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Présentée par
Cao Tri DO

Thèse dirigée par **Ahlame DOUZAL-CHOUAKRIA**,
codirigée par **Michèle ROMBAUT** et
co-encadré par **Sylvain MARIÉ**

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Metric Learning for Time Series Analysis

Thèse soutenue publiquement le **date de soutenance**,
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Prénom NOM
Labo de bidule, Rapporteur, Présidente du jury
Prénom NOM
Labo de bidule, Rapporteur
Prénom NOM
Labo de bidule, Examinateur
Prénom NOM
Labo de bidule, Examinateur
Ahlame DOUZAL-CHOUAKRIA
LIG, Directeur de thèse
Michèle ROMBAUT
GIPSA-Lab, Co-Directeur de thèse

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Thèse dirigée par Ahlame DOUZAL-CHOUAKRIA

préparée au Laboratoire d'Informatique de Grenoble (LIG)

soutenue le date de soutenance

Jury :

Rapporteurs :	Prénom NOM	-	Labo de bidule
	Prénom NOM	-	Labo de bidule
Directeur :	Ahlame DOUZAL-CHOUAKRIA	-	LIG
Co-Directeur :	Michèle ROMBAUT	-	GIPSA-Lab
Encadrant :	Sylvain MARIÉ	-	Schneider Electric
Président :	Prénom NOM	-	Labo de bidule
Examinateur :	Prénom NOM	-	Labo de bidule
	Prénom NOM	-	Labo de bidule

Todo list

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Comment [MR3]: ref application time series (Michèle) 8

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[biblio regression kNN] 17

[biblio kNN pondéré] 17

[biblio fuzzy kNN] 17

Comment [MR5]: + k-NN crédibiliste 17

Comment [CTD6]: réécrire + compléter avec Claude 26

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Prendre le GRAPHIQUE GENERAL et faire le calcul des distances entre les courbes et montrer que pour 2 courbes qui ont des "formes proches", on obtient une valeur de distance faible. 36

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- my parents

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Table of Acronyms

LIG	*Laboratoire d'Informatique de Grenoble*
AMA	*Apprentissage, Méthode et Algorithme*
GIPSA-Lab	*Grenoble Images Parole Signal Automatique Laboratoire*
AGPiG	*Architecture, Géométrie, Perception, Images, Gestes*
A4S	*Analytic for Solutions*
k-**NN**	*k-nearest neighbors*
SVM	*Support Vector Machines*
SVR	*Support Vector Regression*
d_E	*Euclidean distance*
corr	*Pearson correlation*
cort	*Temporal correlation*
dtw	*Dynamic Time Warping*
IoT	*Internet of Things*
Acc	*Classification accuracy*
Err	*Classification error rate*
MAE	*Mean Absolute Error*
RMSE	*Root Mean Square Error*
FAQ	Frequently Asked Questions / Foire Aux Questions

Introduction

Motivation

- Qu'est-ce qu'une série temporelle ? (réponse d'un système dynamique complexe (= pas de modèle du système)
- Motiver l'intérêt des séries temporelles dans les applications aujourd'hui: données de plus en plus présentes dans de nombreux domaines divers et variés
- Les séries temporelles sont impliquées dans des problèmes de classification, régression et clustering
- Pourquoi sont-elles challenging ? (délais, dynamique)
- On fait face à la fois, à un problème de small et big data

Problem statement (with words)

- Dans de nombreux algorithmes de classification ou de régression (kNN, SVM), la comparaison des individus (séries temporelles) reposent sur une notion de distance entre individus (séries temporelles).
- Contrairement aux données statiques, les données temporelles peuvent être comparés sur la base de plusieurs modalités (valeurs, forme, distance entre spectre, etc.) et à différentes échelles. La « métrique idéale », càd, celle qui permettra de résoudre au mieux le problème de classification/régression peut donc impliquer plusieurs modalités.
- Objectif de notre travail : Apprendre une métrique adéquate tenant compte de plusieurs modalités et de plusieurs échelles en vue d'une classification/régression kNN

PhD contributions

- Définition d'un nouvel espace de représentation: la représentation par paires
- Apprentissage d'une métrique multimodale et multi-échelle en vue d'une classification kNN à vaste marge de séries temporelles monovariées.
- Extension/Transposition du problème d'apprentissage de métrique (Metric Learning) dans l'espace des paires

- Comparaison de la méthode proposée avec des métriques classiques sur un vaste jeu de données (30 bases) de la littérature dans le cadre de la classification univariée de séries temporelles
- Extension du framework d'apprentissage de métrique au problème de régression de séries temporelles univariés
- Extension du framework d'apprentissage de métrique au problème de classification/régression de séries temporelles multivariés.
- Donner une solution interprétable.
- Donner un algorithme à la fois pour les small et big data.

Organisation du manuscrit

Présenter les différents chapitres

Note pour Ahlame, Michèle et Sylvain: Pour ajouter des commentaires dans le fichier .TEX, merci de les ajouter sous cette forme:

- dans le texte :
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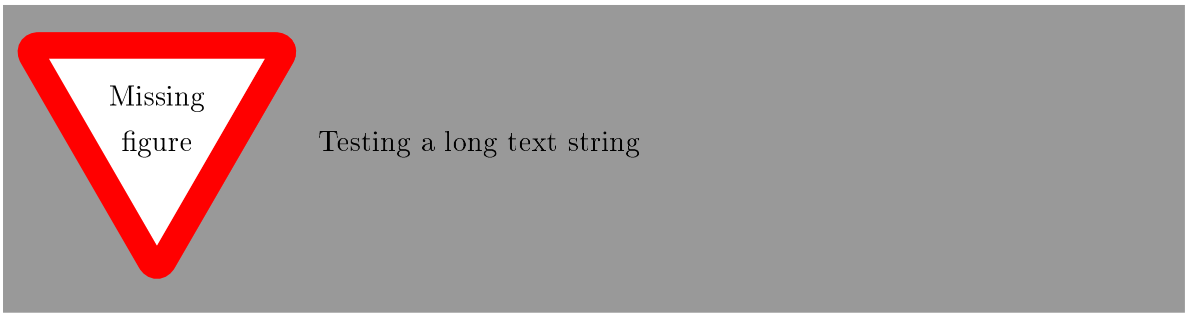
- dans la marge :

Comment [CTD2]: Initial in [CAO] then your comment in the bracket

If you think that they are missing figures, you can add them with a description with this command line :



Notations

$\mathbf{x}_i$	a time series
y_i	a label (discrete or continous)
$\mathbf{X} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$	a set of $n \in \mathbb{N}$ labeled time series
d_E	Euclidean distance
L_q	Minkovski q-norm
$\|\|\mathbf{x}\|\|_q$	q-norm of the vector $\mathbf{x}$
d_A	Value-based distance
$corr$	Pearson correlation
$cort$	Temporal correlation
d_F	Euclidean distance between the Fourier spectrum
D	Distance
$\mathbf{x}_{ij}$	a pair of time series $\mathbf{x}_i$ and $\mathbf{x}_j$
y_{ij}	the pairwise label of $\mathbf{x}_{ij}$
t	time stamp/index with $t = 1, ..., T$
T	length of the time series (supposed fixed)
f	frequential index
F	length of the Fourier transform
ξ	Relaxation term
p	number of metric measure considered in the metric learning process
r	order of the temporal correlation
k	number of nearest neighbors
$K(\mathbf{x}_i, \mathbf{x}_j)$	Kernel function between $\mathbf{x}_i$ and $\mathbf{x}_j$
$\phi(\mathbf{x}_i)$	embedding function from the original space to the Hilbert space
C	Hyper-parameter of the SVM (trade-off)
α	
λ	

Part I

Work positioning

The first part of the manuscript aims to position the work context. Our objective is the comparison and the classification or regression of time series. The first chapter considers time series as static vector data and presents classic machine learning algorithms used to classify them. We note that most of these methods relies on the comparison of objects (time series in our case) through a distance measure. In the second chapter, to cope with the characteristics of time series (amplitude, behavior, frequential spectrum, etc.), we recall some basic metrics used to compare time series. We show that time series may be compared by several modalities and at different granularities. We finally cast that learning an adequate distance based on several modalities and several granularities is a key challenge nowadays to well classify time series using classic Machine Learning algorithms.

Chapter 1

Machine Learning: state of the art

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In this chapter, we first present what a time series is. Then, we vectorize time series, consider them as static data and apply classic Machine Learning algorithms used for classification and regression. We review the protocol used in supervised learning to learn the best fitting of the hyper-parameters and how we evaluate and compare different algorithms performances. Finally, we give some more detailed insights on k-Nearest Neighbors (k-NN) and Support Vector Machine (SVM).

1.1 Definition of a time series

Time series and more generally temporal data are data objects that frequently occur in physical sciences (meteorology, marine science, geophysics), marketing or process control [Cha04]. For physical systems, a time series of length N can be seen as a signal, sampled at a frequency f_e, in a temporal window $[0; \frac{N}{f_e}]$. From a mathematical perspective, a time series is a collection of a finite number of realized normalized observations made sequentially at discrete time instants $t = 1, ..., T$. Note that when $f_e = 1$, $T = N$.

Let $\mathbf{x}_i = (x_{i1}, x_{i2}, ..., x_{iT})$ be a univariate time series of length T. Each observation x_{it} is bounded (i.e., the infinity is not a valid value: $x_{it} \neq \pm\infty$). The time series $\mathbf{x}_i$ is said to be univariate if the collection of observations x_{it} comes from the observations of one variable (i.e., it has been measured by one sensor, the temperature for example). When the observations are made at the same time from Q variables (several sensors such as the temperature, the pressure, etc.), the time series is said multivariate and is denoted $\mathbf{x}_i = (\mathbf{x}_{i,1}, ..., \mathbf{x}_{i,Q}) = (x_{i1,1}, ..., x_{iT,1}, x_{i1,2}, ..., x_{iT,2}, ..., x_{i1,Q}, ..., x_{iT,Q})$. For simplification purpose, we consider in the following univariate time series.

Comment [MR3]: ref application time series (Michèle)

Time series can be found in various emerging applications such as sensor networks, smart buildings, social media networks or Internet of Things (IoT) [Naj+12]; [Ngu+12]; [YG08]. They are involved in many learning problems such as recognizing a human movement in a video, detect a particular operating mode, etc. . In **clustering** problems, one would like to organize similar time series together into homogeneous groups. In **classification** problems, the aim is to assign time series to one of several predefined categories (e.g., different types of defaults in a machine). In **regression** problems, the objective is to predict a continuous value from observed time series (e.g., forecasting the measurement of a power meter from pressure and temperature sensors). Our work focus on classification and regression problems. However, due to their temporal and structured nature, time series constitute complex data to be analyzed by classic Machine Learning approaches.

To overcome this complexity, some authors propose to extract representative features from time series. Fig. 1.1 illustrates a model for time series proposed by Chatfield in [Cha04]. It states that a time series can be decomposed into 3 components: a trend, a cycle (periodic component) and a residual (irregular variations).

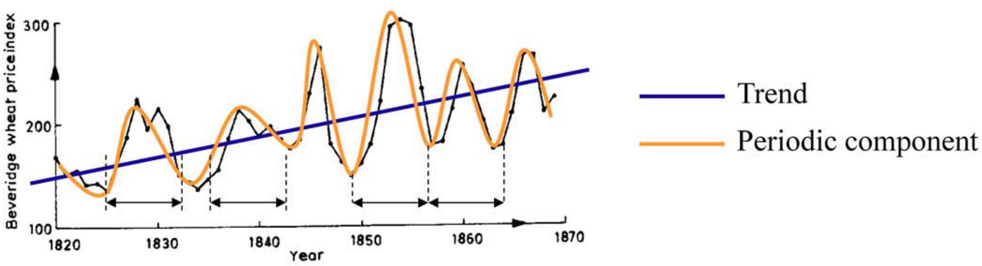

Figure 1.1: The Beveridge wheat price index is the average in nearly 50 places in various countries measured in successive years from 1500 to 1869. [1]

According to Chatfield, most time series exhibit a variation at a fixed period of time (seasonality) such as for example the seasonal variation of temperature. Beyond this cycle, there exists either or both a long term change in the mean (trend) that can be linear, quadratic, and a periodic (cyclic) component. In practice, these 3 features are rarely sufficient for the classification or regression of real time series. In our work, we propose to focus on the raw time series and do not try to extract global features from the time series.

Due to their complexity, other authors made the hypothesis of time independency between the observations x_{it}. They consider time series as a static vector data (samples) and use classic

[1] This time series can be downloaded from `http://www.york.ac.uk/depts/maths/data/ts/ts04.dat`

Machine Learning algorithms [Lia+12]; [CT01]; [HWZ13]; [HHK12].

1.2 Machine Learning framework

In this section, we review some basic terminology in Machine Learning. First, we recall the principle of statistical learning. Then, we detail how to design a framework in the case of supervised learning. After that, we recall how model evaluation is performed. Finally, we take an insight on data pre-processing.

1.2.1 Classification, regression

The idea of Machine Learning (also refer as Pattern Learning or Pattern Recognition) is to imitate with algorithms executed on computers, the ability of living beings to learn from examples. For instance, to teach a child how to read letters, we show him during the training phase labeled examples of letters ('A', 'B', 'C', etc.) written in different styles and fonts. We don't give him a complete and analytic description of the topology of the characters but labeled examples. After the training phase (testing phase), we want the child to be able to recognize and to label correctly the letters that have been seen during the training, and also to generalize to new instances [G. 06].

Let $\mathbf{X} = \{\mathbf{x}_i, y_i\}_{i=1}^{n}$ be a training set of n samples $\mathbf{x}_i$ (time series in our case) and y_i their corresponding labels. The aim of Machine Learning is to learn a relation (model) f between the samples $\mathbf{x}_i$ and their labels y_i based on examples. This relationship can include static relationships, correlations, dynamic relationship, etc. After the training phase based on labeled examples $(\mathbf{x}_i, y_i)$, the model f has to be able to generalize on the testing phase, i.e., to give a correct prediction y_j for new instances $\mathbf{x}_j$ that haven't been seen during the training.

When y_i are class labels (e.g., class 'A', 'B', 'C' in the case of child's reading), learning the model f is a classification problem; when y_i is a continuous value (e.g., the energy consumption in a building), learning f is a regression problem. Both problems corresponds to supervised learning as $\mathbf{x}_i$ and y_i are known during the training phase [Bis06]; [G. 06]; [OE73]. For both problems, when a part of the labels y_i are known and an other part of y_i is unknown during training, learning f is a semi-supervised problem . Note that when the labels y_i are unknown, learning f refers to a clustering problem (unsupervised learning) [JMF99]; [CHY96], not managed in our work.

[biblio semi-supervisé]

1.2.2 Supervised learning framework

A key objective of learning algorithms is to build models f with good generalization abilities, i.e., models f that correctly predict the class labels y_j of new unknown samples $\mathbf{x}_j$. Fig. 1.3 shows a general approach for solving Machine Learning problems. In general, a dataset can be divided into 3 sub-datasets (illustrated in Fig. 1.2):

- A **training set** $X = \{(\mathbf{x}_i, y_i)\}_{i=1}^{n}$ consisting of n samples $\mathbf{x}_i$ whose labels y_i are known. The training set is used to build the supervised model f.

- A **test set** $X_T = \{(\mathbf{x}_j, y_j)\}_{j=1}^{m}$, which consists of m samples $\mathbf{x}_j$ which labels y_j are also known but the model f is applied to predict the label $\hat{y}_j$ of samples $\mathbf{x}_j$. The test is used to evaluate the performance of the learnt model between $\hat{y}_j$ and y_j.

- An **evaluation set** $X_E = \{(\mathbf{x}_l, y_l)\}_{l=1}^{L}$, which consists of L samples $\mathbf{x}_l$ with labels y_l are unknown. The evaluation set is in general a new dataset on which we would like to apply the learnt algorithm.

id	Attribute 1	Attribute 2	Attribute 3	True Class
1	Yes	Large	125	No
2	No	Medium	135	Yes
3	No	Small	256	No
4	Yes	Medium	320	No
5	Yes	Small	128	Yes
6	No	Large	852	Yes
7	No	Medium	963	Yes

Learning Set (ids 1–4)

Validation Set (ids 5–7)

Training Set

id	Attribute 1	Attribute 2	Attribute 3	True Class	Predicted Class
8	No	Large	566	No	?
9	No	Medium	456	Yes	?
10	Yes	Medium	321	No	?
11	No	Small	243	No	?
12	Yes	Small	863	Yes	?
13	No	Large	213	Yes	?
14	Yes	Large	132	Yes	?

Test Set

id	Attribute 1	Attribute 2	Attribute 3	True Class	Predicted Class
15	Yes	Large	874	?	?
16	No	Medium	541	?	?
17	No	Medium	236	?	?
18	No	Large	652	?	?
19	Yes	Small	324	?	?
20	Yes	Small	214	?	?
21	Yes	Medium	222	?	?

Evaluation Set

Figure 1.2: Division of a dataset into 3 datasets: training, test and evaluation.

The errors committed by a classification or regression model are divided into two types: training errors and generalization errors (testing errors). **Training error** is the number of misclassification errors in classification (Root Mean Square Error or other error measures used in regression) committed on training samples $\mathbf{x}_i$, whereas **generalization error** is the expected error of the model f on unseen samples $\mathbf{x}_j$. A good supervised model f must not only fit the training data X well, it must also accurately classify records it has never seen before (test set X_T). In other words, a good model f must have low training error as well as low generalization error. This is important because a model that fits the training data too

Training Set

id	Attribute 1	Attribute 2	Attribute 3	True Class
1	Yes	Large	125	No
2	No	Medium	135	Yes
3	No	Small	256	No
4	Yes	Medium	320	No
5	Yes	Small	128	Yes
6	No	Large	852	Yes
7	No	Medium	963	Yes

Test Set

id	Attribute 1	Attribute 2	Attribute 3	True Class	Predicted Class
8	No	Large	566	No	?
9	No	Medium	456	Yes	?
10	Yes	Medium	321	No	?
11	No	Small	243	No	?
12	Yes	Small	863	Yes	?
13	No	Large	213	Yes	?
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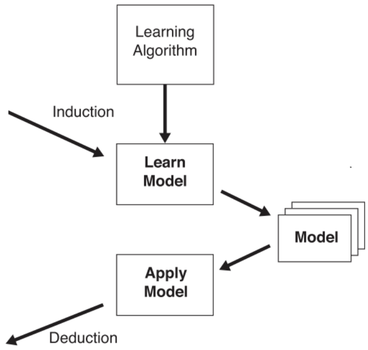

Figure 1.3: General framework for building a supervised (classification/regression) model. Example with 3 features and 2 classes ('Yes' and 'No').

well can have a poorer generalization error than a model with a higher training error. Such a situation is known as model overfitting (Fig. 1.4).

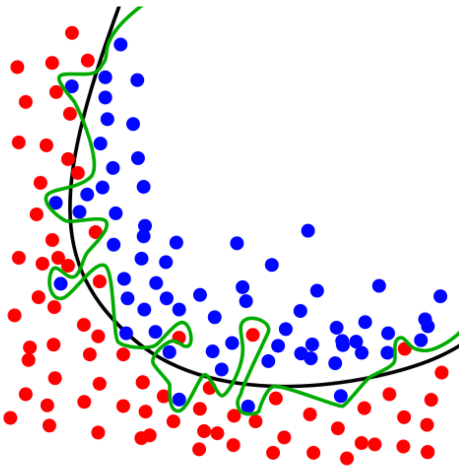

Figure 1.4: An example of overfitting in the case of classification. The objective is to separate blue points from red points. Black line shows a classifier f_1 with low complexity where as green line illustrates a classifier f_2 with high complexity. On training examples (blue and red points), the model f_2 separates all the classes perfectly but may lead to poor generalization on new unseen examples. Model f_1 is often preferred.

In most cases, learning algorithms requires to tune some hyper-parameters. For that, the training set can be divided into 2 sets: a learning and a validation set. Suppose we have two hyper-parameters to tune: C and γ. We make a grid search for each combination (C, γ) of the hyper-parameters, that is in this case a 2-dimensional grid (Fig. 1.5). For each combination (a cell of the grid), the model is learnt on the learning set and evaluated on the validation set.

At the end, the model with the lowest error on the validation set is retained. This process is refered as the model selection.

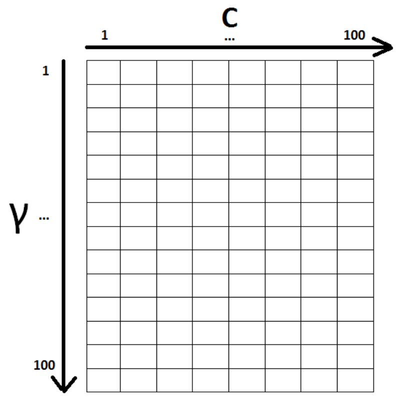

Figure 1.5: Example of a 2 dimensional grid search for parameters C and γ. It defines a grid where each cell of the grid contains a combination (C, γ). Each combination is used to learn the model and is evaluated on the validation set.

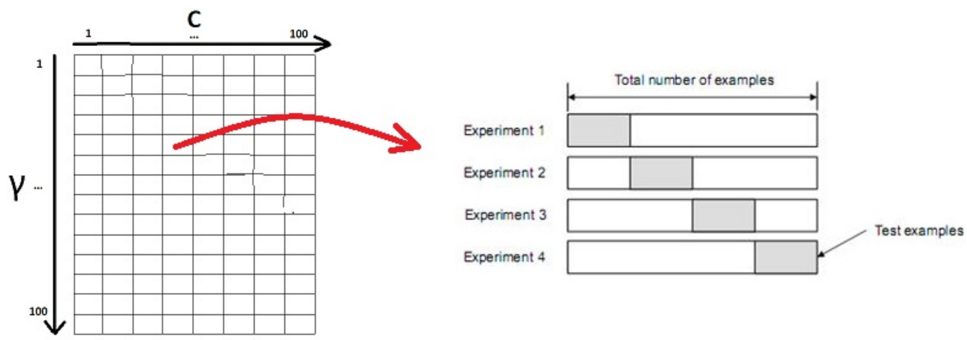

Figure 1.6: v-fold Cross-validation for one combination of parameters. For each of v experiments, use $v-1$ folds for training and a different fold for Testing, then the training error for this combination of parameter is the mean of all testing errors. This procedure is illustrated for $v = 4$.

An alternative is cross-validation with v folds, illustrated in Fig. 1.6. In this approach, we partition the training data into v equal-sized subsets. The objective is to evaluate the error for each combination of hyper-parameters. For each run, one fold is chosen for validation, while the $v-1$ rest folds are used as the learning set. We repeat the process for each fold, thus v times. Each fold gives one validation error and thus we obtain v errors. The total error for the current combination of hyper-parameters is obtained by summing up the errors for all v folds. When $v = n$, the size of training set, this approach is called leave-one-out or Jackknife. Each test set contains only one sample. The advantage is much data are used as possible for training. Moreover, the test sets are exclusive and they cover the entire data set. The drawback is that it is computationally expensive to repeat the procedure n times. Furthermore, since each test set contains only one record, the variance of the estimated performance metric is usually high. This procedure is often used when n, the size training set, is small.

There exists other methods such as sub-sampling or bootstraps [OE73]; [G. 06]. We only use cross-validation in our experiments.

1.2.3 Model evaluation

1.2.3.a Classification

The performance of a classification model is based on the counts of test samples $\mathbf{x}_j$ correctly and incorrectly predicted by the model f. These counts are tabulated in a table called the confusion matrix. Table 1.7 illustrates the concept for a binary classification problem. Each cell f_{ij} the table stands for the number of samples from class i predicted to be of class j. Based on this matrix, the number of correct predictions made by the model is $\sum_{i=1}^{C} f_{ii}$, where C is the number of classes. Equivalently, the number of of incorrect prediction is $1 - \sum_{i=1}^{C} f_{ii}$.

Refaire le tableau

		Predicted Class	
		$Class = 1$	$Class = 0$
Actual	$Class = 1$	f_{11}	f_{10}
Class	$Class = 0$	f_{01}	f_{00}

Figure 1.7: Confusion matrix for a 2-class problem.

To summarize the information, it generally more convenient to use performance metrics such as the classification accuracy (Acc) or error rate (Err). This allows to compare several models with a single number. Note that $Err = 1 - Acc$.

$$Acc = \frac{\text{Number of correct predictions}}{\text{Total number of predictions}} = \frac{\sum\limits_{i=1}^{C} f_{ii}}{\sum\limits_{i,j=1}^{C} f_{ij}} \tag{1.1}$$

$$Err = \frac{\text{Number of wrong predictions}}{\text{Total number of predictions}} = \frac{\sum\limits_{i,j=1,i\neq j}^{C} f_{ij}}{\sum\limits_{i,j=1}^{C} f_{ij}} \tag{1.2}$$

Using these performance metrics allows to compare the performance of different classifiers f. It allows to determine in particular whether one learning algorithm outperforms another on a particular learning task on a given test dataset X_T. However, depending on the size of the test dataset, the difference in error rate Err between two classifiers may not be statistically significant. Snedecor & Cochran proposed in 1989 a statistical test based on measuring the difference between two learning algorithms [Coc77]. It has been used by many researchers [Die97]; [DHB95].

Let consider 2 classifiers f_A and f_B. We test these classifiers on the test set X_T and denote p_A and p_B their respective error rates. The intuition of this statistical test is that when algoithm A classifies an example $\mathbf{x}_j$ from the test set X_T, the probability of misclassification is p_A. Thus, the number of misclassification of m test examples is a binomial random variable with mean $m.p_A$ and variance $p_A(1-p_A)m$. The binomial distribution can be approximated by a normal distribution when m has a reasonable value (Law of large numbers). The difference between two independent normally distributed random variable is also normally distributed. Thus, the quantity $p_A - p_B$ is a normally distributed random variable. Under the null hypothesis (the two algorithm should have the same error rate), this will have a mean of zero and a standard error of:

$$se = \sqrt{\frac{2p(1-p)}{n}} \tag{1.3}$$

where $p = \frac{p_A+p_B}{2}$ is the average of the two error probabilities. From this analysis, we obtain the statistic:

$$z = \frac{p_A - p_B}{\sqrt{2p(1-p)/n}} \tag{1.4}$$

which has (approximatively) a standard normal distribution. We can reject the null hypothesis if $|z| > Z_{0.975} = 1.96$ (for a 2-sided test with probability of incorrectly rejecting the null hypothesis of 0.05).

1.2.3.b Regression

As the concept of classes is restricted to classification problems, the performance of a regression model f is based on metrics that measure the difference between the predicted label $\hat{y}_j$ and the known label y_j. The Mean Absolute Error function (MAE) computes the mean absolute error, a risk metric corresponding to the expected value of the absolute error loss or L1-norm loss.

$$MAE(\hat{y}, y) = \frac{1}{m}\sum_{j=1}^{m} |\hat{y}_j - y_j| \tag{1.5}$$

A commonly used performance metrics is the Root Mean Squared Error function (RMSE) that computes the root of the mean square error, a risk metric corresponding to the expected value of the squared (quadratic) error loss or loss.

$$RMSE(\hat{y}, y) = \sqrt{\frac{1}{m}\sum_{j=1}^{m} (\hat{y}_j - y_j)^2} \tag{1.6}$$

Many works relies on the R^2 function, the coefficient of determination. It provides a measure of how well future samples are likely to be predicted by the model.

$$R^2(\hat{y}, y) = 1 - \frac{\sum_{j=1}^{m}(\hat{y}_j - y_j)^2}{\sum_{j=1}^{m}(\bar{y} - y_j)^2} \tag{1.7}$$

where $\bar{y} = \sum_{j=1}^{m} y_j$ is the mean over the known labels y_j.

1.2.4 Data pre-processing

Real dataset are often subjected to noise or data scaling. Before applying any learning protocol, it is often necessary to pre-process the data when they are numerical. Part 2 of Sarle's Neural Networks FAQ Sarle (1997) [2] explains the importance of theses considerations for neural network but they can be applied to any learning algorithms. The main advantage of scaling is to avoid attributes in greater numeric ranges to dominate those in smaller numeric ranges. Another advantage is to avoid numerical difficulties during the calculation. For example, in the case of SVM, because kernel values usually depend on the inner products of feature vectors, i.e. the linear kernel and the polynomial kernel, large attribute values might cause numerical problems.

In most cases, it is recommended to scale each attribute to the range [-1; +1] or [0; 1]. Many normalization methods have been proposed such as Min/Max normalization, Z-normalization or normalization of the log normalization . Let μ_j and σ_j be the mean and the standard deviation of a variable X_j, applying the Z-normalized variable X_j^{norm} is given by:

références normalization

$$X_j^{norm} = \frac{X_j - \mu_j}{\sigma_j} \tag{1.8}$$

Note that the underlying assumption supposes that the variable X_j is normally distributed: data evolves between $[-\infty; +\infty]$ and are coming from a Gaussian process. In some cases, the data are skewed such as monetary amounts, incomes or distance measures. These data are often log-normally distributed, e.g., the log of the data is normally distributed (Fig. 1.8). The underlying idea is to take the log of the data (X_j^{log}) to restore the symmetry to it, and then, to apply a Z-normalization of this transformation:

$$X_j^{log} = \ln(X_j); \tag{1.9}$$

$$X_j^{log,norm} = \frac{X_j^{log} - \mu_j^{log}}{\sigma_j^{log}} \tag{1.10}$$

$$X_j^{norm} = \exp(X_j^{log,norm}) \tag{1.11}$$

where ln denotes the Natural Logarithm function, μ_j^{log} and σ_j^{log} the mean and the standard

[2] http://www.faqs.org/faqs/ai-faq/neural-nets/

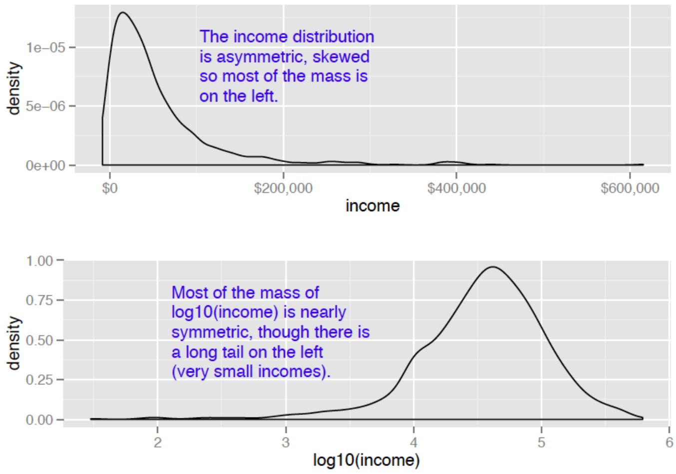

Figure 1.8: A nearly log-normal distribution, and its log [3]

deviation of a variable X_j^{log}.

Finally, we recall some precautions to the practitioner in the learning protocol, experimented by Hsu & al. in [HCL08] in the context of Support Vector Machine (SVM). First, training and testing data must be scaled using the same method. Second, training and testing data must not be scaled separately. Third, the whole dataset must not be scaled together at the same time. These often leads to poorer results. A proper way to do normalization is to scale the training data, store the parameters of the normalization (i.e. μ_i and σ_i for Z-normalization), then apply the same normalization to the testing data.

1.3 Machine Learning algorithms

Many popular algorithms have been proposed in Machine Learning, in the context of supervised learning, such as the Deep neural network, the Decision tree or the Relevance Vector Machine (RVM). We focus on k-Nearest Neighbors (k-NN) and Support Vector Machine (SVM). The interest of these two is that they are based on the comparison of samples (time series in our case) through a distance measure, notion detailed in the next chapters.

1.3.1 k-Nearest Neighbors (k-NN) classifier

Comment [MR4]: principle au la place de approach to classify samples

A simple approach to classify samples is to consider that "close" samples have a great probability to belong to the same class. Given a test sample $\mathbf{x}_j$, one can decide that $\mathbf{x}_j$ belong to the same class of its nearest neighbor in the training set. More generally, we can consider the

[3]source: http://www.r-statistics.com/2013/05/log-transformations-for-skewed-and-wide-distributions-from-practical-data-science-with-r/

k nearest neighbors of $\mathbf{x}_j$. The class y_j of the test sample $\mathbf{x}_j$ is assigned with a voting scheme among them, i.e., using the majority of the class of nearest neighbors. This algorithm is refer as the k-nearest neighbors algorithm (k-NN) [OE73]; [G. 06]. Fig. 1.9 illustrates the concept for a neighborhood of $k = 3$ and $k = 5$.

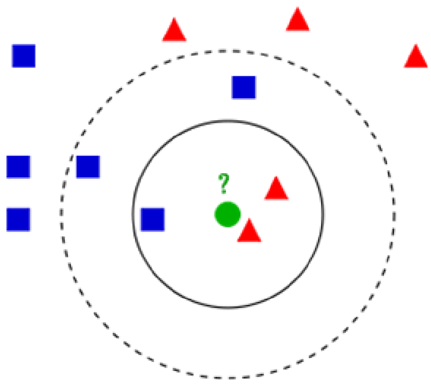

Figure 1.9: Example of k-NN classification. The test sample (green circle) is classified either to the first class (blue squares) or to the second class (red triangles). If $k = 3$ (solid line circle) it is assigned to the second class because there are 2 triangles and only 1 square inside the inner circle. If $k = 5$ (dashed line circle) it is assigned to the first class (3 squares vs. 2 triangles inside the outer circle).

In the k-NN algorithm, the notion of "closeness" between samples is based on the computation of a metric [4]. Let D be a metric. Usually, for static data, standard metrics are the Euclidean distance, the Minkowski distance or the Mahalanobis distance[5]. Solving the 1-NN classification problem is equivalent to solve the optimization problem:
For a new sample $\mathbf{x}_j$, $\forall i \in \{1...n\}$,

$$y_j = y_{i^*} \tag{1.12}$$

where $i^* = \underset{i \in \{1...n\}}{\text{argmin}} D(\mathbf{x}_i, \mathbf{x}_j)$.

The k-NN algorithm can be extended to estimate continous labels (regression problems). The procedure is similar. The label y_j is defined as :

$$y_j = \sum_{i=1}^{k} y_i \tag{1.13}$$

where i corresponds to the index of the k-nearest neighbors. There exists other variants of the k-NN algorithms: in a weighed k-NN, the approach consists in weighting each neighbors labels y_i by a factor equal to the inverse of the distance $\frac{1}{D(\mathbf{x}_i,\mathbf{x}_j)}$; in a fuzzy k-NN, the idea is to assign memberships of samples $\mathbf{x}_j$ to classes. The class membership is a function of the sample's distance $D(\mathbf{x}_i, \mathbf{x}_j)$ from its k-NN training samples;

[biblio regression kNN]

[biblio kNN pondéré]

[biblio fuzzy kNN]

Comment [MR5]: + k-NN crédibiliste

[4] A clarification of the terms metric, distance, dissimilarity, etc. will be given in Chapter 2. For now, we refer all of them as metrics.

[5] A recall of these metrics will be in Chapter 2.

Despite its simplicity, the k-NN algorithm presents many advantages and have been shown to be successful on time series classification problems [Xi+06]; [Din+08]. One main advantage is that a 1-NN classifier can be used to evaluate and compare the efficacy of different metrics [Din+08]. First, the underlying metric is critical in the performance of the 1-NN classifier [TSK05]. Thus, the accuracy of the 1-NN classifier directly reflects the effectiveness of the metric. Second, 1-NN classifier is easy to implement and doesn't need to learn any hyper-parameters, which make it straightforward for anyone to reproduce results. All of this advantages allows one who want to evaluate a benchmark of metrics. Other methods to compare metrics exists such as clustering with small data sets which are not statistically significant, or compare the compactness of the metric [MP07]; [Vla+06]. The 1-NN algorithm will be used in our experiments to compare the performances different metrics used for time series.

However, the k-NN algorithm presents some disadvantages, mainly due to its computational complexity, both in space (storage of the training samples $\mathbf{x}_i$) and time (search) [OE73]. Suppose we have n labeled training samples in T dimensions, and find the closest neighbors to a test sample $\mathbf{x}_j$ ($k = 1$). In the most simple approach, we look at each stored samples $\mathbf{x}_i$ ($i = 1...n$) one by one, calculate its metric to $\mathbf{x}_i$ (D($\mathbf{x}_i$,$\mathbf{x}_j$)) and retain the index of the current closest one. For the standard Euclidean distance, each metric computation is $O(T)$ and thus the search is $O(Tn^2)$. Moreover, using standard metrics (such as the Euclidean distance) uses all the T dimensions in its computation and thus assumes that all dimensions have the same effect on the metric. This assumption may be wrong and can impact the classification performances. Wrong classification due to presence of many irrelevant dimensions is referred as the curse of dimensionality. The importance of defining adapted metrics for time series will be discussed in Chapter 2.

1.3.2 Support Vector Machine (SVM) algorithm

Support Vector Machine (SVM) is a state of the art classification method introduced in 1992 by Boser, Guyon, and Vapnik [BGV92]; [CV95]. The SVM classifier have demonstrate high accuracy, ability to deal with high-dimensional data, good generalization properties and interpretation for various applications from recognizing handwritten digits, to face identification, text categorization, bioinformatics and database marketing [Wan02]; [YL99]; [HHP01]; [SSB03]; [CY11]. SVMs belong to the category of kernel methods, algorithms that depends on the data only through dot-products [SS13].

As SVMs will be used in Chapter 5, we first present an intuition of maximum margin concept. We give the primal formulation of the SVM optimization problem. Then, by transforming the latter formulation into its dual form, the kernel trick can be applied to learn non-linear classifiers. Finally, we detail how we can interpret the obtained coefficients and how SVMs can be extended for regression problems.

Note that this section doesn't aim to give an detailed comprehension of SVMs. It aims to give an overview of the mathematical key points interpretation and comprehension of the method. For more informations, the reader can consult [SS13]; [CY11]; [CV95].

1.3.2.a Intuition

Let consider a classification problem with 2 classes ($y_i = \pm 1$). The objective is to learn a hyperplane, whose equations are $\mathbf{w}.\mathbf{x} + b = 0$, that can separate samples of class $+1$ from the ones of class -1. When the problem is linearly separable such as in Fig. 1.10, there exists an infinite number of hyperplanes. We denote $||\mathbf{w}||_2$, the L2-norm of the vector $\mathbf{w}$.

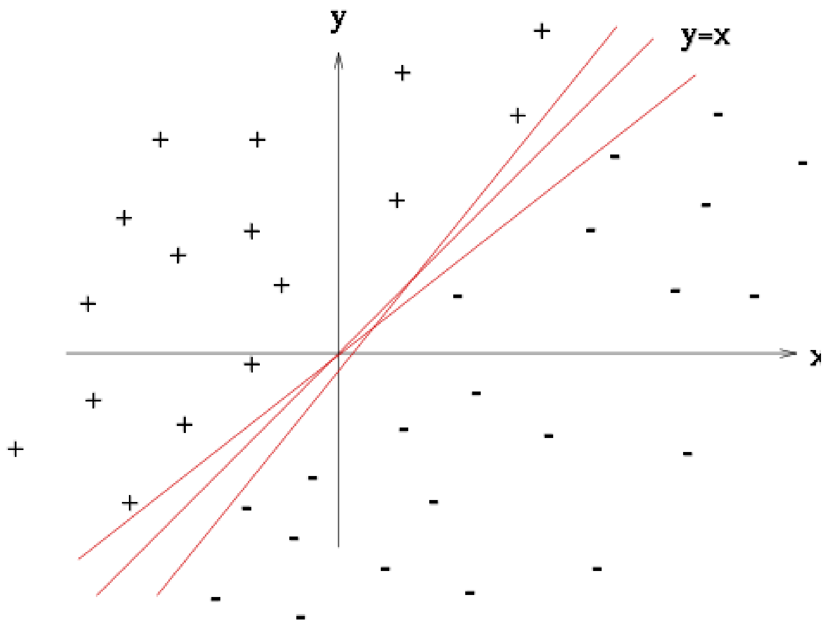

Figure 1.10: Example of linear classifiers in a 2-dimensional plot. For a set of points of classes $+1$ and -1 that are linearly separable, there exists an infinite number of separating hyperplanes corresponding to $\mathbf{w}.\mathbf{x} + b = 0$.

Vapnik & al. [CV95] propose to choose the separating hyperplane that maximizes the margin, e.g. the hyperplane that leaves as much distance as possible between the hyperplane and the closest examples of each class, called the support vectors. This distance is equal to $\frac{1}{||\mathbf{w}||_2}$. The hyperplanes passing through the support vectors of each class are referred as the canonical hyperplanes, and the region between the canonical hyperplanes is called the margin band (Fig. 1.11).

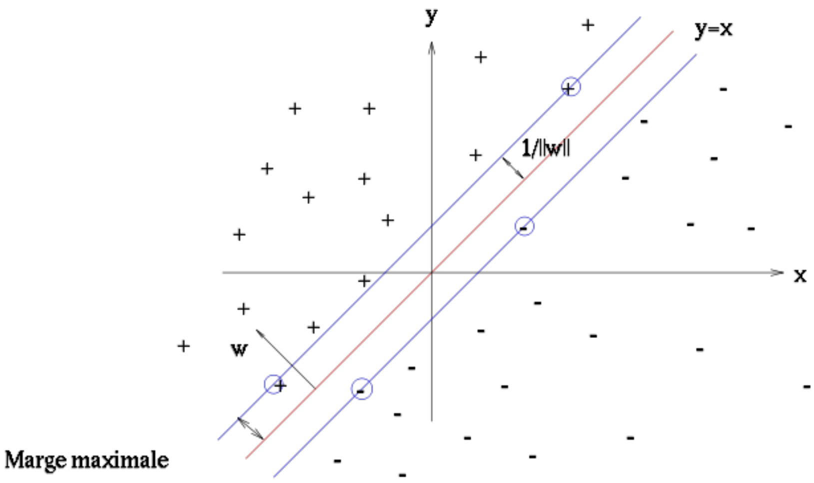

Figure 1.11: The argument inside the decision function of a classifier is $\mathbf{w}.\mathbf{x}+b$. The separating hyperplane corresponding to $\mathbf{w}.\mathbf{x}+b=0$ is shown as a line in this 2-dimensional plot. This hyperplane separates the two classes of data with points on one side labeled $y_i=+1$ ($\mathbf{w}.\mathbf{x}+b \geq 0$) and points on the other side labeled $y_i=-1$ ($\mathbf{w}.\mathbf{x}+b<0$). Support vectors are circled in blue and lies on the hyperplanes $\mathbf{w}.\mathbf{x}+b=+1$ and $\mathbf{w}.\mathbf{x}+b=-1$

1.3.2.b Primal formulation

Finding $\mathbf{w}$ and b by maximizing the margin $\frac{1}{||\mathbf{w}||_2}$ is equivalent to minimizing the norm of $\mathbf{w}$ such that all samples from the training set are correctly classified:

$$\underset{\mathbf{w},b}{\operatorname{argmin}} \frac{1}{2}||\mathbf{w}||_2^2 \tag{1.14}$$

$$\textbf{s.t.} \;\; y_i(\mathbf{w}.\mathbf{x}_i+b) \geq 1 \tag{1.15}$$

This is a constrained optimization problem in which we minimize an objective function (Eq. 1.14) subject to constraints (Eq. 1.15). This formulation is referred as the primal hard margin problem. Many real life datasets are subjected to noise and SVM can lead to poor generalization if it tries to fit to this noise, represented by the constraints in Eq. 1.15. The effects of noise can be reduced by introducing slack variables $\xi_i \geq 0$ to relax the optimization problem:

$$\underset{\mathbf{w},b}{\operatorname{argmin}} \left(\overbrace{\frac{1}{2}||\mathbf{w}||_2^2}^{Regularization} + C \overbrace{\sum_{i=1}^{n} \xi_i(\mathbf{w};b;x_i;y_i)}^{Loss} \right) \tag{1.16}$$

$$\textbf{s.t.} \;\; y_i(\mathbf{w}.\mathbf{x}_i+b) \geq 1-\xi_i \tag{1.17}$$

$$\xi_i \geq 0 \tag{1.18}$$

where $C>0$ is a penalty hyper-parameter.

This formulation is referred as the primal soft margin problem. It is quadratic programming optimization problem subjected to constraints. Thus, it is a convex problem: any local solutions is a global solution. The objective function in Eq. 1.16 is made of two terms. The first one, the regularization term, penalize the complexity of the model and thus, controls the ability of the algorithm to generalize on new samples. The second one, the loss term, is an adaptation term to the data. The hyper-parameter C is a trade-off between the regularization and the loss term. When C tends to $+\infty$, the problem is equivalent to the primal hard margin problem. The hyper-parameter C is learnt during the training phase.

For SVM, the two common loss functions ξ_i are $\max(1-y_i\mathbf{w}.\mathbf{x}_i, 0)$ and $[\max(1-y_i\mathbf{w}.\mathbf{x}_i, 0)]^2$. The former is referred to as L1-Loss and the latter is L2-Loss function. L2-loss function will penalize more slack variables ξ_i during training. Theorically, it should lead to less error in training and poorer generalization in most of the case.

An other thing to specify is the type of regularizer. For SVM, the two common regularizer are $||\mathbf{w}||_2$ and $||\mathbf{w}||_2^2$. The former is referred to as L1-Regularizer while the latter is L2-Regularizer. L1-Regularizer is used to obtain sparser models than L2-Regularizer. Thus, it can be used for variable selection. L2-Regularizer allows to transform the primal formulation into a dual form.

From this, for a binary classification problem, to classify a new sample $\mathbf{x}_j$, the decision function is:

$$f(\mathbf{x}_j) = sign(\mathbf{w}.\mathbf{x}_j + b) \tag{1.19}$$

1.3.2.c Dual formulation

From the primal formulation, using a L2-Regularizer, it is possible to have an equivalent dual form. This latter formulation allows samples $\mathbf{x}_i$ to appear in the optimization problem through dot-products only. Thanks to that, a kernel trick can be applied to extend the methods to learn non-linear classifiers.

First, to simplify the calculation development, let consider the hard margin formulation in Eq. 1.16, 1.17 and 1.18 with a L1-Loss function. As a constrained optimization problem, the formulation is equivalent to the minimization of a Lagrange function $L(\mathbf{w}, b)$, consisting of the sum of the objective function and the n constraints multiplied by their respective Lagrange multipliers $\boldsymbol{\alpha} = [\alpha_1, \ldots, \alpha_n]'$:

$$\underset{\boldsymbol{\alpha}}{\operatorname{argmax}} \left(L(\mathbf{w}, b) = \frac{1}{2}(\mathbf{w}.\mathbf{w}) - \sum_{i=1}^{n} \alpha_i (y_i(\mathbf{w}.\mathbf{x}_i + b) - 1) \right) \tag{1.20}$$

s.t. KKT $\forall i = 1...n$:

$$\alpha_i \geq 0 \tag{1.21}$$

$$y_i(\mathbf{w}.\mathbf{x}_i + b) - 1 \geq 0 \tag{1.22}$$

$$\alpha_i(y_i(\mathbf{w}.\mathbf{x}_i + b) - 1) = 0 \tag{1.23}$$

where $\alpha_i \geq 0$ are the Lagrange multipliers. In optimization theory, Eq. 1.21, 1.22 and 1.23 are called the Karush-Kuhn-Tucker (KKT) conditions. It corresponds to the set of conditions which must be satisfied at the optimum of a constrained optimization problem. The KKT conditions will play an important role in the interpretation of SVM in Section 1.3.2.e.

At the minimum value of $L(\mathbf{w}, b)$, we assume the derivatives with respect to b and $\mathbf{w}$ are set to zero:

$$\frac{\partial L}{\partial b} = \sum_{i=1}^{n} \alpha_i y_i = 0$$
$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i = 0$$

that leads to:

$$\sum_{i=1}^{n} \alpha_i y_i = 0 \tag{1.24}$$
$$\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i \tag{1.25}$$

By substituting $\mathbf{w}$ into $L(\mathbf{w}, b)$ in Eq. 1.20, we obtain the dual formulation (*Wolfe dual*):

$$\underset{\boldsymbol{\alpha}}{\text{argmax}} \left(\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i . \mathbf{x}_j) \right) \tag{1.26}$$
$$\textbf{s.t.} \quad \sum_{i=1}^{n} \alpha_i y_i = 0 \tag{1.27}$$
$$\alpha_i \geq 0 \tag{1.28}$$

The dual objective in Eq. 1.26 is quadratic in the parameters α_i. Adding the constraints in Eq. 1.27 and 1.28, it is a constrained quadratic programming optimization problem (QP). Note that while the primal formulation is minimization, the equivalent dual formulation is maximization. It can be shown that the objective functions of both formulations reach the same value when the solution is found [CY11].
In the same spirit, considering the soft margin primal problem, it can be shown that it leads to the same formulation [CY11] (Eqs. 1.26 and 1.27), except that the Lagrange multipliers α_i are upper bounded by the trade-off C in the soft margin formulation:

$$0 \leq \alpha_i \leq C \tag{1.29}$$

The constraints in Eq. 1.29 are called the Box constraints [CY11]. From the optimal value of α_i, denoted α_i^*, it is possible to compute the weight vector $\mathbf{w}^*$ and the bias b^* at the optimality:

$$\mathbf{w}^* = \sum_{i=1}^{n} \alpha_i^* y_i \mathbf{x}_i \tag{1.30}$$

$$b^* = \sum_{i=1}^{n} (\mathbf{w}.\mathbf{x}_i - y_i) \tag{1.31}$$

At the optimality point, only a few number of datapoints have $\alpha_i^* > 0$ as shown as in Fig. 1.12. These samples are the vector supports. All other datapoints have $\alpha_i^* = 0$, and the decision function is independent of them. Thus, the representation is sparse.

From this, to classify a new sample $\mathbf{x}_j$, the decision function for a binary classification problem is:

$$f(\mathbf{x}_j) = sign(\sum_{i=1}^{n} \alpha_i^* y_i (\mathbf{x}_i.\mathbf{x}_j) + b^*) \tag{1.32}$$

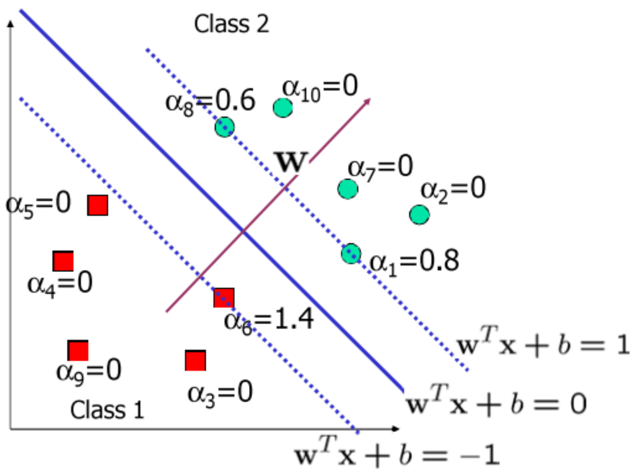

Figure 1.12: Obtained hyperplane after a dual resolution (full blue line). The 2 canonical hyperplanes (dash blue line) contains the support vectors whose $\alpha_i > 0$. Other points have their $\alpha_i = 0$ and the equation of the hyperplane is only affected by the support vectors.

1.3.2.d Kernel trick

The concept of kernels was introduced by Aizerman & Al in 1964 to design potential functions in the context of pattern recognition [ABR64]. The idea was re-introduced in 1992 by Boser & al. for Support Vector Machine (SVM) and has been received a great number of improvements and extensions to symbolic objects such as text or graphs [BGV92].

One theoretical interesting property of SVM if that it has been shown that the generalization error bound does not depend on the dimensionality T of the space [SS13]. From the dual objective in Eq. 1.26, we note that the samples $\mathbf{x}_i$ are only involves in a dot-product. Therefore, we can map these samples $\mathbf{x}_i$ into a higher dimensional hyperspace, called the feature space, through the replacement:

$$(\mathbf{x}_i.\mathbf{x}_j) \rightarrow \Phi(\mathbf{x}_i).\Phi(\mathbf{x}_j) \tag{1.33}$$

where Φ is the mapping function. The intuition behind is that in many datasets, it is not possible to find a hyperplan that can separate the two classes in the input space if the problem is not linearly separable. However, by applying a transformation Φ, data might become linearly separable in a higher dimensional space (feature space). Fig. 1.13 illustrates the idea: in the original 2-dimensional space (left), the two classes can't be separated by a line. However, with a third dimension such that the $+1$ labeled points are moved forward and the -1 labeled moved back the two classes become separable.

In most of the case, the mapping function Φ does not need to be known since it will be defined by the choice of a kernel: $K(\mathbf{x}_i, \mathbf{x}_j) = \Phi(\mathbf{x}_i).\Phi(\mathbf{x}_j)$. We call Gram matrix G, the matrix containing all $K(\mathbf{x}_i, \mathbf{x}_j)$:

$$G = (K(\mathbf{x}_i, \mathbf{x}_j))_{1 \leq i,j \leq n} = \begin{pmatrix} K(\mathbf{x}_1, \mathbf{x}_1) & ... & K(\mathbf{x}_1, \mathbf{x}_n) \\ ... & & ... \\ K(\mathbf{x}_n, \mathbf{x}_1) & ... & K(\mathbf{x}_n, \mathbf{x}_n) \end{pmatrix}$$

Defining a kernel has to follow rules. One of these rules specifies that the kernel function has to define a proper inner product in the feature space. Mathematically, the Gram matrix has to be semi-definite positive (Mercer's theorem) [SS13]. These restricted feature spaces, containing an inner product are called Hilbert space.

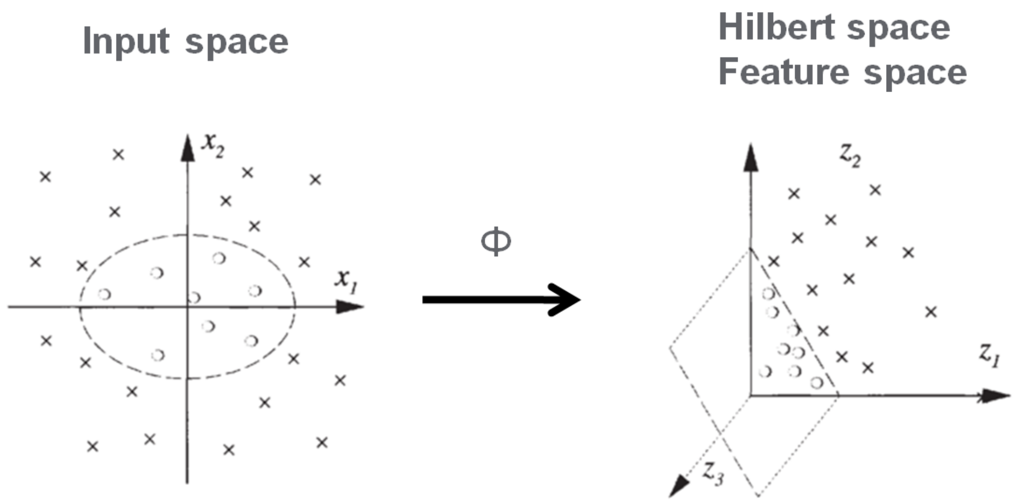

Figure 1.13: Left: in two dimensions these two classes of data are mixed together, and it is not possible to separate them by a line: the data is not linearly separable. Right: using a Gaussian kernel, these two classes of data (cross and circle) become separable by a hyperplane in feature space, which maps to the nonlinear boundary shown, back in input space.

Many kernels have been proposed in the literature such as the polynomial, sigmoid, exponential or wavelet kernels [SS13]. The most popular ones that we will use in our work are respectively the Linear and the Gaussian (or Radial Basis Function (RBF)) kernels:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i.\mathbf{x}_j \tag{1.34}$$

$$K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\frac{||\mathbf{x}_j - \mathbf{x}_i||_2^2}{2\sigma^2}) = \exp(-\gamma||\mathbf{x}_j - \mathbf{x}_i||_2^2) \tag{1.35}$$

where $\gamma = \frac{1}{2\sigma^2}$ is the parameter of the Gaussian kernel and $||\mathbf{x}_j - \mathbf{x}_i||_2$ is the Euclidean distance between $\mathbf{x}_i$ and $\mathbf{x}_j$. Note that the Linear kernel is the identity transformation. In practice, for large scale problem (when T is high), using a Linear kernel is sufficient [FCH08].

The Gaussian kernel computed between a sample $\mathbf{x}_j$ and a support vector $\mathbf{x}_i$ is an exponentially decaying function in the input feature space. The maximum value of the kernel ($K(\mathbf{x}_i, \mathbf{x}_j)$=1) is attained at the support vector (when $\mathbf{x}_i = \mathbf{x}_j$). Then, the value of the kernel decreases uniformly in all directions around the support vector, with distance and ranges between zero and one. It can thus be interpreted as a similarity measure. Geometrically speaking, it leads to hyper-spherical contours of the kernel function as shown in Fig. 1.14 [6]. The parameter γ controls the decreasing speed of the sphere. In practice, this parameter is learnt during the training phase.

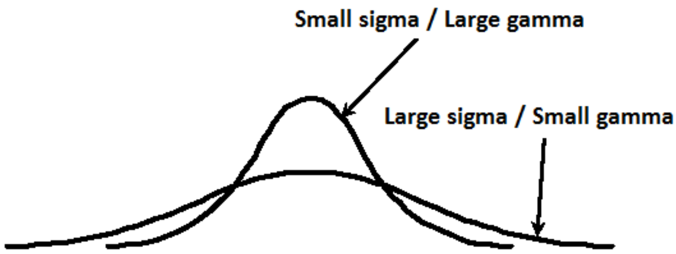

Figure 1.14: Illustration of the Gaussian kernel in the 1-dimensional input space for a small and large γ.

By applying the kernel trick to the soft margin formulation in Eq. 1.26, 1.27 and 1.29, the following optimization problem allows to learn non-linear classifiers:

$$\underset{\boldsymbol{\alpha}}{\text{argmax}} \left(\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i.\mathbf{x}_j) \right) \tag{1.36}$$

$$\textbf{s.t.} \quad \sum_{i=1}^{n} \alpha_i y_i = 0 \tag{1.37}$$

$$0 \leq \alpha_i \leq C \tag{1.38}$$

[6] `https://www.quora.com/Support-Vector-Machines/What-is-the-intuition-behind-Gaussian-kernel-in-SVM`

The decision function f becomes:

$$f(\mathbf{x}_j) = sign(\sum_{i=1}^{n} \alpha_i^* y_i K(\mathbf{x}_i.\mathbf{x}_j) + b^*) \tag{1.39}$$

Note that in this case, we can't recover the weight vector $\mathbf{w}^*$. Let n_{SV} be the number of support vectors ($n_{SV} \leq n$). To recover b^*, we recall that for support vectors $\mathbf{x}_i$:

$$y_j \left(\sum_{i=1}^{n_{SV}} \alpha_i^* y_i K(\mathbf{x}_i, \mathbf{x}_j) + b^* \right) = 1 \tag{1.40}$$

From this, we can solve b^* using an arbitrarily chosen support vector $\mathbf{x}_i$:

$$b^* = \frac{1}{y_j} - \sum_{i=1}^{n_{SV}} \alpha_i^* y_i K(\mathbf{x}_i, \mathbf{x}_j) \tag{1.41}$$

1.3.2.e Complexity and interpretation

Complexity

Comment [CTD6]: réécrire + compléter avec Claude

As the objective is to provide an algorithm for both small and large datasets, let us examine the complexity of SVMs and in the computation of the Gram matrix G [BL07].

In the dual, suppose that we know which samples are not support vectors ($\alpha_i = 0$) and which sample are bounded support vectors ($\alpha_i = C$). The R remaining support vectors are determined by a system of R linear equations. They represent the derivatives of the objective function and requires a number of operations proportional to R^3. Verifying that a vector α is a solution of the SVM problem involves computing the gradient of the dual and checking the optimality conditions. With n samples and n_{SV} support vectors, the number of operations required is equal to $n.n_{SV}$. When C gets large, few support vectors reach the upper bound, the cost is then $R^3 \approx n_{SV}^3$. The term $n.n_{SV}$ is usually larger. The final number of support vectors n_{SV} therefore is the critical component of the computational cost of solving the dual problem. Since the asymptotical number of support vectors n_{SV} grows linearly with the number of samples n, the computational cost of solving the SVM problem has both a quadratic and a cubic component. It grows at least like n^2 when C is small and n^3 when C gets large.

Computing the n^2 components of the kernel matrix $G = \{K(\mathbf{x}_i, \mathbf{x}_j)\}_{i=1}^{n}$ is a quadratic matter. Note that technical issues may arise in practice. For example, the kernel matrix does not fit in memory when n is large.

Interpretation in the primal

We recall that $\mathbf{x}_i$ is a univariate time series of length T. We suppose time in dependency. Thus, the T observations x_{it} can be seen as attributes in the representation $\mathbb{R}^T$. In the primal, the weight vector $\mathbf{w} = [w_1, \ldots, w_T]'$ contains as many elements as there are variables in the dataset, i.e., $\mathbf{w} \in \mathbb{R}^T$. The magnitude of each element in $\mathbf{w}$ denotes the importance of the corresponding variable for the classification problem. If the element of $\mathbf{w}$ for some variable is

0, these variables are not used for the classification problem.

In order to visualize the above interpretation of the weight vector $\mathbf{w}$, let us examine several hyperplanes $\mathbf{w}.\mathbf{x}+b=0$ shown in Fig. 1.15 with $T=2$. Figure (a) shows a hyperplane where elements of $\mathbf{w}$ are the same for both variables $\mathbf{x}_1$ and $\mathbf{x}_2$. The interpretation is that both variables contribute equally for classification of objects into positive and negative. Figure (b) shows a hyperplane where the element of $\mathbf{w}$ for $\mathbf{x}_1$ is 1, while that for $\mathbf{x}_2$ is 0. This is interpreted as that $\mathbf{x}_1$ is important but $\mathbf{x}_2$ is not. An opposite example is shown in figure (c) where $\mathbf{x}_2$ is considered to be important but $\mathbf{x}_1$ is not. Finally, figure (d) provides a 3-dimensional example ($T=3$) where an element of $\mathbf{w}$ for $\mathbf{x}_3$ is 0 and all other elements are equal to 1. The interpretation is that $\mathbf{x}_1$ and $\mathbf{x}_2$ are important but $\mathbf{x}_3$ is not.

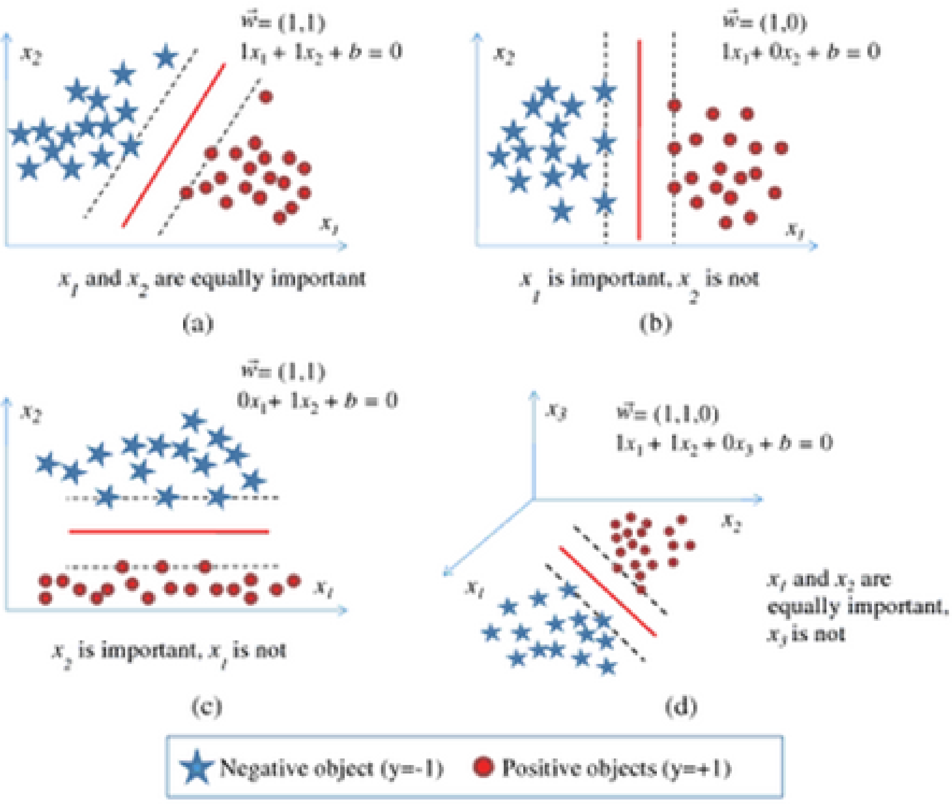

Figure 1.15: Example of several SVMs and how to interpret the weight vector $\mathbf{w}$

Another way to interpret how much a variable contributes in the vector $\mathbf{w}$ is to express the contribution in percentage. To do that, if the variables $\mathbf{X}_j$ of the time series are normalized before learning the SVM model, they evolves in the same range. Thus, the ratio $\frac{w_j}{||\mathbf{w}||_2} \times 100$ defines the percentage of contribution for each variable $\mathbf{X}_j$ in the SVM model.

Geometrically, the vector $\mathbf{w}$ represents the direction of the hyperplane (Fig. 1.16). The bias b is equal to the distance of the hyperplane to the origin point $\mathbf{x} = \mathbf{0}$[7]. The orthogonal projection of a sample $\mathbf{x}_i$ on the direction $\mathbf{w}$ is $P_{\mathbf{w}}(\mathbf{x}_i) = \mathbf{w}.\mathbf{x}_i$. In the soft margin problem, the slack variables ξ_i of the samples $\mathbf{x}_i$ that lies within the two canonical hyperplanes are equal to zero. Outside of these canonical hyperplanes, the slack variables $\xi_i > 0$ are equal to the distance to the hyperplane.

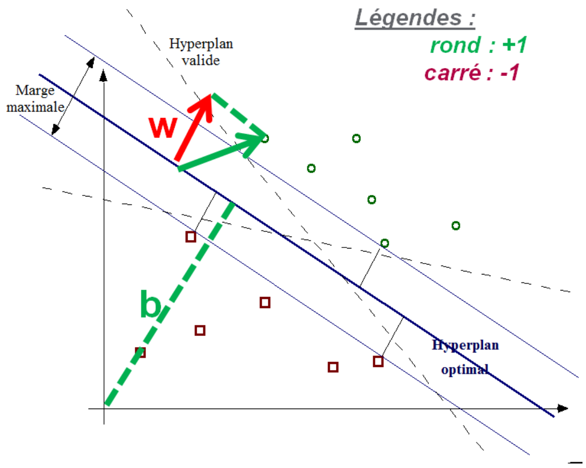

Figure 1.16: Geometric representation of SVM.

Interpretation in the dual

As a constrained optimization, the dual form satisfies the Karush-Kuhn-Tucker (KKT) conditions (Eq. 1.21, 1.22 and 1.23). We recall Eq. 1.23:

$$\alpha_i(y_i(\mathbf{w}.\mathbf{x}_i + b) - 1) = 0$$

From this, for every datapoint $\mathbf{x}_i$, either $\alpha_i^* = 0$ or $y_i(\mathbf{w}.\mathbf{x}_i + b) = 1$. Any datapoint with $\alpha_i^* = 0$ do not appear in the sum of the decision function f in Eq. 1.32 or 1.39. Hence, they play no role for the classification decision of a new sample $\mathbf{x}_j$. The others $\mathbf{x}_i$ such that $\alpha_i^* > 0$ corresponds to the support vector. Looking at the distribution of α_i^* allows also to have either a better understanding of the datasets, or either to detect outliers. The higher is the coefficient α_i^* for a sample $\mathbf{x}_i$, the more the sample $\mathbf{x}_i$ impacts on the decision function f. However, unusual high value of α_i^* among the samples can lead to two interpretations: either this point is a critical point to the decision, either this point is an outlier. In the soft margin formulation, by constraining α_i^* to be inferior to C (Box constraints) the effect of outliers can be reduced and controlled.

1.3.2.f Extensions of SVM

SVM has received many interests in recent years. Many extensions has been developed such as ν-SVM, asymmetric soft margin SVM or multiclass SVM [KU02]; [CS01]. One interesting

[7] $\mathbf{0}$ stands for the null vector: $\mathbf{0} = [0, \ldots, 0]^T$

extension is the extension of Support Vector Machine to regression problems, also called Support Vector Regression (SVR). The objective is to find a linear regression model $f(\mathbf{x}) = \mathbf{w}.\mathbf{x} + b$. To preserve the property of sparseness, the idea is to consider an ϵ-insensitive error function. It gives zero error if the absolute difference between the prediction $f(\mathbf{x}_i)$ and the target y_i is less than ϵ where $\epsilon > 0$ penalize samples that are outside of a ϵ-tube as shown as in Fig. 1.17.

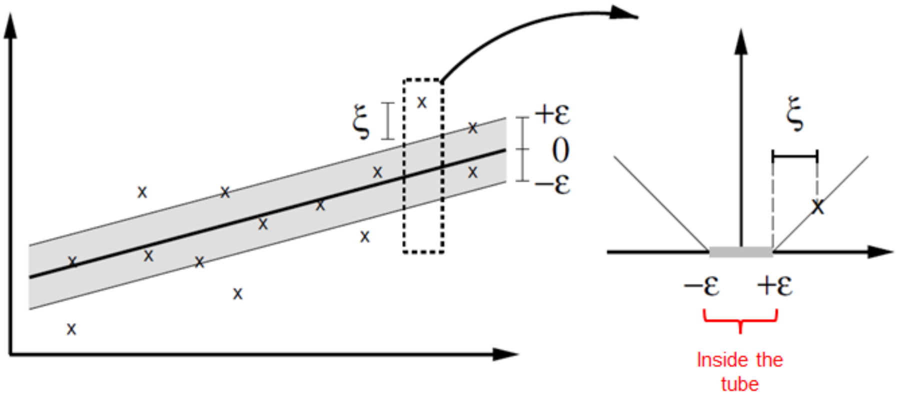

Figure 1.17: Illustration of SVM regression (left), showing the regression curve with the ϵ-insensitive "tube" (right). Samples $\mathbf{x}_i$ above the ϵ-tube have $\xi_1 > 0$ and $\xi_1 = 0$, points below the ϵ-tube have $\xi_2 = 0$ and $\xi_2 > 0$, and points inside the ϵ-tube have $\xi = 0$.

An example of ϵ-insensitive error function E_ϵ is given by,

$$E_\epsilon(f(\mathbf{x}_i) - y_i) = \begin{cases} 0 & \text{if} \quad |f(\mathbf{x}_i) - y_i| < \epsilon \\ |f(\mathbf{x}_i) - y_i| - \epsilon & \text{otherwise} \end{cases} \tag{1.42}$$

The soft margin optimization problem in its primal form is formalized as:

$$\operatorname*{argmin}_{\mathbf{w},b} \left(\overbrace{\frac{1}{2}||\mathbf{w}||_2^2}^{Regularization} \; \overbrace{+C\sum_{i=1}^{n}(\xi_{i_1} + \xi_{i_2})}^{Loss} \right) \tag{1.43}$$

$$\textbf{s.t.} \;\; \forall i = 1 \ldots n :$$

$$y_i - (\mathbf{w}.\mathbf{x}_i + b) \geq \epsilon - \xi_{i_1} \tag{1.44}$$

$$(\mathbf{w}.\mathbf{x}_i + b) - y_i \geq \epsilon - \xi_{i_2} \tag{1.45}$$

$$\xi_{i_1} \geq 0 \tag{1.46}$$

$$\xi_{i_2} \geq 0 \tag{1.47}$$

The slacks variables are divided into 2 slacks variables, one for samples above the decision function f (ξ_{i_1}), and one for samples under the decision function f (ξ_{i_2}). As for SVM, it is possible to have a dual formulation:

$$\underset{\boldsymbol{\alpha}}{\text{argmax}} \left(\sum_{i=1}^{n} y_i(\alpha_{i_1} - \alpha_{i_2}) - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} (\alpha_{i_1} - \alpha_{i_2})(\alpha_{j_1} - \alpha_{j_2})(\mathbf{x}_i.\mathbf{x}_j) \right) \tag{1.48}$$

$$\textbf{s.t.} \;\; \forall i = 1 \ldots n :$$

$$\sum_{i=1}^{n} \alpha_{i_1} = \sum_{i=1}^{n} \alpha_{i_2} \tag{1.49}$$

$$0 \leq \alpha_{i_1} \leq C \tag{1.50}$$

$$0 \leq \alpha_{i_2} \leq C \tag{1.51}$$

As in SVM, we obtain three possible decision functions for a new sample $\mathbf{x}_j$, respectively in its primal, dual, and non-linear form:

$$f(\mathbf{x}_j) = \mathbf{w}.\mathbf{x}_j + b \tag{1.52}$$

$$f(\mathbf{x}_j) = \sum_{i=1}^{n} (\alpha_{i_1}^* - \alpha_{i_2}^*)(\mathbf{x}_i.\mathbf{x}_j) + b \tag{1.53}$$

$$f(\mathbf{x}_j) = \sum_{i=1}^{n} (\alpha_{i_1}^* - \alpha_{i_2}^*) K(\mathbf{x}_i.\mathbf{x}_j) + b \tag{1.54}$$

More informations about the calculation development can be found in [Bis06].

1.3.3 Other classification algorithms

Partie non encore rédigée. A faire à la fin.

- Positionner les travaux par rapport aux autres méthodes d'apprentissage supervisé
- S'intéresser au Deep neural network (à la mode en ce moment)
- RVM, Decision Tree,
- Ne pas trop développer
- Dans notre cas, on ne s'intéressera pas à ce type d'algorithmes (type deep learning) car il ne repose pas sur une notion de distance et les features qui sont trouvés ne sont pas interprétables

1.4 Conclusion of the chapter

To make the classification or regression of time series, a commonly hypothesis is to consider time series as static data and then to apply classical machine learning algorithms, such as a k-Nearest Neighbors (k-NN) or Support Vector Machine (SVM) approach. For that, the practitioner has to be careful on the design of his learning framework: data must be separated into a training and testing set, data have to be normalized depending on their distributions, cross-validation must be operated on the training set to learn the best fitting of the hyper-parameters and finally, performance metrics and statistical tests should be used to compare the performances of different classifiers.

A key aspect in k-NN and SVM relies on the comparison of time series through metrics. Assuming that time series can be reduced to flat data may be too restrictive. Under such hypothesis and using a standard Euclidean distance, time series are only compared on their amplitude at the same time instant. However, time series are more complex. They may exhibit similar behavior or share similar frequential spectrum. Thus, there is a need to consider time series as an ordered object and to define adapted metrics for time series.

Chapter 2

Time series basic metrics

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In this chapter, we review different metrics for time series. In the case of classification, time series are expected to be similar if they belong to the same class. The concept of similarity among time series is directly linked to the concept of metrics.

In the following, we consider time series as an object. We suppose that time series have the same lengths T and have been sampled at the same sampling frequency f_e. They may be compared either on all their observations x_{it}, a part of them or in a window. We first recall the properties of a metric. Then, we review 3 types of metrics (amplitude-based, behavior-based, frequential-based) and kernels adapted to time series. As real time series are subjected to varying delays, we recall the concept of alignment and dynamic programming. Finally, we show how these metrics can be extended to define metrics that can capture local characteristics of time series.

2.1 Properties of a metric

A mapping $D : \mathbb{R}^T \times \mathbb{R}^T \to \mathbb{R}^+$ over a vector space $\mathbb{R}^T$ is called a metric or a distance if for all vectors $\forall \mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_l$, it satisfies the properties:

1. $D(\mathbf{x}_i, \mathbf{x}_j) \geq 0$ (positivity)
2. $D(\mathbf{x}_i, \mathbf{x}_j) = D(\mathbf{x}_j, \mathbf{x}_i)$ (symmetry)
3. $D(\mathbf{x}_i, \mathbf{x}_j) = 0 \Leftrightarrow \mathbf{x}_i = \mathbf{x}_j$ (distinguishability)
4. $D(\mathbf{x}_i, \mathbf{x}_j) D(\mathbf{x}_j, \mathbf{x}_l) \leq D(\mathbf{x}_i, \mathbf{x}_l)$ (triangular inequality)

A mapping D that satisfies properties 1, 2, 3 but not the forth one is called a dissimilarity. A mapping D that satisfies properties 1, 2, 4 and not the third one is called a pseudo-metric. To simplify the discussion in the following, we refer to pseudo-metric and dissimilarity as metrics, pointing out the distinction only when necessary.

Note that for a metric, if a time series $\mathbf{x}_i$ is expected to be closer to $\mathbf{x}_j$ than to $\mathbf{x}_l$, then $D(\mathbf{x}_i, \mathbf{x}_j) \leq D(\mathbf{x}_i, \mathbf{x}_l)$. On the contrary, when the time series $\mathbf{x}_i$ is expected to be closer to $\mathbf{x}_j$ than to $\mathbf{x}_l$ and then $D(\mathbf{x}_i, \mathbf{x}_j) \geq D(\mathbf{x}_i, \mathbf{x}_l)$, the mapping D is called a similarity.

2.2 Unimodal metrics for time series

In this section, we review 3 categories of time series metrics used in our work: amplitude-based, behavior-based and frequential-based. Let $\mathbf{x}_i = (x_{i1}, x_{i2}, ..., x_{iT})$ and $\mathbf{x}_j = (x_{i1}, x_{i2}, ..., x_{iT})$ be two univariate time series of length T.

To illustrate the effect of different metrics, we will consider some toy examples of time series, illustrated in Fig. 2.1. The objective is to determine which time series is closer to $\mathbf{x}_1$. Based on the amplitude of the signals, it is straightforward that $\mathbf{x}_2$ is the closest to $\mathbf{x}_3$. However, if we consider the shape of the signal, $\mathbf{x}_1$ is the closest to $\mathbf{x}_3$. $\mathbf{x}_1$ and $\mathbf{x}_4$ can be considered also as the closest in value if we delete the effect of delays between the two time series. Finally, it seems that $\mathbf{x}_1$ and $\mathbf{x}_5$ share the same frequential components.

Reparler avec Michèle et Sylvain de la figure. J'aimerai pouvoir trouver 5 séries temporelles qui couvrirait ces cas.

2.2.1 Amplitude-based metrics

The most frequent comparison measures are amplitude-based metrics, where time series are compared in the temporal domain on their amplitudes regardless of their behaviors or frequential characteristics. Among these metrics, there are the commonly used Euclidean distance

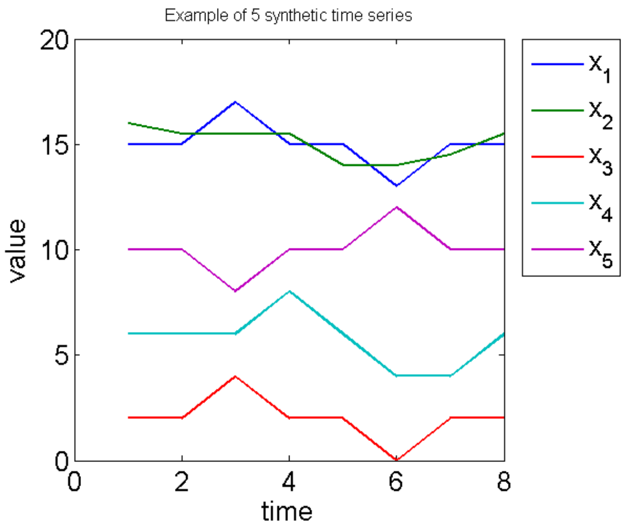

Figure 2.1: An example of 4 time series that can be compared on different distinct modalities. The objective is to determine which time series is closer to $\mathbf{x}_3$.

that compares elements observed at the same time [Din+08]:

$$d_A(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{\sum_{t=1}^{T} (x_{it} - x_{jt})^2} \tag{2.1}$$

Note that the Euclidean distance is a particular case of the Minkowski L_p norm ($p = 2$). An other amplitude-based metric is the Mahalanobis distance [PL12]:

$$d_M(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i - \mathbf{x}_j)'\mathbf{M}(\mathbf{x}_i - \mathbf{x}_j) \tag{2.2}$$

In particular, when $\mathbf{M}$ is a diagonal matrix, the previous formula becomes:

$$M = \begin{pmatrix} M_1 & & & & \\ & \ldots & & 0 & \\ & & M_t & & \\ & 0 & & \ldots & \\ & & & & M_T \end{pmatrix} \tag{2.3}$$

$$d_M(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{\sum_{t=1}^{T} M_t (x_{it} - x_{jt})^2} \tag{2.4}$$

Intuitively, each dimension difference $(x_{it} - x_{jt})$ is weighed by a factor M_t. In the following of the work, we consider the standard Euclidean distance as the amplitude-based distance d_A.

Prendre le GRAPHIQUE GENERAL et faire le calcul des distances entre les courbes et montrer que pour 2 courbes qui ont des "amplitudes proches", on obtient une valeur de distance faible.

2.2.2 Behavior-based metrics

The second category of metrics aims to compare time series based on their shape or behavior despite the range of their amplitudes. By time series of similar behavior, it is generally intended that for all periods $[t, t']$, they increase or decrease simultaneously with the same growth rate. On the contrary, they are said of opposite behavior if for all $[t, t']$, if one time series increases, the other one decreases and (vise-versa) with the same growth rate in absolute value. Finally, time series are considered of different behaviors if they are not similar, nor opposite. Many applications refer to the Pearson correlation [AT10]; [Ben+09] for behavior comparison. A generalization of the Pearson correlation is introduced in [DCA11]:

$$cort_r(\mathbf{x}_i, \mathbf{x}_j) = \frac{\sum (x_{it} - x_{it'})(x_{jt} - x_{jt'})}{\sqrt{\sum (x_{it} - x_{it'})^2}\sqrt{\sum (x_{jt} - x_{jt'})^2}} \tag{2.5}$$

where $|t - t'| \leq r$, $r \in [1, ..., T - 1]$.

It computes the sum of growth rate between $\mathbf{x}_i$ and $\mathbf{x}_j$ between all pairs of values observed at $[t, t']$ for $t' \leq t + r$ (r-order differences). The value $cort_r(\mathbf{x}_i, \mathbf{x}_j) = 1$ signifies that $\mathbf{x}_i$ and $\mathbf{x}_j$ have similar behavior. The value $cort_r(\mathbf{x}_i, \mathbf{x}_j) = -1$ means that $\mathbf{x}_i$ and $\mathbf{x}_j$ have opposite behavior. Finally, $cort_r(\mathbf{x}_i, \mathbf{x}_j) = 0$ expresses that their growth rates are stochastically linearly independent (different behaviors).

When $r = 1$, Eq. (2.5) leads to the temporal correlation coefficient *cort* [DCA11]. When $r = T - 1$, it leads to the Pearson correlation. As $cort_r$ is a similarity measure, it can be transformed into a dissimilarity measure:

$$d_B(\mathbf{x}_i, \mathbf{x}_j) = \frac{1 - cort_r(\mathbf{x}_i, \mathbf{x}_j)}{2} \tag{2.6}$$

Prendre le GRAPHIQUE GENERAL et faire le calcul des distances entre les courbes et montrer que pour 2 courbes qui ont des "formes proches", on obtient une valeur de distance faible.

2.2.3 Frequential-based metrics

Voir Michèle s'il faut réécrire

The third category, commonly used in signal processing, relies on comparing time series based on their frequential properties (e.g. Fourier Transform, Wavelet, Mel-Frequency Cepstral

Coefficients) [SS12]; [TC98]; [BM67]. In our work, we limit the frequential comparison to Discrete Fourier Transform [Lhe+11], but other frequential properties can be used as well. Thus, for time series comparison, first $\mathbf{x}_i$ are transformed into their Fourier representation $\tilde{\mathbf{x}}_i = [\tilde{x}_{i1}, ..., \tilde{x}_{iF}]$, with $\tilde{x}_{if}$ the complex component at frequential index f. The Euclidean distance is then used between their respective complex number modules $\tilde{x}_{if}$, noted $|\tilde{x}_{if}|$:

$$d_F(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{\sum_{f=1}^{F}(|\tilde{x}_{if}| - |\tilde{x}_{jf}|)^2} \tag{2.7}$$

Prendre le GRAPHIQUE GENERAL et faire le calcul des distances entre les courbes et montrer que pour 2 courbes qui ont des "spectres proches", on obtient une valeur de distance faible.

2.2.4 Other metrics and Kernels for time series

A faire à la fin, pas urgent

- Il existe dans la littérature de nombreuses autres métriques pour les séries temporelles (laisser la porte ouverte).
- Certaines métriques sont utilisées dans le domaine temporelle
- D'autres métriques sont utilisés dans d'autres représentations (Wavelet, etc.)
- Certaines combinent la représentation temporelles et fréquentielles (Représentation spectrogramme en temps-fréquence)
- Se baser sur l'article "TSclust : An R Package for Time Series Clustering".
- Fermer le cadre : dans la suite de notre travail, on ne va pas les utiliser mais elles pourront être intégrées dans le framework qui suivra au chapitre suivant

2.3 Time series alignment and dynamic programming approach

In some applications, time series needs to be compared at different time instants t (i.e. energy data [Naj+12]) whereas in other applications, comparing time series on the same time instants t is essential (i.e. gene expression [DCN07]). When time series are asynchronous (i.e. varying delays or dynamic changes), they must be aligned before any comparison or analysis process. The asynchronous effects can be of various natures: time shifting, time compression or time dilatation. For example, in the case of voice recognition (Fig. 2.2), it is straightforward that

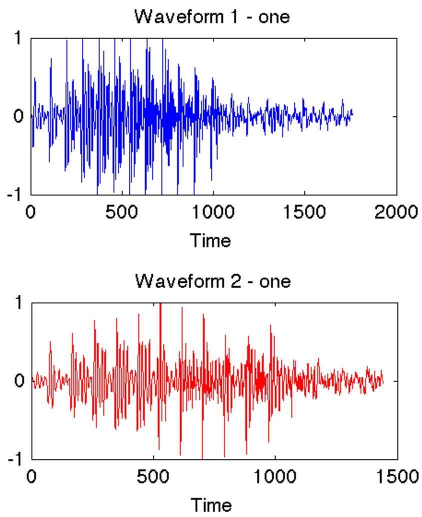

Figure 2.2: Example of a same sentence said by two different speakers. Time series are shifted, compressed and dilatated in the time.

a same sentence said by two different speakers will produce different time series: one speaker may speak faster than the other; one speaker may take more time on some vowels, etc.

Proposer une figure plus évidente ou plus simple?

To cope with delays and dynamic changes, dynamic programming approach has been introduced [BC94b]. Let $\mathbf{x}_i = (x_{i1}, ..., x_{iT})$ and $\mathbf{x}_j = (x_{j1}, ..., x_{jT})$ be two time series of time length T. An alignment $\boldsymbol{\pi}$ of length $|\boldsymbol{\pi}| = m$ between two time series $\mathbf{x}_i$ and $\mathbf{x}_j$ is defined as the set of m $(T \leq m \leq 2T-1)$ couples of aligned elements of $\mathbf{x}_i$ to m elements of $\mathbf{x}_j$:

$$\boldsymbol{\pi} = ((\pi_i(1), \pi_j(1)), (\pi_i(2), \pi_j(2)), \ldots, (\pi_i(m), \pi_j(m))) \tag{2.8}$$

where the applications π_i and π_j defined from $\{1, ..., m\}$ to $\{1, ..., T\}$ obey the following boundary monotocity conditions:

$$1 = \pi_i(1) \leq \pi_i(2) \leq ... \leq \pi_i(m) = T \tag{2.9}$$
$$1 = \pi_j(1) \leq \pi_j(2) \leq ... \leq \pi_j(m) = T \tag{2.10}$$

$\forall l \in \{1, ..., m\}$,

$$\pi_i(l+1) \leq \pi_i(l) + 1 \tag{2.11}$$
$$\text{and} \quad \pi_j(l+1) \leq \pi_j(l) + 1 \tag{2.12}$$
$$\text{and} \quad (\pi_i(l+1) - \pi_i(l)) - (\pi_j(l+1) - \pi_j(l)) \geq 1. \tag{2.13}$$

Intuitively, an alignment $\boldsymbol{\pi}$ defines a way to associate elements of two time series. Alignments can be described by paths in the $T \times T$ grid that crosses the elements of $\mathbf{x}_i$ and $\mathbf{x}_j$ (Fig. 2.3). We denote $\boldsymbol{\pi}$ a valid alignment and A, the set of all possible alignments between $\mathbf{x}_i$ and $\mathbf{x}_j$

($\boldsymbol{\pi} \in A$). To find the best alignment $\boldsymbol{\pi}^*$ between two time series $\mathbf{x}_i$ and $\mathbf{x}_j$, the Dynamic Time Warping (DTW) algorithm has been proposed [KR04]; [SC].

DTW requires to choose a cost function φ to be optimised, such as a dissimilarity function (d_A, d_B, d_F, etc.). Classical DTW uses the Euclidean distance d_E as the cost function [BC94a]. The warp path is optimize for the chosen cost function:

$$\pi^* = \underset{\pi \in A}{\operatorname{argmin}} \frac{1}{|\boldsymbol{\pi}|} \sum_{(t,t') \in \boldsymbol{\pi}} \varphi(x_{it}, x_{jt'})$$

Note that when the cost function φ is a similarity measure, the optimization involves maximization instead of minimization. The warped signal $\mathbf{x}_{i,\boldsymbol{\pi}}$ and $\mathbf{x}_{j,\boldsymbol{\pi}}$ are defined as:

$$\begin{aligned} \mathbf{x}_{i,\boldsymbol{\pi}} &= (x_{i\pi_i(1)}, ..., x_{i\pi_i(m)}) \\ \mathbf{x}_{j,\boldsymbol{\pi}} &= (x_{j\pi_j(1)}, ..., x_{j\pi_j(m)}) \end{aligned}$$

When other constraints are applied on $\boldsymbol{\pi}$, Eq. (2.3) leads to other variants of DTW (Sakoe-Shiba [SC78], Itakura parallelogram [RJ93]).

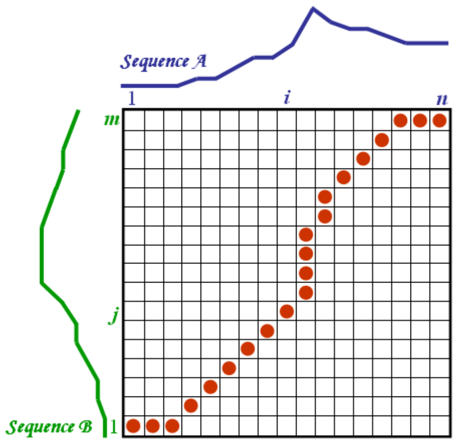

Figure 2.3: Example of DTW grid

The previous metric (amplitude-based d_A, behavior-based d_B) can be then computed on the warped signals $\mathbf{x}_{i,\boldsymbol{\pi}^*}$ and $\mathbf{x}_{j,\boldsymbol{\pi}^*}$. In the following, we suppose that the best alignment $\boldsymbol{\pi}^*$ is found. For simplification purpose, we refer $\mathbf{x}_{i,\boldsymbol{\pi}^*}$ and $\mathbf{x}_{j,\boldsymbol{\pi}^*}$ as $\mathbf{x}_i$ and $\mathbf{x}_j$.

Doit-on développer + sur la DTW comme par exemple, donner l'algorithme?

Prendre le GRAPHIQUE GENERAL et faire le calcul des distances entre les courbes et montrer que pour 2 courbes qui ont des "valeurs proches" mais décalés, on obtient une valeur de distance faible. (prendre DTW standard avec une fonction de coût D_E par exemple)

2.4 Multi-scale aspect

J'ai repris ce que ahlame avait marqué dans le papier PRL mais faudrait il réécrire?

The systematic requisite of the total time series elements in Eqs. 2.1, 2.6 and 2.7, restricts the measures potential to capture local temporal differences, as illustrated in Fig. 2.4. This section provides a multi-scale framework for time series comparison, crucial to capture latent local, as well as global discriminative features. Many methods exist in the literature such as the dichotomy or the sliding window. We detailed here the dichotomy process used in our work.

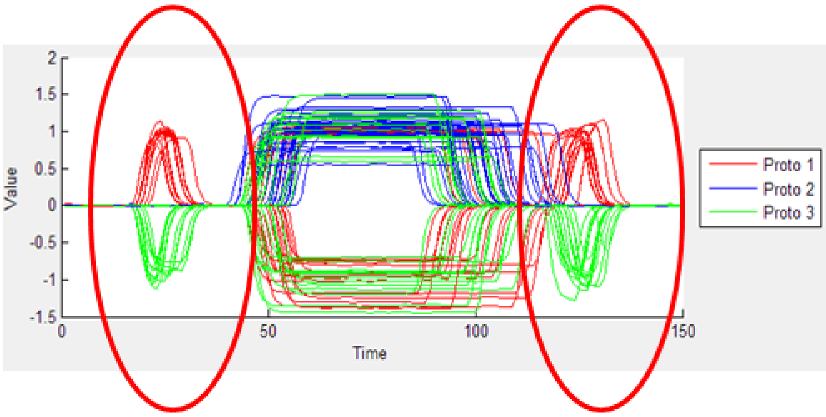

Figure 2.4: UMD dataset. The dataset is made of 3 classes : Up, Middle and Down. The 'Up' class has a characteristic upward bell at the beginning or at the end of the time series. The 'Down' class has a characteristic downward bell at the beginning or at the end of the time series. The 'Middle' class has no characteristic bell. Circle red show the region of interest of these bells. This region are local and standard global metric fails to show these characteristics.

A multi-scale description is obtained by repeatedly segmenting a time series expressed at a given temporal scale to induce its description at a coarser level. The segmentation process refers to different approaches that mainly assume fixed either the number of the segments or their lengths. A multi-scale comparison is then obtained by comparing time series, based on usual measures, through several segments of different temporal granularities. For a multi-scale amplitude-based comparison based on binary segmentation, Figure 2.5 shows the set of involved amplitude-based measures d_A^{Is}. The local behaviors- and frequential- based measures d_B^{Is} and d_F^{Is} are obtained similarly.

2.5 Conclusion of the chapter

To cope with specificities inherent to time series, we review in this chapter several basic metrics dedicated to time series. Depending on the considered modality (amplitude, behavior, frequency), adapted metrics for time series have been proposed in the literature such as the Euclidean distance d_A, the Temporal correlation d_B or the Fourier-based distance d_F.

In practice, real time series may be subjected to delays. Thus, they need to be re-aligned

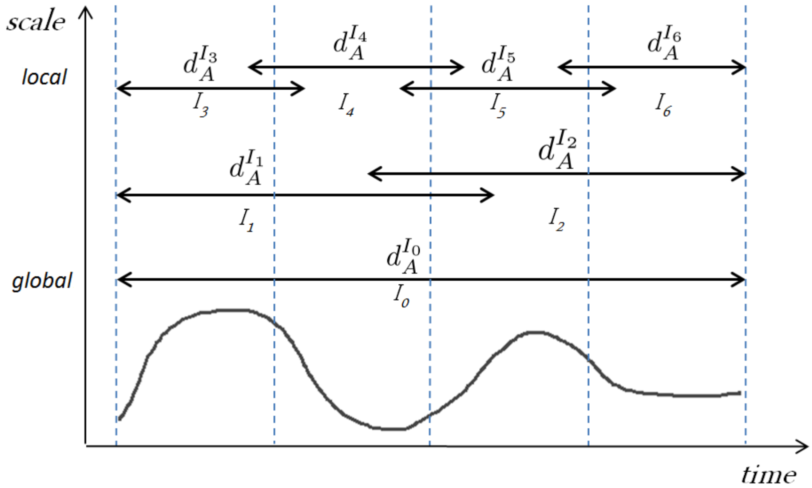

Figure 2.5: Multi-scale amplitude-based measures $d_A^{I_s}$

before any analysis task. For that, the Dynamic Time Warping (DTW) algorithm has been proposed. Finally, to capture local characteristics, the previous metrics (d_A, d_B, d_F) can be computed on smaller intervals. Many strategies exist such as the dichotomy or the sliding window.

However, all of these metrics only include one modality and at a particular scale. Generally, several modalities may be implied. In the next chapter, we review some advanced metrics. First, we recall some combined metrics that have been proposed in the literature. They mainly combine the Euclidean distance d_A and the Temporal correlation d_B. After that, we will take an insight on Metric Learning approaches which aims to learn a metric that makes closer samples that are expected to be similar, and far away those expected to be dissimilar.

Chapter 3

Time series advanced metrics

Sommaire

3.1 Combined metrics for time series **43**
3.2 Metric Learning: state of the art **45**
3.2.1 Intuition 45
3.2.2 Problem formalization 45

Chapeau introductif

- Objectif : Trouver une distance, combinaison des distances basiques qui donne une bonne classification k-NN sur une base de données.
- Pourquoi une distance combinée? Dans le cadre de données réelles, plusieurs modalités peuvent être impliquées (forme, valeur, fréquence), de manière globale ou locale.
- Dans le cadre des données réelles, plusieurs composantes/modalités peuvent être impliqués (forme, valeur, fréquence). = attribut (feature) en traitement du signal. Hypothèse : valeur sur une série complète, sur un intervalle ou sur une fenêtre (dans le cadre des métriques à base fréquentielle).

3.1 Combined metrics for time series

- Certains travaux dans la littérature propose des combinaisons : linéaire, exponentielle, sigmoïde.
- Limites:
  - Implique que 2 modalités et au niveau global. Pour intégrer d'autres modalités et à d'autres échelles, il faut changer la formule et ajouter de nouveaux hyper-paramètres à optimiser → l'apprentissage de ces paramètres est plus long.
  - La combinaison est définie a priori
  - La combinaison est indépendante de la tâche d'analyse.

– Pour répondre à ces problèmes, certains auteurs proposent d'apprendre une métrique en vue de la tâche d'analyse considérée (classification, régression, clustering).

In most classification problems, it is not known in advance if time series of a same class exhibits same characteristics based on their value or behavior components alone. In some cases, both components (value and behavior) may be useful. Given an optimal alignment $\boldsymbol{\pi}^*$, to define a metric D covering both the behavior d_B and amplitude components d_A, some authors proposed some combined models under the form:

$$D(\mathbf{x}_i, \mathbf{x}_j) = f(d_A(\mathbf{x}_i, \mathbf{x}_j), d_B(\mathbf{x}_i, \mathbf{x}_j)) \tag{3.1}$$

where d_A and d_B refers respectively to amplitude and behavior-based metrics defined in section **??** and $f(d_A, d_B)$ is an adaptive function. In the case that f is a linear combination (ref):

$$f(d_A, d_B) = \alpha.d_B + (1 - \alpha).d_A \tag{3.2}$$

where $\alpha \in [0; 1]$ is a parameter that defines the contributions of the behavior and value components. When $\alpha = 0$, the combined metric includes only the value component. For $\alpha = 1$, it includes only the behavior component. A second combined form for f is the geometric combination (ref):

$$f(d_A, d_B) = d_B^{\alpha}.d_A^{1-\alpha} \tag{3.3}$$

In this case, the parameter α has the same interpretation as in the linear combination. A third model for f was proposed by Douzal-Chouakria & Al. in [DCA11]:

$$f(d_A, d_B) = \frac{2.d_A}{1 + exp(\alpha.d_B)} \tag{3.4}$$

where α is a parameter that defines the compromise between behavior and value components. When α is fixed to 0, the metric only includes the value proximity component. For $\alpha \geq 6$, the metric completely includes the behavior proximity component.

Depending on the application, one can choose the compromise α between the value and the behavior component. For a given learning algorithm, the parameter α can be optimized by a grid search procedure. However, these combinations are defined independently from the analysis task at hand. Moreover, only two variables are taking into account in the metric. Finally, in the case of the model D_{sig}, the component $cort_r$ can be seen as a penalizing factor of DTW. It doesn't represent a real compromise between value and behavior components. To overcome these limits, other authors propose to learn the metric D for a robust k-NN classifier.

3.2 Metric Learning: state of the art

- Placer le contexte : travaux réalisés dans le cadre de la classification de données statiques.
- Présenter l'intuition du Metric Learning sur la base des travaux de Weinberger.
- Donner la terminologie (target, imposter, push, pull)
- Objectif : push des imposters et pull des targets
- Formalisation du problème (optimisation)
- Limites:
  - On apprend les poids d'une distance de Mahalanobis
  - L'apprentissage ne prend pas en compte l'aspect multi-modal dans les données

3.2.1 Intuition

3.2.2 Problem formalization

Conclusion of Part I

This first part of the manuscript presents a state of the art of classic Machine Learning framework and algorithms to make the classification or the regression of time series. We note that the considered algorithms (k-Nearest Neighbors (k-NN), Support Vector Machine (SVM)) are based on the comparison of time series through distance measures.

Considering time series as static data lead to compare time series only the comparison of their amplitude and the same time instant between the two considered time series. To take into account other characteristics of time series, other metrics (e.g., the temporal correlation d_B, the frequential-based distance d_F, etc.) and other methods (Dynamic Time Warping DTW, dichomotie) have been proposed to cope with these temporal characteristics.

Learning an adequate metric is a key challenge to well classify time series. Inspired by Metric Learning work for static data, we propose in the following a framework to learn a Multi-modal and Multi-scale Metric for a robust nearest neighbor classifier of time series.

Part II

Metric learning for time series from multiple modalities and multiple scales

The first part has enlightened the importance of combining several modalities and several scales to compare time series in order to make a better classification. We propose, in this part, a framework to learn this metric. For that, the idea is to define a new space representation, the pairwise space, where a vector is a pair of time series which is described by the basic metrics. Then, we formalize the problem of learning the metric as an optimization problem and show its equivalence by solving an adequate SVM problem. In the first chapter, we present this pairwise representation and gives interpretation in this new space. In the second chapter, we formalize the optimization problem and its adapted SVM equivalence. In the third chapter, we present the details of the algorithm. In the final chapter, we experiment our proposed approach on datasets, discuss and interpret the results.

Chapter 4

Projection in the pairwise space

Sommaire

4.1 Pairwise embedding 51
4.2 Interpretation of the pairwise space 51
4.3 Pros & Cons 52

Chapeau introductif

- Le calcul d'une métrique implique toujours 2 individus. On va proposer un changement d'espace, un nouvel espace : la représentation par paire.
- Le cadre : on suppose que l'on a p métriques.

4.1 Pairwise embedding

- Changement de l'espace
- Normalisation de l'espace des paires
- Label des pairwise

4.2 Interpretation of the pairwise space

- Proximity to the origin (les individus sont identiques)
- Proximity of 2 pairwise points in the pairwise space
- Norm in the pairwise space
- Representation of combined metric in the pairwise space

4.3 Pros & Cons

- perte de la classe initiale des individus. L'information qui nous reste est : les 2 individus sont de la même classe ou sont de classes différentes.

CHAPTER 5

M^2TML: formalization

Sommaire

5.1 LP optimization problem **53**
5.2 QP optimization problem **53**
5.3 SVM approximation **53**

Chapeau introductif

- Rappeler : quel problème on résout : pull des targets et push des individus de classes différentes
- Formaliser le problème général avec D

5.1 LP optimization problem

- Formaliser le problème sous forme d'un problème d'optimisation sous contraintes

5.2 QP optimization problem

- Passer de la forme LP (forme primale) et par transformation, arriver à la forme duale
- Montrer les similitudes avec la résolution SVM
- Montrer que l'on peut kerneliser la méthode

5.3 SVM approximation

- Faire remarquer que le problème LP ressemble à un problème SVM
- Faire la démonstration de l'équivalence (ou mettre la démonstration en annexe).

- Expliquer les différences entre la résolution LP/QP et la résolution SVM. (ajout de sur-contraintes dans le problème SVM)
- Expliquer pourquoi on va préférer le cadre SVM. Expliquer mathématiquement et avec des interprétations géométriques.
- Cadre connu
- Utilisation de librairie standard de Machine Learning
- Extension directe à l'apprentissage de métrique non linéaire grâce au kernel trick

Chapter 6

M^2TML: implementation

Sommaire

6.1 **Projection in the pairwise space** **55**
6.2 **M-NN M-diff strategy** **55**
6.3 **Radius normalization** **56**
6.4 **Solving the SVM problem** **56**
6.5 **Definition of the dissimilarity measure** **56**
6.6 **Extension to regression problem** **56**
6.7 **Extension to multivariate problem** **56**

Chapeau introductif :

- Quel problème on résout?
- Donner les étapes principales de résolution (sous forme de puces). Cela doit rester général, clair et concis.
- Développer dans chaque section les puces énumérés précédemment.

6.1 Projection in the pairwise space

- Projection
- Log normalization

6.2 M-NN M-diff strategy

- Expliquer les différentes stratégies (k-NN VS All / M-NN VS M-diff / k-NN VS Imposters)
- Expliquer pourquoi on va choisir une stratégie M-NN VS M-diff

6.3 Radius normalization

- Expliquer le problème de la non-homogénéité des radius.
- Expliquer comment on résout ce problème par une normalisation des radius de chaque voisinage.

6.4 Solving the SVM problem

- Expliquer l'apprentissage avec le SVM.
- Utilisation de la version L1 du SVM pour avoir une solution sparse.

6.5 Definition of the dissimilarity measure

- Produit scalaire
- Papier PR : norme pondérée x fonction exponentielle
- Version Sylvain : norme x fonction exponentielle?

6.6 Extension to regression problem

(To do)

6.7 Extension to multivariate problem

(To do)

Chapter 7

M^2TML: Experiments

Sommaire

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7.3 Results 57
7.4 Discussion 57

Chapeau introductif

- Application sur des bases de séries temporelles univariés de la littérature (Keogh)
- Données Schneider? ou Expliquer les problématiques de Schneider

7.1 Dataset presentation

7.2 Experimental protocol

7.3 Results

7.4 Discussion

Conclusion of Part II

Conclusion and perspectives

- Bilan des apports de la thèse
- Perspectives
  - Multi-pass learning
  - Kernel pour la résolution du problème QP
  - Utilisation de la distance apprise dans d'autres algorithmes de machine learning (Arbre de décision) pour obtenir une interprétabilité?
  - Utilisation d'autres distances (wavelets, etc.)
  - Apprentissage locale de la métrique

Appendix A

Detailed presentation of the datasets

Appendix B

Solver library

Appendix C

SVM librairy

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Mots clés : Série temporelle, Apprentissage de métrique, k-NN, SVM, classification, régression.

Abstract — Lorem ipsum dolor sit amet, consectetur adipiscing elit. Sed non risus. Suspendisse lectus tortor, dignissim sit amet, adipiscing nec, ultricies sed, dolor. Cras elementum ultrices diam. Maecenas ligula massa, varius a, semper congue, euismod non, mi. Proin porttitor, orci nec nonummy molestie, enim est eleifend mi, non fermentum diam nisl sit amet erat. Duis semper. Duis arcu massa, scelerisque vitae, consequat in, pretium a, enim. Pellentesque congue. Ut in risus volutpat libero pharetra tempor. Cras vestibulum bibendum augue. Praesent egestas leo in pede. Praesent blandit odio eu enim. Pellentesque sed dui ut augue blandit sodales. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae; Aliquam nibh. Mauris ac mauris sed pede pellentesque fermentum. Maecenas adipiscing ante non diam sodales hendrerit. Ut velit mauris, egestas sed, gravida nec, ornare ut, mi. Aenean ut orci vel massa suscipit pulvinar. Nulla sollicitudin. Fusce varius, ligula non tempus aliquam, nunc turpis ullamcorper nibh, in tempus sapien eros vitae ligula. Pellentesque rhoncus nunc et augue. Integer id felis.

Keywords: Time series, Metric Learning, k-NN, SVM, classification, regression.

Schneider Electric
Université Grenoble Alpes, LIG
Université Grenoble Alpes, GIPSA-Lab