Classification Techniques for Time Series and Functional Data

Internet Version

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Doctoral Thesis

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Some calculus-tricks are quite easy. Some are enormously difficult. The fools who write the textbooks of advanced mathematics—and they are mostly clever fools—seldom take the trouble to show you how easy the easy calculations are. On the contrary, they seem to desire to impress you with their tremendous cleverness by going about it in the most difficult way.

Being myself a remarkably stupid fellow, I have had to unteach myself the difficulties, and now beg to present to my fellow fools the parts that are not hard. Master these thoroughly, and the rest will follow. What one fool can do, another can.

Silvanus P. Thompson

(from the prologue of *Calculus Made Easy*)

To my family, for the absolute confidence they have always placed in me (even when they did not understand why my —our— salary and holidays were not "like those teachers usually have").

Preface

The following body of work[1] is part of the research that I have done, in collaboration with my advisors, over several academic years at the Universidad Carlos III de Madrid. I am very pleased to have had the opportunity to help with the teaching tasks at the Departamento de Estadística.

This document is a digital version —by common consent of my advisors— of my doctoral thesis, defended on 12^{th} July 2010. Some misprints have been removed and few explanations, remarks, equations and pictures have been included. The margins have been reduced and the interline spacing has been set to one and a half, instead of double. As a result, a lot less pages were needed. Several appendices with auxiliar theory have been included (I am solely responsible for these sections). They contain well-known theory related to the mathematics used —in a more or less direct way— in the previous chapters. Many statisticians are not mathematicians; for this reason, the index has been expanded to make these appendices more accessible. Readers with enough background knowledge will not need to consult them.

This text is organized as follows: the first chapter begins with the basic mathematical notation, followed by the main definitions and classical results, and concludes with general ideas on the statistical problem of *classification* are provided, just before the exposition of our proposals. Chapters two and three are devoted, respectively, to our time series and functional data classification methods; these chapters can be independently consulted. Several possible extensions and forthcoming work are proposed in chapter four. Finally, some conclusions are summarised. In both chapter one and the appendices, the theory included is the "minimum necessary" while being, at the same time, selfcontained.

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Abstract

The main aim of this doctoral thesis is to develop classification techniques for dependent and functional data. Methods for classifying time series and functional data are proposed. Although this work involves several type of data, the functional data play a central role. An important point of both classification methodologies is that the original problems are not directly dealt with: the time series problem is rewritten as a functional data problem while the functional data problem is solved using a multivariate technique. Nevertheless, it is worthwhile noticing the different role of the functional data in the two forthcoming proposals: in the time series problem functional, estimators are constructed; while in the functional data problem, curves are the primary data.

For the classification of time series, their integrated periodograms are considered instead of the time series themselves. Subsequently, a new element is assigned to the group minimizing the distance from its integrated periodogram to the group mean of integrated periodograms. Although the periodogram is defined only for stationary time series, the application of the methodology to nonstationary series is still possible by calculating these periodograms locally. Finally, functional data depth is applied to make the classification robust.

The classification of functional data arises naturally in the previous framework. Moreover, the problem of selecting the most appropriate form (crude functions, their integrals or their derivatives) to express the data is also suggested. Without loss of generality, this second problem is equivalently formulated in terms of functions and their derivatives of different order, without integrals. In this thesis, a single methodology is proposed to cope with these two tasks at the same time. Following the same criterion of classifying a curve by using the distances from the function or its derivatives to group representative (usually the mean) functions or their derivatives, the combination of those distances is proposed in our method. The proposal works with a multivariate variable defined in terms of the distances. Moreover, an automatic form of ranking the original functions and their derivatives by discriminant power is obtained.

Key words: classification, time series data, integrated periodogram, functional data, depth, multivariate data, discriminant analysis, weighted distances.

Chapter 1

Introduction

Summary: The different types of data involved in this thesis are explained with the minimum necessary extension. Although this is a thesis on Statistics, not on Probability, the next sections begin with the theoretical models frequently used to fit the data. Knowing these models is essential in understanding the statistical methods proposed later. Finally, the classification problem is presented in a general form.

Key words: multivariate data, time series, functional data, supervised classification.

1.1 Notation

The following mathematical notation will be used throughout this document:

X	and	x	for a univariate variable
$\mathbf{X}$	and	$\mathbf{x}$	for a multivariate variable
X_t	and	x_t	for a (discrete-time) sequence of variables
$X(t)$	and	$x(t)$	for a (continuous-time) family of variables
$\mathcal{X}(t)$	and	$\chi(t)$	for a function (depending on the variable t)

Upper case letters represent stochastic quantities, while lower case letters represent nonstochastic numeric quantities. The letter Y is used for mathematical objects of the same kind, but with some dependence on the corresponding objects denoted with X.

In addition, for samples the subindex $_e$ denotes the e-th element of a sample of size n, and, when there are K different populations or groups, the superindex $^{(k)}$ denotes the k-th population or group.

For a general matrix $\mathbf{M}$ of size $n_1 \times n_2$, the following notation will be used sometimes:

$$\mathbf{M} = \begin{pmatrix} m_{11} & \cdots & m_{1n_2} \\ \vdots & \ddots & \vdots \\ m_{n_1 1} & \cdots & m_{n_1 n_2} \end{pmatrix} = (m_{ij})_{i,j},$$

where $i = 1, \ldots, n_1,\ j = 1, \ldots, n_2$. Finally,

$D^i\mathcal{X}(t)$ and $D^i\chi(t)$ denote the i-th derivative,

with respect to the real variable t, where $D^0\mathcal{X}(t) \equiv \mathcal{X}(t)$ and $D^0\chi(t) \equiv \chi(t)$.

1.2 Stochastic Vectors

1.2.1 Models

Definition 1 *A* multivariate random variable *or* random vector *of dimension p is defined as*

$$\mathbf{X} = (X_1, \ldots, X_p)^t, \tag{1.1}$$

where X_i are simultaneous univariate random variables (defined in the same probability space).

The previous vector can be represented through the following application

$$\begin{array}{rccc} \mathbf{X}: & \Omega & \longrightarrow & \mathbb{R}^p \\ & \omega & \to & \mathbf{X}(\omega) \end{array}.$$

That is, for fixed ω a value in $\mathbb{R}^p$ is obtained, while a random variable is obtained when the subindex —in the vector— is fixed.

Definition 2 *The* mean vector *of the multivariate random variable* $\mathbf{X}$ *is defined as the (column, in this case) vector*

$$\mu_{\mathbf{X}} = (\mu_1, \ldots, \mu_p)^t = (\mathbb{E}(X_1), \ldots, \mathbb{E}(X_p))^t = \mathbb{E}(\mathbf{X}). \tag{1.2}$$

Definition 3 *The* covariance matrix *of the variable* $\mathbf{X}$ *is defined as*

$$\begin{aligned} \mathbf{\Sigma_X} &= (\sigma_{ij})_{i,j} = (\mathbb{E}((X_i - \mu_i)(X_j - \mu_j)))_{i,j} \\ &= \mathbb{E}\left(((X_i - \mu_i)(X_j - \mu_j))_{i,j}\right) = \mathbb{E}\left((\mathbf{X} - \mu_{\mathbf{X}})(\mathbf{X} - \mu_{\mathbf{X}})^t\right). \end{aligned} \tag{1.3}$$

Although it is implicit in the previous definition,

Definition 4 *Given two univariate variables X_i and X_j, the* covariance *between them is defined as*

$$cov(X_i, X_j) = \mathbb{E}\left((X_i - \mu_{X_i})(X_j - \mu_{-X_j})\right) = \sigma_{ij}. \tag{1.4}$$

As a particular case,

Definition 5 *The* variance *of a univariate variable X_i is defined as*

$$var(X_i) = cov(X_i, X_i) = \sigma_{ii} = \sigma_i^2. \tag{1.5}$$

Definition 6 *A* univariate compound random variable *is defined as*

$$Y = a_1 X_1 + \ldots + a_p X_p = \mathbf{a}^t \mathbf{X}, \tag{1.6}$$

where $\mathbf{a} = (a_1, \ldots, a_p)^t \in \mathbb{R}^p$.

Remark 1 The nomination 'compound variable' is the literal translation of 'variable compuesta', from Cuadras (2007).

Definition 7 *A* multivariate compound random variable *of dimension* q *is defined as*

$$\mathbf{Y} = (Y_1, \ldots, Y_q)^t, \tag{1.7}$$

with

$$Y_j = a_{1j} X_1 + \ldots + a_{pj} X_p = \mathbf{a}_j^t \mathbf{X}, \qquad j = 1, \ldots, q \tag{1.8}$$

or, in matrix notation,

$$\mathbf{Y} = \mathbf{A}^t \mathbf{X}, \tag{1.9}$$

where $\mathbf{A} = (a_{ij})_{i,j}$ *is the* $p \times q$ *matrix of the coefficients.*

For the previous definitions, it holds that

Proposition 1

$$\mu_{\mathbf{Y}} = \mathbf{A}^t \mu_{\mathbf{X}}, \tag{1.10}$$

and, for the particular univariate case, $\mu_Y = \mathbf{a}^t \mu_{\mathbf{X}}$.

Proof.

$$\mu_{\mathbf{Y}} = \mathbb{E}(\mathbf{Y}) = \mathbb{E}(\mathbf{A}^t \mathbf{X}) = \mathbf{A}^t \mathbb{E}(\mathbf{X}) = \mathbf{A}^t \mu_{\mathbf{X}}.$$

□

and

Proposition 2

$$\mathbf{\Sigma}_{\mathbf{Y}} = \mathbf{A}^t \mathbf{\Sigma}_{\mathbf{X}} \mathbf{A}, \tag{1.11}$$

and, for the particular univariate case, $\Sigma_Y = \mathbf{a}^t \mathbf{\Sigma}_{\mathbf{X}} \mathbf{a}$.

Proof.

$$\begin{aligned}
\mathbf{\Sigma}_{\mathbf{Y}} &= \mathbb{E}\left((\mathbf{Y} - \mu_{\mathbf{Y}})(\mathbf{Y} - \mu_{\mathbf{Y}})^t\right) = \mathbb{E}\left((\mathbf{A}^t \mathbf{X} - \mathbf{A}^t \mu_{\mathbf{X}})(\mathbf{A}^t \mathbf{X} - \mathbf{A}^t \mu_{\mathbf{X}})^t\right) \\
&= \mathbb{E}\left(\mathbf{A}^t (\mathbf{X} - \mu_{\mathbf{X}})(\mathbf{X} - \mu_{\mathbf{X}})^t \mathbf{A}\right) = \mathbf{A}^t \mathbb{E}\left((\mathbf{X} - \mu_{\mathbf{X}})(\mathbf{X} - \mu_{\mathbf{X}})^t\right) \mathbf{A} \\
&= \mathbf{A}^t \mathbf{\Sigma}_{\mathbf{X}} \mathbf{A}.
\end{aligned}$$

□

Proposition 3 *If* $Y_1 = \mathbf{a}^t\mathbf{X}$ *and* $Y_2 = \mathbf{b}^t\mathbf{X}$*, it holds that*

$$cov(Y_1, Y_2) = \mathbf{a}^t\mathbf{\Sigma_x}\mathbf{b}, \tag{1.12}$$

where $cov(Y_1, Y_2)$ *is given by 1.4.*

Proof.

$$\begin{aligned} cov(Y_1, Y_2) &= cov(\sum_{i=1}^{p} a_i X_i, \sum_{j=1}^{p} b_j X_j) = \sum_{i=1}^{p} a_i cov(X_i, \sum_{j=1}^{p} b_j X_j) \\ &= \mathbf{a}^t \left(cov(X_1, \sum_{j=1}^{p} b_j X_j), \ldots, cov(X_p, \sum_{j=1}^{p} b_j X_j) \right)^t \\ &= \mathbf{a}^t \left(\sum_{j=1}^{p} b_j \sigma_{1j}, \ldots, \sum_{j=1}^{p} b_j \sigma_{pj} \right)^t = \mathbf{a}^t\mathbf{\Sigma_x}\mathbf{b}. \end{aligned}$$

□

Corollary 1 *If* $Y = \mathbf{a}^t\mathbf{X}$*, it holds that*

$$var(Y) = \mathbf{a}^t\mathbf{\Sigma_x}\mathbf{a}. \tag{1.13}$$

Proof. It is a direct conclusion of either of the two previous propositions.

□

1.2.2 Multivariate Data

In this thesis, numeric variables are quantitative and continuous, and they can be thought of as realizations of random variables.

Definition 8 *A* multivariate variable *of dimension p is defined as the vector*

$$\mathbf{x} = (x_1, \ldots, x_p)^t, \tag{1.14}$$

where x_i *are simultaneous univariate numeric variables.*

Remark 2 This definition makes it clear that the termed Multivariate Analysis deals with the simultaneous relationships among the variables of the vector.

The compound variables are defined as

Definition 9 *A* univariate compound variable *is defined as*

$$y = a_1 x_1 + \ldots + a_p x_p = \mathbf{a}^t \mathbf{x}, \tag{1.15}$$

where $\mathbf{a} = (a_1, \ldots, a_p)^t \in \mathbb{R}^p$.

Definition 10 *A* multivariate compound variable *of dimension* q *is defined as*

$$\mathbf{y} = (y_1, \ldots, y_q)^t, \tag{1.16}$$

with

$$y_j = a_{1j} x_1 + \ldots + a_{pj} x_p = \mathbf{a}_j^t \mathbf{x}, \qquad j = 1, \ldots, q \tag{1.17}$$

or, in matrix notation,

$$\mathbf{y} = \mathbf{A}^t \mathbf{x}, \tag{1.18}$$

where $\mathbf{A} = (a_{ij})_{i,j}$ *is the* $p \times q$ *matrix of the coefficients.*

1.2.3 Statistical Inference

Let us consider that the previous multivariate variable $\mathbf{x} = (x_1, \ldots, x_p)^t$ has taken the values of the following sample of size n, expressed in a matrix

$$(\mathbf{x}_1, \cdots, \mathbf{x}_n) = \begin{pmatrix} x_{11} & \cdots & x_{1n} \\ \vdots & \ddots & \vdots \\ x_{p1} & \cdots & x_{pn} \end{pmatrix} = (x_{ij})_{i,j}, \tag{1.19}$$

where $\mathbf{x}_e$, the e-th column of the matrix, contains the e-th element of the sample of size n. It is supposed that the multivariate variables $\mathbf{x}_e$ are also simultaneous, that is, in this situation there is no interest in the evolution through time. We are relating the e-th column of the sample with the univariate variable x_e of $\mathbf{x}$. Then, some well-known results on the parameter estimation of the models from the samples of data are the following (see, for example, section 2.8 of Mardia et al. [1979]):

Definition 11 *The* covariance *between* x_i *and* x_j *is defined as*

$$cov(x_i, x_j) = n^{-1} \sum_{e=1}^{n} (x_{ie} - \overline{x}_i)(x_{je} - \overline{x}_j), \tag{1.20}$$

where $\overline{x}_i = n^{-1} \sum_{e=1}^{n} x_{ie}$ *and* $\overline{x}_j = n^{-1} \sum_{e=1}^{n} x_{je}$.

Definition 12 *The* variance *of* x_i *is defined as*

$$var(x_i) = cov(x_i, x_i). \tag{1.21}$$

Mean Vector

- The quantity $\mathbb{E}(X_i)$ is estimated by $\overline{x}_i = \frac{1}{n}\sum_{e=1}^{n} x_{ie}$.
- Then, $\mu_{\mathbf{x}}$ is estimated by $\overline{\mathbf{x}} = \frac{1}{n}\sum_{e=1}^{n} \mathbf{x}_e$.
- For the multivariate compound variable $\mathbf{Y}$, the mean $\mu_{\mathbf{Y}}$ is estimated by $\overline{\mathbf{y}} = \mathbf{A}^t\overline{\mathbf{x}}$. For the univariate compound variable Y, the mean μ_Y is estimated by $\overline{y} = \mathbf{a}^t\overline{\mathbf{x}}$.

Covariance Matrix

- The matrix $\mathbf{\Sigma_x} = (\sigma_{ij})_{i,j}$ is estimated with bias by $\hat{\mathbf{\Sigma}}_{\mathbf{x}} = \frac{1}{n}\sum_{e=1}^{n}(\mathbf{x}_e - \overline{\mathbf{x}})(\mathbf{x}_e - \overline{\mathbf{x}})^t = (cov(x_i, x_j))_{i,j}$. With the usual definition $\hat{\sigma}_{ij} = cov(x_i, x_j)$, it holds that $\hat{\sigma}_{ij}$ estimates σ_{ij} and $\hat{\mathbf{\Sigma}}_{\mathbf{x}} = (\hat{\sigma}_{ij})_{i,j}$.
- The matrix $\mathbf{\Sigma_x}$ is estimated without bias by $\mathbf{S}_{\mathbf{x}} = \frac{n}{n-1}\hat{\mathbf{\Sigma}}_{\mathbf{x}}$.
- For the variable $\mathbf{Y}$, the matrix $\mathbf{\Sigma_Y}$ is estimated with bias by $\hat{\mathbf{\Sigma}}_{\mathbf{y}} = \mathbf{A}^t\hat{\mathbf{\Sigma}}_{\mathbf{x}}\mathbf{A}$. For the variable Y, the matrix Σ_Y is estimated with bias by $\hat{\Sigma}_y = \mathbf{a}^t\hat{\mathbf{\Sigma}}_{\mathbf{x}}\mathbf{a}$.
- For the variable $\mathbf{Y}$, the matrix $\mathbf{\Sigma_Y}$ is estimated without bias by $\mathbf{S}_{\mathbf{y}} = \mathbf{A}^t\mathbf{S}_{\mathbf{x}}\mathbf{A}$. For the variable Y, the matrix Σ_Y is estimated without bias by $S_y = \mathbf{a}^t\mathbf{S}_{\mathbf{x}}\mathbf{a}$.

1.2.4 Mathematical Framework

Although it is always necessary to take into account the mathematical aspects of any statistical study, usually they are understood and not mentioned explicitly. For each kind of object, we shall devote a brief section to justify the main mathematical operations.

The sets of multivariate vectors (stochastic or not) of dimension p take values in the set $\mathbb{R}^p$, that is a linear space with the usual operations of sum and product with a real number. With the Euclidean or the Mahalanobis distance, the sets are metric spaces; it is also possible to work in a Banach or in a Hilbert space by considering, respectively, a proper norm or inner product (see sections 2.1.1, 3.1.1, 3.3.1 and 3.4.1 of Kolmogórov and Fomín [1975]).

The set of matrices formed from the previous multivariate vectors are also a linear space with respect to the usual sum and product with a scalar. The product of matrices is a little more complicated, since the set is a noncommutative group.

Remark 3 For concrete data, for example a matrix, it is possible to test some numerical properties. Nonetheless, when the data —numeric or stochastic— are not yet known, although some numerical properties can still be proved (those independent of the concrete values), suppositions like "when the matrix is not singular", for example, are generally needed.

1.2.5 Addendum: Compound Variable Geometry

In this subsection, the geometric interpretation of the univariate compound variable is hightlighted,

$$y = a_1 x_1 + \ldots + a_p x_p = \mathbf{a}^t \mathbf{x}, \tag{1.22}$$

where $\mathbf{a} = (a_1, \ldots, a_p)^t \in \mathbb{R}^p$ is the parameter.

Geometry in $\mathbb{R}^p$

Let $\mathbf{x}$ and $\mathbf{a}$ be (column) vectors, both with origin in $\mathbf{0}$; then, the projection of $\mathbf{x}$ onto the line —one-dimensional linear subspace— determined by $\mathbf{a}$ is obtained as follows. Let $V_{\mathbf{a}}$ be the linear subspace of $\mathbb{R}^p$ generated by $\mathbf{a}$; then any $\mathbf{x} \in \mathbb{R}^p$ can be written uniquely as the sum of the projections on $V_{\mathbf{a}}$ and its complementary $V_{\mathbf{a}}^{\perp}$, that is, symbolically, $\mathbb{R}^p = V_{\mathbf{a}} \oplus V_{\mathbf{a}}^{\perp}$. Since

$$\mathbf{x} = Proj_{V_{\mathbf{a}}}(\mathbf{x}) + Proj_{V_{\mathbf{a}}^{\perp}}(\mathbf{x}) = c\mathbf{a} + Proj_{V_{\mathbf{a}}^{\perp}}(\mathbf{x}), \tag{1.23}$$

after premultiplying by $\mathbf{a}$,

$$\langle \mathbf{a}, \mathbf{x} \rangle = c \langle \mathbf{a}, \mathbf{a} \rangle, \tag{1.24}$$

so, as $\langle \mathbf{a}, \mathbf{a} \rangle \neq 0$,

$$Proj_{V_{\mathbf{a}}}(\mathbf{x}) = c\mathbf{a} = \frac{\langle \mathbf{a}, \mathbf{x} \rangle}{\langle \mathbf{a}, \mathbf{a} \rangle} \mathbf{a} = \left\langle \frac{\mathbf{a}}{\|\mathbf{a}\|_e}, \mathbf{x} \right\rangle \frac{\mathbf{a}}{\|\mathbf{a}\|_e} = \left(\frac{\mathbf{a}^t}{\|\mathbf{a}\|_e} \mathbf{x} \right) \frac{\mathbf{a}}{\|\mathbf{a}\|_e}, \tag{1.25}$$

where $\| \cdot \|_e$ denotes the Euclidean norm in $\mathbb{R}^p$ and $\langle \cdot, \cdot \rangle$ denotes the inner product. Then, the parameter $\mathbf{a}$ of the compound variable can be interpreted geometrically as a parameter determining the direction into which $\mathbf{x}$ is projected.

The linear subspace and the vectors $\mathbf{x}$ and $Proj_{V_{\mathbf{a}}}(\mathbf{x})$ can be represented (literally only for low dimensions) graphically in $\mathbb{R}^p$.

Alternatively, if there is no interest in the interpretation of the "line" (subspace) as a subspace of $\mathbb{R}^p$, this "line" can be seen as an independent axis.

Geometry in $\mathbb{R}$

For compound variables, the interest usually relies on the module of the projection, that is, in the following part

$$\left\langle \frac{\mathbf{a}}{\|\mathbf{a}\|_e}, \mathbf{x} \right\rangle = \frac{\mathbf{a}^t}{\|\mathbf{a}\|_e} \mathbf{x}. \tag{1.26}$$

In addition, if there is no interest in the scale factor of the projection, a characterization is provided by the numeric factor

$$\mathbf{a}^t \mathbf{x} = y. \tag{1.27}$$

Remark 4 Note that this approach justifies the use of the expression 'the premultiplication $\mathbf{a}^t\cdot$ projects $\mathbf{x}$ into a one-dimensional space'.

Another possible geometric interpretation of the compound variable can be obtained by considering a higher-dimensional linear space.

Geometry in $\mathbb{R}^{p+1}$

Using equation (1.27) in another form

$$\mathbf{a}^t\mathbf{x} - y = 0, \tag{1.28}$$

and, considering the new $(p+1)$-dimensional linear space determined by the variables $(\mathbf{x}, y)$, it is clear that the hyperplane (1.28), with director vector $(\mathbf{a}^t, -1)$, projects the multivariate point $\mathbf{x}$ into the last axis, the y axis.

These geometrical interpretations will be reviewed several times in chapter 3 and appendix D, since the choice of $\mathbf{a}$, from the information provided by multivariate data, will be the main objective there. Selecting $\mathbf{a}$ for the compound variable can be interpreted geometrically as selecting (the direction of) a one-dimensional subspace into which the multivariate data will be projected. This choice is usually guided by some explicit criterion. Although in the theoretical compound variable $y = \mathbf{a}^t\mathbf{x}$, the term $\mathbf{x}$ is a multivariate variable and $\mathbf{a}$ is a multivariate parameter, in the empirical selection of the direction of the one-dimensional linear subspace, $\mathbf{a}$ will be temporarily considered a multivariate variable. Finally, let us note that making any restriction on the value of $\mathbf{a}$ is equivalent to making restrictions on the direction into which the compound variable projects the data.

Remark 5 The theory developed in this addendum acquires special importance due to the fact that any finite-dimensional Hilbert space is "structurally identical" (*isomorphic*) to $\mathbb{R}^p$ (see section 3.4.6 of Kolmogórov and Fomín [1975]).

1.3 Stochastic Processes

In this section, only discrete-time univariate stochastic processes are considered.

1.3.1 Models

Definition 13 *A* discrete-time stochastic process *is a sequence of random variables (defined in the same probability space and taking values in the same* state space *S),*

$$(X_t,\ t \in \mathbb{Z}), \tag{1.29}$$

where the index t represents time.

In the previous process, for fixed t the quantity X_t is a random variable, while for fixed ω a *trajectory* is obtained, as represented through the following application

$$\begin{array}{rccc} X_t: & \Omega & \longrightarrow & \mathbb{R}^{\infty} \\ & \omega & \to & X_t(\omega) \end{array}.$$

Note that now the variables are not simultaneous, as those of the multivariate vector (1.1). This mathematical object is defined to study dynamic (univariate) changes in time. On the other hand, another possibility could be to consider multivariate stochastic processes $(\mathbf{X}_t,\ t \in \mathbb{Z})$, where each $\mathbf{X}_t$ is a vector of simultaneous variables.

Two Domains

Stochastic processes can be studied from the *time domain* or, alternatively or additionally, from the *spectral domain*. Time domain uses position or time as index, and the autocovariance —or, equivalently, autocorrelation— function is the natural tool for studying the evolution in the time domain. The previous definition corresponded to the time domain, but the *Fourier Analysis* allows the use of the frequency as variable. The *Spectral Analysis* is the adaptation of the Fourier analysis to deal with stochastic —rather than deterministic— functions of time.

In order to handle processes, some additional structure is assumed under the name of *stationarity*. It implies homogeneity in the time domain, in the form of autocovariance function invariant under time shifts. This similarity with the periodicity of functions will allow the decomposition of processes, under some conditions, in terms of regular underlying oscillations whose magnitudes are random variables; that is, a decomposition into the sum of uncorrelated periodic components. The *spectrum*, the set of frequencies of oscillations, is the natural mathematical tool in the frequency domain.

Definition 14 *The stochastic process* (X_t) *is* strongly stationary *if the random vectors,*

$$(X_{t_1}, \ldots, X_{t_d}) \quad \text{and} \quad (X_{t_1+s}, \ldots, X_{t_d+s}) \tag{1.30}$$

have the same joint distribution for all $t_1, \ldots, t_d$ *and for all* $s > 0$.

Thus, the finite-dimensional distributions of a strongly stationary process are invariant under time shifts. These distributions characterize the whole process. For processes such that $Var(X_t) < \infty,\ \forall t \in \mathbb{Z}$, a weaker condition —implied by the previous— is presented in the following definition.

Definition 15 *The stochastic process* (X_t) *is* weakly *(also termed* second-order *or* covariance*)* stationary *if* $\mathbb{E}(|X_t|^2) < \infty$*, for all* $t \in \mathbb{Z}$*, and*

1. $\mathbb{E}(X_{t_1}) = \mathbb{E}(X_{t_2})$,
2. $cov(X_{t_1}, X_{t_2}) = cov(X_{t_1+s}, X_{t_2+s})$,

for all $t_1, t_2, s \in \mathbb{Z}$ *with* $s > 0$.

Once the stationarity is imposed, the following definitions make sense:

Definition 16 *The* mean function *of a weakly stationary process* (X_t) *is defined as*

$$\mu_t = \mathbb{E}(X_t), \quad t \in \mathbb{Z}. \tag{1.31}$$

Definition 17 *The* autocovariance function *of a weakly stationary process* (X_t) *is defined as*

$$\sigma_s = cov(X_t, X_{t+|s|}), \quad s \in \mathbb{Z}, \tag{1.32}$$

where the *covariance* of any two variables (with finite mean) is defined as

$$cov(X_1, X_2) = \mathbb{E}\left([X_1 - \mathbb{E}(X_1)][X_2 - \mathbb{E}(X_2)]\right). \tag{1.33}$$

The *variance* of any variable X is defined as $var(X) = cov(X, X)$.

From these definitions, it follows that the process (X_t) is weakly stationary if and only if

1. It has a constant mean.

2. Its autocovariance function is invariant under time shifts.

Stationary processes can be described in terms of the autocovariance function (it contains enough information) or, equivalently, in terms of the following rescaled function.

Definition 18 *The* autocorrelation function *of a weakly stationary process* (X_t) *is defined as*

$$\rho_s = \frac{cov(X_0, X_{|s|})}{\sqrt{var(X_0)var(X_{|s|})}} = \frac{\sigma_{|s|}}{\sigma_0}, \quad s \in \mathbb{Z} \tag{1.34}$$

whenever $\sigma_0 = var(X_{|s|}) > 0$.

Classical results linking both domains are provided by the Fourier analysis.

Theorem 1 - *Wold's Theorem.* *A necessary and sufficient condition for a sequence* $\{\rho_s\}$ *to be the autocorrelation function for some discrete-time stationary process* (X_t) *is that there exists a function* $F(\lambda)$*, having the properties of a distribution function on the interval* $(-\pi, +\pi)$*, (i.e.* $F(-\pi) = 0$*,* $F(+\pi) = 1$ *and* $F(\lambda)$ *is nondecreasing), such that*

$$\rho_s = \int_{-\pi}^{+\pi} e^{is\lambda} dF(\lambda), \qquad s \in \mathbb{Z}. \tag{1.35}$$

Proof. See section 4.8.3 of Priestley (1981). □

Definition 19 *If the autocorrelation* ρ_s *satisfies (1.35) then* $F(\lambda)$ *is called the* spectral distribution function *of the process.*

Theorem 2 *Any integrated spectrum $F(\lambda)$ can be written in the form,*

$$F(\lambda) = c_1 F_1(\lambda) + c_2 F_2(\lambda) + c_3 F_3(\lambda), \tag{1.36}$$

where

1. $c_i \geq 0, \quad i = 1, 2, 3 \quad$ *and* $\quad c_1 + c_2 + c_3 = 1$
2. $F_i(\lambda) \geq 0, \quad i = 1, 2, 3 \quad$ *are distribution functions of the following types;*
   (a) $F_1(\lambda)$ *is absolutely continuous with derivative* $F_1'(\lambda)$ *which exists for almost all* λ*, and the density function* $f_1(\lambda)$*, which is such that* $F_1(\lambda) = \int_{-\pi}^{\lambda} f_1(h)dh$*, exists for all* λ*.*
   (b) $F_2(\lambda)$ *is a step function with steps* $\{p_s\}$ *at points* λ_s*, say,* $s = 1, 2 \ldots$*, and* $\sum_s p_s = 1$*.*
   (c) $F_3(\lambda)$ *is a "singular" function with zero derivative almost everywhere.*

Proof. See section 4.9 of Priestley (1981). □

Remark 6 The part $F_3(\lambda)$ in (1.36) is highly pathological and usually ignored.

Definition 20 *A stochastic process* (X_t) *is said to have* purely continuous spectrum *if* $F \equiv F_1$ *in expression (1.36), that is, the other two parts are null.*

Theorem 3 - *Spectral Theorem.* *If* (X_t) *is a discrete-time stationary process with zero mean, unit variance, and spectral distribution function* $F(\lambda)$*, there exists a complex-valued process* $\mathbf{S} = (S(\lambda), \ -\pi < \lambda \leq +\pi)$ *such that*

$$X_t = \int_{-\pi}^{+\pi} e^{it\lambda} dS(\lambda), \quad t \in \mathbb{Z}. \tag{1.37}$$

Furthermore, $\mathbf{S}$ *has orthogonal increments and*

$$\mathbb{E}(|S(v) - S(u)|^2) = F(v) - F(u) \quad \textit{for} \quad u \leq v. \tag{1.38}$$

Proof. See section 9.4 of Grimmett and Stirzaker (2001). □

Purely Continuous Spectrum

A purely indeterministic discrete-time stationary process (X_t) verifies that $\sum_{s=1}^{+\infty} |\rho_s| < \infty$ and, as a consequence, has a purely continuous spectrum. In this case, the spectral distribution function $F(\lambda)$ is absolutely continuous and has density function $f(\lambda)$, named as follows:

Definition 21 *The function* $f(\lambda)$ *is termed* spectral density function.

It holds that

$$F(\lambda) = \int_{-\pi}^{\lambda} f(h)dh, \quad \lambda \in [-\pi, +\pi], \tag{1.39}$$

so

$$F'(\lambda) = \frac{d}{d\lambda}F(\lambda) = f(\lambda), \quad \lambda \in [-\pi, +\pi]. \tag{1.40}$$

Some other consequences are that the expression (1.35) becomes

$$\rho_s = \int_{-\pi}^{+\pi} e^{is\lambda} f(\lambda)d\lambda, \qquad s \in \mathbb{Z}, \tag{1.41}$$

and that the following theorem holds:

Theorem 4 *Let $\{\rho_s\}$ be the autocorrelation function (sequence) of a stationary sequence. If the function $F(\lambda)$ in (1.35) is differentiable with derivative $f(\lambda)$, then*

$$f(\lambda) = \frac{1}{2\pi} \sum_{s=-\infty}^{+\infty} \rho_s e^{-is\lambda} \tag{1.42}$$

at any point $\lambda \in [-\pi, +\pi]$ where $f(\lambda)$ is differentiable.

Proof. See section 9.3 of Grimmett and Stirzaker (2001). □

Remark 7 It is important not to confuse the expression "purely indeterministic", that is, without a deterministic part at all, with the expression "purely random", which is frequently used for referring to the *white noise* or to an independent or uncorrelated sequence or family of variables.

Remark 8 The decomposition of $f(\lambda)$ in trigonometric terms is highlighted when expression (1.42) is written as

$$f(\lambda) = \frac{1}{2\pi}\left(\rho_0 + 2\sum_{s=+1}^{+\infty} \rho_s cos(s\lambda)\right). \tag{1.43}$$

Remark 9 The integrals in (1.35) and (1.41) are deterministic (classical), while the integral in (1.37) is stochastic (although with deterministic integrand; for the definition of this kind of integral see, for example, Grimmett and Stirzaker [2001]: section 9.4 for deterministic integrands and section 13.8 for stochastic ones).

Under some conditions, a stochastic process can be expressed as an infinite combination of white noise. Since the noise always contains the same information, it follows that the information of the process can be encapsulated in a sequence of coefficients. The following theorem is a consequence of the *Wold decomposition* (see Wold [1938]).

Theorem 5 *Any (purely indeterministic) discrete-time stationary process (X_t) can be expressed in the form*

$$X_t = \sum_{s=0}^{+\infty} a_s \epsilon_{t-s}, \quad t \geq 1, \tag{1.44}$$

with $a_0 = 1$, $\sum_{s=0}^{+\infty} a_s^2 < \infty$ and (ϵ_s) a white noise process. The sequences $\{a_s\}$ and (ϵ_s) are uniquely determined.

Proof. See section 10.1.5 of Priestley (1981). □

Remark 10 Due to its similarity with the finite moving-average (MA) models, the expression (1.44) is known as the *MA(∞)-representation* of the process (X_t).

In Practice

Let us note that in a theoretically infinite stochastic process, only a finite quantity of variables can be considered in practice,

$$(X_t, 1 \leq t \leq T) = (X_1, X_2, \ldots, X_T). \tag{1.45}$$

1.3.2 Time Series Data

A time series can be interpreted as a realization of a (generating) stochastic process. For our purposes, a formal enough definition of time series is the following:

Definition 22 *A* time series *is a sequence of numerical variables,*

$$(x_t, 1 \leq t \leq T) = (x_1, \ldots, x_t, \ldots, x_T), \tag{1.46}$$

where the index t represents the time at which x_t is observed.

For this definition to be useful, some dependence among data is supposed. A time series is named *stationary* if its generating stochastic process is supposed stationary.

1.3.3 Statistical Inference

For the stationary time series $(x_t,\ 1 \leq t \leq T)$, the following inferential definitions and properties can be found, for example, in Priestley (1981).

Mean Function

The mean function (in fact, a constant $\mu_t = \mu$) is estimated by

$$\bar{x}_T = \frac{1}{T} \sum_{t=1}^{T} x_t. \tag{1.47}$$

Autocovariance Function

The autocovariance function can be estimated by

$$\hat{\sigma}_\tau = \frac{1}{T} \sum_{t=1}^{T-|\tau|} (x_t - \bar{x}_T)(x_{t+|\tau|} - \bar{x}_T), \quad |\tau| = 0, 1, \ldots, T-1. \tag{1.48}$$

In this expression, to obtain an unbiased estimator some authors prefer using $1/(T - |\tau|)$ instead of $1/T$ (see section 5.3.3 of Priestley [1981]); the expression (1.48) has lower mean square error.

Autocorrelation Function

Thus, the autocorrelation function can be estimated by

$$\hat{\rho}_\tau = \frac{\hat{\sigma}_\tau}{\hat{\sigma}_0}, \qquad |\tau| = 0, 1, \ldots, T-1. \tag{1.49}$$

Spectral Density Function

To estimate the spectral density function, the following concept is defined:

Definition 23 *The* periodogram *of* $(x_t, 1 \leq t \leq T)$ *is defined as*

$$I_T(\lambda) = \frac{1}{2\pi T} \left| \sum_{t=+1}^{T} x_t e^{-it\lambda} \right|^2, \quad \lambda \in [-\pi, +\pi]. \tag{1.50}$$

As estimator of the spectral density function, the periodogram is asymptotically unbiased but its variance does not decrease as n increases, so it is not consistent. There are several ways of constructing —basically by smoothing the periodogram— consistent estimates of the spectral density function.

Spectral Distribution Function

The integration, a sort of smoothing, provides a consistent estimate of the spectral distribution function.

Definition 24 *The* integrated *or* cumulative periodogram *of* $(x_t, 1 \leq t \leq T)$ *is defined as* $F_T(\lambda) = \int_{-\pi}^{\lambda} I_T(h)dh$*, or, with a normalization,*

$$F_T(\lambda) = \frac{1}{c_T} \int_{-\pi}^{\lambda} I_T(h)dh, \quad \lambda \in [-\pi, +\pi], \tag{1.51}$$

where $c_T = \int_{-\pi}^{-\pi} I_T(h)dh$*.*

Fourier Frequencies Set

Previous definitions have been given for $\lambda \in [-\pi, +\pi]$. In practice, only a finite set of values is considered for the estimation. The choice of the set of *Fourier frequencies* provides —among others— some simplification in the algebra (see, for example, sections 6.1.3 of Priestley [1981] and 2.7 of Diggle [1990]):

$$\mathcal{S} = \left\{ \lambda_j = \frac{2\pi j}{T}, \quad j = -\left[\tfrac{T-1}{2}\right], \ldots, -1, 0, +1, \ldots, +\left[\tfrac{T}{2}\right] \right\}. \tag{1.52}$$

In fact, these frequencies are related to efficient ways of computing the periodogram; for example, the *fast Fourier transform*. Then,

$$I_T(\lambda_j) = \frac{1}{2\pi T} \left| \sum_{t=+1}^{T} x_t e^{-it\lambda_j} \right|^2, \quad \lambda_j \in \mathcal{S}, \tag{1.53}$$

and the integrated periodogram takes the form $F_T(\lambda_j) = \sum_{i=1}^{j} I_T(\lambda_i)$, or, in the normalized version,

$$F_T(\lambda_j) = \frac{1}{c_T} \sum_{i=1}^{j} I_T(\lambda_i), \qquad \lambda_i \in \mathcal{S}, \quad \lambda_j \in \mathcal{S}, \tag{1.54}$$

where now $c_T = \sum_{i=1}^{m} I_T(\lambda_i)$, with m being the cardinal of $\mathcal{S}$.

Positive Frequencies Only

Both functions $f(\lambda)$ and $I_T(\lambda)$ are symmetric, so they (as well as set $\mathcal{S}$) could have been defined only in positive values in $[0, +\pi]$.

1.3.4 Mathematical Framework

The sets of sequences of variables (random or not) take values in, symbolically, $\mathbb{R}^\infty = \mathbb{R} \times \mathbb{R} \cdots$, which is a linear space with the usual operations of sum and product with a real number (see sections 2.1.1, 3.1.1, 3.3.1 and 3.4.1 of Kolmogórov and Fomín [1975]).

No more complex structure is required in this piece of work; note that we shall soon pass on functional spaces and the periodograms make sense —as a mathematical object— for any set of variables. Nonetheless, for $1 \leq m < \infty$, the set of m-order summable sequences is defined as

$$l^m = \left\{ (x_t) \in \mathbb{R}^\infty \;\; | \;\; \sum_{t=1}^{\infty} |x_t|^m dt < \infty \right\}. \tag{1.55}$$

With the usual operations for sequences, the set l^m is a linear space. With the distance

$$d_m((x_t^{(1)}), (x_t^{(2)})) = \left(\sum_{t=1}^{\infty} |x_t^{(1)} - x_t^{(2)}|^m \right)^{1/m}, \quad (x_t^{(k)}) \in l^m, \quad k = 1, 2. \tag{1.56}$$

l^m forms the metric space $(l^m, d_m(\cdot, \cdot))$. As this metric can be defined from the norm

$$\|(x_t)\|_m = \left(\sum_{t=1}^{\infty} |x_t|^m \right)^{1/m}, \quad (x_t) \in l^m. \tag{1.57}$$

the pair $(l^m, \|\cdot\|_m)$ is a normed space. These spaces are in general Banach spaces, and only the case $m = 2$ is a Hilbert space, as the norm verifies the parallelogram condition and the following inner product can be defined (see proposition 7 in appendix A.2):

$$\langle (x_t^{(1)}), (x_t^{(2)}) \rangle = \sum_{t=1}^{\infty} |x_t^{(1)} x_t^{(2)}|, \quad (x_t^{(k)}) \in l^2, \quad k = 1, 2. \tag{1.58}$$

1.3.5 Addendum: Locally Stationary Processes

Some causes of nonstationarity —as trend, heteroscedasticity and seasonality— can be removed by applying well-known transformations. A possible approach to nonstationary processes is based

on this removal. The other frequently used approach consists in supposing local stationarity and applying the usual techniques in narrow blocks. The literature includes several definitions of "nonstationary processes", as *locally stationary random processes*, *semistationary processes*, *quasi-stationary processes*, *piecewise stationary processes*, etcetera. For a stochastic process, there are many more ways of being nonstationary than stationary, and it seems that at least the local stationarity assumption is necessary. Perhaps those definitions of Priestley (1965) and Dahlhaus (1996) have been the most successful; see Dahlhaus' paper for a comparison of both spectra. In this section, the approach of Dahlhaus is chronologically presented from several papers.

As there is a dynamic change in time, in the nonstationary framework it is not possible to separate the time and the frequency domains. The strategy of Dahlhaus started with a sort of "spectral representation" definition:

Definition 25 *(Dahlhaus [1996]) A sequence of stochastic processes* $(X_{t,T}\ 1 \leq t \leq T,\ T \geq 1)$ *is called* locally stationary with transfer function A^0 and trend μ *if such a representation exists*

$$X_{t,T} = \mu\left(\frac{t}{T}\right) + \int_{-\pi}^{+\pi} e^{i\lambda t} A^0_{t,T}(\lambda) d\xi(\lambda), \tag{1.59}$$

where

(i) $\xi(\lambda)$ *is a stochastic process on* $[-\pi, +\pi]$ *with* $\overline{\xi(\lambda)} = \xi(-\lambda)$ *and*

$$cum\{d\xi(\lambda_1), \cdots, d\xi(\lambda_k)\} = \eta(\sum_{j=1}^{k} \lambda_j) h_k(\lambda_1, \cdots, \lambda_{k-1}) d\lambda_1 \cdots d\lambda_k,$$

where $h_1 = 0$, $h_2(\lambda) = 1$, $|h_k(\lambda_1, \cdots, \lambda_{k-1})| \leq const_k$ *for all* k, $cum\{\cdots\}$ *denotes the cumulant of* k*-th order and* $\eta(\lambda) = \sum_{j=-\infty}^{+\infty} \delta(\lambda + 2\pi j)$ *is the period* 2π *extension of the Dirac delta function.*

(ii) There is a constant c *and a* 2π*-periodic function* $A : [0,1] \times \mathbb{R} \to \mathbb{C}$ *with* $A(u, -\lambda) = \overline{A(u,\lambda)}$ *and*

$$sup_{t,\lambda} |A^0_{t,T}(\lambda) - A(t/T, \lambda)| \leq cT^{-1},$$

for all T*.*

$A(u,\lambda)$ *and* $\mu(u)$ *are assumed to be continuous in* u*.*

Remark 11 The smoothness of A in u guarantees that the process (in fact, the sequence of processes) has locally "stationary performance".

Definition 26 *(Dahlhaus [1996]) The* (time-varying) spectral density *of the process (sequence of processes) is defined as:*

$$f(u,\lambda) = A(u,\lambda)\overline{A(u,\lambda)} = |A(u,\lambda)|^2. \tag{1.60}$$

For these processes, Dahlhaus (1996) also defines the local covariance of lag k at time u, and gives kernel estimates of it, as well as of the spectral density.

For the locally stationary processes, Dahlhaus and Polonik have more recently given a sort of "MA(∞)-representation", instead of the previous spectral-type definition. Let

$$V(g) = sup\left\{\sum_{k=1}^{m} |g(x_k) - g(x_{k-1})|, \quad \text{where} \quad 0 \leq x_0 < \ldots < x_m \leq m,\ m \in \mathbb{N}\right\} \tag{1.61}$$

be the total variation of a function g on $[0,1]$, and for some $\kappa > 0$, let be

$$l(j) = \begin{cases} 1, & |j| \leq 1, \\ |j| log^{1+\kappa}|j| & |j| > 1. \end{cases} \tag{1.62}$$

Definition 27 *(Dahlhaus and Polonik [2006]) The sequence* $(X_{t,T},\ 1 \leq t \leq T, T \geq 1)$ *is a* locally stationary process *if it has the representation*

$$X_{t,T} = \sum_{j=-\infty}^{+\infty} a_{t,T}(j)\epsilon_{t-j}, \tag{1.63}$$

where the ϵ_t *are identically distributed with* $\mathbb{E}(\epsilon_t) \equiv 0$, $\mathbb{E}(\epsilon_s\epsilon_t) = 0$ *for* $s \neq t$, $\mathbb{E}(\epsilon_t^2) \equiv 1$, *and satisfying the following conditions:*

$$sup_t|a_{t,T}(j)| \leq \frac{K}{\ell(j)} \quad \textit{(with } K \textit{ not depending on } T\textit{)},$$

and there exist functions $a(\cdot, j) : (0,1] \to \mathbb{R}$ *with*

$$sup_u|a(u,j)| \leq \frac{K}{\ell(j)},$$

$$sup_j \sum_{t=1}^{T} \left| a_{t,T}(j) - a\left(\frac{t}{T}, j\right)\right| \leq K,$$

$$V(a(\cdot, j)) \leq \frac{K}{\ell(j)}.$$

This definition is more general than definition 25, since the parameter curves are allowed to have jumps (but bounded variation in time direction). On the other hand, this representation can be transformed easily into the previous time-varying spectral representation. The above conditions are discussed in Dahlhaus and Polonik (2009).

Definition 28 *(Dahlhaus and Polonik [2006]) Let* $(X_{t,T})$ *be a locally stationary process with time--varying spectral density* $f(u,\lambda)$*; then*

$$\sigma_{u,k} = \int_{-\pi}^{+\pi} f(u,\lambda)e^{i\lambda k}d\lambda = \sum_{j=-\infty}^{+\infty} a(u, k+j)a(u,j) \tag{1.64}$$

is the time-varying covariance *of lag* k *at rescaled time* u.

Remark 12 The integral in (1.64) is deterministic, while the integral in (1.59) is stochastic.

Definition 29 *(Dahlhaus and Polonik [2006]) Let* $(X_{t,n})$ *be a locally stationary process. The function*

$$f(u,\lambda) = \frac{1}{2\pi}|A(u,\lambda)|^2 \tag{1.65}$$

with

$$A(u,\lambda) = \sum_{j=-\infty}^{+\infty} a(u,j)e^{-i\lambda j} \tag{1.66}$$

is the time-varying spectral density function*.*

1.4 Stochastic Functions

This type of data appears in many mathematical areas and has been used many times over. In the theory of continuous-time univariate stochastic processes, $(X(t), t \in [0,T])$, for fixed t a random variable $X(t)$ is obtained, while for a given event $\omega \in \Omega$, the *trajectories* $(X(t))$ are in a functional space L, as represented through the application

$$\begin{array}{rccc} X(t,\cdot): & \Omega & \longrightarrow & L \\ & \omega & \to & X(t,\omega) \end{array}.$$

In this case, the characteristics of the space L depends on the properties of $(X(t))$; for example, for the Wiener process the trajectories are —almost surely— continuous everywhere but differentiable nowhere.

1.4.1 Models

The following definition is based on definition 1.1 of Ferraty and Vieu (2006). Let $(\Omega, \mathcal{F}, P)$ be a probability space.

Definition 30 *A* stochastic function *or* functional random variable *is a random variable,* $\mathcal{X} = \mathcal{X}(\omega),\ \omega \in \Omega$*, that takes values in a functional space* L*.*

Let $t \in [0,T]$ be the independent variable of the elements of L, then $\mathcal{X}$ is in fact a bidimensional function, $\mathcal{X}(\omega,t)$, such that for fixed ω a deterministic function is obtained and for fixed t a random variable is obtained (this point of view, instead of the previous definition, is preferred when the dynamic performance is studied). For simplicity, $\mathcal{X}(\omega,t)$ will be written as $\mathcal{X}$, and $\mathcal{X}(t)$ when the membership to the functional space L must be highlighted. The main interest will be in the application:

$$\begin{array}{rccc} \mathcal{X}(t,\cdot): & \Omega & \longrightarrow & L \\ & \omega & \to & \mathcal{X}(t,\omega) \end{array}.$$

As a final comment, let us notice that the classical analysis differentiation makes sense only when ω is fixed. In this situation $D^i\mathcal{X}(t)$ will be denoting the i-th derivative of the real function $\mathcal{X}(t) = \mathcal{X}(\omega, t)$ of real variable t:

$$D^i\mathcal{X}(t) = \frac{d^i\mathcal{X}(t)}{dt^i}, \quad t \in [0, T], \tag{1.67}$$

even when both quantities $\mathcal{X}$ and $D^i\mathcal{X}$ can be considered as stochastic; that is, in our framework D^i can be thought of as an operator in the functional space of nonstochastic functions L or, equivalently, as an operator in the previous functional space of random functions.

Remark 13 The variable t is real and "deterministic" while, in general, ω is not. For some type of random variables, the Stochastic Calculus provides definitions of the derivative operator with respect to ω (see, for example, section 1.2 of Nualart [1995]).

For a general space L of functions, Ferraty and Vieu (2006) propose the following definitions for the functional mean.

Definition 31 *The* mean function *of the model $\mathcal{X}$ is defined as*

$$\mu(t) = \mathbb{E}(\mathcal{X}) = \int_\Omega \mathcal{X}(\omega, t)dP(\omega), \quad t \in [0, T], \tag{1.68}$$

where $(\Omega, \mathcal{F}, P)$ is the probability space.

Ferraty and Vieu (2006) also give definitions for the *median function*, the *mode function* and estimators of them.

More generally, in the literature on random functions, concepts like (*auto*)*correlation function*, *mutual correlation function* (between two functions) or *spectral decomposition* can be found.

In Practice

Let us notice that in this section we have not taken into account the fact that a function is continuously observed in very few cases. In practice a function consists of a pair of vectors $(\mathbf{t}, \mathbf{X})$, with $\mathbf{t} = (t_1, t_2, \ldots, t_T)$ and $\mathbf{X} = (X_1, X_2, \ldots, X_T)$, where t_i is the time at which the X_i value is taken. Moreover, $\mathbf{t}$ could be different in each different element in a sample of functions.

1.4.2 Functional Data

Definition 32 *A* functional datum $\chi(t)$ *is an observation of a functional random variable $\mathcal{X}(\omega)$.*

For functional data, a huge amount of classical theory is available. The most important for us is that on metric, normed and Hilbert spaces, and their topology and calculus. Of special interest is the theory of linear spaces, where under good conditions (mainly numerability and separability of the induced topological space; see appendix A.3) bases of functions can be used to

approximate or represent the elements of the spaces. Some frequently used bases are: the basis of the monomials

$$\{1, t, t^2, t^3, \ldots\}, \tag{1.69}$$

the basis of the trigonometric functions

$$\{1, sin(t), cos(t), sin(2t), cos(2t), \ldots\}, \tag{1.70}$$

basis of the *spline functions*, basis of the *wavelets*, *exponential* and *power bases*, *polynomial bases*, *polygonal basis*, and *step-function basis* or *constant basis*, among others.

The *filtering* techniques for functional data use some basis $\{\psi_i\}$ and therefore work with the multivariate coefficients $\mathbf{c}$ (see the linear combinations of section A.1). Note that in this case the coefficients c_i contain more information than that of mere scalars.

1.4.3 Statistical Inference

Let $\chi_1(t), \ldots, \chi_e(t), \ldots, \chi_n(t)$ be a sample of *functional data*.

Definition 33 *The* sample mean function *of a set of functions is defined as*

$$\bar{\chi}(t) = \frac{1}{n} \sum_{e=1}^{n} \chi_e(t), \quad t \in [a, b] \subset \mathbb{R}, \tag{1.71}$$

and it estimates $\mu(t)$.

Ramsay and Silverman (2006) also give definitions of sample concepts like: *covariance function*, *correlation function*, *cross-covariance function* and *cross-correlation function*.

Remark 14 Although the sample mean can be computed in any linear space of functions, the ideas of approximation and convergence require an additional —stronger— analysis concepts, such as norm or inner product.

Remark 15 Our proposals use the sample mean as an inference tool. A worthwhile observation is that we are allowed to use this representative function due to the smoothness of our functional data, since this function does not reflect, in general, the characteristics of rough data.

1.4.4 Mathematical Framework

Given $I \subset \mathbb{R}$ compact, the set of continuous functions defined on I is denoted by

$$\mathcal{C}(I) = \{\chi : I \to \mathbb{R} \ \mid \chi \text{ is continuous in } t\}. \tag{1.72}$$

For $l \in \mathbb{N} \setminus \{0\}$, a more restrictive set is defined for differentiable functions,

$$\mathcal{C}^l(I) = \left\{\chi : I \to \mathbb{R} \ \mid \exists D^l\chi \text{ and } D^l\chi \in \mathcal{C}(I)\right\}. \tag{1.73}$$

Finally, for $m \in \mathbb{N} \setminus \{0\}$ the set of m-order integrable functions is defined as

$$\mathcal{L}^m(I) = \left\{ \chi : I \to \mathbb{R} \ \mid \ \int_I |\chi(t)|^m dt < \infty \right\}, \tag{1.74}$$

where the previous integration is usually the Lebesgue integral.

With the operations for functions, the three previous sets are linear spaces. Moreover, it holds that

Proposition 4 *For any finite $l \in \mathbb{N} \setminus \{0\}$ and $m \in \mathbb{N} \setminus \{0\}$,*

$$\mathcal{C}^l(I) \subset \mathcal{C}(I) \subset \mathcal{L}^m(I). \tag{1.75}$$

Proof.

The first inclusion holds by definition. In the case of the second, since for a given $\chi(t) \in \mathcal{C}(I)$ a finite constant exists such that $sup_{t\in[0,T]}|\chi(t)| \leq M$ then

$$\int_I |\chi(t)|^m dt \leq \nu(I) M^m < \infty$$

where $\nu(I)$ is the Lebesgue measure of I.

□

Thus, the following statements are given for the more general spaces of integrable functions, since the other two subsets are closed —as linear subspaces— and they inherit the structures.

The set $\mathcal{L}^m(I)$ with the distance

$$d_m(\chi_1, \chi_2) = \left(\int_I |\chi_1(t) - \chi_2(t)|^m dt \right)^{1/m}, \quad \chi_k \in \mathcal{L}^m(I), \quad k = 1, 2. \tag{1.76}$$

form the metric space $(\mathcal{L}^m(I), d_m(\cdot,\cdot))$. As this metric can be defined from the norm

$$\|\chi\|_m = \left(\int_I |\chi(t)|^m dt \right)^{1/m}, \quad \chi \in \mathcal{L}^m(I), \tag{1.77}$$

the pair $(\mathcal{L}^m(I), \|\cdot\|_m)$ is a normed space. These spaces are in general numerable and separable Banach spaces, and only the case $m = 2$ is a Hilbert space, as its norm verifies the parallelogram condition and can be defined (see proposition 7 in appendix A.2) the inner product

$$\langle \chi_1, \chi_2 \rangle = \int_I |\chi_1(t)\chi_2(t)| dt, \quad \chi_k \in \mathcal{L}^2(I), \quad k = 1, 2. \tag{1.78}$$

In general, the functional space determines the allowed operations: proximity, types of convergence, continuity or geometry for example, projection, angle or orthogonality (see sections 2.1.1, 3.1.1, 3.3.1 and 3.4.2 of Kolmogórov and Fomín [1975]).

Expression (1.68) needs the $\mathcal{L}^1(I)$ space while expression (1.71) needs just a linear space structure (both spaces need an overlapped metric structure for the convergence). More generally, Ferraty and Vieu (2006) frequently base definitions and model adjustements on optimization problems, so they usually work in "good" Banach spaces; on the other hand, Ramsay and Silverman (2006) need the more restrictive Hilbert space structure of $(\mathcal{L}^2(I), \langle\cdot,\cdot\rangle)$, as they use the inner product to compute the coefficients of fitted models.

Our Functional Spaces

In this document, the domain of the functions is compact (in $\mathbb{R}$ with the Borel topology): in chapter 2 the interval is $I = [-\pi, +\pi]$ (or the joint of g intervals like this), while in chapter 3 it is $I = [0, T]$. Functions are continuous in t or composed of continuous parts: in chapter 2, due to the integrability of the periodogram and, in chapter 3, due to the differentiability assumptions.

As a distance measurement between two functions we have taken d_1 (defined by [1.76] with $m = 1$), so the metric or normed space of functions into which we shall be working are: the spaces $(\mathcal{C}(I), \|\cdot\|_1)$ or $(\mathcal{L}^1(I), \|\cdot\|_1)$ in chapter 2 and the more restrictive spaces $\left(\mathcal{C}^l(I), \|\cdot\|_1\right)$ in chapter 3. Some other distance could be considered, and in general there is no "best" one. For example, with the usual distance of $\mathcal{L}^2$, big differences between functions would be highlighted and so would be the corresponding values of the independent variable; this distance is usually preferred to develop theory since the square power is a more manageable way of avoiding the sign than the absolute value.

1.4.5 Addendum: Functional Depth

The statistical concept of *depth* is a measurement of the "centrality" of each element inside a sample. This implies, for example, that in a set of points in $\mathbb{R}^m, m \in \mathbb{N} \setminus \{0\}$, the closer a point is to the mass center, the deeper it is. The same general idea applies to other types of data, including functions. Different definitions of depth for functions can be given. In this section we will describe and use the definitions proposed in López-Pintado and Romo (2009).

Band Depth

Let $G(\chi(t)) = \{(t, \chi(t)) \mid t \in [a, b]\}$ denote the graph in $\mathbb{R}^2$ of a function $\chi(t)$; let $\chi_e(t)$, $e = 1, \ldots, n$, be a sample of functions; then a subset of these functions, $\chi_{e_j}(t)$, $j = 1, \ldots, m$, determines the band in $\mathbb{R}^2$ defined as

$$B(\chi_{e_1}(t), \ldots, \chi_{e_m}(t)) = \{(t, y) \mid t \in [a, b], \min_{r=1,\ldots,m} \chi_{e_r}(t) \leq y \leq \max_{r=1,\ldots,m} \chi_{e_r}(t)\}. \tag{1.79}$$

For any function $\chi(t)$, the quantity

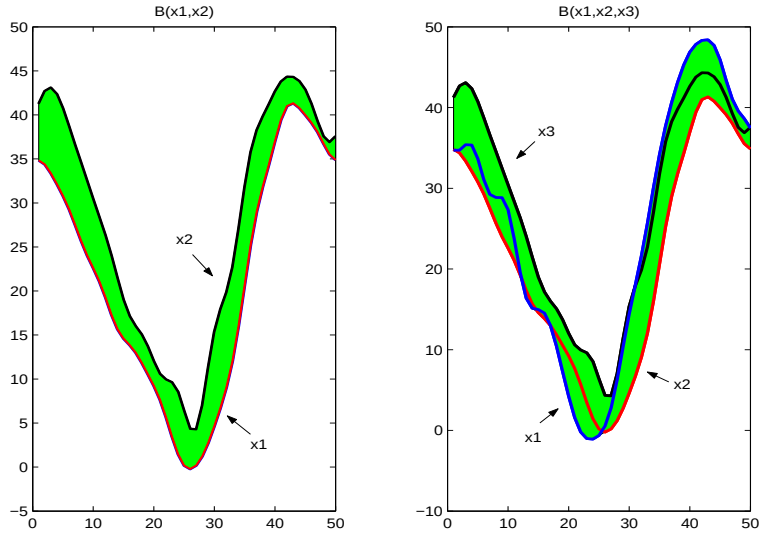
$$BD_n^{(j)}(\chi(t)) = \binom{n}{j}^{-1} \sum_{1 \leq e_1 < e_2 < \ldots < e_j \leq n} \mathbb{I}\{G(\chi(t)) \subset B(\chi_{e_1}(t), \ldots, \chi_{e_j}(t))\}, \qquad j \geq 2, \tag{1.80}$$

expresses the proportion of bands, determined by j different curves, $\chi_{e_1}(t), \ldots, \chi_{e_j}(t)$, containing the graph of $\chi(t)$ (the indicator function takes the value $\mathbb{I}\{A\} = 1$ if A occurs and $\mathbb{I}\{A\} = 0$ otherwise).

Definition 34 *For functions $\chi_e(t)$, $e = 1, \ldots, n$, the* band depth *of any of these curves χ with respect to the sample is*

$$BD_{n,J}(\chi(t)) = \sum_{j=2}^{J} BD_n^{(j)}(\chi(t)), \qquad 2 \leq J \leq n. \tag{1.81}$$

Figure 1.1: Example of functions and their band



If $\mathcal{X}$ is a stochastic process and $\mathcal{X}_e(t)$, $e = 1, \ldots, n$, are copies of it, the population versions of these depth indexes are, respectively,

$$BD^{(j)}(\mathcal{X}) = P\{G(\mathcal{X}) \subset B(\mathcal{X}_{e_1}, \ldots, \mathcal{X}_{e_j})\}, \quad j \geq 2, \tag{1.82}$$

and

$$BD_J(\mathcal{X}) = \sum_{j=2}^{J} BD^{(j)} = \sum_{j=2}^{J} P\{G(\mathcal{X}) \subset B(\mathcal{X}_{e_1}, \ldots, \mathcal{X}_{e_j})\}, \quad J \geq 2. \tag{1.83}$$

Modified Band Depth

A more flexible notion of depth is also defined in López-Pintado and Romo (2009). The indicator function in definition (1.80) is replaced by the length of the set where the function is inside the corresponding band. For any function $\chi(t)$ of $\chi_e(t)$, $e = 1, \ldots, n$, and $2 \leq j \leq n$, let

$$\begin{aligned} A_j(\chi(t)) &\equiv A(\chi(t); \chi_{e_1}(t), \ldots, \chi_{e_j}(t)) \\ &\equiv \{t \in [a,b] \mid \min_{r=1,\ldots,j} \chi_{e_r}(t) \leq \chi(t) \leq \max_{r=1,\ldots,j} \chi_{e_r}(t)\} \end{aligned} \tag{1.84}$$

be the set of points in the interval $[a,b]$ where the function $\chi(t)$ is inside the band. If ν is the Lebesgue measure on the interval $[a,b]$, $\nu_r(A_j(\chi(t))) = \nu(A_j(\chi(t)))/\nu([a,b])$ is the "proportion of time" that $\chi(t)$ is inside the band.

The quantity

$$MBD_n^{(j)}(\chi(t)) = \binom{n}{j}^{-1} \sum_{1 \leq e_1 < e_2 < \ldots < e_j \leq n} \nu_r(A(\chi(t); \chi_{e_1}(t), \ldots, \chi_{e_j}(t))), \quad 2 \leq j \leq n, \tag{1.85}$$

is a modified version of $BD_n^{(j)}$.

Notice that if $\chi(t)$ is always inside the band, the measure $\nu_r(A_j(\chi(t)))$ is 1 and this generalises the definition given in (1.80).

Definition 35 *The* modified band depth *of any of these curves χ with respect to the sample is*

$$MBD_{n,J}(\chi(t)) = \sum_{j=2}^{J} MBD_n^{(j)}(\chi(t)), \qquad 2 \leq J \leq n. \tag{1.86}$$

If $\mathcal{X}_e$, $e = 1, \ldots, n$, are independent copies of the stochastic process $\mathcal{X}$, the population versions of these depth indexes are, respectively,

$$MBD^{(j)}(\mathcal{X}) = \mathbb{E}\left(\nu_r(A(\mathcal{X}; \mathcal{X}_{e_1}, \ldots, \mathcal{X}_{e_j}))\right), \quad 2 \leq J \leq n, \tag{1.87}$$

and

$$MBD_J(\mathcal{X}) = \sum_{j=2}^{J} MBD^{(j)}(\mathcal{X}) = \sum_{j=2}^{J} \mathbb{E}\left(\nu_r(A(\mathcal{X}; \mathcal{X}_{e_1}, \ldots, \mathcal{X}_{e_j}))\right), \quad 2 \leq J \leq n. \tag{1.88}$$

In chapter 2 we have used the value $J = 2$, since it is computationally fast and the modified band depth is very stable in J, providing similar center-outward order in a collection of functions (see López-Pintado and Romo [2006, 2009]).

Robust Inference: Trimmed Mean

Let $\chi_{(e)}(t)$, $e = 1, \ldots, n$ be a sample of functions ordered by decreasing depth, then

Definition 36 *The* sample α-trimmed mean function *is defined as*

$$\overset{\alpha}{\bar{\chi}}(t) = \frac{1}{n - [n\alpha]} \sum_{e=1}^{n-[n\alpha]} \chi_{(e)}(t), \tag{1.89}$$

where $[\cdot]$ is the integer part function.

A kind of "median function", in the sense of the "deepest"curve, is obtained with the previous expression just considering $\alpha = (n-1)/n$. Nevertheless, the α-trimmed mean is robust, like the median, and summarizes the general performance of the functions, like the mean. In our simulation and real data exercises, a value of $\alpha = 0.2$ is used. It means that for each group only the 80% deepest data are considered, while the remaining 20% are left out.

1.5 The Classification Problem

It is frequently necessary to study a set of —abstract or real— objects in order to characterise their heterogeneity, that is, to identify the underlying structure of subsets. This task is known as *classification*, and consists in finding some "properties" —theoretical or approximated— that characterise the differences among subsets. As the elements of each subset must be similar, some kind of "distance", based on the characterising properties, is necessary to evaluate the proximity — between two elements, an element and a group or two groups— and, finally, to apply a "criterion"

for determining the underlying structure. In the rest of this section, a general symbolic notation is used to locate these concepts of "property", "distance" and "criterion".

When there is not previous knowledge about the structure, the problem is termed *unsupervised classification* —or *clustering*— and even the number of subsets is usually unknown and has to be determined. If the structure of subsets is indicated by the membership of the elements in a subset (through labels), the problem is named *supervised classification*. The classification that we address here is of this latter kind.

1.5.1 Theoretical Rule

Let $P^{(k)},\ k = 1, \ldots, K$ be different and disjoint populations of theoretical mathematical objects, where "disjoint" means that any element belongs to only one population, and let $c^{(\cdot)}$ be a property characterising these populations as much as possible; then the classification problem consists in applying a criterion to decide to which population a new element E belongs to, by using the information provided by its property $c_{(E)}$. It is important to notice that the choice of $c^{(\cdot)}$ and $c_{(E)}$ usually depends on the information available or the information that we are capable of knowing. Let us assume that $c^{(\cdot)}$ does characterise the populations in the sense that it is different and unique for each group. Then, it seems natural for the election of $c_{(E)}$ to be as similar as possible to $c^{(\cdot)}$, that is, to capture as much "inherited" information as possible. In the following, it is supposed that the definitions of $c_{(E)}$ and $c^{(\cdot)}$ depend on one another.

Separable Populations

Let us consider the unrealistic case in which the quantity $c_{(E)}$ can contain the same information as $c^{(\cdot)}$, that is, characterizing information. We shall say that these are *separable populations*.

In this case, we can know the exact information of the element and the populations, so the classification is not a problem but a mere deterministic application, $C : \cup_{k=1}^{K} P^{(k)} \to \{1, 2, \ldots, K\}$ such that:

$$C(E) = \begin{cases} k = 1 & \text{if} \quad c_{(E)} = c^{(1)} \\ k = 2 & \text{if} \quad c_{(E)} = c^{(2)} \\ \vdots & \qquad \vdots \\ k = K & \text{if} \quad c_{(E)} = c^{(K)} \end{cases} \tag{1.90}$$

The information contained in $c_{(E)}$ implies that the populations are *separable*.

Nonseparable Populations

In the previous case, $c_{(E)}$ could contain as much information as $c^{(\cdot)}$. Nevertheless, in most situations it happens that $c_{(E)}$ provides useful information but not sufficient information, in general, for a perfect classification. We shall say that these are *nonseparable populations*.

For nonseparable populations, such a naive rule as (1.90) is not available, and some elements cannot be assigned; this can be represented as $C : \cup_{k=1}^{K} P^{(k)} \to \{1, 2, \ldots, K, \emptyset\}$ such that:

$$C(E) = \begin{cases} k = 1 & \text{if} \quad c_{(E)} = c^{(1)} \\ k = 2 & \text{if} \quad c_{(E)} = c^{(2)} \\ \vdots & \vdots \\ k = K & \text{if} \quad c_{(E)} = c^{(K)} \\ k = \emptyset & \text{otherwise} \end{cases}, \tag{1.91}$$

where the element E is assigned to the empty set if it is not equal to one, and only one, model. In this case the rule cannot assign with certainty the element to one population.

In the following we shall consider that $c_{(E)}$, for E belonging to any of the populations, cannot contain in general characterizing information, as in an other case there would be no classification problem. That is, we shall consider the case of nonseparable populations.

1.5.2 Sample Rule

Since in general the theoretical populations are defined to model the reality, the exact information $c^{(k)}$ is not known, and the previous rule has to be substituted by the empirical version, $\hat{C} : \cup_{k=1}^{K} P^{(k)} \to \{1, 2, \ldots, K, \emptyset\}$.

$$\hat{C}(E) = \begin{cases} k = 1 & \text{if} \quad c_{(E)} \approx \hat{c}^{(1)} \\ k = 2 & \text{if} \quad c_{(E)} \approx \hat{c}^{(2)} \\ \vdots & \vdots \\ k = K & \text{if} \quad c_{(E)} \approx \hat{c}^{(K)} \\ k = \emptyset & \text{otherwise} \end{cases} \tag{1.92}$$

where the estimates $\hat{c}^{(k)}$ are constructed from samples of the populations. In practice, the element E is assigned to the closest population. Again, the element is assigned to the empty set if it is not similar to one, and only one, model. In this case the classification rule is less certain than the previous $C(\cdot)$ and a stochastic component is added by the use of samples.

Some Estimators $\hat{c}^{(\cdot)}$

If $E_1^{(k)}, \ldots, E_{n_k}^{(k)}$ is a sample of the k-th population, usually $\hat{c}^{(k)}$ is such that

$$\hat{c}^{(k)} = \frac{1}{n_k} \sum_{e=1}^{n_k} c_{E_e^{(k)}}, \tag{1.93}$$

where the term $c_{E_e^{(k)}}$, of the e-th element $E_e^{(k)}$ of the k-th sample, has both approximative and stochastic characters. The average (1.93) is the sample version of the population quantity $c^{(k)} = \mathbb{E}(c_{E^{(k)}})$, where $E^{(k)}$ follows the theoretical functional distribution of the k-th population and $c_{E^{(k)}}$ is its property.

Nonetheless, before using expression (1.93) it is necessary to be sure that such a mix of information (the sample mean) makes sense and is useful. For example, if the property of the populations were the *range of values* (e.g. of continuous random variables), averaging would be a quite inappropriate way of mixing the information. A more proper estimator would be

$$\hat{c}^{(k)} = [min_{e=1,\dots,n_k}\{c_{E_e^{(k)}}\}, max_{e=1,\dots,n_k}\{c_{E_e^{(k)}}\}] \tag{1.94}$$

1.5.3 Our Classification Frameworks

Minimizing the Distance

The role of the "similarity of the property" has been highlighted in the previous classification criteria, but this similarity (equality and approximation) has to be measured with a distance. The theoretical criteria are, in this case, equivalent to

$$k = argmin_{\{1,\cdots,K\}}\left\{d(c_{(E)}, c^{(k)})\right\}, \tag{1.95}$$

since all the values $d(c_{(E)}, c^{(k)}),\ k = 1, \dots, K$ are constant but one. Then, it seems natural assigning a new element to the population minimizing the distance to the group representative; that is, the sample criteria could be substituted by

$$k = argmin_{\{1,\cdots,K\}}\left\{d(c_{(E)}, \hat{c}^{(k)})\right\}. \tag{1.96}$$

Nevertheless, the exact theoretical information $c_{(E)}$ is usually unknown due to different causes, for example measurement and calculation errors, partial knowledge or computational aspects. In this situation, the approximation $\tilde{c}_{(E)}$ is available. So happens with $\tilde{d}(\cdot,\cdot)$, which denotes the fact that, in general, the exact theoretical distance cannot be computed.

The previous general objects will take the following mathematical meaning for the classification methods proposed in chapters 2 and 3:

Time Series Method

$c^{(k)}$	Curve formed from the spectral distribution function models
$c_{(E)}$	Curve formed in the same way for the time series E
$d(\cdot,\cdot)$	Natural distance of the functional space $\mathcal{L}^1$
$\hat{c}^{(k)}$	Empirical curve estimate formed from integrated periodograms
$\tilde{c}_{(E)}$	Curve formed from the integrated periodogram of the series E
$\tilde{d}(\cdot,\cdot)$	Approximation of the previous distance
$\hat{C}(E)$	Criterion such that $k = argmin_{\{1,2\}}\left\{\tilde{d}(\tilde{c}_{(E)}, \hat{c}^{(k)})\right\}$.

$c^{(k)}$	Univariate variable $Y^{(\cdot)}$ formed from the functional models
$c_{(E)}$	Univariate variable formed in the same way for the function E
$d(\cdot,\cdot)$	Natural distance of $\mathbb{R}$
$\hat{c}^{(k)}$	Empirical value $y^{(k)}$ formed from samples
$\tilde{c}_{(E)}$	Value $y_{(E)}$ formed from the curve E
$\tilde{d}(\cdot,\cdot)$	Approximation of the previous distance
$\hat{C}(E)$	Criterion such that $k = argmin_{\{1,2\}}\left\{\tilde{d}(\tilde{c}_{(E)}, \hat{c}^{(k)})\right\}$.

1.5.4 Stochastic Rule

So far we have relegated some difficult or uncomfortable decisions —e.g. nonseparable populations— to the "otherwise" case of the classification rules. On the other hand, the rules tried to assign a new element with certainty, instead of with partial uncertainty. Finally, the stochastic character of the rule (1.92) has been mentioned only implicitly, while the estimators are random quantities. The previous enunciations of the rules highlighted the similarity of the properties and the certainty in the classification.

For several reasons, and sometimes for necessity, it is usually more convenient an enunciation in terms of probabilities:

$$\hat{C}(E) = \begin{cases} k = 1 & \text{with probability} \quad p_1(c_{(E)}, \hat{c}^{(1)}, \hat{c}^{(2)}, \ldots, \hat{c}^{(K)}) \\ k = 2 & \text{with probability} \quad p_2(c_{(E)}, \hat{c}^{(1)}, \hat{c}^{(2)}, \ldots, \hat{c}^{(K)}) \\ \vdots & \qquad\qquad \vdots \\ k = K & \text{with probability} \quad p_K(c_{(E)}, \hat{c}^{(1)}, \hat{c}^{(2)}, \ldots, \hat{c}^{(K)}) \\ k = \emptyset & \text{with probability} \quad p_0(c_{(E)}, \hat{c}^{(1)}, \hat{c}^{(2)}, \ldots, \hat{c}^{(K)}) \end{cases}, \tag{1.97}$$

with $\sum_{k=0}^{K} p_k(c_{(E)}, \hat{c}^{(1)}, \hat{c}^{(2)}, \ldots, \hat{c}^{(K)}) = 1$. Classifying an element E in terms of proper probabilities is more informative than not classifying it. The similarity and distances can be used to calculate these probabilities, but this is a complex task out of the scope of this discussion. While the election of the probabilities may be simple for separable populations, how to calculate them may be quite complex for nonseparable populations. Finally, let us notice that it is easy to obtain the rule (1.92) as a particular case of this rule (1.97).

1.5.5 Asymptotic Behaviour

If the properties $c^{(k)}$ and $c_{(E)}$, the distance $d(\cdot,\cdot)$, and the estimates $\hat{c}^{(k)}$ are properly defined, the sample classification rule $\hat{C}$ tends to provide the same classification as the theoretical rule C:

$$\hat{C} \underset{n_k \to \infty}{\longrightarrow} C \tag{1.98}$$

This means that the rule $\hat{C}$ converges to C in the sense that asymptotically $\hat{C}$ tends to classify the element E as C would do. Notice that the election of $\hat{c}^{(k)}$ should depend on the previous election of $c^{(k)}$.

Both relations $=$ and $\approx$ can be expressed by the distance $d(\cdot,\cdot)$, and it can be written informally:

$$d(c_{(E)}, c^{(k)}) \leq d(c_{(E)}, \hat{c}^{(k)}) + d(\hat{c}^{(k)}, c^{(k)}),$$

and, analogously,

$$d(c_{(E)}, \hat{c}^{(k)}) \leq d(c_{(E)}, c^{(k)}) + d(c^{(k)}, \hat{c}^{(k)}).$$

Thus, when $d(\hat{c}^{(k)}, c^{(k)}) \to 0$ it is concluded, on the one hand, that $d(c_{(E)}, c^{(k)}) \leq lim\{d(c_{(E)}, \hat{c}^{(k)})\}$ and, on the other hand, that $lim\{d(c_{(E)}, \hat{c}^{(k)})\} \leq d(c_{(E)}, c^{(k)})$, so

$$lim\{d(c_{(E)}, \hat{c}^{(k)})\} = d(c_{(E)}, c^{(k)}). \tag{1.99}$$

Several samples (the data) may not be separable due to the fact that perhaps there are elements that could have been generated by different models and the information available from the property does not characterise the membership. Asymptotically, what usually happens is that the unlimited amount of information in the training samples —of the supervised classification framework— usually facilitates "the separability". Then, in spite of the uncertainty and random components, a classification could be "asymptotically perfect", where *perfect* must be understood in the sense that, for separable populations,

$$\begin{cases} p(\hat{C}(E) = 1) = 1 & \text{if} \quad E \in P^{(1)} \\ p(\hat{C}(E) = 2) = 1 & \text{if} \quad E \in P^{(2)} \\ \vdots & \vdots \\ p(\hat{C}(E) = K) = 1 & \text{if} \quad E \in P^{(K)} \end{cases}, \tag{1.100}$$

and, for nonseparable populations,

$$\begin{cases} p(\hat{C}(E) = 1) = 1 & \text{if} \quad E \in P^{(1)} \cap \{\cup_{k\neq 1} P^{(k)}\}^c \\ p(\hat{C}(E) = 2) = 1 & \text{if} \quad E \in P^{(2)} \cap \{\cup_{k\neq 2} P^{(k)}\}^c \\ \vdots & \vdots \\ p(\hat{C}(E) = K) = 1 & \text{if} \quad E \in P^{(K)} \cap \{\cup_{k\neq K} P^{(k)}\}^c \\ p(\hat{C}(E) = 1) = p_{12}^{(1)} & \text{if} \quad E \in P^{(1)} \cap P^{(2)} \cap \{\cup_{k\neq 1,2} P^{(k)}\}^c \\ p(\hat{C}(E) = 2) = p_{12}^{(2)} & \text{if} \quad E \in P^{(1)} \cap P^{(2)} \cap \{\cup_{k\neq 1,2} P^{(k)}\}^c \\ \vdots & \vdots \end{cases}, \tag{1.101}$$

where the superindex ^{c} denotes the complementary set and, in the place of the second set of vertical points, all possible intersections among the populations must be considered (only the case of the intersection of the two first populations have been included). The election of the probabilities can follow lots of different criteria, e.g. the probabilities being proportional to the likelihood of having been generated by the model of each class.

How close to this "perfect" performance the rule C is depends on its own definition or design.

1.5.6 Theoretical Misclassification Rates

Let the populations be $P^{(k)},\ k = 1, \ldots, K$, an element be $E \in \cup_k P^{(k)}$ and the classification rule be $C : \cup_{k=1}^{K} P^{(k)} \to \{1, 2, \ldots, K\}$. Let us define the successes $\mathcal{E}^{(k)} = \{C(E) \neq k\} \cap \{E \in P^{(k)}\}$, $k = 1, \ldots, K$; that is, $\mathcal{E}^{(k)}$ is the success *misclassifying an element of the k-th population* (chosen at random). By using the conditional probability definition, the probability of $\mathcal{E}^{(k)}$ is

$$p(\mathcal{E}^{(k)}) = p(\{C(E) \neq k\} \cap \{E \in P^{(k)}\}) = p(\{C(E) \neq k\} \mid \{E \in P^{(k)}\}) \cdot p(\{E \in P^{(k)}\}). \quad (1.102)$$

Now the success *misclassifying an element* (chosen at random) is written, from the previous disjoint successes, as

$$\mathcal{E} = \cup_{k=1}^{K} \mathcal{E}^{(k)}, \quad (1.103)$$

so the probability of misclassification can be calculated as

$$p(\mathcal{E}) = \sum_{k=1}^{K} p(\mathcal{E}^{(k)}) = \sum_{k=1}^{K} p(\{C(E) \neq k\} \mid \{E \in P^{(k)}\}) \cdot p(\{E \in P^{(k)}\}). \quad (1.104)$$

For the particular case of two populations ($K = 2$),

$$\begin{aligned} p(\mathcal{E}) &= p(\{C(E) = 2\} \mid \{E \in P^{(1)}\}) \cdot p(\{E \in P^{(1)}\}) \\ &\quad + p(\{C(E) = 1\} \mid \{E \in P^{(2)}\}) \cdot p(\{E \in P^{(2)}\}). \end{aligned} \quad (1.105)$$

Sometimes the quantities involved in this expression can be calculated easily and even without calculations; other times, more or less difficult calculations are necessary. See the models of the simulations exercises in section 3.3.

1.5.7 Example

To illustrate the previous frameworks, let us consider random variables following discrete uniform laws with different and disjoint (nonoverlapping) set of values; these populations are different and disjoint (any variable follows only one of the laws). The groups are characterised by the property *set of values*. For a new variable the most similar information to the set of values is the *single value* of the variable, which is also characterising information. Let us measure the proximity of a single value to a set of values through the minimum of the absolute values of the distances from the single value to the values of the set. Under the knowledge of all the previous information, the criterion (1.90) can be applied without problems. Nevertheless, several complexities arise immediately. On the one hand, we have some limitation in managing numbers and operations, since we can work with a high but limited level of precision; this implies that approximations ($\approx$) must be considered instead of equalities ($=$) in criterion (1.90). On the other hand, when the property *set of values* of the populations is not known, it is necessary to use some estimator of it (notice that in this case an expression like (1.93) makes no sense). If the estimator of the *set of values* is a record of the

values of a sample and the approximations are good enough, asymptotically there will be enough information to classify as stated in (1.100).

On the other hand, if the sets of values of these previous discrete uniform laws are not disjoint, that is, they overlap, then we are in the case of nonseparable populations. The main difference is that the property *single value* of the variable is not characterising, and some rule of the form (1.91) must be considered at the beginning. The technical problems mentioned in the previous paragraph would also remain in this case. Finally, asymptotically and under good conditions a "perfect" classification would take the form (1.101).

Chapter 2

Time Series Classification

Summary: We propose using the integrated periodogram to classify time series. The method assigns a new element to the group minimizing the distance from the element integrated periodogram to the group mean of integrated periodograms. Local computation of these periodograms allows the application of this approach to nonstationary time series. Since the integrated periodograms are functional data, we apply depth--based functional techniques to make the classification robust. The method provides small error rates with both simulated and real data, and shows good computational performance[1].

Key words: time series, classification, integrated periodogram, depth.

2.1 Introduction

Classification of time series is a statistical subject with many applications. Time series can be studied from both time and frequency domains; while the former uses position or time as an index, the latter involves the frequency. With short stationary series, a time domain approach based on usual multivariate techniques can be applied. However, a frequency domain approach is more appropriate with long time series because it provides a reduction of the dimension. Moreover, frequency domain is particularly important for nonstationary series (Huang et al. [2004]). There are many studies on classification methods for stationary processes in both domains (see references in chapter 7 of Taniguchi and Kakizawa [2000]). Several authors have addressed the discrimination analysis of nonstationary time series: Hastie et al. (1995), Shumway (2003), Huang et al. (2004), Hirukawa (2004), Sakiyama and Taniguchi (2004), Chandler and Polonik (2006) and Maharaj and Alonso (2007), among others. Caiado et al. (2006) define a measure based on the normalized periodogram and use it for both clustering and classifying between stationary and nonstationary time series. Our procedure uses the integrated periodograms to classify time series and therefore

[1]MATLAB code is available at `http://www.Casado-D.org/edu/publications.html`.

is a frequency domain approach.

Since the integrated periodogram can be seen as a function, we shall use specific techniques for functional data analysis. There are several studies on the statistical analysis of functional data and, particularly, on their classification. For example, a penalized discriminant analysis is proposed in Hastie et al. (1995); it is adequate for situations with many highly correlated predictors, like those obtained by discretizing a function. Nonparametric tools to classify a set of curves have been introduced in Ferraty and Vieu (2003), where authors calculate the posterior probability of belonging to a given class of functions by using a consistent kernel estimator. A new method for extending classical linear discriminant analysis to functional data has been analysed in James and Hastie (2001); this technique is particularly useful when only fragments of the curves are observed. The problem of unsupervised classification or clustering of curves is addressed in James and Sugar (2003), who elaborate a flexible model-based approach for clustering functional data; it is effective when the observations are sparse, irregularly spaced or occur at different time points for each subject. In Abraham et al. (2003) unsupervised clustering of functions is considered; they fit the data by B-splines and partition is done over the estimated model coefficients using a k-means algorithm. In a related problem, Hall et al. (2001) explore a functional data-analytic approach to performing signal discrimination. Nonetheless, many of these procedures are highly sensitive to outliers. A natural idea for classifying functions is to minimize the distance between the new curve and a reference one from the group. The approach presented in this chapter follows this idea. As a reference function of each group, we shall take the mean of the integrated periodograms of its elements. Later, this curve will be substituted by a more robust representative.

The notion of statistical *depth* was first introduced for multivariate data. It measures the "centrality" or "outlyingness" of an observation within a set of data (or with respect to a probability distribution), providing a criterion for ordering observations from center-outward. This idea of depth has been extended to functional data in several papers (see, e.g. Fraiman and Muniz [2001] and López-Pintado and Romo [2009]). Moreover, López-Pintado and Romo (2006) have used this concept to classify curves. Since robustness is an interesting feature of the statistical methods based on depth, we have applied these ideas to add robustness to our time series classification procedure. Their method considers the α-trimmed mean as a reference curve of each group, which is defined as the average of the $1-\alpha$ proportion of deepest curves from the sample; in other words, it leaves $100\alpha\%$ of the least representative data curves out.

The chapter is organized as follows: in section 2, we include some definitions and explain how depth can be used to make the method robust; in section 3, we describe the classification algorithm; the next two sections, 4 and 5, show the performance of the procedure with simulated and real data, respectively; a brief summary of conclusions is given in section 6.

2.2 The Classification Method

A first and important step in our classification proposal is to transform the time series problem into a functional data problem by considering the integrated periodogram of each time series.

2.2.1 The Integrated Periodogram

The Fourier transform of the correlation function of an absolutely summable stochastic process is known as *spectral density* or *spectrum*; its integration provides the *spectral distribution function* or *cumulative spectrum*. Let (X_t) be a stationary process with autocovariance function $\sigma_s = cov(X_t, X_{t-s})$ satisfying $\sum_{s=-\infty}^{+\infty} |\sigma_s| < +\infty$. Then the spectral density can be expressed in terms of the autocorrelation as $f(\lambda) = \sum_{s=-\infty}^{+\infty} \rho_s \exp(-2\pi i s\lambda)$, and it holds that $\rho_s = \int_{-1/2}^{+1/2} \exp(2\pi i s\lambda) dF(\lambda)$, where $F(\cdot)$ is the spectral distribution function.

The *periodogram* is the sample version of the population concept of spectral density, and it expresses the contribution of the frequencies to the variance of a series. Let $(x_t^{(k)}) = (x_1^{(k)}, \ldots, x_T^{(k)})$ be a time series of the k-th population; the periodogram $I_T^{(k)}$ is obtained as indicated in (1.53):

$$I_T^{(k)}(\lambda_j) = \frac{1}{2\pi T} \left| \sum_{t=1}^{T} x_t^{(k)} e^{-it\lambda_j} \right|^2, \quad \lambda_j \in \mathcal{S}. \tag{2.1}$$

Its cumulative version is the integrated periodogram $F_T^{(k)}$ calculated as indicated in (1.54), that is,

$$F_T^{(k)}(\lambda_j) = \frac{1}{c_{T,k}} \sum_{i=1}^{j} I_T^{(k)}(\lambda_i), \quad \lambda_j \in \mathcal{S}, \quad \lambda_i \in \mathcal{S}, \tag{2.2}$$

where $c_{T,k} = \sum_{i=1}^{m} I_T^{(k)}(\lambda_i)$. The normalized version of the cumulative periodogram takes into account the shape of the curves more than the nonnormalized version, which also considers the scale.

In our case, we propose using the normalized version when the graphs of the functions of the different groups tend to intersect and there is no clear scale pattern, and using the nonnormalized one when the graphs do not tend to intersect.

Some of the advantages of using the integrated periodogram are: it is a nondecreasing and quite smooth curve; it has good asymptotic properties (for example, while the periodogram is an asymptotically unbiased but inconsistent estimator of spectral density, the integrated periodogram is a consistent estimator of spectral distribution); although, in practice, for stationary processes the integrated spectrum is usually estimated via the estimation of the spectrum, from a theoretical point of view, spectral distribution always exists, whereas spectral density exists only under absolutely continuous distributions (see theorem 2); finally, from a theoretical point of view, the integrated spectrum completely determines the stochastic processes.

Since the periodogram is defined only for stationary series, in order to be able to classify nonstationary time series, we shall consider locally stationary series. With this assumption we

can split them into blocks, compute the integrated periodogram of each block and merge these periodograms into a final curve; hence, we approximate the locally stationary processes by piecewise stationary processes. In figure 2.3(b), we illustrate our blockwise spectral distribution estimation of the locally stationary process spectrum. It is worth mentioning that there are two opposite effects as a consequence of splitting: one is that the narrower the blocks are, the closer we are to the locally stationary assumption; the other one is that when the length of the blocks decreases, the quality of the integrated periodogram as an estimator of the integrated spectrum also decreases.

2.2.2 Classifying Functions

When functions need to be classified, a possible criterion is to assign them to the group minimizing some distance from the new data to the group. In our context this criterion means that we classify new series in the group minimizing the distance between the integrated periodogram of the series and a reference curve from the group. As a reference function of each group, we take the mean of its elements, as it summarizes the general performance of the sample. Let $\chi_e^{(k)}(\lambda)$ be the joint integrated periodograms of the blocks for the e-th series —out of n_k— in group k. The mean is defined as:

$$\mathcal{R}^{(k)}(\lambda) = \bar{\chi}^{(k)}(\lambda) = \frac{1}{n_k}\sum_{e=1}^{n_k}\chi_e^{(k)}(\lambda). \tag{2.3}$$

As a distance measurement between two functions we have taken the distance given by expression (1.76) with $m = 1$. Notice that the functions we are working with, that is, the integrated periodograms, belong to the $\mathcal{L}^1[-\pi, +\pi]$ space.

2.2.3 Robustness

Our classification method depends on the group reference curve to which the distance is measured. The mean of a set of functions is not robust to the presence of outliers. Then robustness can be added to the classification procedure by using a robust reference curve. Instead of considering the mean of the integrated periodograms of all the elements of the group, we shall consider the α-trimmed mean, where only the deepest elements are averaged. The trim adds robustness by making the reference curve more resistant to the presence of outliers. In this section, we describe the concept of depth for functional data given by López-Pintado and Romo (2009). Then we propose a robust version of our classification algorithm.

New Reference Function

In order to add robustness, we shall take the group α-trimmed mean of its elements

$$\mathcal{R}^{(k)}(\lambda) = \bar{\chi}^{\alpha\ (k)}(\lambda) = \frac{1}{n_k - [n_k\alpha]}\sum_{e=1}^{n_k-[n_k\alpha]}\chi_{(e)}^{(k)}(\lambda), \tag{2.4}$$

where $[\cdot]$ is the integer part function and $\chi_{(e)}^{(k)}(\lambda)$, $e = 1, \ldots, n_k$, is the k-th sample of functions ordered by decreasing depth.

2.3 Algorithms

We can establish the classification algorithms with the above definitions:

Algorithms 1 and 2

Let $(x_t)_e^{(k)}$, $e = 1, \ldots, n_k$, be a sample containing n_k time series from population $P^{(k)}$, for $k = 1, 2$; the classification method includes the following steps:

1. **From time series to functions.** To this end, each time series is split into G blocks, then a curve associated with each series is constructed by merging the integrated periodograms of the blocks. Concretely, consider $\{\chi_1^{(k)}(\lambda), \ldots, \chi_{n_k}^{(k)}(\lambda)\}$, $k = 1, 2$, where $\chi_e^{(k)}(\lambda) = (F_{1,e}^{(k)}(\lambda) \ldots F_{G,e}^{(k)}(\lambda))$ and $F_{g,e}^{(k)}(\lambda)$ is the integrated periodogram of the g-th block of the e-th series of sample k.
2. **The reference functions $\mathcal{R}^{(k)}$.** Calculate the curve of each group: $\mathcal{R}^{(k)}(\lambda) = \bar{\chi}^{(k)}(\lambda)$, in algorithm 1, or $\mathcal{R}^{(k)}(\lambda) = \overset{\alpha}{\chi}{}^{(k)}(\lambda)$, in algorithm 2, $k = 1, 2$.
3. **The allocation of new series.** Let $\chi(\lambda)$ be the associated curve of a new series (x_t), that is $\chi(\lambda) = (F_1(\lambda) \ldots F_G(\lambda))$; then (x_t) is classified as

$$\begin{cases} k = 1 & \text{if} \quad d(\chi(\lambda), \mathcal{R}^{(1)}(\lambda)) < d(\chi(\lambda), \mathcal{R}^{(2)}(\lambda)) \\ k = 2 & \text{otherwise} \end{cases} . \tag{2.5}$$

Remark 16 An important point of our approach is that it can be interpreted as the fit to locally stationary processes with piecewise stationary processes (see figure 2.3).

Remark 17 To apply the algorithm to stationary series, G can be set equal to 1. We have used a dyadic splitting of the series into blocks in the simulation and real data computations, that is, $g = 2^n, n = 0, 1, \ldots$; but the implementation with blocks of different lengths, as could be suggested by visual inspection of data, is also possible.

Remark 18 The same methodology that we propose in this thesis could be implemented using different classification criterion between curves, reference function —or functions— of each group, or distance between curves.

Remark 19 The same algorithm could be implemented using a different functional depth.

Remark 20 The previous classification criteria can be expressed as

$$k = argmin_{\{1,2\}} \{d(\chi(\lambda), \mathcal{R}^{(k)}(\lambda))\} . \tag{2.6}$$

CODE

In the link given on the first page of this chapter, we have made some code available. It implements our algorithms, methods *DbC* and *DbC*-α. There are two main scripts, one for simulation exercises and another for the application to real data; the former runs a Monte Carlo loop, while the latter adds a leave-m-out cross-validation partition of the real data (the user can choose the value of m, possibly different for each group).

Our code provides previous optional graphics that are based on an additional and independent run of the loop; these graphics use both training and testing data and have a useful prospective and descriptive character.

The code is fast (a particular robustifying process accelerates the computes with *DbC*-α) and easy to execute and extend. The reader can reproduce, apply or extend our results and graphics easily. A helping file is included with the code.

2.4 Simulation Results

In this section, we evaluate —based on simulation studies— the two algorithms that we have introduced and, as a reference, the method proposed in Huang et al. (2004). The results obtained with our two algorithms and Huang et al.'s (2004) method are denoted by *DbC*, *DbC*-α and *SLEXbC*, respectively. Ombao et al. (2001) introduced the SLEX (smooth localized complex exponentials) model of a nonstationary random process, which is based on a set of Fourier-type bases that are at the same time orthogonal and localized in both time and frequency domains. The method of Huang et al. (2004) uses SLEX for classification of nonstationary time series. In a first step, they select from SLEX a basis explaining the difference between the classes of time series as well as possible. In a second step, they construct a discriminant criterion that is related to the SLEX spectra of the different classes: a time series is assigned to the class minimizing the Kullback-Leibler divergence between the estimated spectrum and the spectrum of the class. For the *SLEXbC* method, we have used an implementation provided by the authors (`http://www.stat.uiuc.edu/~ombao/research.html`). To select the parameters for this method, we have carried out a small optimization for each simulation exercise and the results were similar to the values recommended by the authors.

We have used the same models as the ones proposed in Huang et al. (2004). For each model, we have run the steps 1000 times. We generate training and testing sets of each class. Training sets have the same sizes (sample size and series length) as the ones used in Huang et al. (2004). The testing sets always contain 10 series of length determined in each particular simulation exercise. The performance of the different methods are based on exactly the same simulated data.

Simulation Exercise 1. We compare an autoregressive process of order one $X_t^{(1)}$

with a Gaussian white noise $X_t^{(2)}$:

$$X_t^{(1)} = \phi X_{t-1}^{(1)} + \epsilon_t^{(1)} \qquad t = 1, \ldots, T$$

$$X_t^{(2)} = \epsilon_t^{(2)} \qquad t = 1, \ldots, T$$

where ϵ_t are i.i.d. $N(0,1)$, independently generated for the two models. Each training data set has $n = 8$ series of length $T = 1024$. Six comparisons have been run, with the parameter ϕ of the AR(1) model taking the values -0.5, -0.3, -0.1, $+0.1$, $+0.3$ and $+0.5$. Series are stationary in this exercise. The integrated periodograms are represented in the left graph in figure 2.2.

Simulation Exercise 2. We compare two processes, half of each model is white noise and half is an autoregressive process of order one. The value of the AR(1) parameter is -0.1 in the first class and $+0.1$ in the second class:

$$\begin{array}{ll} X_t^{(1)} = \epsilon_t^{(1)} & \text{if } \ t = 1, \ldots, T/2 \\ X_t^{(1)} = -0.1 X_{t-1}^{(1)} + \epsilon_t^{(1)} & \text{if } \ t = T/2+1, \ldots, T \end{array}$$

.

$$\begin{array}{ll} X_t^{(2)} = \epsilon_t^{(2)} & \text{if } \ t = 1, \ldots, T/2 \\ X_t^{(2)} = +0.1 X_{t-1}^{(2)} + \epsilon_t^{(2)} & \text{if } \ t = T/2+1, \ldots, T \end{array}$$

Different combinations of training sample sizes, $n = 8$ and 16, and series lengths, $T = 512$, 1024 and 2048, are considered. In this exercise, the series are piecewise stationary, although the series themselves are not stationary. The integrated periodograms are represented on the right in figure 2.2.

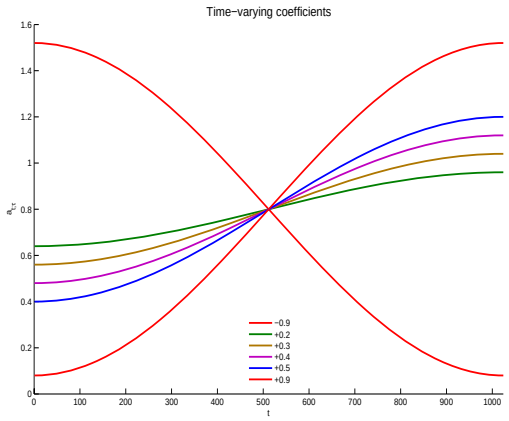
Simulation Exercise 3. In this exercise, the stochastic models of both classes are slowly time-varying second-order autoregressive processes:

$$X_t^{(1)} = a_{t;0.5} X_{t-1}^{(1)} - 0.81 X_{t-2}^{(1)} + \epsilon_t^{(1)} \qquad t = 1, \ldots, T$$

$$X_t^{(2)} = a_{t;\tau} X_{t-1}^{(2)} - 0.81 X_{t-2}^{(2)} + \epsilon_t^{(2)} \qquad t = 1, \ldots, T$$

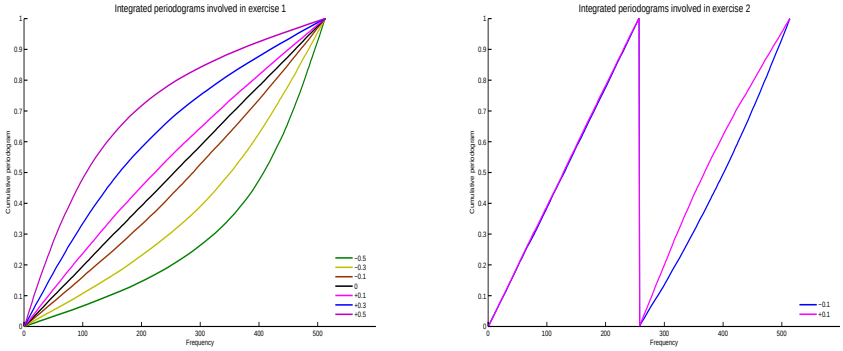
with $a_{t;\tau} = 0.8[1 - \tau \cos(\pi t/1024)]$, where τ is a parameter (see figure 2.1). Each training data set has $n = 10$ series of length $T = 1024$. Three comparisons have been made, the first class always having the parameter $\tau = 0.5$, and the second class having the values $\tau = 0.4$, 0.3 and 0.2, respectively. Notice that a coefficient of the autoregressive structure is not fixed but it varies in time; therefore, the processes are not stationary. We have also proved that, for these values of τ and any value of t, the characteristic polynomial of the autoregressive process has roots outside the unit circle.

Figure 2.1: Time-varying coefficients used in exercise 3



The coefficients $a_{t;\tau}$ are represented in figure 2.1. See figure 2.3(a) for an example of the integrated spectrum corresponding to these processes.

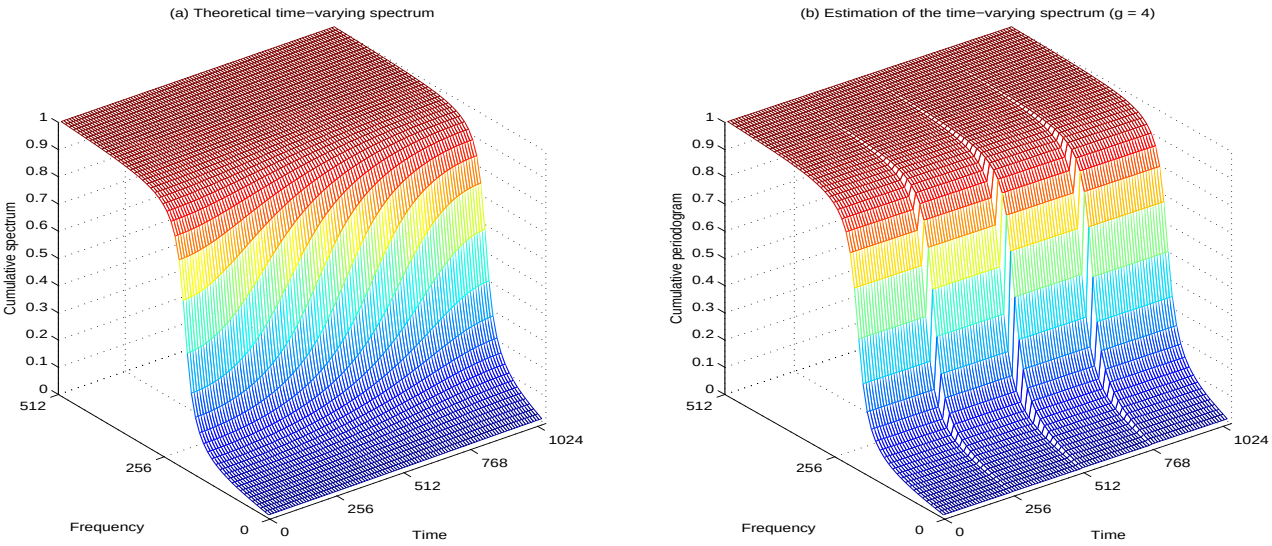
Figure 2.2: Integrated periodograms of the models used in exercises 1 and 2



In order to test the robustness of our classification procedure and the *SLEXbC* method, we perform additional experiments where the training set is contaminated with an outlier. In all cases we contaminate the $P^{(1)}$ population by changing one series for another following a different model. We consider three levels of contamination: one type of weak contamination (A) and two strong contaminations (B and C).

Contamination A. For exercise 1, we replace the autoregressive structure by a moving-average structure, that is, generate an MA(1) instead of an AR(1) model, with the MA parameter equal to the AR parameter. For exercise 2, we make the same substitution of structures in the autoregressive half of one series of a class (the other half remains as a white noise). For exercise 3, we contaminate the set of slowly time--varying autoregressives of parameter +0.5 with a series of the same model but with parameter value +0.2.

Figure 2.3: Time-varying autoregressive model with $\tau = 0.4$



Contamination B. This contamination consists in using a parameter value of $\phi = -0.9$ in exercises 1 and 2 and $\tau = -0.9$ in exercise 3 for one time series instead of the correct value. Therefore, we always use the correct model except for one time series where the parameter value is mistaken.

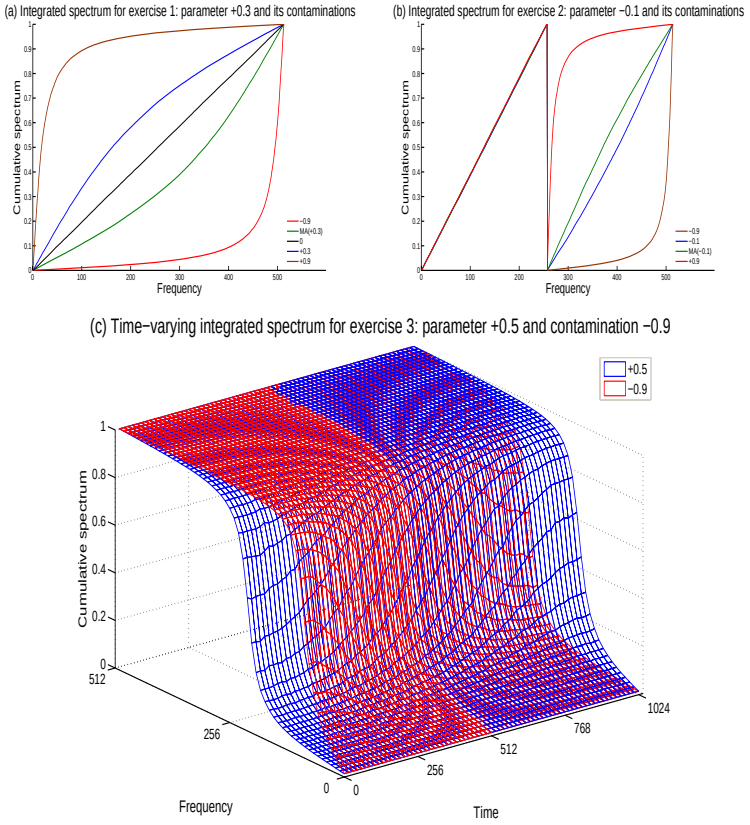
Contamination C. The same as contamination B but using a value +0.9 instead of the value -0.9.

In figures 2.4(a) and 2.4(b), we illustrate the three contaminations for the first two exercises with specific parameter values. Figure 2.4(c) shows contamination B for the third exercise.

The error rate estimates for the first simulation exercise are presented in table 2.1, for the second simulation experiment in tables 2.2, 2.3, 2.4 and 2.5, and for the third simulation experiment in tables 2.6, 2.7, 2.8 and 2.9. Each cell includes the mean and the standard error (in parentheses) of the error rates based on 1000 runs.

Tables 2.10, 2.11 and 2.12 provide the estimates of the computation times of the different classification methods using the simulation exercises previously described. In these tables, each cell contains the average time in seconds to compute 1000 runs. The time is measured from the instant the series are inputted into the algorithm until the moment the method gives the error rate. The time required to generate the training and testing time series is not included in the computation; nevertheless, for our method, the computation does include the construction of functional data from the time series and the calcutation of depth inside groups. Simulation exercises have been run on a personal computer with an AMD Athlon(tm) 64 Processor 3200+, 2.01GHz and 2.00Gb of RAM memory.

Figure 2.4: Examples of contaminations for the three simulation experiments



For all tables, we use the following notation: *DbC* (from *depth-based classification*) for algorithm 1, *DbC*-α for algorithm 2 and *SLEXbC* for the method of Huang et al. (2004). If a number follows *DbC* or *DbC*-α, this represents the number of blocks g into which the series are split. The digits in bold correspond to the minimum misclassification rates (when there is at least one value different from zero).

Figure 2.5: Third simulation with $\tau = 0.3$ and contamination B: some figures when $G = 4$

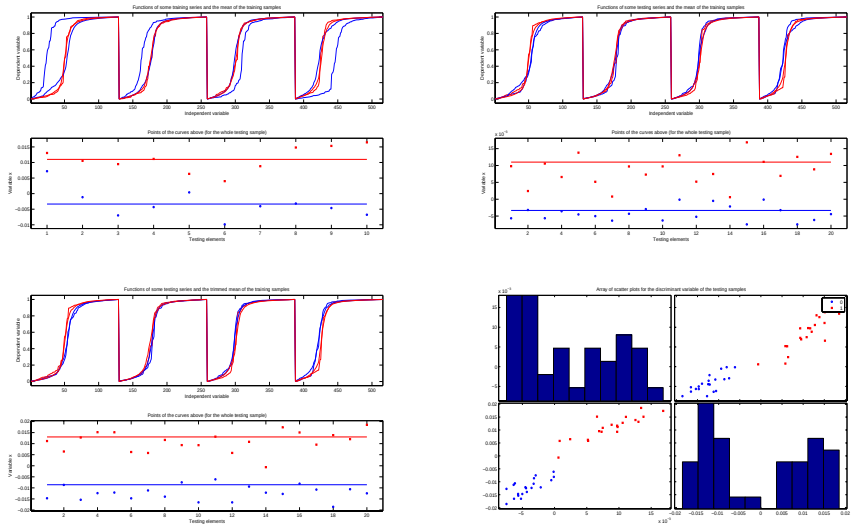
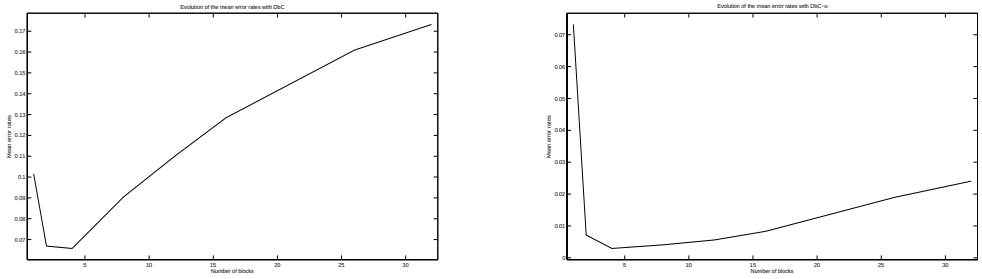


Figure 2.6: Third simulation with $\tau = 0.3$ and contamination B: change of the error rates with G



Comments on Error Rates

Table 2.1 shows the estimates of the misclassification rates for the first simulation exercise. We can observe that when there is no contamination: *DbC* and *DbC*-α provide similar error rates, and they are of lower value (approximately half) of those obtained by *SLEXbC*. As we expected, for *DbC* and *SLEXbC*, error rates increase slightly with contamination A (weak) and notably with contaminations B and C (strong), while changes are negligible for *DbC*-α because the trim keeps the contamination out. When contamination A is applied, *DbC* has about half the errors of *SLEXbC*; whereas, their errors are similar with contaminations B and C. The three methods have no misclassifications for series that are easy to assign, that is, for values of ϕ far from 0. There are some symmetries in table 2.1 for *DbC* and *SLEXbC*: for example, the effect of contamination B with positive (negative) ϕ values of the autoregressive process model is similar to the effect of contamination C with negative (positive) ϕ. In addition, to extend the information provided by the tables, we include some boxplots showing distributions of the misclassification rates. For exercise 1, we only include the plot of one of the two most difficult discrimination settings, which is the comparison of the autoregressive model with $\phi = +0.1$ and the Gaussian white noise (see figure 2.7). The plot shows that *SLEXbC* tends to have a higher median, higher errors above this median, and fewer errors near zero. For the strongest contamination, *DbC* and *SLEXbC* classify almost at random. On the other hand, *DbC*-α is the only method that maintains the same pattern in the models with and without contamination and which has a considerable number of errors close to zero.

Tables 2.2, 2.3, 2.4 and 2.5 provide the results of the second simulation exercise. As expected, the errors decrease when any parameter, n or T, increases. The errors based on our methods, *DbC* and *DbC*-α, are larger than the errors using *SLEXbC* when we consider the whole series (without splitting them into blocks), although these errors fall with the first division. Notice that our methods outperform SLEXbc when series are divided into blocks, achieving the minimum error rates when $g = 2$. As we mentioned earlier, the length of the blocks decreases with g, and this implies that the quality of the estimated periodogram is decreased and the errors increase. This effect is reflected in all the tables and the optimal g is shown to be 2. Moreover, we can see that the increase in error with g is higher for short series than for longer ones. Recall that, like

Table 2.1: Misclassification rate estimates for simulation exercise 1 with and without contamination

	$\phi =$ **-0.5**	$\phi =$ **-0.3**	$\phi =$ **-0.1**	$\phi =$ **+0.1**	$\phi =$ **+0.3**	$\phi =$ **+0.5**
Without contamination						
DbC	0.000 (0.0000)	0.000 (0.0000)	**0.063** (0.0017)	**0.060** (0.0017)	0.000 (0.0000)	0.000 (0.0000)
DbC-α	0.000 (0.0000)	0.000 (0.0000)	0.065 (0.0018)	0.062 (0.0017)	0.000 (0.0000)	0.000 (0.0000)
SLEXbC	0.000 (0.0000)	0.000 (0.0000)	0.131 (0.0024)	0.127 (0.0024)	0.000 (0.0000)	0.000 (0.0000)
Contamination A						
DbC	0.000 (0.0000)	0.000 (0.0001)	0.077 (0.0019)	0.074 (0.0019)	0.000 (0.0001)	0.000 (0.0000)
DbC-α	0.000 (0.0000)	**0.000** (0.0000)	**0.064** (0.0017)	**0.062** (0.0017)	**0.000** (0.0000)	0.000 (0.0000)
SLEXbC	0.000 (0.0000)	0.000 (0.0001)	0.175 (0.0028)	0.172 (0.0029)	0.000 (0.0001)	0.000 (0.0000)
Contamination B						
DbC	0.000 (0.0000)	0.000 (0.0001)	0.300 (0.0028)	0.513 (0.0012)	0.001 (0.0002)	0.000 (0.0000)
DbC-α	0.000 (0.0000)	**0.000** (0.0000)	**0.065** (0.0018)	**0.062** (0.0017)	**0.000** (0.0000)	0.000 (0.0000)
SLEXbC	0.000 (0.0000)	0.001 (0.0002)	0.377 (0.0025)	0.491 (0.0011)	0.002 (0.0003)	0.000 (0.0000)
Contamination C						
DbC	0.000 (0.0000)	0.001 (0.0002)	0.512 (0.0013)	0.300 (0.0027)	0.000 (0.0001)	0.000 (0.0000)
DbC-α	0.000 (0.0000)	**0.000** (0.0000)	**0.064** (0.0017)	**0.062** (0.0017)	**0.000** (0.0000)	0.000 (0.0000)
SLEXbC	0.000 (0.0000)	0.002 (0.0004)	0.490 (0.0011)	0.377 (0.0025)	0.001 (0.0002)	0.000 (0.0000)

Figure 2.7: Boxplot of the misclassification rates in exercise 1, parameters values +0.1 versus 0

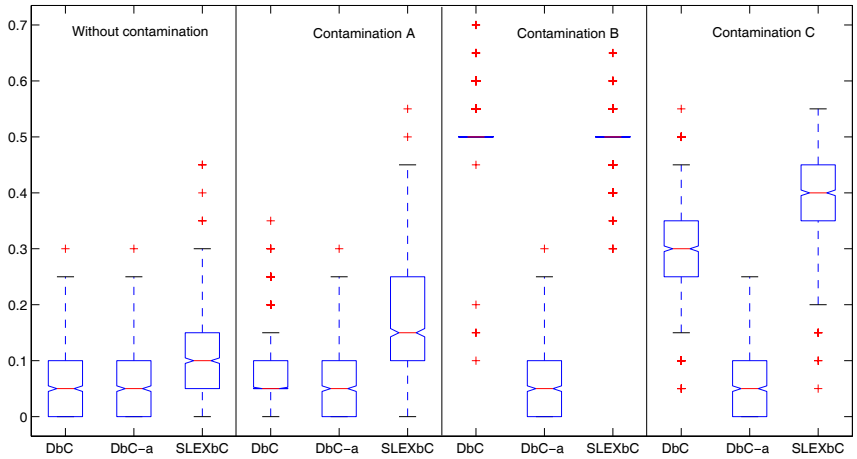


Table 2.2: Misclassification rate estimates for simulation exercise 2 without contamination

	nxT = **8x512**	**16x512**	**8x1024**	**16x1024**	**8x2048**	**16x2048**
DbC **1**	0.141 (0.0024)	0.131 (0.0024)	0.062 (0.0017)	0.060 (0.0017)	0.014 (0.0008)	0.014 (0.0008)
2	**0.066** (0.0017)	**0.061** (0.0017)	**0.015** (0.0009)	**0.014** (0.0008)	**0.001** (0.0003)	**0.001** (0.0003)
4	0.078 (0.0019)	0.069 (0.0018)	**0.015** (0.0009)	0.014 (0.0009)	**0.001** (0.0003)	**0.001** (0.0003)
8	0.090 (0.0020)	0.080 (0.0019)	0.020 (0.0010)	0.018 (0.0009)	0.002 (0.0003)	**0.001** (0.0003)
DbC-α **1**	0.143 (0.0024)	0.132 (0.0024)	0.063 (0.0017)	0.061 (0.0017)	0.015 (0.0009)	0.014 (0.0008)
2	0.069 (0.0018)	0.064 (0.0017)	0.016 (0.0009)	0.015 (0.0009)	**0.001** (0.0003)	**0.001** (0.0003)
4	0.083 (0.0020)	0.073 (0.0018)	0.017 (0.0010)	0.016 (0.0009)	0.002 (0.0003)	**0.001** (0.0003)
8	0.105 (0.0023)	0.088 (0.0020)	0.024 (0.0011)	0.019 (0.0010)	0.002 (0.0004)	0.002 (0.0003)
SLEXbC	0.114 (0.0023)	0.086 (0.0020)	0.038 (0.0014)	0.025 (0.0011)	0.007 (0.0006)	0.003 (0.0004)

our procedure, the *SLEXbC* method implicitly splits the series into blocks. When we consider contaminations in the model, the error rates based on *DbC* and *SLEXbC* increase slightly with contamination A and greatly with contaminations B and C, while *DbC*-α maintains its errors and outperforms the other methods, especially with strong contaminations and $g = 2$. As expected, contaminating a series has major effects when samples sizes are $n = 8$ compared to when $n = 16$. The *DbC* and *SLEXbC* methods are more affected by contamination C than by contamination B, since $\phi = +0.9$ is farther from $\phi = -0.1$ (population $P^{(1)}$) than $\phi = -0.9$.

The boxplots of the error distributions for exercise 2 are represented in figure 2.8. As in the tables, the plots show that *DbC* and *DbC*-α perform better than *SLEXbC* when $g > 1$. The median error rate decreases when $g = 2$ (with respect to $g = 1$) and presents stable performance for g greater than 2. These plots and tables reflect that *DbC*-α, with $g = 2$, tends to provide the best results, except when there is no contamination with which *DbC* with $g = 2$ outperforms all the other methods.

Similar results to the previous ones can be derived for simulation exercise 3 (see tables 2.6, 2.7, 2.8 and 2.9). They show that in our proposal the drawback of splitting too much is not relevant when series are long enough. With the presence of contamination, the best errors are obtained by *DbC*-α for $g = 4$. Contamination A has minor effects. On the other hand, results are very different for contaminations B and C. Notice that since τ has positive values in both populations, contaminating with a time series of parameter $\tau = -0.9$ (contamination B) has a stronger effect than using a series with $\tau = +0.9$ (contamination C).

Finally, in the three experiments a subtle effect can be seen between *DbC* and *DbC*-α. When there is no contamination it is normal for the former to provide slightly better error rates, because *DbC*-α is using only $100(1-\alpha)\%$ of the training data available. Nevertheless, when there is some

Table 2.3: Misclassification rate estimates for simulation exercise 2 with contamination A

	nxT = **8x512**	**16x512**	**8x1024**	**16x1024**	**8x2048**	**16x2048**
***DbC* 1**	0.143 (0.0025)	0.132 (0.0024)	0.063 (0.0017)	0.062 (0.0017)	0.018 (0.0010)	0.015 (0.0008)
2	**0.070** (0.0018)	**0.062** (0.0017)	0.018 (0.0010)	**0.014** (0.0008)	0.002 (0.0003)	**0.001** (0.0003)
4	0.083 (0.0020)	0.071 (0.0019)	0.019 (0.0010)	0.015 (0.0009)	0.002 (0.0003)	**0.001** (0.0003)
8	0.102 (0.0022)	0.083 (0.0020)	0.026 (0.0012)	0.019 (0.0010)	0.003 (0.0004)	0.002 (0.0003)
***DbC*-α 1**	0.145 (0.0025)	0.132 (0.0023)	0.063 (0.0017)	0.061 (0.0017)	0.015 (0.0009)	0.014 (0.0008)
2	0.072 (0.0018)	0.064 (0.0017)	**0.015** (0.0009)	0.015 (0.0009)	**0.001** (0.0002)	**0.001** (0.0003)
4	0.086 (0.0021)	0.073 (0.0018)	0.018 (0.0010)	0.016 (0.0009)	0.002 (0.0003)	**0.001** (0.0003)
8	0.114 (0.0024)	0.089 (0.0021)	0.025 (0.0011)	0.019 (0.0010)	0.003 (0.0004)	0.002 (0.0003)
SLEXbC	0.128 (0.0025)	0.092 (0.0021)	0.050 (0.0016)	0.027 (0.0012)	0.012 (0.0008)	0.004 (0.0004)

Table 2.4: Misclassification rate estimates for simulation exercise 2 with contamination B

	nxT = **8x512**	**16x512**	**8x1024**	**16x1024**	**8x2048**	**16x2048**
***DbC* 1**	0.258 (0.0029)	0.168 (0.0026)	0.252 (0.0029)	0.117 (0.0022)	0.250 (0.0029)	0.065 (0.0018)
2	0.135 (0.0024)	0.082 (0.0020)	0.088 (0.0021)	0.030 (0.0012)	0.049 (0.0016)	0.007 (0.0006)
4	0.137 (0.0025)	0.085 (0.0020)	0.089 (0.0021)	0.031 (0.0012)	0.049 (0.0016)	0.007 (0.0006)
8	0.143 (0.0025)	0.092 (0.0021)	0.093 (0.0022)	0.034 (0.0014)	0.050 (0.0016)	0.007 (0.0006)
***DbC*-α 1**	0.145 (0.0024)	0.134 (0.0024)	0.064 (0.0017)	0.061 (0.0017)	0.015 (0.0008)	0.014 (0.0008)
2	**0.070** (0.0018)	**0.065** (0.0017)	**0.017** (0.0010)	**0.015** (0.0009)	0.003 (0.0006)	**0.001** (0.0003)
4	0.081 (0.0020)	0.071 (0.0019)	**0.017** (0.0010)	0.017 (0.0009)	**0.002** (0.0003)	0.002 (0.0003)
8	0.104 (0.0023)	0.087 (0.0020)	0.023 (0.0011)	0.019 (0.0010)	0.002 (0.0004)	0.002 (0.0003)
SLEXbC	0.239 (0.0031)	0.134 (0.0024)	0.228 (0.0030)	0.081 (0.0020)	0.220 (0.0030)	0.037 (0.0013)

Table 2.5: Misclassification rate estimates for simulation exercise 2 with contamination C

	nxT = **8x512**	**16x512**	**8x1024**	**16x1024**	**8x2048**	**16x2048**
DbC **1**	0.457 (0.0056)	0.162 (0.0027)	0.437 (0.0055)	0.090 (0.0020)	0.445 (0.0047)	0.038 (0.0013)
2	0.147 (0.0036)	0.078 (0.0019)	0.055 (0.0020)	0.028 (0.0012)	0.015 (0.0010)	0.005 (0.0005)
4	0.187 (0.0037)	0.092 (0.0021)	0.068 (0.0022)	0.030 (0.0012)	0.017 (0.0010)	0.006 (0.0005)
8	0.225 (0.0039)	0.107 (0.0022)	0.101 (0.0027)	0.034 (0.0014)	0.024 (0.0011)	0.006 (0.0006)
DbC- α **1**	0.145 (0.0025)	0.133 (0.0024)	0.063 (0.0017)	0.062 (0.0017)	0.015 (0.0009)	0.014 (0.0008)
2	**0.073** (0.0020)	**0.065** (0.0017)	0.018 (0.0013)	**0.015** (0.0009)	0.002 (0.0005)	**0.001** (0.0003)
4	0.083 (0.0020)	0.073 (0.0018)	**0.017** (0.0010)	0.016 (0.0009)	**0.002** (0.0003)	**0.001** (0.0003)
8	0.108 (0.0022)	0.088 (0.0021)	0.024 (0.0011)	0.019 (0.0010)	0.003 (0.0004)	0.002 (0.0003)
SLEXbC	0.376 (0.0036)	0.177 (0.0029)	0.354 (0.0032)	0.098 (0.0023)	0.369 (0.0030)	0.040 (0.0015)

Figure 2.8: Boxplots of the misclassification error rates for simulation exercise 2, training sets with 8 series of length 1024

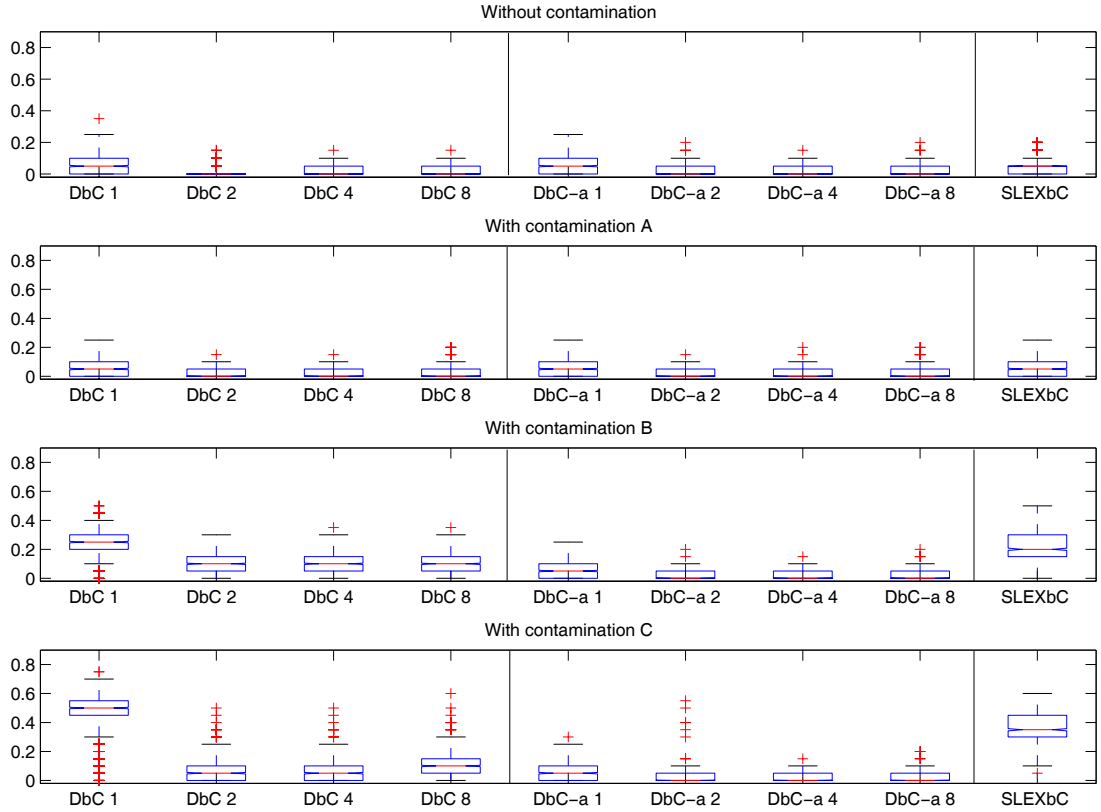


Table 2.6: Misclassification rate estimates for simulation exercise 3 without contamination

	$\tau = \mathbf{0.4}$	$\tau = \mathbf{0.3}$	$\tau = \mathbf{0.2}$
***DbC* 1**	0.218 (0.0031)	0.063 (0.0017)	0.019 (0.0010)
2	0.119 (0.0023)	0.006 (0.0006)	**0.000** (0.0000)
4	**0.101** (0.0022)	**0.002** (0.0003)	**0.000** (0.0000)
8	0.123 (0.0024)	0.003 (0.0004)	**0.000** (0.0000)
***DbC*-α 1**	0.226 (0.0032)	0.065 (0.0018)	0.021 (0.0010)
2	0.128 (0.0023)	0.006 (0.0006)	**0.000** (0.0000)
4	0.112 (0.0023)	**0.002** (0.0003)	**0.000** (0.0000)
8	0.139 (0.0026)	0.004 (0.0004)	**0.000** (0.0000)
SLEXbC	0.181 (0.0031)	0.011 (0.0009)	**0.000** (0.0000)

Table 2.7: Misclassification rate estimates for simulation exercise 3 with contamination A

	$\tau = \mathbf{0.4}$	$\tau = \mathbf{0.3}$	$\tau = \mathbf{0.2}$
***DbC* 1**	0.232 (0.0032)	0.062 (0.0017)	0.019 (0.0009)
2	0.143 (0.0026)	0.006 (0.0006)	**0.000** (0.0000)
4	0.144 (0.0026)	0.004 (0.0004)	**0.000** (0.0000)
8	0.177 (0.0028)	0.005 (0.0005)	**0.000** (0.0000)
***DbC*-α 1**	0.241 (0.0035)	0.065 (0.0018)	0.020 (0.0010)
2	0.131 (0.0025)	0.007 (0.0006)	**0.000** (0.0000)
4	**0.121** (0.0026)	**0.003** (0.0004)	**0.000** (0.0000)
8	0.150 (0.0029)	0.005 (0.0005)	**0.000** (0.0000)
SLEXbC	0.234 (0.0033)	0.016 (0.0011)	**0.000** (0.0000)

Table 2.8: Misclassification rate estimates for simulation exercise 3 with contamination B

	$\tau = \mathbf{0.4}$	$\tau = \mathbf{0.3}$	$\tau = \mathbf{0.2}$
***DbC* 1**	0.254 (0.0029)	0.106 (0.0022)	0.043 (0.0015)
2	0.500 (0.0015)	0.067 (0.0021)	0.001 (0.0002)
4	0.500 (0.0012)	0.062 (0.0020)	0.001 (0.0002)
8	0.499 (0.0013)	0.082 (0.0024)	0.000 (0.0001)
***DbC*-α 1**	0.231 (0.0031)	0.074 (0.0020)	0.026 (0.0012)
2	0.128 (0.0024)	0.007 (0.0006)	**0.000** (0.0000)
4	**0.113** (0.0023)	**0.002** (0.0004)	**0.000** (0.0000)
8	0.141 (0.0026)	0.003 (0.0004)	**0.000** (0.0000)
SLEXbC	0.492 (0.0019)	0.174 (0.0051)	0.015 (0.0009)

Table 2.9: Misclassification rate estimates for simulation exercise 3 with contamination C

	$\tau = \mathbf{0.4}$	$\tau = \mathbf{0.3}$	$\tau = \mathbf{0.2}$
***DbC* 1**	0.257 (0.0029)	0.107 (0.0022)	0.044 (0.0015)
2	0.153 (0.0025)	0.017 (0.0009)	0.000 (0.0001)
4	0.128 (0.0024)	0.007 (0.0006)	**0.000** (0.0000)
8	0.132 (0.0024)	0.006 (0.0006)	0.000 (0.0001)
***DbC*-α 1**	0.234 (0.0031)	0.074 (0.0020)	0.025 (0.0012)
2	0.125 (0.0024)	0.007 (0.0006)	0.000 (0.0001)
4	**0.114** (0.0024)	**0.002** (0.0004)	**0.000** (0.0000)
8	0.138 (0.0026)	0.004 (0.0004)	**0.000** (0.0000)
SLEXbC	0.173 (0.0027)	0.015 (0.0009)	0.000 (0.0001)

Table 2.10: Mean computation times for simulation exercise 1

	$\phi =$ **-0.5**	$\phi =$ **-0.3**	$\phi =$ **-0.1**	$\phi =$ **+0.1**	$\phi =$ **+0.3**	$\phi =$ **+0.5**
DbC	0.027	0.027	0.027	0.027	0.027	0.027
DbC-α	0.044	0.045	0.045	0.044	0.044	0.044
SLEXbC	0.632	0.678	0.724	0.713	0.670	0.619

kind of contamination the best results are given by *DbC-*α.

Comments on Computation Times

Estimates of the computation times are given in tables 2.10, 2.11 and 2.12. The computation time depends on the implementation —not just on the method itself—so we pay closer attention to the qualitative interpretation of the results, as they are less dependent on the programmed code.

Since the chronometer is called after generating the series, it can be expected that the computation times do not depend on the parameters of the stochastic processes. This is what we observed for our algorithms, but not for the *SLEXbC* method. Perhaps this is because this method needs to select a basis of the SLEX library for each series, while our method works only with the graphs of the functions and the computation of the integrated periodograms, which do not depend on the parameters.

Some conclusions that can be derived from the three simulation exercises are the following: it is clear that for our procedures, computation time increases with the number of blocks g; table 2.11 shows that our methods, especially *DbC-*α, depend on sample size; and the computation of depth is moderately time-consuming with the sample size and in less degree with series length. Nonetheless, we have conveniently implemented the notion of depth in López-Pintado and Romo (2006) so it is computationally feasible and applicable to high sample sizes. Table 2.11 illustrates that *DbC-*α computation time increases with size but it is still reasonable and faster than *SLEXbC*. In short, for our approach computation time depends more on the number of blocks g and the sample size n, but not so much on the series length T. In contrast, *SLEXbC* computation time depends on both, n and T, and increases when either of them increases.

2.5 Real Data Example

2.5.1 Explosions and Earthquakes Data

We have evaluated our proposal in a benchmark data set containing eight explosions, eight earthquakes and one extra series —known as *NZ event*— not classified (but being either an earthquake or an explosion). This data set was constructed by Blandford (1993). Each series contains 2048

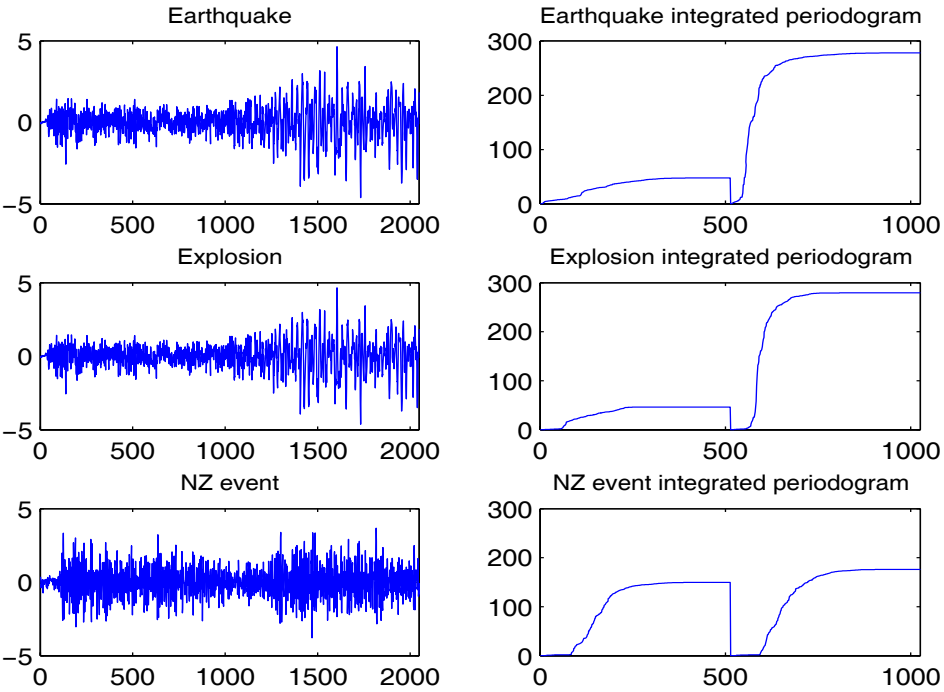
Table 2.11: Mean computation times for simulation exercise 2

	nxT = **8x512**	**16x512**	**8x1024**	**16x1024**	**8x2048**	**16x2048**
***DbC* 1**	0.021	0.028	0.027	0.038	0.044	0.067
2	0.036	0.049	0.043	0.060	0.062	0.087
4	0.066	0.092	0.067	0.094	0.081	0.115
8	0.125	0.180	0.126	0.181	0.129	0.186
***DbC*-α 1**	0.031	0.108	0.044	0.200	0.084	0.463
2	0.046	0.137	0.064	0.237	0.103	0.496
4	0.086	0.280	0.087	0.276	0.123	0.505
8	0.170	0.585	0.171	0.595	0.173	0.602
SLEXbC	0.355	0.517	0.736	1.095	1.681	2.506

Table 2.12: Mean computation times for simulation exercise 3

	τ = **0.4**	τ = **0.3**	τ = **0.2**
***DbC* 1**	0.031	0.030	0.030
2	0.047	0.047	0.048
4	0.074	0.074	0.074
8	0.140	0.140	0.140
***DbC*-α 1**	0.066	0.062	0.063
2	0.083	0.093	0.094
4	0.120	0.121	0.120
8	0.235	0.234	0.235
SLEXbC	0.733	0.685	0.675

Figure 2.9: Real data examples and its curves



points, and its plot clearly shows two different parts — the first half is the part P and the second half is S. This division is an assumption considered by most authors, and it is based on geological reasons. It is also frequently considered that both parts are stationary. Kakizawa et al. (1998) give a list of these measurements. Shumway and Stoffer (2000) included a detailed study of this data set and provide access to the data set on the web site of their book: `http://www.stat.pitt.edu/stoffer/tsa.html`. Figure 2.9 presents examples of an earthquake and an explosion, plus the NZ event.

Following the criterion to choose between normalized and nonnormalized versions of the cumulative periodogram given in section 2.2, we have considered the curve formed by merging the nonnormalized integrated periodograms of parts P and S independently computed; that is, we take $g = 2$. Let us consider the eight earthquakes as group 1 and the eight explosions as group 2. We have used leave-one-out cross validation to classify the elements of these two groups by removing a series at a time and using the rest of the data to train the method for final classification of the series. With this validation procedure, our two algorithms misclassify the first series of group 2 (explosions). Regarding the NZ event, both algorithms agree on assigning it to the explosions group, as described previously by other authors (for example, Kakizawa et al. [1998] and Huang et al. [2004]).

An additional exercise considers an artificial data set constructed by the eight earthquakes plus the NZ event as group 1, and the eight explosions as group 2. Note that our method and most of the published papers classify NZ as an explosion. Therefore, this could be considered an artificial scenario where an outlier is presented in group 1. In this situation, algorithm 1 misclassifies the

first and the third elements of group 2 (explosions), whereas algorithm 2 misclassifies only the first series of group 2. This seems to show the robustness of our second algorithm. Obviously, as we are using leave-one-out cross validation, both algorithms classify the NZ event in the explosions group.

2.6 Conclusions

We propose a new frequency domain approach for time series classification based on the integrated periodograms of the series. When series are nonstationary, they are split into blocks and the integrated periodograms of the blocks are merged to construct a curve. This idea relays on the assumption that series are locally stationary. Since the integrated periodogram is a function, the statistical tools for functional data analysis can be applied. In our classification procedure new series are assigned to the class minimizing the distance between its corresponding curve and the group mean curve. Since the group mean can be affected by the presence of outliers, robustness of the classification method is achieved by substituting the mean curve with the α-trimmed mean, where only the deepest elements are averaged for each group. To evaluate our proposal in different scenarios, we have done simulation exercises containing several models and parameters, with both stationary and nonstationary series, as well as with different types of contamination. We have also illustrated the performance of our procedure in a real benchmark data set. Our proposal provides small error rates, robustness, and good computational performance: properties which make the methodology suitable for time series classification. It also outperforms previous methods proposed in the literature. This chapter suggests that the integrated periodogram contains useful information for classifying time series.

Chapter 3

Functional Data Classification

Summary: A popular approach for classifying functional data is based on the distances from the function or its derivatives to group representative (usually the mean) functions or their derivatives. In this chapter, we propose using a combination of those distances. Simulation studies show that our procedure performs very well, resulting in smaller testing classification errors. Applications to real data show that our procedure performs as well as —and in some cases better than— other classification methods[1].

Key words: functional data, discriminant analysis, weighted distances.

3.1 Introduction

Functional data have great —and growing— importance in Statistics. Nowadays, functional data are present in many areas, sometimes because they are the output of measurement processes, other times for theoretical or practical reasons — functional models are used even for nonfunctional data (see section 1.2 of Ramsay and Silverman [2006]). Most of the classical techniques for the finite- and high-dimensional frameworks have been adapted to cope with the infinite dimensions, but due to the *curse of dimensionality*, new and specific treatments are still required. As with other types of data, statisticians must supervise different steps —registration, missing data, representation, transformation, typicality— and tackle different tasks —modelization, classification or clustering, amongst others. In practice, curves can neither be registered continuously nor at infinite points. Then, techniques dealing with high-dimensional data can sometimes be applied: Hastie et al. (1995), for example, adapt the discriminant analysis to cope with many highly correlated predictors, "such as those obtained by discretizing a function".

Among the approaches specifically designed for functional data classification, the following project the data into a finite-dimensional space of functions and therefore work with the coefficients; this technique is called *filtering*. James and Hastie (2001) model the coefficients with

[1]MATLAB code is available at `http://www.Casado-D.org/edu/publications.html`.

"Gaussian distribution with common covariance matrix for all classes, by analogy with LDA [linear discriminant analysis]"; their classification minimizes the distance to the group mean. The classification method of Hall et al. (2001) maximizes the likelihood, and although they propose a fully nonparametric density estimation, in practice multivariate Gaussian densities are considered, leading to quadratic discriminant analysis. Biau et al. (2003) apply k-nearest neighbour to the coefficients, while Rossi and Villa (2006) apply support vector machines. Berlinet et al. (2008) extend the approach of Biau et al. (2003) to wavelet bases and to more general discrimination rules. Our proposals can imply a higher dimensional reduction, but, on the other hand, the original functional data cannot be recovered (even approximately). Other proposals are designed to make direct use of the continuity of the functional data. Ferraty and Vieu (2003) classify new curves in the group with the highest posterior probability of membership kernel estimate. On the other hand, López-Pintado and Romo (2006) also take into account the continuous feature of the data and propose two classification methods based on the notion of *depth* for curves: in their first proposal new curves are assigned to the group with the closest trimmed mean, while the second method minimizes a weighted average distance to each element in the group. Abraham et al. (2006) extend the moving window rule for functional data classification. Nerini and Ghattas (2007) classify density functions with functional regression trees. Baíllo and Cuevas (2008) provide some theoretical results on the functional k-nearest neighbour classifier, and suggest —as a partial answer— that this method could play the same central role for functional data as Fisher's method for the finite-dimensional case. To use only the most informative parts of the curves, Li and Yu (2008) have proposed a new idea: they use F-statistics to select the place where linear discriminant analysis is applied into small intervals, providing an output that is used as input in a final support vector machines step.

There are several works addressing the unsupervised classification —or clustering— problem. Abraham et al. (2003) fit the functional data by B-splines and apply k-means on the coefficients. James and Sugar (2003) project the data into a finite-dimensional space and consider a random--effects model for the coefficients; their method is effective when the observations are sparse, irregularly spaced or occur at different time points for each subject. The continuous nature of the data is used, in a more direct form, by other works. The proposal of Tarpey and Kinateder (2003) classifies using a k-means algorithm over the probability distributions. A hierarchical descending procedure, using heterogeneity indexes based on modal and mean curves, is presented in Dabo-Niang et al. (2006). Impartial trimming is combined with k-means in Cuesta-Albertos and Fraiman (2007).

Functional data can be transformed in several ways. After the registration, spatial or temporal alignments are sometimes necessary; references on this topic are Wang and Gasser (1997, 1999) and Ramsay and Silverman (2006). On the other hand, Dabo-Niang et al. (2007) use a distance invariant to small shifts. Examples of centering, normalization and derivative transformations are found in Rossi and Villa (2006). The objective of the transformations is to highlight some

features of the data and to allow the information to be used more efficiently. For this kind of data, when they are smooth enough, the most important transformation is taking derivatives. Since the different derivatives can contribute new information, a possible combination of them —or their information— should be taken into account. Mathematical *Functional Analysis* has been working with such combinations for a long time, mainly through some norms (in norm and Sobolev spaces), and Ramsay and Silverman (2006) find them frequently as a consequence of model adjustements or system properties (for Canadian weather stations data, melanoma data or lower lip movement data).

In order to obtain semimetrics, instead of metrics, Ferraty and Vieu (2006) consider derivatives (one at a time) in the distances. This implies theoretical advantages —throughout the topological structure induced by the semimetric— in the small ball probability function, providing a new way to deal with the curse of dimensionality.

We transform the functional data classification problem into a classical multivariate data classification problem. While the filtering techniques encapsulate the functional information into a set of coefficients, we construct a linear combination of variables and coefficients. Given the variables, the *linear discriminant analysis* determines the combination. Our proposal is based on the interpretation as variables of the distances between a new curve and the transformed and untransformed functional data. On the one hand, the classification can be improved, and, on the other hand, the coefficients of the combination provide information about the importance of each data transformation. When a nonnegativeness condition is applied to the coefficients, the combination (discriminant function) can be interpreted as the difference of measurements with a weighted distance. This metric automatically becomes a semimetric when the importance of the distance to the untransformed data is null or insignificant; but the user can force, by considering only the derivatives as input, the method to produce a semimetric as output.

The chapter is organized as follows: in section 2 the classification method is presented and described, from the optimization problem to the classification algorithm; in section 3, our proposal is evaluated using several simulation exercises; two real data sets are classified in section 4; finally, in section 5 a summary of conclusions is given.

3.2 The Classification Method

3.2.1 The Optimization Problem

An Additional Constraint

In order to base the classification on a semimetric or on a metric, one version of our proposal adds another constraint —in fact, several nonnegativity constraints— to the classical Fisher's

discriminant analysis optimization problem:

$$\mathbf{a} = argmax\left\{\mathbf{a}^t\mathbf{B}\mathbf{a}\right\} \quad \text{subject to} \quad \begin{cases} \mathbf{a}^t\mathbf{W}\mathbf{a} = 1 \\ \mathbf{a} \geq \mathbf{0} \end{cases}, \tag{3.1}$$

where $\mathbf{B}$ is the *between-class scatter matrix*, $\mathbf{W}$ is the *within-class scatter matrix*, $\mathbf{a} = (a_1, \ldots, a_p)^t$, and $\mathbf{a} \geq \mathbf{0}$ means $a_i \geq 0,\ i = 1, \ldots, p$ (see appendix D for the definition of $\mathbf{B}$ and $\mathbf{W}$. Notice that $\mathbf{B}$ is positive semidefinite and $\mathbf{W}$ is, by hypothesis, positive definite). This is a nonlinear (quadratic) programming problem with an *equality constraint* and *nonnegativity constraints*. The latter constraints are frequently dealt with in literature, since they appear naturally when considering the dual problems of linear and quadratic programs (see examples 3.4.2 and 3.4.3 of Bertsekas [1999] or sections 4.3 and 4.4 of Boyd and Vandenberghe [2008]). The solution of this new optimization problem can be represented by the pair $(\mathbf{a}_n, \lambda_n)$, with $\mathbf{a}_n^t\mathbf{W}\mathbf{a}_n = 1,\ \ \mathbf{a}_n \geq \mathbf{0}$ and $\lambda_n = \mathbf{a}_n^t\mathbf{B}\mathbf{a}_n$. Let us denote $V_{\mathbf{a}}^* = \{c\mathbf{a},\ \ c \in \mathbb{R},\ \ c \neq 0\}$. Section 3.2.2 contains some theory on obtaining the explicit expression of $\mathbf{a}_n$.

Geometrically, the set $V_{\mathbf{a}} = V_{\mathbf{a}}^* \cup \{\mathbf{a} = \mathbf{0}\}$ is a one-dimensional linear subspace of $\mathbb{R}^p$. When $V_{\mathbf{a}}^*$ intersects the nonnegative orthant $\{\mathbf{a} \in \mathbb{R}^p \mid \mathbf{a} \geq \mathbf{0}\}$ outside the origin, this last optimization problem will provide the same solution as those without the nonnegativity constraints.

Convexity

The cost function $\mathbf{a}^t\mathbf{B}\mathbf{a}$ is convex due to proposition 22(d) and the positive definiteness of the matrix $\mathbf{B}$.

Existence of Solutions

In this new optimization problem, the feasible domain is

$$\mathcal{D} = \left\{\mathbf{a} \in \mathbb{R}^p \mid \mathbf{a}^t\mathbf{W}\mathbf{a} = 1 \ \text{ and } \ \mathbf{a} \geq \mathbf{0}\right\}, \tag{3.2}$$

that is convex, since proposition 23(a) can be applied after writing

$$\mathcal{D} = \{\mathbf{a} \in \mathbb{R}^p \mid \mathbf{a}^t\mathbf{W}\mathbf{a} \leq 1\} \cap \{\mathbf{a} \in \mathbb{R}^p \mid \mathbf{a} \geq \mathbf{0}\}. \tag{3.3}$$

On the other hand, as the inequality constraints are expressed in terms of linear functions, they do not change the performance of the second derivatives of the Lagrangian, that is, do not change the convexity of the cost function of the optimization problem. As a consequence, the existence of solution is guaranteed as in the classical discriminant analysis optimization problem (see appendix D).

Case $K = 2$: Two Populations

In this case, the optimization problem (3.1) is equivalent to the following one (see appendix D):

$$\mathbf{a} = argmax\left\{[\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})]^2\right\} \quad \text{subject to} \quad \begin{cases} \mathbf{a}^t\mathbf{W}\mathbf{a} = 1 \\ \mathbf{a} \geq \mathbf{0} \end{cases}. \tag{3.4}$$

3.2.2 The Discriminant Function

The expression of the discriminant function with our additional constraint, $y = \mathbf{a}_n^t\mathbf{x}$, is more difficult to obtain than in the classical case (see appendix D). Athough the optimization problem can be solved computationally, we present explicit expressions for some specific easy cases (notice that in this work we consider $p = 1$, 2 or 3). A possible different way to obtain such a explicit expression is outlined in section 4.2.2.

Although we are interested in the $K = 2$ case, some of the following calculations are made with the same difficulty for the general K-populations case; that is, for the general problem (3.1) instead of this specific one (3.4). As was mentioned, when the linear subspace $V_{\mathbf{a}}$ of $\mathbb{R}^p$ intersects the nonnegative orthant $\{\mathbf{a} \in \mathbb{R}^p \mid \mathbf{a} \geq \mathbf{0}\}$ outside the origin, that is, when all the components of $\mathbf{a}_F$ have the same sign, the new discriminant function will be

$$y = \mathbf{a}_n^t\mathbf{x} = \alpha\mathbf{a}_F^t\mathbf{x} = \alpha(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t\mathbf{W}^{-1}\mathbf{x}, \tag{3.5}$$

with $\alpha = +1$ or $\alpha = -1$ so that the condition $\alpha\mathbf{a}_F \geq \mathbf{0}$ holds (note that this would avoid the need for calculation of the constrained linear discriminant function).

In general, when all the components of $\mathbf{a}_F$ do not have the same sign, formal calculations are necessary. The *objective function* —of the optimization problem— and the constraints are combined in the *Lagrangian*, and the nonnegativeness is taken into account through the *Karush--Kuhn-Tucker conditions*, that are necessary and sufficient (see proposition 35 in appendix E):

$$\begin{cases} \frac{\partial L}{\partial \mathbf{a}} = \mathbf{0} \\ \frac{\partial L}{\partial \beta} = \mathbf{0} \\ a_i \geq 0,\ \mu_i \geq 0 \ \text{ and } \ \mu_i a_i = 0, \end{cases} \tag{3.6}$$

where the Lagrangian is

$$L(\mathbf{a}, \beta, \mu) = \mathbf{a}^t\mathbf{B}\mathbf{a} + \beta(1 - \mathbf{a}^t\mathbf{W}\mathbf{a}) + \mathbf{a}^t\mu \tag{3.7}$$

and $\mu = (\mu_i, \ldots, \mu_p)^t$ and β are the *multipliers*. It holds that

$$\frac{\partial L}{\partial \mathbf{a}} = 2\mathbf{B}\mathbf{a} - \beta 2\mathbf{W}\mathbf{a} + \mu. \tag{3.8}$$

The conditions (3.6) become

$$\begin{cases} 2(\mathbf{B} - \beta\mathbf{W})\mathbf{a} = -\mu \\ \mathbf{a}^t\mathbf{W}\mathbf{a} = 1 \\ a_i \geq 0,\ \mu_i \geq 0 \ \text{ and } \ \mu_i a_i = 0, \end{cases} \tag{3.9}$$

which are a system with $2p+1$ conditions and variables. Giving an explicit solution of this system is only possible in simple cases.

CASE $p = 1$: ONE VARIABLE

In this case, with only one discriminant variable, the original Fisher's discriminant analysis is trivial, since

$$\lambda(a) = \frac{aBa}{aWa} = \frac{B}{W} = constant. \tag{3.10}$$

CASE $p = 2$: TWO VARIABLES

First of all, when **two populations** are considered, let us denote

$$\mathbf{W} = \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix} \quad \text{and} \quad \mathbf{B} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix},$$

where by definition $w_{12} = w_{21}$ and $b_{12} = b_{21}$.

For two discriminant variables, three nonnull subcases (see the searching strategy mentioned in appendix E) cover the bidimensional positive quadrant where $\mathbf{a}$ is:

(A) Case $a_1 > 0$, $\mu_1 = 0$ and $a_2 = 0$. In this case,

(a1) By hypothesis, $\mu_1 = 0$ and $a_2 = 0$.

(a2) From $\mathbf{a}^t\mathbf{W}\mathbf{a} = 1$ the value $a_1 = |\sqrt{w_{11}^{-1}}|$ is obtained.

(a3) Finally, $2(\mathbf{B}-\beta\mathbf{W})\mathbf{a} = -\mu$ implies that $\beta = w_{11}^{-1}b_{11}$ and $\mu_2 = -2(b_{21}-w_{11}^{-1}b_{11}w_{21})|\sqrt{w_{11}^{-1}}|$.

The discriminant function, if $\mathbf{B} - \beta\mathbf{W}$ is negative semidefinite, would be

$$y_A = \mathbf{a}_n^t\mathbf{x} = |\sqrt{w_{11}^{-1}}|x_1. \tag{3.11}$$

(B) Case $a_1 = 0$, $a_2 > 0$ and $\mu_2 = 0$. In this case,

(b1) By hypothesis, $a_1 = 0$ and $\mu_2 = 0$.

(b2) Thus, $\mathbf{a}^t\mathbf{W}\mathbf{a} = 1$ implies the value $a_2 = |\sqrt{w_{22}^{-1}}|$.

(b3) From $2(\mathbf{B} - \beta\mathbf{W})\mathbf{a} = -\mu$ the values $\beta = w_{22}^{-1}b_{22}$ and $\mu_1 = -2(b_{12} - w_{22}^{-1}b_{22}w_{12})|\sqrt{w_{22}^{-1}}|$ are obtained.

The discriminant function, if $\mathbf{B} - \beta\mathbf{W}$ is negative semidefinite, would be

$$y_B = \mathbf{a}_n^t\mathbf{x} = |\sqrt{w_{22}^{-1}}|x_2. \tag{3.12}$$

(C) Case $a_1 > 0$, $\mu_1 = 0$, $a_2 > 0$ and $\mu_2 = 0$. To study the *interior solutions*,

(c1) By hypothesis $\mu = \mathbf{0}$, the nonnegativity constraint disappears from the Lagrangian and the objective function is again $L(\mathbf{a}) = \lambda(\mathbf{a})$.

(c2) As $(\mathbf{B}-\beta\mathbf{W})\mathbf{a}=\mathbf{0}$, it is necessary that $|\mathbf{B}-\beta\mathbf{W}|=0$; this condition implies, since $\mathbf{W}$ is not singular (by hypothesis), that

$$\beta=\frac{-b\pm\sqrt{b^2-4|\mathbf{W}||\mathbf{B}|}}{2|\mathbf{W}|}, \tag{3.13}$$

with $b=w_{12}b_{21}+w_{21}b_{12}-w_{11}b_{22}-w_{22}b_{11}$. This means that $(\mathbf{W}^{-1}\mathbf{B}-\beta\mathbf{I})\mathbf{a}=\mathbf{0}$, and we are again interested in an eigenvector of an eigenvalue of $\mathbf{W}^{-1}\mathbf{B}$. Nevertheless, now the criterion is not selecting the largest eigenvalue, but selecting the largest one with eigenvectors verifying the nonnegativity constraint (or nonpositiveness, since the scale factor is not a problem).

(c3) Given β, also from $(\mathbf{B}-\beta\mathbf{W})\mathbf{a}=\mathbf{0}$ there will be nontrivial solution if $a_2=\gamma a_1$, or, equivalently, $a_1=\gamma^{-1}a_2$ with

$$\gamma=-\frac{b_{11}-\beta w_{11}}{b_{12}-\beta w_{12}},\quad \text{or, respectively,}\quad \gamma=-\frac{b_{21}-\beta w_{21}}{b_{22}-\beta w_{22}}, \tag{3.14}$$

as $|\mathbf{B}-\beta\mathbf{W}|=0$.

(c4) Finally, the condition $\mathbf{a}^t\mathbf{W}\mathbf{a}=1$ implies that

$$a_1=|\sqrt{[w_{11}+\gamma(w_{12}+w_{21})+\gamma^2w_{22}]^{-1}}|, \tag{3.15}$$

or, respectively,

$$a_2=|\sqrt{[\gamma^{-2}w_{11}+\gamma^{-1}(w_{12}+w_{21})+w_{22}]^{-1}}|, \tag{3.16}$$

so the discriminant function, if $\mathbf{B}-\beta\mathbf{W}$ is negative semidefinite, would be

$$y_C=\mathbf{a}_n^t\mathbf{x}=a_1x_1+\gamma a_1x_2, \tag{3.17}$$

or, respectively,

$$y_C=\mathbf{a}_n^t\mathbf{x}=\gamma^{-1}a_2x_1+a_2x_2, \tag{3.18}$$

with γ (and β) as given above.

Remark 21 In the last expressions it has been implicitly supposed that $\gamma\neq 0$ and $\gamma\neq\infty$. Nevertheless, it is noteworthy that when $\gamma\to 0$ or $\gamma\to\infty$, the discriminant functions of the cases (A) and (B) arise, respectively, as limit cases of (C). As $a_1\longrightarrow|\sqrt{w_{11}^{-1}}|$ when $\gamma\to 0$ and $a_2\to|\sqrt{w_{22}^{-1}}|$ when $\gamma\to\infty$, respectively, then

$$y_C\underset{\gamma\to 0}{\longrightarrow}y_A\qquad\text{and}\qquad y_C\underset{\gamma\to\infty}{\longrightarrow}y_B. \tag{3.19}$$

Remark 22 The parameter γ acquires an important role, since it provides information —under the nonnegativity constraints— about each variable importance for classifying purposes, that is, about each variable discriminant power.

Remark 23 This simple case $p = 2$ (two variables) and $K = 2$ (two populations) can be used to better understand the meaning of the within-class scatter matrix,

$$\mathbf{W} = \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix} = \begin{pmatrix} n_1\hat{\sigma}_{11}^{(1)} + n_2\hat{\sigma}_{11}^{(2)} & n_1\hat{\sigma}_{12}^{(1)} + n_2\hat{\sigma}_{12}^{(2)} \\ n_1\hat{\sigma}_{21}^{(1)} + n_2\hat{\sigma}_{21}^{(2)} & n_1\hat{\sigma}_{22}^{(1)} + n_2\hat{\sigma}_{22}^{(2)} \end{pmatrix}. \tag{3.20}$$

Remark 24 The Karush-Kuhn-Tucker conditions are sufficient due to proposition 35 in appendix E; this means that the previous calculations have led to the local and global minimum. On the other hand, as these conditions are also necessary, due to proposition 33 in appendix E, it holds that

$$\nabla^2_{\mathbf{aa}} L(\mathbf{a}, \beta, \mu) = \frac{\partial^2 L}{\partial \mathbf{a}^2}(\mathbf{a}, \beta, \mu) = 2(\mathbf{B} - \beta\mathbf{W}) \tag{3.21}$$

is a positive semidefinite matrix (in this case, $p = 2$, and under the nonnegativity constraints).

Other Values of p

From the Karush-Kuhn-Tucker conditions of the cases $p = 3$ or $p = 4$, several subcases would arise after some work, providing explicit expressions for $\mathbf{a}_n$ under some conditions on the samples. Nevertheless, since it has been proved that there are no formula for the solution of a five-degree general polinomial equation, for the cases $p \geq 5$ it would be impossible to find —in this way— the explicit expressions for $\mathbf{a}_n$.

3.2.3 The Classification

To classify new elements, the previous discriminant function is applied following the same ideas than in the classical discriminant analysis (see section D.4). Geometrically, the condition $\mathbf{a} \geq 0$ restricts the possible directions into which the data should be projected. We also determine the cutoff point by projecting $\frac{1}{2}(\overline{\mathbf{x}}^{(1)} + \overline{\mathbf{x}}^{(2)})$ with $y = \mathbf{a}_n^t\mathbf{x}$, that is, via the $\mathbf{a}_n^t\cdot$ premultiplication. The method classifies a new element in the population k as follows:

$$\begin{cases} k = 1 & \text{if} \quad y > \frac{1}{2}\mathbf{a}_n^t(\overline{\mathbf{x}}^{(1)} + \overline{\mathbf{x}}^{(2)}) \\ k = 2 & \text{otherwise} \end{cases}, \tag{3.22}$$

where the value $y(\frac{1}{2}\overline{\mathbf{x}}^{(1)} + \frac{1}{2}\overline{\mathbf{x}}^{(2)}) = \frac{1}{2}\mathbf{a}_n^t(\overline{\mathbf{x}}^{(1)} + \overline{\mathbf{x}}^{(2)})$ can be termed the *adjusted cutoff point*. Notice that for the particular case (3.5) the classification is just the same as that of the classical discriminant analysis.

As for $y = \mathbf{a}_F^t\mathbf{x}$, now the classification of a multivariate point is done for $y = \mathbf{a}_n^t\mathbf{x}$ by the simple comparison of its projection with the projection of the semisum of the group means (centroids). The computed with simulated and real data show that the classification provided by the two discriminant functions is similar, while the nonnegativity restriction adds some theoretical advantages.

Remark 25 Rules like (3.22) assign the elements verifying the equality to the group 2. The number of these elements is usually negligible. Nevertheless, the frontier is sometimes not negligible and a possible solution is assigning these elements to a group at random. We observed this effect in some simulation exercises (methods *DFMj*, due to the nature of our discriminant variables), and our code allocated these elements at random.

Remark 26 Rules like (D.40) assign the elements verifying the equality to the group 2. The number of these elements is usually negligible.

3.2.4 Our Discriminant Variables

In order to facilitate understanding of the classification criterion, so far we have used generic discriminant variables $x_1, \ldots, x_p$. Now we define the specific variables and explain how to construct them from the functional data.

If $\chi^{(1)}$ and $\chi^{(2)}$ are (p-1)-order differentiable functions in a functional space L, the quantities $d(D^i\chi^{(1)}, D^i\chi^{(2)})$, for $i = 0, 1, \ldots, p-1$, are numeric when $d(\cdot,\cdot)$ is a (semi)distance and the D^i denotes the i-th derivative ($i = 0$ represents no differentiation).

Assuming that there are two populations, with models $\mathcal{X}^{(1)}$ and $\mathcal{X}^{(2)}$, and let $\chi_1^{(k)}, \ldots, \chi_{n_k}^{(k)}$ be a sample of the population k, respectively; in this situation, for a function χ we define the variables

$$x_i = d(D^{i-1}\chi, \overline{D^{i-1}\chi}^{(1)}) - d(D^{i-1}\chi, \overline{D^{i-1}\chi}^{(2)}), \tag{3.23}$$

for $i = 1, 2, \ldots, p$, where $\overline{D^{i-1}\chi}^{(k)} = n_k^{-1} \sum_{e=1}^{n_k} D^{i-1}\chi_e^{(k)}$, $k = 1, 2$. That is, x_i is the difference between the distances from $D^{i-1}\chi$ to the (i-1)-th derivative of the population means. With these definitions, the discriminant analysis will provide information about the usefulness of each derivative for classification purposes.

From the fact that $d(\cdot,\cdot)$ is a (semi)distance, some qualitative properties of our variables can be deduced. The triangular property implies[2] that

$$|x_i| \leq d(\overline{D^{i-1}\chi}^{(1)}, \overline{D^{i-1}\chi}^{(2)}). \tag{3.24}$$

This means that there is a "natural sample boundary" for the values that each variable can take. A problem can appear when $\overline{D^{i-1}\chi}^{(1)} \approx \overline{D^{i-1}\chi}^{(2)}$, since $|x_i| \approx 0$ and the order of magnitude of variations in x_i can be confused with some computational or approximation inaccuracies — the discriminant variable would lose classification power. Our proposals assign a tiny weight to these variables.

If the triangular property does not hold, some data such that $|x_i| \gg d(\overline{D^{i-1}\chi}^{(1)}, \overline{D^{i-1}\chi}^{(2)})$ might exist; then, the order of magnitude of small variations in x_i could be confused with $d(\overline{D^{i-1}\chi}^{(1)}, \overline{D^{i-1}\chi}^{(2)})$, and the discriminant variable would lose classification power.

[2] $d(a,c) - d(a,b) \leq d(b,c)$ and $d(a,b) - d(a,c) \leq d(c,b) = d(b,c)$, so $|d(a,c) - d(a,b)| \leq d(b,c)$

If $d(\cdot,\cdot)$ were only a semidistance, not a distance, some pairs of different points would be indistinguishable; in the extreme —but possible— case where the original samples were such that $\overline{D^{i-1}\chi}^{(1)} \neq \overline{D^{i-1}\chi}^{(2)}$ with $d(\overline{D^{i-1}\chi}^{(1)}, \overline{D^{i-1}\chi}^{(2)}) = 0$, inequality (3.24) would imply that $x_i \equiv 0$, and the information of the functional transformation D^{i-1} would not be used by our procedures. Notice that, irrelevant of whether $d(\cdot,\cdot)$ is a semidistance or a distance, what may occur is that $\overline{D^{i-1}\chi}^{(1)} = \overline{D^{i-1}\chi}^{(2)}$; in this situation $d(\overline{D^{i-1}\chi}^{(1)}, \overline{D^{i-1}\chi}^{(2)}) = 0$ and, due also to the inequality (3.24), the variables x_j, $j \geq i$, are useless (this effect has been observed in the simulation exercises).

Thus, in our proposals it is important to test how different $\overline{D^{i-1}\chi}^{(1)}$ and $\overline{D^{i-1}\chi}^{(2)}$ are. In the following, let us suppose that these quantities are different enough —this is essential for a method based on the mean function— for the aforementioned problems not to hold (although this does not guarantee good results, since the variability also plays an important role). In our implementations, the variables with negligible variability have been discarded — those with variance smaller than $\sqrt{eps}$, where *eps* is the level of precision of the programming language. Nevertheless, these useless variables are included in the graphical representations of our proposals.

On the other hand, for a unique variable x_i, it is possible for two functions $\chi^{(1)} \neq \chi^{(2)}$ (belonging or not to the same population) to have corresponding univariate variable values holding $x_i^{(1)} = x_i^{(2)}$. Nevertheless, from the theoretical point of view, if the functions were analytical, $D^{i-1}\chi^{(1)} = D^{i-1}\chi^{(2)}$, $\forall i = 0, 1, \ldots$ if, and only, if, $\chi^{(1)} \equiv \chi^{(2)}$; in practice, even for nonanalytical functions $\chi^{(1)} \neq \chi^{(2)}$, the bigger the number of variables is, the more probable it is that the desiderable condition $\mathbf{x}^{(1)} \neq \mathbf{x}^{(2)}$ holds. Thus, one of the advantages of combining the information is that the elements are usually better characterized in the finite-dimensional space. Our proposals involve a drastic reduction of the dimension — from infinite to p (usually 2 or 3).

Remark 27 The following function can be thought of as the representative sample curve of the k-th population,

$$\mathcal{R}_{i-1}^{(k)} = \overline{D^{i-1}\chi}^{(k)}. \tag{3.25}$$

Let us insist on the fact that functions are supposed to be differentiable, so the sample mean is a "good representative" of a collection of smooth functions.

Remark 28 In this document we do not highlight the population version of the concepts, but, in terms of the models $\mathcal{X}^{(1)}$ and $\mathcal{X}^{(2)}$ our discriminant variables are random variables; for a stochastic function $\mathcal{X}$,

$$X_i = d(D^{i-1}\mathcal{X}, \mathbb{E}(D^{i-1}\mathcal{X}^{(1)})) - d(D^{i-1}\mathcal{X}, \mathbb{E}(D^{i-1}\mathcal{X}^{(2)})). \tag{3.26}$$

Since $d(\cdot,\cdot)$ is a (semi)distance, the triangular property implies that

$$|X_i| \leq d(\mathbb{E}(D^{i-1}\mathcal{X}^{(1)}), \mathbb{E}(D^{i-1}\mathcal{X}^{(2)})). \tag{3.27}$$

This means that there is a "natural theoretical boundary" for the values that each variable can take. When $\mathbb{E}(D^{i-1}\mathcal{X}^{(1)}) = \mathbb{E}(D^{i-1}\mathcal{X}^{(2)})$ these variables cannot be used for classification, as the

questions $X_i < 0?$ and $X_i > 0?$ make no sense. When the previous equality holds because $D^{i-1}\mathcal{X}^{(1)} = D^{i-1}\mathcal{X}^{(2)}$, the same will happen for any variable X_j, $j \geq i$. Now, finally the representative population curve of the k-th population would be

$$\mathbf{R}_{i-1}^{(k)} = \mathbb{E}(D^{i-1}\mathcal{X}^{(k)}). \tag{3.28}$$

Remark 29 The previous sample and population boundaries for the variables depend on the (semi)distance $d(\cdot,\cdot)$, not only on the data itself; this means that an inappropriate choice of the distance could take little advantage of important differences between the groups (samples or populations).

Remark 30 Since the derivation, the integration and the addition are linear operations, it holds that $\overline{D^{i-1}\chi}^{(k)} = D^{i-1}\overline{\chi}^{(k)},\ k = 1, 2$ and $\mathbb{E}(D^{i-1}\mathcal{X}^{(k)}) = D^{i-1}\mathbb{E}(\mathcal{X}^{(k)}),\ k = 1, 2$. This highlights the importance of the mean functions in our proposals.

Standardization and Coefficients

At this point, it is advisable to study the relationship between the variables just defined and the interpretation of the coefficientes provided by the general optimization problem (see section D.3.1).

Supposing that a variable t and a function $\chi(t)$ are not dimensionless (scalars without units of measure), nor is $D^1\chi(t) = d\chi(t)/dt$. Moreover, the derivative has a different dimension than its original function, as the term $d\chi(t)$ has the same units as $\chi(t)$, while the term dt does not. As a consequence, all the variables defined in (3.23) are dimensionless only when t and $\chi(t)$ also are.

Regardless, for classification and descriptive purposes the transformation and the standardization of the data must be applied, respectively, as explained in section D.3.1. In our methodology this could be done over the functions (definitions of mean and standard deviation for functional data are given in literature), but it is preferable to operate over the multivariate data, as they are just in the input of the multivariate optimization problem and it is not certain that the changes were preserved in the functional-to-multivariate data transformation step.

3.2.5 Algorithms

Algorithms 3 and 4

Let $\chi_1^{(k)}(t), \ldots, \chi_{n_k}^{(k)}(t),\ k = 1, 2$, be samples of functions from the two populations, then:

1. **From functional to multivariate data.** For each $\chi_e^{(k)}(t),\ e = 1, \ldots, n_k$, the following vector is constructed

$$\mathbf{x}_e^{(k)} = (x_{1,e}^{(k)}, \ldots, x_{p,e}^{(k)})^t, \tag{3.29}$$

where $x_{i,e}^{(k)}$ is obtained by (3.23). These vectors form the multivariate sample

$$(\mathbf{x}_1^{(k)}, \cdots, \mathbf{x}_{n_k}^{(k)}). \tag{3.30}$$

2. **The discriminant function.** These samples are used as input in the optimization problem to obtain the discriminant function:

$$y(\mathbf{x}) = \mathbf{a}^t \mathbf{x}, \tag{3.31}$$

where $\mathbf{x} = (x_1, \ldots, x_p)^t$, and $\mathbf{a} = \mathbf{a}_F$, in algorithm 3, or $\mathbf{a} = \mathbf{a}_n$, in algorithm 4, depending on whether or not the additional constraint was imposed.

3. **The allocation of new curves.** To classify a new curve $\chi(t)$, its multivariate vector is constructed,

$$\mathbf{x} = (x_1, \ldots, x_p)^t, \tag{3.32}$$

again using expression (3.23), and finally the value $y(\mathbf{x})$ is used to assign the curve $\chi(t)$ to one of the two populations, as mentioned in subsections 3.2.3 and D.4.

These steps have been represented in figure 3.5. Several versions of this algorithm have been implemented and compared in the following sections.

Remark 31 As a distance measurement between two functions we have taken the distance given in expression (1.76) for $m = 1$.

Remark 32 The possible outliers in the samples of functions could be extracted with the same methodology used in section 2.2.3.

Code

In the link given on the first page of this chapter, we have made some code available. It implements the methods *DFM0,...*, *DFM(p-1)*, *WI* and *WD* (defined below, in the sections with computes). There are two main scripts, one for simulation exercises and another for the application to real data; the former runs a Monte Carlo loop, while the latter adds a leave-m-out cross-validation partition of the real data (the user can choose the value of m, possibly different for each group). The code can be executed without any derivative, that is, only with the crude functions, and can manage as many derivatives as desired — the limit can come from the hardware, the software (we have tested up to a differentiation of order 30) or the theory (with many discriminant variables, the sample pooled covariance matrix can be singular).

Our code provides previous optional graphics that are based on an additional and independent run of the loop; these graphics use both training and testing data and have a useful prospective and descriptive character.

The code is fast and easy to execute and extend. The reader can reproduce, apply or extend our results and graphics easily. A helping file is included with the code.

3.2.6 Weighted Semidistances or Distances

Let us substitute, for a function $\chi(t)$, the discriminant variables into the expression of the discriminant function:

$$\begin{aligned} y(\mathbf{x}) &= \mathbf{a}^t\mathbf{x} = \sum_{i=1}^{p} a_i x_i \\ &= \sum_{i=1}^{p} a_i d(D^{i-1}\chi, \overline{D^{i-1}\chi}^{(1)}) - \sum_{i=1}^{p} a_i d(D^{i-1}\chi, \overline{D^{i-1}\chi}^{(2)}) \\ &= \zeta(\chi, \overline{\chi}^{(1)}) - \zeta(\chi, \overline{\chi}^{(2)}), \end{aligned} \tag{3.33}$$

where

$$\zeta(\chi, \overline{\chi}^{(k)}) = \sum_{i=1}^{p} a_i d(D^{i-1}\chi, \overline{D^{i-1}\chi}^{(k)}) = \sum_{i=1}^{p} a_i d(D^{i-1}\chi, D^{i-1}\overline{\chi}^{(k)}). \tag{3.34}$$

More generally, for any curves χ_1 and χ_2 the weighted sum $\zeta(\chi_1, \chi_2) = \sum_{i=1}^{p} a_i d(D^{i-1}\chi_1, D^{i-1}\chi_2)$ can be considered. The values a_i play a role in determining the properties that $\zeta(\cdot,\cdot)$ inherits from the distance $d(\cdot,\cdot)$.

An important general property of $\zeta(\cdot,\cdot)$ is that it takes into account —with different importance and at the same time— the functions, their smoothness, their curvature, etcetera. Some qualitative information can be deduced by doing for $\zeta(\cdot,\cdot)$ the same qualitative analysis done for $d(\cdot,\cdot)$ in subsection 3.2.4.

For $\zeta(\cdot,\cdot)$ to take nonnegative values, our additional restrictions ($a_i \geq 0$) are necessary; then, only the function $y = \mathbf{a}_n^t\mathbf{x}$ —not the classical linear discriminant function— can be seen as providing a classification based on the minimization of a weighted (semi)distance. In this situation, the triangular property implies that

$$|y| \leq \zeta(\overline{\chi}^{(1)}, \overline{\chi}^{(2)}). \tag{3.35}$$

Thus, there is a "natural sample boundary" for the values that the discriminant function can take. This inequality would also imply that $|y| \approx 0$ when $\overline{\chi}^{(1)} \approx \overline{\chi}^{(2)}$, leading to a problem when the order of magnitude of variations in y can be confused with some computational or approximation inaccuracies — the discriminant variable would lose classification power. Nevertheless, $\overline{\chi}^{(1)}$ and $\overline{\chi}^{(2)}$ were supposed different enough in section 3.2.4.

When $\zeta(\cdot,\cdot)$ is not a (semi)distance, the triangular property does not hold; so some data such that $|y| \gg \zeta(\overline{\chi}^{(1)}, \overline{\chi}^{(2)})$ might exist, and the order of magnitude of small variations in y could be confused with $\zeta(\overline{\chi}^{(1)}, \overline{\chi}^{(2)})$, leading to a loss of classification power of the discriminant function. This seems to indicate that our restrictions could improve the classification when data are such that the classical Fisher's discriminant function tends to take quite different values —smaller or bigger— than $\zeta(\overline{\chi}^{(1)}, \overline{\chi}^{(2)})$. In this case, our constraints would prevent extreme values that could deteriorate the classification.

As in a space of functions the derivation can imply a loss of information, then $\zeta(\cdot,\cdot)$ with $a_i \geq 0$ can be interpreted as measurements with a weighted distance if and only if $a_1 \neq 0$ (in practice, if and only if a_1 is significant) and $d(\cdot,\cdot)$ is a distance; otherwise, if $a_1 = 0$ or $d(\cdot,\cdot)$ is a semidistance, it can be interpreted as a measurement with a weighted semidistance, since two functions can differ in a constant and verify that $\zeta(\mathcal{X}^{(1)}, \mathcal{X}^{(2)}) = 0$. When $\zeta(\cdot,\cdot)$ is only a semidistance, not a distance, some pairs of different points would be indistinguishable; in the extreme —but possible— case where the original samples were such that $\overline{\chi}^{(1)} \neq \overline{\chi}^{(2)}$ with $\zeta(\overline{\chi}^{(1)}, \overline{\chi}^{(2)}) = 0$, it would hold that $y \equiv 0$, and the discriminant function would be useless (notice that $\overline{\chi}^{(1)} \neq \overline{\chi}^{(2)}$ was supposed in section 3.2.4). Finally, irrelevant of whether $\zeta(\cdot,\cdot)$ is a semidistance or a distance, for any two curves (belonging or not to the same population) the unlikely case where $\chi^{(1)} \neq \chi^{(2)}$ with $y(\mathbf{x}^{(1)}) = y(\mathbf{x}^{(2)})$ could occur.

Remark 33 The "natural theoretical boundary" of the random variable Y would be

$$|Y| \leq \zeta(\mathbb{E}(\mathcal{X}^{(1)}), \mathbb{E}(\mathcal{X}^{(2)})). \tag{3.36}$$

3.3 Simulation Results

In order to illustrate the performance of our two procedures, we perform a Monte Carlo study using three different settings. In all cases we consider two functional populations in the space $\mathcal{C}[0,1]$ of continuous functions defined in the interval $[0,1]$. The methods used to classify are the following:

- Distance to the sample functional mean, calculated using the functions in the training set (*DFM0*). That is, using the rule

$$\begin{cases} k = 1 & \text{if} \quad x_1 < 0 \\ k = 2 & \text{otherwise} \end{cases}. \tag{3.37}$$

- Distance to the sample functional mean, calculated using the first derivatives of functions in the training set (*DFM1*). That is, using the rule

$$\begin{cases} k = 1 & \text{if} \quad x_2 < 0 \\ k = 2 & \text{otherwise} \end{cases}. \tag{3.38}$$

- Weighted indicator (*WI*) obtained using our first procedure (algorithm 3). Using the algorithm with $\mathbf{x} = (x_1, x_2)^t$ and without our additional constraint.

- Weighted distance (*WD*) obtained using our second procedure (algorithm 4). Then, for the algorithm with $\mathbf{x} = (x_1, x_2)^t$ and the nonnegativity constraint.

We generate 200 functions from each population. The training set consists of the first 100 functions from each population, and the remaining 100 observations from each sample are the testing set. For each setting we run 1000 replications, so the results are based on 1000 estimates of the misclassification rates. The functions have been evaluated in 30 points between 0 and 1. With the code that we have distributed, the reader can reproduce these exercises easily.
Thus, we describe the three considered settings.

Simulation Exercise 1. We consider the following two functional data generating models:

Model B1. $\mathcal{X}_e^{(1)} = t + U_e$, where U_e is a uniform random variable on the interval $(0, 1)$.

Model R1. $\mathcal{X}_e^{(2)} = t + V_e$, where V_e is a uniform random variable on the interval $(1/2, 3/2)$.

Remark 34 Figure 3.1(a) displays a random sample for these two models. Notice that models B1 and R1 differ in level when U_e takes value in $(0, 1/2)$ and V_e in $(1, 3/2)$ but they coincide when U_e and V_e take values in $(1/2, 1)$. This intersection causes a theoretical misclassification rate equal to 25% when the method *DFM0* is used. Moreover, the first derivative of models $\mathcal{X}^{(1)}$ and $\mathcal{X}^{(2)}$ coincides, so method *DFM1* will have a misclassification rate equal to 50%.

Simulation Exercise 2. We consider the following two functional data generating models:

Model B2. $\mathcal{X}_e^{(1)} = (t+U_e)^2$, where U_e is a uniform random variable on the interval $(0, 1)$.

Model R2. $\mathcal{X}_e^{(2)} = t^2 + V_e$, where V_e is a uniform random variable on the interval $(0, 1)$.

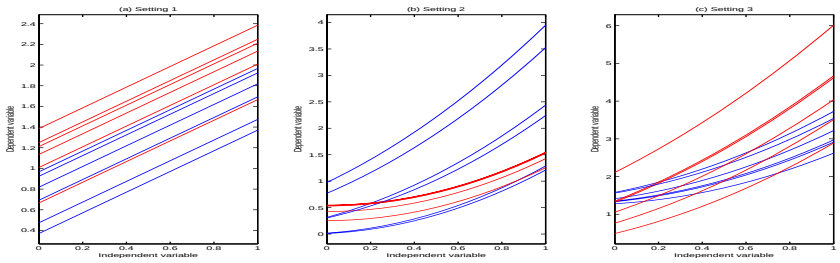
Remark 35 Figure 3.1(b) displays a random sample for these two models. Notice that models B2 and R2 generate functional observations that cross one another; but if we consider the first derivative, $D^1\chi^{(1)}$ and $D^1\chi^{(2)}$, then they have significant level differences. The theoretical misclassification rate is equal to 12.5% when the method *DFM1* is used.

Simulation Exercise 3. We consider the following two functional data generating models:

Model B3. $\mathcal{X}_e^{(1)} = (t + U_e)^2 + 5/4$, where U_e is a uniform random variable on the interval $(0, 1)$.

Model R3. $\mathcal{X}_e^{(2)} = (t+V_e)^2$, where V_e is a uniform random variable on the interval $(1/2, 3/2)$.

Figure 3.1: Plots of samples from the three simulation settings: (a) Functions following models B1 and R1; (b) Functions following models B2 and R2; (c) Functions following models B3 and R3.



Remark 36 Figure 3.1(c) displays a random sample for these two models. Notice that models B3 and R3 also generate functional observations that cross one another (the term 5/4 in $\mathcal{X}^{(1)}$ is added in order to maximize the crossing) but if we consider the first derivatives, $D^1\chi^{(1)}(t)$ and $D^1\chi^{(2)}(t)$, then these have level differences in the same way as $\chi^{(1)}(t)$ and $\chi^{(2)}(t)$ generated by models B1 and R1, respectively. So, we have a theoretical misclassification rate equal to 25% when the method *DFM1* is used. In order to evaluate the derivatives of second order, in this exercise the method *DFM2* (defined in the following section) has been included, and an additional variable has been considered in the methods *WI* and *WD* through $\mathbf{x} = (x_1, x_2, x_3)^t$.

In figure 3.2 we present the results for the first simulation setting. Figure 3.2(a) gives the boxplots of the misclassification rate estimates for the four methods. As expected, the method *DFM0* has a misclassification rate of around 25% and the method *DFM1* is useless (it classifies almost at random) in this setting. Figures 3.2(b) and 3.2(c) give the boxplots of the estimated weights for methods *WI* and *WD*. Both methods give positive weights for the variable associated to $\chi^{(1)}$ and $\chi^{(2)}$ and zero weights for the variable associated to $D^1\chi^{(1)}$ and $D^1\chi^{(2)}$. Notice that in this case the variable $D^1\chi^{(1)} - D^1\chi^{(2)}$ has variance equal to zero since $D^1\chi_e^{(1)}(t) = D^1\chi_e^{(2)}(t) = 1$ for all e. In this simulation setting, methods *DFM0*, *WI* and *WD* have the same performance.

In figure 3.3, we present the results for the second simulation setting. Figure 3.3(a) gives the boxplots of the misclassification rate estimates for the four methods. In this case, method *DFM0* is outperformed by method *DFM1*, which obtains misclassification rates around the expected 12.5%. Method *WD* has similar performance to *DFM1*, and both are outperformed by method *WI*. Figures 3.3(b) and 3.3(c) give the boxplots of the estimated weights for methods *WI* and *WD*. In this case, method *WI* gives positive weights for the variable associated to $\chi^{(1)}$ and $\chi^{(2)}$ and negative (but higher in module) weights for the variable associated to $D^1\chi^{(1)}$ and $D^1\chi^{(2)}$, so the classification rule with *WI* is not based on a distance. Once we impose the positiveness on the weights, method *WD* gives positive weights for the variable associated to $D^1\chi^{(1)}$ and $D^1\chi^{(2)}$ and zero weights for the variable associated to $\chi^{(1)}$ and $\chi^{(2)}$. So, the classification rule with *WD* is a semidistance. In this setting and in the previous one, method *WD* selects the variable that has lower misclassification rates.

Figure 3.2: First simulation setting results: (a) Boxplots of the misclassification rates for methods *DFM0*, *DFM1*, *WI* and *WD*; (b) Boxplots of the weights obtained for method *WI*; (c) Boxplots of the weights obtained for method *WD*.

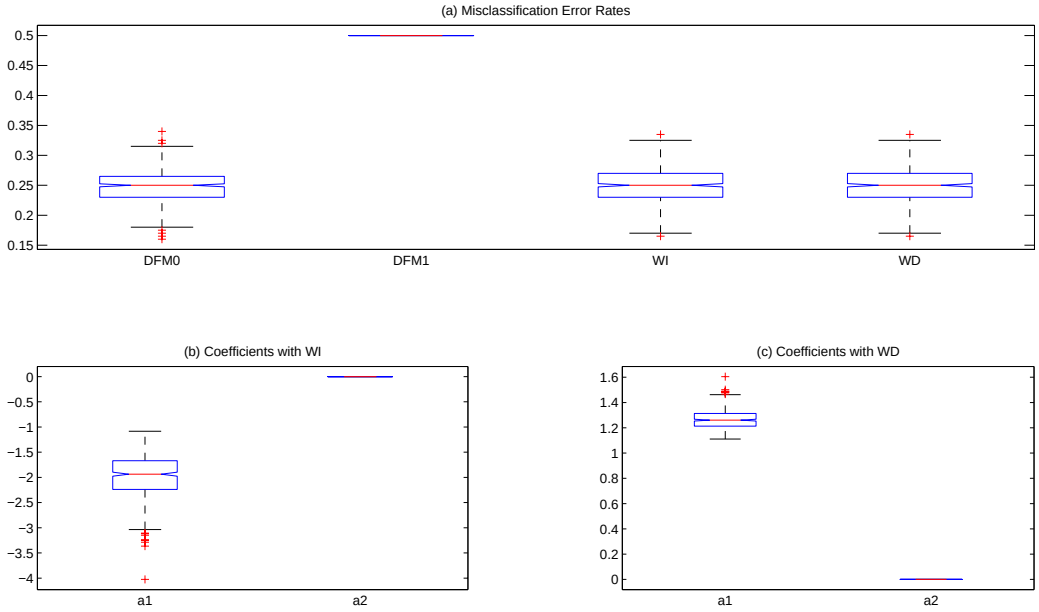
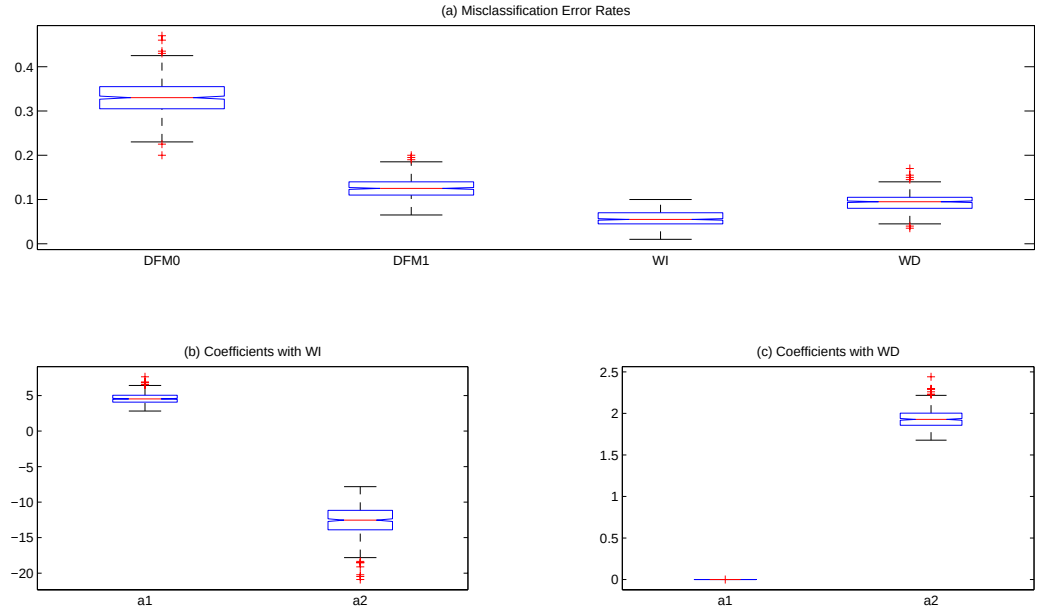


Figure 3.3: Second simulation setting results: (a) Boxplots of the misclassification rates for methods *DFM0*, *DFM1*, *WI* and *WD*; (b) Boxplots of the weights obtained for method *WI*; (c) Boxplots of the weights obtained for method *WD*.



We have considered up to the second derivative in this exercise. Figure 3.4, containing the scatter plots of the three discriminant variables, indicates that the combination of the two first discriminant variables has a good discriminant power. The histograms of this figure show that x_2 is the variable with the highest discriminant power, as the weights (coefficients) will confirm in the boxplots of this exercise. In figure 3.5 a bi- and three-dimensional representations of the functional data are given, as well as the plot of the discriminant functions provided by our methods. Finally, in figure 3.6 we present the results for the third simulation setting. Figure 3.6(a) gives the boxplots of the misclassification rate estimates for the methods. In this case, method *DFM0* is again outperformed by method *DFM1*, which obtains misclassification rates around the expected 25%. Both methods perform worse than the weighted procedures, *WI* and *WD*; method *WI* has the best performance. Here, the improvement comes from the combination of variables associated to functions and their first derivatives. Derivatives of higher order are useless, although the presence of these variables does not affect the performance of our proposals. As expected, the method *DFM2* classifies at random. Figures 3.6(b) and 3.6(c) give the boxplots of the estimated weights for methods *WI* and *WD*. In this case, method *WI* gives positive weights for the variable associated to $\chi^{(1)}$ and $\chi^{(2)}$ in more than 25% of the replications and negative weights in the remaining ones. In all replications, *WI* gives negative weights for the variable associated to $D^1\chi^{(1)}$ and $D^1\chi^{(2)}$. For those replications where there are sign differences, the classification rule with *WI* is not a distance. This "inconvenience" is avoided by using the method *WD*. In this setting, the classification rule with *WD* is a semidistance in all cases and a distance in 75% of the replications.

3.3.1 Theoretical Misclassification Rates

The models of the previous simulation exercises were chosen to calculate these quantities easily; nevertheless, the complex and formal way is also included. Notice that, to evaluate the global error rate, e is usually chosen at random from the populations with the same probability (if $n_1 = n_2$; the empirical counterpart is that the testing samples would have the same size, $m_1 = m_2$).

Simulation Exercise 1

The misclassification rate for method *DFM0* was calculated as

$$p(\mathcal{E}) = \left(\frac{1}{2}\frac{1}{2}\right) \cdot \frac{1}{2} + \left(\frac{1}{2}\frac{1}{2}\right) \cdot \frac{1}{2} = \frac{1}{4}. \tag{3.39}$$

On the other hand, for *DFM1*,

$$p(\mathcal{E}) = \frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{2}. \tag{3.40}$$

These rates can be calculated in a more explicit way by using the following complementary probabilities.

Since $\mathbb{E}(\mathcal{X}^{(1)}) \neq \mathbb{E}(\mathcal{X}^{(2)})$, the variable X_1 can be used to classify.

Figure 3.4: Third exercise: prospective plots for the first three discriminant variables

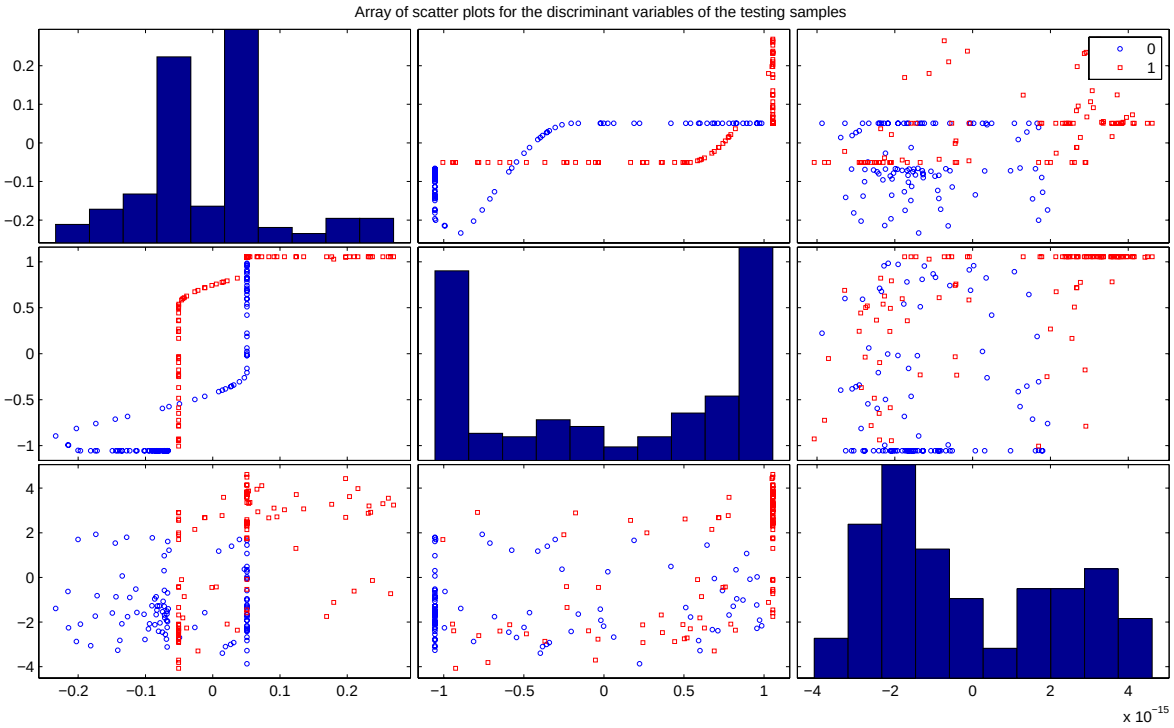


Figure 3.5: Third exercise: descriptive figures

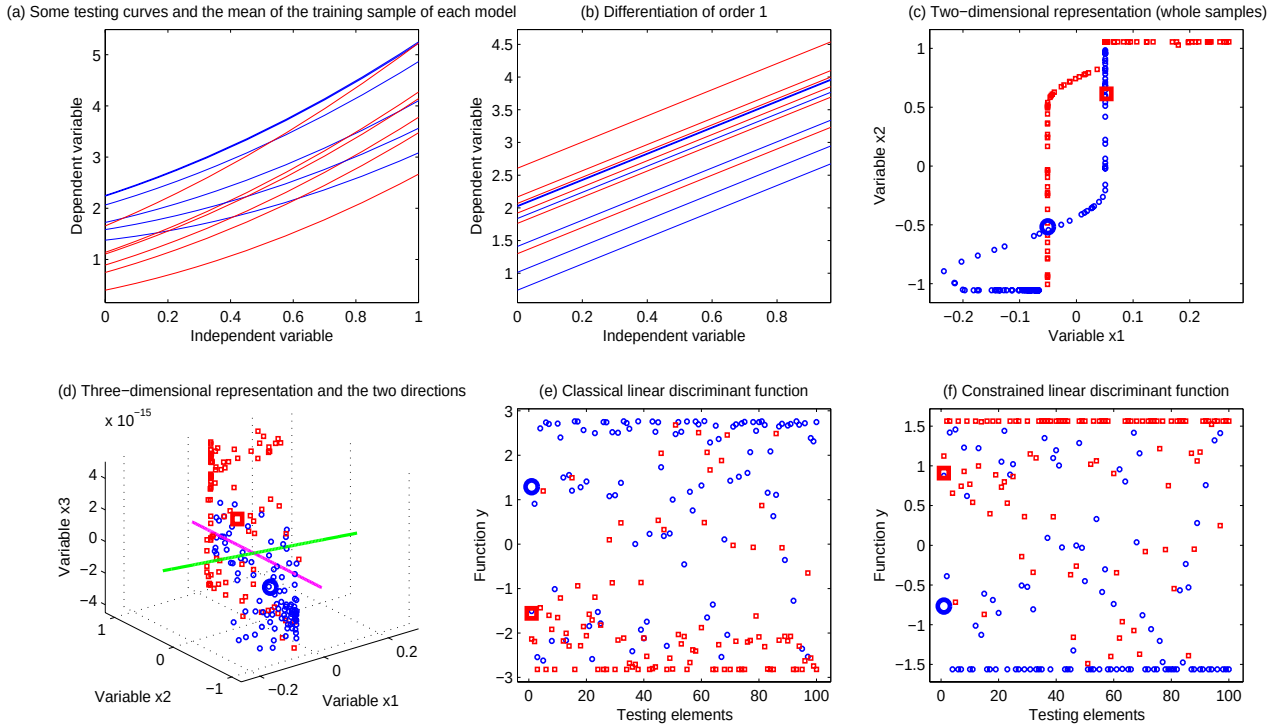
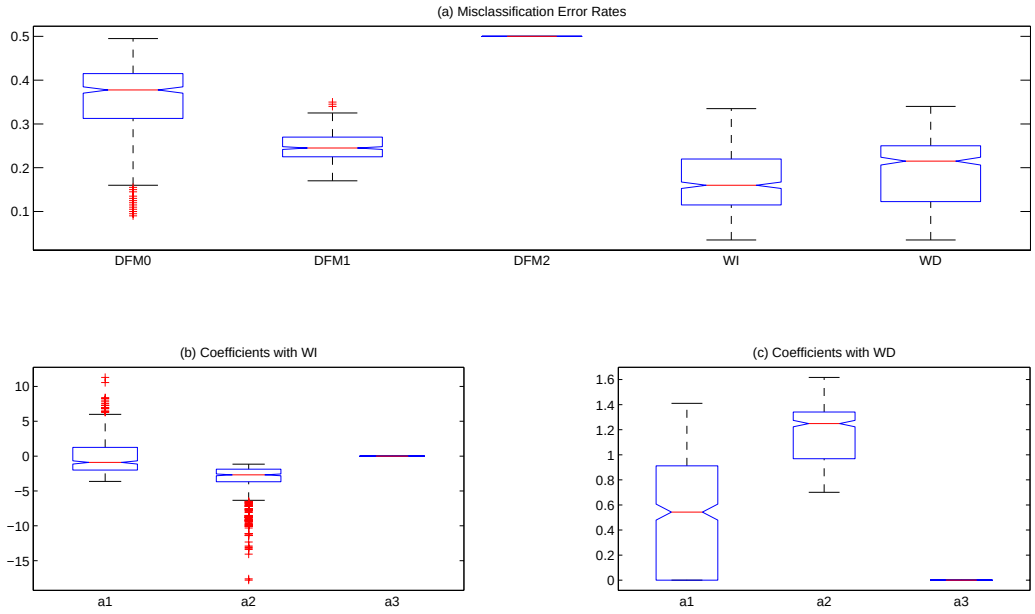


Figure 3.6: Third simulation setting results: (a) Boxplots of the misclassification rates for methods *DFM0*, *DFM1*, *DFM2*, *WI* and *WD*; (b) Boxplots of the weights obtained for method *WI*; (c) Boxplots of the weights obtained for method *WD*.



The probability of classifying **correctly** an element of $P^{(1)}$ with *DFM0* is:

$$\begin{aligned} p\left(X_1 < 0 \;\middle|\; \mathcal{X} \in P^{(1)}\right) &= p\left(d(\mathcal{X}, \mathbb{E}(\mathcal{X}^{(1)})) < d(\mathcal{X}, \mathbb{E}(\mathcal{X}^{(2)})) \;\middle|\; \mathcal{X} \in P^{(1)}\right) \\ &= p\left(\int_0^1 |t + U - t - \frac{1}{2}|dt < \int_0^1 |t + U - t - 1|dt \;\middle|\; U \sim U(0,1)\right) \\ &= p\left(|U - \frac{1}{2}| < |U - 1| \;\middle|\; U \sim U(0,1)\right) = \frac{3}{4} \end{aligned} \tag{3.41}$$

(Hint: Do not calculate anything in the last step, draw a segment.)

The probability of classifying **correctly** an element of $P^{(2)}$ with *DFM0* is:

$$\begin{aligned} p\left(X_1 > 0 \;\middle|\; \mathcal{X} \in P^{(2)}\right) &= p\left(d(\mathcal{X}, \mathbb{E}(\mathcal{X}^{(1)})) > d(\mathcal{X}, \mathbb{E}(\mathcal{X}^{(2)})) \;\middle|\; \mathcal{X} \in P^{(2)}\right) \\ &= p\left(\int_0^1 |t + V - t - \frac{1}{2}|dt > \int_0^1 |t + V - t - 1|dt \;\middle|\; V \sim U(1/2, 3/2)\right) \\ &= p\left(|V - \frac{1}{2}| > |V - 1| \;\middle|\; V \sim U(1/2, 3/2)\right) = \frac{3}{4} \end{aligned} \tag{3.42}$$

Now, supposing that the element is chosen at random from both populations with the same probability

$$p(\mathcal{E}) = \left(1 - \frac{3}{4}\right) \cdot \frac{1}{2} + \left(1 - \frac{3}{4}\right) \cdot \frac{1}{2} = \frac{1}{4}. \tag{3.43}$$

On the other hand, since $\mathbb{E}(D\mathcal{X}^{(1)}) = \mathbb{E}(D\mathcal{X}^{(2)})$, the variable X_2 cannot be used to classify; due to the fact that $|X_2| \leq d(\mathbb{E}(D\mathcal{X}^{(1)}), \mathbb{E}(D\mathcal{X}^{(2)})) = 0$, the questions $X_2 < 0?$ and $X_2 > 0?$ make no sense. The same happens for any variable X_j, $j \geq 2$.

Simulation Exercise 2

The rate for method *DFM1* was calculated as

$$p(\mathcal{E}) = \frac{1}{4} \cdot \frac{1}{2} + 0 \cdot \frac{1}{2} = \frac{1}{8}. \tag{3.44}$$

These rates can be calculated —or tried— in a more explicit way by using the following complementary probabilities.

Since $\mathbb{E}(\mathcal{X}^{(1)}) \neq \mathbb{E}(\mathcal{X}^{(2)})$, the variable X_1 can be used to classify.

The probability of classifying **correctly** an element of $P^{(1)}$ with *DFM0* is:

$$\begin{aligned} p\,(X_1 < 0 \quad | \quad \mathcal{X} \in P^{(1)}) &= p\,(d(\mathcal{X}, \mathbb{E}(\mathcal{X}^{(1)})) < d(\mathcal{X}, \mathbb{E}(\mathcal{X}^{(2)})) \ \mid \mathcal{X} \in P^{(1)}) \\ &= p\left(\int_0^1 |(t+U)^2 - (t+\frac{1}{2})^2| dt < \int_0^1 |(t+U)^2 - t^2 - \frac{1}{2}| dt \ \mid U \sim U(0,1)\right) \\ &= p\left(\int_0^1 |2Ut - t + U^2 - \frac{1}{4}| dt < \int_0^1 |2Ut + U^2 - \frac{1}{2}| dt \ \mid U \sim U(0,1)\right) \\ &= p\left(\int_0^1 |2Ut + U^2 - \frac{1}{2} + (\frac{1}{4} - t)| dt \right. \\ &\quad \left. < \int_0^1 |2Ut + U^2 - \frac{1}{2}| dt \ \mid U \sim U(0,1)\right) \end{aligned} \tag{3.45}$$

The probability of classifying **correctly** an element of $P^{(2)}$ with *DFM0* is:

$$\begin{aligned} p\,(X_1 > 0 \ \mid \mathcal{X} \in P^{(2)}) &= p\,(d(\mathcal{X}, \mathbb{E}(\mathcal{X}^{(1)})) > d(\mathcal{X}, \mathbb{E}(\mathcal{X}^{(2)})) \ \mid \mathcal{X} \in P^{(2)}) \\ &= p\left(\int_0^1 |t^2 + V - (t+\frac{1}{2})^2| dt > \int_0^1 |t^2 + V - t^2 - \frac{1}{2}| dt \ \mid V \sim U(0,1)\right) \\ &= p\left(\int_0^1 |V - t - \frac{1}{4}| dt > \int_0^1 |V - \frac{1}{2}| dt \ \mid V \sim U(0,1)\right) \\ &= p\left(\int_0^1 |V - \frac{1}{2} + (\frac{1}{4} - t)| dt > |V - \frac{1}{2}| \ \mid V \sim U(0,1)\right) \end{aligned} \tag{3.46}$$

Since $\mathbb{E}(D\mathcal{X}^{(1)}) \neq \mathbb{E}(D\mathcal{X}^{(2)})$, the variable X_2 can be used to classify.

The probability of classifying **correctly** an element of $P^{(1)}$ with *DFM1* is:

$$\begin{aligned} p\,(X_2 < 0 \ \mid \mathcal{X} \in P^{(1)}) &= p\,(d(D\mathcal{X}, \mathbb{E}(D\mathcal{X}^{(1)})) < d(D\mathcal{X}, \mathbb{E}(D\mathcal{X}^{(2)})) \ \mid \mathcal{X} \in P^{(1)}) \\ &= p\left(\int_0^1 |2(t+U) - 2(t+\frac{1}{2})| dt < \int_0^1 |2(t+U) - 2t| dt \ \mid U \sim U(0,1)\right) \\ &= p\,(|2U - 1| < |2U| \ \mid U \sim U(0,1)) = \frac{3}{4} \end{aligned} \tag{3.47}$$

The probability of classifying **correctly** an element of $P^{(2)}$ with *DFM1* is:

$$\begin{aligned} p\,(X_2 > 0 \ \mid \mathcal{X} \in P^{(2)}) &= p\,(d(D\mathcal{X}, \mathbb{E}(D\mathcal{X}^{(1)})) > d(D\mathcal{X}, \mathbb{E}(D\mathcal{X}^{(2)})) \ \mid \mathcal{X} \in P^{(2)}) \\ &= p\left(\int_0^1 |2t - 2(t+\frac{1}{2})| dt > \int_0^1 |2t - 2t| dt \ \mid V \sim U(0,1)\right) \\ &= p\,(1 > 0 \ \mid V \sim U(0,1)) = 1 \end{aligned} \tag{3.48}$$

Now,

$$p(\mathcal{E}) = \left(1 - \frac{3}{4}\right) \cdot \frac{1}{2} + (1-1) \cdot \frac{1}{2} = \frac{1}{8}. \tag{3.49}$$

Since $\mathbb{E}(D^2\mathcal{X}^{(1)}) = \mathbb{E}(D^2\mathcal{X}^{(2)})$, the variable X_3 cannot be used to classify. The same happens for any variable X_j, $j \geq 3$.

Simulation Exercise 3

Finally, the rate for method *DFM1* can be calculated as

$$p(\mathcal{E}) = \frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{2}. \tag{3.50}$$

Again, these rates can be calculated —or tried— more explicitly by using the following probabilities.

Since $\mathbb{E}(\mathcal{X}^{(1)}) \neq \mathbb{E}(\mathcal{X}^{(2)})$, the variable X_1 can be used to classify.

The probability of classifying **correctly** an element of $P^{(1)}$ with *DFM0* is:

$$\begin{aligned}
p\left(X_1 < 0 \quad | \quad \mathcal{X} \in P^{(1)}\right) &= p\left(d(\mathcal{X}, \mathbb{E}(\mathcal{X}^{(1)})) < d(\mathcal{X}, \mathbb{E}(\mathcal{X}^{(2)})) \;\; | \; \mathcal{X} \in P^{(1)}\right) \\
&= p\left(\int_0^1 |(t+U)^2 + \frac{5}{4} - (t+\frac{1}{2})^2 - \frac{5}{4}|dt < \int_0^1 |(t+U)^2 + \frac{5}{4} - (t+1)^2|dt \;\; | \; U \sim U(0,1)\right) \\
&= p\left(\int_0^1 |(2t+U+\frac{1}{2})(U-\frac{1}{2})|dt < \int_0^1 |(2t+U+1)(U-1) + \frac{5}{4}|dt \;\; | \; U \sim U(0,1)\right) \\
&= p\left(\int_0^1 |2(U-\frac{1}{2})t + U^2 - \frac{1}{4}|dt < \int_0^1 |2(U-1)t + U^2 + \frac{1}{4}|dt \;\; | \; U \sim U(0,1)\right)
\end{aligned} \tag{3.51}$$

The probability of classifying **correctly** an element of $P^{(2)}$ with *DFM0* is:

$$\begin{aligned}
p\left(X_1 > 0 \quad | \quad \mathcal{X} \in P^{(2)}\right) &= p\left(d(\mathcal{X}, \mathbb{E}(\mathcal{X}^{(1)})) > d(\mathcal{X}, \mathbb{E}(\mathcal{X}^{(2)})) \;\; | \; \mathcal{X} \in P^{(2)}\right) \\
&= p\left(\int_0^1 |(t+V)^2 - (t+\frac{1}{2})^2 - \frac{5}{4}|dt > \int_0^1 |(t+V)^2 - (t+1)^2|dt \;\; | \; V \sim U(1/2, 3/2)\right) \\
&= p\left(\int_0^1 |(2t+V+\frac{1}{2})(V-\frac{1}{2}) - \frac{5}{4}|dt > \int_0^1 |(2t+V+1)(V-1)|dt \;\; | \; V \sim U(1/2, 3/2)\right) \\
&= p\left(\int_0^1 |2(V-\frac{1}{2})t + V^2 - \frac{3}{2}|dt > |2(V-1)t + V^2 - 1| \;\; | \; V \sim U(1/2, 3/2)\right)
\end{aligned} \tag{3.52}$$

Since $\mathbb{E}(D\mathcal{X}^{(1)}) \neq \mathbb{E}(D\mathcal{X}^{(2)})$, the variable X_2 can be used to classify.

The probability of classifying **correctly** an element of $P^{(1)}$ with *DFM1* is:

$$\begin{aligned}
p\left(X_2 < 0 \quad | \quad \mathcal{X} \in P^{(1)}\right) &= p\left(d(D\mathcal{X}, \mathbb{E}(D\mathcal{X}^{(1)})) < d(D\mathcal{X}, \mathbb{E}(D\mathcal{X}^{(2)})) \;\; | \; \mathcal{X} \in P^{(1)}\right) \\
&= p\left(\int_0^1 |2(t+U) - 2(t+\frac{1}{2})|dt < \int_0^1 |2(t+U) - 2(t+1)|dt \;\; | \; U \sim U(0,1)\right) \\
&= p\left(|2U-1| < |2U-2| \;\; | \; U \sim U(0,1)\right) = \frac{3}{4}
\end{aligned} \tag{3.53}$$

The probability of classifying **correctly** an element of $P^{(2)}$ with *DFM1* is:

$$\begin{aligned} p\left(X_2 > 0 \quad | \quad \mathcal{X} \in P^{(2)}\right) &= p\left(d(D\mathcal{X}, \mathbb{E}(D\mathcal{X}^{(1)})) > d(D\mathcal{X}, \mathbb{E}(D\mathcal{X}^{(2)})) \ \mid \mathcal{X} \in P^{(2)}\right) \\ &= p\left(\int_0^1 |2(t+V) - 2(t+\frac{1}{2})|dt > \int_0^1 |2(t+V) - 2(t+1)|dt \ \mid V \sim U(1/2, 3/2)\right) \\ &= p\left(|2V-1| > |2V-2| \ \mid V \sim U(1/2, 3/2)\right) = \frac{3}{4} \end{aligned} \tag{3.54}$$

Finally,

$$p(\mathcal{E}) = \left(1 - \frac{3}{4}\right) \cdot \frac{1}{2} + \left(1 - \frac{3}{4}\right) \cdot \frac{1}{2} = \frac{1}{4}. \tag{3.55}$$

Since $\mathbb{E}(D^2\mathcal{X}^{(1)}) = \mathbb{E}(D^2\mathcal{X}^{(2)})$, the variable X_3 cannot be used to classify. The same happens for any variable X_j, $j \geq 3$.

3.4 Real Data Examples

In this section we illustrate the performance of our proposal in two benchmark data sets: (**a**) *Spectrometric data set*, consisting of 215 near-infrared spectra of meat samples obtained by a Tecator Infratec Food and Feed Analyzer; (**b**) *Growth curves data set*, consisting of the height (in centimeters) of 44 girls and 39 boys measured at a set of 31 different instances between the ages 1 and 18.

In both examples, the original data was smoothed using a cubic smoothing spline with smoothing parameter equal to $1/(1+h^3/6)$, where h is the average spacing of the data sites (see De Boor [1978]).

In this section, the nomenclature for the different versions of the algorithm is that used in the previous section. Furthermore,

- *DFM2* denotes the classification with the distance to the sample functional mean, calculated using the second derivatives of functions in the training set. That is, using the rule

$$\begin{cases} k = 1 & \text{if} \quad x_3 < 0 \\ k = 2 & \text{otherwise} \end{cases}. \tag{3.56}$$

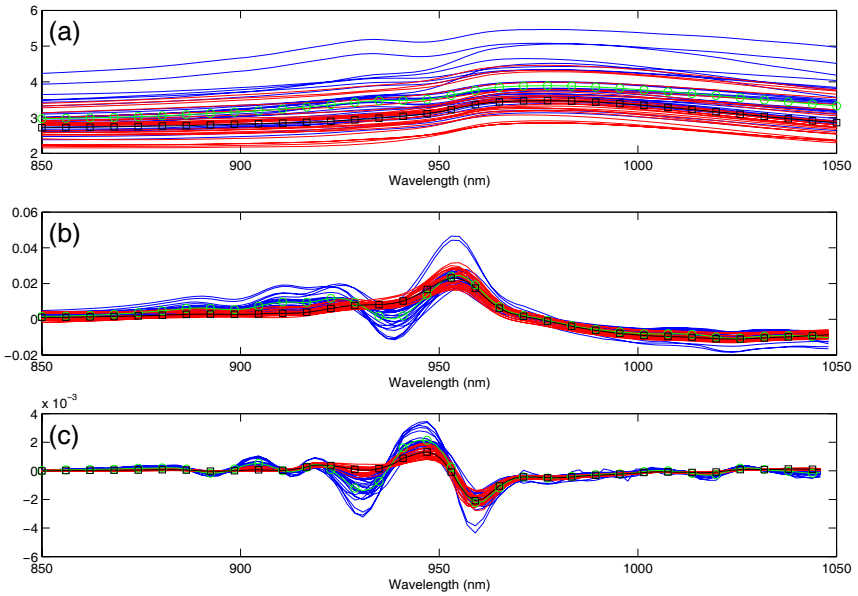
- Now the weighted approaches (algorithms 3 and 4) take into account up to the second derivative by considering

$$\mathbf{x} = (x_1, x_2, x_3)^t. \tag{3.57}$$

3.4.1 Spectrometric Data

The classification problem in the spectrometric data set consists in separating meat samples with a high fat content (more than 20%) from samples with low fat content (less than 20%). Among the 215 samples, 77 have high fat content and 138 have low fat content. Figure 3.7 shows a sample of

Figure 3.7: Sample from the spectrometric data set (wavelengths 850–1050 nm): (a) Data; (b) First derivative; (c) Second derivative.



these 100-channel absorbance spectrum in the wavelength 850–1050 nm and the first and second derivatives.

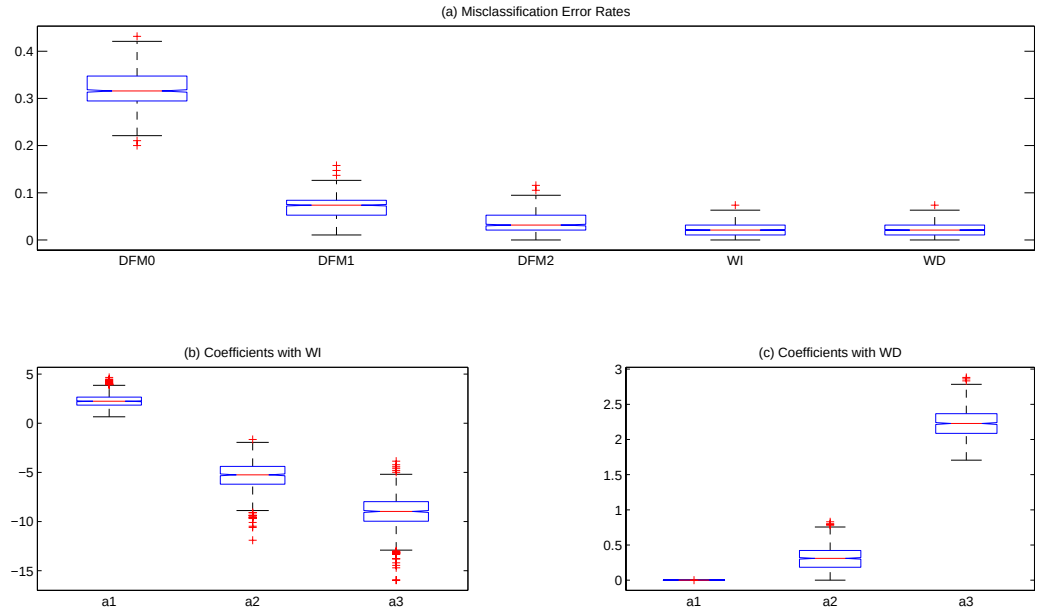
Among others, Ferraty and Vieu (2003), Rossi and Villa (2006) and Li and Yu (2008) had considered the original spectrum and its derivatives for classification purpose and had concluded that the second derivative produces the lower misclassification rates.

In order to evaluate the performance of our proposal, we will split the data set into 120 spectra for training and 95 spectra for testing as in Rossi and Villa (2006) and Li and Yu (2008). The classification results shown in figure 3.8 are based on 1000 replications. Methods *WI* and *WD* obtain a mean misclassification rate equal to 2.02% and 2.32%, respectively. They improve the classification rule based on the second derivative, *DFM2*, which obtains 3.70%.

In this example, method *WI* gives positive weights to the variable associated with $\chi^{(1)}$ and $\chi^{(2)}$, and negative —but higher in module— weights for the variables associated with $D^1\chi^{(1)}$ and $D^1\chi^{(2)}$ and with $D^2\chi^{(1)}$ and $D^2\chi^{(2)}$; so the classification rule with *WI* is not based on a distance. Method *WD* gives positive weights to the variables associated with $D^1\chi^{(1)}$ and $D^1\chi^{(2)}$ and with $D^2\chi^{(1)}$ and $D^2\chi^{(2)}$, and zero weights for the variable associated with $\chi^{(1)}$ and $\chi^{(2)}$. Notice that both procedures give the higher weights to the variable associated with $D^2\chi^{(1)}$ and $D^2\chi^{(2)}$, which is consistent with the results of Ferraty and Vieu (2003), Rossi and Villa (2006) and Li and Yu (2008).

The functional support vector machine proposed by Rossi and Villa (2006) obtains 3.28% (7.5%) using a linear (Gaussian) kernel and the spectra, and a 2.6% (3.28%) using a Gaussian (linear) kernel and the second derivative of the spectra.

Figure 3.8: Spectrometric data set classification results: (a) Boxplots of the misclassification rates for methods *DFM0*, *DFM1*, *DFM2*, *WI* and *WD*; (b) Boxplots of the weights obtained for method *WI*; (c) Boxplots of the weights obtained for method *WD*.

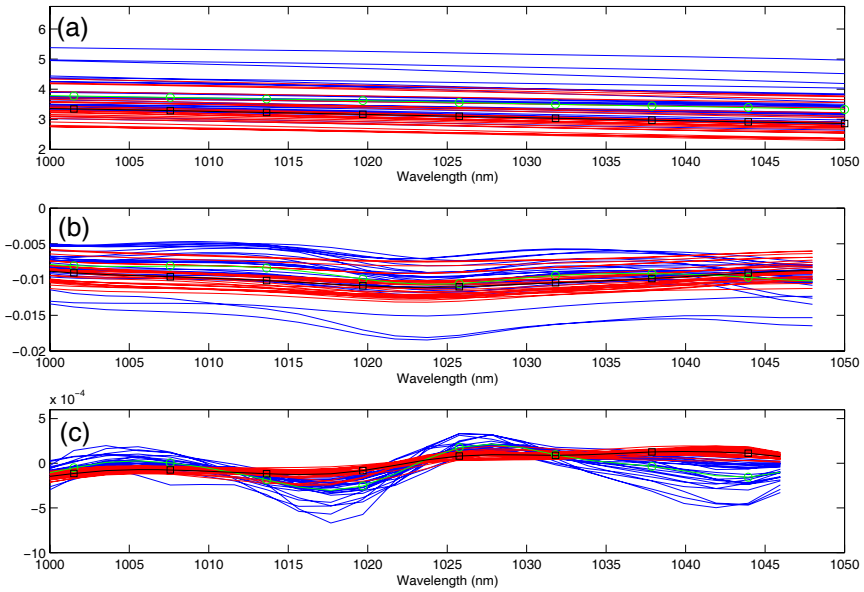


The nonparametric functional method proposed by Ferraty and Vieu (2003) obtains a mean error of around 2% using the second derivative. Notice that Ferraty and Vieu (2003) use a training set with 160 spectra. In that setting, our mean misclassification rates are equal to 1.89% and 2.27%, respectively.

Li and Yu (2008) obtain 3.98%, 2.91% and 1.09% using the raw data, the first derivative and the second derivative, respectively. Notice that Li and Yu's method selects the data segments where the two populations have large differences, and then it combines the linear discriminant as a data reduction tool and the support vector machine as a classifier. These authors' method has three tuning parameters: number of segments, separation amongst segments and the regularization parameter of the support vector machine.

If we repeat our procedures using the channels in the wavelengths 1000–1050 nm, then we obtain 1.49% and 1.30%, using *WI* and *WD*, respectively. Notice that these results show that in some cases the additional nonnegative constraints improve the performance of our algorithm 3. Figure 3.9 shows a sample of these spectrum in the wavelength 1000–1050 nm and the first and second derivatives. This segment, 1000–1050 nm, was obtained by cross-validation through a grid search. The design of a segmentation approach for selecting more than one segment is beyond the scope of this thesis and probably deserves a separate body of research.

Figure 3.9: Sample from the spectrometric data set (wavelengths 1000–1050 nm): (a) Data; (b) First derivative; (c) Second derivative.



3.4.2 Growth Data

The classification problem in the growth data set consists in separating samples by sex, taking the growth curves as variables. Figure 3.10 shows a sample of these curves, measured in ages ranging from 1 to 18, and their first and second derivatives. López-Pintado and Romo (2006) had considered the growth curves (but not their derivatives) for classification purpose.

In order to evaluate the performance of our proposal, we will split the data set into 60 curves for training and the remaining 33 for testing. The classification results shown in figure 3.11 are based on 1000 replications. Weighted methods *WI* and *WD* have similar performance, with means misclassification rates equal to 3.65% and 3.75%, respectively. They improve the classification rules based on the raw data, on the first derivative or on the second derivative, which obtain 31.08%, 5.30% and 18.85%, respectively. The best result with the depth-based classification procedure proposed by López-Pintado and Romo (2006) was 14.86%.

In this example, method *WI* gives positive weights for the variable associated to $D^2\chi^{(1)}$ and $D^2\chi^{(2)}$ and negative (but higher in module) weights for the variables associated to $D^1\chi^{(1)}$ and $D^1\chi^{(2)}$; so the classification rule with *WI* is not based on a distance. Method *WD* gives positive weights for the variables associated to $\chi^{(1)}$ and $\chi^{(2)}$ and to $D^1\chi^{(1)}$ and $D^1\chi^{(2)}$; then, the classification rule is based on a distance. Moreover, these weights of *WD* indicate that it is not necessary to use x_3 (second derivative) when a combination of x_1 and x_2 (raw data and first derivative) is considered.

Figure 3.10: Sample from the growth data set: (a) Data; (b) First derivative; (c) Second derivative.

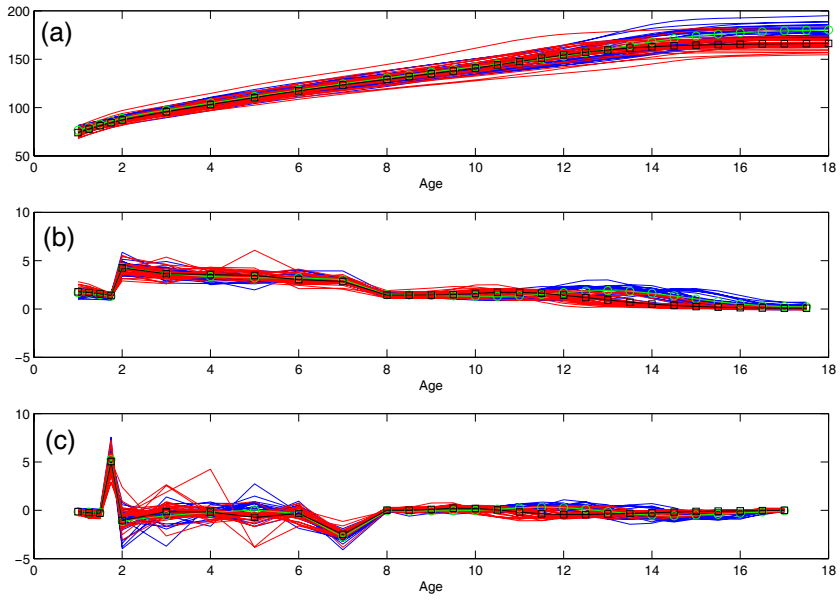
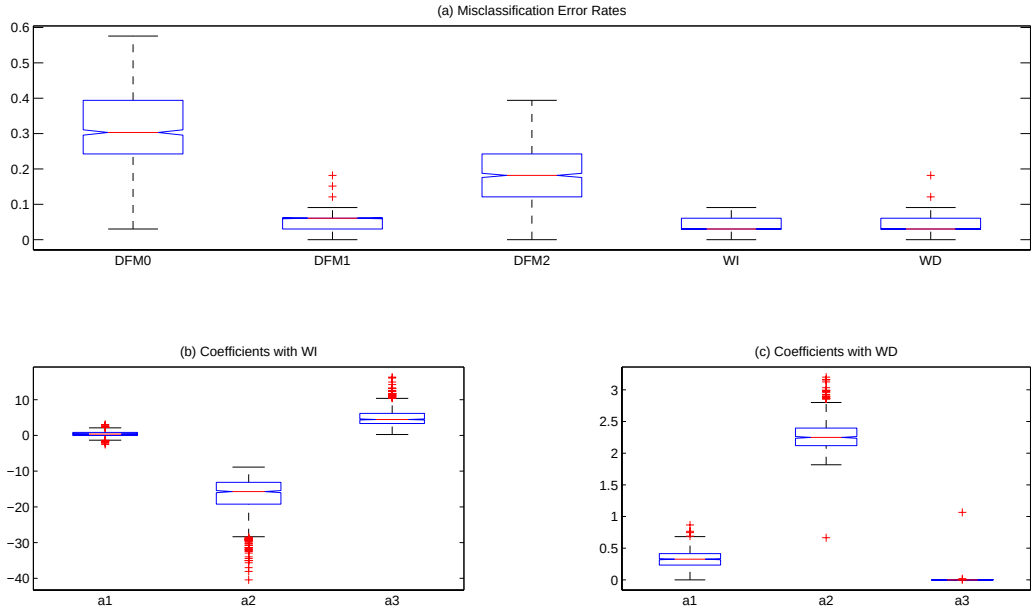


Figure 3.11: Growth data set classification results: (a) Boxplots of the misclassification rates for methods *DFM0*, *DFM1*, *DFM2*, *WI* and *WD*; (b) Boxplots of the weights obtained for method *WI*; (c) Boxplots of the weights obtained for method *WD*.



3.5 Conclusions

In this chapter we have proposed a new approach for discriminating functional data. This method involves the use of distances to a representative function and its successive derivatives. Our simulation studies and our applications show that the method performs very well, resulting in small training and testing classification errors. Applications to real data show that our procedure performs as well as —and in some cases better than— other classifications methods. In addition, our methodology provides, through the weights, information about the importance of each data transformation. Finally, some adaptability of our methodology to the different types of functional data can be achieved by selecting the distance $d(\cdot, \cdot)$ or the multivariate classification technique.

Chapter 4

Extensions and Further Work

Summary: In this chapter, possible generalisations and forthcoming work, for both classification methods, are itemised and outlined briefly.

There is much theory available on multivariate, time series and functional data, so techniques from the three frameworks can be applied, respectively, to the original time series and curves or to the constructed curves and variables: graphical representations, transformations, inference, typicality and robustness, etcetera. For example, graphical methods can be used for the detection of outliers, through the representation of the curves —in our first proposal— or our multivariate variables —in the second.

Nevertheless, a great complexity appears if we want to connect both theories, taking into account the fact that in our cases the functional or multivariate characters come, respectively, from original time series and functional data, with transformations and distance measurements.

4.1 Time Series Method

4.1.1 More than Two Populations

The generalisation to a K-group classification, with $K > 2$, is trivial. In the algorithms of section 2.3, it is enough to consider the reference curves of the K groups and apply the classification rule

$$k = argmin_{\{1,\dots,K\}} \{d(\chi(\lambda), \mathcal{R}^{(k)}(\lambda))\} \tag{4.1}$$

with $\mathcal{R}^{(k)}(\lambda) = \bar{\chi}^{(k)}(\lambda)$ or $\mathcal{R}^{(k)}(\lambda) = \overset{\alpha}{\bar{\chi}}{}^{(k)}(\lambda)$, respectively.

4.1.2 Clustering

From our first proposal it is concluded that the spectral distribution function contains information which is useful for the supervised classification of time series. The same information can be used

for the unsupervised classification —or clustering— of time series, by tackling the corresponding/associated functional data problem in the frequency domain: some references on this subject are mentioned at the end of section 8.6 of Ramsay and Silverman (2006) and —with extension and in the nonparametric framework— in chapter 9 of Ferraty and Vieu (2006).

4.1.3 Other Depth Definitions

Other different definitions of depth can be considered, for example: Fraiman and Muniz (2001), or Cuevas et al. (2007).

4.2 Functional Data Method

4.2.1 Classical Assumptions

Some interesting questions are related to the fulfilment of the linear discriminant analysis assumptions, the performance when there are departures from them, and possible corrections of these departures or extensions in order to deal with them. In general, the linear discriminant analysis, when used for classification, is quite robust to departures from the assumptions, especially for large sample sizes. In practice the multivariate techniques can be applied to our discriminant variables, but it would be very interesting to do some simulations studying the distribution of these variables for different functional models and distances.

The normality assumption can be tested, that is, how far from the normal distribution our variables $X_1, \ldots, X_p$ are. Under normality, the method becomes optimal; otherwise, functional or multivariate transformations to achieve normality could be considered. The normality of the discriminant variables implies the normality of the discriminant functions, so the rejection of one normality would imply the rejection of the other. On the other hand, since the discriminant analysis is somewhat affected by the presence of atypical values, multivariate or functional techniques could be used to leave these values out.

Equally important is testing the homoscedasticity assumption, that is, if $\mathbf{\Sigma}_{\mathbf{X}}^{(k)} = \mathbf{\Sigma}_{\mathbf{X}}$, $\forall k$, in order to combine or not the information in a unique pooled estimator of the covariance matrix. When the equality is rejected, quadratic —instead of linear— discriminant analysis should be used in our approach. Nevertheless, the quadratic analysis is more sensitive to the normality assumption. On the other hand, if the equality holds, the use of the quadratic version implies a loss of efficiency.

When it is not possible to reject the equality of the covariance matrices, it is important to test the equality of the means, that is, the hyphotesis $\mu_{\mathbf{X}}^{(k)} = \mu_{\mathbf{X}}$, $\forall k$. If this equality cannot be rejected either, it is difficult to ensure from the samples that, in fact, there are two different underlying populations.

Finally, if high correlations were observed in the multivariate samples (induced by correlations in the functional samples), the linear discriminant analysis can be substituted by the *penalized discriminant analysis* of Hastie et al. (1995), a variant of the classical discriminant analysis specifically designed to cope with correlations.

4.2.2 Additional Constraint Embedding

The quadratic-form optimization problem arises frequently in literature. When there is a constraint, a known approach consists in finding an equivalent optimization problem without the constraint. This is done by embedding the constraint into the quadratic form; analitically, by introducing the constraint multipliers in the matrix of the quadratic form. For example, Jagannathan and Ma (2003) transform the minimum variance portfolio optimization problem

$$\mathbf{a} = argmin\left\{\mathbf{a}^t\mathbf{S}\mathbf{a}\right\} \quad \text{subject to} \quad \begin{cases} \sum_i a_i = 1 \\ 0 \leq a_i \leq \bar{a} \end{cases} \tag{4.2}$$

into the equivalent problem

$$\mathbf{a} = argmin\left\{\mathbf{a}^t\tilde{\mathbf{S}}\mathbf{a}\right\} \tag{4.3}$$

by considering $\tilde{\mathbf{S}} = \mathbf{S} + (\delta\mathbf{1}^t + \mathbf{1}\delta^t) - (\lambda\mathbf{1}^t + \mathbf{1}\lambda^t)$, where $\mathbf{1}$ is the column vector of ones.

For our optimization problem

$$\mathbf{a} = argmax\left\{\frac{\mathbf{a}^t\mathbf{B}\mathbf{a}}{\mathbf{a}^t\mathbf{W}\mathbf{a}}\right\} \quad \text{subject to} \quad \mathbf{a} \geq \mathbf{0} \qquad [3.1]$$

we would be interested in defining new matrices $\tilde{\mathbf{B}}$ and $\tilde{\mathbf{W}}$ so as to obtain the equivalent optimization problem

$$\mathbf{a} = argmax\left\{\frac{\mathbf{a}^t\tilde{\mathbf{B}}\mathbf{a}}{\mathbf{a}^t\tilde{\mathbf{W}}\mathbf{a}}\right\}. \tag{4.4}$$

This would allow using all the theory of the Fisher's discriminant analysis; for example, the expression of the discriminant function for $K = 2$ (two populations), when $\tilde{\mathbf{W}}$ is nonsingular, will be:

$$y = \mathbf{a}_n^t\mathbf{x} = (\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t\tilde{\mathbf{W}}^{-1}\mathbf{x}. \tag{4.5}$$

More generally, for this unconstrained optimization problem general theory could be considered or developed, as that of McDonald (1979) and Kiers (1995) for quotients of quadratic forms. Thus, this constraint embedding problem has general theoretical interest.

4.2.3 Additional Constraint Avoidance

As we have mentioned in section 3.2.6, we introduced the nonnegativeness constraints for theoretical reasons. Perhaps the same theoretical advantage could sometimes be achieved through a different way; for example, by applying a transformation $\mathbf{t} : \mathbb{R}^p \to \mathbb{R}^p$ to the $\mathbf{a}_F$ coefficients,

instead of imposing the additional constraint. That is, by transforming the classical discriminant function in the following way:

$$\tilde{y} = \mathbf{t}(\mathbf{a}_F)^t \mathbf{x} = \sum_{i=1}^{p} t_i(\mathbf{a}_F) x_i, \tag{4.6}$$

where $\mathbf{t} = (t_1, \ldots, t_p)^t$ with $t_i : \mathbb{R}^p \longrightarrow \mathbb{R}$ such that $t_i(\mathbf{a}) \geq 0, \quad \forall i = 1, \ldots, p.$

Advantages

It seems that this approach would add several advantages. On the one hand, the core optimization problem of the methodology would again be the classical Fisher's problem, so the usual interpretation of $\mathbf{a}_F$ and the available software could be accessed. On the other hand, several transformations, $\mathbf{t}(\cdot)$, could be tested without having to solve the optimization problem again, that is, without computing $\mathbf{a}_F$ again.

Disadvantages

Let us notice that the election of $\mathbf{t}(\cdot)$ is an ad hoc election, while the optimization problem —with the nonnegativeness restriction— is based on a general and transparent criterion.

Deformation of the Scale

Some tools of the vectorial calculus, concretely the divergence, indicate that in this transformation there is an implicit deformation (in the sense of contraction or dilatation of volumes) of the mathematical space $\mathbb{R}^p$, measured by:

$$div(\mathbf{t}) = \nabla^t \cdot \mathbf{t} = \sum_{i=1}^{p} \frac{\partial t_i}{\partial a_i}. \tag{4.7}$$

See section 3.4 of Marsden and Tromba (1991) for mentioned physical interpretation of the divergence (in section 8.4 of the same book there is a different interpretation in terms of fluxes and integrals).

Some Cases

1. Isotropic: If $\mathbf{t} = (t, \ldots, t)^t$
2. Anisotropic: If $\mathbf{t} = (t_1, \ldots, t_p)^t$
3. Unidimensional components: If $\mathbf{t} = (t_1(a_1), \ldots, t_p(a_p))^t$, that is, with $t_i : \mathbb{R} \to \mathbb{R}$.

Geometrical Interpretation

Following the geometrical interpretations of section 1.2.5, the isotropic substitution

$$(a_1, \ldots, a_p) \qquad \longrightarrow \qquad (t(\mathbf{a}), \ldots, t(\mathbf{a})) \tag{4.8}$$

is interpreted as a subsequent change —guided by $t(\cdot)$— of the projection direction (with, in general, an implicit homothecy).

For the anisotropic case, it can be written

$$t_i(\mathbf{a})x_i = t(\mathbf{a})\tilde{x}_i, \tag{4.9}$$

for some $t(\cdot)$, and the substitution

$$(a_1, \ldots, a_p) \qquad \longrightarrow \qquad (t_1(\mathbf{a}), \ldots, t_p(\mathbf{a})) \tag{4.10}$$

is now interpreted as a subsequent change —guided by $t(\cdot)$— of the projection direction (with, in general, an implicit homothecy) followed by a rescaling in the axes —determined by $\tilde{\mathbf{x}} = (\tilde{x}_1, \ldots, \tilde{x}_p)^t$— to obtain a new reference system.

The Classification

In the previous cases, the classification rule would be

$$\begin{cases} k = 1 & \text{if} \quad \tilde{y} > \mathbf{t}(\mathbf{a}_F)^t \frac{1}{2}(\overline{\mathbf{x}}^{(1)} + \overline{\mathbf{x}}^{(2)}) \\ k = 2 & \text{otherwise} \end{cases}, \tag{4.11}$$

where the value $\mathbf{t}(\mathbf{a}_F)^t \frac{1}{2}(\overline{\mathbf{x}}^{(1)} + \overline{\mathbf{x}}^{(2)})$ would be the new cutoff point.

Remark 37 Under normality (of the multivariate variables), it is not possible that the classification with (4.11) would improve the classification with (D.40) of appendix D.4, as in this case $\mathbf{t}(\mathbf{a}_F)$ would have probably been found first, instead of $\mathbf{a}_F$; nevertheless, some improvement can be achieved when the normality does not hold.

Remark 38 After the coefficients have been transformed, $\tilde{y}$ is still a linear application, so the statements of remark 61 in appendix D still hold. Nonetheless, the transformation implies a change of the subspace into which data are projected; then, the role of the different variables also changes, implying that the classification rule (4.11) is different to the classical rule (D.40) in appendix D.

4.2.4 Transformation Importance

Our methodology provides information about the usefulness of the different function derivatives for classification purposes. In the same way, we could try to obtain information over data transformations different from derivation, that is, using the following discriminant variables instead of (3.23),

$$x_i = d(T_i(\chi), \overline{T_i(\chi^{(1)})}) - d(T_i(\chi), \overline{T_i(\chi^{(2)})}), \tag{4.12}$$

for $i = 1, 2, \ldots, p$, where $\overline{T_i(\chi^{(k)})} = \frac{1}{n_k}\sum_{e=1}^{n_k} T_i(\chi_e^{(k)})$, $k = 1, 2$, with $T_i(\cdot)$ being an application between two functional spaces.

Notice that the information of different transformations could be combined (indirectly, through the distances) using an expression similar to (3.33), that is, with

$$\begin{aligned} y(\mathbf{x}) &= \mathbf{a}^t\mathbf{x} = \sum_{i=1}^{p} a_i x_i \\ &= \sum_{i=1}^{p} a_i d(T_i(\chi), \overline{T_i(\chi^{(1)})}) - \sum_{i=1}^{p} a_i d(T_i(\chi), \overline{T_i(\chi^{(2)})}). \end{aligned} \tag{4.13}$$

Remark 39 In some cases it might be convenient to substitute the reference function

$$\mathcal{R}^{(k)}(\lambda) = \overline{T_i(\chi^{(k)})} \tag{4.14}$$

with a more proper one.

4.2.5 Distance Importance

Given a data set, which characteristics are the important ones depends on the aim of the study for which the data are being used. For example, a peak in smooth curves can indicate the presence of an event, and depending on whether or not there is interest in this event —or even in avoiding it— one particular distance should be used: $\|\chi\| = \max_{t\in I}\chi(t)$ or $\|\chi\| = \int_I \chi(t)dt$. Moreover, as mentioned in remark **??**, an inappropriate choice of the distance can imply a severe loss of efficiency.

Then, similarly as in the previous subsection, the importance of several different distances can be studied using the variables

$$x_i = d_i(\chi, \overline{\chi^{(1)}}) - d_i(\chi, \overline{\chi^{(2)}}) \tag{4.15}$$

for $i = 1, 2, \ldots, p$, where $d_i(\cdot,\cdot)$ are different distances and $\overline{\chi} = \frac{1}{n_k}\sum_{e=1}^{n_k}\chi_e^{(k)}$, $k = 1, 2$.

An important fact is that, again with an expression similar to (3.33), combinations of distances can be constructed:

$$\begin{aligned} y(\mathbf{x}) &= \mathbf{a}^t\mathbf{x} = \sum_{i=1}^{p} a_i x_i \\ &= \sum_{i=1}^{p} a_i d_i(\chi, \overline{\chi^{(1)}}) - \sum_{i=1}^{p} a_i d_i(\chi, \overline{\chi^{(2)}}). \end{aligned} \tag{4.16}$$

Remark 40 Again, in some cases it might be convenient to substitute the reference function

$$\mathcal{R}^{(k)}(\lambda) = \overline{\chi^{(k)}} \tag{4.17}$$

with a more proper one.

4.2.6 Several Discriminant Functions

The few two or three discriminant variables considered by us justified the use of only one discriminant function; in fact, for two-group classification, no more functions can be considered. In a K--group classification problem, some of the previous extensions could require several discriminant variables; for example, when many discriminant variables are considered or when more information needs to be captured. In this case, a multivariate compound variable $\mathbf{y}$ has to be constructed in several consecutive steps, as in the classical discriminant analysis. Then, a possible classification rule would be

$$k = argmin_{\{1,\dots,K\}} \left\{ d(\mathbf{y}(\mathbf{x}), \mathbf{y}(\overline{\mathbf{x}}^{(k)})) \right\}, \tag{4.18}$$

where now $d(\cdot,\cdot)$ is a distance in $\mathbb{R}^q$ (here q is the lenght of $\mathbf{y}$).

4.2.7 Other Classification Methods

The use of the linear discriminant analysis in the algorithms 3 and 4 (section 3.2.5) is not compulsory, and this technique can be substituted with another one. That is, once the multivariate variables are defined they can be used for any other multivariate classification technique.

If the new method constructs a multivariate compound variable $\mathbf{y}$, the classification criterion can again be (4.18). Finally, if the weights in $\mathbf{y}$ are nonnegative, our additional constraint would be unnecessary.

Conclusions

Although our proposals are not based on complex ideas, the theory included in the first chapter is necessary for a deep understanding of the second and third chapters. The different types of mathematical objects have been explained, including the basic statistical tools for inducing general information (models) from particular samples (data). At the end of the opening chapter, the problem of *classification* was presented in a way that the basic concepts of "property", "distance" and "criterion" were highlighted.

In chapter two we have proposed a new frequency domain approach for time series classification based on the integrated periodograms of the series. When series are nonstationary, they are split into blocks and the integrated periodograms of the blocks are merged to construct a curve. This idea rests on the assumption that series are locally stationary; an example definition of *locally stationary processes* has been given. Since the integrated periodogram is a function, the statistical tools for functional data analysis can be applied; concretely, the concept of *depth*, applied to functions, allows the use of a robust version of the functional mean. In our classification procedure, new series are assigned to the class minimizing the distance between its corresponding curve and the group mean curve. Since the group mean can be affected by the presence of outliers, robustness of the classification method is achieved by substituting the mean curve with the α-trimmed mean, where for each group only the deepest elements are averaged. To evaluate our proposal in different scenarios, we have done simulation exercises containing several models and parameters, with both stationary and nonstationary series, as well as with different types of contamination. We have also illustrated the performance of our procedure in a real benchmark data set. Our proposal provides small error rates, robustness, and good computational performance: properties which make the methodology suitable for time series classification. The procedure suggests that the integrated periodogram contains useful information for classifying time series.

This leads to both the functional data classification and the search of a procedure for selecting the derivative (or the crude functions) with the highest discriminant power. In chapter three we have proposed a new approach for discriminating functional data. This method involves the use of distances to a representative function and its successive derivatives. Since the information useful for discriminating is summarized in multivariate data, the appendix D is devoted to the most classical linear discriminant analysis. This method inspires the classificatory method and the introduction of an additional requirement that provides theoretical advantages. Our simulation

studies and our applications show that the method performs very well, resulting in small training and testing classification errors. Applications to real data show that our procedure performs as well as —and in some cases better than— other classifications methods. Moreover, our methodology provides, through the weights, information about the importance of each data transformation. Some adaptability of our methodology to the different types of functional data can be achieved by selecting the distance $d(\cdot, \cdot)$, the transformation $T(\cdot)$ or the multivariate classification technique providing y.

Finally, our proposals are quick and easy to understand. In Statistics, there is no method which is considered to be "the best", and ours have shown good performance in several scenarios. In chapter four, many possible extensions and further work has been outlined.

Appendix A

Mathematical Structures

Although they are usually tacitly supposed, in this section we include the main theoretical underlying structures involved in this document. Let E be a set of mathematical objects (here they are numbers, vectors, matrices, sequences or functions). Briefly speaking, the algebra structures allow the operations among the elements of E; the topological and analysis structures introduce ideas about proximity, convergence and limits; while the inner product allows geometrical operations such as projections, angles or orthogonality; finally, the theory-measure structures provide a framework where measuring the size of the subsets of E that are of interest. The different kinds of structures are usually overlapped and some compatibility conditions are neccesary.

A.1 Algebra Structures

A.1.1 Group

Definition 37 *Given a set G and an inner operation $\odot$ defined on $G \times G$, then G is said to be* closed *with respect to the operation if $g_1 \odot g_2 \in G, \quad g_i \in G, \ i = 1, 2$.*

Definition 38 *Given a set G, the pair $(G, +)$ is a* group *with respect to a well-defined sum (that is, with G being closed) if*

(1g+) *Associativity:* $(g_1 + g_2) + g_3 = g_1 + (g_2 + g_3), \quad g_i \in G, \ i = 1, 2, 3.$

(2g+) *Identity or neutral element: There is an element* 0_G *such that* $g + 0_G = 0_G + g = g, \quad g \in G.$

(3g+) *Inverse element: For all $g \in G$ there is an element, denoted by $-g$, such that* $(-g) + g = g + (-g) = 0_G$.

Definition 39 *A pair $(G, +)$ is a* commutative group *with respect to $+$ if it is a group and*

(4g+) *Commutativity:* $g_1 + g_2 = g_2 + g_1, \quad g_i \in G, \ i = 1, 2.$

Definition 40 *Given a set G, the pair $(G, *)$ is a* group *with respect to a (well-defined) product if*

(1g)* *Associativity:* $(g_1 * g_2) * g_3 = g_1 * (g_2 * g_3), \quad g_i \in G, \ i = 1, 2, 3.$

(2g)* *Identity or neutral element: There is an element* 1_G *such that* $1_G * g = g * 1_G = g, \quad g \in G.$

(3g)* *Inverse element: For* $g \in G$ *there is an element, denoted by* g^{-1}*, such that* $g * g^{-1} = g^{-1} * g = 1_G$.

Definition 41 *A pair $(G, *)$ is a* commutative group *with respect to $*$ if is a group and*

(4g)* *Commutativity:* $g_1 * g_2 = g_2 * g_1, \quad g_i \in G, \ i = 1, 2.$

A.1.2 Field

Definition 42 *Given a set K and any two closed operations, the triple $(K, +, *)$ is a* field *if*

(1f) *$(K, +)$ is a commutative group.*

(2f) *$(K, *)$ is a commutative group.*

(3f) $(k_1 + k_2) * k_3 = k_1 * k_3 + k_2 * k_3, \quad k_i \in K, \ i = 1, 2, 3.$

A.1.3 Linear Space

Definition 43 *Given a set E, an outer operation $\cdot K$ defined on $K \times E$, where K is a field, is said to be* closed *if* $k \cdot e \in E, \quad k \in K, \ e \in E.$

Definition 44 *Given a set E and two (well-defined) operations, an inner sum operation $+$ and an outer product operation $\cdot K$, where K is a field (usually $K = \mathbb{R}$ or $K = \mathbb{C}$); then the triple $(E, +, \cdot K)$ is a* linear *—or* vectorial*—* space *if*

(1s) *$(E, +)$ is a commutative group.*

(2s) *$(E, \cdot K)$ verifies*

(2f.1) $1_K \cdot e = e, \quad \forall e \in E.$

(2f.2) $k_1 \cdot (k_2 \cdot e) = (k_1 \cdot k_2) \cdot e, \quad k_i \in K, \ i = 1, 2, \quad \forall e \in E.$

(3s) $(k_1 + k_2) \cdot e = k_1 \cdot e + k_2 \cdot e, \quad k_i \in K, \ i = 1, 2, \quad \forall e \in E.$

(4s) $k \cdot (e_1 + e_2) = k \cdot e_1 + k \cdot e_2, \quad k \in K, \quad \forall e_i \in E, \ i = 1, 2.$

Linear Combinations

Definition 45 *In the linear space* $(E, +, \cdot K)$*, a* (finite) linear combination *is any expression of the form*

$$\sum_{i}^{n} k_i \psi_i, \tag{A.1}$$

where $\psi_i \in E$ *and* $k_i \in K$*, for* $i = 1, \ldots, n$*.*

Thus, to be able to work with linear combinations of elements (belonging to the same space), a linear space structure is necessary.

Linear Independence

Definition 46 *In the linear space* $(E, +, \cdot K)$*, a set of* n *elements* $\{\psi_i\} \subset E$ *is said to be* linearly independent *if*

$$\sum_{i}^{n} k_i \psi_i = 0_E, \tag{A.2}$$

where $k_i \in K$*,* $i = 1, \ldots, n$*, implies that* $k_i = 0_K$ *for all* i*.*

This means that 0_E can be obtained from $\psi_i \in E$, $i = 1, \ldots, n$, only by multiplying each ψ_i for "zero", that is, for 0_K, the neutral element of the field with respect to the sum.

Generation

Definition 47 *In the linear space* $(E, +, \cdot K)$*, a set of* n *elements* $\{\psi_i\} \subset E$ *form a* generator set *of the space if any element* $e \in E$ *can be expressed as a linear combination*

$$e = \sum_{i} k_i \psi_i, \tag{A.3}$$

with $k_i \in K$*,* $i = 1, \ldots, n$*.*

Bases

Definition 48 *A set* $\{\psi_i\}$ *of elements of* E *form a* basis *of the space if they are both a linearly independent set and a generator set. The basis of a space is not usually unique. The size of a basis —possibly infinite— is the* dimension *of the space, denoted by* $dim(E)$*.*

The vectors and matrices of this thesis are related to finite-dimensional spaces, whose theory is "simple". To study sequences and functions, more "complex" infinite-dimensional spaces are necessary.

Approximations

Sometimes an approximation of the element e is sufficient to work with, and —in spaces of dimension greater than p— combinations of the form

$$\tilde{e} = \sum_{i=1}^{p} c_i \psi_i = \mathbf{c}^t \psi, \tag{A.4}$$

are used, where $\mathbf{c} = (c_1, c_2, \ldots, c_p)^t$ and $\psi = (\psi_1, \psi_2, \ldots, \psi_p)^t$.

The concept of *convergence* (defined in sections A.2 and A.3) is closely related to these approximations. At the same time, to quantify the accuracy of an approximation, some additional analysis structure is necessary. In general, in linear spaces the coefficients $\mathbf{c}$ are not easy to calculate, even in normed spaces (defined below), and the inner product operation, which will be defined for the pre- and Hilbert spaces (also defined below), is quite useful (see next section).

Linear Subspaces

Definition 49 *Given a linear space $(E, +, \cdot K)$, the subset $V \subset E$ is a* linear subspace *if $(V, +, \cdot K)$ is also a linear space.*

As the linear subspace inherits all the properties of the linear space, the only requirement is that the subset must be closed with respect to the operations, that is

(1ss) $v_1 + v_2 \in V, \quad v_i \in V, \ i = 1, 2.$

(2ss) $k \cdot v \in V, \quad \forall k \in K, \quad \forall v \in V.$

Definition 50 *Given two linear subspaces V_1 and V_2 of a linear space E, their* sum *is defined as*

$$V_1 + V_2 = \{v_1 + v_2 \mid v_i \in V_i, \ i = 1, 2\}. \tag{A.5}$$

Definition 51 *A linear space E is the* direct sum *of two linear subspaces V_1 and V_2 if*

(1ds) $V_1 + V_2 = E,$

(2ds) $V_1 \cap V_2 = \{0_E\}$

and it is denoted as $E = V_1 \oplus V_2$.

Proposition 5 *Given two linear subspaces V_1 and V_2 of E, it holds that $E = V_1 \oplus V_2$ if and only if any element $e \in E$ can be expressed uniquely as $e = v_1 + v_2$ with $v_i \in V_i, \ i = 1, 2$.*

Proof. If there were another expression, $v_1 + v_2 = e = v_1' + v_2'$, then $V_1 \ni v_1 - v_1' = v_2' - v_2 \in V_2$, so $v_1 - v_1' = 0_E = v_2' - v_2$, which implies that $v_1 = v_1'$ and $v_2' = v_2$.

On the other hand, if $e \in V_1 \cap V_2$ then e could be expressed as $0_E + e = e + 0_E$, and, as the decomposition is unique, it is concluded that $e = 0_E$.

□

A.2 Analysis Structures

In this section, the categories of spaces are shown in order of generality from highest to lowest.

A.2.1 Semimetric and Metric Spaces

Definition 52 *The application $d(\cdot,\cdot) : E \times E \to \mathbb{R}^+$ is a* semidistance *—or* semimetric*— if*

(1m) $d(e,e) = 0, \quad \forall e \in E.$

(2m) $d(e_1,e_2) = d(e_2,e_1), \quad e_i \in E,\ i = 1,2.$

(3m) $d(e_1,e_2) \leq d(e_1,e_3) + d(e_3,e_2), \quad e_i \in E,\ i = 1,2,3.$

Definition 53 *A* distance *—or* metric*— $d(\cdot,\cdot)$ is a semidistance —or semimetric— that verifies*

(4m) $d(e_1,e_2) = 0 \ \Rightarrow\ e_1 = e_2, \quad e_i \in E,\ i = 1,2.$

Remark 41 When condition (4m) does not hold, some pairs of elements are not distinguishable (by taking the distance between them); nevertheless, the elements of E can be grouped into distinguishable classes of equivalence. The same will happen for the norms and the inner products defined below.

Definition 54 *A set E equipped with a semimetric $d(\cdot,\cdot)$ forms a* semimetric space*, and equipped with a metric $d(\cdot,\cdot)$ forms a* metric space*. In both cases, the space is denoted by $(E, d(\cdot,\cdot))$.*

The concept of *distance* allows us to quantify how close two elements are, and, as a consequence, the definition of a sequence of elements approximating to an element. Moreover, this concept will also provide some good topological properties (see section A.3).

Definition 55 *A sequence $\{e_n,\ n \geq 1\}$ of elements of a metric space is said to* converge *to an element e if for all $\epsilon > 0$ there exists $n_0 \in \mathbb{N}$ such that if $n > n_0$ then $d(e_n, e) < \epsilon$.*

Definition 56 *A sequence $\{e_n,\ n \geq 1\}$ of elements of a metric space is a* Cauchy sequence *if for all $\epsilon > 0$ there exists $n_0 \in \mathbb{N}$ such that if $n > n_0$ and $m > n_0$ then $d(e_n, e_m) < \epsilon$.*

It is easy to prove that convergent sequences are Cauchy sequences; the contrary is generally not true.

Definition 57 *A metric space is* complete *if any convergent sequence is a Cauchy sequences.*

In this case, the limit belongs to the space; that is, the space is closed with the topology (this concept is defined below) induced by the distance.

A.2.2 Seminormed and Normed Spaces

Let $(E, +, \cdot K)$ be a linear space.

Definition 58 *The application* $\|\cdot\| : E \to \mathbb{R}^+$ *is a* seminorm *if*

(1n) $\|ce\| = |c|\|e\|, \quad \forall c \in \mathbb{R},\ \forall e \in E.$

(2n) $\|e_1 + e_2\| \leq \|e_1\| + \|e_2\|, \quad e_i \in E,\ i = 1, 2.$

Definition 59 *A* norm *is a seminorm that verifies*

(3n) $\|e\| = 0 \ \Rightarrow\ e = 0_E\ ,$

where 0_E *denotes the null element of* E*.*

Remark 42 A semidistance —or a distance— can be defined from a seminorm —or norm— by taking

$$d(e_1, e_2) = \|e_1 - e_2\|. \tag{A.6}$$

In this case $d(e, 0_E) = \|e - 0_E\| = \|e\|$.

Definition 60 *A set* E *equipped with a seminorm* $\|\cdot\|$ *forms a* seminormed space*, and equipped with a norm* $\|\cdot\|$ *forms a* normed space*. In both cases, the space is denoted by* $(E, \|\cdot\|)$*.*

Definition 61 *A* Banach space *is a normed linear space that is complete.*

Linear Combinations and Approximations

As in any linear space, combinations of the form (A.4) can be considered as a mathematical operation. Nonetheless, only under "good conditions" the coefficients c_j exist, are unique and can be obtained (for example, by considering an optimization problem or projections) for any element e.

Theorem 6 *A finite-dimensional subspace of a normed vector space contains at least one point of minimum distance from a given point.*

Proof. See section 6.6 of Cohen (2003). □

Also from Cohen's book:

Definition 62 *A normed space* E *is said to be* strictly convex *if the equation*

$$\|e_1 + e_2\| = \|e_1\| + \|e_2\|, \tag{A.7}$$

for nonnull elements $e_i \in E$*,* $i = 1, 2$*, holds only when* $e_1 = ce_2$ *for some (real) positive number* c*.*

As Cohen states: *However equality can hold in the triangle inequality in some normed spaces in cases other that this, as we show below for $\mathcal{C}[a,b]$, so such spaces are not strictly convex.*

Now we can put a few things together.

Theorem 7 *If E is a strictly convex normed space, then a finite-dimensional subspace of E contains a unique best approximation of any point in E.*

Proof. See section 6.6 of Cohen (2003). □

A.2.3 Pre-Hilbert and Hilbert Spaces

Let $(E, +, \cdot K)$ be a linear space.

Definition 63 *The application $\langle \cdot, \cdot \rangle : E \times E \to \mathbb{R}$ is an* semiinner product *if*

(1h) $\langle e, e \rangle \geq 0, \quad \forall e \in E$, *and* $\langle 0_E, 0_E \rangle = 0$.

(2h) $\langle e_1, e_2 \rangle = \langle e_2, e_1 \rangle, \quad \forall e_i \in E,\ i = 1, 2$.

(3h) $\langle c_1 e_1 + c_2 e_2, e_3 \rangle = c_1 \langle e_1, e_3 \rangle + c_2 \langle e_2, e_3 \rangle, \quad e_i \in E,\ i = 1, 2, 3, \quad \forall c_i \in \mathbb{R},\ i = 1, 2$.

Definition 64 *An* inner product *is a semiinner product that verifies*

(4h) $\langle e, e \rangle = 0$ *if and only if* $e = 0_E$.

Definition 65 *Two nonnull elements of E are* orthogonal *if* $\langle e_1, e_2 \rangle = 0$.

Proposition 6 *If $\{e_j\}_1^n$ are nonnull and orthogonal elements of E, they are linearly independent.*

Proof. See section 3.4.1 of Kolmogórov and Fomín (1975). □

Definition 66 *A set E equipped with an inner product $\langle \cdot, \cdot \rangle$ forms a* pre-Hilbert space*, denoted by $(E, \langle \cdot, \cdot \rangle)$.*

Remark 43 Given an inner product, a norm —and then, a distance— can be defined from it by considering

$$\|e\| = (\langle e, e \rangle)^{1/2} = \sqrt{\langle e, e \rangle}. \tag{A.8}$$

Proposition 7 *A given norm can be defined from an inner product if and only if it verifies the parallelogram identity,*

$$\|e_1 + e_2\|^2 + \|e_1 - e_2\|^2 = 2\left(\|e_1\|^2 + \|e_2\|^2\right). \tag{A.9}$$

Proof. See section 3.4.8 of Kolmogórov and Fomín (1975). □

Remark 44 For the norms verifying the previous condition an inner product can be recovered or defined through

$$\langle e_1, e_2 \rangle = \frac{1}{4} \left(\|e_1 + e_2\|^2 - \|e_1 - e_2\|^2 \right). \tag{A.10}$$

Definition 67 *A* Hilbert space *is a pre-Hilbert space that is complete.*

Hilbert spaces are of great importance, not only for their completeness but also for the richness provided by the inner product of the pre-Hilbert structure.

Definition 68 *A basis of a linear space is* orthogonal *if any pair of its elements are orthogonal.*

Proposition 9 is devoted to the existence of orthogonal bases.

Linear Combinations

When the elements of the basis are orthogonal, and under "good conditions" (see theorem 9 below), the coefficients c_j of expression (A.4) exist (for any e) and are easy to find:

$$\langle e, \psi_j \rangle = \langle \sum_i c_i \psi_i, \psi_j \rangle = \sum_i c_i \langle \psi_i, \psi_j \rangle = c_j \langle \psi_j, \psi_j \rangle \tag{A.11}$$

so, when $\langle \psi_j, \psi_j \rangle \neq 0$,

$$c_j = \frac{\langle e, \psi_j \rangle}{\langle \psi_j, \psi_j \rangle}. \tag{A.12}$$

The scalar c_j is the coefficient of the projection of e into the linear subspace of E determined by ψ_j, say V_{ψ_j}, in the sense that $Proj_{V_{\psi_\mathbf{j}}}(e) = c_j \psi_j$.

Approximations via Truncation

The *Fourier Analysis* and the extension to more general pre- and Hilbert spaces provide easy theory on truncations (in this case, projections into the first elements of a properly ordered basis) like

$$Proj_{V_\psi}(e) = \sum_{i=1}^{p} c_i \psi_i = \mathbf{c}^t \psi, \tag{A.13}$$

where $\mathbf{c} = (c_1, c_2, \ldots, c_p)^t$ and $\psi = (\psi_1, \psi_2, \ldots, \psi_p)^t$. This corresponds to projecting the element e into the linear subspace generated by ψ, say V_ψ.

Least Squares Approximation

From Cohen's (2003) book: *In [a previous section] we considered the problem of best approximation in a normed space. In [a theorem], we stated that a unique solution exists to this problem when the space is strictly convex. [...] It is therefore very pleasing that we can show that any inner product space is strictly convex. This is the content of our first theorem below. We then deduce a simple formula that gives the best approximation and apply this in a further discussion of least squares polynomial approximations. The term* least squares approximation *is used generally for approximation problems in inner product spaces, for a reason that will become apparent.*

Theorem 8 *Inner product spaces are strictly convex.*

Proof. See section 8.3 of Cohen (2003). □

This implies that theorem 7 can be invoked.

Definition 69 *A basis* $\{\psi_j\}$ *of elements of* E *is* orthonormal *if it is orthogonal and each element verifies that* $1 = \|\psi_j\| = \sqrt{\langle \psi_j, \psi_j \rangle}$.

Moreover,

Theorem 9 *A finite-dimensional subspace* V *of an inner product space* E *contains a unique best approximation of any point* $e \in E$. *If* $\{\psi_i\}_1^n$ *is a basis for* V *and is orthonormal, then the best approximation of* e *is*

$$\sum_1^n \langle e, \psi_j \rangle \psi_j. \tag{A.14}$$

Proof. See section 8.3 of Cohen (2003). □

Remark 45 Expression (A.14) is the same as expression (A.12), where now the orthogonality of the basis implies that $\langle \psi_j, \psi_j \rangle = 1$.

In the proof of the previous theorem it is obtained that

$$\|e - \sum_1^n \langle e, \psi_j \rangle \psi_j\|^2 = \sum_1^n |c_j - \langle e, \psi_j \rangle|^2 + \|x\|^2 - \sum_1^n |\langle e, \psi_j \rangle|^2, \tag{A.15}$$

which is least when $c_j = \langle e, \psi_j \rangle$ for each j. See Cohen's book for the geometrical interpretation of this theorem.

Finally, the following theorem provides a way to determine the best least squares approximation.

Theorem 10 *Let* $\{\psi_i\}_1^n$ *be a basis for a subspace* V *of an inner product space* E. *Let* $e \in E$ *be given; if* $\sum_1^n c_j \psi_j$ *is the best least squares approximation in* V *of* e, *then*

$$\sum_{j=1}^n c_j \langle \psi_j, \psi_i \rangle = \langle e, \psi_i \rangle, \quad i = 1, \ldots, n. \tag{A.16}$$

Proof. See section 8.3 of Cohen (2003). □

Previous equations, called the *normal equations*, are a system of n linear equations in n unknowns, from which the coefficients c_j, $j = 1, \ldots, n$, may be obtained.

Decomposition

Definition 70 *Given a linear subspace V of E, its* orthogonal complement *is defined as*

$$V^{\perp} = \{e \in E \mid \langle e, v \rangle = 0 \ \forall v \in V\}. \tag{A.17}$$

Proposition 8 *Given a Hilbert space E, it holds that for any closed linear subspace $V \subset E$, $E = V \oplus V^{\perp}$.*

Proof. See section 21 of Jost (1998). □

These results and proposition 5 imply that any $e \in E$ can be uniquely decomposed, for any linear subspace V of E, as a sum of its two projections into V and $V^{\perp}$:

$$e = Proj_V(e) + Proj_{V^{\perp}}(e). \tag{A.18}$$

Remark 46 Kolmogórov and Fomín (1975) include theory on possible infinite-dimensional linear spaces, a situation which is quite more complicated and usually not included in basic text on Linear Algebra. In their book the reader can notice, for example, the importance of the existence of a countable and everywhere dense set, in order to apply an orthogonalization method for constructing an orthogonal countable everywhere dense set (see section 3.8.3 of this reference).

Proposition 9 *In any separable (with a countable and everywhere dense subset, as defined also in section A.3) pre- or Hilbert space there is at least one orthogonal basis.*

Proof. See section 3.4.3 of Kolmogórov and Fomín (1975). □

A.3 Topological Structures

The area of Mathematics known as *Topology* generalises some ideas of the Analysis. Specifically, the theory of functions between topological and measure spaces provides foundation for the definition of random variables.

A.3.1 Topological Space

Definition 71 *A collection $\mathcal{T} = \{\tau\}$ of subsets of E is a* topology *if:*

(1t) For the empty set and the whole space: $\emptyset \in \mathcal{T}$ and $E \in \mathcal{T}$.

(2t) For the union of any collection of subsets: $\cup_i \tau_i \in \mathcal{T}, \quad \forall \tau_i \in \mathcal{T}$.

(3t) For finite intersections of subsets: $\cap_i^n \tau_i \in \mathcal{T}, \quad \forall \tau_i \in \mathcal{T}, \ i = 1, 2, \ldots, n$.

Any element of $\mathcal{T}$ is termed an open *set, while any subset of E not belonging to the topology is a* closed *set.*

Definition 72 *A set E equipped with a topology $\mathcal{T}$ forms a* topological space*, and is denoted by $(E, \mathcal{T})$.*

Definition 73 *A collection of open sets $\{B_i\} \subset \mathcal{T}$ is a* basis *of $\mathcal{T}$ if for any open $\tau \in \mathcal{T}$ and any point $e \in \tau$, a set B_i exists such that $e \in B_i$.*

Definition 74 *Given $e \in E$, a* neighbourhood *of the point e is any subset $N(e) \subset E$ satisfying the conditions: (i) $e \in N(e)$; (ii) there exists $\tau \in \mathcal{T}$ such that $e \in \tau \subset N(e)$.*

For a topological structure, the convergence of a sequence can be defined as follows.

Definition 75 *A sequence of elements of a topological space, $\{e_n,\ n \geq 1\}$, is said to* converge *to an element e if for all neighbourhood $N(e)$ of e, there exists $n_0 \in \mathbb{N}$ such that if $n > n_0$ then $e_n \in N(e)$.*

Nevertheless, the topology is usually a much too general structure and, in order to achieve properties similar to those of the metric spaces, some additional conditions are required, such as separability and numerability axioms. Briefly, the former conditions are related to the distinguishableness or identificability of two different points of the space, while the latter axioms concern the possibility of approximating any element of the space with sequences of other elements of the space (the separability guarantees the uniqueness of the limit).

Separability

Definition 76 *A topological space $(E, \mathcal{T})$ is said to satisfy the* first separability axiom *if for any two points of E, e_1 and e_2, two neighbourhoods exist, $N(e_1)$ and $N(e_2)$, such that $e_2 \notin N(e_1)$ and $e_1 \notin N(e_2)$.*

Definition 77 *A topological space $(E, \mathcal{T})$ is said to satisfy the* second separability *—or* Hausdorff*—* axiom *if for any two points of E, e_1 and e_2, two neighbourhoods exist, $N(e_1)$ and $N(e_2)$, such that $N(e_1) \cap N(e_2) = \emptyset$.*

A space satisfying the second separability axiom also satisfies the first; that is, the second axiom is a stronger condition than the first one, while the converse is not true in general.

Numerability

Definition 78 *The family $\{B(e)\}$ of the neighbourhoods of a point $e \in E$ is called the* basis of the neighbourhood system *of e if there is an element from this family in each neighbourhood of the point e.*

Definition 79 *A topological space* $(E, \mathcal{T})$ *is said to satisfy the* first numerability —*or* countability— axiom *if the neighbourhood system of any point possesses a countable basis.*

Definition 80 *A topological space* $(E, \mathcal{T})$ *is said to satisfy the* second numerability —*or* countability— axiom *if a countable basis exists in the topology* $\mathcal{T}$*.*

A space satisfying the second numerability axiom also satisfies the first; that is, the second axiom is a stronger condition than the first one; the converse is not true in general.

Definition 81 *Let* e *be a point of* $S \subset E$*. A point* e *is said to be* interior *if a neighbourhood* $N(e)$ *exists such that* $N(e) \subset S$*. A point* e *is* isolated *if there is a neighbourhood* $N(e)$ *such that it does not contain any other point of* S*. A point* e *is termed* boundary *if it is neither interior nor isolated.*

Interior points of S can always be approximated by sequences of elements of S (then, of E). When the first numerability axiom is satisfied, any boundary point —of any subset of the space— can be represented as the limit of a sequence of elements of E.

Separability and Numerability

Definition 82 *Given a subset* $S \subset E$*, the* closure *of* S*, denoted by* $\bar{S}$*, is the intersection of all the closed sets containing* S*.*

Definition 83 *A topological space* $(E, \mathcal{T})$ *is* separable *if it has a countable subset such that* $\bar{S} = E$*.*

The importance of the second numerability axiom is that it implies the separability of the topological space, that is, the existence of a numerable dense subset such that $\bar{S} = E$; this means that any element of E is surrounded by elements of S.

Metric Spaces

The existence of a distance provides particularly good topological properties for the metric spaces. Some of them are the following:

- **Induced Topology**. Not any topological space can be placed in a metric space in a natural manner, but, on the contrary, a topological space can be defined from a metric by taking the following set of neighbourhoods of $e \in E$,

$$D_\epsilon(e) = \{\tilde{e} \mid d(e, \tilde{e}) < \epsilon\}. \tag{A.19}$$

  The subset $D_\epsilon(e)$ is an *open ball* of radius ϵ and with center at e. The topology formed in such way is the *topology induced* by the metric $d(\cdot, \cdot)$.

- Any metric space satisfies the first axiom of numerability (it is enough to consider the system $\{D_\epsilon(e),\ \epsilon \in \mathbb{Q}\}$, with $D_\epsilon(e)$ as given by A.19).
- For metric spaces, the separability also implies the second numerability axiom (it is enough to consider the system $\{D_{1/k}(e_n)\},\ k \in \mathbb{N}$, with $D_\epsilon(e)$ as given by A.19 and $\{e_n\}$ a countable and everywhere dense set).

Linear Spaces

With the topology constructed from the distance induced by the norm of a linear space, E, the pair $(E, \mathcal{T}_{\|\cdot\|})$ becomes a *topological linear space*.

Our Framework

The spaces in which we work in this document have —as usual in applied mathematics— good properties, in these cases due to the fact that they —$\mathbb{R}^p$, $\mathbb{R}^\infty$ and $\mathcal{C}(I)$— are separable metric spaces.

A.4 Measure-Theory Structures

Let $\mathcal{P}(E)$ be the set of all possible subsets of E; the next structure is an algebraic structure related to theory-set operations among subsets of E.

A.4.1 Measurable Space

Definition 84 *A collection $\mathcal{F} = \{f\}$ of subsets of E (that is, $\mathcal{F} \subset \mathcal{P}(E)$) is called a* σ-algebra *if:*

(1mt) $\emptyset \in \mathcal{F}$.

(2mt) For the complementary: $f^c \in \mathcal{F}, \quad \forall f \in \mathcal{F}$.

(3mt) For sequences of subsets: $\cup_i f_i \in \mathcal{F}, \quad \forall f_i \in \mathcal{F},\ i = 1, 2, \ldots$

Any element of $\mathcal{F}$ is termed a measurable *set.*

Definition 85 *A set E equipped with a* σ-algebra $\mathcal{F}$ *forms a* measurable space*, denoted by $(E, \mathcal{F})$.*

A.4.2 Measure Space and Probability Space

Definition 86 *Given a measurable space $(E, \mathcal{F})$, a* measure *with domain $\mathcal{F}$ is a function $\nu : \mathcal{F} \to \mathbb{R}$ verifying*

(i) It is nonnegative: $\nu(f) \geq 0, \quad \forall f \in \mathcal{F}$.

(ii) For the empty set: $\nu(\emptyset) = 0$.

(iii) For sequences of disjoint subsets: $\nu\left(\cup_i f_i\right) = \sum_i \nu(f_i), \quad f_i \in \mathcal{F},\ i = 1, 2, \ldots$

Definition 87 *A measurable space* $(E, \mathcal{F})$ *equipped with a measure* ν *forms a* measure space, *denoted by the triple* $(E, \mathcal{F}, \nu)$.

Definition 88 *A measure space* $(E, \mathcal{F}, \nu)$ *is* finite *if* $\nu(E) < \infty$.

Definition 89 *A* probability *is a measure* P *such that* $P(E) = 1$.

Remark 47 For a finite measure space, a probability P can be defined from a measure ν by considering

$$P(f) = \frac{\nu(f)}{\nu(E)}, \quad \forall f \in \mathcal{F}. \tag{A.20}$$

Definition 90 *A measurable space* $(\Omega, \mathcal{F})$ *equipped with a probability* P *forms a* probability space, *denoted by the triple* $(\Omega, \mathcal{F}, P)$.

A.4.3 Measurable Function and Random Variable

Definition 91 *A function* $g : (E_1, \mathcal{F}_1) \to (E_2, \mathcal{F}_2)$ *between measurable spaces is* measurable *if*

$$g^{-1}(f_2) \in \mathcal{F}_1, \quad \forall f_2 \in \mathcal{F}_2. \tag{A.21}$$

Remark 48 A measurable function $g(\cdot)$ from a measure space $(E_1, \mathcal{F}_1, \nu_1)$ to a measurable space $(E_2, \mathcal{F}_2)$ induces a measure ν_2 in the latter space by considering

$$\nu_2(f_2) = \nu_1(g^{-1}(f_2)), \quad \forall f_2 \in \mathcal{F}_2 \tag{A.22}$$

Definition 92 *For* $E = \mathbb{R}$, *the smallest* σ-algebra *containing all the intervals of the form* $I = (a, b)$, *with* $a, b \in \mathbb{R}$, *is the* Borel σ-algebra, *and the corresponding measurable space is denoted by* $(\mathbb{R}, \mathcal{B})$.

Definition 93 *Given a probability space* $(\Omega, \mathcal{F}, P)$, *a* random variable *is a measurable function* X *from* $(\Omega, \mathcal{F}, P)$ *to* $(\mathbb{R}, \mathcal{B})$.

This application can be represented as

$$\begin{array}{rccc} X: & \Omega & \longrightarrow & \mathbb{R} \\ & \omega & \to & X(\omega) \end{array}.$$

Remark 49 The measurable space $(\mathbb{R}, \mathcal{B})$ becomes a measure space $(\mathbb{R}, \mathcal{B}, P_X)$ with the induced probability

$$P_X(I) = P(X^{-1}(I)), \quad \forall I \in \mathcal{B}. \tag{A.23}$$

Appendix B

Matrix Algebra

Definition 94 *A square $p \times p$ matrix $\mathbf{M} = (m_{ij})_{i,j}$ is symmetric if it is equal to its transpose matrix, that is, if $\mathbf{M} = \mathbf{M}^t$; or, in terms of its elements, if $m_{ij} = m_{ji},\ \forall i, j$.*

Definition 95 *A symmetric $p \times p$ matrix $\mathbf{M}$ is positive definite if $\mathbf{x}^t\mathbf{M}\mathbf{x} > 0$ for all nonnull $\mathbf{x} \in \mathbb{R}^p$; and it is positive semidefinite —or nonnegative definite— if $\mathbf{x}^t\mathbf{M}\mathbf{x} \geq 0$ for all $\mathbf{x} \in \mathbb{R}^p$.*

Proposition 10

(a) A square symmetric matrix is positive semidefinite (respectively, positive definite) if and only if all its eigenvalues are nonnegative (respectively, positive).

(b) The inverse of a symmetric positive definite matrix is symmetric and positive definite.

Proof. See appendix A.4 of Bertsekas (1999). □

Proposition 11 *The sum $\mathbf{M} = c_1\mathbf{M}_1 + c_2\mathbf{M}_2,\ c_i > 0$, of two positive semidefinite (respectively, positive definite) matrices $\mathbf{M}_1$ and $\mathbf{M}_2$ is also a positive semidefinite (respectively, positive definite) matrix.*

Proof. By hypothesis $\mathbf{x}^t\mathbf{M}_i\mathbf{x} \geq 0,\ i = 1, 2$, so

$$\mathbf{x}^t\mathbf{M}\mathbf{x} = \mathbf{x}^t(c_1\mathbf{M}_1 + c_2\mathbf{M}_2)\mathbf{x} = c_1\mathbf{x}^t\mathbf{M}_1\mathbf{x} + c_2\mathbf{x}^t\mathbf{M}_2\mathbf{x} \geq 0.$$

(For positive definite matrices, '$\geq$' must be substituted with '$>$'.)

□

Proposition 12 *A full-rank positive semidefinite matrix, $\mathbf{M}$, is positive definite.*

Proof. By hypothesis $\mathbf{x}^t\mathbf{M}\mathbf{x} \geq 0$, but the system of equations $\mathbf{x}^t\mathbf{M}\mathbf{x} = 0$ has the unique solution $\mathbf{x} = \mathbf{0}$.

□

Appendix C

Vector Analysis

C.1 A Philological Note

Priestley (1981) makes the difference between the meanings of *multivariate* and *multidimensional* clear (see section 1.2 and the introduction of chapter 9):

Multivariate: "Of course, in a similar way we may have to consider the simultaneous variation of two, three, four, ..., or any number of related quantities, and such 'collections' of records are called *multivariate processes*".

Multidimensional: "Generally, if a quantity depends on several variables it is termed a *multidimensional process*".

In the same way, it would seem reasonable and coherent naming as:

$f : \mathbb{R} \to \mathbb{R}$	Univariate unidimensional function
$f : \mathbb{R}^p \to \mathbb{R}$	Univariate multidimensional function
$\mathbf{f} : \mathbb{R} \to \mathbb{R}^p$	Multivariate unidimensional function
$\mathbf{f} : \mathbb{R}^p \to \mathbb{R}^p$	Multivariate multidimensional function

C.2 Univariate Multidimensional Functions

C.2.1 Differentiation

Let $f : \mathbb{R}^p \to \mathbb{R}$ be a differentiable function depending on the variables $\mathbf{x} = (x_1, \ldots, x_p)^t$, then

Definition 96

$$\frac{\partial f}{\partial \mathbf{x}} = \left(\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_p} \right)^t. \tag{C.1}$$

Proposition 13 *If $f = \mathbf{x}^t\mathbf{c} = c_1x_1 + \ldots + c_px_p$, where $\mathbf{c} = (c_1, \ldots, c_p)^t$, then it holds that*

$$\frac{\partial f}{\partial \mathbf{x}} = \frac{\partial(\mathbf{x}^t\mathbf{c})}{\partial \mathbf{x}} = \mathbf{c} \tag{C.2}$$

and, since $f^t = f$,

$$\frac{\partial f^t}{\partial \mathbf{x}} = \frac{\partial (\mathbf{c}^t \mathbf{x})}{\partial \mathbf{x}} = \mathbf{c}. \tag{C.3}$$

Proof. See section 10 of Lütkepohl (1996).

□

Proposition 14 *If* $f = \mathbf{x}^t \mathbf{C} \mathbf{x}$, *where* $\mathbf{C}$ *is a square matrix, then it holds that*

$$\frac{\partial f}{\partial \mathbf{x}} = \frac{\partial (\mathbf{x}^t \mathbf{C} \mathbf{x})}{\partial \mathbf{x}} = (\mathbf{C} + \mathbf{C}^t)\mathbf{x} \tag{C.4}$$

and, when $\mathbf{C}$ *is symmetric,*

$$\frac{\partial f}{\partial \mathbf{x}} = \frac{\partial (\mathbf{x}^t \mathbf{C} \mathbf{x})}{\partial \mathbf{x}} = 2\mathbf{C}\mathbf{x}. \tag{C.5}$$

Proof. See section 10 of Lütkepohl (1996).

□

Let be the differentiable functions $g : \mathbb{R}^p \to \mathbb{R}$ and $h : \mathbb{R}^p \to \mathbb{R}$. Then

Proposition 15 *If* $f = g \cdot h$, *then*

$$\frac{\partial f}{\partial \mathbf{x}} = \left(\frac{\partial g}{\partial \mathbf{x}} h + g \frac{\partial h}{\partial \mathbf{x}} \right)^t \tag{C.6}$$

and, as a particular case,

$$\frac{\partial f^2}{\partial \mathbf{x}} = \left(2f \frac{\partial f}{\partial \mathbf{x}} \right)^t. \tag{C.7}$$

Proof. See section 10 of Lütkepohl (1996).

□

Proposition 16 *If* $f = g/h$, *then*

$$\frac{\partial f}{\partial \mathbf{x}} = \left(\frac{1}{h^2} \left(\frac{\partial g}{\partial \mathbf{x}} h - g \frac{\partial h}{\partial \mathbf{x}} \right) \right)^t. \tag{C.8}$$

Proof. See section 10 of Lütkepohl (1996).

□

An equivalent definition, with different notation, is the following:

Definition 97 *The* gradient *of the function* f *is defined as the (column) vector*

$$\nabla f = \left(\frac{\partial f}{\partial \mathbf{x}} \right) = \left(\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_p} \right)^t. \tag{C.9}$$

When there are several multivariate variables with respect to which the gradient would be considered, a subindex is added in the notation — for example, $\nabla_\beta f = \left(\frac{\partial f}{\partial \beta}\right)$.

Proposition 17 *When $\nabla f \neq \mathbf{0}$, it indicates —as a vector— the maximum variation direction of f.*

Proof. See section 2.5 of Marsden and Tromba (1991). □

Remark 50 This notation is preferred in Optimization theory (perhaps for the geometric interpretation of the gradient), while the previous, in terms of partial derivatives, is preferable in Multivariate Analysis.

Definition 98 *The* Hessian matrix *of the function f is defined as*

$$\nabla^2 f = \left(\frac{\partial^2 f}{\partial x_i \partial x_j}(\mathbf{x})\right)_{i,j}. \tag{C.10}$$

C.2.2 Operators

The previous definitions can be rewritten in terms of the the following operators:

Definition 99 *The (vectorial)* gradient *operator (that applies on univariate multidimensional functions) is defined as*

$$\nabla = \left(\frac{\partial}{\partial \mathbf{x}}\right) = \left(\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_p}\right)^t. \tag{C.11}$$

Definition 100 *The (scalar)* Laplacian *operator (that applies on univariate multidimensional functions) is defined as*

$$\nabla^2 = \nabla \cdot \nabla = \left(\frac{\partial}{\partial \mathbf{x}}\right)^t \left(\frac{\partial}{\partial \mathbf{x}}\right) = \sum_{i=1}^{p} \frac{\partial}{\partial x_i}, \tag{C.12}$$

where the dot $\cdot$ represents the canonical scalar product in $\mathbb{R}^p$.

C.2.3 Theoretical Results

Proposition 18 ***(Mean Value Theorem)*** *If $f : \mathbb{R}^p \to \mathbb{R}$ is continuously differentiable over the linear segment from $\mathbf{x}$ to $\mathbf{y}$, then an intermediate point in the segment exists, ξ, such that*

$$f(\mathbf{y}) - f(\mathbf{x}) = \nabla f(\xi)^t (\mathbf{y} - \mathbf{x}). \tag{C.13}$$

Proposition 19 ***(Second Order Expansions)*** *Let $f : \mathbb{R}^p \to \mathbb{R}$ be twice continuously differentiable over an open sphere $\mathcal{S}$ centered at a vector $\mathbf{x}$. Then*

(a) For all $\mathbf{y}$ such that $\mathbf{x} + \mathbf{y} \in \mathcal{S}$,

$$f(\mathbf{x} + \mathbf{y}) = f(\mathbf{x}) + \mathbf{y}^t \nabla f(\mathbf{x}) + \frac{1}{2}\mathbf{y}^t \left(\int_0^1 \left(\int_0^t \nabla^2 f(\mathbf{x} + \tau \mathbf{y}) d\tau\right) dt\right) \mathbf{y}. \tag{C.14}$$

(b) For all $\mathbf{y}$ *such that* $\mathbf{x}+\mathbf{y} \in \mathcal{S}$*, there exists an* $\alpha \in [0,1]$ *such that*

$$f(\mathbf{x}+\mathbf{y}) = f(\mathbf{x}) + \mathbf{y}^t \nabla f(\mathbf{x}) + \frac{1}{2}\mathbf{y}^t \nabla^2 f(\mathbf{x}+\alpha\mathbf{y})\mathbf{y}. \tag{C.15}$$

(c) For all $\mathbf{y}$ *such that* $\mathbf{x}+\mathbf{y} \in \mathcal{S}$*, there holds*

$$f(\mathbf{x}+\mathbf{y}) = f(\mathbf{x}) + \mathbf{y}^t \nabla f(\mathbf{x}) + \frac{1}{2}\mathbf{y}^t \nabla^2 f(\mathbf{x})\mathbf{y} + o(\|\mathbf{Y}\|^2). \tag{C.16}$$

Proof. See appendix A.5 of Bertsekas (1999). □

C.3 Multivariate Multidimensional Functions

Let $\mathbf{f} : \mathbb{R}^p \to \mathbb{R}^p$ be a differentiable function, $\mathbf{f} = (f_1, \ldots, f_{m_f})^t$.

C.3.1 Differentiation

Definition 101 *The* gradient matrix *of a multivariate multidimensional function* $\mathbf{f}$ *is defined as the matrix whose columns are* ∇f_j*, that is,*

$$\nabla \mathbf{f} = \left(\nabla f_1 \cdots \nabla f_{m_f}\right)_j = \left(\left(\frac{\partial f_1}{\partial \mathbf{x}}\right) \cdots \left(\frac{\partial f_{m_f}}{\partial \mathbf{x}}\right)\right)_j. \tag{C.17}$$

Remark 51 Instead of this definition, some *matricial differentiation* can be defined as the *vectorial differentiation* of section C.2.

Definition 102 *The* Jacobian *of a function is defined as the transpose of the gradient.*

C.3.2 Operators

Definition 103 *The (scalar)* divergence *operator (that applies on multivariate multidimensional functions) could be defined as*

$$\nabla \cdot = \left(\frac{\partial}{\partial \mathbf{x}}\right) \cdot = \left(\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_p}\right)^t \cdot, \tag{C.18}$$

where $\cdot$ *represents the canonical scalar product in* $\mathbb{R}^p$*.*

Definition 104 *The (vectorial)* rotational *operator (that applies on multivariate multidimensional functions) could be defined as*

$$\nabla \times = \left(\frac{\partial}{\partial \mathbf{x}}\right) \times = \left(\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_p}\right)^t \times, \tag{C.19}$$

where $\times$ *represents the canonical vectorial product in* $\mathbb{R}^p$*.*

With these operators, the following could be defined:

Definition 105 *The (vectorial)* divergence *of* $\mathbf{f}$ *is defined as*

$$div(\mathbf{f}) = \nabla^t \cdot \mathbf{f}. \tag{C.20}$$

Definition 106 *The (vectorial)* rotational *of* $\mathbf{f}$ *is defined as*

$$rot(\mathbf{f}) = \nabla \times \mathbf{f}. \tag{C.21}$$

Remark 52 Definitions, applications and the interpretation can be found in sections 3.3, 3.4 and 8.4 of Marsden and Tromba (1991).

Appendix D

Linear Discriminant Analysis for two groups ($K = 2$)

In this appendix, the Linear Discriminant Analysis is presented in the original Fisher's (1936) form, in the sense of not assuming either normality or equality of the group covariances; that is, nonparametrically and with possible heteroscedasticity. These two assumptions were introduced later also under the denomination *Linear Discriminant Analysis*. This classification method is defined as an optimization problem from matrices that expresses the sample variability information. The analytical solution, the geometrical interpretation and the assignment of new elements to a population are explained. The two-group classification case is specially considered, so only one discriminant function will be considered.

D.1 Motivation

D.1.1 The Problem

Let $\mathbf{X} = (X_1, \ldots, X_p)^t$ be a random vector with mean $\mu_{\mathbf{X}} = (\mathbb{E}(X_1), \ldots, \mathbb{E}(X_p))^t$ and covariance matrix $\mathbf{\Sigma_X} = (\sigma_{ij})_{i,j} = (cov(X_i, X_j))_{i,j} = \mathbb{E}\left((\mathbf{X} - \mu_{\mathbf{X}})(\mathbf{X} - \mu_{\mathbf{X}})^t\right)$. When there are $P^{(k)}$, $k = 1, \ldots, K$, populations where the vector is $\mathbf{X}^{(k)} = (X_1^{(k)}, \ldots, X_p^{(k)})^t$, with parameters $\mu_{\mathbf{X}}^{(k)}$ and $\mathbf{\Sigma}_{\mathbf{X}}^{(k)}$, respectively, capturing the differences between the groups from the distribution of $\mathbf{X}$ is a subject of great interest.

On the other hand, it is frequently convenient or necessary to summarize the information of a vector in a shorter one; that is, to consider $\mathbf{Y} = (Y_1, \ldots, Y_q)^t$, with $q < p$, instead of $\mathbf{X} = (X_1, \ldots, X_p)^t$.

The previous two tasks can be done simultaneously via the following multiple transformation, where the coefficients can be interpreted as weights (in the sense explained in section D.3.1):

$$Y_j^{(k)} = a_{j1}X_1^{(k)} + \ldots + a_{jp}X_p^{(k)} = \mathbf{a}_j^t\mathbf{X}^{(k)}, \qquad j = 1, \ldots, q \tag{D.1}$$

or, in matrix notation,

$$\mathbf{Y}^{(k)} = \mathbf{A}^t \mathbf{X}^{(k)}, \tag{D.2}$$

where $\mathbf{A} = (a_{ij})$ is the $p \times q$ matrix of the coefficients. Notice that $\mathbf{A}$ is independent of k, that is, independent of the population. The superscript $^{(k)}$ has been maintained in the notation to highlight that the new vector $\mathbf{Y}$ also has a different distribution in each population, and that the election of $\mathbf{A}$ must preserve or increase this difference so that $\mathbf{Y}$ is suitable for discrimination. The covariance matrix of $\mathbf{Y}^{(k)}$ is $\mathbf{\Sigma}_{\mathbf{Y}}^{(k)} = \mathbf{A}^t \mathbf{\Sigma}_{\mathbf{X}}^{(k)} \mathbf{A}$.

Remark 53 Functions given by (**??**) are linear by definition, which will imply that this document is devoted to the linear —not quadratic— discriminant analysis.

D.1.2 Data

When the model-versus-datum approach is applied, usually the unknown theoretical information must be inferred from samples. Let us consider, for each population k, the sample

$$(\mathbf{x}_1^{(k)}, \cdots, \mathbf{x}_{n_k}^{(k)}) = \begin{pmatrix} x_{11}^{(k)} & \cdots & x_{1n_k}^{(k)} \\ \vdots & \ddots & \vdots \\ x_{p1}^{(k)} & \cdots & x_{pn_k}^{(k)} \end{pmatrix}, \quad k = 1, \ldots, K \tag{D.3}$$

where $\mathbf{x}_j^{(k)}$, the j-th column of the matrix, containts the j-th element of the sample, with $n = \sum_{k=1}^{K} n_k$ and $p \leq min\{n_k\}$. There are techniques in the literature on discriminant analysis to test the significance of each discriminant variable. In the following subsections some known theory of this multivariate framework is given in order to motivate Fisher's method criterion.

D.1.3 Parameter Estimation

The parameters of the distributions can be estimated —for each population— as explained in section 1.2.3. In addition, when homoscedasticity hypothesis holds, $\mathbf{\Sigma}_{\mathbf{X}}^{(k)} = \mathbf{\Sigma}_{\mathbf{X}}$, $k = 1, \ldots, K$, the sample information can be combined and the matrix $\mathbf{\Sigma}_{\mathbf{X}}$ is estimated with bias by $\hat{\mathbf{\Sigma}}_{\mathbf{x}} = \sum_{k=1}^{K} \frac{n_k}{n} \hat{\mathbf{\Sigma}}_{\mathbf{x}}^{(k)}$ and without bias by $\mathbf{S}_{\mathbf{x}} = \frac{n}{n-K} \hat{\mathbf{\Sigma}}_{\mathbf{x}}$.

D.1.4 Variability Information

Information about the within- and between-group variabilities are provided, respectively, by the *within-class scatter matrix*

$$\mathbf{W} = \sum_{k=1}^{K} \sum_{e=1}^{n_k} (\mathbf{x}_e^{(k)} - \overline{\mathbf{x}}^{(k)})(\mathbf{x}_e^{(k)} - \overline{\mathbf{x}}^{(k)})^t \tag{D.4}$$

and the *between-class scatter matrix*

$$\mathbf{B} = \sum_{k=1}^{K} n_k (\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}})(\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}})^t, \tag{D.5}$$

where $\overline{\mathbf{x}} = n^{-1} \sum_{k=1}^{K} n_k \overline{\mathbf{x}}^{(k)}$ is the global mean. The *total scatter matrix*,

$$\mathbf{T} = \sum_{k=1}^{K} \sum_{e=1}^{n_k} (\mathbf{x}_e^{(k)} - \overline{\mathbf{x}})(\mathbf{x}_e^{(k)} - \overline{\mathbf{x}})^t, \tag{D.6}$$

expresses the total variability and is the sum of the previous quantities, $\mathbf{W} + \mathbf{B} = \mathbf{T}$.

These three matrices are, by definition, symmetric and positive semidefinite. In addition, $\mathbf{W}$ is usually nonsingular (full rank) if $n > p$, and, as a consequence, positive definite (see proposition 12).

Remark 54 The discriminant analysis is a supervised classification technique where the membership information is exploited through these variability matrices.

Remark 55 An important observation is that from definition (D.4) it holds that

$$\mathbf{W} = \sum_{k=1}^{K} n_k \hat{\mathbf{\Sigma}}_{\mathbf{x}}^{(k)} = n \hat{\mathbf{\Sigma}}_{\mathbf{x}} = (n - K) \mathbf{S}_{\mathbf{x}}. \tag{D.7}$$

This implies that any of the matrices $\mathbf{W}$, $\hat{\mathbf{\Sigma}}_{\mathbf{x}}$ and $\mathbf{S}_{\mathbf{x}}$ could be used in the statements of this document. A positive constant factor does not change the optimization problems that will be considered. Nevertheless, we shall use $\mathbf{W}$ since it maintains its meaning as variability matrix, while the matrices $\hat{\mathbf{\Sigma}}_{\mathbf{x}}$ and $\mathbf{S}_{\mathbf{x}}$ make sense as estimators only under the fulfilment of the equal group variability assumption (homoscedasticity). Although we shall find the solution of an optimization problem and we shall not include an analysis of the quality of $y = \mathbf{a}^t \mathbf{x}$, the discriminant power of this linear function is strongly related to the fulfilment of the homoscedasticity condition — given $\mathbf{T}$, the bigger $\mathbf{W}$ is, the smaller $\mathbf{B}$ and the between-group variability are. This is why most authors use $\mathbf{S}_{\mathbf{x}}$ in their statements.

Remark 56 Another expression of $\mathbf{W}$ can be obtained by using some inference concepts already defined and the relation of remark 55

$$\mathbf{W} = (w_{ij})_{i,j} = \left(\sum_{k=1}^{K} \sum_{e=1}^{n_k} (x_{ie}^{(k)} - \overline{x}_i^{(k)})(x_{je}^{(k)} - \overline{x}_j^{(k)}) \right)_{i,j}. \tag{D.8}$$

Compound Variables

Given a compound variable $\mathbf{y} = \mathbf{A}^t \mathbf{x}$, it is important to establish the relation between the scatter matrices of $\mathbf{y}$ —say $\mathbf{W}_{\mathbf{y}}$, $\mathbf{B}_{\mathbf{y}}$ and $\mathbf{T}_{\mathbf{y}}$— and those of $\mathbf{x}$ —say $\mathbf{W}$, $\mathbf{B}$ and $\mathbf{T}$.

Proposition 20 *If* $\mathbf{y} = \mathbf{A}^t \mathbf{x}$, *then*

1. $\mathbf{W}_{\mathbf{y}} = \mathbf{A}^t \mathbf{W} \mathbf{A}$.
2. $\mathbf{B}_{\mathbf{y}} = \mathbf{A}^t \mathbf{B} \mathbf{A}$.

3. $\mathbf{T}_{\mathbf{y}} = \mathbf{A}^t\mathbf{T}\mathbf{A}$.

Proof. Let $\mathbf{y}_e^{(k)}$ be the e-th element of the k-th sample; then

$$\begin{aligned}
\mathbf{W}_{\mathbf{y}} &= \sum_{k=1}^{K}\sum_{e=1}^{n_k}(\mathbf{y}_e^{(k)} - \overline{\mathbf{y}}^{(k)})(\mathbf{y}_e^{(k)} - \overline{\mathbf{y}}^{(k)})^t \\
&= \sum_{k=1}^{K}\sum_{e=1}^{n_k}(\mathbf{A}^t\mathbf{x}_e^{(k)} - \mathbf{A}^t\overline{\mathbf{x}}^{(k)})(\mathbf{A}^t\mathbf{x}_e^{(k)} - \mathbf{A}^t\overline{\mathbf{x}}^{(k)})^t \\
&= \sum_{k=1}^{K}\sum_{e=1}^{n_k}\mathbf{A}^t(\mathbf{x}_e^{(k)} - \overline{\mathbf{x}}^{(k)})(\mathbf{x}_e^{(k)} - \overline{\mathbf{x}}^{(k)})^t\mathbf{A} \\
&= \mathbf{A}^t\left(\sum_{k=1}^{K}\sum_{e=1}^{n_k}(\mathbf{x}_e^{(k)} - \overline{\mathbf{x}}^{(k)})(\mathbf{x}_e^{(k)} - \overline{\mathbf{x}}^{(k)})^t\right)\mathbf{A} = \mathbf{A}^t\mathbf{W}\mathbf{A}, \qquad \text{(D.9)}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{\mathbf{y}} &= \sum_{k=1}^{K} n_k(\overline{\mathbf{y}}^{(k)} - \overline{\mathbf{y}})(\overline{\mathbf{y}}^{(k)} - \overline{\mathbf{y}})^t \\
&= \sum_{k=1}^{K} n_k(\mathbf{A}^t\overline{\mathbf{x}}^{(k)} - \mathbf{A}^t\overline{\mathbf{x}})(\mathbf{A}^t\overline{\mathbf{x}}^{(k)} - \mathbf{A}^t\overline{\mathbf{x}})^t \\
&= \sum_{k=1}^{K} n_k\mathbf{A}^t(\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}})(\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}})^t\mathbf{A} \\
&= \mathbf{A}^t\left(\sum_{k=1}^{K} n_k(\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}})(\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}})^t\right)\mathbf{A} = \mathbf{A}^t\mathbf{B}\mathbf{A}, \qquad \text{(D.10)}
\end{aligned}$$

and

$$\mathbf{T}_{\mathbf{y}} = \mathbf{W}_{\mathbf{y}} + \mathbf{B}_{\mathbf{y}} = \mathbf{A}^t\mathbf{W}\mathbf{A} + \mathbf{A}^t\mathbf{B}\mathbf{A} = \mathbf{A}^t(\mathbf{W} + \mathbf{B})\mathbf{A} = \mathbf{A}^t\mathbf{T}\mathbf{A}. \qquad \text{(D.11)}$$

□

Positiveness

The previous calculations include a proof of the following statement:

Proposition 21 *Given a multivariate variable* $\mathbf{x}$*, its scatter matrices* $\mathbf{W}$*,* $\mathbf{B}$ *and* $\mathbf{T}$ *are positive semidefinite.*

Proof. It can be written

$$\mathbf{y}_e^{(k)} = (y_{e,1}^{(k)}, \ldots, y_{e,q}^{(k)}) \qquad \text{(D.12)}$$

$$\overline{\mathbf{y}}^{(k)} = \frac{1}{n_k}\sum_{e=1}^{n_k}\mathbf{y}_e^{(k)} = \left(\frac{1}{n_k}\sum_{e=1}^{n_k}y_{e,1}^{(k)}, \ldots, \frac{1}{n_k}\sum_{e=1}^{n_k}y_{e,q}^{(k)}\right) \qquad \text{(D.13)}$$

$$\overline{\mathbf{y}} = \frac{1}{n}\sum_{k=1}^{K} n_k \overline{\mathbf{y}}^{(k)} = \left(\frac{1}{n}\sum_{k=1}^{K}\sum_{e=1}^{n_k} y_{e,1}^{(k)}, \ldots, \frac{1}{n}\sum_{k=1}^{K}\sum_{e=1}^{n_k} y_{e,q}^{(k)} \right). \tag{D.14}$$

The positiveness is obtained by looking to both (D.9) and (D.10) from the bottom up and considering the univariate case $y = \mathbf{a}^t\mathbf{x}$:

$$\begin{aligned} \mathbf{a}^t\mathbf{W}\mathbf{a} &= \sum_{k=1}^{K}\sum_{e=1}^{n_k} (y_e^{(k)} - \overline{y}^{(k)})(y_e^{(k)} - \overline{y}^{(k)})^t \\ &= \sum_{k=1}^{K}\sum_{e=1}^{n_k} \left(y_e^{(k)} - \frac{1}{n_k}\sum_{e=1}^{n_k} y_e^{(k)} \right)^2 \geq 0 \end{aligned} \tag{D.15}$$

and

$$\begin{aligned} \mathbf{a}^t\mathbf{B}\mathbf{a} &= \sum_{k=1}^{K} n_k (\overline{y}^{(k)} - \overline{y})(\overline{y}^{(k)} - \overline{y})^t \\ &= \sum_{k=1}^{K} n_k \left(\frac{1}{n_k}\sum_{e=1}^{n_k} y_e^{(k)} - \frac{1}{n}\sum_{k=1}^{K}\sum_{e=1}^{n_k} y_e^{(k)} \right)^2 \geq 0. \end{aligned} \tag{D.16}$$

Finally, the matrix $\mathbf{T}$ is positive semidefinite as a consequence of being the sum of positive semidefinite matrices (see proposition 11).

□

Splitting Criterion

Given a unique sample with elements of both populations, minimizing a functional of $\mathbf{W}$ or maximizing a functional of $\mathbf{B}$ would be a reasonable criterion for splitting the sample from the information provided by the vector $\mathbf{x}$. Many techniques are based on this idea. On the one hand, the smaller $\mathbf{W}$ is, the more similar between them the elements of the subgroups are; on the other hand, the bigger $\mathbf{B}$ is, the more differences there are within the subgroups.

Although the subgroups are made in the supervised classification framework, it is still reasonable to choose the coefficients $\mathbf{A}$ so as the functions $\mathbf{Y}$ minimize $\mathbf{W}_\mathbf{y}$ or maximize $\mathbf{B}_\mathbf{y}$. Notice that given $\mathbf{T}$, the bigger $\mathbf{W}$ is, the smaller $\mathbf{B}$ and the between-group variability are — a trade-off between these two criteria is necessary.

D.1.5 Case $q = 1$: One Function

Some methods in literature choose —with different criteria— the linear combinations $y_j^{(k)}$ one at a time. Moreover, in a K-group classification problem, q must be no bigger that $K-1$; since we have worked in the two-group classification case, only one discriminant function could be considered in this thesis:

$$y^{(k)} = a_1 x_1^{(k)} + \ldots + a_p x_p^{(k)} = \mathbf{a}^t\mathbf{x}^{(k)}, \quad k = 1, 2, \ldots, K, \tag{D.17}$$

with $\mathbf{a} = (a_1, \ldots, a_p)^t$. For this new compound variable, $\overline{y}^{(k)} = \mathbf{a}^t\overline{\mathbf{x}}^{(k)}$ and $(s_y^{(k)})^2 = \mathbf{a}^t\mathbf{S}_{\mathbf{x}}^{(k)}\mathbf{a}$, where $\mathbf{S}_{\mathbf{x}}^{(k)}$ is the within-group sample covariance matrix. For classifying purposes, the variable $y^{(k)}$ must discriminate as much as possible. Following the idea of the aforementioned splitting criterion, the interest is in finding $\mathbf{a}$ so as to minimize the within-group dispersion, $W_y = \mathbf{a}^t\mathbf{W}\mathbf{a}$, or to maximize the between-group dispersion, $B_y = \mathbf{a}^t\mathbf{B}\mathbf{a}$. Then, the choice of $\mathbf{a}$ can be formulated as an *optimal weighting problem*.

D.2 The Optimization Problem

A general fraction increases either when the numerator increases or the denominator decreases; that is, two criteria are combined and taken into account at the same time. Fisher's proposal is based on a trade-off criterion between maximizing B_y and minimizing W_y, as it maximizes the —sometimes termed— *(generalised) Rayleigh quotient*: $\lambda = B_y/W_y$ (this greek letter has no relation with the λ used in chapter 2). This nonnegative quantity makes sense —mathematically— only when $W_y > 0$, that is, when $\mathbf{W}$ is positive definite, or, equivalently in this case, is a nonsingular matrix: then, **this hypothesis is necessary** throughout this appendix and chapter 3. To add each consecutive compound function, this method also maximizes this quantity but with the imposition of uncorrelation with the previous combination.

Of special interest is the case of one *discriminant function* y and several *discriminant variables* $x_1, \ldots, x_p$, consisting in finding $\mathbf{a} \in \mathbb{R}^p$ such that:

$$\mathbf{a} = argmax\left\{\lambda(\mathbf{a})\right\} = argmax\left\{\frac{B_y}{W_y}\right\} = argmax\left\{\frac{\mathbf{a}^t\mathbf{B}\mathbf{a}}{\mathbf{a}^t\mathbf{W}\mathbf{a}}\right\}. \tag{D.18}$$

This is an unconstrained ($\mathcal{D} = \mathbb{R}^p$) *nonlinear (quadratic) optimization problem*. Both $\mathbf{a}^t\mathbf{B}\mathbf{a}$ and $\mathbf{a}^t\mathbf{W}\mathbf{a}$ are polinomial (quadratic) differentiable functions in $\mathbf{a}$.

The analytical resolution of the problem is obtained by solving

$$\mathbf{0} = \frac{\partial\lambda}{\partial\mathbf{a}} = \frac{2[\mathbf{B}\mathbf{a}(\mathbf{a}^t\mathbf{W}\mathbf{a}) - (\mathbf{a}^t\mathbf{B}\mathbf{a})\mathbf{W}\mathbf{a}]}{(\mathbf{a}^t\mathbf{W}\mathbf{a})^2} = \frac{2[\mathbf{B}\mathbf{a} - \lambda\mathbf{W}\mathbf{a})]}{\mathbf{a}^t\mathbf{W}\mathbf{a}}, \tag{D.19}$$

so the expression

$$\mathbf{0} = \mathbf{B}\mathbf{a} - \lambda\mathbf{W}\mathbf{a} = (\mathbf{B} - \lambda\mathbf{W})\mathbf{a} \tag{D.20}$$

is the eigenequation of the problem. For a nonnull solution to exist, it is necessary for $|\mathbf{B} - \lambda\mathbf{W}| = 0$. As $\mathbf{W}$ is invertible (nonsingular) by hypothesis,

$$\mathbf{0} = \mathbf{W}^{-1}(\mathbf{B} - \lambda\mathbf{W})\mathbf{a} = (\mathbf{W}^{-1}\mathbf{B} - \lambda\mathbf{I})\mathbf{a}. \tag{D.21}$$

The interest is in the eigenvectors of the largest eigenvalue of the matrix $\mathbf{W}^{-1}\mathbf{B}$. In general, $\mathbf{W}^{-1}\mathbf{B}$ has $min\{p, K-1\}$ nonzero eigenvalues (section 11.5 of Mardia et al. [1979]).

Set of Solutions

As $\lambda(c\mathbf{a}) = \lambda(\mathbf{a}),\ \ \forall c \in \mathbb{R},\ c \neq 0$, that is, $\lambda(\mathbf{a})$ is *homogeneous*, the existing solution will not be a unique vector but an infinite family of them, denoted by

$$V_{\mathbf{a}}^* = \{c\mathbf{a} \mid c \in \mathbb{R},\ \ c \neq 0\}. \tag{D.22}$$

If $\mathbf{a}$ is a nonnull eigenvector of λ, so is any element of $V_{\mathbf{a}}^*$; that is, the set of eigenvectors is the solution to (D.21): mathematically it is necessary to include the null vector as solution of the equation, but this vector makes no sense in the optimization problem. Let us denote the solution of this optimization problem by the pair $(V_{\mathbf{a}_F}^*, \lambda_F)$.

Geometrically, the set $V_{\mathbf{a}} = V_{\mathbf{a}}^* \cup \{\mathbf{a} = \mathbf{0}\}$ is a one-dimensional linear subspace of $\mathbb{R}^p$.

Another Interpretation

Another interesting interpretation arises when the generalised Rayleigh quotient is written as

$$\lambda(\mathbf{a}) = \frac{B_y}{W_y} = \frac{\mathbf{a}^t\mathbf{B}\mathbf{a}}{\mathbf{a}^t\mathbf{W}\mathbf{a}} = \frac{\mathbf{a}^t(\mathbf{B}+\mathbf{W}-\mathbf{W})\mathbf{a}}{\mathbf{a}^t\mathbf{W}\mathbf{a}} = \frac{\mathbf{a}^t\mathbf{T}\mathbf{a}}{\mathbf{a}^t\mathbf{W}\mathbf{a}} - 1. \tag{D.23}$$

This decomposition shows that the previous maximization problem can be interpreted as maximizing the total variability while minimizing the within-class variability.

D.2.1 Equivalent Problems

Usually the previous optimization problem is solved via equivalent constrained problems.

Inequality Constrained Problem

For fixed $\mathbf{a}$, since $\|c\mathbf{a}\| = |c|\|\mathbf{a}\|$ the scalar c can always be chosen so that the set of solutions $V_{\mathbf{a}}^*$ has a "representative" as close to the origin $\mathbf{0}$ as desired. This means that the search can be restricted to any domain $\mathcal{D}$ having the origin as an interior point; concretely, the compact (p-1)-dimensional sphere $\{\mathbf{a}^t\mathbf{W}\mathbf{a} \leq 1\}$ can be considered.

On the other hand, as $\mathbf{W}$ is positive semidefinite, by proposition 22(d) (in appendix E), the function $h(\mathbf{a}) = \mathbf{a}^t\mathbf{W}\mathbf{a}$ is convex; thus, from proposition 23(c) (in appendix E) the set $\{\mathbf{a} \in \mathbb{R}^p \mid h(\mathbf{a}) = \mathbf{a}^t\mathbf{W}\mathbf{a} \leq 1\}$ is convex; finally, these facts and proposition 24 provide the equivalence —under existence— of the following optimization problem:

$$\mathbf{a} = argmax\left\{\mathbf{a}^t\mathbf{B}\mathbf{a}\right\} \quad \text{subject to} \quad \mathbf{a}^t\mathbf{W}\mathbf{a} \leq 1, \tag{D.24}$$

where the feasible domain is $\mathcal{D} = \{\mathbf{a} \in \mathbb{R}^p \mid \mathbf{a}^t\mathbf{W}\mathbf{a} \leq 1\}$.

For fixed λ, the solutions $\mathbf{a}$ can be interpreted geometrically in $\mathbb{R}^p$ as the intersection of a one-dimensional linear subspace and the volume (sphere) whose frontier is $\mathbf{a}^t\mathbf{W}\mathbf{a} = 1$, that is, $V_{\mathbf{a}} \cap \{\mathbf{a}^t\mathbf{W}\mathbf{a} \leq 1\}$ (strictly, the point $\mathbf{a} = \mathbf{0}$ must be excluded).

Equality Constrained Problem

The original optimization problem and the previous one, due to (D.22), do not guarantee the uniqueness of the solution. To avoid the arbitrary scale factor and obtain a unique solution, usually the constraint is added in the form:

$$\mathbf{a} = argmax \left\{ \mathbf{a}^t \mathbf{B} \mathbf{a} \right\} \quad \text{subject to} \quad \mathbf{a}^t \mathbf{W} \mathbf{a} = 1, \tag{D.25}$$

whose solution is $(\mathbf{a}_F, \lambda_F)$, with $\mathbf{a}_F^t \mathbf{W} \mathbf{a}_F = 1$ and $\lambda_F = \mathbf{a}_F^t \mathbf{B} \mathbf{a}_F$. Thus, the feasible region is $\mathcal{D} = \{\mathbf{a} \in \mathbb{R}^p \mid \mathbf{a}^t \mathbf{W} \mathbf{a} = 1\}$. The calculations leading to the explicit expression of $\mathbf{a}_F$ are given in section D.3. On the one hand, the constraint is only fixing the value of the constant c (defined in [D.22]); on the other hand, $V_{\mathbf{a}}^*$ is generated by any of its elements — this justifies the fact that the two optimization problems are equivalent.

More formally, the previous *inequality constrained problem* is equivalent to this *equality constrained problem* due to proposition 25 with $\{\mathbf{a} \in \mathbb{R}^p \mid \mathbf{a}^t \mathbf{W} \mathbf{a} \leq 1\}$ as closed convex bounded from below set. This is the way in which the optimization problem has been considered in this text.

As in the previous case, for fixed λ the solutions $\mathbf{a}$ can be interpreted geometrically in $\mathbb{R}^p$ as the intersection of a one-dimensional linear subspace and the p-dimensional surface determined by $\mathbf{a}^t \mathbf{W} \mathbf{a} = 1$, that is $V_{\mathbf{a}} \cap \{\mathbf{a}^t \mathbf{W} \mathbf{a} = 1\}$ (strictly, the point $\mathbf{a}$ must be excluded).

Convexity

In these problems, the objective function is convex due to proposition 22(d) (in appendix E) and the positive definiteness of the matrix $\mathbf{B}$.

D.2.2 Existence of Solutions

Weierstrass Theorem

The search for a solution can be tackled via the previous equivalent optimization problems. In the first one, the feasible region is compact and, as $\lambda(\mathbf{a})$ is continuous, the Weierstrass theorem implies the existence of a solution.

D.2.3 Fractional Programming

The optimization problem (D.18) can be seen as a particular case of *fractional optimization*, that is, the optimization of a quotient of functions. To see how these problems can be turned into nonfractional equality constrained problems, see proposition 36 (in appendix E).

D.2.4 Case $K = 2$: Two Populations

We have taken into special consideration classification into two populations. It is well-known that this case can be written as an equivalent linear regression problem; nevertheless, we have not used

this interpretation here.

On the other hand, since

$$(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}) = \frac{n_2}{n}(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)}) \tag{D.26}$$

and

$$(\overline{\mathbf{x}}^{(2)} - \overline{\mathbf{x}}) = \frac{n_1}{n}(\overline{\mathbf{x}}^{(2)} - \overline{\mathbf{x}}^{(1)}) = -\frac{n_1}{n}(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)}), \tag{D.27}$$

it follows that

$$\begin{aligned}
\mathbf{a}^t\mathbf{B}\mathbf{a} &= \mathbf{a}^t \left[\sum_{k=1}^{K} n_k(\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}})(\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}})^t\right] \mathbf{a} \\
&= \mathbf{a}^t \frac{n_1 n_2}{n}(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t\mathbf{a} \\
&= \frac{n_1 n_2}{n}[\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})][\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})]^t \\
&= \frac{n_1 n_2}{n}[\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})]^2.
\end{aligned} \tag{D.28}$$

Thus, the previous optimization problems are equivalent, respectively, to the following ones:

$$\mathbf{a} = argmax \left\{ \frac{[\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})]^2}{\mathbf{a}^t\mathbf{W}\mathbf{a}} \right\} \tag{D.29}$$

and

$$\mathbf{a} = argmax \left\{ [\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})]^2 \right\} \quad \text{subject to} \quad \mathbf{a}^t\mathbf{W}\mathbf{a} = 1. \tag{D.30}$$

Remark 57 Notice that with this formulation (for two populations) the numerator highlights the objective of the optimization problem — maximizing the difference between the means under control of the variability.

Remark 58 The quantity $[\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})]^2$ can be written as $\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t\mathbf{a}$.

D.3 The Discriminant Function

For two populations, the resolution of the optimization problem, with and without the classical constraint (when $\mathbf{a}^t\mathbf{W}\mathbf{a} = 1$ or $\beta = 0$, respectively), is given at the same time by

$$\begin{aligned}
\mathbf{0} &= \frac{\partial}{\partial \mathbf{a}} \left(\frac{[\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})]^2}{\mathbf{a}^t\mathbf{W}\mathbf{a}} - \beta(\mathbf{a}^t\mathbf{W}\mathbf{a} - 1) \right) \\
&= \frac{\partial}{\partial \mathbf{a}} \left(\frac{[\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})]^2}{\mathbf{a}^t\mathbf{W}\mathbf{a}} \right) - \frac{\partial}{\partial \mathbf{a}} \left(\beta(\mathbf{a}^t\mathbf{W}\mathbf{a} - 1) \right) \\
&= \frac{2\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})\mathbf{a}^t\mathbf{W}\mathbf{a} - [\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})]^2 2\mathbf{W}\mathbf{a}}{(\mathbf{a}^t\mathbf{W}\mathbf{a})^2} \\
&\quad -\beta 2\mathbf{W}\mathbf{a}
\end{aligned} \tag{D.31}$$

so

$$\frac{\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})\mathbf{a}^t\mathbf{W}\mathbf{a}}{[\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})]^2 + \beta(\mathbf{a}^t\mathbf{W}\mathbf{a})^2}(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)}) = \mathbf{W}\mathbf{a} \tag{D.32}$$

and, if $\mathbf{W}$ is invertible,

$$\mathbf{a} = \frac{\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})\mathbf{a}^t\mathbf{W}\mathbf{a}}{[\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})]^2 + \beta(\mathbf{a}^t\mathbf{W}\mathbf{a})^2}\mathbf{W}^{-1}(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)}). \tag{D.33}$$

Since $\mathbf{a}^t(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})$ and $\mathbf{a}^t\mathbf{W}\mathbf{a}$ are numbers, irrelevant of whether the constraint $\mathbf{a}^t\mathbf{W}\mathbf{a} = 1$ is imposed or not, the solution for the classical linear discriminant analysis is that y is proportional to $(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t\mathbf{W}^{-1}$, and, without loss of generality:

$$y = \mathbf{a}_F^t\mathbf{x} = (\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t\mathbf{W}^{-1}\mathbf{x}. \tag{D.34}$$

See section 1.2.5 for a discussion of the negligible role of a possible scalar factor in this expression. Since $y \in \mathbb{R}$, it is sometimes written as $y = y^t = \mathbf{x}^t\mathbf{a}_F = \mathbf{x}^t\mathbf{W}^{-1}(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})$ in literature.

D.3.1 Interpretation of the Coefficients

Usually the variables of the vector $\mathbf{x}$ have been measured using different scales: localization, variability or even units of measure. In this case, the mathematical solution of the optimization problem provides values a_i not taking into account this fact. The function

$$y = a_1x_1 + \ldots + a_px_p = \mathbf{a}^t\mathbf{x}, \tag{D.35}$$

with $\mathbf{a} = (a_1, \ldots, a_p)^t$, can still be used for classifying.

A possible transformation that can be applied to the previous values is a translation so that the origin of the axes coincides with the global centroid of the samples and a homothecy so that the coordinates refer to the standard deviation of each axis. Then,

$$\tilde{y} = b_0 + b_1x_1 + \ldots + b_px_p = b_0 + \mathbf{b}^t\mathbf{x}, \tag{D.36}$$

with $\mathbf{b} = (b_1, \ldots, b_p)^t$, where b_i can be interpreted as regression coefficients. When these values are obtained from crude data, they are termed *nonstandardized coefficients*, that represent the (absolute) contribution of the variables to the function but are not comparable amongst them. Regardless, $\tilde{y}$ is also used for classifying. On the other hand, the typification of variables solves, at the same time, the aforementioned scale problems —localization, variability and units. So if $\mathbf{b}$ is obtained from typified —not crude— variables, this vector contains the *standardized coefficients*, that represent the relative contribution of the variables to the function and are comparable amongst them. Nevertheless, now the function (D.36) cannot be used for classifying, as the important information has been lost (in this case $b_0 = 0$, for example).

Our proposal has been described in terms of the function (D.35) suggested by the optimization problem; nevertheless, the interpretation of the coefficients —through the figures— has been based on the function

$$y = \mathbf{a}^t\mathbf{x} = \mathbf{a}^t\mathbf{D}\mathbf{D}^{-1}\mathbf{x} = \mathbf{a}^t\mathbf{D}\tilde{\mathbf{x}}, \tag{D.37}$$

where $\tilde{\mathbf{x}} = \mathbf{D}^{-1}\mathbf{x}$, with $\mathbf{D}$ being the diagonal matrix with elements $\sigma_1, \ldots, \sigma_p$, where σ_i is the standard deviation of the variable x_i. After applying this *univariate standardization*, the new dimensionless variables have variance equal to one:

$$\tilde{\mathbf{x}} = \mathbf{D}^{-1}\mathbf{x} = (\sigma_1^{-1}x_1, \ldots, \sigma_p^{-1}x_p) \quad \Rightarrow \quad Var(\tilde{x_i}) = Var(\sigma_i^{-1}x_i) = 1. \tag{D.38}$$

Note that the previous transformation does not change the mean of each variable. Thus, for the interpretation we have considered the coefficients defined by $\mathbf{a}^t\mathbf{D}$, that is, the quantities

$$\mathbf{a}^t\mathbf{D} = (a_1\sigma_1, \ldots, a_p\sigma_p). \tag{D.39}$$

The vector $\mathbf{a} = (a_1, \ldots, a_p)^t$ determines a direction in $\mathbb{R}^p$; for our two algorithms and when $p = 2$ or $p = 3$, the code draws the version of these two directions that contains the global centroid of the data (in green for the first algorithm and in magenta for the second [see figure 3.5(d)]).

Finally, there are in literature different methods to measure the contribution of each discriminant variable in the discriminant functions. The coefficients are related to the descriptive character of the linear discriminant analysis, while the discriminant functions are related to the predictive character.

D.4 The Classification

Geometrically, the Fisher's discriminant analysis projects the data into one-dimensional linear subspaces (see addendum 1.2.5). For the first direction, this operation is analytically done by the $y = \mathbf{a}_F^t\mathbf{x}$ operation; that is, the multivariate vector $\mathbf{x}$ is projected by the $(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t\mathbf{W}^{-1}$ premultiplication. The method classifies a new element in the population k as follows:

$$\begin{cases} k = 1 & \text{if} \quad y(\mathbf{x}) > \frac{1}{2}(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t\mathbf{W}^{-1}(\overline{\mathbf{x}}^{(1)} + \overline{\mathbf{x}}^{(2)}) \\ k = 2 & \text{otherwise} \end{cases} \tag{D.40}$$

with the value $\frac{1}{2}(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t\mathbf{W}^{-1}(\overline{\mathbf{x}}^{(1)} + \overline{\mathbf{x}}^{(2)})$, the *cutoff point*, determined by the equation

$$(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t\mathbf{W}^{-1}\mathbf{x} - \frac{1}{2}(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t\mathbf{W}^{-1}(\overline{\mathbf{x}}^{(1)} + \overline{\mathbf{x}}^{(2)}) = 0, \tag{D.41}$$

where the equality determines a hyperplane. By writing

$$\frac{1}{2}(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t\mathbf{W}^{-1}(\overline{\mathbf{x}}^{(1)} + \overline{\mathbf{x}}^{(2)}) = (\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t\mathbf{W}^{-1}\frac{1}{2}(\overline{\mathbf{x}}^{(1)} + \overline{\mathbf{x}}^{(2)}) \tag{D.42}$$

we see that the cutoff point is the projection of the midpoint between the two population sample averages, $\frac{1}{2}(\overline{\mathbf{x}}^{(1)} + \overline{\mathbf{x}}^{(2)})$, into the same subspace.

Thus, for $y = \mathbf{a}_F^t \mathbf{x}$ the classification of a multivariate point is made by the simple comparison of its projection with the projection of the semisum of the group means (centroids). It is well-known that the decision boundaries of the linear discriminant analysis are linear; in (D.40) the equality has been included in the "otherwise" case (in practice this case is usually negligible).

Remark 59 Expressions (D.34) and (D.40) lead to the —also named in literature— *(sample) linear discriminant function*

$$\begin{aligned} L(\mathbf{x}) &= (\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t \mathbf{W}^{-1} \mathbf{x} - \frac{1}{2}(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t \mathbf{W}^{-1}(\overline{\mathbf{x}}^{(1)} + \overline{\mathbf{x}}^{(2)}) \\ &= y(\mathbf{x}) - \frac{1}{2}(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t \mathbf{W}^{-1}(\overline{\mathbf{x}}^{(1)} + \overline{\mathbf{x}}^{(2)}) \end{aligned} \tag{D.43}$$

Notice that the second factor does not depend on the variables $\mathbf{x}$. See, for example, section 12.2.2 of Krzanowski (2000).

Remark 60 The use of data and the previous optimization problem provide a value for $\mathbf{a}$. Then, if there is interest in the stochastic character of the vectors $\mathbf{X}$ and Y (see the motivation at the beginning of this appendix), the following discriminant function

$$Y = Y(\mathbf{X}) = \hat{\mathbf{a}}^t \mathbf{X} = \mathbf{a}_F^t \mathbf{X} = (\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t \mathbf{W}^{-1} \mathbf{X} \tag{D.44}$$

and classification rule

$$\begin{cases} k = 1 & \text{if} \quad Y > \frac{1}{2}(\overline{\mathbf{x}}^{(1)} - \overline{\mathbf{x}}^{(2)})^t \mathbf{W}^{-1}(\overline{\mathbf{x}}^{(1)} + \overline{\mathbf{x}}^{(2)}) \\ k = 2 & \text{otherwise} \end{cases} \tag{D.45}$$

can be considered instead of (D.34) and (D.40), where $\mathbf{X}$ and Y are random variables again. This appendix can be interpreted in the classification framework of section 1.5. Some population information is unknown and the use of samples allows us to infer it; the sample rule (D.40) is obtained; on the other hand, an underlying theoretical rule can be obtained by substituting the corresponding population quantities into it.

Remark 61 The point $\mathbf{r} = \frac{1}{2}(\overline{\mathbf{x}}^{(1)} + \overline{\mathbf{x}}^{(2)})$ can be considered to be a reference global p-dimensional point of the samples; in the same way, the cutoff point can be seen as a global reference point in the unidimensional subspace, that is, $r = y(\mathbf{r})$. Then, the classification criterion (D.40) becomes

$$\begin{cases} k = 1 & \text{if} \quad y > r \\ k = 2 & \text{otherwise} \end{cases} . \tag{D.46}$$

Another interpretation of the classification criterion arises when, for each k, the centroid of each group is interpreted as a representative multivariate point of the group, $\mathbf{r}^{(k)} = \overline{\mathbf{x}}^{(k)}$, and, equivalently, the projection of the centroid is thought of as a representative univariate point, $r^{(k)} = y(\mathbf{r}^{(k)})$.

Since $y(\mathbf{x})$ is a linear application in $\mathbb{R}^p$, on the one hand $y(\hat{\mathbf{x}}) = \hat{y}$, and, on the other hand, geometrically, the point $\mathbf{r}$ is the midpoint of the p-dimensional segment from $\mathbf{r}^{(1)}$ to $\mathbf{r}^{(2)}$, so r is the midpoint of the unidimensional segment from $r^{(1)}$ to $r^{(2)}$. Analytically, this can be proved from the fact that, for any points $\mathbf{x}_j \in \mathbb{R}^p$, $j = 1, 2$, it holds that $|\Delta y| = |y(\mathbf{x}_2) - y(\mathbf{x}_1)| = |\mathbf{a}_F^t(\mathbf{x}_2 - \mathbf{x}_1)| = |\mathbf{a}_F^t \Delta \mathbf{x}|$. Regardless, the important conclusion is that the rules (D.40) and (D.46) can be expressed, respectively, as

$$k = argmin_{\{1,2\}} \left\{ d(y(\mathbf{x}), y(\mathbf{r}^{(k)})) \right\} = argmin_{\{1,2\}} \left\{ d(y, r^{(k)}) \right\} \tag{D.47}$$

and finally as

$$k = argmin_{\{1,2\}} \left\{ |\mathbf{a}_F^t \mathbf{x} - \mathbf{a}_F^t \overline{\mathbf{x}}^{(k)}| \right\}. \tag{D.48}$$

Remark 62 For two populations, a rule like (D.46) is possible; this rule makes a simple comparison with the midpoint and does not need to take into account the magnitude of the distance to the point r. For more than two populations, a rule like (D.47) would be needed; this rule takes into account the magnitude of the distances to the points $r^{(k)}$.

Remark 63 For one discriminant function ($q = 1$) a rule like (D.46) is possible; for more discriminant functions a rule like (D.47), with multivariate $\mathbf{y}$, would be needed.

Remark 64 In the literature on discriminant analysis, there are other ways to classify that are not directly based on the discriminant functions.

D.4.1 Theoretical Misclassification Rates

For two populations ($K = 2$) and $e = \mathbf{x}$, and when e is chosen —to evaluate the global error rate— from the populations with the same probability (if $n_1 = n_2$; the empirical counterpart is that the testing samples would have the same size, $m_1 = m_2$),

$$\begin{aligned} p(\mathcal{E}) &= p(C(e) = 2 \mid e \in P^{(1)}) \cdot p(e \in P^{(1)}) \\ &\quad + p(C(e) = 1 \mid e \in P^{(2)}) \cdot p(e \in P^{(2)}) \\ &= \frac{1}{2} p(y(\mathbf{x}) < r \mid \mathbf{x} \in P^{(1)}) + \frac{1}{2} p(y(\mathbf{x}) > r \mid \mathbf{x} \in P^{(2)}). \end{aligned} \tag{D.49}$$

Sometimes the quantities involved in this expression can be calculated easily and even without calculations; other times, more or less difficult calculations are necessary.

Under Normality

As a final and general theoretical comment, when the distributions of $\mathbf{X}^{(k)}$ are normal, Fisher's approach is optimal in the sense of minimizing the misclassification probability.

Appendix E

Optimization Theory

All the contents of this section can be found in Bertsekas (1999). Let be $\mathcal{D} \subset \mathbb{R}^p$ and the differentiable function $f : \mathcal{D} \to \mathbb{R}$ depending on the variables $\mathbf{x} = (x_1, \ldots, x_p)^t$, where $p \in \mathbb{N} \setminus \{0\}$ and $\mathbb{R}^p$ is equipped with the usual Euclidean norm $\|\cdot\| = \|\cdot\|_p$. Notice that since the function f is supposed to be differentiable, gradients and Taylor series can be used to study the performance and the conditions in the neighbourhood of the extreme points.

E.1 Some Definitions

E.1.1 Minima

Definition 107 *The point $\mathbf{x}_0 \in \mathcal{D}$ is said to be a* constrained relative *—or* local*— minimum if*

$$f(\mathbf{x}_0) \leq f(\mathbf{x}), \quad \forall\ \mathbf{x} \in D_\epsilon(\mathbf{x}_0), \tag{E.1}$$

where $D_\epsilon(\mathbf{x}_0) = \{\mathbf{x} \mid \|\mathbf{x}_0 - \mathbf{x}\| < \epsilon\}$, for some $\epsilon > 0$ such that $D_\epsilon(\mathbf{x}_0) \subset \mathcal{D}$.

Definition 108 *The point $\mathbf{x}_0 \in \mathcal{D}$ is said to be a* constrained global minimum *if*

$$f(\mathbf{x}_0) \leq f(\mathbf{x}), \quad \forall\ \mathbf{x} \in \mathcal{D}. \tag{E.2}$$

E.1.2 General Problem

A general *constrained optimization (minimization) problem* with *feasible* or *admissible domain* $\mathcal{D}$ consists in searching for the point $\mathbf{x}$ such that

$$\mathbf{x} = argmin\,\{f(\mathbf{x})\} \qquad \text{subject to} \qquad \mathbf{x} \in \mathcal{D}, \tag{E.3}$$

where f is the *objective* —or *cost*— *function*. Usually, $\mathcal{D}$ is expressed through some conditions on differentiable multivariate functions $\mathbf{h} = (h_1, \ldots, h_{m_h})^t$ and $\mathbf{g} = (g_1, \ldots, g_{m_g})^t$; for example, the *equality constraints* $\mathbf{h}(\mathbf{x}) = \mathbf{0}$ and the *inequality constraints* $\mathbf{g}(\mathbf{x}) \leq \mathbf{0}$, that would provide

$$\mathcal{D} = \{\mathbf{x} \in \mathbb{R}^p \mid \mathbf{h}(\mathbf{x}) = \mathbf{0} \ \text{ and } \ \mathbf{g}(\mathbf{x}) \leq \mathbf{0}\}. \tag{E.4}$$

The points of $\mathcal{D}$ are termed *feasible* points.

E.1.3 Existence of Solutions

It is well-known, due to the *Weierstrass theorem*, that there is at least one global minimum if f is a continuous function and $\mathcal{D}$ is compact (with the usual topology of $\mathbb{R}$ — the *Borel topology*).

On the other hand, there is also an optimal solution when f is continuous, $\mathcal{D}$ is closed and $f(\mathbf{x_k}) \to \infty$ for any $\{\mathbf{x_k}\}_k \subset \mathcal{D}$ such that $\|\mathbf{x_k}\| \to \infty$.

Some other results on the existence of optimal solutions are in section 2.1.2 of Bertsekas (1999) and below in this appendix.

E.1.4 Maximization Problem

Local and global maximum are defined in the same way, just by substituting $\leq$ by $\geq$ in (E.1) and (E.2).

The general minimization problem (E.3) is equivalent to the following maximization one:

$$\mathbf{x} = argmax\,\{-f(\mathbf{x})\} \quad \text{subject to} \quad \mathbf{x} \in \mathcal{D}. \tag{E.5}$$

In this case, all the forthcoming theory can be reformulated by replacing the concepts related to minimum and convexity of f with the corresponding concepts of maximum and concavity of f.

E.1.5 Convexities

Definition 109 *The subset $\mathcal{D} \subset \mathbb{R}^p$ is said to be* convex *if*

$$c\mathbf{x}_1 + (1-c)\mathbf{x}_2 \in \mathcal{D} \tag{E.6}$$

for all $\mathbf{x}_i \in \mathcal{D},\ i = 1, 2$ and all $c \in [0, 1]$.

In the following, the domain $\mathcal{D}$ is supposed to be convex, although some results also hold for an open set containing the minimum.

Definition 110 *For a convex domain $\mathcal{D}$, a function $f : \mathcal{D} \to \mathbb{R}$ is* convex *if*

$$f(c\mathbf{x}_1 + (1-c)\mathbf{x}_2) \leq cf(\mathbf{x}_1) + (1-c)f(\mathbf{x}_2) \tag{E.7}$$

for all $\mathbf{x}_i \in \mathcal{D},\ i = 1, 2$ and all $c \in [0, 1]$, and f is strictly convex *if the previous inequality holds with $<$ instead of $\leq$, for all $\mathbf{x}_i \in \mathcal{D},\ i = 1, 2$ with $\mathbf{x}_1 \neq \mathbf{x}_2$ and all $c \in (0, 1)$.*

Proposition 22 *Let $\mathcal{D} \subset \mathbb{R}^p$ be a convex set and let $f : \mathcal{D} \to \mathbb{R}$ be twice continuously differentiable, then*

(a) If $\nabla^2 f(\mathbf{x})$ is positive semidefinite for all $\mathbf{x} \in \mathbb{R}^p$, then f is convex over $\mathcal{D}$.

(b) If $\nabla^2 f(\mathbf{x})$ is positive definite for every $\mathbf{x} \in \mathbb{R}^p$, then f is strictly convex over $\mathcal{D}$.

(c) If $\mathcal{D} = \mathbb{R}^p$ and f is convex, then $\nabla^2 f(\mathbf{x})$ is positive semidefinite for all $\mathbf{x} \in \mathcal{D}$.

(d) The quadratic function $f(\mathbf{x}) = \mathbf{x}^t\mathbf{M}\mathbf{x}$, where $\mathbf{M}$ is a symmetric $p \times p$ matrix, is convex if and only if $\mathbf{M}$ is positive semidefinite. Furthermore, f is strictly convex if and only if $\mathbf{M}$ is positive definite.

Proof. See appendix B.1 of Bertsekas (1999). □

Proposition 23

(a) For any collection $\{\mathcal{D}_i \mid i \in I\}$ of convex sets, the set intersection $\bigcap_{i \in I} \mathcal{D}_i$ is convex.

(b) The image of a convex set under a linear transformation is convex.

(c) If $\mathcal{D}$ is a convex set and $f : \mathcal{D} \to \mathbb{R}$ is a convex function, the level sets $\{\mathbf{x} \in \mathcal{D} \mid f(\mathbf{x}) \leq c\}$ and $\{\mathbf{x} \in \mathcal{D} \mid f(\mathbf{x}) < c\}$ are convex for all scalars c.

Proof. See appendix B.1 of Bertsekas (1999). □

E.2 Convexities and Optimization

Taking into account the fact that an unconstrained problem is a particular case of a constrained one, with $\mathcal{D} = \mathbb{R}^p$, the following statements concern both situations.

Definition 111 *An optimization problem is* convex *if f and $\mathcal{D}$ are convex.*

The importance of this definition is that, in a convex problem, the local minimum —when it exists— is the global minimum.

Proposition 24 *If f is a convex function and $\mathcal{D}$ is also convex, then a local minimum of f over $\mathcal{D}$ is a global minimum. If in addition f is strictly convex over $\mathcal{D}$, then at most one global minimum of f over $\mathcal{D}$ exists.*

Proof. See section 2.1 of Bertsekas (1999). □

Definition 112 *The point $\mathbf{x}_0 \in \mathcal{D} \subset \mathbb{R}^p$ is an* extreme *—or* frontier*— point if for any neighbourhood $N(\mathbf{x}_0)$ such that $\mathbf{x}_0 \in N(\mathbf{x}_0) \subset \mathcal{D}$ there are both a point belonging to $\mathcal{D}$ and a point not belonging to $\mathcal{D}$.*

Proposition 25 *Let f be convex, let $\mathcal{D}$ be closed convex bounded from below, then if f attains a maximum over $\mathcal{D}$, it attains a maximum at some extreme point of $\mathcal{D}$.*

Proof. See appendix B.4 of Bertsekas (1999). □

As in the unconstrained optimization, the first order variation $\nabla f(\mathbf{x}_0)^t \Delta\mathbf{x}$, due to a small feasible variation $\Delta\mathbf{x}$, is expected to be nonnegative at a local minimum $\mathbf{x}_0$. Due to the convexity of $\mathcal{D}$, the feasible variations are of the form $\Delta\mathbf{x} = \mathbf{x} - \mathbf{x}_0$, with $\mathbf{x} \in \mathcal{D}$.

Proposition 26 ***(First Order Necessary Condition)***

(a) If $\mathbf{x}_0$ is a local minimum of f over $\mathcal{D}$, then

$$\nabla f(\mathbf{x}_0)^t(\mathbf{x} - \mathbf{x}_0) \geq 0, \quad \forall \mathbf{x} \in \mathcal{D}. \tag{E.8}$$

(b) If f is convex over $\mathcal{D}$, then the condition of part (a) is also sufficient for $\mathbf{x}_0$ to minimize f over $\mathcal{D}$.

Proof. See section 2.1 of Bertsekas (1999). □

Remark 65 In the unconstrained situation, when f is convex the first order condition $\nabla f(\mathbf{x}_0) = 0$ (given in equation [E.18]) is also sufficient for optimality.

Proposition 27 ***(Second Order Necessary Condition)*** *If $\mathbf{x}_0$ is a local minimum of the twice continuously differentiable function $f : \mathbb{R}^p \to \mathbb{R}$ over the convex set $\mathcal{D}$, then*

$$(\mathbf{x} - \mathbf{x}_0)^t \nabla^2 f(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0) \geq 0 \tag{E.9}$$

for all $\mathbf{x} \in \mathcal{D}$ such that $\nabla f(\mathbf{x}_0)^t(\mathbf{x} - \mathbf{x}_0) = 0$.

Proof. See exercise 2.1.10 of Bertsekas (1999). □

With respect to sufficient conditions, the following result holds:

Proposition 28 ***(Second Order Sufficient Condition)*** *If $\mathbf{x}_0$ is a local minimum of the twice continuously differentiable function $f : \mathbb{R}^p \to \mathbb{R}$ over the convex set $\mathcal{D}$, then*

$$\nabla f(\mathbf{x}_0)^t(\mathbf{x} - \mathbf{x}_0) \geq 0 \qquad \forall \mathbf{x} \in \mathcal{D} \tag{E.10}$$

and one of the following three conditions holds:

1. *$\mathcal{D}$ is polyhedral and it follows that*

$$(\mathbf{x} - \mathbf{x}_0)^t \nabla^2 f(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0) > 0 \tag{E.11}$$

   for all $\mathbf{x} \in \mathcal{D}$ satisfying $\mathbf{x} \neq \mathbf{x}_0$ and $\nabla f(\mathbf{x}_0)^t(\mathbf{x} - \mathbf{x}_0) = 0$.

2. *It follows that $\bar{\mathbf{x}}^t \nabla^2 f(\mathbf{x}_0)\bar{\mathbf{x}} > 0$ for all nonzero $\bar{\mathbf{x}}$ that are in the closure of the set $\{d \mid d = \alpha(\mathbf{x} - \mathbf{x}_0),\ \mathbf{x} \in \mathcal{D},\ \alpha \geq 0\}$ and satisfy $\nabla f(\mathbf{x}_0)^t \bar{\mathbf{x}} = 0$.*

3. *For some $\gamma > 0$, we have*

$$(\mathbf{x} - \mathbf{x}_0)^t \nabla^2 f(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0) > \gamma \|\mathbf{x} - \mathbf{x}_0\|^2, \quad \mathbf{x} \in \mathcal{D}. \tag{E.12}$$

Proof. See exercise 2.1.11 of Bertsekas (1999). □

E.2.1 Consequences of the Convexities

It is worthwhile noting how, due to the monotony of a convex function and the topology of a convex domain, the optimization problem is simplified in two directions:

1. **Minimum**. A local minimum is also a global minimum: see proposition 24.
2. **Maximum**. There is an extreme (or frontier) point of the domain where the maximum —when it exists— is attained: see proposition 25.

E.3 Unconstrained Problem

The unconstrained situation is a particular case of the constrained situation with $\mathcal{D} = \mathbb{R}^p$. Nevertheless, this particular case is of great importance, as one of the approaches towards solving the constrained optimization problem consists in tackling an equivalent unconstrained problem. Minima are now defined as

Definition 113 *The point* $\mathbf{x}_0 \in \mathbb{R}^p$ *is said to be an* unconstrained relative —*or* local— minimum *if*

$$f(\mathbf{x}_0) \leq f(\mathbf{x}), \quad \forall \mathbf{x} \in D_\epsilon(\mathbf{x}_0), \tag{E.13}$$

where $D_\epsilon(\mathbf{x}_0) = \{\mathbf{x} \mid \|\mathbf{x}_0 - \mathbf{x}\| < \epsilon\}$, *for some* $\epsilon > 0$.

Definition 114 *The point* $\mathbf{x}_0 \in \mathbb{R}^p$ *is said to be a* unconstrained global minimum *if*

$$f(\mathbf{x}_0) \leq f(\mathbf{x}), \quad \forall \mathbf{x} \in \mathbb{R}^p. \tag{E.14}$$

E.3.1 Necessary Conditions

Small variations $\Delta\mathbf{x}$ from $\mathbf{x}_0$ yield, up to first order, a cost variation

$$f(\mathbf{x}_0 + \Delta\mathbf{x}) - f(\mathbf{x}_0) \approx \nabla f(\mathbf{x}_0)^t \Delta\mathbf{x} \tag{E.15}$$

and, up to second order,

$$f(\mathbf{x}_0 + \Delta\mathbf{x}) - f(\mathbf{x}_0) \approx \nabla f(\mathbf{x}_0)^t \Delta\mathbf{x} + \frac{1}{2}\Delta\mathbf{x}^t \nabla^2 f(\mathbf{x}_0) \Delta\mathbf{x}. \tag{E.16}$$

It is expected that if $\mathbf{x}_0$ is an unconstrained local minimum, the first order cost variation due to small variation $\Delta\mathbf{x}$ is nonnegative

$$\nabla f(\mathbf{x}_0)^t \Delta\mathbf{x} = \sum_{i=1}^{p} \frac{\partial f(\mathbf{x}_0)}{\partial x_i} \Delta x_i \geq 0, \tag{E.17}$$

and, in particular, by taking $\Delta\mathbf{x}$ to be positive and negative multiples of the unit coordinate vectors, we obtain $\frac{\partial f(\mathbf{x}_0)}{\partial x_i} \geq 0$ and $\frac{\partial f(\mathbf{x}_0)}{\partial x_i} \leq 0$, respectively, so the equivalent necessary condition

$$\nabla f(\mathbf{x}_0) = 0 \tag{E.18}$$

is obtained.

On the other hand, it is also expected that the second order cost variation due to small $\Delta\mathbf{x}$ must be nonnegative

$$\nabla f(\mathbf{x}_0)^t \Delta\mathbf{x} + \frac{1}{2}\Delta\mathbf{x}^t \nabla^2 f(\mathbf{x}_0)\Delta\mathbf{x} \geq 0,$$

that becomes (by applying equation [E.18])

$$\Delta\mathbf{x}^t \nabla^2 f(\mathbf{x}_0)\Delta\mathbf{x} \geq 0, \tag{E.19}$$

which implies that the matrix

$$\nabla^2 f(\mathbf{x}_0) \tag{E.20}$$

is positive semidefinite.

Proposition 29 *Let $\mathbf{x}_0$ be an unconstrained local minimum of $f : \mathbb{R}^p \to \mathbb{R}$ and assume that f is continuously differentiable in an open set $\mathcal{D}$ containing $\mathbf{x}_0$; then*

$$\nabla f(\mathbf{x}_0) = 0 \tag{E.21}$$

and if, in addition, f is twice continuously differentiable within $\mathcal{D}$, the

$$\nabla^2 f(\mathbf{x}_0) \quad \textit{is positive semidefinite.} \tag{E.22}$$

Proof. See section 1.1 of Bertsekas (1999). □

E.3.2 Sufficient Conditions

If $\mathbf{x}_0$ is such that

$$\nabla f(\mathbf{x}_0) = 0 \tag{E.23}$$

and

$$\nabla^2 f(\mathbf{x}_0) \quad \text{is positive definite} \tag{E.24}$$

then for all $\Delta\mathbf{x} \neq \mathbf{0}$ it holds that

$$\Delta\mathbf{x}^t \nabla^2 f(\mathbf{x}_0)\Delta\mathbf{x} > 0, \tag{E.25}$$

implying that at $\mathbf{x}_0$ the second order variation of f due to small nonzero variation $\Delta\mathbf{x}$ is positive. Thus, the function f tends to increase strictly with small departures from $\mathbf{x}_0$, suggesting that the conditions (E.23) and (E.24) are sufficient for local optimality.

Proposition 30 *Let $f : \mathbb{R}^p \to \mathbb{R}$ be twice continuously differentiable in an open set $\mathcal{D}$; suppose that $\mathbf{x}_0 \in \mathcal{D}$ satisfies the conditions*

$$\nabla f(\mathbf{x}_0) = 0 \tag{E.26}$$

and

$$\nabla^2 f(\mathbf{x}_0) \quad \textit{is positive definite (not only semidefinite)}; \tag{E.27}$$

then $\mathbf{x}_0$ *is a strict unconstrained local minimum of* f*. In particular, scalars* $\gamma > 0$ *and* $\epsilon > 0$ *exist such that*

$$f(\mathbf{x}) \geq f(\mathbf{x}_0) + \frac{\gamma}{2}\|\mathbf{x} - \mathbf{x}_0\|^2 \quad \forall \mathbf{x} \;\; \textit{such that} \;\; \|\mathbf{x} - \mathbf{x}_0\| < \epsilon. \tag{E.28}$$

Proof. See section 1.1 of Bertsekas (1999). □

E.4 Constrained Problem: Equality Constraints

Under some conditions, the *constrained* optimization problem (E.3) can be solved by way of an *unconstrained* optimization problem. Let be

$$\mathcal{D} = \{\mathbf{x} \in \mathbb{R}^p \mid \mathbf{h}(\mathbf{x}) = \mathbf{0}\}. \tag{E.29}$$

E.4.1 Necessary Conditions

Proposition 31 ***(Lagrange Multiplier Theorem)*** *Let* $\mathbf{x}_0$ *be the local minimum of* f *subject to* $\mathbf{h}(\mathbf{x}) = \mathbf{0}$*, and assume that the vectors* $\nabla h_i(\mathbf{x}_0),\ i = 1, \ldots, m_h$ *are linearly independent. Then there is a unique (column) vector* β_0*, called a* Lagrange multiplier vector*, such that*

$$\nabla f(\mathbf{x}_0) + \sum_{i=1}^{m_h} \beta_i \nabla h_i(\mathbf{x}_0) = 0. \tag{E.30}$$

If in addition f *and* $\mathbf{h}$ *are twice continuously differentiable, we have*

$$\mathbf{x}^t \left(\nabla^2 f(\mathbf{x}_0) + \sum_{i=1}^{m_h} \beta_i \nabla^2 h_i(\mathbf{x}_0) \right) \mathbf{x} \geq \mathbf{0} \tag{E.31}$$

for all $\mathbf{x} \in V(\mathbf{x}_0) = \{\mathbf{x} \mid \nabla h_i(\mathbf{x}_0)^t \mathbf{x} = 0,\ i = 1, \ldots, m_h\}$.

Proof. See section 3.1 of Bertsekas (1999). □

Both local minima and local maxima —and possible other points— may satisfy the first order necessary conditions. In this situation, the second order necessary conditions are used to find local minima.

E.4.2 The Lagrangian

It is useful to combine the objective function and the constraints in the following function.

Definition 115 *The* Lagrangian *of the optimization problem (E.3) with domain (E.29) is given by*

$$F(\mathbf{x}, \beta) = f(\mathbf{x}) + \beta^t \mathbf{h}(\mathbf{x}), \quad \mathbf{x} \in \mathcal{D}. \tag{E.32}$$

where $\beta = (\beta_1, \ldots, \beta_{m_h})^t$ *are the* multipliers.

Remark 66 It does not matter whether the second term is added as $+\beta^t \mathbf{h}(\mathbf{x})$ or $-\beta^t \mathbf{h}(\mathbf{x})$, since $\mathbf{h}(\mathbf{x}) = \mathbf{0}$ if and only if $-\mathbf{h}(\mathbf{x}) = \mathbf{0}$.

E.4.3 Sufficient Conditions

Proposition 32 ***(Second Order Conditions)*** *Let f and $\mathbf{h}$ be twice continuously differentiable, and let $\mathbf{x}_0 \in \mathbb{R}^p$ and $\beta_0 \in \mathbb{R}^{m_h}$ such that*

$$\nabla_{\mathbf{x}} F(\mathbf{x}_0, \beta_0) = \mathbf{0} \quad \text{and} \quad \nabla_{\beta} F(\mathbf{x}_0, \beta_0) = \mathbf{0} \tag{E.33}$$

and

$$\mathbf{x}^t \nabla^2_{\mathbf{xx}} F(\mathbf{x}_0, \beta_0) \mathbf{x} \geq \mathbf{0} \quad \text{for all} \quad \mathbf{x} \neq \mathbf{0} \quad \text{with} \quad \nabla \mathbf{h}(\mathbf{x}_0)^t \mathbf{x} = 0. \tag{E.34}$$

Then $\mathbf{x}_0$ is a strict local minimum of f subject to $\mathbf{h}(\mathbf{x}) = \mathbf{0}$. In fact, scalars $\gamma > 0$ and $\epsilon > 0$ exist such that

$$f(\mathbf{x}) \geq f(\mathbf{x}_0) + \frac{\gamma}{2} \|\mathbf{x} - \mathbf{x}_0\|^2 \quad \forall \mathbf{x} \quad \text{such that} \quad \mathbf{h}(\mathbf{x}) = \mathbf{0} \quad \text{and} \quad \|\mathbf{x} - \mathbf{x}_0\| < \epsilon.$$

Proof. See section 3.2 of Bertsekas (1999). □

E.4.4 Equivalent Unconstrained Problem

In short, the constrained optimization problem can be studied via the following unconstrained optimization problem

$$\mathbf{x} = argmin \left\{ F(\mathbf{x}, \beta) \right\}. \tag{E.35}$$

E.5 Constrained Problem: Inequality Constraints

Let the feasible domain be given by

$$\mathcal{D} = \left\{ \mathbf{x} \in \mathbb{R}^p \mid \mathbf{h}(\mathbf{x}) = \mathbf{0} \text{ and } \mathbf{g}(\mathbf{x}) \leq \mathbf{0} \right\}. \tag{E.36}$$

E.5.1 The Lagrangian

In this situation, the Lagrangian takes the form

Definition 116 *The* Lagrangian *of the optimization problem (E.3) with domain (E.36) is given by*

$$F(\mathbf{x}, \beta, \mu) = f(\mathbf{x}) + \beta^t \mathbf{h}(\mathbf{x}) + \mu^t \mathbf{g}(\mathbf{x}), \quad \mathbf{x} \in \mathcal{D}. \tag{E.37}$$

where $\beta = (\beta_1, \ldots, \beta_{m_g})^t$ and $\mu = (\mu_1, \ldots, \mu_{m_h})^t$ are the multipliers.

Remark 67 The sign of the added terms is usually taken as positive; for example, the last term is usually taken as $+\mu^t \mathbf{g}(\mathbf{x})$, instead of $-\mu^t \mathbf{g}(\mathbf{x})$; nevertheless, we have used the latter form in chapter three due to the particular function $\mathbf{g}(\mathbf{x}) = -\mathbf{x}$.

There are several ways of dealing with the inequality constraints problem; one of them is based on the previous equality constraints framework (see section 3.3.2 of Bertsekas [1999]). The following approach is not the most general, since some regularity conditions are needed, but it is the most direct generalization of the previous theory (notice that the generalised Rayleigh quotient $\lambda(\mathbf{a})$ fulfils the regularity conditions).

E.5.2 Necessary Conditions

The following proposition generalises the Lagrange multiplier theorem (proposition 31).

Proposition 33 ***(Karush-Kuhn-Tucker Conditions)*** *Let $\mathbf{x}_0$ be the local minimum of f subject to $\mathbf{h}(\mathbf{x}) = \mathbf{0}$ and $\mathbf{g}(\mathbf{x}) \leq \mathbf{0}$, where f, $\mathbf{h}$ and $\mathbf{g}$ are continuously differentiable functions, and assume that $\nabla h_i(\mathbf{x}_0),\ i = 1, \ldots, m_h$ and $\nabla g_i(\mathbf{x}_0),\ i = 1, \ldots, m_g$ are linearly independent; then unique Lagrange multiplier vectors β_0 and μ_0 exist such that*

$$\nabla_{\mathbf{x}} F(\mathbf{x}_0, \beta_0, \mu_0) = 0 \tag{E.38}$$

$$\mu \geq \mathbf{0} \quad \text{with} \quad \mu_i = 0 \ \text{ when } \ g_i(\mathbf{x}_0) < 0. \tag{E.39}$$

If in addition f, $\mathbf{h}$ and $\mathbf{g}$ are twice continuously differentiable, there holds

$$\mathbf{x}^t \nabla^2_{\mathbf{xx}} F(\mathbf{x}_0, \beta_0, \mu_0)\mathbf{x} \geq \mathbf{0} \tag{E.40}$$

for all $\mathbf{x}$ such that $\nabla h_i(\mathbf{x}_0)^t \mathbf{x} = 0,\ i = 1, \ldots, m_h$, and $\nabla g_i(\mathbf{x}_0)^t \mathbf{x} = 0$ when $g_i(\mathbf{x}_0) = 0$.

Proof. See section 3.3 of Bertsekas (1999). □

E.5.3 Searching Strategy

As Bertsekas (1999) states: *One approach for using necessary conditions to solve inequality constrained problems is to consider separately all the possible combinations of constraints being active or inactive* (an inequality constraint $g_i(\mathbf{x}) \leq 0$ is active at point $\mathbf{x}$ if the equality holds, and inactive otherwise).

E.5.4 Sufficient Conditions

Proposition 34 ***(Second Order Conditions)*** *Let f, $\mathbf{h}$ and $\mathbf{g}$ be twice continuously differentiable, and let $\mathbf{x}_0 \in \mathbb{R}^p$, $\beta_0 \in \mathbb{R}^{m_h}$ and $\mu_0 \in \mathbb{R}^{m_g}$ such that*

$$\nabla_{\mathbf{x}} F(\mathbf{x}_0, \beta_0, \mu_0) = \mathbf{0}, \qquad \mathbf{h}(\mathbf{x}_0) = \mathbf{0}, \qquad \mathbf{g}(\mathbf{x}_0) \leq \mathbf{0} \tag{E.41}$$

$$\mu \geq \mathbf{0} \quad \text{with} \quad \mu_i = 0 \ \text{ when } \ g_i(\mathbf{x}_0) < 0. \tag{E.42}$$

$$\mathbf{x}^t \nabla^2_{\mathbf{xx}} F(\mathbf{x}_0, \beta_0, \mu_0)\mathbf{x} > \mathbf{0} \tag{E.43}$$

for all $\mathbf{x}$ *such that* $\nabla h_i(\mathbf{x}_0)^t\mathbf{x} = 0,\ i = 1, \ldots, m_h$, *and* $\nabla g_i(\mathbf{x}_0)^t\mathbf{x} = 0$ *when* $g_i(\mathbf{x}_0) = 0$. *Assume also that*

$$\mu_i > 0 \quad when \quad g_i(\mathbf{x}_0) = 0. \tag{E.44}$$

Then $\mathbf{x}_0$ *is a strict local minimum of* f *subject to* $\mathbf{h}(\mathbf{x}) = \mathbf{0}$ *and* $\mathbf{g}(\mathbf{x}) \leq 0$.

Proof. See section 3.3 of Bertsekas (1999). □

This result is based on the transformation of the problem to one with equality constraints, but there are stricter versions of sufficient conditions.

Remark 68 Again from Bertsekas (1999): *The sufficient conditions that we have discussed so far* [previous proposition] *involve second derivatives and Hessian positive definiteness assumptions. Our experience with unconstrained problems suggests that the first order Lagrange multiplier conditions together with convexity assumptions should also be sufficient for optimality. Indeed this is so, as we will demonstrate shortly. In fact we will not need to impose convexity or even differentiability assumptions explicitly. A minimization condition on the Lagrangian function turns out to be sufficient.*

Proposition 35 ***(General Conditions)*** *Let the problem be*

$$\mathbf{x} = argmin\,\{f(\mathbf{x})\} \quad subject\ to \quad \mathbf{x} \in \mathcal{S} \quad and \quad \mathbf{g}(\mathbf{x}) \leq \mathbf{0}, \tag{E.45}$$

where f *and* $\mathbf{g}$ *are real valued functions on* $\mathbb{R}^p$ *and* $\mathcal{S}$ *is a given subset of* $\mathbb{R}^p$. *Let* $\mathbf{x}_0$ *be a feasible point which together with* $\mu_0 \in \mathbb{R}^{m_g}$ *satisfies*

$$\mu \geq \mathbf{0} \quad with \quad \mu_i = 0 \quad when \quad g_i(\mathbf{x}_0) < 0 \tag{E.46}$$

and minimizes the Lagrangian function $F(\mathbf{x}, \mu_0)$ *over* $\mathbf{x} \in (S)$, *that is:*

$$\mathbf{x}_0 = argmin\{F(\mathbf{x}, \mu_0)\}; \tag{E.47}$$

then $\mathbf{x}_0$ *is a global minimum of the problem.*

Proof. See section 3.3 of Bertsekas (1999). □

Remark 69 Note that the function f of this proposition can be a Lagrangian that implicitly takes equality constraints into account.

E.5.5 Equivalent Unconstrained Problem

In short, the constrained —in $\mathbf{x}$— optimization problem can be studied through the following unconstrained —in $\mathbf{x}$— optimization problem

$$\mathbf{x} = argmin\,\{F(\mathbf{x}, \beta, \mu)\} \quad \text{subject to} \quad \mu \geq \mathbf{0} \ \text{ with } \ \mu_i = 0 \ \text{ when } \ g_i(\mathbf{x}) < 0. \tag{E.48}$$

E.5.6 Karush-Kuhn-Tucker Conditions

From the previous propositions, it is clear that the following definition is quite useful for referring to the necessary and sufficient conditions.

Definition 117 *The Karush-Kuhn-Tucker conditions (of first order) are given by*

$$\begin{cases} \nabla_{\mathbf{x}} F = \mathbf{0} \\ \nabla_{\beta} F = \mathbf{0} \\ \mathbf{g}(\mathbf{x}) \leq \mathbf{0},\ \mu \geq \mathbf{0} \quad \textit{and} \quad \mu^t \mathbf{g}(\mathbf{x}) = \mathbf{0} \end{cases} \tag{E.49}$$

or, in the usual differentiation notation, by

$$\begin{cases} \frac{\partial F}{\partial \mathbf{x}} = \mathbf{0} \\ \frac{\partial F}{\partial \beta} = \mathbf{0} \\ \mathbf{g}(\mathbf{x}) \leq \mathbf{0},\ \mu \geq \mathbf{0} \quad \textit{and} \quad \mu^t \mathbf{g}(\mathbf{x}) = \mathbf{0} \end{cases} . \tag{E.50}$$

Note that the two first are related to minimizing the Lagrangian.

E.5.7 Nonnegativity Constraints

For the particular case $\mathbf{g}(\mathbf{x}) = -\mathbf{x}$, that is, when the inequality constraints are $\mathbf{x} \geq \mathbf{0}$, the conditions are given by

$$\begin{cases} \frac{\partial F}{\partial \mathbf{x}} = \mathbf{0} \\ \frac{\partial F}{\partial \beta} = \mathbf{0} \\ x_i \geq 0,\ \mu_i \geq 0 \ \text{ and } \ \mu_i x_i = 0. \end{cases} \tag{E.51}$$

E.6 Some Particular Problems

In this section, some frequent problems similar to those of our framework are included.

E.6.1 Fractional Programming

Of special interest for our optimization problem is the following situation:

Proposition 36

$$\mathbf{x} = argmin \left\{ \frac{f(\mathbf{x})}{g(\mathbf{x})} \right\} \qquad \textit{subject to} \qquad \mathbf{x} \in \mathcal{D}, \tag{E.52}$$

where f and g are real functions on $\mathbb{R}^p$ and $\mathcal{D}$ is a given subset such that $g(\mathbf{x}) > 0$ for all $\mathbf{x} \in \mathcal{D}$. For $\beta \in \mathbb{R}$, it can be defined

$$Q(\beta) = min_{\mathbf{x} \in \mathcal{D}} \left\{ f(\mathbf{x}) - \beta g(\mathbf{x}) \right\}. \tag{E.53}$$

Suppose that a scalar β_0 and a vector $\mathbf{x}_0$ satisfy $Q(\beta_0) = 0$ and

$$\mathbf{x}_0 = argmin_{\mathbf{x} \in \mathcal{D}} \left\{ f(\mathbf{x}) - \beta_0 g(\mathbf{x}) \right\}, \tag{E.54}$$

respectively; then $\mathbf{x}_0$ is an optimal solution to the original problem.

Proof. See exercise 2.1.17 of Bertsekas (1999). □

Remark 70 Using this fact, it is possible to reduce the problem to an equivalent problem without quotient of functions.

E.6.2 Linear and Quadratic Problems

Also of special interest is:

Proposition 37 ***(Existence of Solutions)*** *Let* $\mathbf{Q}$ *be a positive semidefinite symmetric* $p \times p$ *matrix; let* $\mathbf{c}$ *and* $\mathbf{a}_1, \ldots, \mathbf{a}_m$ *be vectors in* $\mathbb{R}^p$*; and let* $b_1, \ldots, b_m$ *be scalars. Assume that the optimal value of the problem*

$$\mathbf{x} = argmin \left\{ \mathbf{x}^t \mathbf{Q} \mathbf{x} + \mathbf{c}^t \mathbf{x} \right\} \quad subject\ to \quad \mathbf{a}_j^t \mathbf{x} + b_j \leq 0,\ j = 1, \ldots, m, \tag{E.55}$$

is finite. Then the problem has at least one optimal solution.

Proof. See section 2.1 of Bertsekas (1999). □

E.6.3 Nonconvex Quadratic Problems

Finally:

Proposition 38 ***(Existence of Solution)*** *Let* $\mathbf{Q}$ *be a symmetric —not necessarily positive semidefinite— $p \times p$ matrix, let* $\mathbf{c} \in \mathbb{R}^p$ *and a set* $\mathcal{D} \subset \mathbb{R}^p$*. Assume that the optimal value of the problem*

$$\mathbf{x} = argmin \left\{ \mathbf{x}^t \mathbf{Q} \mathbf{x} + \mathbf{c}^t \mathbf{x} \right\} \quad subject\ to \quad \mathbf{x} \in \mathcal{D} \tag{E.56}$$

is finite; then an optimal solution in each of the following two cases exists:

1. *$\mathcal{D}$ is specified by linear inequalities as in proposition 37.*
2. *$\mathcal{D}$ is the vector sum of a compact set and a closed cone.*

Proof. See exercise 2.1.19 of Bertsekas (1999). □

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