrix. page-48 video wiki example

Crisp label Labels point from an object to a class. They are assigned by an expert or estimated during automatic classification. If there is no uncertainty or ambiguity such a label is unique and symbolic. It just contains the name of the class. See also soft labels. page-48

Cross-validation An evaluation system in which the design set is repeatedly split into a training set and a test set. Each time the system is trained and tested. Next, the roles of training and test sets are reversed, and the obtained performance estimates are averaged.

In n-fold cross-validation the design set is split into n partitions. In n rounds $n-1$ partitions are used for training and one for testing. Afterwards all performance estimates are averaged. Common values for n are 5 or 10. As the result depends on the random partition, n-fold cross-validation is sometimes repeated a number of times to get a more stable result, needed for a reliable comparison of different training systems. page-57 paper paper video wiki example

Curse of dimensionality Statistics in high-dimensional spaces tend to be bad. This is related to Rao's paradox, the peaking phenomenon and to overtraining. page-42 paper quora wiki example

Decision forest A combined classifier constituted by of a large set of decision tree classifiers. Some or all might be very simple, weak classifiers like the decision stump. Also random forest. page-54 paper wiki

Decision function A function of observable variables that makes a crisp choice between two or more options. A classifier is a decision function. page-49

Decision stump A weak classifier based on a decision tree consisting of just a single decision step, usually optimized for a random subset of features and/or a random subset of the training set. See decision forest and adaboost. paper wiki example

Decision tree A classifier based on a sequence of elementary decisions (usually thresholds on a feature) that can be understood as a graph tree. At the root the object to be classified comes in. By the sequence of decisions it arrives at an end node that is assigned to one of the classes. page-53 page-76 paper tutorial wiki

Dendrogram A graph tree used for visualizing the results of hierarchical clustering. The tope node stands for the entire dataset. Downward nodes show splits into smaller clusters. Bottom nodes may correspond to the individual objects. The lengths of the edges can be related to the clustering strength. page-70 page-76 wiki example example

Density Often used as a short for probability density. page-77

Density estimation The estimation of a probability density function (PDF), usually in a vector space, on the basis of a training set. PDFs are used in the Bayes classifier. This results in classifiers like Bayes normal, Parzen and naive Bayes, depending on the procedures and assumptions used for estimating the density. page-48 wiki wiki example

Design set The total set of objects that is available for the designer of a pattern recognition system. It may be split (repeatedly) into subsets like the training set, validation set and test set. page-19 page-29 page-57

Dimension reduction Transformation of a given vector representation, usually a feature space into another one with a lower dimension then the original one, while maintaining the information content. This content is either expressed in the object variability (unsupervised) or the class separability (supervised). page-42 section 6.3 wiki

Dipping The phenomenon that the learning curve of some classifier for a particular classification problem shows an optimum for some size of the training set. paper example

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Discriminant A function that decides between two possibilities, in pattern recognition usually between two classes. Decision function and classifier are more commonly used than 'discriminant'. The latter is mainly found in Fisher's Linear Discriminant (FLD) and Linear Discriminant Analysis (LDA). wiki example

Dissimilarity A measure for the difference between two objects. This can be a proper metric but may also violate the triangle inequality or be asymmetric. The main characteristics of a dissimilarity measure are usually: (1) the property of identity holds: it is zero if and only if the objects are identical, and (2) it is monotonic: the more different the objects the larger the dissimilarity. See dissimilarity representation and dissimilarity space. post

Dissimilarity representation In this representation objects are represented by pairwise dissimilarities to other objects, either directly computed from the real world observations or from another representation, e.g. features or graphs. The next step may be the postulation of a dissimilarity space or embedding. page-34 page-40 post paper paper tutorial

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Dissimilarity space The vector space defined by the dissimilarities to a representation set of objects. The vector length (space dimensionality) is thereby equal to the size of the representation set. This set can be the entire training set, a selection of these objects, but possibly also a set of entirely different objects. Classifiers in this space can be trained in a similar way as in a feature space. page-40 post paper tutorial example

Eigenvalue decomposition The decomposition of a square matrix X into a diagonal matrix D and a full matrix V such that XV = VD. The diagonal elements of D are the eigenvalues and the row vectors of V constitute a set of orthonormal eigenvectors.

An important application in pattern recognition is the eigenvalue decomposition of the covariance matrix of some vector representation of the objects. If the eigenvectors are ranked according to decreasing eigenvalues then the first n eigenvectors constitute the linear subspace for which the sum of the squared distances of the objects to this subspace is minimal. It is assumed that the dataset mean has been shifted to the origin first. See also eigenspectrum. page-74 wiki example

Eigenspectrum A plot of the ranked eigenvalues. Usually applied to the covariance matrix of a vector representation of a set of objects. It shows the data variances in the directions of the eigenvectors. Often the cumulative eigenspectrum is preferred for visualization purposes. page-77 paper example example

Embedding The computation of a set of vectors in an Euclidean space for which the distances are equal to a given set of dissimilarities or the inner products are equal to a given set of similarities (isometric embedding), see Euclidean geometry and MDS. page-41 wiki wiki

Ensemble classifier A subset of the family of combined classifiers. In an ensemble all base classifiers are of the same type, e.g. decision stumps used in adaboost. wiki tutorial example example

Error estimation Procedure to estimate the classification error of a classifier, e.g. by using a test set or cross-validation. page-55 section 8.1 paper paper example

Euclidean geometry A geometry based on Euclid's axiomatic system, the Elements. The traditional vector representation in pattern recognition is usually equipped with a Euclidean geometry. Distances are based on the Euclidean metric. page-41 wiki wiki

Evaluation Test of the performance of (a part of) a pattern recognition system. This may best be done by an independent test set. page-18 page-55 chapter 8 short-tutorial long-tutorial video example

Feature A symbolic or numeric property of a real world object that might be useful to determine its class. The word 'attribute'is used for this as well. Different objects however may have different numbers of attributes, while usually for all objects in the same problem the same features can be measured. Thereby objects may be represented by a feature vector, or by a set of attributes. page-19 page-23

Feature curve A plot that shows the performance of a trainable system (e.g. a classifier) as a function of the number of features used for training. page-62 page-78 section 8.3 example example

Feature extraction The process of determining good features for a feature representation of objects.

This may refer to raw data like images or time signals, but also to already given representation. In the latter case the aim is to simplify the representation, e.g. by dimension reduction. Examples are PCA and LDA. page-28 page-42 tutorial video wiki example

Feature representation The representation of objects by features resulting in a feature space. page-37

Feature scaling See scaling. page-35 wiki example

Feature selection Reducing the dimensionality of a feature space by the selecting of a subset of the features. Procedures for feature selection consist of a criterion (a filter approach or a wrapper) and a strategy (e.g. individual selection, forward selection, backward selection, branch and bound, floating search). page-43 paper paper post tutorial video video wiki example example

Feature space The vector space defined by the feature vectors. This concept is so familiar in statistical pattern recognition and machine learning that sometimes also vector spaces used for object representation but created otherwise, are also called feature spaces. Examples are the kernel space and the dissimilarity space which are defined by functions of input features or distances between objects. page-12

Feature vector The vector storing all relevant properties of a real world object in a particulary well defined order. It may also be the unfolded set of image pixels (pixel space) or a sampling of a spectrum or a time signal. If feature vectors are used to represent a set of objects in a vector space it is necessary that the images, spectra or signals are converted to the same size before sampling.

Filter In general a filter transforms an input (stream) by a fixed procedure into an output (stream). In relation with feature selection it has the specific meaning that it refers to criteria that are different, usually less complex, than the final classifier to be used after feature selection. The latter would be the wrapper approach, which is more focussed to the final use of the features to be selected. The filter approach, however, has the advantage that it might be faster (more simple to compute) and may avoid overtraining. Filtering is especially important if feature selection is done because the computation of the target classifier

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is troublesome for the given feature size. page-45 paper wiki example

Fisher classifier Usually called Fisher's Linear Discriminant (FLD). This is the traditional linear classifier optimizing the between scatter w.r.t. the within scatter. This classifier is based on the same criterion as Linear Discriminant Analysis (LDA). Also the classifier is thereby occasionally called LDA. page-51 paper paper video wiki example

Fisher mapping The orthonormal transformation of a feature space that maximizes the class between scatter w.r.t. the average class within scatter. It is also called LDA. video wiki example

FLD **Fisher's Linear Discriminant**, see Fisher classifier page-51 paper video wiki example

Forward search See forward selection.

Forward selection The selection of features or prototypes on the basis of the performance increase after addition to an already selected set. The selection is started with the best performing individual. See also feature selection. page-44 example example

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Floating search A forward selection procedure of features or prototypes including backward steps. See also feature selection. page-45 paper

Gaussian distribution See normal distribution. page-48 tutorial video wiki example

Generalization Generalization is the step from the observations of a set of objects to their common properties or concept. In logic this is called induction. In pattern recognition it is the process of finding clusters, classes or typical objects. If for a new object, that was not used in the generalization, its most similar cluster, class or typical object can now be determined. Thereby a property may be predicted that has not been measured. page-7 page-18 page-47 chapter 7 wiki wiki

Graph A symbolic representation of data: nodes (or vertices) connected by edges. In pattern recognition used for visualization, representation (see graph representation) and generalization (see hierarchical clustering and decision trees). page-75 wiki

Graph tree A connected graph in which any two nodes (vertices) are connected by exactly one path. page-75 wiki

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Graph representation A structural object representation by a set of nodes partially connected by edges. Nodes (vertices) and edges may be attributed. page-25 page-33 paper paper wiki

Grid search A way to find an optimal parameter setting, e.g. hyperparameters used for regularization. The possibly multi-dimensional domain of the parameters (e.g. of a classifier) is sampled by a grid and for every parameter vector on the grid a criterion (e.g. the performance of the classifier) is determined. The best parameter vector is used. page-54 wiki

Hierarchical clustering A clustering procedure in which small clusters (initially possibly single objects) are iteratively merged into large ones, eventually into a single large cluster. Hierarchical clustering may be visualized by a dendrogram. page-69 subsection 9.1.1 paper tutorial video wiki example example

Hold-out error The classification error of a classifier trained by the available design set, estimated by the classification error found for a classifier trained by a randomly chosen subset of the design set by applying it to the unused part of the design set (the hold-out set). Sometimes the subsets have equal size and the roles of the two sets is reversed as well and results are averaged: 2-fold cross-validation. page-57 paper wiki example

Image A one-, two-, or multi-dimensional set of pixels. For many pattern recognition applications it is relevant that the assumption holds that neighboring pixels have a higher correlation than more remote ones. This information is lost by a straight forward pixel representation. page-24

Individual selection The selection of features or prototypes on the basis of their individual contribution to some performance measure. See also feature selection. page-44 example example

Intrinsic dimensionality Formally this is the number of variables to represent a signal. For vector representations of objects this corresponds the dimensionality of the, possibly nonlinear, subspace that spans these objects with sufficient accuracy. wiki example

Input space Machine learning terminology for the space of the given (vector) representation. It is usually used in relation with kernel representations as it refers to the input space for which kernels are computed. The input space is in this case identical to what is called feature space in pattern recognition. paper

Invariant A property, often a (possible) feature, that has no relation with a particular class. Objects of that class may have all values of the invariant. For example, rotation angle is an invariant for most character classes, but not for the numbers '6' and '9', as they will be confused by rotation. page-36

Iris dataset A classical dataset in pattern recognition. It is one of the first real world datasets used to illustrate (by R.A. Fisher) the operation and performance of a classifier (Fisher's Linear Discriminant). data paper wiki example

Kernel A function $K(x, y)$ of two objects x and y. It is either computed from a representation like a feature space, or from the raw data of x and y directly. A training set of m objects is converted by the kernel in an $m \times m$ matrix. This may be used directly as a representation, but much more often the kernel trick is used (when possible) to train classifiers in kernel space. See also dissimilarity representation and dissimilarity space. page-53 example

Kernels are also used in non-parametric density estimation, e.g. Parzen, and in the classifiers based on it. page-52 example

Kernel space If a kernel is separable, i.e. if $K(x, y) = \phi(x)\phi(y)$ then the space $\phi(x)$ and $\phi(y)$ refer to is the kernel space. If the kernel satisfies the Mercer conditions, e.g. a Gaussian kernel (a radial basis kernel) or a polynomial kernel, this space is a Hilbert space. In support vector machines the kernel space is only used implicitly by the kernel trick. paper tutorial wiki wiki

Kernel trick If a kernel is separable, i.e. if $K(x, y) = \phi(x)\phi(y)$, which is the case if $K()$ fulfills the Mercer conditions, then the kernel may be interpreted as the inner product in the kernel space. As some transformations and classifiers, in particular the support vector machines, can be written in terms of inner products only, they implicitly base their result on a virtual kernel space, which might be of an infinite dimensionality. See also the Wikipedia article on this topic. page-53post tutorial video wiki

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KLT **The Karhunen-Loeve Transform**. It is sometimes used as an alternative name for PCA. In some toolboxes it is used for a slightly different use of PCA, e.g. PCA based on the averaged class covariance matrix instead of the overall covariance matrix. page-74 example

***k*NN** **The *k*-nearest neighbor** classifier. New objects are assigned to the majority class of the k nearest neighbors in the training set. page-52 example

KPCA **Kernel PCA**, an extension of PCA by using the kernel trick. Consequently a non-linear subspace is found, depending on the choice of the kernel. Often this subspace is 2D and the purpose is visualization by a scatter plot. page-75 wiki example

Label In general this is a tag or a pointer assigned to some entity in order to link it to some other entity. In a pattern recognition context it is often a short for class label as it links an object to a class by the name of that class. page-19

Labeled object An object with a known class label. It may be used in a training set for training a classifier or in a test set for error estimation. page-48

LDA **Linear Discriminant Analysis** stands for both, the linear transformation to the sub-space of a vector space under consideration for which the class between scatter is maximized w.r.t. the average class within scatter, as well as for the classifier that assigns new objects to the class with the highest posterior probability under the assumption of Gaussian class distributions with equal covariance matrices. LDA is also called Fisher mapping. page-44 page-52 page-74 paper paper post tutorial wiki example

Learner Sometimes used as alternative for an untrained classifier: the learning rule to find a classifier from data. It is especially used in discussions on weak and strong classifiers (learners).

Learning curve A plot that shows the performance of a trainable system (e.g. a classifier) as a function of the size of the training set. page-59 page-78 section 8.2 example example

Learning from examples This is the general goal of pattern recognition. One may gain knowledge from a teacher, but if this is not available one should learn from experience, from the observations as they arise: learning from examples. page-9 page-47

LOO **Leave-One-Out** cross-validation. A cross-validatio procedure which uses as many folds as objects in the design set. In each fold a classifier is trained on n-1 objects and tested on the remaining object. As this is a systematic procedure, repeating makes no sense as it will result in the same error estimate. page-59 example

LOO-error The classification error as estimated by LOO cross-validation. page-59

Mahalanobis distance The distance in a vector space between two sets of objects, or two distributions A and B, defined by their means μ_A and μ_B and their common covariance matrix Σ.

$$D(A, B) = \sqrt{(\mu_A - \mu_B)^T \Sigma^{-1} (\mu_A - \mu_B)}$$

Using the same metric also the distance between an object x and a set or distribution of objects A may be defined:

$$D(A, B) = \sqrt{(x - \mu)^T \Sigma^{-1} (x - \mu)}$$

.

or between two objects x and y within a set or distribution with covariance matrix Σ

$$D(A, B) = \sqrt{(x - y)^T \Sigma^{-1} (x - y)}$$

Note that if Σ equals the identity matrix the Mahalanobis distance equals the Euclidean distance. page-63 wiki

MDS **Multi-Dimensional Scaling** is a nonlinear technique for embedding a set of objects with a given dissimilarity matrix in a Euclidean vector space such that the distances in this space correspond to the given matrix. Often this vector space is 2D and the purpose is visualization by a scatter plot. page-74 wiki example

Mode seeking A clustering procedure based on the local maxima (modes) of the probability density function of all objects. page-72 subsection 9.1.3 paper paper wiki example

MST **Minimal Spanning Tree**: A graph tree representing a set of objects as the nodes of the tree used for visualization the dataset. The length of the edges are the distances between the connected objects. The sum of all represented lengths is minimized. page-76 video wiki

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Multi-class classification A classification problem in which a number of classes classes (two or more) have to be distinguished. Not all classifiers are able to distinguish directly more than two classes. Such binary classifiers need to a one-against-one or a one-against-rest strategy to solve a general multi-class problem. page-49 paper paper tutorial wiki example

Naive Bayes Used for classification procedures based on the Bayes classifier and the assumption that all features are independent. Consequently, the density functions can be estimated feature by feature, followed by a multiplication. Usually histograms are used for estimating the feature densities. page-52post tutorial video wiki

Nearest mean Classification rule in which objects are assigned to the class of the nearest class mean derived from the training set. page-51 paper example

Nearest neighbor The closest object in a set of objects (usually the training set) of a given object (e.g. a test object). The 1-nearest-neighbor rule (1-NN) is one of the traditional classifiers. The kNN classifier, which selects the majority class among the k nearest neighbors in the training set, approximates the Bayes classifier for an appropriate choice of k. The optimization of k is based on the assumption that the training set is selected according to the true class density distributions. page-51 paper scholar video wiki wiki example

Neural network Originally designed as a simulation of the nervous system. In pattern recognition it is a flexible trainable tool for defining non-linear subspaces and non-linear classifiers. It consists of a large set of simple units, called neurons, combining many inputs into a single output. Usually they are organized in layers. A non-linear neural network has at least three layers: the input layer (connected to the features), a hidden layer and an output layer (the class confidences). A very simple, degenerated neural network is the perceptron, consisting out of a single neuron. Neural networks are usually trained sequentially. page-53 paper tutorial wiki wiki

Non-parametric estimation Model estimation, e.g. a probability density function, not based on optimizing a parametric model, e.g. a normal distribution, but on a non-parametric function of all observations, e.g. a kernel density estimator

(Parzen). See also parametric estimation. page-48 tutorial wiki example

Normal distribution A very common bell shaped one-dimensional or multi-dimensional distribution. It is very common as for many other distributions holds that the means of a set of independently randomly drawn random variables asymptotically approximate a normal distribution. The normal distribution, $f(x, \mu, \Sigma)$ depends on just the class mean μ and the covariance matrix Σ: wiki

$$f(x, \mu, \Sigma) = \frac{1}{(2\pi)^{k/2}\sqrt{|\Sigma|}} e^{-(x-\mu)^T \Sigma^{-1} (x-\mu)/2}$$

Normal distributions with the given parameters are symbolically denoted by $N(\mu, \Sigma)$. The Bayes normal classifiers are based on the assumption of normally distributed classes. Normal distributions are also named Gaussian distributions. page-48 tutorial video wiki example

Normalization Used to describe the process of removing object differences that are not relevant for the classification, e.g. rotation or size. page-36 example

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Object A real world entity that can be physically observed. Also used for a representation of such an entity. Examples are 2-dimensional items like photos, characters, plotted curves; 3-dimensional items like chair, tables, cells, airplanes; but also time dependent events like speech, gestures, movies. More abstract entities like a voice, a persons identity, style of writing, a composition are sometimes called an object. Another way to phrase it is that an object is a realization of a concept, which corresponds to the pattern recognition terminology: a member (element) of a class (set). page-12 page-19 page-23 page-26

Object label A pointer to the class to which an object belongs or may belong, e.g. its name. Note the inconsistency in terminology: a class label is often used in way: the same pointer from an object to a class.

Object representation A formal description of an object that facilitates the comparison of objects and the generalization of sets of similar objects to a class. Examples are the feature representation, pixel representation, dissimilarities, kernels and graphs. page-33 section 6.1 paper

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Object variability A measure that expresses how much the objects in a given set differ in general.

Observation A single measurement or a set of measurements made from a single object. page-8 page-23

One-against-one A scheme for solving the multi-class classification problem in which binary classifiers (discriminants) are trained between all pairs of classes. On a second level these classifiers are combined. page-49 example

One-against-rest A scheme for solving the multi-class classification problem in which binary classifiers (discriminants) are trained between all single classes and the remaining ones. On a second level these classifier are combined. page-49 example

One-class classification A classification problem in which a boundary around a single class has to be found. paper paper thesis website wiki

Overfitting Classifiers and transformations that are optimized too long or by a too sensitive procedure may adapt to the noise in the data instead of to the for generalization relevant information. Such

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procedures may be qualified as overtraining, the result as overfitting. wiki example

Overtraining Originally overtraining refers to training a neural network too long, by which it adapts to the noise in the data. Now overtraining is also used for any classifier that by bad parameter settings, too small training sets, too many dimensions or too many parameters to be optimized adapts to the noise. Other terms for (about) the same phenomenon are curse of dimensionality, overfitting, peaking and Rao's paradox. page-42 page-56 page-63 post paper wiki example

Parametric estimation Model estimation, e.g. a probability density function, based on optimizing a parametric model, e.g. a normal distribution, and not on a non-parametric function of all observations, e.g. a kernel density estimator (Parzen). See also non-parametric estimation. page-48 tutorial wiki wiki

Partitional clustering A clustering procedure which starts with an initial, possibly random, clustering with the desired number of clusters. Iteratively it is optimized according to some specific criterion. Examples are k-Means, k-Centers and

Expectation-Maximization (EM) clustering. page-71 subsection 9.1.2 paper wiki example

Parzen Kernel based procedures for non-parametric density estimation. Usually a spherical normal distribution is used as kernel. Its width, also called the smoothing parameter, should be adapted to size of the training set. If done properly the Parzen classifier, which is based on the Parzen density estimates, is asymptotically a Bayes classifier. page-48 page-52 paper paper post paper tutorial example example

Pattern The word 'pattern' is overly used for slightly different but related concepts. The main one is the subset of similar objects in a larger set (a class or a cluster). It is however also used for the entire similarity structure in a collection of objects as well as for a single object which is typical for a set of similar objects.

Pattern recognition This is the process or ability of finding patterns in a set of objects. It also refers to the scientific domain that studies such processes as well as to the technology of creating artificial systems that can do this. The main sub-domains are representation and generalization. Pattern recognition is related to but slightly different from the fields of artificial intelligence and machine learning. As pattern recognition refers to both, a human ability as well as a research domain, it may be labeled as an art as well as a science. page-9 paper tutorial wiki

PCA **Principal Component Analysis** finds a orthogonal transformation for a vector space that decorrelates a specified covariance matrix C. It results in a set of eigenvectors (the new axes) V and the variances (diagonal terms) of the transformed covariance matrix D, also called eigenvalues. Thereby

$$V^{-1}CV = D$$

The orthonormal transformation is $V^T = V^{-1}$ as the covariance matrix of the transformed space is

$$\mathrm{E}[V^T x(V^T x)^T] = V^T \mathrm{E}(xx^T)V = V^{-1}CV = D$$

It is assumed without loss of generality that x has zero mean.

In practical applications often just the eigenvectors corresponding the the largest eigenvalues are used as they stand for the main directions of variance. Other directions are then neglected under the assumption that they correspond to noise. As this is effectively a type of averaging it may improve accuracy.

PCA is related to the Karhunen-Loeve Transform KLT and to LDA or Fisher mapping. page-44 page-74 post tutorial wiki example

Peaking phenomenon The phenomenon that the expected classification performance computed for a constant size of the training set as a function of the number of features (the feature curve) may show an optimum for some small number of features. See also overtraining and curse of dimensionality post paper paper example

Perceptron A simple neural network classifier consisting out of a single neuron. The perceptron classifier is linear and trained sequentially. It is sometimes used as a weak classifier. wiki example

Pixel representation Images can be represented by their pixels. The unfolded 1-dimensional vector constructed from 2-dimensional or even multi- dimensional images is then used for building a feature space. There are two problems with this approach: it results in very high-dimensional spaces and small shifts or rotations of the image may result into a large jump of the representing vector. A good property of the pixel representation is that all information available in the image is preserved, in contrast to features measured from the image. page-38 example

Pixel space Sometimes used as a short for 'feature space based on pixels'. Objects like images and spectra are in this way represented by a feature vector with all pixels or samples as elements. A set of 64x64 grey value images is thereby represented by a set of vectors in a 4096 dimensional space. page-40 example

Posterior probability In classification this is the probability $P(\omega|x)$ that a particular object, given by an observation x, belongs to the class ω. page-51 paper wiki

Prior knowledge All knowledge of measurements, models and probabilities that may be helpful to classify a particular object x, except any measurement on x itself. wiki

Prior probability In classification this is the probability $P(\omega)$ for a particular class ω of an object x

without taking into account any measurement on x itself. page-48 tutorial video example

Probability A number between 0 and 1 which is the likeliness that a particular event will occur. It is thereby the expectation of the fraction of the number of times that this event occurs in the total number of events under consideration. See also probability density. wiki

Probability density This is used for describing the probability of events given by a (set of) continuous variable(s). If the probability density of an event x is $f(x)$ then the probability that x is in the interval $[x - \triangle, x + \triangle]$ is $\int_{x-\triangle,x+\triangle} f(x)dx$. $f(x)$ is also named probability density function (PDF), probability distribution or just density. See density estimation for the relation with classifiers. page-48 tutorial wiki

Prototype In general, something that is typical for a larger class. In pattern recognition it is often used for objects that are representative for a class or for a classification problem. page-50 example

QDA **Quadratic Discriminant Analysis** is used for the Bayes normal classifier allowing different covariance matrices for the classes. page-52 tutorial wiki example

Random forest A combined classifier based on an ensemble of decision tree trained by a random subset of the training set and a random subset of the features. See also decision forest. page-54

Recognition In the strict sense the recognition of an object is equivalent to its classification. In a broader sense it includes the (development of the) representation as well of the classifier. page-6

Recognition problem The application for which a pattern recognition system has to be designed. The problem may include not only representation and generalization, but also the choice of sensors and the collection of a design set. wiki

Regularization A general term for the various ways to avoid overtraining in optimizing a classifier, e.g. adding noise to the data, adding noise to an optimization step, restrictions on the size of the step, adding a cost term to the criterion and early stopping (a limit on the number of optimization steps). page-65 video wiki example

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Reject Classification option by which no class is assigned to the input object. Instead it is rejected, i.e. returned for a better classifier, a human specialist or just put aside. Reasons for rejection can be that the object is for every class an outlier, or it is a borderline case. page-48 paper paper example example

Representation The representation of an object is a description of that object in terms of measurable observations that enables the a numeric or logic comparison with other objects in the same problem. page-12 page-17 page-27 chapter 6 post tutorial

Representation set The representation set is a set of objects used in a dissimilarity representation to represent other objects by their dissimilarities to the objects in the representation set. page-40 paper

Resubstitution error The classification error estimated by resubstituting the training set used for training the classifier. Also apparent error or training error. page-56 example

Scaling Used to modify feature spaces in such a way that the variability of features (e.g. their variances, mean class variances or domains) become equal. page-14 page-35 post wiki

Scatter matrix The scatter is a synonym for the estimated variance or covariance matrix, based on observed data points. If the set of data points has been split into subsets, the scatter of the total set is split into the between scatter and the within scatter. See also LDA and Fisher classifier. wiki

Scatter plot A plot that shows the vector locations of object representation in a 2D or 3D space, or a projection of a higher dimensional vector space. page-12 page-73 subsection 9.2.1 example

Segmentation The isolation of an object to be recognized from a larger observation containing other objects and/or a disturbing background. Examples are a single character on a page with more text and images, a phoneme in a speech signal, a face in an picture from a street with more people. page-25 page-34 wiki wiki wiki

Semantic gap The jump in the processing of observations, from physical phenomena, senses, nervous system to understanding. What first was just a physically measurable signal gets suddenly a meaning. page-9 wiki

Similarity A measure expressing how much two objects are equal. Usually similarities are positive, sometimes even restricted to the [0,1] interval. See also dissimilarity. page-7 scholar wiki

Soft label Labels point from an objects to a class. They are assigned by an expert or estimated during automatic classification. In both cases there might be uncertainty or ambiguity. This can be solved by replacing the traditional crisp labels by soft labels, usually numbers between 0 and 1. Every object has a soft label value for every class. They don't necessarily sum to one. They might be interpreted in several ways: uncertainties, probabilities or fuzzy class membership. See also crisp label. scholar wiki

Strong classifier This is a classifier that, after training, is expected to perform significantly better than random assignment, also called a strong learner. The opposite of a strong classifier is a weak classifier (weak learner). wiki

Structural representation The representation of an object by some structural means, e.g. (sequences of) symbols or a graph. page-33 paper paper

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Supervised learning This is learning from examples under supervision of a teacher. This almost always refers to a teacher who assigns desired class labels to the example objects. page-44 wiki

SVM **Support Vector Machine**. A linear classifier or regression function that is optimized for a distance based criterion as a linear function of a subset of the given vectors (training objects), the support vectors. Thanks to the kernel trick also non-linear classifiers can be trained. The result depends on the choice of the kernel. page-53 tutorial wiki example

Template matching A classification rule in which objects are assigned to the most similar object example. Such examples are usually selected by the teacher or found automatically by a prototype selection procedure. Originally templates are used for the recognition of simple objects like characters by optical comparison. page-50 wiki

Teacher The application expert who is able to collect examples, label them, and define a representation, e.g. suggesting features or defining a dissimilarity measure. page-47

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Testing Evaluation of a system by a test set, preferably selected independent from the training set. See evaluation and error estimation. page-56 example

Test error The classification error as estimated by a test set. page-55 example

Test set A set of objects with given class labels used for the evaluation of a classifier. A good test set is representative for the set of objects to be classified later by the classifier and is not used during training. page-19 page-30 page-55 page-57 example

Trained classifier A classifier trained by a training set, ready for evaluation by a test set or to be applied in practice. A trained classifier might be just a linear function. The way it is trained (the untrained classifier) may not be visible anymore. page-47

Training The optimization of a mapping or a classifier for a given set of objects, the training set. There are several types of training procedures, e.g. analytically, based on a single estimate of the parameter (e.g. the Fisher classifier), iteratively, by

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optimizing a criterion based on the entire training set (e.g. SVM), or sequentially, object by object (e.g. perceptron) page-47

Training error The classification error of a classifier based on the set of objects used for training the classifier, its training set. example

Training set The set of objects used for optimizing a mapping or a classifier. page-15 page-19 page-30 page-48 page-56 example

True classification error The classification error as made by the classifier on the objects of the problem for which it was trained. This error can be estimated by a test set randomly sampled from these objects. page-56

tSNE **t-distributed Stochastic Neighbor Embedding**. It is a low-dimensional embedding of objects such that similar objects are modeled by nearby points and dissimilar objects are modeled by distant points with a high emphasis on the first. Usually objects are embedded in a 2D subspace and the purpose is visualization by a scatter plot. page-75 wiki example

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Unseen objects This expression refers to objects in the design set that are different from all objects in the training set.

Unsupervised learning This is learning from examples without the supervision of a teacher. This almost always refers to a learning from objects for which no class labels have been given. Examples are cluster analysis and PCA. page-68 page-44 wiki

Untrained classifier A classifier for which the functional form and a criterion are given but for which the parameters have not yet been specified. They need to be optimized by the use of a training set.

Validation Synonym for evaluation and for testing. page-31

Validation set A subset of the design set, usually different from the training set, used to optimize some training step. page-30

Vector representation An object representation by a vector space. This is the most popular representation as there are many tools to analyze sets of vectors. page-36 section 6.2

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Visualization Various tools are used to demonstrate in some graphical way the data, the processing and the results of pattern recognition problems or the properties of the algorithms to tackle them: scatter plots, graphs, decision trees, dendrograms, learning curves and feature curves. page-73 section 9.2

Weak classifier This is a classifier that, after training, is expected to perform just slightly better than random assignment, also called a weak learner. Usually such classifiers can be trained fast and store just a few parameters. They are thereby popular as a base classifiers in combined classifiers like adaboost. The opposite of a weak classifier is a strong classifier (strong learner). page-54 wiki example

Within scatter The estimated variance or covariance of a set of data points. There is formally no difference with just the scatter. By within scatter, however, the difference with between scatter is emphasized as it restrict itself to the scatter of a single set, while the between scatter expresses the scatter between sets. page-44 paper paper wiki

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Wrapper The is an approach in feature selection in which as criterion the performance of the target classifier is used. For each feature set to be evaluated this performance has to be estimated, usually by cross-validation. This makes the procedure computationally intensive and may result in overtraining, especially if the performance is estimated by data that is also used in designing the final classifier. If this danger exist, e.g. when the original feature size is large, the so-called filter approach may be preferred, which is based on the use of a more simple criterion. page-45 paper wiki example

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