Graduate Program in Electrical Engineering

# TRANSDUCTION BASED APPROACHES FOR DATASET SHIFT PROBLEMS

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Nous ne pouvons pas construire un monde meilleur sans améliorer les individus. Dans ce but, chacun de nous doit travailler à son propre perfectionnement, tout en acceptant dans la vie générale de l'Humanité sa part de responsabilités.

---

Marie Curie, in *Madame Curie*, by Ève Curie (1937)

# ABSTRACT

*Dataset Drift* problems occur in every field that extract or adjust models from data. It is named *drift* the phenomena which causes the training and testing datasets to differ, and may also appear at any time during the model real application. In this context, approaches using Transductive learning were proposed to solve classification problems under some *Dataset Drift* scenarios. Two strategies were defined, and present satisfactory results with some limitations. The first one is based on an Essentially Transductive Approach that uses genetic algorithm to optimize data entropy. The other one is a strategy oriented to two-dimensional spatial datasets based on Gabriel Graphs for the estimation of Gaussian Mixture Models. However, the correct analysis if the model under a drift is not systematically performed, thus the experimentation of the methods was done with study cases.

# RESUMO

O problema do *Dataset Drift* ocorre em toda e qualquer área que utilize dados para criar ou ajustar modelos. É chamado de *drift* o fenômeno que faz com que haja alguma diferença entre os dados de treinamento e os de teste, além de se manisfestar em qualquer momento no ambiente de aplicação real do modelo. Nesse contexto são sugeridas abordagens utilizando aprendizado transdutivo para lidar com o *Dataset Drift*. Duas estratégias foram definidas e apresentam resultados satisfatórios com algumas limitações. A primeira é baseada em uma Abordagem Essencialmente Transdutiva que utiliza um algoritmo genético para a otimização da entropia dos dados. A outra é uma estratégia orientada a problemas espaciais bidimensionais, baseada em Grafos de Gabriel para a estimação de Modelos de Mistura Gaussiana. No entanto, a análise da qualidade dos modelos perante a presença do *drift* ainda não é realizada de forma sistemática, dessa forma os experimentos foram feitos com estudos de caso.

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# 1 INTRODUCTION

The future is already here - it's just not very evenly distributed.

Willian Gibson, *"The Science in Science Fiction" on Talk of the Nation, NPR (30 November 1999, Timecode 11:55)*

Data, at present, is generated in great amounts and with great speed. The systems which generate these data have become complex in such way that their modelling require advanced techniques and methodologies that extract information from data itself. Strategies to learn from data are present in a large variety of research fields such as Machine Learning, Data Mining, Statistics, System Identification, among others, and have application in vast range of problems including biomedical, financial, information science, ecology, industrial automatic control, computer vision, game development and entertainment. In this context, the importance of correct information extraction from data is widely related to the efficiency of the final application, which could be the diagnosis of a certain disease, credit approval system, optimal automation of an industrial plant, visual recognitions for video game consoles such as Kinect, etc.

Machine Learning methods allows automated models building, with the knowledge extracted directly from data. In this science field, the machine, or computer, is able to learn information through data analysis, unveiling hidden insights, which could not be immediately perceived, without necessarily being explicitly programmed for that. Usually, in this field, it is desired to generate a model that is capable of imitating an unknown system with the objective of: (a) label unknown data as the original system would, which defines classification models; (b) return de output for a given input according to the original system function, which occurs in function regression or time series prediction; or (c) grouping data according to its intrinsic characteristics, which is performed by unsupervised clustering algorithms. There are several methods and strategies for each of these types of machine learning algorithms, nevertheless all of them have as a common characteristic the fact that they all extract information from data and create stochastic models. Additionally, several other fields extract information from data, although each one have different objectives to reach.

Learning from data, either in Machine Learning or any other field, has a number of particularities that must be properly managed regarding its stochastic characteristics. As data itself, even if generated from the same system, tends not to be stationary, the modelling of the system needs strategies to either adapt to data as it is provided or to be robust to any variations of the data, whatsoever they may be. In real world scenarios, non-stationarity is an issue which occurs naturally in most of systems, intrinsic characteristics or even external factor might change its behaviour and, thus, the data it generates. Considering modelling strategies that uses data to generate its models, this variation implies that the model will eventually become inadequate.

In a broad definition, the phenomena where the data generated by any system changes, either slowly or abruptly, is named *Dataset Shift*. This becomes a serious issue since the model created for these systems become unfit for its actual application. In Machine Learning contexts, some initial data is required to create the model that will be applied, later, to the system, either to classify new data, cluster new sets or mimic the system output values according to its function regression. The model is then, created according

to a very specific set of data and, if the application, or testing, data was actually generated differently the classification, clustering or regression are simply wrong and may not lead to the correct outputs.

*Dataset Drifting* problem is a serious issue in several applications, since it causes models response to degrade in the application space, not because of an internal degeneration, but due to a modification in the input and output relation. Despite the existence of robust and adaptive methods, which work well for some specific scenarios, the drifting context more comprehensive then noise issues or an systematic input variation. More forebodingly, dataset drift might occur in data in unexpected manners but, still, the models should be able to extract the necessary information. It is precisely the nature of this needed information that defines if a simpler robust or adaptive is enough or a more complex approach for dataset drift is necessary. Defining and setting the modelling methodology depends on what is needed to be known and the drifts affects it.

The dataset shifting may occur for several reasons, the system could be non-stationary and gradually suffers changes in time, which is common in industrial plants where there are sensors and actuators degradation. Another situations occurs when the training data is obtained in a context different from the actual application data, for instance an image recognition system which was trained with different lighting conditions from the application. The speed of the shift also raises an important issue, since it interferes in the difficulty of actually detecting or adapting to it. When the data suffers a fast unexpected change it is called abrupt and a tendency which slowly changes data is named a gradual shift, they can both occur in the same system simultaneously, for instance a greenhouse or a clean room temperature control system has to adapt to the weather of all the seasons of the year, which gradually raises and lowers the temperature consisting in a gradual shift, however any possible fault on a fan or air conditioning would be an abrupt shift that should be considered in the system.

Despite all of the reasons and forms of shifts, they can be defined statistically according to its distribution characteristics. Thus, a systematic approach for detecting and adapting or disregarding it could be properly designed. This work premise is that, with an appropriate employment of statistical data distribution testing and statistical model adaptation, the dataset shift issue could be minimized, as an intermediate stage, for different modelling strategies and methods from different fields.

Given that different types of dataset shifts can be categorized according to their effects over the data statistical distributions, in disregard of the reason or the velocity of the shift, not only the occurrence of a given shift can be detected but also the identification of which type of shift can performed. There is a consequential relation between shift types and their reason for appearing, thus the identification of shift lead to the unveiling of its possible causes and, hence, might allow the correction, or the control, of the shift itself instead of its consequences.

Probability density estimation methods define the characteristics and parameters of a dataset distributions adjusting it to a known statistical distribution type, thereby it is possible, for instance to define the dataset distribution in different points and assert whether they are similar or if a shift occurred. Nonetheless, the comparison between distributions is not simple, and recognizing the specific difference between them might not even be possible, however measuring, in a quantitative manner, how similar they are can be promptly solved. The measure of the distance between two distributions can be achieved by their dissimilarity, analogously the similarity can be defined according to the distributions proximity.

Despite the categorization of the causes that lead to *Dataset Shifting*, the shift can be also defined according to its manifestation over the data statistical distribution and its effect on the model output, disregarding its specific cause. This allows particular methods and techniques to perform reasonably well for several types of Dataset Shifts even though their cause might differ. It can, then, be said that the shift reason is transparent to the model as it receives only raw data and perceives only the statistical information observable in it. In this context, the principal characteristic of the *Dataset Shift* is whether it occurs abruptly or gradually. Expressly, if changes on data distributions occur very fast in specific instants, thus being abrupt, or if it is a slow and constant deviation that affects data gradually.

However, there remains the need to define systematically how well the selected model is able to perform in different *Dataset Shift* conditions. Considering this, the main objective of this work is to delineate a series of procedures to test whether a model of interest behave under data shifting and measure the effect of different types of shifts on the models output. In this matter, a systematic quantitative measurement of the effects of the shift on the model enables a efficient analysis of the model components which, in fact, interfere in the performance of the model. For instance, it is possible to define if either the modelling methodology, or the metrics used, had any significance on the results achieved by the model. This topic does not have conclusive nor significant approaches in the literature, thus in this work it is proposed an strategy to systematically analyse models performance when subject to dataset drifting scenarios, based on stability criteria.

Considering the characteristics of the drifting problem, it is expected that semi-supervised and transductive approaches that uses both the training labelled and unlabelled testing or working datasets might lead to improved models. In this context, a transductive method in which a model is defined to work specifically in the current working set. In contrast to the traditional inductive approach, a general model is not generated from the particular testing data and for each working set a new model is defined. Thereby, a transductive method with statistical similarity metrics was implemented envisaging an improved performance in dataset drifting scenarios.

This thesis will be divided in six chapters, in which the first one is this introduction and the next chapters will have the following structure: the second chapter is a literature survey and will include an

comprehensive presentation of the Dataset Shift issues and approaches in literature and the necessary informations about the methods employed in this work; chapter 3 consists in the description and justifications of the approaches used to design the proposed methods for solving classification with data drifting; 4 chapter describes the proposed analysis strategies for experimental methodology; the fifth chapter contains results obtained by the test designed in previous chapters and also provides valid statistical analysis of results; in the last chapter, are the conclusions of this work and the future work.

# 2 LITERATURE REVIEW

Time is not a line but a dimension, like the dimensions of space

Margaret Atwood, *Cat's eye*

## 2.1 DATASET SHIFT

The formalization of machine learning methods according to statistical premisses and formulations is of great importance because it allows definitions of learning quality and risk. While stochastic methods, as most of Machine Learning methods are, can easily fall under computational methods with performance empirically proven, the incorporation of statistical learning theories to the field, for instance with [100], allows, then, theoretical foundations and analysis standardization. The risk limits concepts, can be used both as model training parameters or as criteria for model selection. This relation with statistical fundamentals require the statistical premisses to be met as well, however in real-world problems, these dependences might not be true as the datasets might not be easily defined, for instance the data distribution is commonly not defined and sometimes can not be well estimated. In this context, an issue that has been studied in recent years is the Dataset Shift, which defines the phenomena when the training dataset differs from the testing or application datasets.

Regarding learning problems, the main objective of function estimation is selecting a model capable of producing correctly the expected responses of a given system, usually named supervisor, according to specified inputs. Which is done, however, having as reference a limited set of examples of the supervisor behaviour [9], thus, the necessary and available components for modelling are:

1. A generator of random vectors $\mathbf{x}$, defined by a fixed and unknown distribution $P(x)$.
2. A supervisor which generates an output $y$ given an input $\mathbf{x}$, according to a fixed and unknown conditional distribution function $P(y|\mathbf{x})$;
3. A machine that implements a set of functions $f(\mathbf{x},\mathbf{w}), \mathbf{w} \in \Lambda$.

A machine learning problem consists in a correct function selection, within the set $f(\mathbf{x},\mathbf{w}), \mathbf{w} \in \Lambda$, that more accurately imitates the supervisor behaviour. In this context, the training set should be composed of independent identically distributed(i.i.d.) samples according to the distribution $P(\mathbf{x},y) = P(\mathbf{x})P(y|\mathbf{x})$ and should be sufficiently large to guarantee data representativeness.

The risk and loss functions relation is measured according to differences between the supervisor response - $y$ given $\mathbf{x}$ - and results provided by the learning machine - $f(\mathbf{x},\mathbf{w})$. Risk limits allow a consistent analysis of the learning premisses and, thus, allow several statistical learning method, at some degree, to be primarily assessed by a theoretical criteria. The real risk functional $R(\mathbf{w})$ can be represented by Equation 1. [102, 77, 67]

$$R(\mathbf{w}) = \int L(y, f(\mathbf{x},\mathbf{w}))p(\mathbf{x},y)dxdy \tag{1}$$

in which $L(y, f(\mathbf{x},\mathbf{w}))$ is a loss function or discrepancy, the approximation function is $f(\mathbf{x},\mathbf{w})$, and $(\mathbf{x},y)$ are pairs of inputs and outputs that must be completely described by a model. The joint probability

density function (pdf) given by $p(\mathbf{x}, y)$ should be known a priori. However, since the joint probability density function is usually unknown and only a limited set of input/output pairs $(\mathbf{x}, y)$ is actually available for evaluation, it is, then, necessary using an empirical risk function.

Furthermore, it exists another important reservation regarding PDFs used by machine learning model estimators. In real-world problems, training data and test data densities might significantly differ. Which characterizes a set of issues observed in machine learning and data mining named *Dataset Shift*. In this context, it is possible to notice a significant limitation in methods which premises consider training and test data to be i.i.d.. Breaking such premise imply in creating a model with a training set which is not representative of the actual testing data and, thus, the machine itself is not adequate for the final application [77, 67].

When considered the empirical risk of the Equation 2, proposed by [38], it is possible to define the sampling error and the approximation error according to the Equation 3. In this case, the *Dataset shift* should cause a distortion in the expected value $E[y|\mathbf{x}]$. Hence, it is expected a deterioration of the sampling and approximation errors.

$$R_{emp} = \frac{1}{N}\sum_{i=1}^{N}(y_i - f(\mathbf{x}_i, \mathbf{w}))^2 \tag{2}$$

$$E\left[(y - f(\mathbf{x}, \mathbf{w}))^2\right] = E\left[(y - E[y|\mathbf{x}])^2\right] + E\left[(f(\mathbf{x}, \mathbf{w}) - E[y|\mathbf{x}])^2\right] \tag{3}$$

in which the first term, given by $E\left[(y - E[y|\mathbf{x}])^2\right]$, is the sampling error and the second one, $E\left[(f(\mathbf{x}, \mathbf{w}) - E[y|\mathbf{x}])^2\right]$ represents the approximation error.

In case there is a shift in $p(y, \mathbf{x})$ there will be also a shift in the expected value of $y$, $E[y|\mathbf{x}]$, and therefore, a degradation in sampling and approximation errors given by Equation 3. This situation will happen when $P_{train}(y, \mathbf{x}) \neq P_{test}(y, \mathbf{x})$ [77, 67] as a result of dataset shift. Considering that the system is stationary, so $P(y|\mathbf{x})$ does not change, a shift in $P(y, \mathbf{x})$ can only be due to $P_{train}(\mathbf{x}) \neq P_{test}(\mathbf{x})$, characterized by a dataset shift, due to Equation 4.

$$P(y, \mathbf{x}) = P(y|\mathbf{x})P(\mathbf{x}) \tag{4}$$

There are several types of *Dataset Shift* which can be defined according to the differences between $P_{train}(y|\mathbf{x})$ and $P_{test}(y|\mathbf{x})$ or between $P_{train}(\mathbf{x})$ and $P_{test}(\mathbf{x})$ [67]. Other forms of "*shift*" might be related to the differences in mechanisms which causes differences in the data, for instance: the source that generated the training and test data might be slightly different, even if the data generated are intended to be the same; the data domain could have its significance or interpretation changed when the context changes from training to testing; the sampling my not be representative of the overall dataset; or even the class imbalance problem can be considered a type of *dataset shift* [77].

One important observation regarding the study of *Dataset Shift* is related to its nomenclature, there is a lack of agreement on names and terms used to appoint the same problems. In the machine learning context, *Dataset Shift* was widespread by [77]. However, other therms, such as *concept drift*, *concept shift*, *data fracture*, *reject inference*, among others, are used in different areas, as Statistics and Data Mining, to denominate very similar or even the same class of problems. Therefore, achieving a complete and extensive bibliographic review is rather overstraining [67].

The matter of a better agreement between the models, obtained through machine learning, and the real problems is of great importance on the field of computer intelligence, since it allows not only a better understanding of the real-world but also increases the control possibilities for these real systems. In the real-world the environment and the time are non-stationary, thus the *Dataset Shift* is natural and is present in several applications. However, in the Machine Learning field this subject has several limitations, for instance, the detection and automatic classification of the different types of shift that may appear in a problem is understudied, on the same context the methods that can deal simultaneously with more than one shift are very rare.

### 2.1.1 Types of Dataset Shift

The dataset shifting is a general problem that may affect several types of data very differently. Strictly, drifting occurs when the model training data form and intensity differ from the data that is actually used during the model testing or its real employment. More directly, shifting is considered when the phenomena that generates data undergoes some change in time.

The difference in the data distribution can unfold in very distinct manners, for instance, two different density functions can show a distribution of the same type but with other coefficients, or the distribution average and dispersion might be equivalent but the shape of the distribution could differ. In this context, a variety of different shifts exist and have particular characteristics, usually three categories are defined: covariate shift, prior-probability shift and concept shift.[82]

#### *Covariate Shift*

Covariate is a designation of the explanatory variable $x$. When the covariates future values are different from past observations, it occurs a specific type of dataset shift, named *Independent Covariate Shift* or simply *Covariate Shift* [90, 86]. This type of shifting occurs when only the distribution of $\mathbf{x}$ suffers some variation, and all the other probabilities are kept equal, thus, according to Equation 4, $P_{train}(y|\mathbf{x}) = P_{test}(y|\mathbf{x})$ but $P_{train}(\mathbf{x}) \neq P_{test}(\mathbf{x})$ As seen in Fig. 2.1, the relation between the target $y$ and the covariate $x$ remains the same for both classes, but the distribution of de covariate $P(\mathbf{x})$ changes. [86, 90, 77, 67].

In a streaming scenario this change could occur in any given time after the training, which was performed in a reference time instant $T$. Thus the covariate shift occurs when it is perceived a change in sampled data distribution between two consecutive time instants $P_{t-T}(y|\mathbf{x}) = P_{t+1-T}(y|\mathbf{x})$ but $P_{t-T}(\mathbf{x}) \neq P_{t+1-T}(\mathbf{x})$ [25].

This mismatch is very common and is considered a fundamental form of *Dataset Shift*. It could be said that it occurs when the mechanism that generates the data suffers some type of change in $P(x)$ between the training moment and the testing. Therefore it has a strong relation with time series prediction problems. In real-world prediction problems, it is common that the mechanism that generates data suffer changes in time, thus modifying the covariate density. However, it is not as likely that the phenomena which produces the output given the input, the conditional probability $P(y|\mathbf{x})$, suffer such changes. Moreover, simple survey experiments tend to also show this sort of issue, since $P_{train}(\mathbf{x})$ is determined by sampling schemes and $P_{test}(\mathbf{x})$ is set by the population [77, 86].

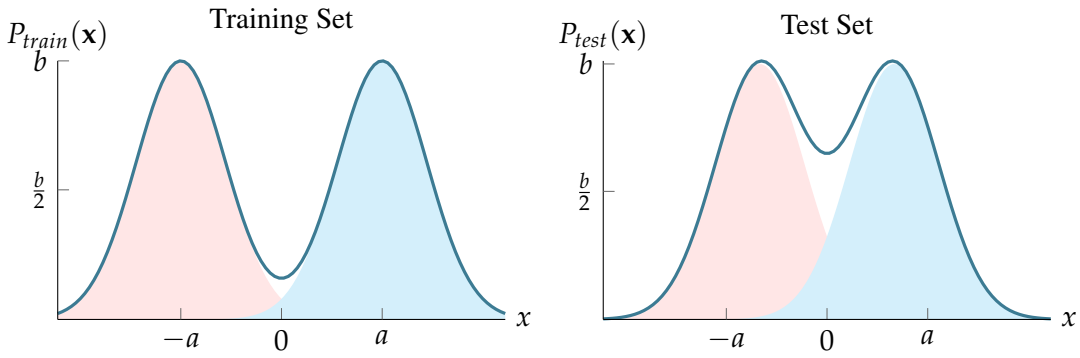



**Figure 2.1:** Covariate Shift: $P_{train}(y|\mathbf{x}) = P_{test}(y|\mathbf{x})$ and $P_{train}(\mathbf{x}) \neq P_{test}(\mathbf{x})$, where the distribution of class 0, $P(\mathbf{x}|y=0)P(y=0)$, is given in red and the distribution of class 1,$P(\mathbf{x}|y=1)P(y=1)$, is given in blue.

The covariate shift can be understood as a causal model where the covariate $x$ value has influence on the distribution of the targets $y$. In this case the prediction function and the noise model for the training and testing data, but the typical position of the data provided during the training is different from that applied to the tests. In figure 2.2, it is illustrated a causal model which training data are the dark dots and the test data are the lighter ones. In this example the principal data generating function is basically the same, but the covariate, $x$, position of the training data is different from the position of the testing data, which would lead to very different estimated models.

Referring to eq. 1 it is straight forward that the risk changes with covariate shift since the integration of the loss function $\mathcal{L}$ is performed with respect to a different portion of the input space. Let the model

risk be calculated over $m$ different datasets, which allows it to be understood as a random variable $\mathbf{R}$, with mean and variance:

$$E[\mathbf{R}] = E\left[(y - f(\mathbf{x}, \mathbf{w}))^2\right] = \frac{m-1}{m}\mu_2 \tag{5}$$

$$var(\mathbf{R}) = var\left[(y - f(\mathbf{x}, \mathbf{w}))^2\right] = \frac{(m-1)^2}{m^3}\mu_4 - \frac{(m-1)(m-3)}{m^3}\mu_2^2 \tag{6}$$

where

$$\mu_n = \int_{-\infty}^{\infty} (y - f(\mathbf{x}, \mathbf{w}))^n dP(x, y) \tag{7}$$

The integral of the power of the residual is performed with respect to the probability density, which, in the case of covariate shift, is understood as $P(x, y) = P(y|\mathbf{x})/P(\mathbf{x})$. Thus, the risk expected value and variance might converge to a different value, due to their dependence to the PDF of $\mathbf{x}$. Furthermore, in shift problems, the model might not be well defined for the input $x_test$, causing the loss function results to be unbounded and resulting in a larger variance.

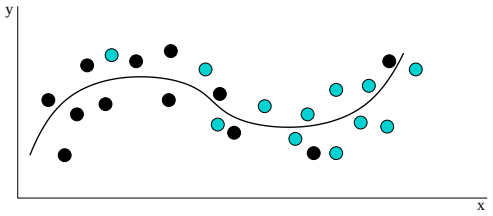
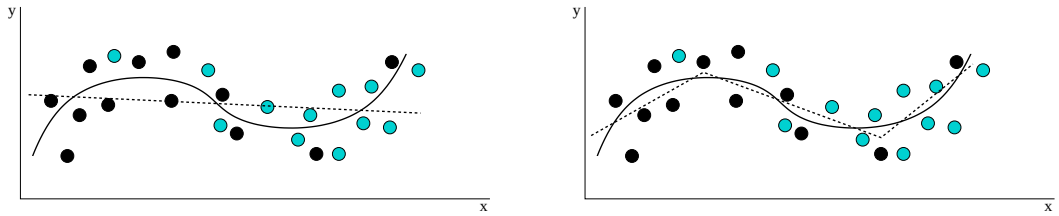



**Figure 2.2:** Dataset with causal relation between $x$ and $y$, in which training data are the darker dots and testing data are the lighter ones. This variation in the abscissa axis characterizes a covariate shift[77].

In this context, estimating a linear global model according to the training set would result in a very poor descriptor of the overall data, specially the test set. As seen in Figure 2.3a, the global estimation with a linear model of the dark dots training data, represented by the dashed line, is a poor fit for the overall data. Meanwhile, the linear local fits of the testing data, represented by the dashed lines in 2.3b, comprises of a completely different linear model. Shifts in the position of covariates in the input domain could lead to different models, since data might be restricted to a limited space in the domain. For instance, if the two dark dots farther left did not exist, the third local model would not exist as is. Nonetheless, a global model based on local linear models, here, still leads to a better estimation. Thus, in such cases, the local estimation of multiple models in the function domain could minimize error caused by shifts in the covariate placement.

Misspecified models occur when the covariate used for training the model are not representative of the testing set, furthermore, even if the models selected may not usually be completely representative of the global original system, it is possible to select a local model suitable for the testing data if the right region of the system domain is chosen. As seen in Figure 2.3, the sinusoidal function is not correctly defined by the model in 2.3a, even with data distributed in all of its domain because a linear model is a very poor fit.

However, even a linear fit would create an appropriate model to predict the test data if just the covariates in the correct range were used [77].




**(a)** The dashed line represents a global estimation of a linear model, and the solid line represents the causal generating function.

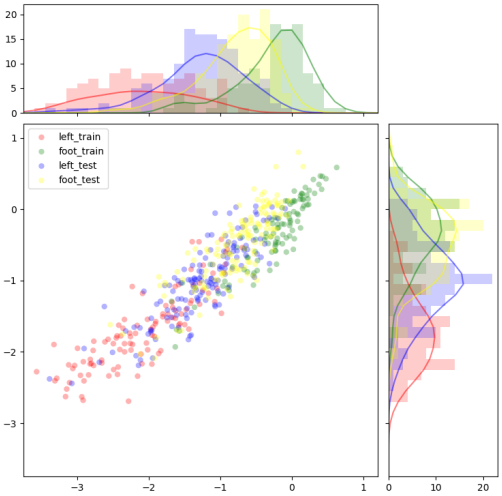
**(b)** Global model based on local linear models is shown in the dashed line, and the solid line is the representation of the generating function.

**Figure 2.3:** Misspecified models caused by covariate shift[77], Here, darker dots are the training set and the lighter ones are the test set.

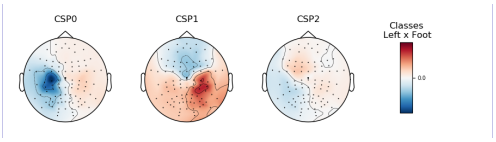
A typical example of covariate shift is its occurrence in the diagnosis of an individual future diseases given one's lifestyle. If someone has a drastic lifestyle change, it is possible that one's risk of developing certain diseases also change, however the probability that drives the development of these diseases within the population itself does not change. For instance, if a man becomes less sedentary it is more likely that his risk of developing a cardiovascular condition decreases, however the risk for sedentary people in general of developing such diseases does not change. Similarly, a health condition survey done within an university campus would not reflect the health status of the country population in general, since students tend to be in a healthier age range [77].

Brain-Computer Interfaces (BCIs) based in electroencephalograms (EEG) are another typical example often associated with covariate shift. In these systems, electrode placement, external stimuli, attention level, user fatigue and other endogenous factors may influence brain activity reading causing signals to be highly variable [83, 80, 84]. Furthermore, due to the complexity of training protocols and to pre-processing procedures, BCI systems are trained off-line. In [74] an ensemble based classifier was used to solve the problem in Fig. 2.4. EEG based BCI models tend to perform well if they are segmented into local models based in the covariate input space, therefore ensemble methods tend to outperform single models [60]. A typical example, in fig. 2.4, would be the Dataset IVc of the BCI Competition III [26, 55], where data of training and test sets were obtained with an interval between them.

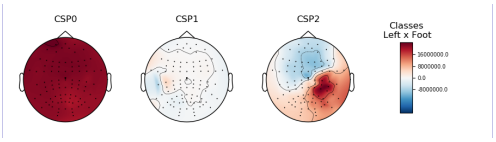
The *covariate shift* is a broadly studied in the literature. A purely discriminative solution for classification problems with *covariate shift* is proposed by [9], in which the learning was defined as an integrated optimization problem.




**(a)** Spatial distribution of the 2 principal features obtained with a Common Spatial Pattern filter for both classes in the training and test sets.




**(b)** Spatial representation of brain activity with Common Spatial Patterns features relative to the training set.




**(c)** Spatial representation of brain activity with Common Spatial Patterns features relative to the test set.

**Figure 2.4:** The distribution of each class differs greatly between training and testing.

### *Prior Probability Shift*

The prior probability shift is a type of *Dataset Shift* that occurs in models that have the assumption of a causal relation of the data, as it is the case of the Naive Bayes Classifier. In such cases the probability density function $P(y|\mathbf{x})$ is inferred through $P(\mathbf{x}|y)P(y)$. In this context, the a priori probability $P(y)$ might suffer some modification between the training and testing steps [77, 67]. More straightforwardly,

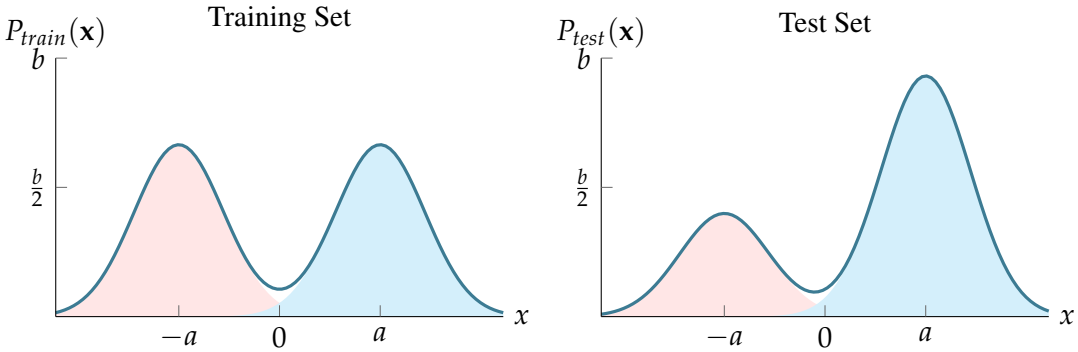
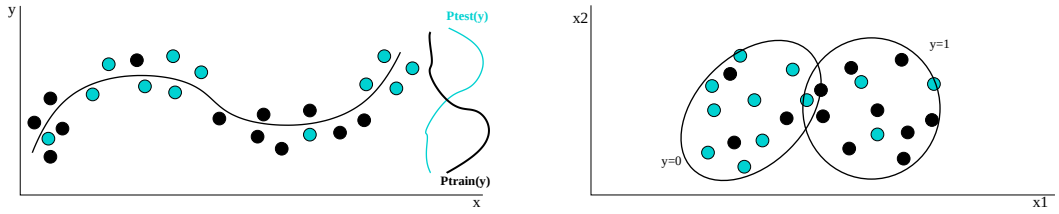



**Figure 2.5:** Prior Probability Shift: $P_{train}(\mathbf{x}|y=0) = P_{test}(\mathbf{x}|y=0)$ and $P_{train}(\mathbf{x}|y=1) = P_{test}(\mathbf{x}|y=1)$ but $P_{train}(y=0) \neq P_{test}(y=0)$ and $P_{train}(y=1) \neq P_{test}(y=1)$. Here, the distribution of class 0, $P(\mathbf{x}|y=0)P(y=0)$, is given in red and the distribution of class 1,$P(\mathbf{x}|y=1)P(y=1)$, is given in blue.

a prior probability shift occurs when the covariates $x$ are somehow dependent on the predictors $y$, thus causing the models vary according to any drifts between the distribution of the predictor during training

$P_{train}(y)$ and testing $P_{test}(y)$. According to Figure 2.6, a causal relation between the predictor $y$, interferes in the accuracy of a model if the predictor changes how the data is scattered in the domain between training and testing steps, i.e. even with similar $x$ covariates, the models for the training and testing data are different because the $y$ predictions do not have the same distribution in both cases. In Fig. 2.5, it is represented how the dependence of the covariate $x$ to the predictor $y$ causes a distortion on the covariate distribution according to changes in the predictor probability distribution, even if the distribution along the covariate $x$ has not changed.




**(a)** Prior Probaility Shift in a continuous funcion regrassion regression problem.

**(b)** Prior Priobability Shift in a conditional classification classification problem.

**Figure 2.6:** Graphical representation of prior probability shifts in datasets, where darker dots are the training set, the lighter ones are the test set. [77]

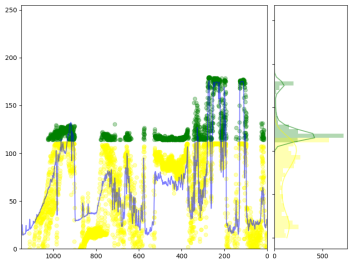
Since, in general, the priori probability of the test set is not known in most real-world problems, the prediction methods that are based in the Bayes Theorem are usually faulty and inadequate. Techniques of *cost -sensitive learning* present a strong relation to this type of *Dataset Shift*, therefore, with this approach, there are techniques more appropriated in dealing with problems that fall under this category. [67]

In practice, prior probability shifts in classification problems relate to differences in class balance between training and testing [40], and regression problem is represented in Fig. 2.7a.

Image capture systems often face overexposure or light saturation problems, which cause bright/dark spots in the image with low or even none information. In any light sensing system, the sensors are subject to saturation, and, despite the scene actually having more information, it can not be translated by the sensors. Prior probability shift occurs here, since information between test and training differ according to the luminance output, as in Fig. 2.7. A practical example is remote sensing applications with UAVs and image classification, where drift might occur due to various factors [1, 96, 95, 113, 97, 16].

### *Concept Shift*

Concept shifting is widely associated with data streaming and spam filtering, basically this type of drift is related to learning in non-stationary environments or in domains that have hidden contexts which causes



**(a)** Normalized luminance of a section of the image, saturated values were discarded. The blue line is the average of the real image 2.7d, the training data is yellow and the test data is green.

**(b)** Overexposed training image.

**(c)** Underexposed test image.

**(d)** Real image with correct exposure.

**Figure 2.7:** The information distribution depends on the target value, characterizing prior-probability shift. Here training data is represented by 2.7b and test data by 2.7c.

changes over time or seasons. In this class of problems it is said that drifts occur in the target concepts [19, 29, 22, 30].

The "Concept", itself, is an abstract interpretation of the information that are learned by the machine, e.g. as the relation between a given covarite and its class. Thus, in terms of probability density distributions, concepts are, then, related to the knowledge of a priori probabilities or covariate density probabilities or conditional probabilities. Any of these are required to establish an concept learning scenario based in the joint probability distribution in equation 4.

The *Concept Shift* is a different problem in which both the a priori probability and the $\mathbf{x}$ data PDF are usually kept the same, however there is a "*Shift*" in the relation between the input data and the output results. With this, the inequality $P_{train}(y|\mathbf{x}) \neq P_{test}(y|\mathbf{x})$ (or $P_{train}(\mathbf{x}|y) \neq P_{test}(\mathbf{x}|y)$ for Bayesian models) implies a variation of the test data generating mechanism in regarding the training data and, thus, $P_{train}(y,\mathbf{x}) \neq P_{test}(y,\mathbf{x})$. This is considered an extremely complex type of *Dataset Shift* [67]. In

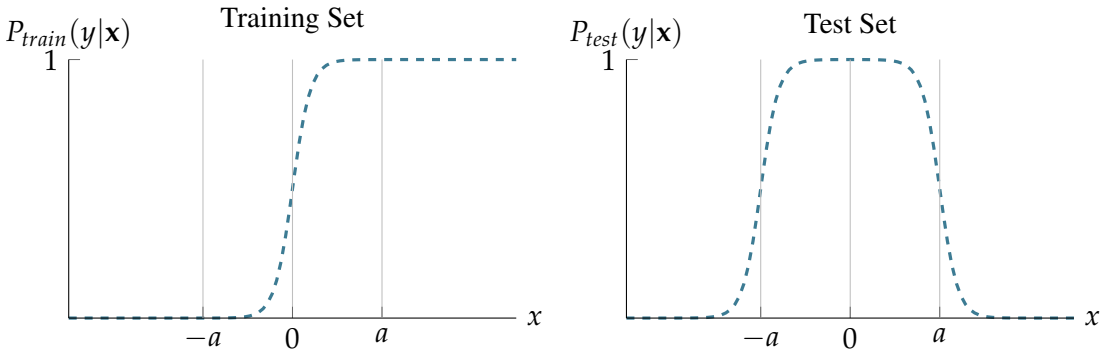
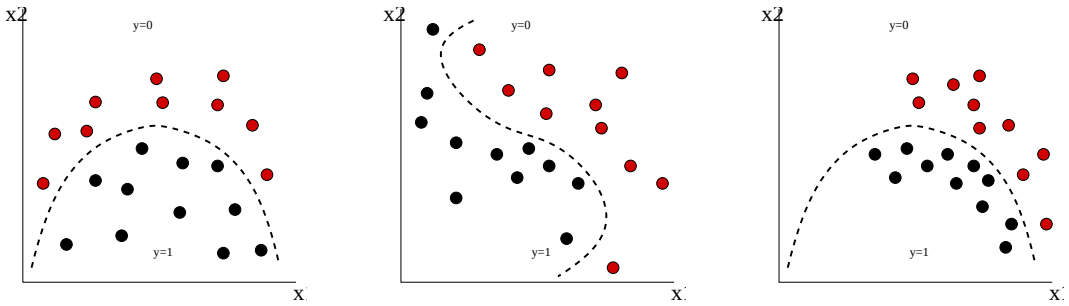



**Figure 2.8:** Concept Shift:$P_{train}(\mathbf{x}) = P_{test}(\mathbf{x})$ but $P_{train}(y|\mathbf{x}) \neq P_{test}(y|\mathbf{x})$

Fig. 2.8, the probability distribution of the covariate is equal in both cases as it is not dependent on the conditional probability $P(y|\mathbf{x})$. However the difference of the predictor probability $y$ given $x$ indicates that the classes definitions changed, i.e. the predictor output is different for the same input.

It is often considered that there are two types of concept drifts:

- Real concept drift: refer to changes in the conditional distribution $P_{train}(y|\mathbf{x}) \neq P_{test}(y|\mathbf{x})$, which is named *concept shift* [36].
- Virtual concept drift: occurs when the distribution of the incoming covariate data changes $P_{train}(\mathbf{x}) \neq P_{test}(\mathbf{x})$ [36]. In fact, the Virtual concept drift is not actually a concept shift, but actually it is an interpretation of the *Covariate Shift*, from a cognitive learning stand point.




**(a)** Training Dataset. **(b)** Real concept shift. **(c)** Virtual concept shift.

**Figure 2.9:** Graphical representation of real and virtual of covariate drifts. Here, circles represent instances and different colours represent different classes.[36]

The variability of data exists in most of the real-world data problems, regarding this matter the factors that lead to this variation are documented and grouped according to the mechanism that result in a drifting. Since stochastic models in general have great dependency in both the data generation mechanism and the sampling method, any variation in any step of the data processing, i.e. generation, acquisition, sampling, precessing, etc., would cause one or more types of shifting. Knowing some of the main causes of drifts favour the design of methods to detect them, and solve any eventual difficulty caused by it.

Spam filtering is often considered concept shifting problems because the interpretation of unwanted or harmful messages that should be learned by the machine is a function that depends on the overall messages that are received according to the spam definitions. Thus the concept in such case can be, for instance, the probability density function of spam given all messages received. In this case, several approaches that acknowledge the dataset shift have been proposed: [19, 31, 9, 85].

Another example would be the training of a system with specific operational set-points, but during application the behaviour of the system is different. Thus, covariate shift occurs if set-points differ from expected and, in case of some fault, concept shifts are as in 2.10.

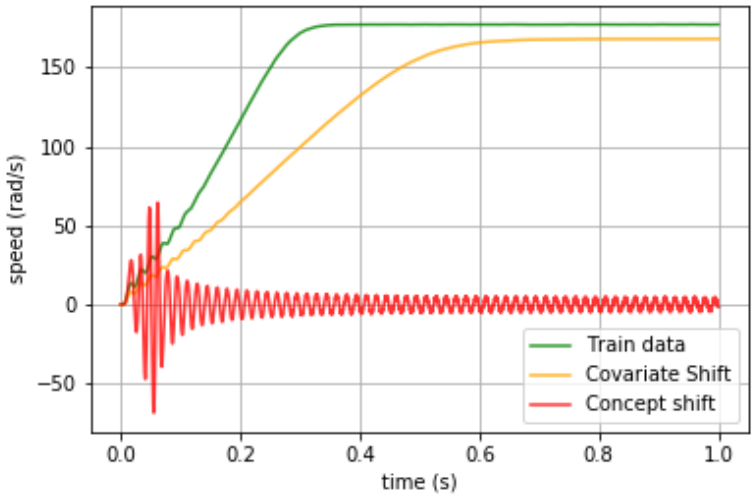



**Figure 2.10:** This is the graph of the speed of a three-phase electric motor. The training data is the motor speed for a controlled training set-point. The orange data is the motor working with a covariate shift, i.e. a shifted set-point. The red plot is the output of the system for the same set-point as the training data but the motor has a short-circuit phase fault

### 2.1.2 Dataset Shift Characteristics in Time

The most common scenario for dataset shift occurs when the machine is constantly submitted to new data in time, in form of streams or batches. Ultimately, the main assumption is that data for either training or testing can be received by the machine at different time points. In this context, it is straightforward to define drifting characteristics of temporal nature.

Consider the streaming scenario previously discussed in which the data probability density function is dependent on time and is given by:

$$P(y, \mathbf{x}, t) = P((y|\mathbf{x}), t)P(\mathbf{x}, t) \tag{8}$$

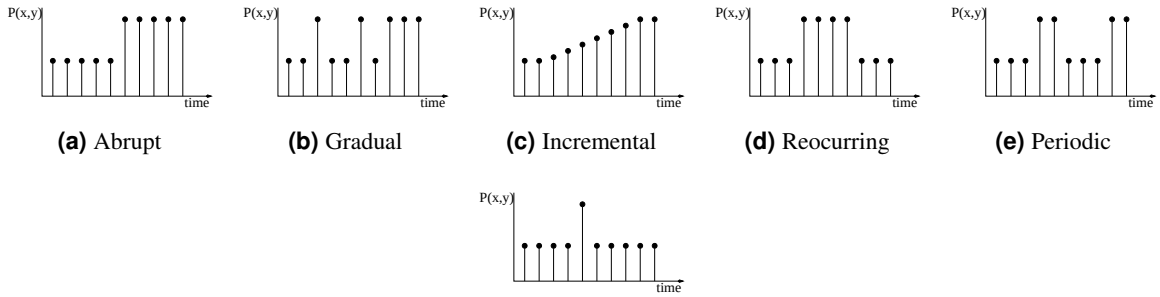
As any function in time there are a few characteristics that can be observed regarding the changes pattern and constraints. The duration of shifts can be defined as the time taken for data to leave a initial stable state $A$ and reach the final stable state $B$ [108], if data leaves state $A$ in $t = s$ and reaches $B$ in $t = e$, then the duration of the drift is:

$$D = e - s \tag{9}$$

And the traditional 2 types of drift, Abrupt and Gradual, can be defined according to a threshold $\delta$ that depends on the application as in [108]:

$$\text{Type} = \begin{cases} \text{Abrupt} & \text{if } D \leq \delta \\ \text{Gradual} & \text{if } D > \delta \end{cases} \tag{10}$$

### *Patterns of Change in Time*




**(a)** Abrupt **(b)** Gradual **(c)** Incremental **(d)** Reocurring **(e)** Periodic

**(f)** Outlier (not shift)

**Figure 2.11:** Graphical representation different dataset shift behaviours in time [36].

The first thing that need to be observed in any changing data is its speed, i.e. whether it is a tendency or a step [25, 118]. Overall, there are two principal patterns of shift regarding its speed:

**ABRUPT** An abrupt shift occurs when there is a sudden change in the data behaviour, such as the fault of a sensor in the plant. In this case, the probability distribution of the data $P(y, \mathbf{x}, t)$ is very different from $P(y, \mathbf{x}, t+1)$. In linear systems theory, this would be equivalent to a step disturbance.

A straightforward shift that occurs abruptly is the implementation of a system trained with a similar case or a simulation. This is often the case of Mobile Ad-hoc Networks (MANETs) [37], but might appear other system identification and control problems. A example of this issue would be a learning machine of an audio system, which was trained with data collected indoors but the testing and application was outdoors with different equipment, as seen in Fig.2.12.

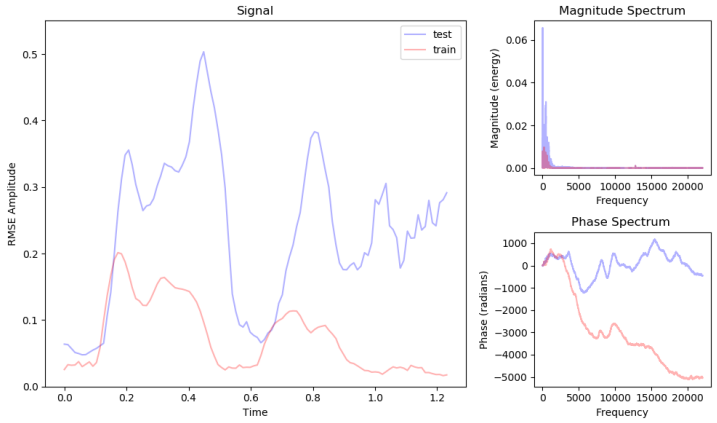



**Figure 2.12:** Example of audio data collected indoors(red) and outdoors(blue), where street noise had a expressive impact on the overall data. A machine trained for with the indoor data should compensate possible background noise.

**GRADUAL** Gradual changes are subtle and can be perceived as a trend in data, in real-world scenarios this would be observed in sensors ageing or thermal effects. Often, gradual shifts comprise of a change between two concepts that is not concluded in a single transition. Consider the case where a concept drifts from $A$ towards $B$ with an oscillation between these two states, which causes the concept to change from $A$ to $B$ and back to $A$. The shift is said to be gradual if it progressively stays less time in $A$ and more in $B$, remaining there at the end of change. Gradual changes are regularly too subtle to be noticed in subsequent moments and $P(y, \mathbf{x}, t)$ might appear to be similar to $P(y, \mathbf{x}, t+1)$, however the shift trend is present and becomes visible in a larger time spam or with a smaller threshold for changes. However the observation of gradual shifts require balance, since increasing the observed time spam might cause the system to perceive the changes too slowly, and a smaller threshold might make it too sensible to noise. The equivalent signal for an gradual shift, in linear systems theory, is the ramp.

A practical problem would be the identification of people in pictures from multiple stages of their lives, as in Fig. 2.13, but with a limited set labeled pictures. This could be applied to face identification in social media pictures or even in missing children cases [78, 91].


**Figure 2.13:** Incremental Shift represented by pictures of a person in her infancy (Initial State $A$), childhood, teenage and adulthood (Final State $B$), The L2 distance to the $A$ state was calculated with OpenFace[4].

Otherwise, if data is generated by different sources, this might cause targets to differ for the same covariate, depending on the source that generated the data. Thus, shifts could occur with data collected at the exact same time. Take, for instance, a market research problem, in this case, consumer patterns change depending on their living area or niches, [8], thus shifts occur geographically when using a model trained for a specific market across the others. Another example is the TeleECG of Federal University of Minas Gerais [72], which is part of a semi-automatic health program. In this system, electrocardiograms exams are made in hundreds of remote locations and diagnostics evaluation is centralized with automatic triage. Since several exams are made simultaneously and exams conditions may change, due to nurse technicians' ability or equipment condition etc., then shifts appear both in time and geographically.

The trend of the change is precisely the information about the shift that needs to be incorporated to the machine learning model in order the improve its performance. Thus, other complementary pattern interpretations can be derived from these two main patterns to better explain the shifts behaviour [118]:

**INCREMENTAL** Incremental drift occurs when sudden changes causes a trend in data. It can be seen as a "staircase", where each step is an abrupt change, but overall there is a gradual shift trend.

**REOCCURRING** The shift recurrence defines whether the change shifts towards a novel concept or if it returns to previously visited, or reoccurring, ones.

**PERIODIC** Periodic shifts can be understood as reoccurring shift in which the concepts are revisited according to a temporal pattern:

$$P(y, \mathbf{x}, t) = P(y, \mathbf{x}, t + nT) \quad \forall n \tag{11}$$

where $T$ is a constant period.

**OUTLIER** An outlier, otherwise, is a type of change in where a novel concept is visited without, however, sustaining that state, nor indicating any trend or recurrence characteristics. Since an actual statistical reflex does not exist, outliers are not considered dataset shifts.

#### *Time Constraints of Shifts*

The time constraints of the drift define whether it is:

**PERMANENT** A dataset shift is permanent if effects of the drift remain over the data distribution for an unlimited amount of time.

**TRANSIENT** In this case the effects of the dataset shift vanishes after a particular amount of time.

### 2.1.3 Causes of Dataset Shift

Through the stand point of the implementation of algorithms which target dataset shifting problems, the first step is to define the causes of the drift. Overall machine learning methods should ideally be robust to the data generators and retrieve any knowledge from the data itself. However, it is often common pre processing data to deliver more significant or better conditioned information or features, for instance

through feature selection methods. These strategies do tend to improve models in machine learning and should be smartly applied, so understanding the phenomena which causes any type of change in data is the very first step to solve dataset shifting problems.

Knowing what type of dataset shift is present in data, or even if any type occurs at all, can be a very challenging. However there are several situations that typically leads to one or more types of shift. In this section we will briefly discuss some of them in order to facilitate the analysis of popular current approaches for dataset shifting.

### *Sample Selection Bias*

A common cause of *Dataset Shift* is related to the selection of a uniform, or biased, sample for training. In this case, the training set choice is often obtained according to the conditional probability in Equation 12, with influence of a sampling decision variable $s$. Meanwhile, the test set is not subject to this decision variable and is defined by the probability in Equation 13 [77, 67]. Specifically, the training data selection is not performed randomly, and, instead, characteristics from the data targets $y$ and covariates $x$ are used to decide whether the data should be used or not.

$$P_{train}(s = 1|\mathbf{x}, y) \tag{12}$$

$$P_{test}(y, \mathbf{x}) \tag{13}$$

Where the sample are selected when $s = 1$ and discarded when $s = 0$.

The choice of an adequate data sample in fact require some knowledge of the system targets and covariates, because simple covariate shifts and prior probability shifts might occur when the training data do not properly define the input space. For instance, *Dataset Shift* ensues when part of the system domain where the test covariates, lighter dots displayed in Figure 2.14, would most likely be is actually excluded by the arbitrary selection function defined by $s$, hence resulting in a misspecified model caused by covariate shift. Another shift scenario is the " regression to the mean ", that occurs when the choice of the sample is based upon the targets but is done naively.

The *Sample Selection Bias* problem might occur in three distinct manners: $P_{train}(s = 1|\mathbf{x})$, $P_{train}(s = 1|y)$ e $P_{train}(s = 1|\mathbf{x}, y)$ [67]. A sampling system is denominated *MAR (Missing at Random)* occurs when the sample selection depends on $x$, i.e. $P_{train}(s = 1|\mathbf{x})$, which characterizes *covariate shift*. Similarly, *prior probability shift* occurs when the sample choice is related to $y$, causing $P_{train}(s = 1|y)$. The lack independence regarding both to $x$ and $y$ is a sampling system denominated *MNAR (Missing not at Random)*, which might lead to any type of *Dataset Shift*, or even to several of them[77, 67].

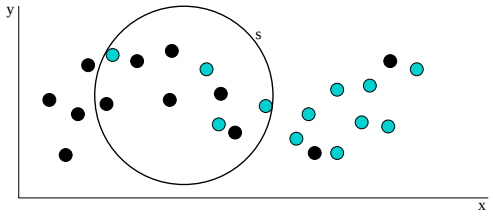



**Figure 2.14:** The selection variable $s$ and its selection function given by the equiprobable contour define which data are sampled [77]. Where darker dots are the training set, the lighter ones are the test set and the contour is the boundary of the selection function.

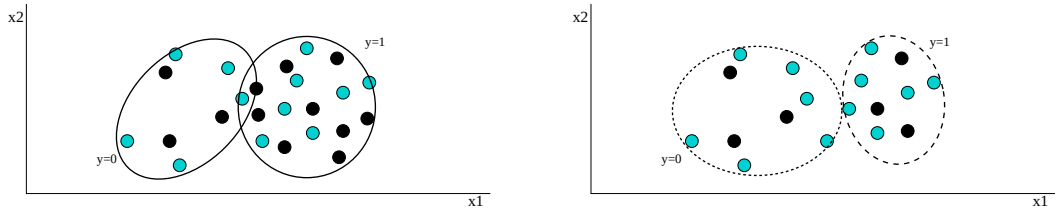
The issue of bias in estimators may be induced by unequal selection probabilities at any stage of sampling. This problem was addressed by [75], where consistent estimators were obtained by weighting the model estimation using the reciprocals of the selection probabilities at each sampling stage.

### *Imbalanced Datasets*

A common problem in data classification, specially in multi-class cases, is the quantity of data patterns presented by each class, named data balance. Unbalanced datasets are defined when one or more classes present much fewer data then the others. However, this is problematic since the correct classification of smaller classes becomes significantly harder when their rarity of increases [32, 58, 59]. Differences in balance between testing and training sets in classification problems are a prior probability shift scenario, thus imbalanced datasets can use methods aimed to prior probability shifts to mitigate the problem [2, 43]. However, in *Dataset Shift* context, another important issue arises when attempts of class balancing are made, since they tend to induce a *sample selection bias* with known *bias*. The dataset shift occurs when, in order to rebalance data, patterns of the more populous class are discarded in a manner that the training data distribution becomes different from the test set distribution [77].

In order to minimizes possible *Dataset Shifts*, the authors in [59] balance the classes through partition of the dataset using *"Distribution optimally balanced stratified cross-validation"*. The same authors, in [58], solves the problem of unbalanced classes using different intrinsic characteristics of the data. The hepatitis dataset [21] was used as an example of this issue in Fig.2.16.

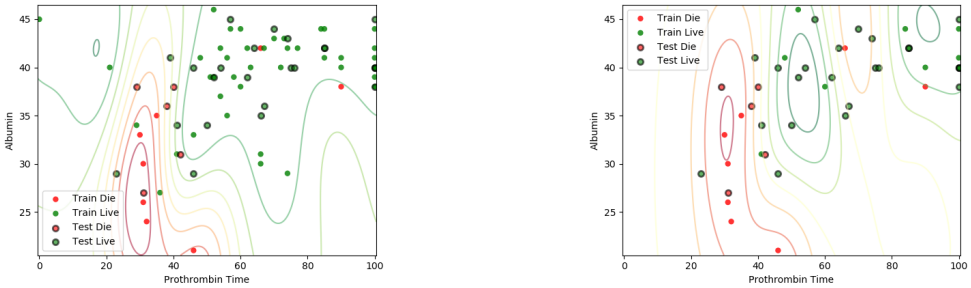
Model generation and selection is hindered when the training data is heavily unbalanced since most modelling process tends to favour the dominant class. Ideally both classes should have a comparable amount of data, thus a common practice is to exclude patterns from the most populous class. This strategy is often used since it is usually extremely costly to obtain enough rare cases to equalize both classes [32, 58, 59, 98]. For instance, in the two class classification problem in Figure 2.15, the training set, represented by the lighter dots, has been under sampled in order to rebalance the classes, represented by the circular contours, however in the test data, in darker shade, the imbalance still exists.




**(a)** Imbalanced datasets with a classification model(solid lines).

**(b)** Under sampling conditional model to rebalance data, causisng missepecified models (dashed lines).

**Figure 2.15:** Dataset shift caused by class rebalance for a two class case example, where the darker dots are training data and lighter ones are test data [77].




**(a)** Original Imbalanced datasets with a Gaussian SVM classifier, with 85% cccuray for the test set (dots black border).

**(b)** Under sampled rebalanced data with a Gaussian SVM classifier, with 63% accuray for the test set.

**Figure 2.16:** Projection of the features Albumin and Prothrombin Time from the Hepatitis dataset. Class Live (green) has significantly more instances than class Die (red in Fig 2.15a. The under sampling process dependent on values of other features, such as Malaise, Age and Histology, resulted in the misspecified models in 2.15b, with the class contours significantly different.

The work in [107] is a systematic study regarding imbalanced classes and dataset drift. In it, there are compelling comparison and analysis of state-of-art methods when applied to class imbalance problems with concept drift in one-by-one on-line learning. This paper verifies six different methods to handle either data imbalance, drift or both.

### *Non-Stationary Environments*

Real problems are, in general, never completely stationary in time and space. In addition, the environment is not usually completely controlled or modelled, which causes data extracted from the system to present variations between training and testing. Sometimes these changes are known and can be observed, however adjusting the model at every moment, even for a known shift, can be very costly. In other scenarios, changes can be unexpected, unobservable or even unknown which forbids tuning the model at any point [67]. In both cases learning strategies that intrinsically consider these changes in data are appropriate solutions.

Learning in non-stationary environments is greatly related to streaming and on-line problems, but not exclusively. The data generating process of non stationary environments is often characterized by evolving phenomenon. In this subject, [25] is a comprehensive survey on non-stationary environments that should be addressed for further information on the topic.

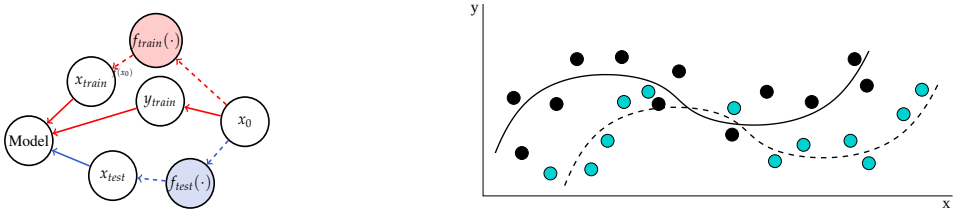
### *Domain Shift*

*Domain Shift*, in particular, occurs when the measurement system, the metrics or even the description of the data generator changes. This *shift* is illustrated by the currency devaluation in a prices prediction system, or the visual classification of images with lighting changes.

A domain is considered when the input covariate $x$ is not directly the latent variable, named here $x_0$, but is, instead, an observation of this latent variable by a function, $x = f(x_0)$. When the function $f(x_0)$ suffer some change the covariate $x$ perceived by the model is different even if the latent variable $x_0$ remains the same. Then, a difference between the training and testing domains could take place even if the latent variable $x_0$ and its relation to $y$ remains constant, because the targets distribution $P(y|x_0)$ depends on the latent variable $x_0$ while the model selection input depends on a function $x = f(x_0)$.

For instance, in the image classification example, the model inputs are not the scenes themselves, they are, instead, photographies taken with very specific settings. In this case, the photographies are outputs of an observation function and a shift in this function could be represented by different lighting settings. Thus, the photographies, or covariate $x$, taken with poorer illumination are very different from the ones taken in a brighter environment, even if the scene remains the same.

The difference in lighting problem was assessed by [15], where a semi-supervised discriminant analysis uses unlabelled data to include the knowledge of the intrinsic geometric structure of data. This allowed the method to generate a smooth discriminant function.




**(a)** Diagram representing the causal model in domain shifts.

**(b)** Domain shift due variation on mapping function $x = f(x_0)$, where the darker dots are training data and lighter ones are test data.

**Figure 2.17:** Representation of Domain Shift regarding the modelling structure and data distribution [77].

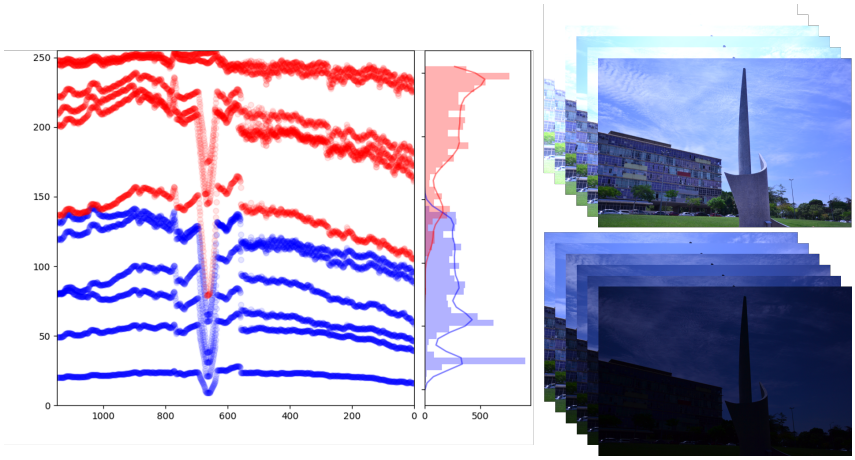



**Figure 2.18:** Representation of image capture problem where domain shift occurs due variation in camera settings. The plot displays the average luminance of the pictures columnwise. The training data is in red and the test in blue.

Domain shift is illustrated in Figure 2.17, in which a model, represented by the dashed line, is selected according to the covariates $x$, an observation of a mapping function of the latent variable $x = f(x_0)$. However the there occurs a change in the observation $f(x_0)$ between the training and test, darker dots, sets, leading to a divergence between the selected model and the ideal model for the test set, solid line, even though the distribution $P(y|x_0)$ remains the same. The distribution of the lighter and darker marks changes because the function $f(x_0)$ is different not because it varied between sets [77].

Another circumstance for domain shift occurs when the model is trained with data from a specific source domain but, later, it is placed in a different target domain [6]. This problem occurs in the real world scenarios since it can be costly to train and test models beforehand in the real industrial plants, thus the modelling can be made with data from equivalent plants.

### *Source Component Shift*

The source of any real-world data is subject to variations, moreover data is often generated from multiple different sources, and each of them is prone to disturbances. In this case, the overall distribution of the covariates can easily differ between training and testing, thus a correct model selection becomes difficult.

**MIXTURE COMPONENT SHIFT** When a problem data is generated by a certain number of sources, each one is responsible for different amount of data, it is possible that the proportions of data from each source change amid the test and the training sets. Given that the source for each data is, in fact, unknown this problem might be featured as *prior probability shift*[77].

**FACTOR COMPONENT SHIFT** In a problem in which the probability of the data is influenced by factors that might be decomposed in *form* and *strength*, if the *form* of the factor remains constant but its strength changes from the training to the test sets, it is characterized the *Factor Component Shift*[77].

**MIXING COMPONENT SHIFT** In this case, there are several similarities with the *Mixture Component Shift*, since both relate to the same context. However, in the *Mixing Component Shift* the data are aggregated so that it is observed an average of $\mathbf{x}$ of a population which could present a great variability[77].

The EEG problem in Fig.2.4 is a typical example of Source component shift. Since brain activity is extremely complex and noisy, several electrodes need to be used and the data dimensionality is usually through filters and feature extraction methods [69], which causes shift due to data aggregation. Shift also occurs in EEG itself since each electrode measures an average stimuli in a brain region. Because of it, small deviations in electrodes placement aggravate dataset shifts.

## 2.1.4 Learning Strategies for Shifting Datasets

Nearly all learning strategies for dataset shift are based in two approaches, named active and passive. Essentially, active approaches detect shifts and adapt the model learning according to changes in data, meanwhile passive approaches are overall robust to shifts that may occur to the data[25].

However, in machine learning, there are numerous other possibilities to solve *Dataset Shift* problems. For instance, the methodology in [93] performs the mining of rules the governs dataset shifts. There, the authors draw these rules with the aid of a mining tree, named Concept Drift Rule mining Tree (CDR-Tree). In this case, classification models are created directly by the extraction of the drift rules for each data configuration.

### *Active Approach*

Adaptive learning models have the prerogative of updating their parameters whenever a change in data is detected. With this approach, the model can be optimized for the data it receives at any given moment. For this, two important structures must exist in the leaning process: a Change Detector and a Adaptation Mechanism[25], as seen in Figure 2.19.

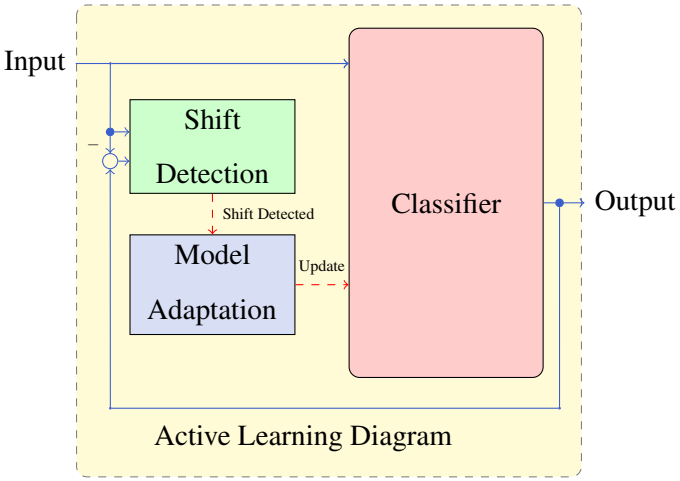



**Figure 2.19:** Active approaches use a change detector to inspect the inputs and/or classification error over the labelled samples. The detector signs the adaptation mechanism to update the classifier[25].

**SHIFT DETECTION** Shift detectors are one of the main components of active approaches. It observes the data and, through tests or other comparison methodologies, indicates if a change in data has happened. Among numerous shift detection methods, statistical hypothesis testing on the multivariate data is a straightforward well established method. However, most of these statistics tests depends on a fixed set of characteristics from the underlying distribution. If the drift causes small changes on the properties observable by the statistics methods, the detector tends to perform poorly[27].

Three adaptive detection methods were proposed by [27], in which the first one uses a rank statistic based on the density estimates of a binary data representation. The other two uses support vector machines (SVM) in their implementation, one compares the average margins of linear classifiers induced by 1-norm SVM, and the last one examines the average zero-one, sigmoid or stepwise linear error rate of SVM classifiers.

The authors of [81, 82] introduce a series of methods employing an *exponentially weighted moving average (EWMA)* for the detection of some *Dataset Shift* problems, in particular the *covariate shift*. For electroencephalogram(EEG) based Brain-Computer Interfaces(BCIs), [83, 80] used the *covariate shift* detection based on an exponential weighted moving average to identify drifts in the principal component analysis of features extracted from motor imagery-based brain electrical responses.

A simple detection system was proposed in [35], where the error of the learning system is monitored in two stages. If it surpasses a warning threshold, the system verifies if the error increases until reaching a drift threshold. When the drift is then detected the learning system is retrained according to the samples received between the warning and the drift points.

A semi-supervised approach that monitors efficiently changes in the classifier confidence to detect shift was proposed by [41]. This approach exploits dynamic programming and selective executions of the detection module in order to make the method feasible.

Dynamic systems modelling are used in [17] to create detection mechanisms for high frequency data streaming. It is argued that supervised and semi-supervised strategies are infeasible for such scenarios, thus the authors propose unsupervised methods based on dynamic models. This paper proposes four different strategies using phase spaces, among them is their comparison using the Gromov-Hausdorff distance, and the application of Cross Recurrence Plot and Recurrence Quantification Analysis to detect drift in consecutive phases.

### *Passive Approach*

Another possibility to solve problems with *Dataset Shift* is modelling with an underlying assumption that data will change, thus the model itself adapts for every new data it receives despite of actually occurring a drift or not. These methods tend to be specially robust on gradual or incremental shifting scenarios.

An early approach was proposed in [44], where the intrinsic mode functions of the model are adaptive. The method is based in the empirical decomposition of the data, allowing a well-behaved Hilbert transform for each function. Since this decomposition concerns local characteristic time scales of the data, at singular time instants the method can be considered a passive adaptive approach.

The method proposed in [47] modifies da data window used in order to minimize the estimated generalization error. Though this method can be used to somewhat detect drifts according to the window size, it is actually a passive approach since the windows sizes are adjusted with every batch input given to the system. Furthermore, this method is similar to cross-validation, where several models with all possible widows sizes are trained, then the window size with the lower estimated error is chosen.

Through a simple analysis of the problem, the parameters of multinomial random variables can be estimated with regard to the first and second moments according to principles of stochastic learning, as done in [70]. Though this paper explanation of the method application in machine learning be quite brief, it is presented examples with pattern recognition problems.

Another possible passive approach is the preprocessing of data, making it possible for traditional learning algorithms to track drifting data. This framework is proposed by [110], where a computational

framework for extending incomplete labelled data stream (FEILDS) transforms the original data stream with a few labelled data into a new one that incorporates the concept drift.

### 2.1.5 Popular Approaches for Dataset Shifting Problems

#### *Transductive and Semi-Supervised Learning*

Transductive and semi-supervised approaches use unlabelled data in combination with labelled datasets to improve classification. These methods are interesting to solve a variety of shifts, since they are capable of using the test data to incorporate more knowledge into the model and, thus, retrieve information that might have changed between the training and test sets.

Transduction classifies and perform regression of data without an induced general model, by considering both training and test data to compute every output. Therefore this method is able to intrinsically handle several types of divergences without requiring an active mechanism to detect or track any types of drifts. Moreover, the overall test error of this method is not affected by differences between training and test sets since the joint error 3 is related particularly to induced models. Thus, transductive learning strategies are very intuitive for passive approaches, since they are robust to dataset changes without reacting to detected shifts.

Approaches that incorporate Support Vector Machines (SVM) with transductive and semi-supervised strategies, such as Transductive Support Vector Machine (TSVM), have been greatly studied in the literature [7]. The TSVM method, despite of incorporating large margin classification and information from unlabelled data, might present lower performance then the traditional SVM if not well tuned[104]. An application for TSVM was proposed by[12], where a specific procedure for binary transductive SVM was proposed for remote-sensing classification with ill-posed data and small-sample sizes.

In this context [24] proposed an ensemble algorithm with transductive learning, named TRANSE, in order to solve the drift problem by assuming that the test data is sample i.i.d. of an unknown distribution.

However, since transductive learning might be very costly, active approaches can also be implemented. In [83, 80], a system is updated according to a transductive learning strategy whenever the covariate shift detector signs a drift. The learning approach is based on a probabilistic K-nearest neighbour (KNN) method and defines a knowledge base according to euclidean distance between the labelled and unlabelled data points. This base obtained through the transductive approach at each covariate detection is combined with the existing knowledge base. Then, the inductive classifier function of the model is adapted according to the final knowledge base.

Semi-supervised approaches, in a broad sense, consists of usually inductive modelling strategies that use both labelled and unlabelled data during training. In [15], a semi-supervised discriminant analysis

was proposed from a Linear Discriminant Analysis (LDA) stand point. In this approach, the classifier is obtained by maximizing the inter-class covariance and minimizing the intra-class. Consider that, for small training sample sizes, the covariance matrix of each class may not be accurately estimated. Thus a semi-supervised approach was proposed in order to include the knowledge from unlabelled data of the intrinsic geometric structure of data.

An application subject to concept changes is voice recording studied in [111], where it was modelled as covariate shift. In this paper, it is proposed a semi-supervised method that comprises of weighted versions of kernel logistic regression and cross validation approach.

In real-world scenarios, the drift in sensors are present in several types of applications, specially caused by sensor ageing or cumulative residuals. Drifts in artificial olfaction were investigated by [18], where semi-supervised methods were applied to long-term on-field continuous operation of chemical multisensory devices with drift-induced performance degradation.

### *Incremental and On-line Learning*

In a scenario where data is constantly changing, an incremental learning approach, in which the model is continuously updated in order to expand the model knowledge, holds great value since, by definition, it is adaptable to data changes [54, 25]. Incremental learning approaches can be passive, as it may consist of dynamic techniques that incorporate new knowledge to the model as data becomes available despite of it being shifted or not.

However, some solutions for *concept drift* were studied in [109], under an aspect of on-line incremental learning. It was proposed that trusted contexts are memorized so that they can be used when they appear again. This paper applies a heuristic to constantly monitors the behaviour of the system, which characterizes an active approach to a concept drift.

The Learn $++$.NSE is an incremental learning algorithm which works with batches of data. For every new batch, it creates a new classifier that is integrated to an ensemble of classifiers according to an age-adjusted dynamic error based weighted majority voting [29, 22, 30]. The Learn $++$.NSE has showed to be able to track changing environments and is capable of accepting additions and subtractions of classes. Also, further studies have shown that this method is robust to class imbalance when combined with Synthetic Minority Over-sampling Technique (SMOTE).

An Extreme Learning Machine was proposed in [57]. Named Forgetting Parameters Extreme Learning Machine (FP-ELM), it defines a mechanism of on-line learning that decreases the importance of older chunks or batches of data as new ones arrive. In this method the weight attributed to older chunks is shrunk by a forgetting parameter in order to guarantee the method performance for the most recent data

context. This method has shown to perform comparably and to be equivalent to more complex and costly ensemble methods.

[87], proposes a kernel ensemble learning method that updates the system whenever the true labels are available. This method redefines the boundaries of the classes in the feature space whenever it receives new labelled data.

An active incremental learning strategy was proposed by [85], where a window-based technique estimates the score of concept drift for each unknown email. The model, then, continuously incorporates new spam keywords and updates the filtering decision process.

Specifically for regression problems, in 2015 a second order on-line method was proposed in [68]. Regression models tend to have more consolidate approaches based on adaptive filtering and control methods, thence this paper regards particularly an on-line machine learning by incorporating two adaptive approaches: (i) an adaptive covariance reset to forget older contexts, and (ii) a last-step min-max optimization of the predictor.

The on-line learning approach was systematically studio regarding the problem of class imbalance with dataset shift by [107]. In this paper the techniques presented in [105], [106], [13], [103], [65] and [39, 71].

### *Transfer Learning and Domain Adaptation*

There is a great relation between the *Dataset shift* and the *transfer learning*, given that this type of learning considers that the training can be performed with barely a limited amount the possible settings of the training data, in such a manner that the prediction for specific settings is improved. Hence the survey in [73] might be an interesting view of the matter.

Strictly the approach proposed by [110], is a possible framework for transfer learning, as it attempts to learn and encode invariances from a limited set of labelled data prior the learning stage.

In a similar context, *Domain adaptation* consists in the adjustment of a given classifier created in an initial context, *source domain*, into a new one, *target domain*, without the necessity of data from the new context or using a very reduced amount. The papers [51], [62] and [114] have proposals with such approach.

The strategy proposed in [46], exploits bias in data during training as it accounts for biased vectors weights, associated with individuals datasets, and *visual world weights*, common to all datasets. The *visual world weights* are retrieved by withdrawing the bias weights from each dataset, which allows a model training with an essentially unbiased datasets.

Another approach to domain adaptation was proposed in [66]. In this paper the performance of an existing classifier was improved with the feature extraction of a new dataset with a genetic based algo-

rithm. In this case a classifier for biological laboratory data for cancer diagnostics was improved with the incorporation of data from a different laboratory that uses the same protocols.

### *Ensemble Learning*

Model misspecification often occur because the data has different behaviours throughout the input domain, leading to drift when de data used for testing is limited to particular domain regions. A possible and effective approach, as seen in Fig. 2.3b, is to define multiple local models throughout different regions the input domain. In machine learning, this strategy can be achieved through ensemble learning methods [54, 76].

Ensemble learning techniques are often intrinsically capable of defining the current data context. Usually, each model within the ensemble committee is related to a given context, which allows this method to define the current context and the best model for such context. However, for this approach, the contexts should be know a priori. In [94], for instance, a dynamic integration of classifiers is performed so that the local accuracy of each classifier with regard to the instance tested is used to select the best classifier or set of weighted classifiers.

The characteristics of diversity on ensemble learners has been studied in [63, 64], there it was observed that, though more diverse ensembles present lower test errors shortly after the drift, afterwards the diversity becomes less important and do not allow faster recovery in long-term.

In [48], some methods are implemented to trace context shifts using on-line learning and dynamic weighted majority to define an ensemble of learners. This papers results showed an overall high accuracy, also the ensemble method have shown to be capable of learning drifting contexts with almost the same accuracy as the base algorithms learn each concept individually. In [49], the same authors proposed an additive expert ensemble algorithm, named *AddExp*, which is a method that can be applied to any on-line learner for drifting contexts.

A semi-supervised approach was used, in [23], for solving non-stationary environments, it updates the weights of an ensemble classifier using unlabelled data unknown distributions. In [24], an ensemble approach was used integrated with transductive learning.

The Learn ++.NSE [29, 22, 30], which was previously addressed, is an incremental learning algorithm that generates dynamic ensembles according to the data batches that become available.

More recently, in 2015, a method to create an ensemble of subset on-line sequential extreme learning machine (ESOS-ELM) was proposed by [65]. This framework consists of an active approach as it includes a change detection mechanism, ir comprises as well a short-term memory system in its main ensemble and a long-term memory structure in an information storage module.

An ensemble method based on the Random Forest Algorithm was proposed by [116]. A Accuracy Weighted Ensemble (AWE) method was implemented in which the majority voting weights use base learners accuracy and intrinsic proximity measure of Random Forest.

Kernel ensembles were also applied to evolving concepts in data stream in [87]. The authors propose a multiple kernel learning approach where the boundaries of classes in the feature space of combined kernels are specified in order to reduce memory usage. And the evolving of the kernels is performed whenever new labelled data is available, by changing to the class boundaries previously defined.

### *Active Learning*

Regarding predictive models, the active learning approach attempts to select the minimum possible amount of labelled data required to develop an accurate model. As to dataset drifting, the predictive models need to adapt to changes in data, which is addressed in [117]. In this paper, a framework for active learning that explicitly handle concept shifts was proposed. For this, dynamic allocation of labelling and randomization of the search space are performed.

The active learning applied to solve the *covariate shift* in *Dataset Shift* is approached in [96, 95]. This paper explores remote sensing image classification, in which shift occur simultaneously for two different reasons Sample Selection Bias and Domain Shift. In this scenario, the image is classified accord to sampled pixels in the image, which addresses the first cause for shifting. In order to improve this issue, the author attempt to select the pixels in an intelligent manner. The domain shift is characterized in changes in illumination or geometry which hinder transfer classification models. Therefore an active approach was proposed to adapt the models to similar images, herein the known distribution is adapted according to model uncertainties criteria and the unknown classes are included according to a clustering criteria. The active sampling was decisive to permit a fast convergence and an optimal adaptation.

### *Weighted Approaches for Covariate Shift*

Several methods attempt to solve dataset shift related problems by weighting data intrinsic characteristics, such as the inputs, the probability densities, [86] proposes a method that deals with the *covariate shift* using a function log-similarity with weighed input samples, thus this method is adequate in situation in which the pdf of the observed samples do not correspond to the total population.

For binary classification, [88] solve the bias in cross validation caused by covariate shift through an importance weighted cross validation method, where the ratio between both classes is used to remove almost completely the bias in cross validation risk. The importance is also addressed in [89], where direct importances are estimated without any probability density estimation.

The detection of covariate shift through *exponentially weighted moving average (EWMA)* was vastly studied by [81, 83, 82, 80]. This method uses statistical process control charts to detect shifts in the input covariate.

## 2.2 STATISTICAL DISTRIBUTIONS COMPARISON

In order to asses a divergence between two populations, e.g. training and testing datasets, it is necessary to choose the appropriate measure to compare them. The selection of suitable measurement coefficients depend on the objectives of the comparison, which should be rather precisely stated. For the purpose of clustering, and thus partially the drifting issue, a large class of measures may lead to similar conclusions. Therefore, the consistence of the final conclusions could be verified using a set of two or more possible measures [79]

### 2.2.1 Dissimilarities and Similarities Measures

Another approach for comparing two different distributions is defining how similar they are, instead of measuring their difference. In this case, there are similarities coefficients

#### *Kullback-Leibler Divergence*

The Kullback-Leibler Divergence is a metric based in Entropy, thus also being named relative entropy, proposed by [53]. The paper "On Information and Sufficiency" the authors investigate the measurement of the distance or, more accurately, divergence between statistical populations with the use of the Kullback-Leibler divergence to retrieve information, for statistical discrimination problems.

The equation 14 is the definition of the divergence for continuous random variables $X_i$ and $X_j$. Where probabilities $p_i(x)$ $p_j(x)$ exist, if there are available observations of the probability functions $P_i$ and $P_j$ over the set $X$ comprised of $X_i$ and $X_j$ observations. KL divergence, then, is defined as equation 15, in which $dP/dQ$ is the Radon–Nikodym derivative.

$$D_{KL}\left(P_i \| P_j\right) = \int_{-\infty}^{\infty} p_i(x) \log \frac{p_i(x)}{p_j(x)} dx \tag{14}$$

$$D_{KL}\left(P_i \| P_j\right) = \int_{X} \log \frac{dP_i}{dP_j} dP_i \tag{15}$$

The equation 16 is the KL divergence for discrete probability distributions $P_i(k)$ $P_j(k)$:

$$D_{KL}\left(P_i \| P_j\right) = \sum_{k} P_i(k) \log \frac{P_i(k)}{P_j(k)} \tag{16}$$

Observing equation 14, it is possible to notice that the Kullback-Leibler divergence is not symmetric, nor is bounded to always be finite. Hence, the relative entropy is not reflexive, not being considered, then, a distance metric. However, it does measure the difference between the informations in two different distributions.

The Kullback-Leibler divergence is not restricted to parametric formulations of probability distributions, however, it is convenient to define the divergence for the comparison of two Normal distributions with dimension $n$:

$$D_{KL}\left(\mathcal{N}_i \| \mathcal{N}_j\right) = \frac{1}{2}\left(\operatorname{tr}\left(\Sigma_j^{-1}\Sigma_i\right) + \left(\mu_j - \mu_i\right)^{\top}\Sigma_j^{-1}(\mu_j - \mu_i) - n + \ln\left(\frac{\det\Sigma_j}{\det\Sigma_i}\right)\right). \tag{17}$$

In statistical inference, the minimization of the Kullback-Leibler divergence between a observed coordinate to a specific point is the maximum likelihood estimator at that point [3]

### *Fisher Information Metric*

The Fisher Information Metric is a smooth statistical manifold, more specifically, it is a particular case of the Riemannian metric. In practice it allows the calculation of the information difference between two measurements, since its points are probability measures defined on a common probability space. This measure is represented in matrix form, thus being, firstly, known as Fisher Information matrix.

Given a random variable $X$ with observations $x$, with probability normalized according to:

$$\int_X p(x,\theta)dx = 1 \tag{18}$$

Let $\Theta = (\theta_1, \theta_2, \theta_3, \ldots, \theta_n)$ be the coordinates of a Riemannian space, that forms a smooth manifold which the metric tensor $g_{ij}$ is defined by the Fisher information matrix [3]. Then, on order to retrieve the dissimilarity information between two coordinates, the Fisher metric takes the following form:

$$g_{ij} = \int_x \frac{\partial \log p\left(x,\theta\right)}{\partial\theta_i}\frac{\partial \log p\left(x,\theta\right)}{\partial\theta_j} p\left(x,\theta\right) dx \tag{19}$$

It can be observed that, in a metric context, the Fisher Information metric is the second derivative of the relative entropy, therefore it is the Hessian of the Kullback–Leibler divergence. Thus, the Fisher information is a symmetric positive, semi definite matrix. In this context, for discrimination between distributions, the $\theta$ are considered parameters of the probability distributions fisher equation could be written as:

$$g_{ij} = \int_x \frac{\partial \log p_i\left(x\right)}{\partial\theta_i}\frac{\partial \log p_j\left(x\right)}{\partial\theta_j} p\left(x,\theta\right) dx \tag{20}$$

### *Jensen Shannon Divergence*

Kullback-Leibler Divergency, however, is not symmetric, which might cause it not to be adequate in several applications, including in distance measure. In this context, the Jensen-Shannon Divergence is a symmetrized and smoothed version of $D_{KL}$ [56, 33], where:

$$D_{JS}\left(P_i \| P_j\right) = \frac{1}{2} D_{KL}\left(P_i \| M\right) + \frac{1}{2} D_{KL}\left(P_j \| M\right) \tag{21}$$

with

$$M = \frac{1}{2}\left(P_i + P_j\right) \tag{22}$$

In the scope of mixture models or joint distributions, the Jensen-Shannon Divergence could be generalized as:

$$D_{JS}\left(P_i \| P_j\right) = H\left(\pi_i P_i + \pi_j P_j\right) - \pi_i H\left(P_i\right) - \pi_j H\left(P_j\right) \tag{23}$$

with *weights* $\pi_i, \pi_j \geq 0$ and $\pi_i + \pi_j = 1$, and $H$ is the Shannon Entropy, which is defined for a *discrete random variable* $X$, with probability mass function $p(x)$ as:

$$H\left(X\right) = \mathbb{E}\left[-\log\left(p(X)\right)\right] \tag{24}$$

And the conditional entropy between two random variables $X_i$ and $X_j$ is:

$$H(X_i|X_j) = -\sum_k \sum_m p(x_{ik}, x_{jm}) \log \frac{p(x_{ik}, x_{jm})}{p(x_{jm})} \tag{25}$$

with $p(x_i, x_j)$ being the probability of $X_i = x_i$ and $X_j = x_j$.

In [56], is defined that the Jensen-Shannon Divergence is, then, bounded:

$$D_{JS}\left(P_i \| P_j\right) \leq H\left(\pi_i, \pi_j\right) \leq 1 \tag{26}$$

Still in this context, the Jensen-Shannon Divergence is related to mutual information of discrete variables in defined in equation 27.Consider that the random variable $X$ is composed by a mixture of distributions $P_i$ and $P_j$, with weights $\pi_i$ and $\pi_j$. And a binary variable $Z$ defines from which distribution each realization of $X$ is derived, choosing $P_i$ when $Z = 0$ and $P_j$ when $Z = 1$.

$$I \equiv \sum_k \sum_m p\left(x_{ik}, x_{jm}\right) \log_2 \frac{p(x_{ik}, x_{jm})}{\pi_j p(x_{ik})} \tag{27}$$

$$\begin{aligned} I(X;Z) &= H(X) - H(X|Z) \\ &= \frac{1}{2} \sum P_i \left(\log P_i - \log M\right) + \frac{1}{2} \sum P_j \left(\log P_j - \log M\right) \\ &= \mathrm{D_{JS}}(P_i \| P_j) \end{aligned} \tag{28}$$

## 2.3 TRANSDUCTIVE LEARNING

In transductive settings, particular values of a functional dependence are directly estimated, without necessarily having to estimate the general function itself. In this context, this estimation can be performed by a number of different techniques, for instance, the approach for transductive learning proposed by [61] uses statistical premisses. This thesis was the main reference for this work.

The general learning problem of model induction can be represented according to the functionality of the four components of Figure 2.20. In the figure, there is a data generator ($DG$), which selects random samples $x \in \chi \subset \Re^n$, drawn independently from an unknown but fixed probability distribution function $F(\mathbf{x})$. There is an oracle – or supervisor – ($O$), which returns an output value $y \in Y$ for every input sample $x$ according to an unknown but fixed conditional distribution function $F(y|\mathbf{x})$. There is an evaluator ($E$) capable of implementing a set of functions $f(\mathbf{x}, \alpha), \alpha \in \Lambda$, where $\Lambda$ is an arbitrary set of parameters that governs the behaviour of the function. Notice that by making $\Lambda$ arbitrary, $f(\mathbf{x}, \alpha)\ \alpha \in \Lambda$ may actually be any set of functions. Finally, there is a learning machine module ($LM$), that is capable to select from the set of functions $f(\mathbf{x}, \alpha)\ \alpha \in \Lambda$ the one that best represents oracle's response for a given training set, which is a finite set of samples

$$(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_\ell, y_\ell), \tag{29}$$

drawn *i.i.d.* by $DG$ and $O$ with respect to the joint density $F(\mathbf{x}, y) = F(\mathbf{x})F(y|\mathbf{x})$.

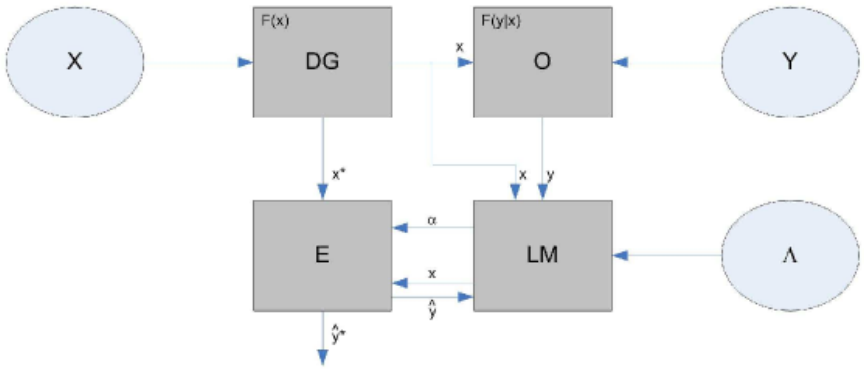



**Figure 2.20:** Learning model based on inductive inference, where a function that best approximates the unknown functional dependence is selected from the set of all possible functions based on the given training data.

Once the machine is trained, the value $\alpha_0 \in \Lambda$ is determined and produces the function $f(\mathbf{x}, \alpha_0)$ through $E$ that best approximates the unknown functional dependence. This approximation may then be used by $E$ to estimate unknown values $\hat{y}^*$ at arbitrary points $x^* \in \chi$. This representation is similar to the

classic one described in computational learning theory [45] . The difference between them is that here $LM$ and $E$ are represented as different functional blocks.

Notice that, at anytime during training, $LM$ may present any sample $\mathbf{x} \in \chi$ to $E$ and expect a response $\hat{y} = f(\mathbf{x}, \alpha)$. For samples $x$ in the set (29), $\hat{y}$ may be compared to the answer $y$ provided by the oracle $O$. This comparison is the basis of the selection mechanism that determines the approximation of the functional dependence, and it is measured by a loss or discrepancy function $L(y, f(x, \alpha))$ that yields the estimation of the risk functional

$$R(\alpha) = \int L(y, f(x, \alpha)) dF(x, y), \tag{30}$$

referred to as the *expected risk*.

The solution of the learning problem, implemented by $LM$, may hence be described as finding the function $f(\mathbf{x}, \alpha_0)$ which minimizes the expected risk [100]. In other words, find the function $f(\mathbf{x}, \alpha_0)$ that minimizes the risk functional $R(\alpha)$ over the class of functions $f(\mathbf{x}, \alpha), \alpha \in \Lambda$, where $F(\mathbf{x}, y)$ is unknown and the only data available is the training set (29).

The main issue here is whether or not the estimated risk yielded by the training set approximates the *expected risk* as defined by Equation 30. Since only a restricted training set is available, the general risk functional is then approximated by the empirical risk functional by making it discrete with respect to the training set (29):

$$R_{emp}(\alpha) = \frac{1}{\ell} \sum_{i=1}^{\ell} Q(z_i, \alpha), \qquad \alpha \in \Lambda. \tag{31}$$

where $Q(z_i, \alpha)$ is a loss function calculated over the training samples.

Notice that Equation 31 does not depend on any knowledge about the joint densities, so $R_{\text{emp}}(\alpha)$ is fixed for a particular choice of $\alpha$ and for a particular training set (29) [14]. Assume that $\alpha_0$ and $\alpha_1$ are the optimal parameter sets for the empirical functional risk and functional risk, respectively. We have that $R_{\text{emp}}(\alpha_0)$ and $R_{\text{emp}}(\alpha_1)$ will converge to the same value as the number of samples $N$ tends to infinity.

Despite being theoretically sound, the ERM principle is not well suited to deal with small data samples, since convergence is achieved only when $N$ is very large. This motivated the development of the so-called Structural Risk Minimization (SRM) inductive principle [99]. The SRM principle, as the ERM principle, also attempts to minimize the empirical risk. The SRM principle, though, simultaneously attempts to minimize the confidence interval given by the bounds on the risk functional [100]. As a result, the SRM principle is able to consider both the quality of the approximation of the data as well as the complexity of the approximating function. Although an additional control of function approximation can be made by SRM, it also depends on dataset size and representativeness. Since all the possible functions $f(\mathbf{x}, \alpha), \alpha \in \Lambda$ can be searched for model selection, there is always an expectation that the outcome with SRM will be close to the optimal solution.

We now examine the transductive setting of the learning problem, on which one is not interested in estimating the unknown functional dependence from a set of functions $f(\mathbf{x}, \alpha), \alpha \in \Lambda$ [115] [50]. Rather, the goal is to estimate the values of this functional dependence at given points using a function $f(\mathbf{x}, \alpha^*)$ from the set $f(\mathbf{x}, \alpha), \alpha \in \Lambda$. In order to accomplish the estimation for the specific points, one should be able to use the information conveyed by these given points.

As with inductive inference, it is possible to obtain a learning model based on the same four components for transductive inference (Figure 2.21). Three of these components, $DG$, $O$, $E$, are identical to the inductive case. The difference relies on the learning machine $LM^T$, which now not only takes as input the original training set (29), but also a so-called working set $D_W$

$$(x_{\ell+1}, \ldots, x_{\ell+k}), \tag{32}$$

also drawn *i.i.d.* by $DG$.

The working set represents the $k$ points of interest where one wishes to estimate the values $\hat{y}^* = f(\mathbf{x}^*, \alpha^*)$ of the unknown functional dependence, where $\mathbf{x}^* \in (\mathbf{x}_{\ell+1}, \ldots, \mathbf{x}_{\ell+k})$. Finally, the communication between $DG$ and $E$ becomes restricted, since $E$, despite being the same as in the inductive model, is now only able to properly estimate values either on the training set (29) or on the working set (32). The obtained model is not generic anymore. Notice that, as opposed to the inductive case, it is not necessary for the unknown functional dependence to be a function of the set $f(\mathbf{x}, \alpha), \alpha \in \Lambda$ since now the search is through a restricted set of functions aimed at the working set only.

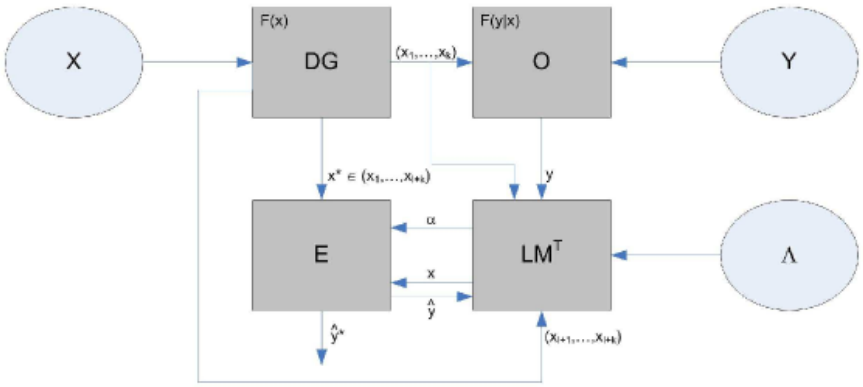



**Figure 2.21:** Learning model based on transductive inference. A modified learning machine takes both training and working sets as inputs, and the evaluator is only able to estimate values on either of these sets.

In the transductive inference setting, the solution to the learning problem, implemented by $LM^T$, may be described as finding the function which minimizes the *overall risk*. More formally, $LM^T$ must

find the function $f(\mathbf{x}, \alpha^*)$ that, with probability $1 - \eta$, minimizes the overall risk of estimating values $\hat{y}^* = f(\mathbf{x}^*, \alpha^*)$ for $\mathbf{x}^* \in (\mathbf{x}_{\ell+1}, \ldots, \mathbf{x}_{\ell+k})$. This is analogous to minimizing the functional

$$R_\Sigma(\alpha) = \frac{1}{k} \sum_{i=1}^{k} L(y_{\ell+i}, f(x_{\ell+i}, \alpha)), \tag{33}$$

where $L(y, f(x, \alpha))$ is a generic loss function.

Notice how the measurement of risk differs from the inductive to the transductive settings of the learning problem. In the inductive case, the risk functional (30) assesses the risk with respect to the joint distribution function $F(x, y)$ for the whole space of the unknown functional dependence. In the transductive case, the risk functional (33) only assesses the risk with respect to the given points of interest, i.e. the working set $D_W = (x_{\ell+1}, \ldots, x_{\ell+k})$. The analysis of Equations 30 and 33 helps to understand how the risk is calculated in both inductive and transductive settings. Since $D_W \in \chi$, a tighter bound for transductive learning risk could be expected. In fact, after Vapnik's original work on error bounds for TL [101], other authors have also pointed out to tighter bounds for TL risk [20, 5]. In practice, risk bounds yield an estimate of the test error by minimizing the risk bound function, and are valuable to choose an algorithm or a model. A tighter bound for TL may suggest, therefore, a better performance on the working set.

Structural minimization of the overall risk is, in fact, the same as the inductive method of structural risk minimization. The key difference lies in the availability, a priori, of the given points of interest where one must estimate the values of the unknown functional dependence:

$$\mathbf{x}_1, \ldots, \mathbf{x}_\ell, \mathbf{x}_{\ell+1}, \ldots, \mathbf{x}_{\ell+k}. \tag{34}$$

When estimating functions, one must determine the structure on a (possibly infinite) set of functions $f(\mathbf{z}, \alpha), \alpha \in \Lambda$ given the set itself and the domain of definition of its members. When estimating values at given points, a structure $S_1 \subset S_2 \subset \cdots \subset S_n$ on the set $f(\mathbf{z}, \alpha), \alpha \in \Lambda$ may be defined on the equivalence classes of the set. A set is decomposed by a finite number of equivalence classes through a set of indicator functions, where two indicator functions are said to be equivalent when they classify elements of the complete sample given in (34) in the same way.

## 2.4 GABRIEL GRAPHS GAUSSIAN MIXTURE MODELS

Gabriel Graphs were proposed in[34] as an approach to analyze geographic variations. The strategy developed in that paper considered the difficulties of estimating fitted contour lines for trends throughout a given region, thus it proposed the categorization of geographic variations.

In summary, Gabriel Graph is similar to Voronoi Diagrams, in fact, it is a subset of them. It consists of a graph which adjacent vertexes must be in opposing sides of a circumference, which contains no other vertexes within it. Thus, the bisections of the all the edges of the graph can be used to define adjacent exclusive regions [92]

### 2.4.1 Gabriel Graphs

In general, graphs $\mathcal{G}(\mathcal{V},\mathcal{E})$ are data representation in the form of connected diagrams. Here, let it be defined by a set of $n$ vertexes $\mathcal{V}$, which correspond to the data points, and by the $m$ edges $\mathcal{E}$, that are connected unordered pairs of vertexes in $\mathcal{V}$. [34]

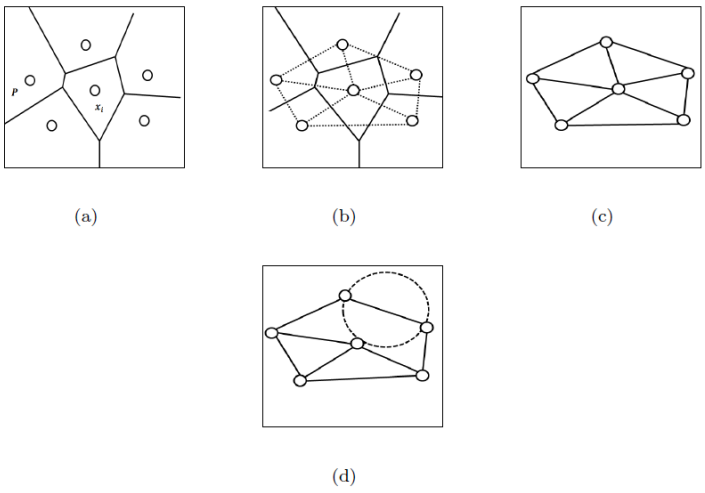



**Figure 2.22:** Gabriel Graph based on Voronoi Diagram. (a) Voronoi diagram. (b) Voronoi diagram dual graph. (c) Delaunay triangulation. (d) Pair of points from Voronoi diagram with an edge of a Gabriel graph.

Gabriel Graphs $\ddot{\mathcal{G}}$ is a subset of the Voronoi Digram and, also a subgraph of the Delaunay Triangulation [92]. Voronoi diagram is a division of the plane into convex polygons, named Voronoi cells, as seen on 2.22 [28]. Consider a set of points $\mathcal{S}$ in $\mathbb{R}^2$, where each of them is related to a cell of the Voronoi diagram. Then, the boundaries of each Voronoi cell is the bisection of the line connecting two adjacent points, as represented in Figure 2.22(a). Any given point $\mathbf{p}$ in $\mathbb{R}^2$ belongs to a Voronoi cell $v(i)$ if, and only if, its distance $\delta(\cdot)$ to $\mathbf{x}_i$ is smaller than to any other point, or, formally:

$$\mathbf{p} \in v(i) \iff \delta(\mathbf{p},\mathbf{x}_i) \leq \delta(\mathbf{p},\mathbf{x}_j), \quad \mathbf{x}_i,\mathbf{x}_i \in \mathcal{S}, \forall j \neq i \tag{35}$$

The dual graph of the Voronoi Diagram is named Delaunay Triangulation. In this case, instead of defining adjacent regions in the form of convex polygons, the points in $\mathcal{S}$ are the vertexes $\mathcal{V}$ of a planar graph [92]. The edges $\mathcal{E}$ of the dual graph are given by pairs of vertexes that are in neighboring Voronoi

cells, as seen in Figure 2.22(b). Finally, Figure 2.22(c) represents the Delaunay Trangulation resulting from the dual of the Voronoi Diagram in Figure 2.22(a).

Gabriel graphs are an specific type of graphs within the Delaunay triangulation definition, which allows an edge between to vertexes to exist if, and only if, an hypersphere that contains just both vertexes and all other points are external to it, as Figure 2.22(d). Specifically, given a set of points $\mathcal{S}$, a Gabriel Graph $\ddot{\mathcal{G}}(\mathcal{V},\mathcal{E})$, with vertexes set $\mathcal{V}=\mathcal{S}$ and edges set $\mathcal{E}$, is defined by:

$$(\mathbf{v}_i,\mathbf{v}_j)\in\mathcal{E} \iff \delta^2(\mathbf{v}_i,\mathbf{v}_j)\leq\left[\delta^2(\mathbf{v}_i,z)+\delta^2(\mathbf{v}_j,z)\right]\forall z\in\mathcal{V},\quad \mathbf{v}_i,\mathbf{v}_j\neq z \tag{36}$$

where $\delta$ is the euclidean distance operator[92]. Thus, any types of points in space, such as geographical coordinates, can be represented as a Gabriel Graph.

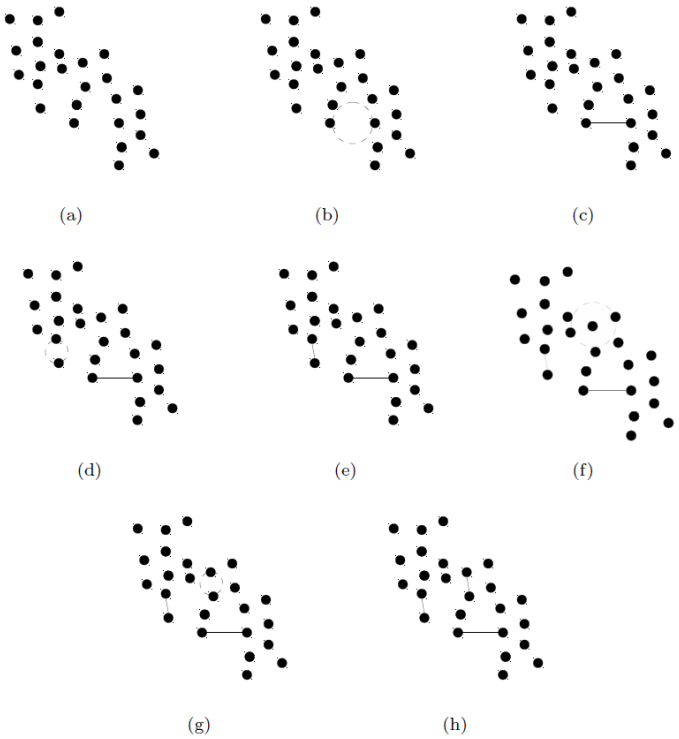



**Figure 2.23:** Visualization of the construction of a Gabriel Graph, in successive steps from (a) to (h). The dots are the scattered vertexes while the edges in solid lines are being creates. Each dashed circle represents the hypersphere of the criteria in Eq. 36

The construction of a Gabriel Graph $\ddot{\mathcal{G}}$ is represented in 2.23, where artificial data points are spatially scattered in a plane. The $\ddot{\mathcal{G}}$ can be constructed by verifying whether each pair of points meets the premise in Equation 36. For instance, the pairs tested in Figure 2.23 (b), (d) and (g) are connected by an edge, but the vertexes chosen in 2.23(f) do not meet the criteria. This intuitive algorithm to construct a Gabriel Graph has complexity order $O(n^3)$, however if the implementation is based on Delaunay triangulation, the complexity to create the graph is $O(n)$ [92].

### 2.4.2 Geometric Parametrization of Gaussian Mixture Models

Gaussian Mixture Models are a very useful tool to define a probability density function of complex data distributions, with appropriate choices of mean vectors $\boldsymbol{\mu}$, covariance matrix $\boldsymbol{\Sigma}$ and weight $\mathbf{w}$ of the Gaussian functions. In geographical analysis problems, GMMs can be defined as a composition of bivariate normal distributions, which are defined as:

$$P(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{2\pi\left|\boldsymbol{\Sigma}\right|^{1/2}} \exp\left[-\frac{1}{2}\left(\mathbf{x}-\mu\right)^{T}\boldsymbol{\Sigma}^{-1}\left(\mathbf{x}-\mu\right)\right]. \tag{37}$$

Let the covariance matrix be given $\Sigma = I_2\sigma^2$, where $I_2$ is a identity matrix $2\times 2$. Thus $|\Sigma| = \sigma^4$ and $\Sigma^{-1} = 1/\sigma^2$, allowing the distribution to be rewritten as:

$$P(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\sigma}) = \frac{1}{2\pi\boldsymbol{\sigma}^2} \exp\left[-\frac{1}{2}\left(\frac{\|\mathbf{x}-\mu\|^2}{\sigma^2}\right)\right]. \tag{38}$$

In this case, data can be appropriately represented by a given normal distribution if it falls within $3\sigma$ of deviation around the mean $\mu$. Consider that the probability value for $\mathbf{x} = \mu + 3\sigma$ is given by $p(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = z$, which is arbitrarily small with $z \approx 0$. With the independent constants removed from Equation 38, we have:

$$P(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\sigma}) = \exp\left[-\frac{1}{2}\left(\frac{\|\mathbf{x}-\mu\|^2}{\sigma^2}\right)\right], \tag{39}$$

in which the $\sigma$ can be isolated, resulting in

$$\sigma = \sqrt{-\frac{1}{2}\left(\frac{\|\mathbf{x}-\mu\|^2}{\ln(z)}\right)}, \tag{40}$$

where $z$ is the solution of Equation 38 with $\mathbf{x} = \mu + 3\sigma$, $\mu = 0$ and $\sigma = 1$, resulting in $z = \exp(-9)/2\pi$.

Specifically in a binary classification problems, each class can be defined according to its density distribution, enabling a the classification of unlabeled points according to its membership probability of each class. However, an adequate selection of parameters can be a challenge as the most used method, the Expectation Maximization, can may have some limitations[10]. In this context of binary classification, [92] proposed a methodology to automatically select Gaussian Mixture Models parameters using Gabriel Graphs.

In order to estimate the Gaussian Mixture Model of a Class in binary classification problems, a Gabriel Graph is created using all available points of both classes. Then, all vertexes from one class that have a link with the other are marked as Geometrical Vertexes $\mathcal{GV}$, and the edges between them are named Geometrical Edges $\mathcal{GE}$. The GMM is, then, estimated for each class, where the centers $\mu$ are defined as the Geometrical Vertexes of the class being estimated. Additionally, the radius are given according to Equation 40. Finally, the weights $w$ can be estimated through the inverse of the distance between support vectors, also being subject to $\sum_{n_{\mathcal{G}}}^{j=1} w_j = 1$, where $n_{\mathcal{G}}$ is the number of $\mathcal{GV}$.

## 2.5 SPATIAL CLUSTERING BASED ON DELAUNAY TRIANGULATION

Spatial clustering extracts information from unsupervised bidimensional data in order to create spatially coherent clusters. In this case, the information obtained from graphs can be used to infer structural characteristics of data [112]. In NSCABDT (Novel Spatial Clustering Algorithm Based on Delaunay Triangulation), proposed in [112], the spatial clustering is performed using Delaunay Triangulation and is able to discriminate clusters based on data density. The NSCABDT algorithm consists of:

1. Create Delaunay Triangulation graph $\mathcal{D}$
2. Calculate the Global Mean and Standard Deviation:

$$\text{Global Mean}(\mathcal{D}) = \frac{\sum_{sum(\mathcal{E}_D)}^{j=1} len(e_j)}{sum(\mathcal{E}_D)}. \tag{41}$$

   where $\mathcal{E}_D$ is the whole set of edges of $\mathcal{D}$ and $len(e)$ are the edges lengths.

$$\text{Global Sta}(\mathcal{D}) = \sqrt{\frac{\sum_{\mathcal{E}_D}^{j=1}(\text{Global Mean}(\mathcal{D}) - len(e_j))^2}{sum(\mathcal{E}_D)}}. \tag{42}$$

3. For each vertex $v_i$ in $\mathcal{D}$ calculate:

$$\text{Local Mean}(v_i) = \frac{\sum_{d(v_i)}^{j=1} len(e_j)}{d(v_i)}. \tag{43}$$

   where $d(v_i)$ is the graph degree of each vertex and $e$ are the edges associated with the vertex $v_i$.

$$\text{F}(v_i) = \text{Global Mean}(\mathcal{D}) \left(1 + \frac{\text{Global Sta}(\mathcal{D})}{\text{Local Mean}(v_i)}\right). \tag{44}$$

4. Each edge in $v_i$ that $len(e_i) > F(v_i)$ is removed.
5. If $d(v_i) = 0$ the node is discarded, else it is added to the current cluster in the clusters set $\mathbf{C}$.
6. Iteratively calculate all vertex the connects do $v_i$.
7. Extract the boundary of current cluster in $\mathbf{C}$ and remove bridges.
8. If no more vertexes connects to $v_i$, repeat process with next unprocessed vertex creating a new cluster in $\mathbf{C}$ until all data are processed.

The authors propose a strategy to eliminate bridges between clusters based on the effective region of each vertex, defined by a fixed radius $r$ around each vertex. The boundary of each cluster in $\mathbf{C}$ is defined according to the border of the region formed by all the connected effective regions of the vertexes in a cluster. The vertexes which effective region do not connected to the rest of the cluster are discarded.

# 3 PROPOSED METHODS

It is change, continuing change, inevitable change, that is the dominant factor in society today. No sensible decision can be made any longer without taking into account not only the world as it is, but the world as it will be ...

Isaac Asimov, *"My Own View" in The Encyclopedia of Science Fiction (1978)*

## 3.1 ESSENTIALLY TRANSDUCTIVE LEARNING WITH GENETIC OPTIMIZATION

Given that the *Dataset Shift* problem can be defined directly from probability distributions of the training and testing sets, it is intuitive that the risk functional, presented in equation 1, is directly affected when there are any type of shift. Hence, the empirical risk and the joint model error also have their values altered on the occurrence of a shift. The use of a essentially transductive method might have the capacity of diminishing errors in the context of *Dataset Shift* problems.

The essentially-trasnductive methods can be defined as binary classifiers. By minimizing the overall risk according to information theory methods, the said binary classifier can be estimated form the risk function 1. If it is considered the functional (33), the problem formulation for solving essentially-transductive learning problems takes the form of the following minimization problem:

$$\begin{aligned} \arg \min_{\{y_{\ell+1},\ldots,y_{\ell+k}\}} \quad & \frac{1}{k}\sum_{i=\ell+1}^{\ell+k} \Phi(f(\boldsymbol{x}_i),\theta,\tau), \\ & \theta = \{(\boldsymbol{x}_1,y_1),\ldots,(\boldsymbol{x}_\ell,y_\ell)\}, \\ & \tau = \{\boldsymbol{x}_{\ell+1},\ldots,\boldsymbol{x}_{\ell+k}\}, \end{aligned} \tag{45}$$

in which there is a training set $\theta = \{(\boldsymbol{x}_1,y_1),\ldots,(\boldsymbol{x}_\ell,y_\ell)\}$, a working set $\tau = \{\boldsymbol{x}_{\ell+1},\ldots,\boldsymbol{x}_{\ell+k}\}$, $X$ is the range of the problem, and its goal is to estimate the values $y_{\ell+1},\ldots,y_{\ell+k}$ associated with each point in the working set.

The expression generalization for the continuous case has the risk asserted for the whole range of the problem:

$$\begin{aligned} \arg \min_{\{y_{\ell+1},\ldots,y_{\ell+k}\}} \quad & \int_X \Phi(f(\boldsymbol{x}),\theta,\tau)d\boldsymbol{x}, \\ & \theta = \{(\boldsymbol{x}_1,y_1),\ldots,(\boldsymbol{x}_\ell,y_\ell)\}, \\ & \tau = \{\boldsymbol{x}_{\ell+1},\ldots,\boldsymbol{x}_{\ell+k}\}. \end{aligned} \tag{46}$$

In this continuous version, the transductive risk is not assessed at each of the given points of interest, but over the whole range of the problem. Notice that the problem still retains its transductivity properties, as the loss function $\Phi$ interprets and takes into consideration $\theta$ and $\tau$, which remain discrete. Therefore, the estimates for $f(\boldsymbol{x})$, defined only for the points in $\tau$ (where $\tau \in \chi$), are given by $\Phi$ considering both $\theta$ and $\tau$. Hence, the solution is achieved based on the general minimum risk over the whole range of the problem.

According to Minimum Discrimination Information principle, the Kullback-Leibler divergence between two probability distributions, may be used as discrimination information on the occurrence of new

facts [52]. That is, given a binary classification problem, in which classes underlying probability densities are known, the dissimilarity properties can be used to classify the unknown data according to how its incorporation disturbs the information drawn from the known data. In this context, two strategies were used: Minimizing the Intra-Class Information Degeneration and Maximizing Inter-Class Information Degeneration.

### 3.1.1 Minimizing Intra-Class Information Degeneration

Consider a classification problem in which the classes $A$ and $B$ have known underlying probabilities $P_A$ and $P_B$, respectively. A given pattern $\boldsymbol{x}_i$ should be classified considering the disturbance it causes to each classes information, regarding its relative entropy. Thus, $\boldsymbol{x}_i$ could be incorporated in either of the two following sets, since it is a binary classification problem:

$$A' = \{A \cup \boldsymbol{x}_i\}, \quad i = \ell + 1 \dots \ell + k \tag{47}$$

$$B' = \{B \cup \boldsymbol{x}_i\}, \quad i = \ell + 1 \dots \ell + k \tag{48}$$

where $A$ and $B$ contain the $\ell$ labelled samples and the extended sets includes the other $k$ samples.

With the probabilities $P_A$ and $P_B$ known already, it is possible to calculate de the information gain for both of the classes $D_{KL}(A\|A')$ and $D_{KL}(B\|B')$. The sample is assigned to the class which it caused lesser disturbance, that is, the class with smaller divergence to its extended set permanently incorporate the new sample. The decision making rules with the Kullback-Leibler divergence is, then:

$$y_i = \begin{cases} A & \text{if } D_{KL}(A\|\{A \cup \boldsymbol{x}_i\}) < D_{KL}(B\|\{B \cup \boldsymbol{x}_i\}), \\ B & \text{if } D_{KL}(A\|\{A \cup \boldsymbol{x}_i\}) > D_{KL}(B\|\{B \cup \boldsymbol{x}_i\}), \\ \text{undetermined} & \text{if } D_{KL}(A\|\{A \cup \boldsymbol{x}_i\}) = D_{KL}(B\|\{B \cup \boldsymbol{x}_i\}), \end{cases} \tag{49}$$

where the undetermined values obtained at the equality may be biased to either $A$ or $B$.

When we employ the Kullback-Leibler divergence and its setting given in (49) to the continuous risk functional (46), we end up with a transductive learning method that may be solved as a multi-objective optimization problem.

$$\begin{aligned} \arg \min_{\{y_{\ell+1},\dots,y_{\ell+k}\}} \quad & (D_{KL}(A(\theta)\|A'(\theta,\tau)), D_{KL}(B(\theta)\|B'(\theta,\tau))), \\ & \theta = \{(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_\ell, y_\ell)\}, \\ & \tau = \{\boldsymbol{x}_{\ell+1}, \dots, \boldsymbol{x}_{\ell+k}\}. \end{aligned} \tag{50}$$

since $A$ and $B$ are composed with elements in $\theta$, and $A'$ and $B'$ also include $\tau$.

To obtain a specific solution, instead of the traditional optimal Pareto front from the multi-objective optimization, a decision maker can be created according to arbitrary bias, as defined in (49).

### 3.1.2 Maximizing Inter-Class Information Degeneration

If the same binary classification problem, in which the $A$ and $B$ classes samples have known density distributions, occur in such manner that both classes should be the most different as possible, the model is obtained by maximizing the dissimilarity between them. Differently from the previous approach when the information gain between the extended sets ($A'$,$B'$) and their respective classes original distributions ($A$,$B$) are calculated. In this case, each unlabelled sample can be assigned exclusively to one class and the relative entropy between the extended sets $A'$ and $B'$ are calculated, regarding each other. Since, the extended sets are mutually exclusive for the new data samples, they can be, now, represented as:

$$A' = \{A \cup (\boldsymbol{x}_i | \hat{y}_i \in A)\}, \quad i = \ell + 1 \ldots \ell + k \tag{51}$$

$$B' = \{B \cup (\boldsymbol{x}_i | \hat{y}_i \in B)\}, \quad i = \ell + 1 \ldots \ell + k \tag{52}$$

An estimation of $\hat{y}_i$ defines the extended sets, which allows an optimization problem for the classes divergence maximization to be given by:

$$\begin{aligned} \arg \max_{\{y_{\ell+1},\ldots,y_{\ell+k}\}} \quad & D_{KL}(A' \| B'), \\ & A \cup B = \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_\ell, y_\ell)\}, \\ & (A' \cup B') = (A \cup B) \cup \{\boldsymbol{x}_{\ell+1}, \ldots, \boldsymbol{x}_{\ell+k}\}, \end{aligned} \tag{53}$$

The optimization problem equation (46) can be directly transformed into the minimization problem in (45):

$$\begin{aligned} \arg \min_{\{y_{\ell+1},\ldots,y_{\ell+k}\}} \quad & - D_{KL}(A'(\theta, \tau) \| B'(\theta, \tau)), \\ & \theta = \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_\ell, y_\ell)\}, \\ & \tau = \{\boldsymbol{x}_{\ell+1}, \ldots, \boldsymbol{x}_{\ell+k}\}, \end{aligned} \tag{54}$$

### 3.1.3 Implementation Aspects

#### *Kulback-Leibler Divergence Objective Function*

The Kullback-Leibler divergence is a measure that does not depends on parametric values of the distribution, thus, in order to provide a versatile algorithm, a Kernel Density Estimation was used to calculate the

probability at each point of interest, i.e. the working/testing set patterns. The KLD is, then, calculated according to the estimated probability density and an objective function for minimization was defined according to Algorithm 1.

**Algorithm 1:** Kulback-Leibler Divergence Objective Function

**Data:** Training set patterns and labels $X_l, Y_l$ and working set patterns $X_u$ and estimated labels $\hat{Y}$

**Result:** Objective Function $f$ based on the negative KLD

**begin**

*KDE is calculates for all the $X_u$ in relation to the patterns in each class*

$kdeA \leftarrow \text{KDE}\left(X_u, \{X_l \mid Y_L = 1\} \cup \{X_u \mid \hat{Y} = 1\}\right)$

$kdeB \leftarrow \text{KDE}\left(X_u, \{X_l \mid Y_L = 0\} \cup \{X_u \mid \hat{Y} = 0\}\right)$

*Since the KLD is not symmetric, it was calculated for both cases*

$kld_A \leftarrow \sum kdeA \cdot \log\left(\frac{kdeA}{kdeB}\right)$

$kld_B \leftarrow \sum kdeB \cdot \log\left(\frac{kdeB}{kdeA}\right)$

$f \leftarrow -\left(kld_A + kld_B\right)$

### *Parallel Genetic Algorithm Classification Strategy*

The method implemented attempts to minimize the Kullback-Leibler divergence negative with regard to the working/testing set labels. That is, an optimization strategy was implemented in order to define testing/working set classification that would lead to the minimum $-KLD$ value. Since the optimization problem input can be defined as a *bit-string* and the objective function is hardly covex or unimodal, it was decided to use an genetic algorithm approach.

However, for working/testing sets of average size the search space can increase very rapidly, since the number of possible solutions for 2 classes is $2^N$, with $N$ being the number of unlabelled patterns. Moreover, the probability density estimation for large quantities of data can be computationally demanding. Thus, it was decided to use a parallel approach, based on divide and conquer strategies. With this approach, the working set was divided into smaller sets which were classified according to the KLD genetic algorithm minimization. When all the subsets are classified, a greedy local search is performed in the whole set, in order to improve the minimization starting from the solution obtained by the parallel GA step, as shown in Algorithm 2.

**Algorithm 2:** Essentially Transductive Classification

**Data:** Training set patterns and labels $X_l, Y_l$ and working set patterns $X_u$

**Result:** Working set estimated labels $\hat{Y}$

**begin**

*Working set is arbitrarily divided into k subsets according to the points distance from each other*

$\{X_{u1}, X_{u2}, \ldots, X_{uk}\} \leftarrow aX_u$

**for** $i \leftarrow 1$ *to* $k$ **do**

*For all subsets a GA minimization is performed in parallel*

$\hat{Y}_i \leftarrow \mathrm{GA}(X_l, Y_l, X_{ui})$

*A greedy local search is performed for all* $X_u$

$\hat{Y} \leftarrow \text{Greedy Local Search}\left(X_l, Y_l, X_u, \hat{Y}_{1,2,\ldots,k}\right)$

**Algorithm 3:** Optimal Labelling Genetic Algorithm

**Data:** Training set patterns and labels $X_l, Y_l$ and working set patterns $X_u$

**Result:** Working set estimated labels $\hat{Y}$

**begin**

*Working set is arbitrarily divided into k subsets according to the points distance from each other*

$\{X_{u1}, X_{u2}, \ldots, X_{uk}\} \leftarrow aX_u$

**for** $i \leftarrow 1$ *to* $k$ **do**

*For all subsets a GA minimization is performed in parallel*

$\hat{Y}_i \leftarrow \mathrm{GA}(X_l, Y_l, X_{ui})$

*A greedy local search is performed for all* $X_u$

$\hat{Y} \leftarrow \text{Greedy Local Search}\left(X_l, Y_l, X_u, \hat{Y}_{1,2,\ldots,k}\right)$

## 3.2 TRANSDUCTIVE APPROACH BASED ON GABRIEL GRAPHS

Transductive learning is a intuitive approach for dataset shift and other problems where the knowledge within the unlabelled data is relevant for the problem. For instance, in dataset shift problems, where the training and testing sets differ, considering the unlabelled data itself to define the targets of the machine, increase its accuracy and generalization power. Other scenarios to be considered are datasets where very few data is unknown and/or there is severe imbalance between classes, this signifies that a very large part of the domain main be invisible to the labelled data – the traditional training set. The transductive approach is intrinsically capable of incorporating information from the parts of interest of the domain by including the unlabeled data in the classification process.

As we have been studying, essentially transductive learning, however, can be very costly to classify datasets with mare than a couple of hundred unlabeled data. The ability of training data in scenarios where very few knowledge of the targets are known is one of the main advantages of transduction, this characteristic is a great drawback.

Thus a different method is proposed here for bidimensional spatial datasets. This approach can be used in a variety of real world problem that are often prone to dataset shift conditions, such as biological and environmental data sets. The proposed method uses both labelled and unlabelled data to create an structure that can be used to transductively label data based on the probability density of the data. Furthermore, here is proposed a hybrid method which uses the structure used to define a semi-supervised classifier. Thus, ultimately, the method is divided in two parts:

1. Transductive Labelling
2. Structural Classifier Selection

### 3.2.1 Transductive Labelling

In this first part, the main objective of the method is to attribute labels to the most significant parts of data, through a transductive approach. Overall, probability density of data is estimated for labelled and unlabeled data, and the labelling is performed according to dissimilarity criteria.

In this context, this methodology relies on the strategy proposed in [92] to define the density functions through Gaussian Mixture Models using Gabriel Graphs. Since this strategy uses pairwise distance between points, a straightforward base of comparison for all data was the use of a Delaunay Triangulation graph based spatial clustering of unlabelled data, as proposed in [112]. This approach defines groups of

data that are more likely to have the same class and discards data that can be regarded as noise and do not consistently belong to any cluster or class.

For the labelling process, the Gaussian Mixture models are defined for the binary classes, with clusters aggregated towards the classes. This cluster aggregation is defined according to the maximization of Jensen-Shannon Dissimilarity between both classes. The labelling process based on entropy is favoured by the spatial clustering, since the evaluation of the dissimilarity can be performed over clusters of data and noise is disregarded.

In summary, the method proposed creates an unified data representation for labelled and unlabelled data, which allows a geometrical estimation of the parameters of a Gaussian Mixture Model. Then, the choice of ideal labels for each clusters is an optimization process that defines the maximum dissimilarity between classes. Thereby, the structure of the Transductive Labelling is given by the Algorith 4. The main novelty of this work is the Unified Structure $\mathcal{TG}$, which was made as in Algorithm 5

With this the support vertexes are concentrated around either the points labelled in classes, case were obtained from the $\mathcal{GG}$, or around a cluster otherwise. The label of each cluster can be attributed to one of the classes, then a density function can be estimated using the method proposed in [92]. The correct choice of labels for each cluster can be defined according to the optimization of a statistical test, such as minimizing Jensen-Shannon Dissimilarity.

### 3.2.2 Structural Classifier Selection

In order to create a classifier, a model that creates a separation surface should be implemented, which is not in the scope of Transductive Learning. However, the proposed methodology admits noise data that might hinder the method capability of classifying new data. Thus, the incorporation of a inductive model at this point is interesting, since it generalizes the output for the whole input space and creates a fast classification response for new data. In fact, any classifier algorithm could be implemented at this point, however, in this paper, a methodology that uses the data structure already created was proposed.

In this context, the structure created to allow the Tranductive Labelling could be used to generalize an inductive classification model based on a Bayesian approach. The classifier is obtained with the probability density function calculated for both classes, according to the method proposed in [92]. At this point is possible to reuse the graph structures to define the Gaussian Mixture Models. Then, a Naive Bayes approach is used to properly define a classifier. This approach is named here as Transductive Gabriel Graph Classifier or TGG.

**Algorithm 4:** Transductive Labelling

**Data:** Training set patterns and labels $X_l, Y_l$ and working set patterns $X_u$

**Result:** Working set estimated labels $\hat{Y}$

**begin**

*Create Gabriel Graph of the labelled data based on [92]*

$\mathcal{GG} \leftarrow$ Gabriel Graph$(X_l, Y_l)$

*Create Spatial Clusters with only unlabelled data, based on [112]*

$\mathcal{DU} \leftarrow$ Gabriel Graph$(X_u)$

*Create Spatial Clusters with both labelled and unlabelled data, based on [112]*

$\mathcal{DW} \leftarrow$ Gabriel Graph$(X_l, X_u)$

*Define unified structures to Parametrize GMMs*

$\mathcal{TG} \leftarrow$ Unified Structure$(\mathcal{GG}, \mathcal{DU}, \mathcal{DW})$

*From $\mathcal{TG}$ is possible to extract structural information such as:*

$Cl \leftarrow$ Ordered Clusters$(\mathcal{TG})$

$N_{clusters} \leftarrow$ Number of Clusters$(\mathcal{TG})$

$N_{clusters}$ *is limited arbitrarily and the smaller ones are considered noise*

*All cluster combinations are defined*

$N_{combination} \leftarrow 2^{N_{clusters}}$

**for** $i \leftarrow 1$ *to* $N_{combination}$ **do**

*For all possible combinations the clusters receive a label*

$\mathbf{L} \leftarrow$ Binary Vector$(i)$

**for** $j \leftarrow 1$ *to* $N_{clusters}$ **do**

$\hat{Y}_n \leftarrow \mathbf{L}_j \quad \forall \quad n \in Cl_j$

*The PDFs are calculated as in [92]*

$P_0 \leftarrow \text{PDF}(Cl, L = 0)$

$P_1 \leftarrow \text{PDF}(Cl, L = 1)$

*The dissimilarity is calculated as in 28:*

$JSD \leftarrow D_{JS}(P_0 \| P_1)$

$\hat{Y} \leftarrow arg\max(JSD)$

**Algorithm 5:** Unified Structure

**Data:** Supervised Gabriel Graph $\mathcal{GG}$ and Unsupervised Delaunay Triangulation Spatial Cluster Graphs $\mathcal{DU}$,$\mathcal{DW}$

**Result:** Unified Transductive Cluster Graph Structure $\mathcal{TG}$

**begin**

*All points that were bridges in $\mathcal{DU}$ and $\mathcal{DW}$ are considered support vertexes, analogously to the support vertexes proposed in [92].*

*Both $\mathcal{DU}$ and $\mathcal{DW}$ are superposed.*

*All points that were considered noise or were in too small agglomerates in both $\mathcal{DU}$ and $\mathcal{DW}$ do not have edges.*

*The resulting graph is superposed with $\mathcal{GG}$*

*All points considered support vertexes in $\mathcal{DU}$ or $\mathcal{DW}$ or $\mathcal{GG}$ are considered support vertexes.*

The prediction for this model is performed as as a simple comparison of the probability of pertinence to each class. Since the proposed method calculates the density function for both classes, the probability for a given point can be calculated straightforwardly for both classes and the highest one is chosen.

# 4 | EXPERIMENTAL DESIGN

It is not clear that intelligence has any long term survival value.

---

Stephen Hawking, *Lecture "Life in the Universe" (1996)*

## 4.1 GENETIC ESSENTIALLY TRANSDUCTIVE LEARNING EXPERIMENTAL DESIGN

The transductive approach implemented in this work is similar to semi-supervised methods, as it uses both, labelled and unlabelled data to perform the classification. In this case, the proposed method is expected to reach better results then supervised methods when very few labelled data is available in comparison to the existing unlabelled data.

In this case, it is necessary to define how the amount of information in the training set affects the models robustness and performance. Therein, reducing the quantity of training data reflects on the learning algorithm aptitude to generate an acceptable model in the presence of incomplete or inconformable data.

Furthermore, this intrinsic characteristic of using information present in unlabelled data allows robustness to *Dataset Shift* scenarios. Thus this characteristic was tested with shifting synthetic datasets.

The proposed method should, then, be compared with popular state of the art methods, such as the Support Vector Machine (SVM) and its semi-supervised adaptation, the Transductive Support Vector Machine (TSVM). In this cases the methods performance was assessed for reduced training data conditions for both synthetic and real-world problems.

### 4.1.1 Imbalanced Datasets

An important issue that is observed, specially when there are limited training patterns, is the imbalanced dataset. Differently from the Imbalance Dataset problem presented in Section 2.1.3, the issue here relates to the methods robustness to an imbalanced training set when no balancing technique is attempted. In the literature there are several techniques specifically designed for treating imbalanced datasets, however that is not the objective at this moment.

Consider, then, a scenario in which the training set and its amount of labelled patterns from each class is uncertain, and the developer do not have much access to the labelled data itself. In this context, the training could be performed with heavily imbalanced data. Again, in a reduced training set situation, this imbalance causes, often, training sets with only one labelled class, which preclude most of the usual supervised methods and a few of the accepted semi-supervised strategies. The proposed method, however, is still permitted in this cases.

#### *Experimental Design*

Some aspects that could have some effect on the methods accuracy were considered:

- Dataset.
- Quantity of training data set.
- Ration between both classes in training data (Imbalanced Data).

The tests performed in this work were intended to evaluate the methods performance when the training data is both small and imbalanced. Actually, the imbalance analysis here is related to uncertainties in the training, since it is desired to learn if the methods are robust to significant differences in the training set. This robustness allows the method to work under some types of *dataset drifting*.

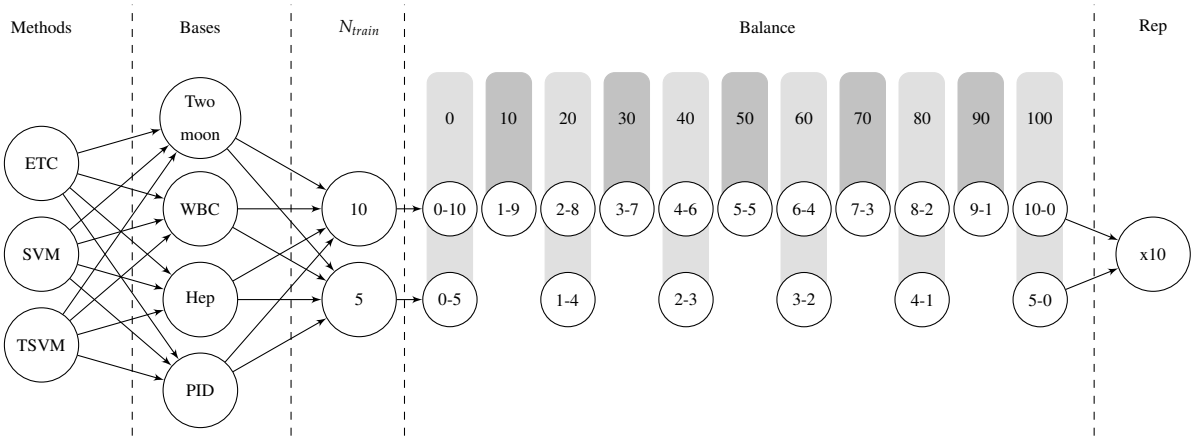



**Figure 4.1:** Diagram of the Transductive Experiment

This experimental design is represented in the diagram in Figure 4.1. The parameters of the methods were obtained beforehand through exhaustive search.

Observe that it was chosen not to work particularly with proportions between training and working/testing sets because, in a real scenario this proportion might be unknown or, at least, harder to obtain then the absolute amount of data.

### *Datasets Description*

The datasets used are described in Table 4.1

**Table 4.1:** Datasets Description

| Name | Features | Patterns | | | Description |
|---|---|---|---|---|---|
| | | Total | Class A | Class B | |
| Two-Moon(tmoon) | 2 | 500 | 250 | 250 | Two entangled semi-circles . |
| Wisconsin Breast Cancer (wbc) | 9 | 699 | 241 | 458 | Clinical data of breast cancer diagnostics from the University of Wisconsin Hospitals, Madison, from Dr. William H. Wolberg [11]. |
| Hepatitis (hep) | 19 | 155 | 123 | 32 | Clinical data of Hepatites diagnostics. |
| Pima Indian Diabetes (hep) | 19 | 155 | 123 | 32 | Clinical data of Diabetes diagnostics from the National Institute of Diabetes and Digestive and Kidney Diseases [11]. |

### *Performance metrics*

In order to assess the performance of the methods the following metrics were employed:

**ACCURACY** The accuracy is given by:

$$Acc = \frac{TPR + TNR}{N} \tag{55}$$

in which N, *TPR* and *TNR* are, respectively, the total number of patterns, the true positive and the true negative rates.

**GMEAN** The geometric mean is given by:

$$GMEAN = \sqrt{TPR \times TNR} \tag{56}$$

in which*TPR* and *TNR* are, respectively, the true positive and true negative rates.

### 4.1.2 Dataset Drift

Another interesting test is the robustness in the presence of concept drifts. Some tests were performed in order to evaluate the accuracy of the traditional Support Vector Machines, the Transductive variation of the SVM and the proposed Essentially Transductive Learning method.

Differently from the previous one, this experiment aims to observe directly the effects of a shift in data between training and test sets. In this scenario, off-line learning strategies are analyzed, therefore shifted data do not have any labels. Thus this experiment assumed a very simple form, with the accuracy analysis of the proposed method and its comparison with state-of-art methods.

#### *Experimental Design*

The experiment in this part is designed more simple. The aim of this experiment is to define the accuracy of the methods when data provided differs between training and testing sets. Thus, the data used as subject to *Dataset Shifts*.

Here, the accuracy was measured for several replications of the classification problem with shift. With this, the variability of the method's accuracy was affect by the variation of the differences between testing and training distributions, as defined in equations (5) to (7). In this case the balance and size of samples were kept equal in order to isolate the shift problem.

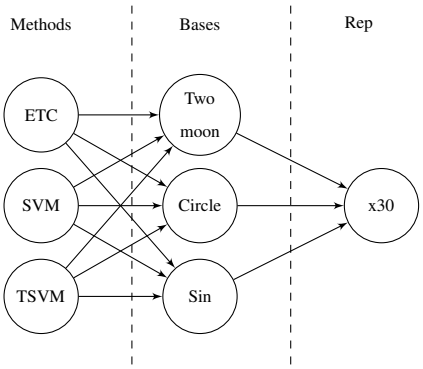



**Figure 4.2:** Diagram of the Transductive Experiment

This experimental design is represented in the diagram in Figure 4.2. The parameters of the methods were obtained beforehand through exhaustive search.

#### *Datasets Description*

**TWO MOON** The first test is a modification of the two moon dataset with the labelled data distribution is biased. Here, in the labelled set, there is a greater data distribution in the central region of the moons, which causes a covariate shift in the dataset.

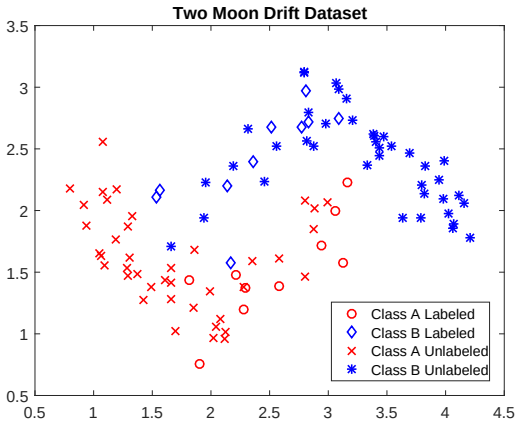



**Figure 4.3:** Graphical representation of the Two Moon Dataset with Covariate Shift.

**CIRCLE** The second test is a circle which centre $c$ and radius $r$ differ between the labelled and the unlabelled sets. It is based in an artificial data set containing one concept drift, proposed by [63].

**SINE** The third test is a plane divided by sinusoidal wave which amplitude $a$, frequency $f$ and offset $o$ changed between the labelled and unlabelled sets. This dataset was also proposed by [63].

**Table 4.2:** Description of the datasets with concept drift

| Name | Features | Patterns | | | | Drift |
|---|---|---|---|---|---|---|
| | | Labelled | | Unlabelled | | |
| | | Class A | Class B | Class A | Class B | |
| Two-Moon (tmoon) | 2 | 10 | 10 | 40 | 40 | $P(x)_L \neq P(x)_U$ |
| Circle (circ) | 2 | 100 | 100 | 100 | 100 | $c_L = [3.5, 3.5]$ and $r_L = 0.5$; $c_U = [4, 4]$ and $r_U = 1$ |
| Sine (sin) | 2 | 100 | 100 | 100 | 100 | $a_L = 1, f_L = 1$ and $o_L = 0$; $a_U = 2$, $f_U = 2$ and $o_U = 1$ |

## 4.2 GABRIEL GRAPH TRANSDUCTIVE APPROACH EXPERIMENTAL DESIGN

The proposed method involved two different parts, the trasnductive labelling and the proposed classifier, thus tests were performed in order to compare:

1. The Proposed Classifier with State of Art Methods
2. State of Art Methods using and not using Transductive Labeling

The transductive labeling, at this point is deterministic and for the same data would return the same result. Thus, in order to compare the performance of the method, different datasets were used. And for each datasets instance used, the performance of the proposed method and of state-of-art methods with and without transductive labeling were assessed. The design of the experiment is illustrated in Figure 4.4.

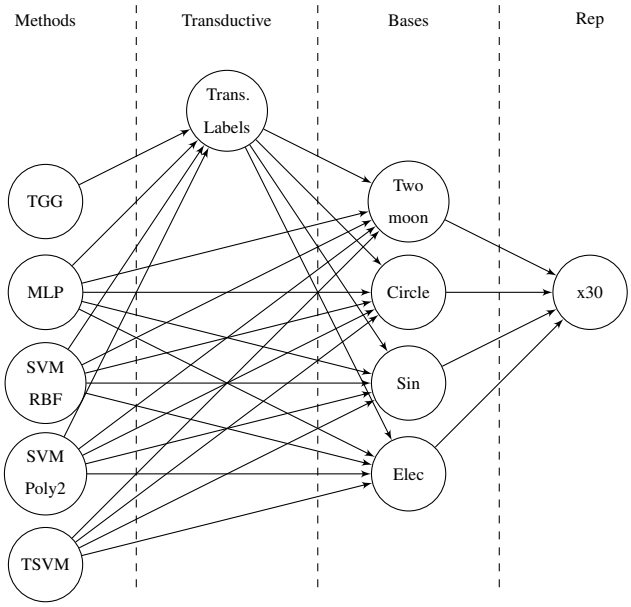



**Figure 4.4:** Diagram of the Transductive Experiment

The datasets used in this part of the experiment were the same used in 4.1.2, with the addition of the Elec2 dataset proposed in [42], which is traditionally used in Dataset Shift Problems. However, since the proposed method is limited to bidimensional spatial datasets, only features 4 and 6 were used.

# 5 EXPERIMENTAL RESULTS

True ignorance is not the absence of knowledge, but the refuse to acquire it.

Karl Popper, *As quoted by Mark Damazer in "In Our Time's Greatest Philosopher Vote" at In Our Time (BBC 4)*

The tests were performed according to the methodology in 4. The proposed methods performance was assessed in contrast to Support Vector Machine models, with the intention of comparing the proposed methods to state of the art ones, additionally it is possible to verify the experimental methodology effectiveness by using a well known method.

## 5.1 GENETIC ESSENTIALLY TRANSDUCTIVE LEARNING EXPERIMENTS RESULTS

### 5.1.1 Imbalanced Datasets

The methods – Essentially Transductive Classifier (ETC), Support Vector Machine (SVM) and Transductive Support Vector Machine (TSVM) – presented comparable classification accuracies, as seen in Figure 5.1, thus it was used an statistical method to compare them further. However when observing the behavior of the methods for imbalanced datasets, they show significant differences, as seen in Figures 5.2 and resultsBAL2.

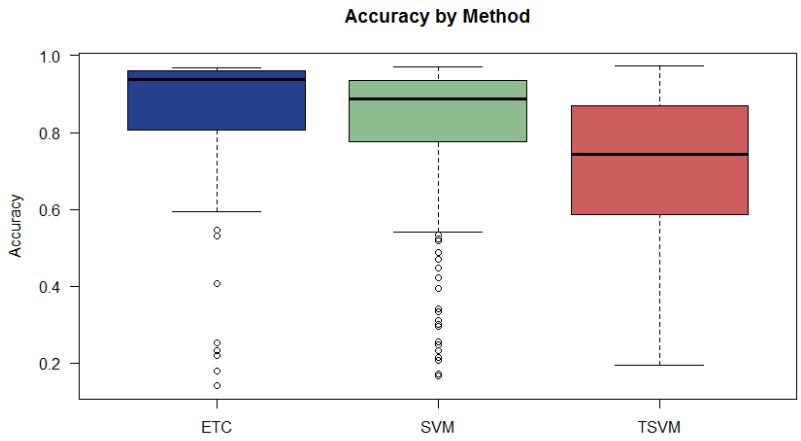
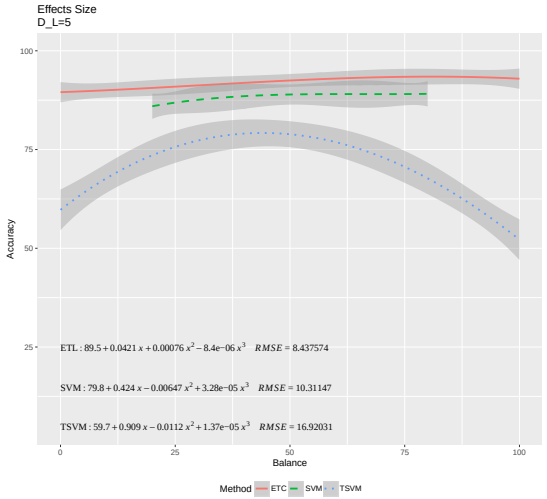
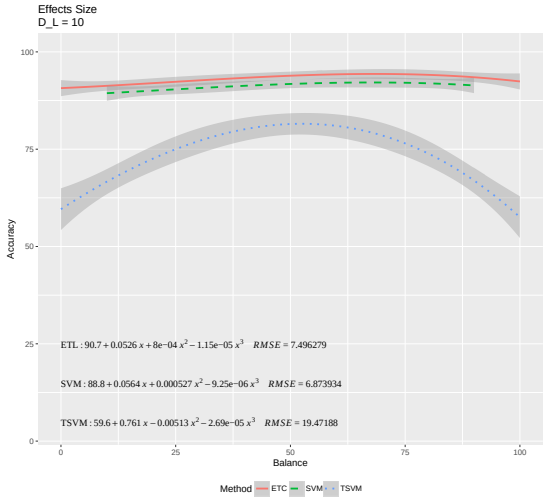



**Figure 5.1:** Accuracy comparison of the ETC with Inter-Class maximization, SVM and the TSVM.

Since residuals distribution is not normal, homoscedastic nor real independent, the Wilcoxon Signed Rank test was performed with a confidence interval of 95% for the methods combined pairwise for each dataset and number of patterns in the training set, and is graphically represented in Figure 5.4. The experiment was performed with paired observations, which also indicated the necessity of a test that considered it.

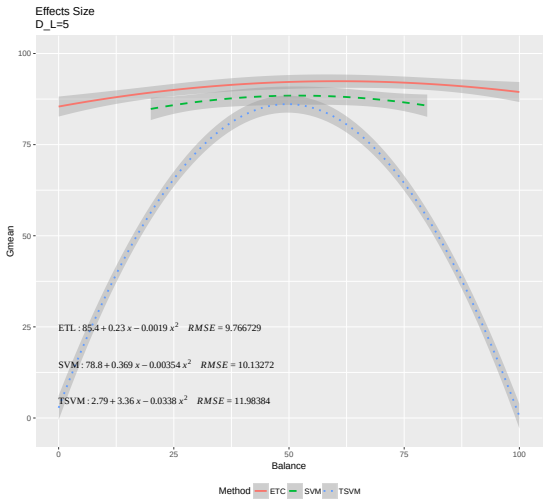



**(a)** Accuracy per balance for $\overline{D_L} = 10$.

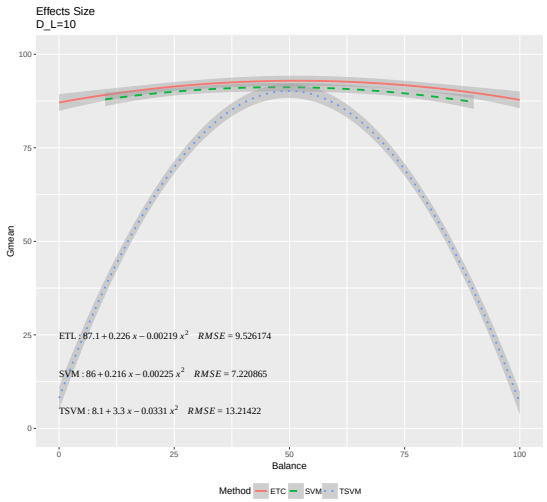



**(b)** Accuracy per balance for $\overline{D_L} = 5$.

**Figure 5.2:** Normalized Accuracy of SVM, TSVM and ETL for **hepatitis**, **Pima Indian diabetes**, **Wisconsin breast cancer** and **two moons** datasets, with $\overline{D_L} = 10$ and 5. The balance varies from 0% (only positive class) to 100% (only negative class) by 10% and 20% for $\overline{D_L} = 10$ and 5, respectively.



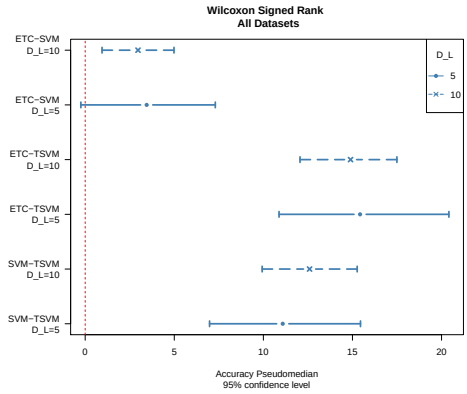

**(a)** GMEAN per balance for $\overline{D_L} = 10$.



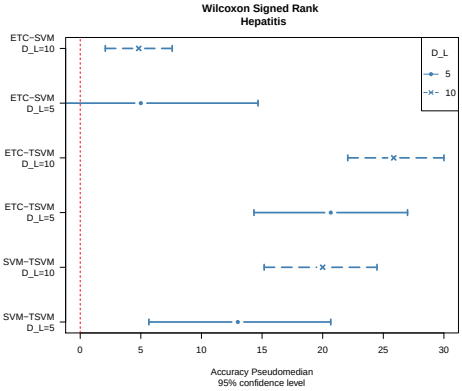

**(b)** GMEAN per balance for $\overline{D_L} = 5$.

**Figure 5.3:** Normalized GMEAN of SVM, TSVM and ETL for **hepatitis**,**Pima Indian diabetes**, **Wisconsin breast cancer** and **two moons** benchmark datasets, with $\overline{D_L}$ equal to 10 and $\overline{D_L}$ equal to 5. The balance varies from 0% (data only from positive class) to 100% (data only from positive class) by 10% for $\overline{D_L} = 10$ and by 20% for $\overline{D_L} = 5$.

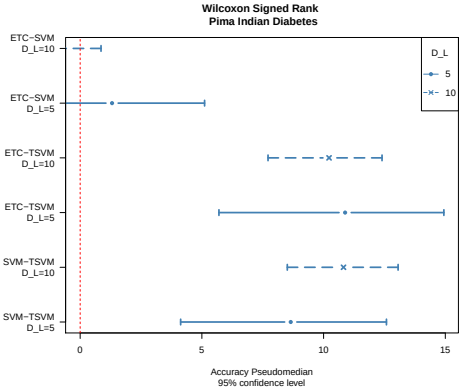
The results in Figure 5.4 indicate that, not only, all the methods results are different between each other, since most cases failed to meet the null hypothesis that distributions were the same. But, it also imply that if ETL approach dos not have a higher accuracy rate than the other two it is at least statistically



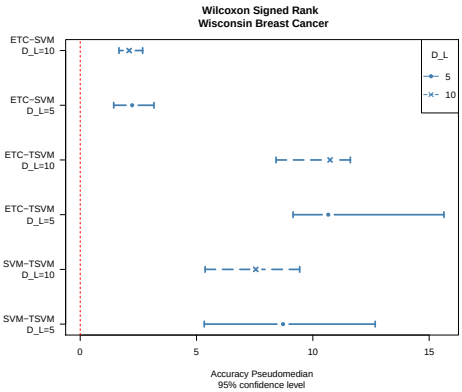

**(a)** All Datasets Wilcoxon Signed Rank Test.



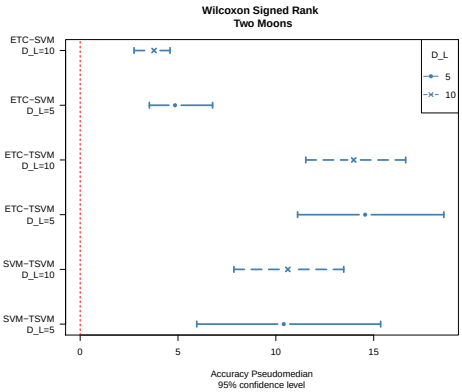

**(b)** Hepatites Wilcoxon Signed Rank Test.




**(c)** Pima Indian Diabetes Wilcoxon Signed Rank Test.




**(d)** Wisconsin Breast Cancer Wilcoxon Signed Rank Test.



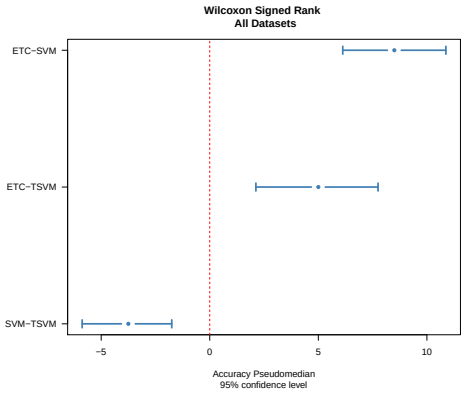

**(e)** Two Moon Wilcoxon Signed Rank Test.

**Figure 5.4:** Pairwise Wilcoxon Rank Sum Test with 95% confidence level of SVM, TSVM and ETL for **hepatitis**, **Pima Indian diabetes**, **Wisconsin breast cancer** and **two moons** benchmark datasets. Results after 90 executions of each combination with distinct unbiased samplings for $\overline{D_L}$ equal to 10 and after 40 executions for $\overline{D_L}$ equal to 5.

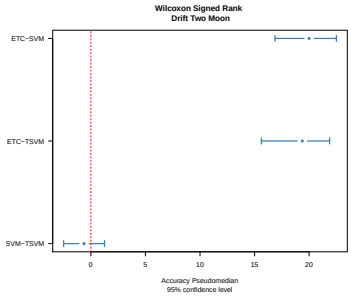
similar, since the pseudo medians of the differences are greater than zero and the 95% confidence interval either does not cross the zero or crosses it in a small margin.

### 5.1.2 Dataset Drift

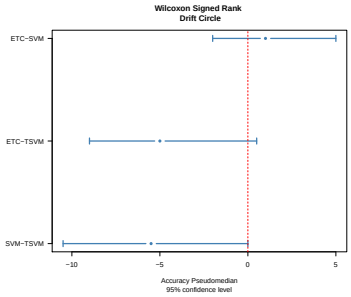
Tests have shown that the transductive approach is intrinsically robust to drifts without the need to adaptive learning models. This method, that is not based in the construction of a model, is naturally capable of classifying patterns in uncertain and restricted regions of the domain. According to Figure 5.5, the transductive methods were always better than the SVM.



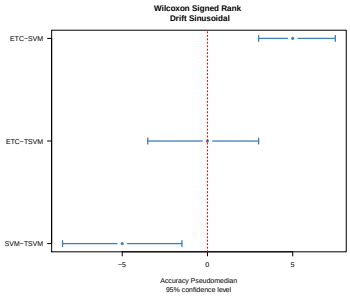

**(a)** All Datasets Wilcoxon Signed Rank Test




**(b)** Two Moons Wilcoxon Signed Rank Test




**(c)** Circle Wilcoxon Signed Rank Test




**(d)** Sinusoidal Wilcoxon Signed Rank Test

**Figure 5.5:** Pairwise Wilcoxon Rank Sum Test with 95% confidence level of SVM, TSVM and ETL for **Two Moons**, **Circle** and **Sinusoidal** benchmark datasets with Drift. Results after 30 executions of each.

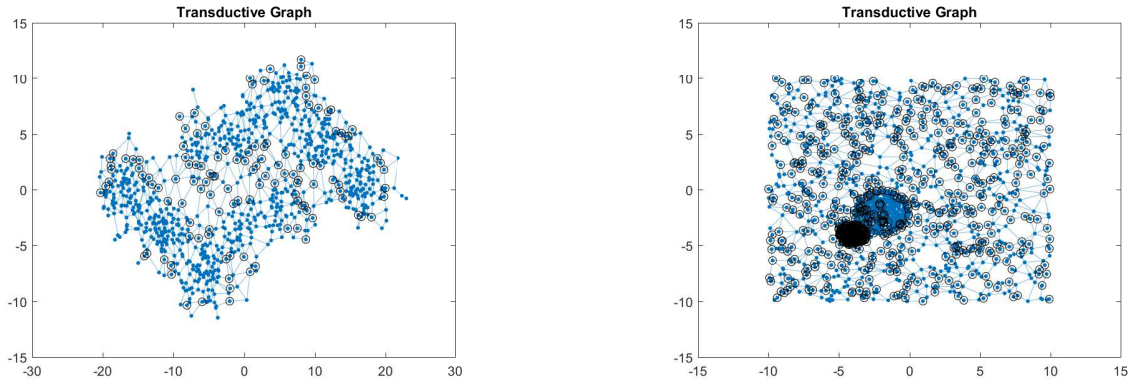
These results show that the performance of different learning approaches is heavily dependent upon the intrinsic characteristics of the data, including how much of it is available in the labeled and unlabeled sets. Therefore, in cases where one does not wish to induce a separating margin and estimation is limited to a given set of points known *a priori*, transductive learning may indeed be the best approach, although this cannot be assumed universally for all datasets or samples.

## 5.2 GABRIEL GRAPH TRANSDUCTIVE APPROACH EXPERIMENTAL RESULTS

### 5.2.1 Graphical Example

The method was evaluated using the following graphical bi-dimensional dataset in order to exemplify its behaviour. This experiment allows the analysis of how the method works under the presence of dataset shifts, with an intuitive example.

In Fig. 5.6, the resulting graph of the unified structure to calculate GMMs of the proposed strategy. The support vertexes are marked with black circles, and is interesting to observe that the supervised Gabriel Graph guarantees, in this case, a separation between both classes in the region defined in the training class. Meanwhile the Spatial Clusters include support vertexes around the classes. A specific scenario might occur when one of the classes ir highly concentrated while te other is spread throughout the space, which is the case of the Circle dataset. In this case, the method identifies that the is a class characterized by the data density, which allows an appropriate classification even with dataset shift. This is possible since the method is will define the highly dense class as a single class and the other one as noise. Fig. 5.7 and 5.8 represent $\mathcal{DW}$ and $\mathcal{DU}$, respectively.

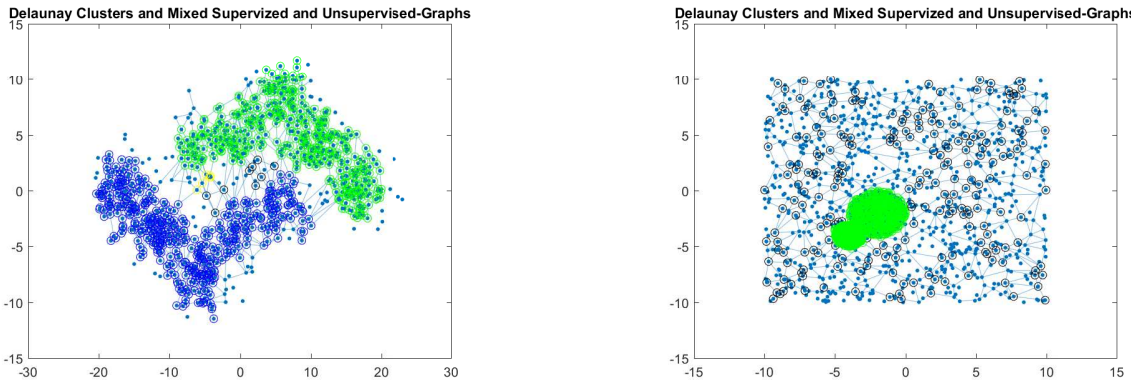



**(a)** Two Moon Dataset

**(b)** Circle Dataset

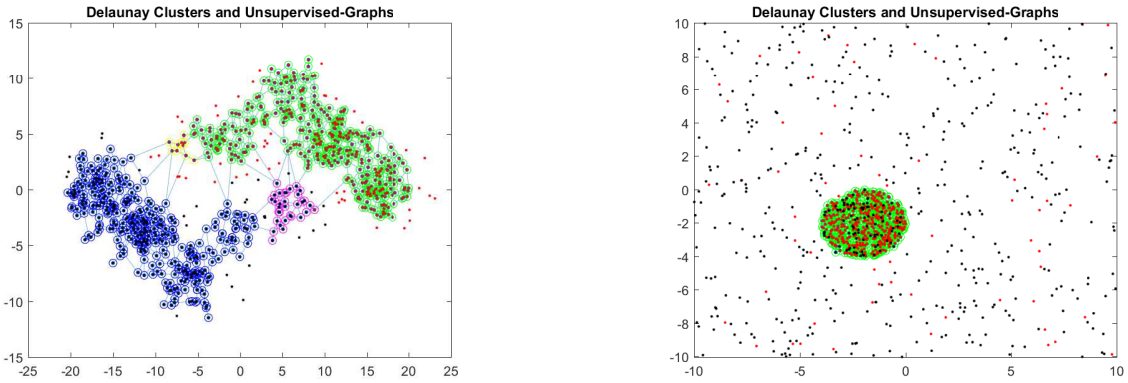
**Figure 5.6:** Transductive Resulting Graph

The output of the transductive labelling is exemplified in Fig. 5.9, there the labels attributed by the method are represented along the originally labeled ones and the resulting graph obtained in Item **??**. In this image is possible to observe the labelling according to the structure, even in a region that was not represented in the domain of training data points.



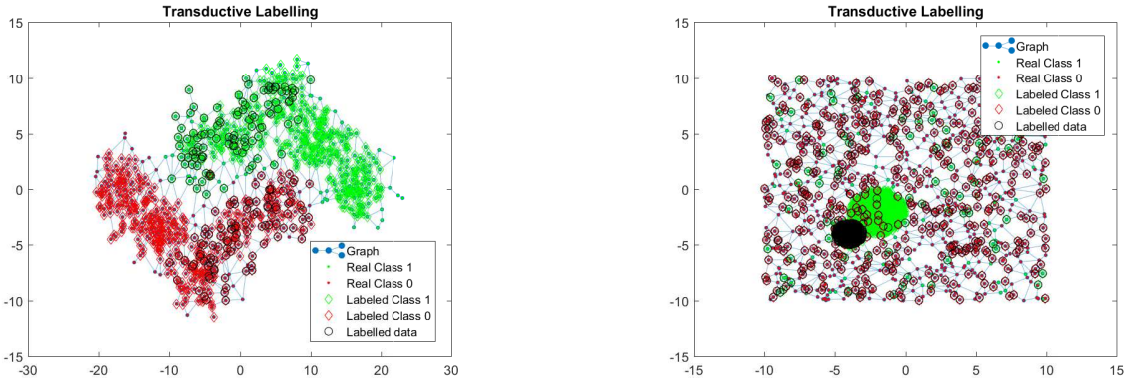

**(a)** Two Moon Dataset **(b)** Circle Dataset

**Figure 5.7:** Spatial Cluster for Working data




**(a)** Two Moon Dataset **(b)** Circle Dataset

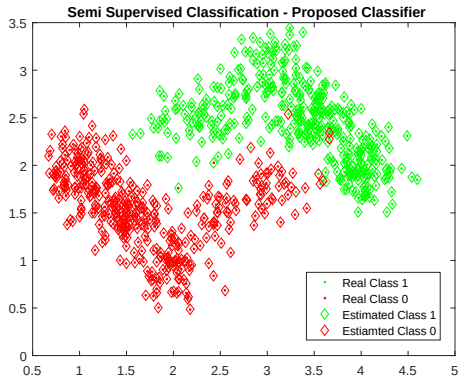
**Figure 5.8:** Spatial Cluster for Unsupervised data



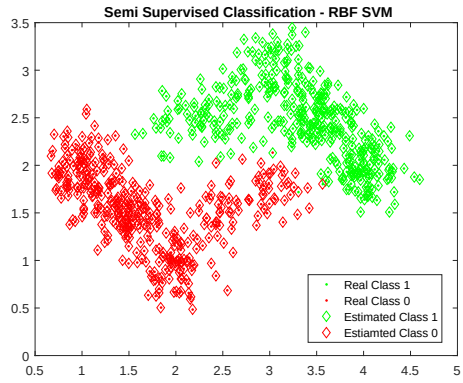

**(a)** Two Moon Dataset **(b)** Circle Dataset

**Figure 5.9:** Transductive Labels with resulting Graph

The result obtained by the classifiers are represented in Fig. 5.10a and 5.10b, the first one shows the results of the proposed method and the last one of a SVM with RBF kernel, using the Transductive labels as input.

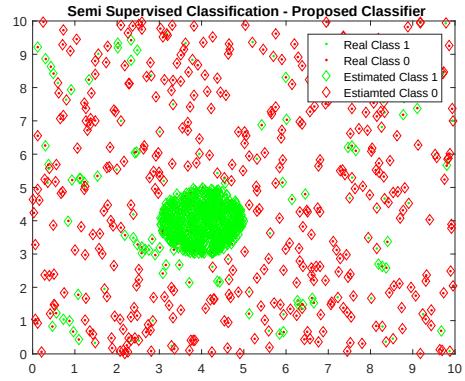



**(a)** Classification of unlabelled data using proposed classifier

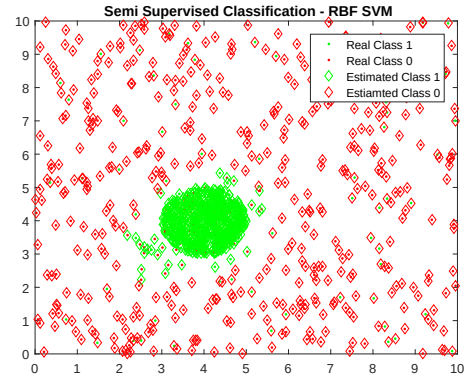



**(b)** Classification of unlabelled data using SVM with RBF kernel

**Figure 5.10:** The classification of the Two Moon Dataset performed by the proposed method in comparison to SVM Classifier, both using the Transductive Labeling as input




**(a)** Classification of unlabelled data using proposed classifier




**(b)** Classification of unlabelled data using SVM with RBF kernel

**Figure 5.11:** The classification of the Circle Dataset performed by the proposed method in comparison to SVM Classifier, both using the Transductive Labeling as input

### 5.2.2 Comparison with State of Art methods

In this experimental setting, the proposed method is compared to state of art methods, with two distinct conditions:

1. Using the data labelled by the transductive approach to generate the classifiers.

2. Only using the originally labelled data set to generate the classifiers.

The datasets used in this experiment are the Two-Moon, shown in the previous section, the Circle from [63] and Elec2 from [42], but since this method is intended for spatial analysis only features 4 and 6 were used. With this experiment, the improvement of classification of datasets with shift is observed when the Transductive Labelling is applied to the whole working data. Also, it is possible to observe that methods integrate well with this labelling strategy. Furthermore, the proposed method that uses the labelling structure have a satisfactory behaviour in comparison to state-of-art methods, as observed in Figure 5.12. Furthermore, it is possible to observe a significant improvement of classification when the transductive labelling strategy is used alongside the state-of-art classifiers, as observed in Figure 5.12.

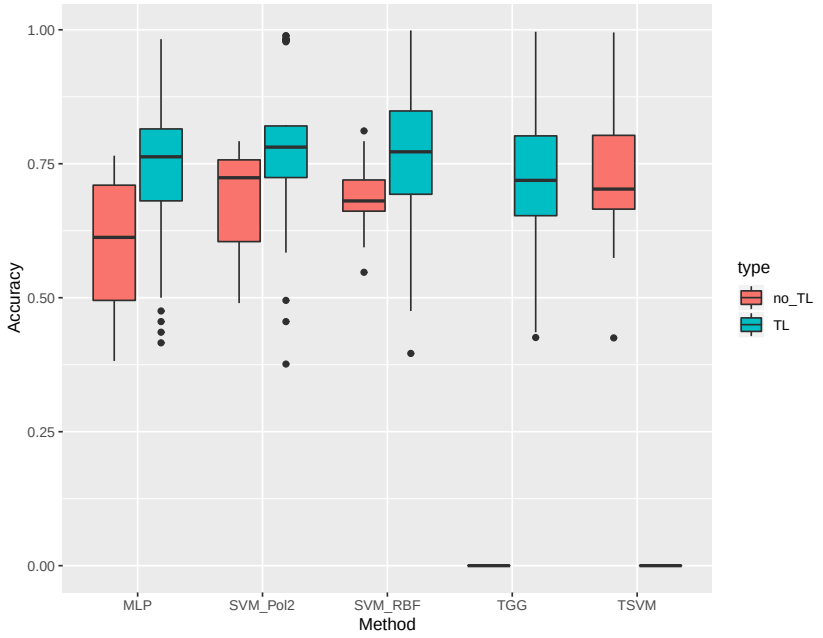
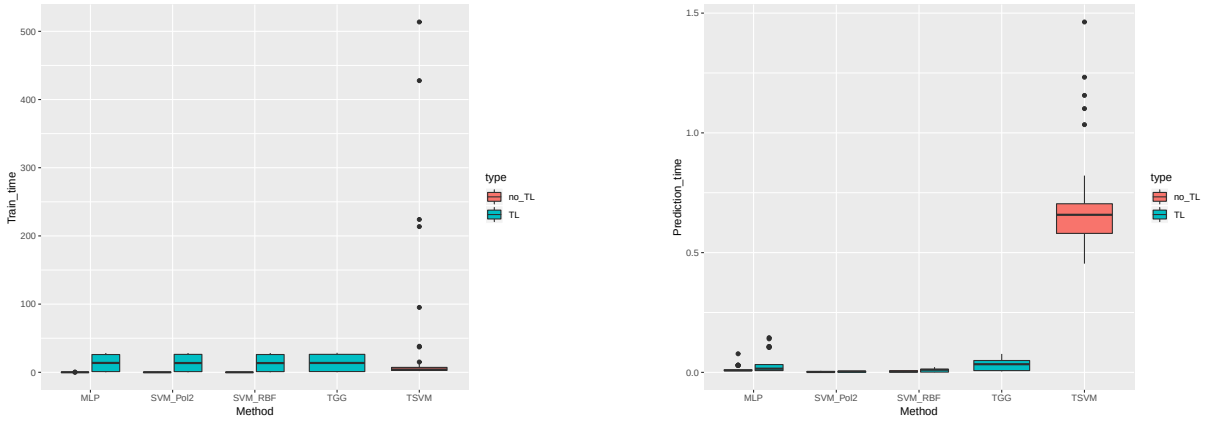



**Figure 5.12:** Accuracy comparison of the Transductive Gabriel Graph with State-of-Art Methods, using Transductive Labelling and Not using it, and the Transductive SVM.

In the matter of training and prediction time, Transductive approaches tend to perform much poorer then inductive models. In this context, in Figure 5.13a it is possible to notice a slower performance of Transductive approaches, including the TSVM that has a large ammount of outliers. Considering the Prediction Time, the proposed classification method is slower then other state-of-art approaches, but the hybrid solutions that are integrated with Transductive labelling have competitive performance.




**(a)** Training Time

**(b)** Prediction Time

**Figure 5.13:** Computational Training and Prediction Time for the Transductive Gabriel Graph compared to State-of-Art Methods, using Transductive Labelling and Not using it, and Transductive SVM

# 6 CONCLUSION

We live in a society absolutely dependent on science and technology and yet have cleverly arranged things so that almost no one understands science and technology. That's a clear prescription for disaster.

Carl Sagan and Anne Kalosh, *Bringing Science Down to Earth (1994)*

It was expected that the transductive approach would present a better result under situations were the data, or real knowledge about the data distribution, is restricted. Even though the method presented results near to the SVM, the actual rank of the classifier was higher. Regarding this comparison, there are two main advantages of the Essentially Transductive Classifier in relation to the Support Vector Machine Classifier. Firstly, for the used databases, the ETC presented a consistent, or at least a higher consistency, to the classification performance for different training set imbalance configurations. This tendency was present including cases where only a single class was presented, which is not possible with a SVM classifier. The other advantage is that, in case of a dataset shift, a transductive approach is able to redefine the system characteristics for the interest points during the application of the method. This however require an appropriate memory of the data previously classified.

Furthermore, the SVM theoretically obtain results statistically close to the dataset limits for unambiguous classification due to its large margin optimization formulation. When the training data presented to the SVM is reduced, the classifier margin is shifted from the optimal classification point. Thus, a slightly better performance is, in fact, reaching small surplus open for improvement in the classification performance.

However, the estimation of probability density of data is extremely costly to be performed at the rate necessary tor the essentially transductive method. It required that the entropy of multiple data combinations was estimated but the calculation of entropy itself needs the estimation of data probability densities. In this case, attempts to optimize data set PDFs estimation were not successful since the problem itself that was the target of this research is based on the deviation of the data structure from pre-setted considerations. Therefore, the ETC strategy initially proposed is not scalable, resulting in prohibitively slow performances when the datasets increased both in instances and features. Thus, the approach based in Gabriel Graphs and spatial clustering was proposed for two dimensional data. This approach attempts to optimization of the statistical tests, by creating a deterministic structure that can integrate both labelled and unlabelled data, and by predifining possible spatial clusters prior calculation of the probability density functions, which greatly reduces the search space.

Dataset shift comprises of a large variety of problems that are a challenge to any strategy that attempts to learn a system behaviour from data. However, this consists of a large variety of problems and, therefore, all cases are not likely to be all solved by a single approach. Thus, different methods have been proposed in order to solve problems with specific contexts. In this sense, the Gabriel Graph Transductive Approach attempts to be easily integrated to other classifiers, in order to be more easily integrated in different applications.

The notion of the adequate similarity between classes can differ depending on the application and type of shift, in this case the comparison between the distribution of both lasses should be adapted. In

this context, the proposed methods are adequate for several different problems, since they use statistical tests in order to evaluate the ideal labelling. Thus, if necessary, a different type of statistical test can be implemented to adapt the labelling process to specific characteristics of data for problems with different contexts.

Finally, solutions for dataset shifting still do not have any consensus and are not systematically being used in real-world systems and applications. In the context of uncertainties in the training set, and thus the primary assumption of dataset drift, the ETC method has shown to be an appropriate alternative of classification learning methods, however it has shown to be a prohibitively slow method. The Gabriel Graph Transductive Approach is a more promising method since it allows an faster transductive step and have an structurally integrated inductive classification method, which allows faster classification of novel data. Also, the creation of novel methods that can be easily integrated to current systems might promote a better development of more complete solutions in the future.

Overall, dataset shift problems affects any modelling strategy that are based on data. Therefore, transductive approaches might theoretically hold some advantage since they do not attempt to define induced general models. Instead, they generate a local transductive solution, based on all available data. However, such approaches have great disadvantages when the time performance is considered, specially when new data is provided, since the transductive solution must be calculated from the beginning. In this context, hybrid solutions can be a better approach for real-world problems. In this scenario, solutions oriented to the problems they are solving might be a more adequate strategy. Therefore, the Gabriel Graphs Trasnductive Approach is an appropriate solution for specific problems with two dimensional data, such as epidemics analysis, some images analysis, ecology, biodiversity and geology problems etc.

# References

# 1 BIBLIOGRAPHY


[1] AHAMED, T., TIAN, L., ZHANG, Y., AND TING, K. A review of remote sensing methods for biomass feedstock production. *Biomass and Bioenergy 35*, 7 (2011), 2455 – 2469.

[2] ALAÍZ-RODRÍGUEZ, R., GUERRERO-CURIESES, A., AND CID-SUEIRO, J. Class and subclass probability re-estimation to adapt a classifier in the presence of concept drift. *Neurocomputing 74*, 16 (2011), 2614–2623.

[3] AMARI, S.-I. *Differential-Geometrical Methods in Statistics*, vol. 28 of *Lecture Notes in Statistics*. Springer, 1985.

[4] AMOS, B., LUDWICZUK, B., AND SATYANARAYANAN, M. Openface: A general-purpose face recognition library with mobile applications. Tech. rep., CMU-CS-16-118, CMU School of Computer Science, 2016.

[5] BÉGIN, L., GERMAIN, P., LAVIOLETTE, F., AND ROY, J. PAC-Bayesian Theory for Transductive Learning. *Proceedings of the Seventeenth Conference on Antificial Intelligence and Statistics (AISTATS) 33* (2014).

[6] BEN-DAVID, S., AND BLITZER, J. Analysis of representations for domain adaptation. In *Advances in Neural Information Processing Systems* (feb 2007), vol. 19, IEEE, pp. 137–144.

[7] BENNETT, K. P., AND DEMIRIZ, A. Semi-supervised support vector machines. In *Proceedings of the 1998 Conference on Advances in Neural Information Processing Systems II* (Cambridge, MA, USA, 1999), MIT Press, pp. 368–374.

[8] BERRY, S., LEVINSOHN, J., AND PAKES, A. Differentiated products demand systems from a combination of micro and macro data: New car market. *Journ. Politic. Econ. 112*, 1 (2004), 68–105.

[9] BICKEL, S., BRÜCKNER, M., AND SCHEFFER, T. Discriminative Learning Under Covariate Shift. *Journal of Machine Learning Research 10* (2009), 2137—-2155.

[10] BISHOP, C. M. *Pattern Recognition and Machine Learning (Information Science and Statistics)*. Springer, 2006.

[11] BLAKE, C. L., AND MERZ, C. J. UCI repository of machine learning databases, 1998.

[12] BRUZZONE, L., CHI, M., AND MARCONCINI, M. A novel transductive SVM for semisupervised classification of remote-sensing images. *IEEE Transactions on Geoscience and Remote Sensing 44*, 11 (2006), 3363–3372.

[13] BRZEZINSKI, D., AND STEFANOWSKI, J. Prequential auc for classifier evaluation and drift detection in evolving data streams. In *New Frontiers in Mining Complex Patterns* (2015), A. Appice, M. Ceci, C. Loglisci, G. Manco, E. Masciari, and Z. W. Ras, Eds., Springer International Publishing, pp. 87–101.

[14] BURGES, C. J. C. A tutorial on support vector machines for pattern recognition. *Data Mining and Knowledge Discovery 2*, 2 (1998), 121–167.

[15] CAI, D., HE, X., AND HAN, J. Semi-supervised discriminant analysis. In *2007 IEEE 11th International Conference on Computer Vision* (Oct 2007), pp. 1–7.

[16] CHEN, Y., LI, W., SAKARIDIS, C., DAI, D., AND VAN GOOL, L. Domain adaptive faster r-cnn for object detection in the wild. In *IEEE Conf. Comp. Vision and Pattern Recognition* (2018), pp. 3339–3348.

[17] DA COSTA, F. G., RIOS, R. A., AND DE MELLO, R. F. Using dynamical systems tools to detect concept drift in data streams. *Expert Systems with Applications 60* (2016), 39–50.

[18] DE VITO, S., FATTORUSO, G., PARDO, M., TORTORELLA, F., AND DI FRANCIA, G. Semi-supervised learning techniques in artificial olfaction: A novel approach to classification problems and drift counteraction. *IEEE Sensors Journal 12*, 11 (2012), 3215–3224.

[19] DELANY, S. J., CUNNINGHAM, P., TSYMBAL, A., AND COYLE, L. A case-based technique for tracking concept drift in spam filtering. *Knowledge-Based Systems 18*, 4-5 (2005), 187–195.

[20] DERBEKO, P., EL-YANIV, R., AND MEIR, R. Explicit learning curves for transduction and application to clustering and compression algorithms. *Journal of Artificial Intelligence Research 22*, 1 (July 2004), 117–142.

[21] DHEERU, D., AND KARRA TANISKIDOU, E. UCI machine learning repository, 2017.

[22] DITZLER, G., AND POLIKAR, R. An ensemble based incremental learning framework for concept drift and class imbalance. In *2010 International Joint Conference on Neural Networks (IJCNN)* (July 2010), pp. 1–8.

[23] DITZLER, G., AND POLIKAR, R. Semi-supervised learning in nonstationary environments. In *2011 Int. Joint Conf. Neural Net.* (July 2011), pp. 2741–2748.

[24] DITZLER, G., ROSEN, G., AND POLIKAR, R. Transductive learning algorithms for nonstationary environments. In *2012 Int. Joint Conf. Neural Net.* (July 2012), pp. 10–15.

[25] DITZLER, G., ROVERI, M., ALIPPI, C., AND POLIKAR, R. Learning in nonstationary environments: A survey. *IEEE Computational Intelligence Magazine 10*, 4 (Nov 2015), 12–25.

[26] DORNHEGE, G., BLANKERTZ, B., CURIO, G., AND MULLER, K. . Boosting bit rates in noninvasive eeg single-trial classifications by feature combination and multiclass paradigms. *IEEE Trans. Bio. Eng. 51*, 6 (June 2004), 993–1002.

[27] DRIES, A., AND RÜCKERT, U. Adaptive concept drift detection. *Statistical Analysis and Data Mining: The ASA Data Science Journal 2*, 5-6 (2009), 311–327.

[28] DUCZMAL, L. H., MOREIRA, G. J., BURGARELLI, D., TAKAHASHI, R. H., MAGALHÃES, F. C., AND BODEVAN, E. C. Voronoi distance based prospective space-time scans for point data sets: a dengue fever cluster analysis in a southeast brazilian town. *International Journal of Health Geographics 10*, 1 (2011), 29.

[29] ELWELL, R., AND POLIKAR, R. Incremental learning of variable rate concept drift. In *Multiple Classifier Systems* (Berlin, Heidelberg, 2009), J. A. Benediktsson, J. Kittler, and F. Roli, Eds., Springer Berlin Heidelberg, pp. 142–151.

[30] ELWELL, R., AND POLIKAR, R. Incremental Learning of Concept Drift in Nonstationary Environments. *IEEE Transactions on Neural Networks 22* (2011), 1517–1531.

[31] FDEZ-RIVEROLA, F., IGLESIAS, E. L., DÍAZ, F., MÉNDEZ, J. R., AND CORCHADO, J. M. Applying lazy learning algorithms to tackle concept drift in spam filtering. *Expert Systems with Applications 33*, 1 (2007), 36–48.

[32] FERNANDEZ, A., GARCIA, S., AND HERRERA, F. Addressing the Classification with Imbalanced Data : Open Problems and New Challenges on Class Distribution In many applications , there exists a significant difference between the class prior Addressing the Classification with Imbalanced. *Hybrid Artificial Intelligent Systems 6678* (2011), 1–10.

[33] FUGLEDE, B., AND TOPSOE, F. Jensen-shannon divergence and hilbert space embedding. In *International Symposium on Information Theory* (2004), IEEE, p. 31.

[34] GABRIEL, K. R., AND SOKAL, R. R. A new statistical approach to geographic variation analysis. *Systematic Zoology 18*, 3 (sep 1969), 259.

[35] GAMA, J., MEDAS, P., CASTILLO, G., AND RODRIGUES, P. Learning with drift detection. In *Advances in Artificial Intelligence – SBIA 2004* (Berlin, Heidelberg, 2004), A. L. C. Bazzan and S. Labidi, Eds., Springer Berlin Heidelberg, pp. 286–295.

[36] GAMA, J. A., ŽLIOBAITĖ, I., BIFET, A., PECHENIZKIY, M., AND BOUCHACHIA, A. A survey on concept drift adaptation. *ACM Computing Surveys 46*, 4 (Mar. 2014), 44:1–44:37.

[37] GAO, B., MAEKAWA, T., AMAGATA, D., AND HARA, T. Environment-adaptive malicious node detection in manets with ensemble learning. In *2018 IEEE 38th International Conference on Distributed Computing Systems (ICDCS)* (July 2018), pp. 556–566.

[38] GEMAN, S., BIENENSTOCK, E., AND DOURSAT, R. Neural Networks and the Bias/Variance Dilemma. *Neural Computation 4*, 1 (Jan. 1992), 1–58.

[39] GHAZIKHANI, A., MONSEFI, R., AND SADOGHI YAZDI, H. Recursive least square perceptron model for non-stationary and imbalanced data stream classification. *Evolving Systems 4*, 2 (Jun 2013), 119–131.

[40] GONZÁLEZ, P., CASTAÑO, A., CHAWLA, N. V., AND COZ, J. J. D. A review on quantification learning. *ACM Computing Surveys 50*, 5 (2017), 74.

[41] HAQUE, A., KHAN, L., BARON, M., THURAISINGHAM, B., AND AGGARWAL, C. Efficient handling of concept drift and concept evolution over Stream Data. In *2016 IEEE 32nd Int. Conf. Data Eng.* (may 2016), pp. 481–492.

[42] HARRIES, M., CSE TR, U. N., AND WALES, N. S. Splice-2 comparative evaluation: Electricity pricing, 1999.

[43] HOFER, V., AND KREMPL, G. Drift mining in data: A framework for addressing drift in classification. *Computational Statistics & Data Analysis 57*, 1 (2013), 377–391.

[44] HUANG, N. E., SHEN, Z., LONG, S. R., WU, M. C., SHIH, H. H., ZHENG, Q., YEN, N.-C., TUNG, C. C., AND LIU, H. H. The empirical mode decomposition and the hilbert spectrum for nonlinear and non-stationary time series analysis. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences 454*, 1971 (1998), 903–995.

[45] KEARNS, M. J., AND VAZIRANI, U. V. *An Introduction to Computational Learning Theory*. MIT Press, Cambridge, MA, USA, 1994.

[46] KHOSLA, A., ZHOU, T., MALISIEWICZ, T., EFROS, A. A., AND TORRALBA, A. Undoing the damage of dataset bias. *Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics) 7572 LNCS* (2012), 158–171.

[47] KLINKENBERG, R., AND JOACHIMS, T. Detecting concept drift with support vector machines. In *Seventeenth International Conference on Machine Learning* (2000), vol. 11, Morgan Kaufmann, pp. 487–494.

[48] KOLTER, J. Z., AND MALOOF, M. A. Dynamic weighted majority: a new ensemble method for tracking concept drift. In *Third IEEE International Conference on Data Mining* (Nov 2003), pp. 123–130.

[49] KOLTER, J. Z., AND MALOOF, M. A. Using additive expert ensembles to cope with concept drift. In *22Nd International Conference on Machine Learning* (New York, NY, USA, 2005), ICML '05, ACM, pp. 449–456.

[50] KONG, X., NG, M. K., AND ZHOU, Z.-H. Transductive multilabel learning via label set propagation. *IEEE Transactions on Knowledge and Data Engineering 25*, 3 (2013), 704–719.

[51] KULIS, B., SAENKO, K., AND DARRELL, T. What you saw is not what you get: Domain adaptation using asymmetric kernel transforms. In *2011 IEEE Conference of Computer Vision and Pattern Recognition* (June 2011), IEEE, pp. 1785–1792.

[52] KULLBACK, S. Minimum discrimination information estimation and application. Tech. rep., Department of Statistics, George Washington University, 1972.

[53] KULLBACK, S., AND LEIBLER, R. A. On information and sufficiency. *The Annals of Mathematical Statistics 22*, 1 (03 1951), 79–86.

[54] KUNCHEVA, L. I. Classifier ensembles for changing environments. In *Multiple Classifier Systems* (Berlin, Heidelberg, 2004), F. Roli, J. Kittler, and T. Windeatt, Eds., Springer Berlin Heidelberg, pp. 1–15.

[55] LI, Y., KAMBARA, H., KOIKE, Y., AND SUGIYAMA, M. Application of covariate shift adaptation techniques in brain–computer interfaces. *IEEE Trans. Bio. Eng. 57*, 6 (June 2010), 1318–1324.

[56] LIN, J. Divergence measures based on the shannon entropy. *IEEE Transactions on Information theory 37*, 1 (1991), 145–151.

[57] LIU, D., WU, Y., AND JIANG, H. Fp-elm: An online sequential learning algorithm for dealing with concept drift. *Neurocomputing 207* (2016), 322 – 334.

[58] LÓPEZ, V., FERNÁNDEZ, A., GARCÍA, S., PALADE, V., AND HERRERA, F. An insight into classification with imbalanced data: Empirical results and current trends on using data intrinsic characteristics. *Information Sciences 250* (Nov. 2013), 113–141.

[59] LÓPEZ, V., FERNÁNDEZ, A., AND HERRERA, F. On the importance of the validation technique for classification with imbalanced datasets: Addressing covariate shift when data is skewed. *Information Sciences 257* (Feb. 2014), 1–13.

[60] LOTTE, F., CONGEDO, M., LÉCUYER, A., LAMARCHE, F., AND ARNALDI, B. A review of classification algorithms for eeg-based brain–computer interfaces. *Jour. Neural Eng. 4*, 2 (2007).

[61] MAIA, T. T. *Aprendizado transdutivo baseado em teoria dainformação e teoria do aprendizado estatístico*. PhD thesis, UFMG School of Engineering, 7 2007.

[62] MATASCI, G., VOLPI, M., TUIA, D., AND KANEVSKI, M. F. Transfer component analysis for domain adaptation in image classification. In *Image and Signal Processing for Remote Sensing XVII* (2011).

[63] MINKU, L. L., WHITE, A. P., AND YAO, X. The impact of diversity on online ensemble learning in the presence of concept drift. *IEEE Transactions on Knowledge and Data Engineering 22*, 5 (May 2010), 730–742.

[64] MINKU, L. L., AND YAO, X. Ddd: A new ensemble approach for dealing with concept drift. *IEEE Transactions on Knowledge and Data Engineering 24*, 4 (April 2012), 619–633.

[65] MIRZA, B., LIN, Z., AND LIU, N. Ensemble of subset online sequential extreme learning machine for class imbalance and concept drift. *Neurocomputing 149* (2015), 316 – 329. Advances in neural networks Advances in Extreme Learning Machines.

[66] MORENO-TORRES, J. G., LLORÀ, X., GOLDBERG, D. E., AND BHARGAVA, R. Repairing fractures between data using genetic programming-based feature extraction: A case study in cancer diagnosis. *Information Sciences 222* (2013), 805–823.

[67] MORENO-TORRES, J. G., RAEDER, T., ALAIZ-RODRÍGUEZ, R., CHAWLA, N. V., AND HERRERA, F. A unifying view on dataset shift in classification. *Pattern Recognition 45*, 1 (Jan. 2012), 521–530.

[68] MOROSHKO, E., VAITS, N., AND CRAMMER, K. Second-order non-stationary online learning for regression. *Journal of Machine Learning Research 16* (2015), 1481–1517.

[69] NICOLAS-ALONSO, L. F., AND GOMEZ-GIL, J. Brain computer interfaces, a review. *Sensors 12*, 2 (2012), 1211–1279.

[70] OOMMEN, B. J., AND RUEDA, L. Stochastic learning-based weak estimation of multinomial random variables and its applications to pattern recognition in non-stationary environments. *Pattern Recognition 39*, 3 (2006), 328 – 341.

[71] PAGE, E. S. Continuous inspection schemes. *Biometrika 41*, 1-2 (1954), 100–115.

[72] PALHARES, D. M. F., MARCOLINO, M. S., SANTOS, T. M. M., DA SILVA, J. L. P., GOMES, P. R., RIBEIRO, L. B., MACFARLANE, P. W., AND RIBEIRO, A. L. P. Normal limits of the electrocardiogram derived from a large database of brazilian primary care patients. *BMC Card. Disord. 17*, 1 (Jun 2017).

[73] PAN, S. J., AND YANG, Q. A Survey on Transfer Learning. *IEEE Transactions on Knowledge and Data Engineering 22*, 10 (Oct. 2010), 1345–1359.

[74] PARK, S.-H., LEE, D., AND LEE, S.-G. Filter bank regularized common spatial pattern ensemble for small sample motor imagery classification. *IEEE Trans. Neural Sys. Rehab. Eng. 26*, 2 (Feb 2018), 498–505.

[75] PFEFFERMANN, D., SKINNER, C. J., HOLMES, D. J., GOLDSTEIN, H., AND RASBASH, J. Weighting for unequal selection probabilities in multilevel models. *Journal of the Royal Statistical Society. Series B (Statistical Methodology) 60*, 1 (1998), 23–40.

[76] POLIKAR, R. *Ensemble Learning*. Springer US, Boston, MA, 2012, pp. 1–34.

[77] QUIÑONERO CANDELA, J., SUGIYAMA, M., SCHWAIGHOFER, A., AND LAWRENCE, N. D. *Dataset Shift in Machine Learning*. The MIT Press, Feb. 2009.

[78] RAMANATHAN, N., CHELLAPPA, R., AND BISWAS, S. Computational methods for modeling facial aging: A survey. *Jour. Vis. Lang. & Comp. 20*, 3 (2009), 131 – 144.

[79] RAO, C. R. Diversity and dissimilarity coefficientes: a unified approach. *Theoretical Population Biology 21*, 1 (1982), 24–43.

[80] RAZA, H., CECOTTI, H., LI, Y., AND PRASAD, G. Adaptive learning with covariate shift-detection for motor imagery-based brain–computer interface. *Soft Computing 20*, 8 (Aug 2016), 3085–3096.

[81] RAZA, H., PRASAD, G., AND LI, Y. Dataset shift detection in non-stationary environments using EWMA charts. *Proceedings - 2013 IEEE International Conference on Systems, Man, and Cybernetics, SMC 2013* (2013), 3151–3156.

[82] RAZA, H., PRASAD, G., AND LI, Y. EWMA model based shift-detection methods for detecting covariate shifts in non-stationary environments. *Pattern Recognition 48*, 3 (Mar. 2015), 659–669.

[83] RAZA, H., PRASAD, G., LI, Y., AND CECOTTI, H. Covariate shift-adaptation using a transductive learning model for handling non-stationarity in eeg based brain-computer interfaces. In *2014 IEEE International Conference on Bioinformatics and Biomedicine (BIBM)* (Nov 2014), pp. 230–236.

[84] RAZA, H., RATHEE, D., ZHOU, S., CECOTTI, H., AND PRASAD, G. Covariate shift estimation based adaptive ensemble learning for handling non-stationarity in motor imagery related eeg-based brain-computer interface. *CoRR abs/1805.01044* (2018).

[85] SHEU, J.-J., CHU, K.-T., LI, N.-F., AND LEE, C.-C. An efficient incremental learning mechanism for tracking concept drift in spam filtering. *PLOS ONE 12*, 2 (02 2017), 1–17.

[86] SHIMODAIRA, H. Improving predictive inference under covariate shift by weighting the log-likelihood function. *Journal of Statistical Planning and Inference 90* (2000), 227–244.

[87] SIAHROUDI, S. K., MOODI, P. Z., AND BEIGY, H. Detection of evolving concepts in non-stationary data streams: A multiple kernel learning approach. *Expert Systems with Applications 91* (2018), 187 – 197.

[88] SUGIYAMA, M., KRAULEDAT, M., AND MÜLLER, K.-R. Covariate Shift Adaptation by Importance Weighted Cross Validation. *The Journal of Machine Learning Research 8* (Dec. 2007), 985–1005.

[89] SUGIYAMA, M., NAKAJIMA, S., KASHIMA, H., BUENAU, P. V., AND KAWANABE, M. Direct Importance Estimation with Model Selection and Its Application to Covariate Shift Adaptation. In *Advances in Neural Information Processing Systems 20* (dec 2008), J. C. Platt, D. Koller, Y. Singer, and S. T. Roweis, Eds., Curran Associates, Inc., pp. 1433–1440.

[90] SUGIYAMA, M., AND STORKEY, A. J. Mixture Regression for Covariate Shift. In *Advances in Neural Information Processing Systems 19* (2007), B. Schölkopf, J. C. Platt, and T. Hoffman, Eds., MIT Press, pp. 1337–1344.

[91] TAISTER, M. A., HOLLIDAY, S. D., AND BORRMMAN, H. Computational methods for modeling facial aging: A survey. *Forensic Sci. Com.* (2000).

[92] TORRES, L. C. B., CASTRO, C. L., AND BRAGA, A. P. Gabriel graph for dataset structure and large margin classification: A bayesian approach. In *Proceedings of the European Symposium on Neural Networks* (2015), pp. 237–242.

[93] TSAI, C. J., LEE, C. I., AND YANG, W. P. Mining decision rules on data streams in the presence of concept drifts. *Expert Systems with Applications 36*, 2 PART 1 (2009), 1164–1178.

[94] TSYMBAL, A., PECHENIZKIY, M., CUNNINGHAM, P., AND PUURONEN, S. Dynamic integration of classifiers for handling concept drift. *Information Fusion 9*, 1 (2008), 56–68.

[95] TUIA, D., PASOLLI, E., AND EMERY, W. Using active learning to adapt remote sensing image classifiers. *Remote Sensing of Environment 115*, 9 (2011), 2232 – 2242.

[96] TUIA, D., PASOLLI, E., AND EMERY, W. J. Dataset shift adaptation with active queries. In *2011 Joint Urban Remote Sensing Event* (April 2011), pp. 121–124.

[97] TUIA, D., PERSELLO, C., AND BRUZZONE, L. Domain adaptation for the classification of remote sensing data: An overview of recent advances. *IEEE Geosci. Remote Sens. 4*, 2 (June 2016), 41–57.

[98] TURHAN, B. On the dataset shift problem in software engineering prediction models. *Empirical Software Engineering 17*, 1-2 (2012), 62–74.

[99] VAPNIK, V. N. Principles of Risk Minimization for Learning Theory. *Advances in Neural Information Processing Systems 4* (1992), 831–838.

[100] VAPNIK, V. N. *The nature of statistical learning theory*. Springer-Verlag, jun 1995.

[101] VAPNIK, V. N. *Statistical Learning Theory*. John Wiley & Sons, Inc., New York, 1998.

[102] VAPNIK, V. N. An Overview of Statistical Learning Theory. *IEEE Transactions on Neural Networks 10*, 5 (Sept. 1999), 988–999.

[103] WANG, H., AND ABRAHAM, Z. Concept drift detection for streaming data. In *2015 International Joint Conference on Neural Networks (IJCNN)* (July 2015), pp. 1–9.

[104] WANG, J., SHEN, X., AND PAN, W. On Transductive Support Vector Machines. *Prediction and Discovery*, 1998 (2005).

[105] WANG, S., MINKU, L. L., GHEZZI, D., CALTABIANO, D., TINO, P., AND YAO, X. Concept drift detection for online class imbalance learning. In *The 2013 International Joint Conference on Neural Networks (IJCNN)* (Aug 2013), pp. 1–10.

[106] WANG, S., MINKU, L. L., AND YAO, X. Resampling-based ensemble methods for online class imbalance learning. *IEEE Transactions on Knowledge and Data Engineering 27*, 5 (May 2015), 1356–1368.

[107] WANG, S., MINKU, L. L., AND YAO, X. A systematic study of online class imbalance learning with concept drift. *IEEE Transactions on Neural Networks and Learning Systems PP*, 99 (2018), 1–20.

[108] WEBB, G. I., HYDE, R., CAO, H., NGUYEN, H. L., AND PETITJEAN, F. Characterizing concept drift. *Data Min. Knowl. Discov. 30*, 4 (jul 2016), 964–994.

[109] WIDMER, G., AND KUBAT, M. Learning in the presence of concept drift and hidden contexts. *Machine Learning 23*, 1 (1996), 69–101.

[110] WIDYANTORO, D. H., AND YEN, J. Relevant data expansion for learning concept drift from sparsely labeled data. *IEEE Transactions on Knowledge and Data Engineering 17*, 3 (March 2005), 401–412.

[111] YAMADA, M., SUGIYAMA, M., AND MATSUI, T. Semi-supervised speaker identification under covariate shift. *Signal Processing 90*, 8 (Aug. 2010), 2353–2361.

[112] YANG, X., AND CUI, W. A novel spatial clustering algorithm based on delaunay triangulation. *JSEA 3* (01 2010), 141–149.

[113] YUAN, C., ZHANG, Y., AND LIU, Z. A survey on technologies for automatic forest fire monitoring, detection, and fighting using unmanned aerial vehicles and remote sensing techniques. *Can. Journ. of Forest Res. 45*, 7 (2015), 783–792.

[114] ZHANG, K., SCHÖLKOPF, B., MUANDET, K., AND WANG, Z. Domain adaptation under target and conditional shift. In *30th International Conference on Machine Learning* (2013), pp. 819–827.

[115] ZHAO, X. Face recognition algorithm based on transductive learning classifier. In *Proceedings of the 2010 International Conference on Measuring Technology and Mechatronics Automation - Volume 02* (Washington, DC, USA, 2010), ICMTMA '10, IEEE Computer Society, pp. 212–215.

[116] ZHUKOV, A. V., SIDOROV, D. N., AND FOLEY, A. M. Random forest based approach for concept drift handling. In *Analysis of Images, Social Networks and Texts* (Cham, 2017), D. I. Ignatov, M. Y. Khachay, V. G. Labunets, N. Loukachevitch, S. I. Nikolenko, A. Panchenko, A. V. Savchenko, and K. Vorontsov, Eds., pp. 69–77.

[117] ŽLIOBAITĖ, I., BIFET, A., PFAHRINGER, B., AND HOLMES, G. Active learning with drifting streaming data. *IEEE Transactions on Neural Networks and Learning Systems 25*, 1 (Jan 2014), 27–39.

[118] ŽLIOBAITĖ, I., PECHENIZKIY, M., AND GAMA, J. *An Overview of Concept Drift Applications*. Springer International Publishing, 2016, pp. 91–114.