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Optimization Methods for Piecewise Affine Model Fitting

Tesi di Laurea Specialistica di

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Abstract

Given numerical data sampled from a real, unknown process the problem of Model Fitting is to find a model that best *fits* the data, i.e., a mathematical function which is able to approximate the data as accurately as possible.

In this work we investigate *Piecewise Affine Models*, which are attracting considerable attention in a variety of fields. A Piecewise Affine Model is described by k affine functions each one associated to a subdomain $\mathcal{D}_j \subseteq \mathbb{R}^n$, with $1 \leq j \leq k$, where $\{\mathcal{D}_1, ..., \mathcal{D}_k\}$ is a partition of $\mathbb{R}^n$. The problem of *k-Piecewise Affine Model Fitting* (k-PAMF) amounts to identifying k linear submodels $\hat{f}_j : \mathcal{D}_j \to \mathbb{R}$, together with their definition domains $\mathcal{D}_j$, so as to minimize an objective function which represents the overall approximation error with respect to the data.

Typically the problem is solved in two distinct phases. In the first phase the data points are partitioned in k subsets and a linear submodel is fitted to each subset, while in the second phase the subdomains $\mathcal{D}_j$ are defined. We propose a novel approach that combines the two aspects in a single phase.

The thesis is organized as follows. In Chapter 1 we give an overview of previous work on the subject and explain the novelty of our approach. The problem of k-PAMF is described in detail and the subproblems Hyperplane Clustering and Multi-category Classification are discussed. In Chapter 2 we

propose a novel Mixed-Integer Linear Programming formulation for k-PAMF. We describe the generation of ad-hoc cuts in a Branch&Cut framework to break symmetries and speed up the solution time. Moreover, we use a *Combinatorial Benders' Cuts* approach to get rid of the big-M coefficients. In Chapter 3 we propose two heuristics to tackle large-size instances: an adaptation of k-means and an adaptive point reassignment algorithm. In Chapter 4 we report and discuss computational results obtained from randomly generated and real-world instances, and we compare the methods we propose. The refined exact formulations yield optimal solutions for instances up to 150 points in low-dimensional spaces while the adaptive point reassignment method provides good solutions in a short computing time. Finally, in Chapter 5 we draw some conclusions and mention ideas for future work.

Riassunto

Nel problema del *Model Fitting*, dato un insieme $\mathcal{A}$ di punti $\mathbf{a}_i \in \mathbb{R}^n$ e i loro cosiddetti valori osservati $y_i \in \mathbb{R}$, si vuole identificare un modello, cioè una funzione $\hat{f} : \mathcal{D} \subseteq \mathbb{R}^n \to \mathbb{R}$, che approssimi nel miglior modo possibile il processo reale $f(\cdot)$ che ha generato i dati y_i.

In questa tesi si studia il problema di *k-Piecewise Affine Model Fitting*, che prevede l'approssimazione di funzioni non lineari con modelli lineari (affini) a tratti. Il problema è di attuale rilevanza in molti ambiti applicativi, ad esempio nei modelli Piecewise AutoRegressive eXogenous (PWARX).

Un modello $\hat{f}$ lineare a tratti (in generale non continuo) è descritto da un numero k di funzioni lineari ciascuna delle quali è associata ad un proprio dominio $\mathcal{D}_j \subseteq \mathbb{R}^n$. Il problema di k-PAMF consiste nel trovare k sottomodelli affini $\hat{f}_j : \mathcal{D}_j \to \mathbb{R}$ che minimizzano una funzione obiettivo che rappresenta l'errore di approssimazione sui dati. Una tipica funzione che viene usata allo scopo è la somma dei moduli delle differenze fra le osservazioni y_i e il valore calcolato dal modello: $\sum_{i=1}^{m} |\hat{f}_j(\mathbf{a}_i) - y_i|^p$, dove $\hat{f}_j$ è il sottomodello lineare nel cui dominio giace il punto $\mathbf{a}_i$. La scelta nel nostro caso è la norma ℓ_1, $p = 1$, ovvero la minimizzazione della somma dei valore assoluti degli errori di approssimazione per ogni punto.

Il problema da risolvere comprende non solo la stima dei parametri dei sottomodelli lineari, ma anche l'identificazione dei loro domini $\mathcal{D}_j$. Ciò che

viene tipicamente fatto nell'approccio classico è dividere il problema in due fasi: nella prima vengono partizionati i punti e si trovano gli iperpiani che meglio approssimano tali sottoinsiemi di punti, mentre la determinazione dei domini dei sottomodelli lineari viene svolta solamente in seconda battuta. L'approccio che proponiamo in questo lavoro prevede un'unica formulazione che contemporaneamente lavora sulla minimizzazione dell'errore sui dati e sulla partizione del dominio continuo in k regioni corrispondenti ai sotto-modelli lineari.

Nel Capitolo 1 è descritto il problema di k-Piecewise Affine Model Fitting con rimandi a precedenti lavori sull'argomento, mostrando la novità dell'approccio proposto. Inoltre vengono introdotti due problemi ad esso collegati, l'Hyperplane Clustering e la Multi-category Classification. In effetti k-PAMF può essere visto come una loro combinazione. Nel Capitolo 2 viene presentata una formulazione esatta di k-PAMF come un problema di programmazione lineare misto-intera. Esso prevede allo stesso tempo la detereminazione dei parametri e dei domini dei modelli lineari. Descriviamo lo studio e l'implementazione di metodi che cercano di ridurre la complessità del problema affrontando due aspetti critici della formulazione: le simmetrie e i big-M. Nel primo caso consideriamo la generazione di una classe di tagli che permettono la rottura delle simmetrie con un netto miglioramento dell'efficienza. Nel secondo caso evitiamo l'utilizzo dei coefficienti big-M medienta una decomposizione basata sui *Combinatorial Benders' Cuts*. Nel Capitolo 3 sono proposte due euristiche: una procedura iterativa simile a k-means ed un algoritmo che è basato sull'individuazione di punti candidati ad essere riassegnati. Entrambi gli algoritmi, che prevedono diverse varianti, forniscono delle soluzioni (subottimali) di buona qualità in tempi brevi. Il Capitolo 4 riporta e discute i test computazionali che sono stati effettuati su

istanze reali e generate aleatoriamente. Infine, nel Capitolo 5 sono contenute delle conclusioni ed alcuni sviluppi futuri.

Chapter 1

Introduction

Given a set $\mathcal{A}$ of m points $\mathbf{a}_i \in \mathbb{R}^n$ and their corresponding observations $f(\mathbf{a}_i) = y_i \in \mathbb{R}$, where $f(\cdot)$ is an unknown, possibly nonlinear, function, the problem of Model Fitting is to find a mathematical function $\hat{f}(\cdot)$ which best approximates the unknown function by minimizing the error on the data points.

The fundamental issue of Model Fitting is the choice of the model and its complexity. Typically real-world data exhibit nonlinearties and are affected by errors (see Figure 1.1). A model which is too *simple* (e.g., affine models) might lack the ability to extract all the information provided by the data. On the other hand, a model which is too involved might be too complicated to use efficiently or overfit the data (e.g., reproduce even noise). This is consistent with Occam's principle, which states that, when a choice is possible, the simplest model has to be preferred.

In this work we investigate *Piecewise Affine Models*, also called *Piecewise Linear Models*. The choice of piecewise affine models is motivated by the difficulty that lies in the identification and the use of nonlinear models. While basic affine models are often *too* simple to cope with the actual complexity

of real data, piecewise affine functions are considered to be general enough to work well in practice, while maintaining most of the practical advantages given by linear models.

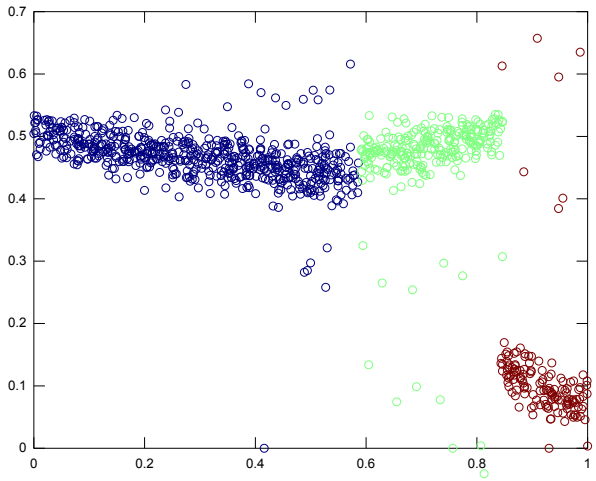


Figure 1.1: A set of points that exhibit highly nonlinear behaviour and can be fitted accurately with 3 affine submodels.

The Piecewise Affine Model Fitting problem requires to find a model $\hat{f} : \mathcal{D} \subseteq \mathbb{R}^n \to \mathbb{R}$, composed by a given number k of affine submodels $\hat{f}_j$ such that the overall approximation error is minimized. Each affine submodel $\hat{f}_j : \mathcal{D}_j \to \mathbb{R}$, for $j = 1 \dots k$, is described by a linear function $\hat{f}_j(\mathbf{x}) = \mathbf{w}_j^T \mathbf{x} - \gamma_j$ and a definition domain $\mathcal{D}_j \subseteq \mathcal{D}$: in each region one would like to identify a hyperplane that best fits the data. We impose no constraints on the continuity of the model. An example of piecewise linear noncontinuous model is reported in Figure (1.2).

If the partitioning of the domain is known a priori, i.e., the definition domains of the submodels are known, the problem can be reduced to a fixed number of linear model fitting problems, which can be easily solved with robust regression techniques. This however requires some deep knowledge of the function that we are approximating, and it is not always the case. Indeed,

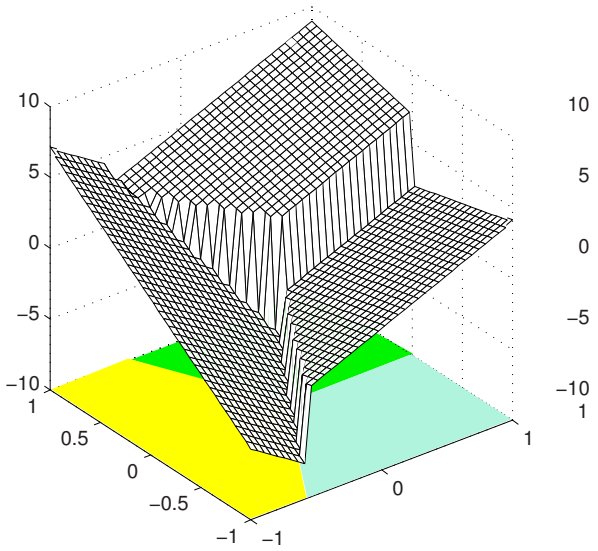


Figure 1.2: A piecewise linear discontinuous model with 3 submodels.

it is likely that we just have an indication of the number of submodels k. Often we might have no *a priori* knowledge that can help in the model fitting process, thus both the number of the linear submodels and their definition domains $\mathcal{D}_j$ (a polyhedral partition of the continuous domain $\mathcal{D}$) have to be completely identified from the raw data.

1.1 Classical approach

The problem of Piecewise Affine Model Fitting arises in a variety of fields, and a number of different methods exist. Classical techniques typically work in two phases. The first phase involves partitioning and fitting the data points: the algorithm looks for coplanarity in the discrete space of the data points. Then, in a second phase, the definition regions $\mathcal{D}_j$ of the affine submodels are derived. However, the affine subspaces that have been found in the first phase might not induce a feasible partition on the continuous domain $\mathcal{D}$: some points might therefore be assigned to a subdomain $\mathcal{D}_j$ that is different

from the one that corresponds to the submodel they contributed to define. An example is reported in Figure 1.3. This is a flaw that our novel approach aims to repair (see Section 1.2).

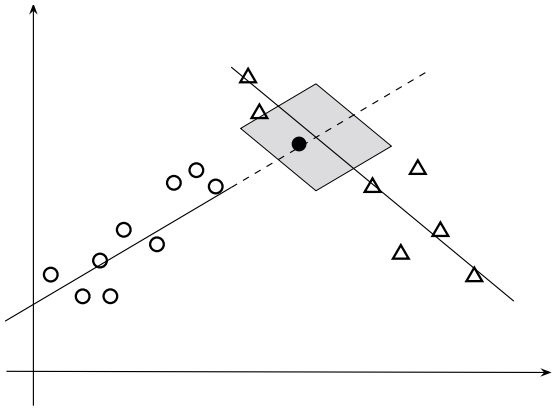


Figure 1.3: Example showing two intersecting linear submodels. According to the point-hyperplane y-distance, the black point would be assigned to the submodel on the left. However, the resulting sets are not linearly separable in the continuous domain (the x-axis), hence we would like the black point to be assigned to the submodel on the right.

In the context of system identification the problem is usually referred to as hybrid system estimation, and the models are called Piecewise AutoRegressive eXogenous (PWARX) models. An overview of a number of techniques for hybrid systems identification is proposed in [PJFTV07], that contains references to several works on Piecewise Affine Model Fitting. Identification procedures described in the paper include an algebraic approach, a Bayesian procedure and a clustering-based method. The continuous domain partition is achieved in a second phase by means of multi-category classification, that is performed with Support Vector Machines (SVM, [Vap98]) or Robust Linear Programming (RLP, [BB99]).

In [AM02] the authors tackle piecewise linear model fitting as a Min-PFS problem, which requires to find a partition of a given linear system in a

minimum number of feasible subsystems (with a maximum noise tolerance ε). The problem is $\mathcal{NP}$-hard, and an effective greedy algorithm is proposed in the paper. The method does not account for the continuous domain partition: in [BGPV03] the authors introduce a second phase that derives the subdomains via multicategory classification, performed with SVM or RLP.

In [FTMLM03] the data points are first clustered in feature space via k-means and then the parameters for each model are computed. The partition is derived at a later stage via SVM or RLP. In [FTM02] the fitting is performed with a 3-layers neural network which models a piecewise linear function. The subdomains are not explicitly derived. [MB09] use an iterative algorithm for estimating *max-affine* models: even in this case the domains of the submodels are not explicit, as a linear model is active in a region if it is maximal compared to the other ones. The resulting piecewise model is, by definition, continuous, while our formulation is more general since the model can be discontinuous.

1.2 Novelty of our approach

In this thesis we propose a novel approach that follows in the footsteps of the work in [CI06], where a single-phase formulation for k-Piecewise Linear Model Fitting is introduced. What distinguishes this approach from most of the previous work on the subject is the fact that we do not focus first on fitting discrete points, then on determining the domains of the submodels. On the contrary, we attempt to solve both problems simultaneously.

The drawbacks of previous, two-phase, approaches are evident especially in cases where distinct submodels are almost coplanar, or when we have intersecting submodels. As an example we display in Figure 1.4 a small

instance that shows the advantage of our approach.

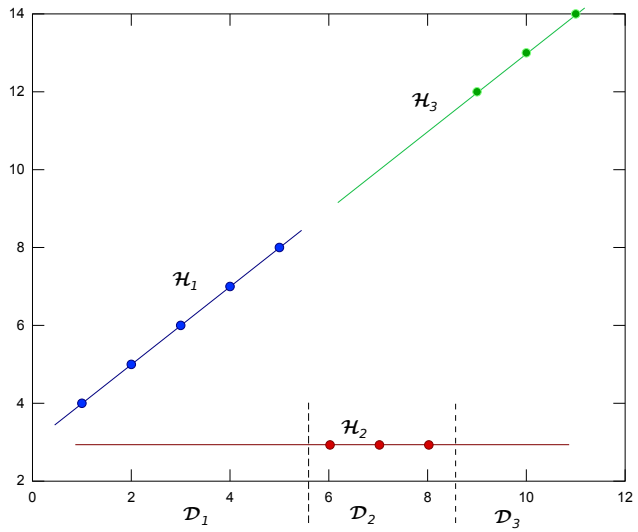


Figure 1.4: Output of the single-phase k-PAMF formulation that we propose.

The blue and the green points lie on the same line, however they are not part of the same submodel. Our method simultaneously partitions the points and the domain, hence it is able to identify the three separate submodels, and it correctly determines the three definition regions on the continuous domain, which in this case is the x-axis.

On the other hand, if we look for linear submodels not taking into account the continuous subdomains, we identify one model for the red points and only one model that includes both the green and the blue points (see Figure 1.5). In the second phase, when it comes to determining the domains for the linear submodels, no meaningful linear partition of the domain can be found: the two clusters are not linearly separable in $\mathcal{D}$. The result will be a single linear model with domain $\mathcal{D}_1$ which is completely unable to correctly predict the value of the red function.

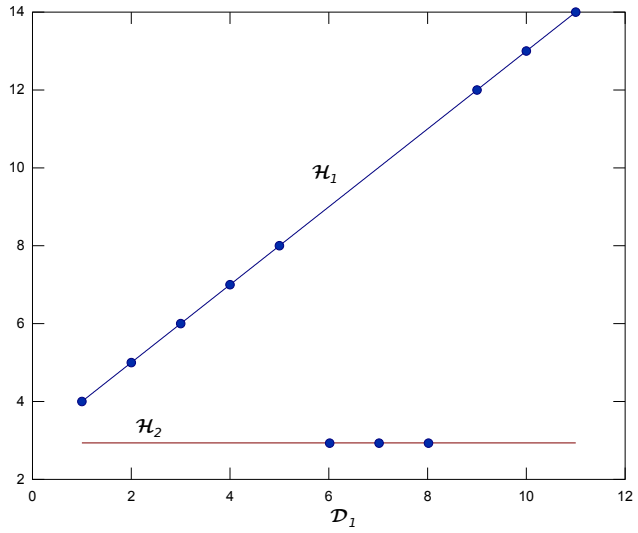


Figure 1.5: Output of a classical k-PAMF method working in two distinct phases. It is unable to induce suitable definition regions for the submodels. All points are considered part of the domain of $\mathcal{H}_1$.

1.3 k-Piecewise Affine Model Fitting

Let $\mathcal{A}$ be a set of m points $\mathbf{a}_i \in \mathbb{R}^n$ and $f(\mathbf{a}_i) = y_i \in \mathbb{R}$ the observations associated to the points $\mathbf{a}_i$, where $f(\cdot)$ is an unknown nonlinear function. The problem of k-Piecewise Affine Model Fitting amounts to finding a model $\hat{f} : \mathcal{D} \subseteq \mathbb{R}^n \to \mathbb{R}$, composed by a given number k of linear submodels $\hat{f}_j$ such that the overall approximation error is minimized. For each affine submodel it is necessary to identify a linear function $\hat{f}_j(\mathbf{x}) = \mathbf{w}_j^T\mathbf{x} - \gamma_j$ and a definition domain $\mathcal{D}_j \subseteq \mathcal{D}$.

To have a formal mathematical formulation for k-PAMF we have to introduce a metric to measure the discrepancy between the model and the data values. Typically this objective function is defined as a norm of the vector containing the approximation errors for each point, i.e., a function of the form:

$$\sum_{i=1}^{m} |\hat{f}_{j(i)}(\mathbf{a}_i) - y_i|^p,$$

where $j(i)$ indicates the index of the submodel in whose domain the data point lies.

In this work we define the objective function of k-PAMF as:

$$\sum_{i=1}^{m} |\hat{f}_{j(i)}(\mathbf{a}_i) - y_i|, \tag{1.1}$$

taking $p = 1$, that is the sum of the absolute values of the approximation errors. In other words, the error function for the problem is expressed in terms of the norm ℓ_1 of the vector containing the approximation errors: this translates easily into a linear mathematical program. Moreover with ℓ_1 we expect the formulation to be less sensitive to outliers than using a norm with $p > 1$, like the ℓ_2 norm.

According to this definition of the problem it is possible to derive a first nonlinear mathematical formulation for k-PAMF:

$$\min \sum_{j=1}^{k} \sum_{i=1}^{m} x_{ij} d_{ij} \tag{1.2}$$

$$\sum_{j} x_{ij} = 1 \quad \forall i \in [m] \tag{1.3}$$

$$d_{ij} = |\hat{f}_j(\mathbf{a}_i) - y_i| \quad \forall i \in [m], j \in [k] \tag{1.4}$$

$$\hat{f}_j(\mathbf{a}_i) = \mathbf{w}_j^T \mathbf{a}_i - \gamma_j \quad \forall i \in [m], j \in [k] \tag{1.5}$$

$$x_{ij} = 1 \Leftrightarrow \mathbf{a}_i \in \mathcal{D}_j \quad \forall i \in [m], j \in [k] \tag{1.6}$$

$$x_{ij} \in \{0, 1\} \quad \forall i \in [m], j \in [k] \tag{1.7}$$

$$d_{ij}, \gamma_j \in \mathbb{R} \quad \forall i \in [m], j \in [k] \tag{1.8}$$

$$\mathbf{w}_j \in \mathbb{R}^n \quad \forall j \in [k] \tag{1.9}$$

$$\bigcup_{j=1}^{k} \mathcal{D}_j = \mathcal{D}, \quad \mathcal{D}_j \cap \mathcal{D}_l = \varnothing \quad \forall j \neq l \tag{1.10}$$

The binary variables x_{ij} indicate whether the point i is assigned to the model j. Hence the objective function accounts for the approximation error d_{ij} only if x_{ij} has value 1, since we are not interested in the error regarding the submodels where a point does not belong. It is important to stress that the subdomains $\mathcal{D}_j$ are not fixed: they have to be derived so that a point $\mathbf{a}_i$ can be assigned to a submodel $\hat{f}_j$ only if it belongs to $\mathcal{D}_j$. Constraints (1.10) ensure that the subdomains are a partition of $\mathcal{D}$, i.e., they are disjoint and their union forms $\mathcal{D}$. In this formulation it is still not explicit how the domains $\mathcal{D}_j$ should be treated in practice. Mixed-Integer Linear Programming (MILP) formulations for the problem are the object of Chapter 2.

1.4 Subproblems

Piecewise Affine Model Fitting can be seen as the combination of three different subproblems.

In the first subproblem, which is combinatorial, the points have to be partitioned so that each one is assigned to one (and only one) linear submodel, as expressed by the binary assignment variables x_{ij}.

In the second subproblem, which is continuous, the hyperplanes parameters $(\mathbf{w}_j, \gamma_j)$ have to be determined such that they minimize the sum of the absolute errors between the *predicted* values $\hat{f}_j(\mathbf{a}_i)$ and the observations y_j in each data point $\mathbf{a}_i$.

Together these two subproblems form a variant of what is called k-Hyperplane Clustering [ACD09].

In the third subproblem the domain $\mathcal{D}$ has to be partitioned so that each point belongs to the domain $\mathcal{D}_j$ corresponding to the submodel $\hat{f}_j(\cdot)$ it is assigned to. This can be seen as a multi-category classification problem,

that is to find a discriminating function that induces a polyhedral partition on the continuous domain $\mathcal{D}$ which is consistent with the assignments of the data points to the submodels.

In the next sections we describe in detail the Hyperplane Clustering problem and the Multi-category Classification problem.

1.4.1 Hyperplane Clustering

Clustering is the problem of discovering clusters, or groups, of *similar* elements in a dataset. Similarity in itself is a rather vague term, hence the problem can be defined, and thus solved, in many different ways. Usually two points are considered similar according to a metric defined on the space they lie in, e.g., the Euclidean distance. The desired result of a clustering process is generally a minimal number k of clusters with high infra-cluster and low inter-cluster similarity.

In Hyperplane Clustering the focus is not on the proximity between points but on their collinearity (or coplanarity). This is to say that the aim is clustering data such that elements of the same group are close to the same linear subspace of dimension $n-1$ (a hyperplane, hence the name). In other words, given a set of m points $\mathcal{A} = \{\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_m\}$ belonging to $\mathbb{R}^n$, we seek to determine a minimal number k of hyperplanes

$$\mathcal{H}_j = \{\mathbf{x} \in \mathbb{R}^n | \mathbf{w}_j^T \mathbf{x} = \gamma_j, \mathbf{w}_j \in \mathbb{R}^n, \gamma_j \in \mathbb{R}\} \tag{1.11}$$

and an assignment of the points of $\mathcal{A}$ to the hyperplanes $\mathcal{H}_j$ such that the resulting clusters minimize an overall error (an objective function) which depends on the aggregated orthogonal distance between the points and their corresponding hyperplanes (see Figure 1.6). For a comprehensive discussion

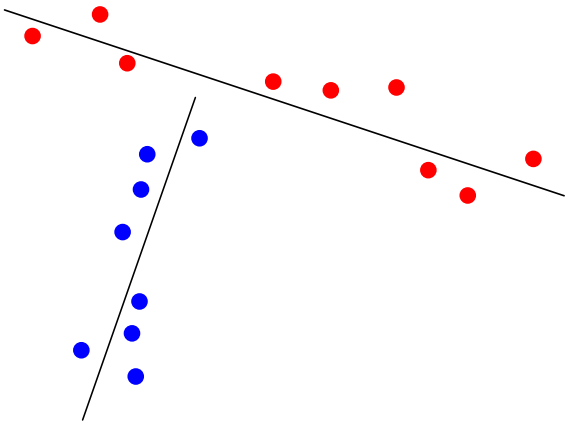


Figure 1.6: In kHC we look for a number k of hyperplanes that minimize the sum of the square orthogonal point-hyperplane distances.

on most aspects of the problem see [ACD09].

A MILP formulation of Hyperplane Clustering with a fixed number k of clusters (k-HC) is the following:

$$\min \sum_{j=1}^{k} \sum_{i=1}^{m} x_{ij} d_{ij} \tag{1.12}$$

$$\sum_{j} x_{ij} = 1 \quad \forall i \in [m] \tag{1.13}$$

$$d_{ij} = \frac{|\mathbf{w}_j^T \mathbf{a}_i - \gamma_j|}{\|\mathbf{w}_j\|_2} \quad \forall i \in [m], j \in [k] \tag{1.14}$$

$$x_{ij} \in \{0, 1\} \quad \forall i \in [m], j \in [k] \tag{1.15}$$

$$\mathbf{w}_j \in \mathbb{R}^n \quad \forall j \in [k] \tag{1.16}$$

$$d_{ij}, \gamma_j \in \mathbb{R} \quad \forall i \in [m], j \in [k] \tag{1.17}$$

This formulation adopts a 2-norm distance:

$$d_{ij} = \frac{|\mathbf{w}_j^T \mathbf{a}_i - \gamma_j|}{\|\mathbf{w}_j\|_2}. \tag{1.18}$$

and an objective function that takes into account for each cluster the sum of all point-hyperplane distances. The binary variables x_{ij} have value 1 when the point $\mathbf{a}_i$ is assigned to the cluster j and 0 otherwise. It is necessary to point out that this formulation is rather naive, as it involves many non-linearties that could be avoided or reformulated in a form better suited for mathematical programming.

1.4.2 Hyperplane Clustering and Piecewise Affine Model Fitting

The similarities between Piecewise Affine Model Fitting and Hyperplane Clustering are many and not difficult to see, since both require to partition the data and to identify k hyperplanes.

An important difference between the PAMF and HC lies in the objective function. In Hyperplane Clustering the aim is of minimizing an aggregate distance function which depends on the orthogonal distance of the points from the hyperplanes,

$$d_i = \frac{|\mathbf{w}_{j(i)}^T \mathbf{a}_i - \gamma_{j(i)}|}{\|\mathbf{w}_{j(i)}\|_2}. \tag{1.19}$$

In PAMF, on the contrary, we seek the minimum sum of the absolute values of the residuals $\sum_i |\varepsilon_i|$, where ε_i is defined as the difference between the observed value y_i and the *estimated* value $\hat{f}_{j(i)}(\mathbf{x}_i) = \mathbf{w}_{j(i)}^T \mathbf{x}_i - \gamma_{j(i)}$. Formally:

$$\varepsilon_i := \hat{f}_{j(i)}(\mathbf{a}_i) - y_i = \mathbf{w}_{j(i)}^T \mathbf{a}_i - \gamma_{j(i)} - y_i. \tag{1.20}$$

In both cases $j(i)$ identifies the cluster that $\mathbf{a}_i$ has been assigned to. Figure 1.7 shows the difference between the distance functions of the two problems.

By replacing the objective function of (1.12)-(1.17) we can write a pro-

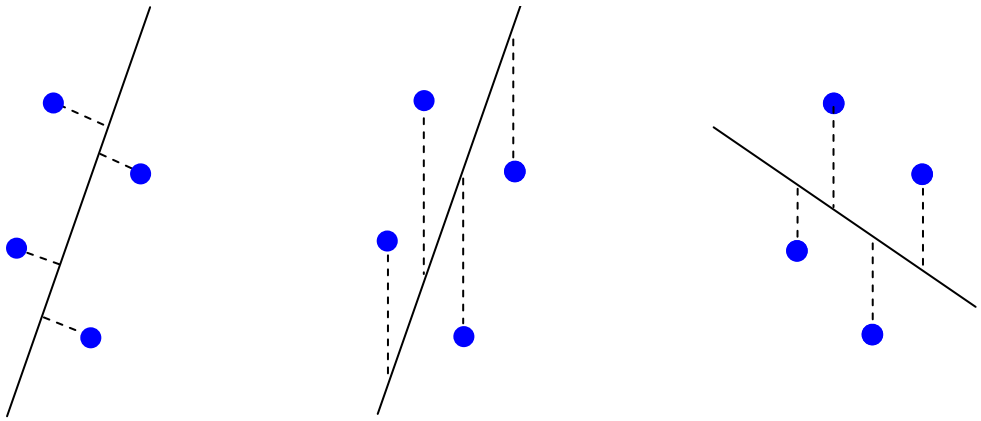


Figure 1.7: On the left we show a plane minimizing the orthogonal distance of the blue points, but that does not translate in an optimal solution on the y-axis (center). The plane on the right correctly minimizes the sum of the absolute values of residuals.

gram which is very similar to k-PAMF, although it lacks the continuous domain partitioning.

$$\min \sum_{j=1}^{k} \sum_{i=1}^{m} x_{ij} \tilde{d}_{ij} \tag{1.21}$$

$$\sum_{j} x_{ij} = 1 \quad \forall i \in [m] \tag{1.22}$$

$$\tilde{d}_{ij} = |\mathbf{w}_j^T \mathbf{a}_i - \gamma_j - y_j| \tag{1.23}$$

$$x_{ij} \in \{0, 1\} \tag{1.24}$$

We can work to write it in a better form. This program can be rephrased as a Mixed-Integer Linear Programming (MILP) problem removing all nonlinearities, first by noticing that the objective function can be written as:

$$\min \sum_{j=1}^{k} \sum_{i=1}^{m} \tilde{d}_{ij} \tag{1.25}$$

with the additional implications

$$x_{ij} = 0 \Rightarrow \tilde{d}_{ij} = 0 \tag{1.26}$$

$$x_{ij} = 1 \Rightarrow \tilde{d}_{ij} = |\mathbf{w}_j^T \mathbf{a}_i - \gamma_j - y_j| \tag{1.27}$$

thus making the objective linear. Now the conditional constraints can be easily transformed in linear constraints using the well known big-M technique (see Section 2.3 for a discussion on it). Then we can remove the absolute norm by introducing two sets of linear inequalities

$$d_{ij} \geq \mathbf{w}_j^T \mathbf{a}_i - \gamma_j - y_j \tag{1.28}$$

$$d_{ij} \geq -\mathbf{w}_j^T \mathbf{a}_i + \gamma_j + y_j \tag{1.29}$$

which are equivalent to the original equations provided that we are dealing with a minimization problem. The resulting MILP problem is the following, where for convenience we introduce the auxiliary variables d_{ij}:

$$\min \sum_{j=1}^{k} \sum_{i=1}^{m} \tilde{d}_{ij} \tag{1.30}$$

$$\sum_{j} x_{ij} = 1 \quad \forall i \in [m] \tag{1.31}$$

$$\tilde{d}_{ij} \leq M x_{ij} \quad \forall i \in [m], j \in [k] \tag{1.32}$$

$$\tilde{d}_{ij} \geq d_{ij} - M(1 - x_{ij}) \quad \forall i \in [m], j \in [k] \tag{1.33}$$

$$d_{ij} \geq \mathbf{w}_j^T \mathbf{a}_i - \gamma_j - y_j \quad \forall i \in [m], j \in [k] \tag{1.34}$$

$$d_{ij} \geq -\mathbf{w}_j^T \mathbf{a}_i + \gamma_j + y_j \quad \forall i \in [m], j \in [k] \tag{1.35}$$

$$x_{ij} \in \{0, 1\} \quad \forall i \in [m], j \in [k] \tag{1.36}$$

$$\mathbf{w}_j \in \mathbb{R}^n \quad \forall j \in [k] \tag{1.37}$$

$$d_{ij}, \gamma_j \in \mathbb{R} \quad \forall i \in [m], j \in [k] \tag{1.38}$$

For a pair (i, j), given a sufficiently large value of M, when $x_{ij} = 0$ the Inequality (1.32) is active and $\tilde{d}_{ij}$ is bound to be 0. Viceversa, if $x_{ij} = 1$ the Constraint (1.33) has to be satisfied ($\tilde{d}_{ij} \geq d_{ij}$).

This is a MILP which is very closely related to k-PAMF, yet it is not enough to fully express the problem. In PAMF we intend not only to partition the given discrete dataset $\mathcal{A}$, but also to guarantee that the partitioned points be linearly separable and to compute a partition of the continuous domain $\mathcal{D}$. This is done by adding classification constraints with the purpose of linearly separating the data and at the same time determining the k subdomains where the linear submodels are defined. Such constraints are meant to avoid the point-cluster assignments which would not translate into a feasible linear partition of the underlying domain $\mathcal{D}$. The partition of $\mathcal{D}$ can be achieved through multi-category linear classification, as in [CI06], that

will be discussed in the next section.

1.4.3 Classification

Given two sets of points $\mathcal{A}_1, \mathcal{A}_2$ in the n-dimensional space $\mathbb{R}^n$, *classification* is the problem of identifying a function capable of discriminating the data according to their classes.

If a linear function is enough to discriminate the two classes, it is sufficient to find an $(n-1)$-dimensional hyperplane $\mathcal{H}$ defined as

$$\mathcal{H}: \ \mathbf{w}^T\mathbf{x} - \gamma = 0 \tag{1.39}$$

where $\mathbf{w}$ is the normal to the plane and γ the distance from the origin, and such that for each point $\mathbf{a}_i$ it fulfils the constraints

$$\mathbf{w}^T\mathbf{a}_i - \gamma > 0 \text{ if } \mathbf{a}_i \in \mathcal{A}_1 \tag{1.40}$$

$$\mathbf{w}^T\mathbf{a}_i - \gamma < 0 \text{ if } \mathbf{a}_i \in \mathcal{A}_2. \tag{1.41}$$

If such a separating plane exists, the points are said to be linearly separable. In this case in general there are infinitely many planes that separate the two classes.

A common approach to deal with this problem in practice is introducing the following nonomogeneous inequalities.

$$\mathbf{w}^T\mathbf{a}_i - \gamma \geq +1 \text{ if } \mathbf{a}_i \in \mathcal{A}_1 \tag{1.42}$$

$$\mathbf{w}^T\mathbf{a}_i - \gamma \leq -1 \text{ if } \mathbf{a}_i \in \mathcal{A}_2 \tag{1.43}$$

These constraints do not only define a hyperplane separating the data

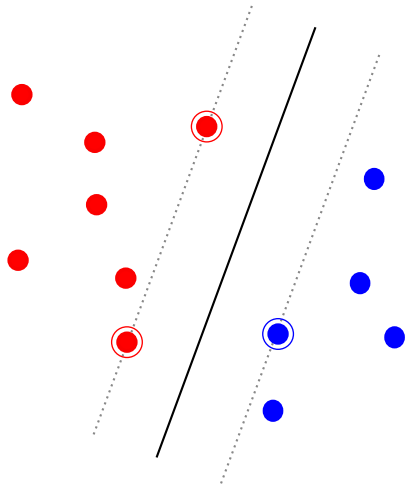


Figure 1.8: A linear separation bound. The points on the margin ρ are the support vectors.

points, but in fact two parallel hyperplanes that keep a margin between the points belonging to different classes. In particular, the distance between the two hyperplanes is $2/\|\mathbf{w}\|$, that represents in fact the minimum distance between two points belonging to different classes. The points lying on the hyperplanes that define the margin between the classes are called Support Vectors (see Figure 1.8), and a well-known and powerful classification method, called Support Vector Machines (SVM), is based on the maximization of the geometric margin $\rho = 2/\|\mathbf{w}\|$.

This technique requires a quadratic minimization problem, and the obvious drawback of this method is the potential complexity of the optimization. Moreover, when dealing with sets which are not completely separable with a linear function, it is important to find a result that discriminates best according to some criterion other than the maximal separation margin. A formulation that naturally accounts for misclassification errors and just requires the solution a linear problem is Robust Linear Programming (RLP,

[BB99]):

$$\min \sum_{i=1}^{m} e_i \tag{1.44}$$

$$\mathbf{w}^T \mathbf{a}_i - \gamma + e_i \geq +1 \quad \text{if } \mathbf{a}_i \in \mathcal{A}_1 \tag{1.45}$$

$$\mathbf{w}^T \mathbf{a}_i - \gamma - e_i \leq -1 \quad \text{if } \mathbf{a}_i \in \mathcal{A}_2 \tag{1.46}$$

$$\mathbf{w} \in \mathbb{R}^n, \gamma \in \mathbb{R} \tag{1.47}$$

$$e_i \geq 0 \tag{1.48}$$

that amounts to minimizing the sum of the misclassification errors e_i.

1.4.4 Multi-category Classification: M-RLP

What was described in the previous section is valid for a binary classification, but can be extended to multi-class problems, where $k > 2$. Given k sets $\mathcal{A}_1, ..., \mathcal{A}_k$ we want to find a classification function capable of discriminating them.

A typical technique is subdividing the k-category classification problem in k binary discrimination problems, i.e., for each set $\mathcal{A}_i$ the method builds a function that discriminates that class from the remaining $k-1$ (one-versus-all). Then, when a new point has to be classified, k binary decisions have to be made, and the highest output wins. This procedure has been vastly adopted both in SVM and RLP contexts with the name k-SVM and k-RLP [BB99].

These methods require the identification of a set of parameters $(\mathbf{w}_1, \gamma_1), \ldots (\mathbf{w}_k, \gamma_k)$ such that for each class $\mathcal{A}_j$ and for each $\mathbf{a}_i \in \mathcal{A}_j$

$$\mathbf{w}_j^T \mathbf{a}_i - \gamma_j > \mathbf{w}_l^T \mathbf{a}_i - \gamma_l \qquad \forall l \in [k], l \neq j \tag{1.49}$$

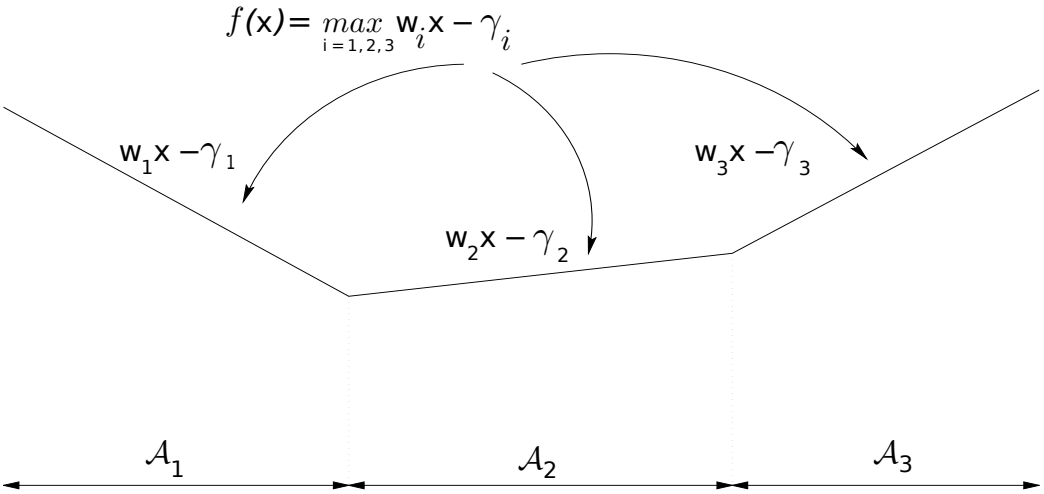


Figure 1.9: Example of a piecewise discriminating function for three classes.

A point $\mathbf{a}_i$ is classified as belonging to $\mathcal{A}_j$ if the above inequalities hold. In other words, the class of a point is determined by the index of the pair $(\mathbf{w}_j, \gamma_j)$ that maximizes the function $f_j(\mathbf{a}_i) = \mathbf{w}_j^T \mathbf{a}_i - \gamma_j$. Indeed, the discriminating function can be expressed as the piecewise linear function (an example in Figure 1.9):

$$g(\mathbf{x}) = \max_{j \in [k]} \{\mathbf{x}^T \mathbf{w}_j - \gamma_j\}$$

where the classification function is

$$c(\mathbf{x}) = \arg\max_{j \in [k]} \{\mathbf{x}^T \mathbf{w}_j - \gamma_j\}.$$

The separating plane of a class $\mathcal{A}_j$ from a class $\mathcal{A}_l$ can be defined as the points satisfying

$$(\mathbf{w}_j - \mathbf{w}_l)^T \mathbf{x} - (\gamma_j - \gamma_l) = 0, \tag{1.50}$$

where the parameters are computed so that $(\mathbf{w}_j - \mathbf{w}_l)^T \mathbf{a}_i - \gamma_j + \gamma_l > 0$ for each points belonging to the set $\mathcal{A}_j$ and viceversa $(\mathbf{w}_j - \mathbf{w}_l)^T \mathbf{a}_i - \gamma_j + \gamma_l < 0$ for each point in $\mathcal{A}_l$.

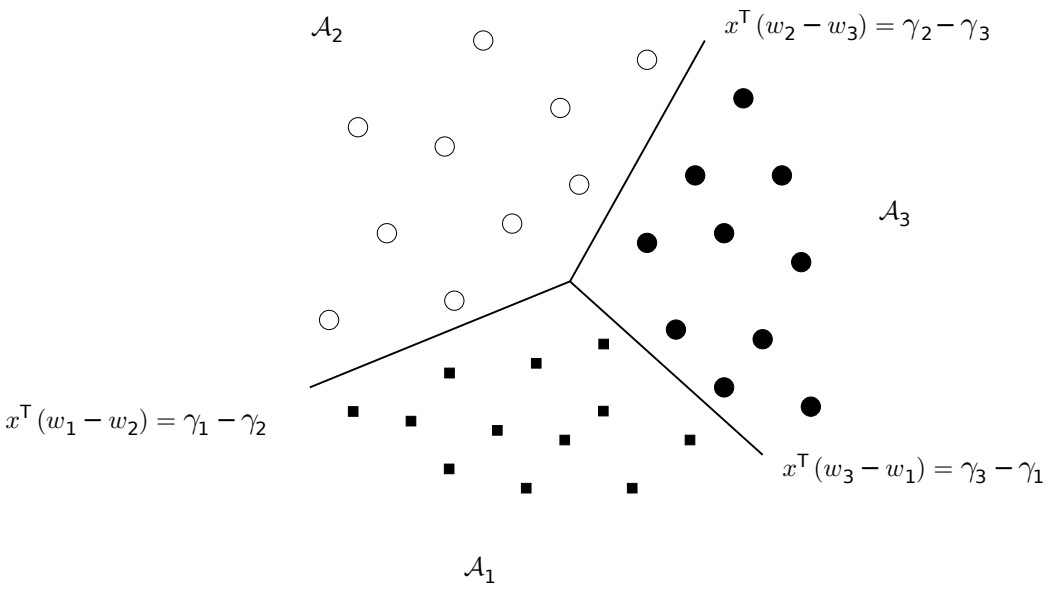


Figure 1.10: Example of a piecewise linear separator for three classes.

If the inequalities are perfectly satisfied, the sets of points are said to be piecewise-linearly separable (Figure 1.10).

A different approach is proposed by Bennett and Mangasarian in [BM94]. The formulation introduced in the paper is a generalization of RLP called M-RLP and requires only a single linear optimization in contrast to the k problems of k-SVM and k-RLP. First we introduce the equivalent nonomogeneous inequalities

$$(\mathbf{w}_j - \mathbf{w}_l)^T \mathbf{a}_i - \gamma_j + \gamma_l \geq 1 \tag{1.51}$$

for each point $\mathbf{a}_i \in \mathcal{A}_j$ and for all $l \neq j$. Accordingly to the proposed inequalities, a point assigned to a class $\mathcal{A}_j$ is considered misclassified if there exists an $l \neq j$ such as $(\mathbf{w}_j - \mathbf{w}_l)^T \mathbf{a}_i - \gamma_j + \gamma_l - 1 \leq 0$. We can therefore consider the negative quantity $(\mathbf{w}_j - \mathbf{w}_l)^T \mathbf{a}_i - \gamma_j + \gamma_l - 1$ as a misclassification error, while, if positive, it measures the "strength" of the classification. It is straightforward to define the misclassification error for $\mathbf{a}_i \in \mathcal{A}_j$ with respect

to $\mathcal{A}_l$ as:

$$e_{ijl} = \max\{0, -(\mathbf{w}_j - \mathbf{w}_l)^T \mathbf{a}_i + \gamma_j - \gamma_l + 1\}, \tag{1.52}$$

where we have inverted the sign of the expression to have a non-negative quantity. The sum of the errors e_{ijl} is the quantity to be minimized in order to find the separator which best discriminates between the two classes $\mathcal{A}_j$ and $\mathcal{A}_l$. This can be generalized with an aggregate error function which accounts for the misclassification errors of each point.

$$\min \sum_{j=1}^{k} \sum_{\substack{l=1 \\ l \neq j}}^{k} \sum_{i:\mathbf{a}_i \in \mathcal{A}_j} e_{ijl} \tag{1.53}$$

$$e_{ijl} \geq -(\mathbf{w}_j - \mathbf{w}_l)^T \mathbf{a}_i + \gamma_j - \gamma_l + 1 \quad \forall j, l \neq j \in [k], i : \mathbf{a}_i \in \mathcal{A}_j \tag{1.54}$$

$$e_{ijl} \geq 0 \quad \forall j, l \in [k], i : \mathbf{a}_i \in \mathcal{A}_j \tag{1.55}$$

$$\mathbf{w}_j \in \mathbb{R}^n \quad \forall j \in [k] \tag{1.56}$$

$$e_{ijl}, \gamma_j \in \mathbb{R} \quad \forall j \in [k] \tag{1.57}$$

If the optimal objective is 0, then the dataset is piecewise-linearly separable. Otherwise, the positive values of the variables e_{ijl} represent the magnitude of the misclassification error of the point $\mathbf{a}_i$.

M-RLP variant: max-error

In the context of this work a slightly different objective function has been adopted. Working within a Piecewise Affine Model Fitting context, we are often interested in setting a misclassification error tolerance rather than minimizing such errors. Moreover, as will be clear further on, the classification will be made on classes that are not fixed *a priori*. We adopt a formulation

with a simpler objective function:

$$\min \sum_{i=1}^{m} \bar{e}_i \tag{1.58}$$

$$\bar{e}_i \geq e_{ijl} \quad \forall j, l \in [k], i : \mathbf{a}_i \in \mathcal{A}_j \tag{1.59}$$

$$e_{ijl} \geq -(\mathbf{w}_j - \mathbf{w}_l)^T \mathbf{a}_i + \gamma_j - \gamma_l + 1 \quad \forall j, l \neq j \in [k], i : \mathbf{a}_i \in \mathcal{A}_j \tag{1.60}$$

$$\bar{e}_i \geq 0 \quad \forall i \in [m] \tag{1.61}$$

$$e_{ijl} \geq 0 \quad \forall j, l \in [k], i : \mathbf{a}_i \in \mathcal{A}_j \tag{1.62}$$

$$\mathbf{w}_j \in \mathbb{R}^n \quad \forall j \in [k] \tag{1.63}$$

$$\gamma_j \in \mathbb{R} \quad \forall j \in [k] \tag{1.64}$$

This program amounts to minimizing the sum of the maximum misclassification errors $\bar{e}_i$ for each point $\mathbf{a}_i$ rather then minimizing the sum of all the misclassification errors for each point [CI06].

In this formulation the presence of the classification constraints depends on the *class labels* of the points $\mathbf{a}_i$. As long as the sets $\mathcal{A}_j$ are known a priori, as it is the case in a classic supervisioned learning problem, the system of inequalities can be written easily. We now introduce a different, but equivalent, formulation that is better suited for the use that will be made in k-PAMF. We add a number $m \times k$ of binary parameters $x_{ij} \in \{0, 1\}$ which express the assignment of a point $\mathbf{a}_i$ to the class $\mathcal{A}_j$. These assignments have to satisfy $\sum_j x_{ij} = 1$ and allow us to declare Constraint (1.60) as:

$$x_{ij} = 1 \Rightarrow e_{ijl} \geq -(\mathbf{w}_j - \mathbf{w}_l)^T \mathbf{a}_i + \gamma_j - \gamma_l + 1 \tag{1.65}$$

Again, we deal with the conditional constraint with the big-M method:

$$\min \sum_{i=1}^{m} \bar{e}_i \tag{1.66}$$

$$\bar{e}_i \geq e_{ijl} - M(1 - x_{ij}) \quad \forall j, l \in [k], i \in [m] \tag{1.67}$$

$$e_{ijl} \geq -(\mathbf{w}_j - \mathbf{w}_l)^T \mathbf{a}_i + \gamma_j - \gamma_l + 1 \quad \forall j, l \neq j \in [k], i \in [m] \tag{1.68}$$

$$\bar{e}_i \geq 0 \quad \forall i \in [m] \tag{1.69}$$

$$e_{ijl} \geq 0 \quad \forall j, l \in [k], i \in [m] \tag{1.70}$$

$$\mathbf{w}_j \in \mathbb{R}^n \quad \forall j \in [k] \tag{1.71}$$

$$\gamma_j \in \mathbb{R} \quad \forall j \in [k] \tag{1.72}$$

When $x_{ij} = 0$ inequality 1.67 is deactivated and $\bar{e}_i$ assumes value 0. The variable e_{ijl} is auxiliary and is used for readability purpose, but could be omitted with a simple substitution obtaining:

$$e_i \geq -(\mathbf{w}_j - \mathbf{w}_l)^T \mathbf{a}_i + \gamma_j - \gamma_l + 1 - M(1 - x_{ij}) \tag{1.73}$$

The value of M is once again crucial, as it has to be big enough (ideally $+\infty$) but could cause numerical instabilities if too large.

Chapter 2

Exact MILP formulations for k-PAMF

In this chapter we present a MILP formulation for k-PAMF which includes not only clustering and linear regression on the data points, but also multi-category classification that directly induce a partition on the domain $\mathcal{D}$.

With our mixed-integer formulation it is possible to find a global optimum to the Piecewise Affine Model Fitting problem with no previous information on the unknown function $f(\cdot)$ that we want to approximate. The only parameter that the method requires is the number k of affine submodels.

The devised MILP program is hard to solve to optimality. We show methods which exploit the peculiarities of the formulation and apply some promising recent results from the literature to cope with the complexity of the problem.

2.1 Mixed integer formulation

Our mixed integer formulation of k-PAMF combines all aspects of Piecewise Affine Model Fitting in one single program. A first part of the formulation follows from what has been discussed in Section 1.4.2 about Hyperplane Clustering and how it is related to PAMF: we seek an assignment to the k clusters such that the distance of each cluster member from the corresponding model is minimal. In other words, we look for a partition of the discrete set of points $\mathcal{A}$ in subsets associated to k submodels. The objective function is the sum of the absolute values of the residuals, i.e., the difference d_{ij} between the observed value y_i of each point and the value $\hat{f}_j(\mathbf{a}_i)$ given by the affine submodel (hyperplane). In Section 1.4.2 we discussed the following MILP, that is a modification of a k-HC program where we have replaced the geometric ℓ_2-norm objective function with the ℓ_1-norm algebraic distance of

PAMF (which we repeat for greater readability):

$$\min \sum_{j=1}^{k} \sum_{i=1}^{m} \tilde{d}_{ij} \tag{2.1}$$

$$\sum_{j} x_{ij} = 1 \quad \forall i \in [m] \tag{2.2}$$

$$\tilde{d}_{ij} \leq M x_{ij} \quad \forall i \in [m], j \in [k] \tag{2.3}$$

$$\tilde{d}_{ij} \geq d_{ij} - M(1 - x_{ij}) \quad \forall i \in [m], j \in [k] \tag{2.4}$$

$$d_{ij} \geq \mathbf{w}_j^T \mathbf{a}_i - \gamma_j - y_j \quad \forall i \in [m], j \in [k] \tag{2.5}$$

$$d_{ij} \geq -\mathbf{w}_j^T \mathbf{a}_i + \gamma_j + y_j \quad \forall i \in [m], j \in [k] \tag{2.6}$$

$$x_{ij} \in \{0, 1\} \quad \forall i \in [m], j \in [k] \tag{2.7}$$

$$\tilde{d}_{ij} \geq 0 \quad \forall i \in [m], j \in [k] \tag{2.8}$$

$$\mathbf{w}_j \in \mathbb{R}^n \quad \forall j \in [k] \tag{2.9}$$

$$\gamma_j \in \mathbb{R} \quad \forall i \in [m], j \in [k] \tag{2.10}$$

What is yet to be added is a second part which performs simultaneously a multi-category classification on the continuous domain $\mathcal{D}$ based on the assignments x_{ij} – which are not fixed. What usually happens with supervised learning is that we have points assigned to classes and we look for a separation of the domain such as the points belonging to different categories are accordingly classified. In contrast, in our formulation of k-PAMF we have a shift of paradigm: we do have a classification problem, but the *supervision* labels, or characteristic vectors, x_{ij} are not known a priori. Instead, they are variables that assume a value according to the remaining constraints.

The M-RLP formulation chosen to be included in the k-PAMF program

is the following (see Section 1.4.4):

$$\min \sum_{i=1}^{m} \bar{e}_i \tag{2.11}$$

$$\bar{e}_i \geq e_{ijl} - M(1 - x_{ij}) \quad \forall j, l \in [k], i \in [m] \tag{2.12}$$

$$e_{ijl} \geq -(\mathbf{w}_j - \mathbf{w}_l)^T \mathbf{a}_i + \gamma_j - \gamma_l + 1 \quad \forall j, l \neq j \in [k], i \in [m] \tag{2.13}$$

$$\bar{e}_i \geq 0 \quad \forall i \in [m] \tag{2.14}$$

$$e_{ijl} \geq 0 \quad \forall j, l \in [k], i \in [m] \tag{2.15}$$

which is convenient because it is straightforward to change the role of the characteristic vectors $\mathbf{x}_i$ from parameters to binary variables. We replace the minimization term with a tolerance η on each $\bar{e}_i$, and we obtain the following exact MILP formulation for k-PAMF:

$$\min \sum_{j=1}^{k} \sum_{i=1}^{m} \tilde{d}_{ij} \tag{2.16}$$

$$\sum_{j} x_{ij} = 1 \quad \forall i \in [m] \tag{2.17}$$

$$\tilde{d}_{ij} \leq M x_{ij} \quad \forall i \in [m], j \in [k] \tag{2.18}$$

$$\tilde{d}_{ij} \geq d_{ij} - M(1 - x_{ij}) \quad \forall i \in [m], j \in [k] \tag{2.19}$$

$$d_{ij} \geq \mathbf{w}_j^T \mathbf{a}_i - \gamma_j - y_j \quad \forall i \in [m], j \in [k] \tag{2.20}$$

$$d_{ij} \geq -\mathbf{w}_j^T \mathbf{a}_i + \gamma_j + y_j \quad \forall i \in [m], j \in [k] \tag{2.21}$$

$$\bar{e}_i \leq \eta \quad \forall i \in [m] \tag{2.22}$$

$$\bar{e}_i \geq e_{ijl} - M(1 - x_{ij}) \quad \forall j, l \in [k], i \in [m] \tag{2.23}$$

$$e_{ijl} \geq -(\mathbf{w}_j^c - \mathbf{w}_l^c)^T \mathbf{a}_i + \gamma_j^c - \gamma_l^c + 1 \quad \forall j, l \neq j \in [k], i \in [m] \tag{2.24}$$

$$x_{ij} \in \{0, 1\} \quad \forall i \in [m], j \in [k] \tag{2.25}$$

$$\tilde{d}_{ij} \geq 0 \quad \forall i \in [m], j \in [k] \tag{2.26}$$

$$d_{ij} \geq 0 \quad \forall i \in [m], j \in [k] \tag{2.27}$$

$$\mathbf{w}_j, \mathbf{w}_j^c \in \mathbb{R}^n \quad \forall j \in [k] \tag{2.28}$$

$$\gamma_j, \gamma_j^c \in \mathbb{R} \quad \forall j \in [k] \tag{2.29}$$

$$\bar{e}_i \geq 0 \quad \forall i \in [m] \tag{2.30}$$

$$e_{ijl} \geq 0 \quad \forall j, l \in [k], i \in [m] \tag{2.31}$$

As in [CI06] we add a superscript c to distinguish the parameters of the classification hyperplanes from the regression hyperplanes. The objective is the minimization of the approximation error, while we impose a tolerance η on the error committed by the multi-category classification. The additional RLP constraints *validate* only the assignments x such that the clusters in $\mathcal{A}$

can be linearly separated in the underlying continuous domain $\mathcal{D}$. In other words, a configuration x is not accepted unless it induces piecewise-linearly separable classes on $\mathcal{D}$.

2.1.1 Issues of the formulation

The formulation appears complex for several reasons, such as the strong combinatorial aspect of the problem and the rather large amount of variables and constraints. It can be simplified, removing unnecessary variables and constraints, yielding a more compact formulation:

$$\min \sum_{i=1}^{m} \tilde{d}_i \tag{2.32}$$

$$\sum_{j} x_{ij} = 1 \quad \forall i \in [m] \tag{2.33}$$

$$d_i \geq \mathbf{w}_j^T \mathbf{a}_i - \gamma_j - y_j - M(1 - x_{ij}) \quad \forall i \in [m], j \in [k] \tag{2.34}$$

$$d_i \geq -\mathbf{w}_j^T \mathbf{a}_i + \gamma_j + y_j - M(1 - x_{ij}) \quad \forall i \in [m], j \in [k] \tag{2.35}$$

$$\eta \geq -(\mathbf{w}_j^c - \mathbf{w}_l^c)^T \mathbf{a}_i + \gamma_j^c - \gamma_l^c + 1 - M(1 - x_{ij}) \quad \forall j, l \in [k], i \in [m] \tag{2.36}$$

$$x_{ij} \in \{0, 1\} \quad \forall i \in [m], j \in [k] \tag{2.37}$$

$$d_i \geq 0 \quad \forall i \in [m] \tag{2.38}$$

$$\mathbf{w}_j, \mathbf{w}_j^c \in \mathbb{R}^n \quad \forall j \in [k] \tag{2.39}$$

$$\gamma_j, \gamma_j^c \in \mathbb{R} \quad \forall j \in [k] \tag{2.40}$$

We have $m(k+1) + 2k(n+1)$ variables, mk of those are integer, and $k^2m + 2mk + m$ linear inequalities, all of them involving binary variables.

The columns of the matrix x can be permuted yielding equivalent solutions: this causes issues in branching, since we can find duplicate solutions due to symmetry. Moreover, the symmetry and the big-M terms are known

to be responsible for weak LP relaxation: indeed the relaxation appears to give poor results, as we experience that the problem always appears to have a fractional solution with objective value 0.

In the next sections we describe an attempt to solve the problem as efficiently as possible applying recent promising results from research on integer programming. The focus will be on methods to break symmetries in problems with partitioning constraints [KP08] and the use of Combinatorial Benders' Cuts [CF06] to avoid numerical instabilities and introduce better bounds than those obtained with big-M.

2.2 Symmetry breaking techniques

An integer mathematical program is said to be symmetric if some of its variables can be permuted without changing the structure of the problem. The symmetry group $\mathfrak{G}$ of an IP problem is the set of all permutations π of the n binary variables mapping each feasible solution on a distinct feasible solution having the same objective value.

Symmetries appear in a vast number of classical problems in optimization, especially in those that exhibit a strong combinatorial aspect (graph coloring or partitioning, job scheduling). A symmetric group makes generally a problem harder to solve with classical branch-and-bounds algorithm: first, symmetries lead to an unnecessarily large search tree, because equivalent (isomorphic) solutions are discovered again and again. Hence great part of the effort may be wasted enumerating instances that were already considered. Second, the quality of LP relaxations of such programs typically is extremely poor [Marg10].

One big class of symmetric problem is related to partitioning or packing

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \qquad \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

Figure 2.1: The two matrices are obviously different but, due to symmetry, they describe the same clusters in k-PAMF

problems, that consists in partitioning (or packing) a set $\mathcal{A}$ in at most a number k of subsets having to meet the same requirements – the subsets have to be interchangeable. This is exactly the case in k-PAMF, where all clusters are equivalent and we have a set of partitioning constraints (also called *row-sum* equations) for the binary decision variables x_{ij}:

$$\sum_j x_{ij} = 1 \quad \forall i \in [m] \tag{2.41}$$

k-PAMF is indeed symmetric: given a solution, any permutation π of the clusters, i.e., the columns of x (viewed as a $m \cdot k$ matrix), results in a feasible solution with the same objective function value. In other words, two solutions are equivalent when for each pair $\mathbf{a}_i, \mathbf{a}_{i'}$ the two points belong to the same cluster in a solution if and only if they belong to the same set also in the other one. Figure 2.1 shows two equivalent x matrices for k-PAMF. If we permute the variables x, to have an equivalent solution obviously all the other variables have to permute in a similar way so that only the indices related to their column change. The symmetric group $\mathfrak{G}$ of order k acts on the solutions (by permuting the columns of x) in such a way that the objective function is constant along every orbit of the group action. Each orbit corresponds to a symmetry class of feasible solutions.

The weakness of the LP-bound mentioned above is due to the fact that in many cases the symmetry is responsible for the feasibility of relaxed solutions of poor quality. For example, in the classical IP formulation of the *graph coloring* problem [GJ79], that is widely considered as one of the hardest problems in combinatorial optimization, the LP relaxation is weak since it gives a solution with all $x^*_{ij} = 1/k$, where k is the maximum number of colors that can be used: the solution represents the barycenter of the orbit of any x that satisfies the partitioning inequalities [KP08].

Several methods that deal with symmetries in integer mathematical programming have been developed during the years: typically the focus is either in detecting symmetries in general problems or in developing ad-hoc breaking techniques that work on specific families of problems. A good survey on the topic is [Marg10], where the author reviews and discusses most of the approaches that have been proposed in the recent past. The line that we follow in this work is the idea of finding symmetry-breaking inequalities that describe a polytope containing only non-equivalent solutions for the partitioning Constraints (2.33).

2.2.1 Lexicographic ordering

A solution to the symmetry problem is trying to partition the feasible region in equivalence classes under that symmetry and cut off as large part of the orbits as possible. This is done by adding inequalities to the MIP problem – yet we have to keep at least one representative of each feasible orbit lest valid solutions be missed. In [MDZ01] Méndez-Díaz and Zabala introduce symmetry-breaking constraints that have been proved to leave out all equivalent solutions from each orbit except for one element, which is the solution that is maximal with respect to a lexicographic ordering of the columns of x.

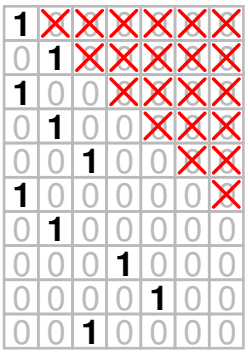


Figure 2.2: A matrix with columns in decreasing lexicographic order. Under partitioning constraints (only one 1-entry per row), the elements over the main diagonal are bound to be 0.

Definition. A vector $v \in R^n$ is lexicographically smaller than a vector $w \in R^n$ if for some $1 \leq p \leq n$ we have $v_i = w_i$ for $i = 1, ..., p-1$ and $v_p < w_p$ (resp. $v_p > w_p$). This is denoted by:

$$v \prec w \tag{2.42}$$

A solution of the integer problem is chosen as a representative if and only if its columns are in non-increasing lexicographic order, i.e., if it is $\prec$-maximal[1] in its symmetry orbit. An example of a matrix with columns in decreasing lexicographic order is reported in Figure 2.2. The authors show that this kind of symmetry-breaking constraints performs well in some situations. The strongest constraints that are introduced in the article are the following inequalities (from now on called MZ inequalities):

$$x_{ij} \leq \sum_{p=1}^{i-1} x_{p,j-1} \tag{2.43}$$

When applied to our problem, the inequalities ensure that a point $\mathbf{a}_i$ can be assigned to a hyperplane $\mathcal{H}_j$ only if all clusters $j' < j$ contain at least a

[1] lexicographically maximal

point with $i' < i$ (see fig. 2.3). Assigning the first vector to the first cluster, by imposing $x_{1,1} = 1$, and adding the symmetry-breaking Constraints (2.43) we ensure that the matrix x has to be lexicographically sorted. When $k = 2$, just by fixing of the variable $x_{1,1}$ to 1 the matrix is obviously lexicographically sorted.

2.2.2 Orbitopes: notation and definitions

In [KP08] Kaibel and Pfetsch derive a linear description of the *convex hull* of all $\prec$-maximal feasible solutions. It involves using an exponential number of constraints that can be seen as both a generalization and a strengthening of the symmetry-breaking inequalities formerly described. The convex hulls of 0/1-matrices with exactly one 1 per row and lexicographically sorted columns are called *partitioning orbitopes* and are a recent research topic.

We introduce some preliminary notations and definitions. We call $\mathcal{M}_{m.k}$ the set of $m \times k$ matrices whose elements can assume only binary values (0 or 1). Then we define:

$$\mathcal{M}^{=}_{m,k} := \{x \in \mathcal{M}_{m,k} : \sum_{j=1}^{k} x_{ij} = 1\} \tag{2.44}$$

as all matrices that satisfy the partitioning constraints (row-sum equations).

Let $\mathfrak{G}_k$ be the group of all permutations acting on $\mathcal{M}_{m,k}$ by permuting columns (*symmetric group*). We denote with $\mathcal{M}^{max}_{m.k}(\mathfrak{G}_k)$ the set of matrices in $\mathcal{M}_{m.k}$ that are $\prec$-maximal within their orbits under the action of their symmetry group (i.e., the set of all 0/1 matrices that are lexicographically sorted).

We define:

$$\mathcal{I}_{m,k} := \{(i, j) \in [m] \times [k] : i \geq j\} \tag{2.45}$$

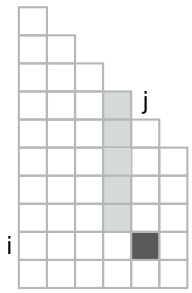


Figure 2.3: The elements in grey form the set $col(i-1, j-1)$ and their sum represents the right-hand side of the inequality in 2.43. Notice that we take into account only the entries under the main diagonal, i.e., with with $i \leq j$.

as the set of valid indices of a matrix in $\mathcal{M}^{max}_{m.k}(\mathfrak{G}_k) \cap \mathcal{M}^{=}_{m.k}$. This is derived from the observation that, in a $\prec$-maximal 0/1 matrix x satisfying the partitioning constraints (one 1-entry per row), all entries x_{ij} with $i > j$ have to be equal to 0 (see Figure 2.2). Accordingly we define:

$$row_i := \{(i,1),(i,2),...,(i,\min\{i,k\})\} \tag{2.46}$$

$$col_j := \{(j,j),(j+1,j),...,(m,j)\} \tag{2.47}$$

$$col(i,j) := \{(j,j),(j+1,j),...,(i,j)\} \tag{2.48}$$

For convenience, given a set of indices $\mathcal{S} \subseteq [m] \times [k]$ and a matrix $x \in \mathbb{R}^{m \times k}$, we write:

$$x(\mathcal{S}) := \sum_{(i,j)\in\mathcal{S}} x_{ij} \tag{2.49}$$

It is now possible to formally define the object on which the following results are based.

Definition. (Partitioning orbitope) The partitioning orbitope associated with the group $\mathfrak{G}_k$ is:

$$\mathcal{O}^{=}_{m,k}(\mathfrak{G}_k) := conv(\mathcal{M}^{max}_{m.k}(\mathfrak{G}_k) \cap \mathcal{M}^{=}_{m.k}) \tag{2.50}$$

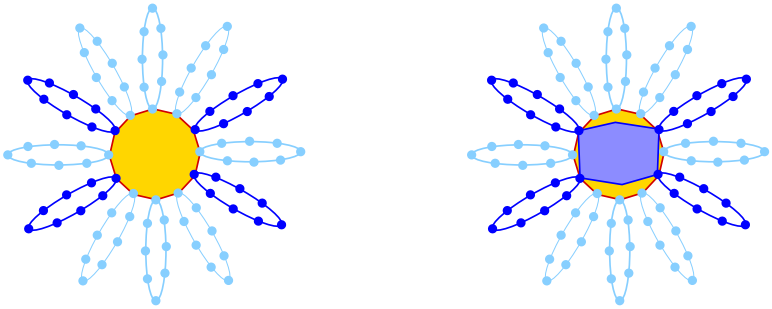


Figure 2.4: The points represent the solutions of a symmetric problems. Darker, the feasible ones. The orbits contain distinct solutions that are equivalent, i.e., with the same objective value. The orbitope, in yellow, describes the convex hull of the lexicographic maxima. Combining the orbitope with the remaining constraints of the problem we have a tighter feasible set with no symmetries. Figure from [KP08].

A partitioning orbitope $\mathcal{O}^{=}_{m,k}(\mathfrak{G}_k)$ is the convex hull of all the $\prec$-maximal 0/1 matrices that satisfy the partitioning constraints. The orbitope contains exactly one representative for each orbit with respect to the symmetry group $\mathfrak{G}_k$. Combining the orbitope with the remaining constraints of a concrete problem, we completely remove the symmetry associated with the permutation of the columns of x (see Figure 2.4).

2.2.3 Shifted Column Inequalities

A first step towards the full description of the orbitope consists in the following generalization of MZ inequalities:

Definition. For a $(i,j) \in \mathcal{I}_{m.k}$ and the set $\mathcal{B} = \{(i,j),(i,j{+}1),\ldots,(i,min\{i,q\}\}$ called *bar* of (i,j), we define the *Column Inequality*:

$$x(\mathcal{B}) \leq x(col(i-1,j-1)) \tag{2.51}$$

Column inequalities are tightenings of the MZ symmetry-breaking in-

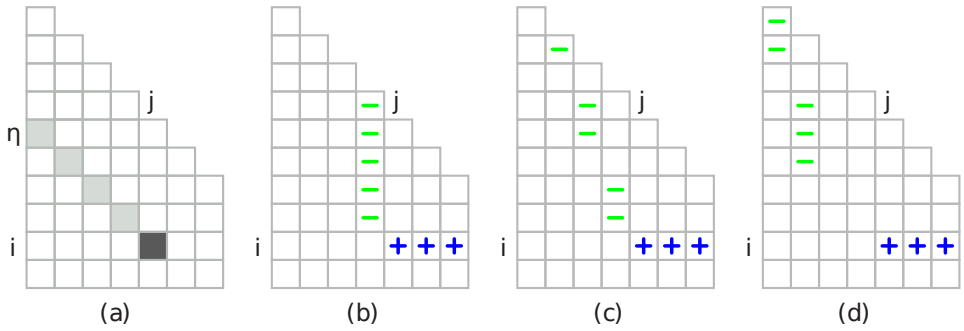


Figure 2.5: (a) shows how diagonal coordinates work. (c), (d) display two possible shiftings of the column $(i, j-1)$ in (b). The shifted columns represent the right-hand side of SCIs with *leader* (i, j).

equalities. It can be demonstrated that an integer solution $x \in \{0,1\}^{m\times k}$ belongs to $\mathcal{O}^{=}_{m,k}(\mathfrak{G})$ if and only if it satisfies all column inequalities and the partitioning constraints. Column inequalities are stronger yet they do not suffice to completely define $\mathcal{O}^{=}_{m,k}(\mathfrak{G}_k)$. In order to do that, we have to introduce the Shifted Column Inequalities. First, it is useful to use a different system of coordinates to indicate the elements in $\mathcal{I}_{m,k}$:

$$\langle \eta, j\rangle = (j+\eta-1, j) \qquad \text{for } j \in [k], \quad 1 \le \eta \le m-j+1 \tag{2.52}$$

We denote with $\langle \eta, j\rangle$ the element contained in the j-th column and η-th diagonal counting from the top (see Figure 2.5).

Definition. A set $\mathcal{S} = \{\langle 1, c_1\rangle, \langle 2, c_2\rangle, \ldots, \langle \eta, c_\eta\rangle\}\} \subset \mathcal{I}_{m,k}$ with $\eta > 1$ and $c_1 \le c_2 \le \ldots \le c_\eta$ is called a *shifted column*. It is a *shifting* of each of the columns

$$col\langle \eta, c_\eta\rangle, col\langle \eta, c_\eta + 1\rangle, \ldots, col\langle \eta, k\rangle, \tag{2.53}$$

A *shifting* can be seen as a column whose elements have been moved diagonally towards the upper-left position (Figure 2.5).

Definition. For $(i, j) = \langle \eta, j\rangle \in \mathcal{I}_{m.k}$, the set $\mathcal{B} = \{(i, j), (i, j+1), ..,$

$(i, min\{i, q\}\}$ and a shifting $\mathcal{S}$ of $col\langle \eta, j-1 \rangle$, we define the *Shifted Column Inequality*:

$$x(\mathcal{B}) \leq x(\mathcal{S}) \tag{2.54}$$

where $\mathcal{B}$ is called the *bar* of the Shifted Column and (i, j) is the *leader* of the SC.

All Column Inequalities are included, since they are Shifted Column Inequalities with a trivial (null) shifting. The family of SCIs is considerably larger: indeed, it contains an exponential number of inequalities (in k).

The final result provided in [KP08] is the following theorem:

Theorem (*Orbitope description*)**.** The partitioning orbitope $\mathcal{O}^{=}_{m,k}(\mathfrak{G}_k)$ is completely described by the nonnegativity constraints, the row-sum equations, and the shifted column inequalities:

$$\begin{aligned}\mathcal{O}^{=}_{m,k}(\mathfrak{G}_k)) = \{x \in \mathbb{R}^{m \times k} | x \geq 0, \sum_{j=1}^{k} x_{ij} = 1 \text{ for } i \in [m], \\ x(\mathcal{B}) \leq x(\mathcal{S}) \text{ for all SCIs}\}\end{aligned} \tag{2.55}$$

Having a full description for the convex hull of $\prec$-maximal partitioning matrices is a powerful result. However, in order to use this characterization of the orbitope $\mathcal{O}^{=}_{m,k}(\mathfrak{G}_k)$ in practice it is not possible to think of adding all SCIs (exponentially many) to the MIP model. It is therefore crucial to have a separation algorithm that adds violated inequalities in a cutting plane fashion.

2.2.4 Separation algorithm for SCIs

A sketch of an efficient algorithm for the separation problem resulting from SCIs is described again in [KP08]. Given a solution x^*, it is possible via

dynamic programming to compute a set of maximally violated cuts.

The algorithm builds two $m \times k$ tables: a matrix $w \in \mathbb{R}^{m \times k}$ that contains the value $x(\mathcal{S})$ of the minimal shifting for each $\langle \eta, j \rangle \in \mathcal{I}_{m,k}$ and a support structure $\tau \in \{0,1\}^{m \times k}$ that allows the reconstruction of the corresponding Shifted Column.

Comparing the values of the minimal shiftings in w with the values of the respective *bars* $x(\mathcal{B})$, with $\mathcal{B} = \{(i, j+1), \ldots, (i, min\{i, q\}\}$, it is possible to identify the SCIs which are violated in $O(mk)$ time. Since the construction of the data structures is done in $O(mk)$ and the reconstruction of a Shifted Column in $O(m)$, we have a separation algorithm that takes an overall linear time with respect to the dimension $m \times k$ of the matrix x. For further details on the algorithm see Appendix A.

2.2.5 Extended formulation for orbitopes

A further step is described by Faenza and Kaibel in [FK09]: they show that there exists an extended formulation for the partitioning orbitope, i.e., a linear description of a higher dimensional polytope that can be projected down to the orbitope $\mathcal{O}^{=}_{m,k}(\mathfrak{G}_k)$. Rather than solving an optimization problem over the orbitope in the original space, where exponentially many inequalities are needed, one may solve it over a simpler polyhedron of which the first one is an orthogonal projection.

The basic idea of the extended formulation for partitioning orbitopes is to assign to each vertex of $\mathcal{O}^{=}_{m,k}$ a directed path in a certain acyclic digraph constructed on the matrix (Figure 2.6). A number of additional variables in the extended formulations are used to suitably express these paths - from here the need of additional dimensions. After a series of transformations, the

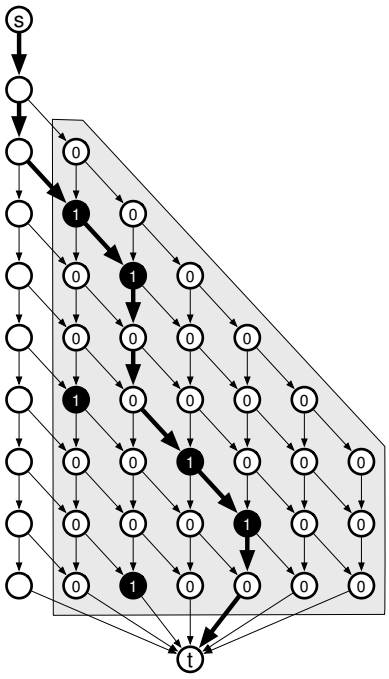


Figure 2.6: A vertex of $\mathcal{O}^{=}_{m,k}$ and its associated s-t path [FK09].

final and most compact form is expressed by the following inequalities:

$$x_{ij} = z_{ij} - z_{i,j+1} \quad \forall (i,j) \in \mathcal{I}_{m,k} \tag{2.56}$$

$$u_{i,j} - u_{i-1,j} \geq 0 \quad \forall (i,j) \in \mathcal{I}_{m,k} \tag{2.57}$$

$$u_{i,j} - u_{i+1,j+1} \geq 0 \quad \forall (i,j) \in \mathcal{I}_{m,k} \tag{2.58}$$

$$u_{m,1} \leq 1 \tag{2.59}$$

$$u_{i,j} - u_{i-1,j} - z_{ij} + z_{i,j+1} \leq 0 \quad \forall (i,j) \in \mathcal{I}_{m,k} \tag{2.60}$$

$$z_{ij} - u_{i,j} \leq 0 \quad \forall (i,j) \in \mathcal{I}_{m,k} \tag{2.61}$$

$$u_{i,j} \geq 0 \quad \forall i \in [m], j = \min\{k, i\} \tag{2.62}$$

$$u_{1,1} = 1 \tag{2.63}$$

The formulation introduces $2mk$ new variables u_{ij}, z_{ij} and about $4mk$ inequalities. The constraints define an integral polyhedron $\mathcal{P}^{=}_{mk}$ whose pro-

jection onto the original space is proved to be the partitioning orbitope $\mathcal{O}^{=}_{m,k}(\mathfrak{G}_k)$. In practice, by including the variables u_{ij}, z_{ij} and the associated inequalities in a problem with packing or partitioning constraints column symmetries are removed at the cost of adding a number of continuous variables and constraints which is linear in mk.

This formulation implies that the optimization over the partitioning orbitope can be solved in polynomial time. The existence of a polynomial description of $\mathcal{O}^{=}_{m,k}(\mathfrak{G}_k)$ is consistent with the result of Grötschel, Lovàsz and Schrijver, that show in [GLS88] how the optimization problem on a polyhedron can be solved in polynomial time if and only if the corresponding separation problem can be solved in polynomial time. Since we have a polynomial separation algorithm for SCI inequalities, the polynomial description of the orbitope is not unexpected.

2.3 Dealing with Big-M

As previously mentioned, one of the major problems involved in modelling a k-PAMF problem is dealing with the conditional constraints, i.e., the inequalities which are active only if an associated binary variable x_{ij} assumes value 1. The most common way to solve this issue is adding a term weighted by a large-valued constant M that acts in practice as an implication. Specifically, we translate:

$$x_{ij} = 1 \Rightarrow \tilde{d_{ij}} \geq d_{ij} \tag{2.64}$$

into:

$$\tilde{d_{ij}} \geq d_{ij} - M(1 - x_{ij}) \tag{2.65}$$

When $x_{ij} = 1$, the big-M term cancels out and the inequality holds. When $x_{ij} = 0$, the large value of M makes the constraint unrelevant, ideally becoming $\tilde{d_{ij}} \geq -\infty$.

However, introducing a coefficient with a value much larger than the rest of the coefficients in the problem might not be advisable, since it can lead to ill-conditioning and numerical instabilities which are hard to manage. See Section 4.2.3 for details on the choice of M in practice.

On the other hand, setting too low values of M is often not possible due to the high values not only in the data vectors, that can be normalized, but in the RLP variables as well (for example, on some instances γ^c tends to assume large values). In these situations the solutions are suboptimal or just plain inconsistent.

2.3.1 Introduction to Combinatorial Benders' Cuts

Combinatorial Benders' Cuts (CBC for short), as proposed by Codato and Fischetti in [CF06], are a family of cuts that have the purpose of removing the drawbacks of the big-M technique. CBC are to be used in a decomposition method similar to classical Benders' [NW]: the MIP problem we want to solve is decomposed in a Master problem, which is an ILP that contains only the integer variables, and a sequence of Slave problems which allow the generation of cuts that determine the feasibility and, possibly, the optimality of the incumbent solution.

Given a general MILP problem with conditional constraints, we call $\mathbf{y}$ the continuous variables, and $\mathbf{x}$ the integer 0/1 variables which control the implications as in:

$$x_i = 1 \Rightarrow \mathbf{a}_i^T \mathbf{y} \leq b_i. \tag{2.66}$$

Let $\mathbf{x}^*$ be an integer solution of the Master problem. The associated Slave problem works only on the variables $\mathbf{y}$. The Slave is an LP program that includes only the conditional inequalities which are active according to the current $\mathbf{x}^*$. Thus the problem of modelling implications disappear: the Slave linear problem is constructed given a fixed solution $\mathbf{x}^*$, so when we build it the active inequalities are included in the system, while inactive ones are not – no need for big-Ms.

If the Slave happens to be infeasible, it means that the current $\mathbf{x}^*$ is not feasible. Therefore we add cuts that are based on Irreducible Infeasible Subsystems (IIS) of the inequalities in the Slave. Doing so, we attempt to cut off the configurations of $\mathbf{x}$ that generated the infeasibility. This is somehow similar to the concept of *no-goods* in Constraint Programming, where one tries to learn from failures and record them as new constraints.

The difference is that with a Combinatorial Benders' Cut we rule out not only one, but a class of solutions.

2.3.2 Combinatorial Benders' Cuts for k-PAMF

The method in [CF06] can be generalized to a vast family of MILP, where integer and/or continuous variables appear either in the objective function or in the system of inequalities. Here we describe only a variant of the technique that is applicable to our k-PAMF formulation. Consider the k-PAMF formulation in (2.32) rewritten as:

$$\min \mathbf{c}^T \mathbf{y} \tag{2.67}$$

$$\sum_{j=1}^{k} x_{ij} = 1 \quad \forall i \in [m] \tag{2.68}$$

$$\mathbf{M}\mathbf{x} + \mathbf{A}\mathbf{y} \leq \mathbf{b} \tag{2.69}$$

$$x_{ij} \in \{0, 1\}$$

where $\mathbf{y}$ is a vector containing all the continuous variables $(d_i, \gamma_j, \gamma_j^c, w_j, w_j^c)$ and the matrices $\mathbf{M}, \mathbf{A}$ express the inequalities in (2.32). It has to be noticed that only *conditional* constraints appear in the formulation, justifying Inequality (2.69). The matrix $\mathbf{M}$ in every row contains exactly one big-M constant associated to a binary variable x_{ij} as in:

$$M x_{ij} + \mathbf{a}_i^T \mathbf{y} \leq b_i. \tag{2.70}$$

The problem can then be split in two subproblems. The first, or MASTER problem, is a purely combinatorial ILP and contains constraints on the binary

variables x_{ij} only:

$$\min 0^T \mathbf{x} \tag{2.71}$$

$$\sum_{j=1}^{k} x_{ij} = 1 \quad \forall i \in [m] \tag{2.72}$$

$$x_{ij} \in \{0, 1\}.$$

The second, the SLAVE problem, is an LP depending on a vector $\tilde{\mathbf{x}}$ of 0/1 parameters:

$$\text{SLAVE}(\tilde{\mathbf{x}}) = \begin{cases} \min \mathbf{c}^T \mathbf{y} \\ \mathbf{A}\mathbf{y} \leq \mathbf{b} - \mathbf{M}\tilde{\mathbf{x}} \end{cases} \tag{2.73}$$

All conditional constraints are moved to the Slave problem, while the Master initially contains only the partitioning constraints. What is more, in our case the objective function is in the Slave, since it only involves continuous variables $\mathbf{y}$. Therefore optimality cannot be ensured by the Master problem: the cuts that we want to generate have to contain not only information on the feasibility of the solutions but on their optimality as well. Combinatorial Benders' cuts translate these requirements from the Slave problem to the Master problem, that only has combinatorial information. It is necessary to stress that the big-M notation has been used in (2.73) for convenience, but it is not used in practice, where we just select the rows of $\mathbf{A}\mathbf{y} \leq \mathbf{b}$ that are *active* according to $\tilde{\mathbf{x}}$ and discard the others.

To start the CBC iterative procedure, we solve the Master problem at integrality: let $\mathbf{x}^*$ be a feasible integer solution for MASTER.

If the linear system SLAVE($\mathbf{x}^*$) is feasible, let $\mathbf{y}^*$ be its optimal solution. The objective value $\mathbf{c}^T\mathbf{y}^*$ represents the optimal value with respect to the

current integer $\mathbf{x}^*$. The solution $(\mathbf{x}^*, \mathbf{y}^*)$ is feasible but it is not guaranteed to be optimal for the whole problem P.

In order to achieve optimality it is necessary to impose it via an upper bound on the slave problem, that is the best value $B = \mathbf{c}^T\mathbf{y}^*$ found so far:

$$\mathbf{c}^T\mathbf{y} \leq B - \epsilon \tag{2.74}$$

With this additional constraint, if a solution does not improve the current best, it is not considered feasible. If SLAVE($\mathbf{x}^*$) is feasible also with respect to the bound inequality, we update the current best incumbent by $(\mathbf{x}^*, \mathbf{y}^*)$ and store a tighter bound B on the objective value.

When the linear system SLAVE($\mathbf{x}^*$) turns out to be infeasible, it means that $\mathbf{x}^*$ is infeasible for P, hence we reject it generating a cut as follows. In the separation problem we look for an Irreducible Infeasible Subsystem of SLAVE($\mathbf{x}^*$). This set will include a number of rows of $\mathbf{Ay} \leq \mathbf{b}$ which, combined, form an irreducible infeasible system of inequalities. A subsystem is an Irreducible Infeasible Subsystem when it is infeasible, but every proper subsystem of it is feasible – i.e., removing just one of the inequalities in the IIS yields a feasible system.

If we denote with $\mathcal{C} \subseteq [m]\times[k]$ the set of indices of $\mathbf{x}$ associated to the constraints in a IIS of SLAVE($\mathbf{x}^*$), we can generate the following *Combinatorial Benders' Cut*:

$$\sum_{(i,j)\in\mathcal{C}_0} x_{ij} + \sum_{(i,j)\in\mathcal{C}_1} (1 - x_{ij}) \geq 1 \tag{2.75}$$

where $\mathcal{C} = \{\mathcal{C}_0 \cup \mathcal{C}_1\}$, $\mathcal{C}_0$ contains the pairs (i, j) such that $x^*_{ij} = 0$ and $\mathcal{C}_1$ those for $x^*_{ij} = 1$. The cut is motivated by the fact that at least one of the binary variables indexed by $\mathcal{C}$ has to be changed in order to disable a constraint in the IIS and break the infeasibility. The current $\mathbf{x}^*$ violates the

CB Inequality (2.75) since by definition of $\mathcal{C}_0$ and $\mathcal{C}_1$:

$$\sum_{(i,j)\in\mathcal{C}_0} x^*_{ij} + \sum_{(i,j)\in\mathcal{C}_1} (1 - x^*_{ij}) = 0.$$

The method will halt when the Master is infeasible: as soon as we generate a CB inequality which results in infeasibility of MASTER, it means that any further improvement of the solution by changing $\mathbf{x}$ is impossible, hence the current incumbent $(\mathbf{x}^*, \mathbf{y}^*)$ is the optimum for P.

CBC PROCEDURE

repeat
  if MASTER($\mathbf{x}$) infeasible
    return $(\mathbf{x}^*, \mathbf{y}^*)$
  $\mathbf{x}^* \leftarrow$ MASTER($\mathbf{x}$)
  if SLAVE($\mathbf{y}; \mathbf{x}^*$) not infeasible
    $\mathbf{y}^* \leftarrow$ SLAVE($\mathbf{y}; \mathbf{x}^*$)
    $B \leftarrow \mathbf{c}^T\mathbf{y}^*$
    Add Upper Bound to SLAVE:
      $\mathbf{c}^T\mathbf{y} \leq B - \epsilon$
  repeat //SLAVE *is infeasible*
    $\mathcal{C} \leftarrow$ IIS of SLAVE($\mathbf{y}; \mathbf{x}^*$)
    Add CB cut to MASTER:
      $\sum_{(i,j)\in\mathcal{C}_0} x_{ij} + \sum_{(i,j)\in\mathcal{C}_1}(1 - x_{ij}) \geq 1$

2.3.3 Irreducible Infeasible Subsystems

The separation problem which is required for the generation of CB cuts involves the search of an Irreducible Infeasible Subsystem. Looking for a minimal-weight IIS of a system of inequalities is known to be a $\mathcal{NP}$-hard

problem [APT03]. However, there are efficient techniques to find Irreducible Infeasible Subsystems in polynomial time. Gleeson and Ryan demonstrated a correspondence between the IISs of a linear system $\mathbf{Ay} \leq \mathbf{b}$ and the nonzero components of the vertices of a related polyhedron. The result presented in [GR90] shows that given an *infeasible* linear problem:

$$\min 0^T \mathbf{y} \tag{2.76}$$

$$\mathbf{Ay} \leq \mathbf{b} \tag{2.77}$$

$$\mathbf{y} \in \mathbb{R}^n \tag{2.78}$$

the indices of its Irreducible Infeasible Subsystems correspond to the supports (nonzero components) of the vertices of the so-called *alternative polyhedron*. To define this polyhedron we start from the set defined by the dual problem, that is:

$$\max \lambda^T \mathbf{b} \tag{2.79}$$

$$\lambda^T \mathbf{A} = 0 \tag{2.80}$$

$$\lambda \leq 0 \tag{2.81}$$

In this situation, given an infeasible primal, the dual problem cannot be infeasible too, as $\lambda = 0$ is always a solution – here we are not interested in primal objective function, but only in its feasibility, so all primal objective coefficients can be considered to be 0. Therefore for every $k \geq 0$ there is a λ^* such that $\mathbf{b}^T \lambda^* > k$: the dual is unbounded.

The *alternative polyhedron* is obtained by bounding the dual variables

with the normalization constraint

$$\lambda^T \mathbf{b} = 1 \tag{2.82}$$

(where any other positive constant would work). The purpose of the normalization constraint is to cut what would otherwise be a cone: we want to look for the support sets of the vertices, which define IIS. The problem to solve becomes the following:

$$\max \lambda^T \mathbf{w} \tag{2.83}$$

$$\lambda^T \mathbf{A} = 0 \tag{2.84}$$

$$\lambda^T \mathbf{b} = 1 \tag{2.85}$$

$$\lambda \leq 0 \tag{2.86}$$

This program amounts to finding a linear combination λ^* of the rows of $\mathbf{Ay} \leq \mathbf{b}$ that certificates its infeasibility. In fact, from $\mathbf{Ay} \leq \mathbf{b}$ and $\lambda \leq 0$ it follows that $\lambda^{*T}\mathbf{Ay} \geq \lambda^{*T}\mathbf{b}$: the left-hand side is equal to 0 (2.84), while $\lambda^T \mathbf{b}$ is strictly positive (in this case 1). If the primal is indeed infeasible, the existence of a solution λ^* is guaranteed by Farkas' Lemma, and it is not unbounded due to the normalization constraint.

Once we have a vertex solution λ^*, its nonzero components identify a Irreducible Infeasible Subsystem for $\mathbf{Ay} \leq \mathbf{b}$, obtained just by solving a LP problem. The vector $\mathbf{w}$ in the Objective Function (2.83) is set to values that are arbitrarily defined. The choice of $\mathbf{w}$ can drive the solution towards different vertices, and by setting nonnegative values we hope to obtain IIS with low cardinality (since we are maximizing and $\lambda \leq 0$). This IIS search is fast because it allows us to find several alternative IIS just by modifying the

weights $\mathbf{w}$ and solving the problem again. To do that, we adopt two different techniques attempting to guarantee diversity in IIS we find:

- start with all costs $w_i = 1$;
- set $w_i = \xi > 0$ for inequalities belonging to the previously identified IIS, attempting to reduce overlap between consecutive generated IISs. We use $\xi = 2$

or, in alternative, a strategy inspired by [BR09]:

- start with all costs $w_i = 1$;
- if inequality i belongs to the currently identified IIS, increase w_i by ξ

so to have coefficients $w_i = 1 + \xi \cdot m_i$ where m_i is the number of the previously identified IIS containing the constraint i.

Chapter 3

Heuristics

The exact mixed-integer formulation for k-PAMF allows to fit a Piecewise Affine Model which is optimal with respect to the sum of the absolute values of the approximation errors. For larger instances the problem is hard to solve to optimality, even if we apply symmetry-breaking methods. It is therefore useful in practice to devise fast techniques that yield good feasible solutions, though not guaranteed to be optimal. The obtained solutions can also help solve the exact formulation providing an upper bound.

We propose two heuristics for the problem of k-Piecewise Affine Model Fitting as defined in Chapter 2: the aim is the minimization of the sum of the absolute values of the errors from the observed values y_i, the norm ℓ_1 of the error vector, while at the same time we want to directly induce a partition on the continuous domain $\mathcal{D}$ via multi-category classification.

3.1 Three-Step PAMF Heuristic

We describe a heuristic algorithm that finds feasible solutions for k-PAMF efficiently. The algorithm, called Three-Step Piecewise Affine Model Fitting

heuristic (3-PAMF for short), is an adaptation of an algorithm for k-HC described by Mangasarian and based on classical k-means.

3.1.1 k-Plane Clustering

The original method proposed in [BM00] is called k-Plane Clustering (k-PC). It is an adaptation of k-means to the case of Hyperplane Clustering.

k-means is a classic clustering algorithm that works in two steps to be repeated until a stable configuration is reached. At the beginning of the algorithm, the clusters are randomly generated. The first step is the assignment of points to the cluster with the closest mean. In the second step the cluster means are recomputed. In the case of Hyperplane Clustering, means are replaced by hyperplanes, and the points are assigned to the plane that has the smallest point-hyperplane orthogonal distance.

The k-PC algorithm starts with k random hyperplanes and it keeps alternating between the following two steps:

Assignment

Assign each vector to the closest hyperplane $\mathcal{H}_j$.
The set of points assigned to $\mathcal{H}_j$ is $\mathcal{A}_j = \{\mathbf{a}_i : i = \arg\min_i \frac{|\mathbf{w}_j^T \mathbf{a}_i - \gamma_j|}{\|\mathbf{w}_j\|_2}\}$

Update

Compute the new hyperplane parameters $(\mathbf{w}_j, \gamma_j)$ for all $j \in [k]$ that minimize the sum of the squared orthogonal distances from the points in the corresponding cluster.

The algorithm proceeds until it reaches a steady state, i.e., when the assignments (and consequently the hyperplane parameters) stops changing. Clearly it is a heuristic algorithm, without any guarantees of optimality. Usually it stops after a small number of iterations, although certain sets of points are

known where the runtime takes an exponential time. The parameter update step can be implemented efficiently in closed form as described in [BM00] and [CI06].

3.1.2 3-PAMF

The main idea behind the Three-Step heuristic is that the k-PC algorithm can be adapted to the Piecewise Affine Model Fitting problem.

The adaptation required by the switch from the Hyperplane Clustering problem to the current task has to deal with the different objective function. In k-PAMF we have a ℓ_1-norm minimization, while k-HC involves the minimization of the sum of the squared orthogonal distances. Hence both the Reassignment and the Parameter Update step have to be modified.

It is also necessary to add a third step, which is required in order to induce the partition on the domain $\mathcal{D}$. The 3-PAMF algorithm iteratively solves the sequence of three subproblems:

1. hyperplane parameter update
2. point assignment
3. partition of the domain $\mathcal{D}$

After the points have been assigned to their closest plane, an RLP (see Section 1.4.4) is performed and a partition of $\mathcal{D}$ is computed according to the clusters that were formed in the previous step. Moreover, if such sets are not piecewise-linearly separable, the algorithm picks the points which are misclassified and reassign them according to the subdomain $\mathcal{D}_j$ they lie in.

The RLP step at each iteration drives the search towards solutions that induce suitable linear partitions on the continuous domain. At the same time,

it avoids drifting towards solutions which are good in the discrete space of data points but do not translate well in linear submodels. This comes at the cost of a harder problem to solve, since with the additional RLP step we implicitly add constraints that limit to 0 the misclassification error on $\mathcal{D}$.

An outline of the algorithm follows. The approximation error mentioned in the algorithm is the sum of the absolute values of the residuals, consistent with the formulation of k-PAMF (see Section 1.4.2).

Start Assign the m points to k hyperplanes with randomly generated parameters $(\mathbf{w}_j, \gamma_j)$.

Repeat as long as the overall approximation error decreases:

Update Step

For each hyperplane $\mathcal{H}_j$ compute the new parameters $(\mathbf{w}_j, \gamma_j)$ such that they minimize the approximation error (absolute deviation) on the corresponding points.

Assignment Step

Assign each vector to the closest hyperplane $\mathcal{H}_j$, the cluster of points assigned to $\mathcal{H}_j$ is:

$$\mathcal{A}_j = \{\mathbf{a}_i : i = \arg\min_i |(\mathbf{w}_j^T \mathbf{a}_i - \gamma_j) - y_i|\}.$$

RLP Step

Identify the k discriminating hyperplanes defined by $(\mathbf{w}_j^c, \gamma_j^c)$ solving the M-RLP formulation. For each misclassified point $\mathbf{a}_i$, reassign it to the cluster $j = c(\mathbf{a}_i)$ given by the classification function.

3.1.3 Algorithm analysis

Parameter update

For each hyperplane $\mathcal{H}_j$ we identify the parameters $(\mathbf{w}_j, \gamma_j)$ that minimize the quantity:

$$\sum_{i:\mathbf{a}_i \in \mathcal{A}_j} |(\mathbf{w}_j^T \mathbf{a}_i - \gamma_j) - y_i| \tag{3.1}$$

By defining:

$$\mathbf{A}_j = \left[\begin{array}{c|c} \mathbf{a}_1^T & -1 \\ \vdots & \vdots \\ \mathbf{a}_{m_j}^T & -1 \end{array}\right], \quad \mathbf{y}_j = \begin{bmatrix} y_1 \\ \vdots \\ y_{m_j} \end{bmatrix}, \quad \bar{\mathbf{w}}_j = \begin{bmatrix} \mathbf{w}_j \\ \gamma_j \end{bmatrix} \tag{3.2}$$

where the row of the matrix $\bar{\mathbf{A}}_j \in \mathbb{R}^{m_j \times n}$ represent the points assigned to the j-th hyperplane with an additional final term -1, the vector $\mathbf{y}_j \in \mathbb{R}^{m_j}$ contains the value of the observations y_i associated to the points and $\bar{\mathbf{w}}_j$ is the vector holding the pair $(\mathbf{w}_j, \gamma_j)$, we have the the following Parameter Update problem:

$$\min_{\bar{\mathbf{w}}_j} \|\bar{\mathbf{A}}_j \bar{\mathbf{w}}_j - \mathbf{y}_j\|_1. \tag{3.3}$$

Due to the use of the ℓ_1-norm this amounts to the following linear mathematical program:

$$\min \sum_{i \in \mathcal{I}_j} d_{ij} \tag{3.4}$$

$$d_{ij} \geq \mathbf{w}_j^T \mathbf{a}_i - \gamma_j - y_j \quad \forall i \in \mathcal{I}_j \tag{3.5}$$

$$d_{ij} \geq -\mathbf{w}_j^T \mathbf{a}_i + \gamma_j + y_j \quad \forall i \in \mathcal{I}_j \tag{3.6}$$

$$\mathbf{w}_j, \gamma_j \in \mathbb{R},$$

where $\mathcal{I}_j$ is the set of the indices i s.t. $\mathbf{a}_i$ is assigned to $\mathcal{H}_j$.

Assignment Step

Each point is assigned to the hyperplane with smallest approximation error $|(\mathbf{w}_j^T \mathbf{a}_i - \gamma_j) - y_i|$. To select the best submodel, for each point all hyperplanes have to be considered and for each of them the residual has to be computed.

RLP Step

The third step consists in solving a M-RLP problem as described in equation 1.66, where we use as *labels* the point-hyperplane assignments that follow from the previous steps. The result of the optimization will be the classification hyperplanes $(\mathbf{w}_j^c, \gamma_j^c)$ that generate a linear partition of the domain $\mathcal{D}$ in k subdomains.

If the classification problem has an optimal objective value equal to 0 it follows that the classes are linearly separable and we need no further action. On the other hand, a solution greater than 0 means that at least one point is misclassified: a vector $\mathbf{a}_i$ is considered misclassified if it is assigned to a hyperplane $\mathcal{H}_j$ but is actually contained in the subdomain of a different hyperplane $\mathcal{H}_{j'}$. In short, $\mathbf{a}_i$ is assigned to $\mathcal{H}_j$ but $c(\mathbf{a}_i) = j' \neq j$.

The algorithm then proceeds to remove the misclassifications: it picks each point which is misclassified according to the M-RLP separation bounds and assign it to the cluster j' that corresponds to the domain $\mathcal{D}_{j'}$ where it belongs.

3.1.4 Complexity

We can analyze the worst-case runtime of a single iteration.

The update of the parameters of an hyperplane $\mathcal{H}_j$ with an ℓ_1-norm is performed by solving k linear programs with $O(m+n)$ variables and at most

$2m$ constraints.

The point reassignment step requires for each point to find the nearest hyperplane, comparing its approximation error $|(\mathbf{w}_j^T \mathbf{a}_i - \gamma_j) - y_i|$ (computed in $O(n)$ time) for each one of the k submodels. This yields an overall complexity of $O(mnk)$.

The RLP phase requires the solution of an LP problem (M-RLP) with $O(kn + m)$ variables and $O(k^2 m)$ constraints, and the reassignment of the misclassified points. The classification function requires the computation of the value $\mathbf{a}_i^T \mathbf{w}_j^c - \gamma_j^c$ for each j, an overall time of $O(kn)$. In the worst case all points may be misclassified, therefore the whole reassignment phase would have a complexity of $O(mkn)$. However, in most cases we expect this quantity to be significantly lower, as only a (hopefully small) fraction of the points is misclassified.

3.1.5 Multi-start

The 3-PAMF algorithm is very efficient in finding feasible solutions but, as a stand-alone method, performs poorly in terms of quality. Its results depend highly on the random initial assignment, and thus the solutions obtained in different runs of the algorithm can vary substantially. This behaviour is typical of similar iterative algorithms such as k-means and k-PC. On k-PAMF this is even more true, as the exact update combined with a larger amount of constraints may cause the algorithm to be stuck in local optima with a high probability.

Results can be significantly improved by using randomized variants of the algorithm, such as a multi-start technique. This feature is a global search that uses a local algorithm, such as our 3-PAMF procedure, starting from several initial solutions. It requires the execution of the algorithm for a finite

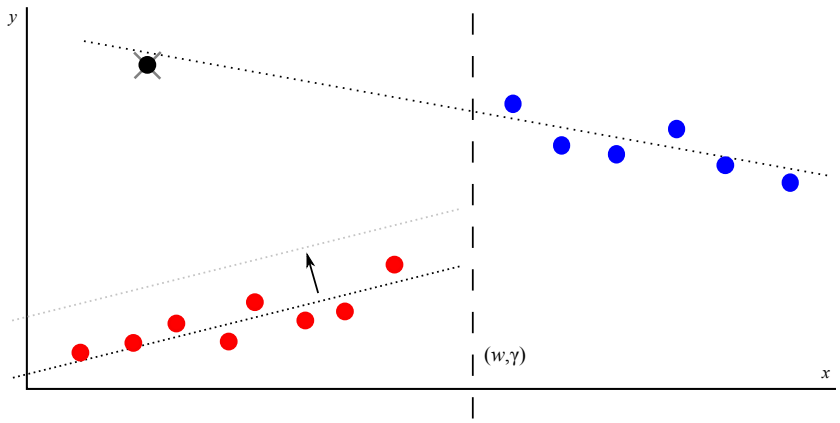


Figure 3.1: The black point cannot be assigned to the blue cluster with a linear classification on the x-axis. Hence RLP flags it as misclassified and it is reassigned to the red cluster. However, a parameter update for the red cluster that includes the black point would result in a model (light grey) which is clearly worse than what we have by leaving out the black point (outlier).

number (possibly large) of iterations. The best solution found over the i iterations is kept as the final solution.

3.1.6 3-PAMF Variants

Selective Parameter Update

We propose a variant of the algorithm in which the Parameter Update Phase for a submodel j is not performed using all data points assigned to it, but only with a *reliable* subset of them.

When the error resulting from the M-RLP optimization is not null, there are points which are misclassified according to the piecewise linear discriminating function. Given a set of vectors $\mathbf{a}_i$ assigned to a hyperplane $\mathcal{H}_j$, we store a list $\mathcal{S}$ of the points with $c(\mathbf{a}_i) \neq j$. The algorithm will then reassign those points to the class indicated by the classification function, in order to have a feasible solution with all points in the correct subdomain. One could

think that the points that were misclassified might not really be relevant with respect to the new submodel they have been reassigned to. Hence, in the next iteration, we update the parameters $(\gamma_j, \mathbf{w}_j)$ of the approximation hyperplanes skipping the vectors that are contained in $\mathcal{S}$, i.e., those that had been previously misclassified. An example of SPU is reported in Figure 3.1. We expect that, with this technique, the objective function will not necessarily decrease: leaving out some points might result in a bigger error on the data, since the update step does not take into account some points which are on the contrary considered when computing the objective value. However, we believe that the true accuracy of the obtained model will improve: the fitting hyperplanes are computed only on points which are supposed to be significant for that submodel. The model therefore will likely be closer to them, and further from the points which happen to be in the subdomain but do not truly belong to that linear model. In a way, we try to identify *outliers* in the data as the points misclassified by M-RLP.

2-Norm Parameter Update

k-PAMF is defined as an ℓ_1 minimization problem, and the update of the hyperplane parameters needs the solution of k linear programs (see Section 3.1.3).

Notice that, choosing to minimize the sum of the squared errors instead of the ℓ_1-norm, the Parameter Update problem results in a typical Least Squares minimization problem:

$$\min_{\bar{\mathbf{w}}_j} \|\bar{\mathbf{A}}_j \bar{\mathbf{w}}_j - \mathbf{y}_j\|_2^2. \tag{3.7}$$

that can be efficiently solved in closed form. Since the matrix $\bar{\mathbf{A}}_j$ might

be very ill-conditioned, due to the extreme proximity of the points in the dataset, using a robust linear regression method is required. The ℓ_2-norm update move is *not* exact for the k-PAMF problem we have defined, but an approximation: we solve a ℓ_2-norm LS problem in the context of an ℓ_1-norm minimization problem. Nevertheless, it could be reasonable to use such approximate update, if motivated by a greater computational efficiency and comparable solutions.

It is therefore possible to have a variant of 3-PAMF replacing the exact Parameter Update with an approximate one that involves the minimization of the ℓ_2-norm, and we expect it to be faster. It is important to stress that it is an approximation: even if the update is performed as a LS problem, the assignment phase is still performed minimizing the sum of the absolute values of the approximation errors and the objective function is computed using the ℓ_1-norm.

3.2 Adaptive Point-Reassignment Heuristic

We propose a refined heuristic for k-PAMF based on the reassignments of points that are considered most likely to be ill-assigned. The algorithm is called Adaptive Point-Reassignment Heuristic (APR for short). It is an iterative procedure and is inspired by the one described in [AC09], that works for k-HC.

At each iteration a parameter α determines the quantity of points to be reassigned following a given criterion. An RLP problem is solved to make sure that the assignments induce linearly-separable domains on $\mathcal{D}$.

Repeat until time limit is reached:

Parameter update

Update the hyperplane parameters $(\mathbf{w}_j, \gamma_j)$ for each $j \in [k]$ so that they minimize the approximation error on the assigned points.

Ill-assigned identification

For each $\mathcal{H}_j$ identify $\alpha \cdot m_j$ points likely to be ill-assigned.

Ill-assigned reassignment

Reassign each ill-assigned point to the closest hyperplane different from the currently assigned.

Global reassignment

Reassign all remaining points to the $\mathcal{H}_j$ with smaller distance $|(\mathbf{w}_j^T \mathbf{a}_i - \gamma_j) - y_i|$.

RLP classification

Perform RLP, partition $\mathcal{D}$ and reassign misclassified points.

The crucial feature of the algorithm is the decision of which and how many points have to be reassigned. We consider likely to be ill-assigned the points

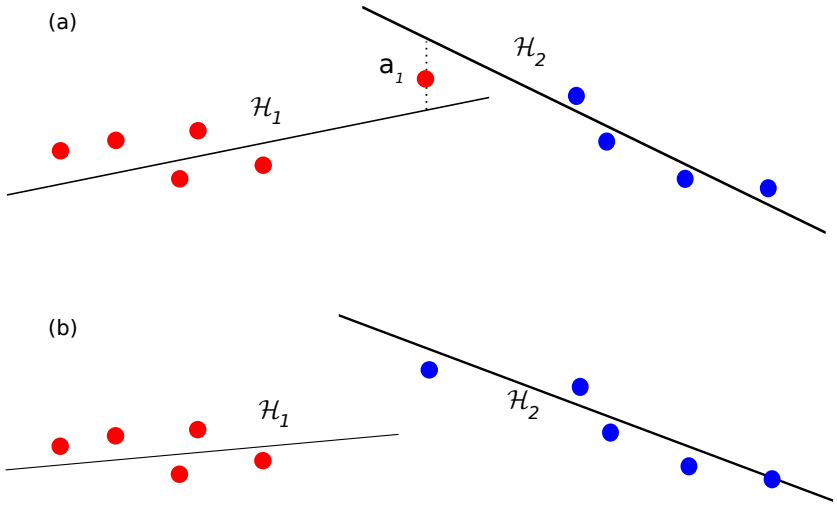


Figure 3.2: (a) The point $\mathbf{a}_1$, closer to $\mathcal{H}_1$, is likely to be ill-assigned since it has a high ratio d_{11}/d_{12} - the distance from the two hyperplanes is nearly the same. (b) The reassignment of $\mathbf{a}_1$ gives a solution with a better objective value (after the parameters have been updated).

that do not have a hyperplane which is *considerably* closer than all the others. In other words, we are interested in the ratio between the distance of a point to the current hyperplane and the shortest distance to the other hyperplanes:

$$r_{ij} = \frac{d_{ij}}{\min_{j' \neq j} d_{ij'}} \tag{3.8}$$

When this quantity is big, the likelihood of being ill-assigned is supposedly high. While in 3-PAMF each point is always assigned to its closest hyperplane, in APR a point may be reassigned even if its current hyperplane is actually the nearest.

3.2.1 PR-Local Search

The core of the algorithm follows the steps given in the outline, but some additional features are included as we attempt to avoid being stuck in local minima.

POINT-REASSIGNMENT LOCAL SEARCH(α_0, s_0)

$\mathcal{L} \leftarrow \varnothing$, $\mathcal{T} \leftarrow \varnothing$
$\alpha_t \leftarrow \alpha_0$
repeat
    $\alpha_t \leftarrow \alpha_t \rho$
    foreach $\mathcal{H}_j$
        update the parameters $\mathbf{w}_j$,γ_j
    foreach $\mathcal{H}_j$
        add to $\mathcal{L}$ the first $\alpha_t \cdot m_j$ points assigned to $\mathcal{H}_j$ with larger d_{ij}
    foreach $\mathbf{a}_i \in \mathcal{L}$
        reassign $\mathbf{a}_i$ from the current $\mathcal{H}_j$ to $\mathcal{H}_{j'}$ with $j' = \arg\min d_{ij}$
        such that $j \neq j'$ and $((i, j') \notin \mathcal{T}$ or $d_{ij'} < d^T_{ij'})$
        if $d_{ij} < d_{ij'}$
            add (i, j) to $\mathcal{T}$
    foreach $\mathbf{a}_i \in \mathcal{A} \backslash L$
        Assign $\mathbf{a}_i$ to $\mathcal{H}_{j'}$ with $j' = \arg\min d_{ij}$
    perform RLP and build list of misclassified points $\mathcal{M}$
    foreach $\mathbf{a}_i \in \mathcal{M}$
        assign $\mathbf{a}_i$ to $\mathcal{H}_{j'}$ with $j' = c(\mathbf{a}_i)$
    $v \leftarrow$ current solution objective value
    if $v < v_{min}$
        $v_{min} \leftarrow v$
        store current solution $\mathbf{s}_t$
    foreach $v_{old} \in \mathcal{O}$
        if $v_{old} = v$
            $i \leftarrow i + 1$
    add v to $\mathcal{O}$
until ($\alpha_t = 0$ **and** no change occurs) **or** ($i > \zeta$)
return v_{min}

The parameter $\alpha_0 \in (0, 1)$ is passed to the procedure from the outside. The algorithm starts from a feasible solution s_0.

Once in the loop, at each iteration a set of moves is performed to find a *neighbour* solution which improves the current. The parameter α_t is progressively reduced: at each iteration the parameter is multiplied by a factor $\rho \in (0, 1)$ that drives it towards 0, so that the search process is stabilized. Indeed, when α_t reaches 0 we fall in the previous case of 3-PAMF, and after some iterations the procedure will converge to a local minimum.

The Parameter Update phase has to be performed as explained for 3-PAMF, hence we have to solve k linear programs to minimize the ℓ_1-norm of the errors for each hyperplane.

The list $\mathcal{L}$ contains the points that are likely to be ill-assigned. $\mathcal{L}$ is built going through each submodel $\mathcal{H}_j$ and ranking its point according to the ratio $\frac{d_{ij}}{\min_{j' \neq j} d_{ij'}}$. This could in principles be replaced by other kinds of criteria which give insight on the reliability of the assignments. Once we have sorted the points assigned to the hyperplane $\mathcal{H}_j$, only a fraction of them is included in $\mathcal{L}$ (the first $\alpha_t \cdot m_j$). When $\mathcal{L}$ has been constructed, each point in it is reassigned to a hyperplane that has to be different from the one they are currently assigned to. The new submodel must have minimal distance $d_{ij'}$ among the hyperplanes with $j \neq j'$.

A Tabu List $\mathcal{T}$ of finite length l is introduced in order to avoid cycling in the reassignment phase. This feature does not allow the reassignment of a point $\mathbf{a}_i$ from $\mathcal{H}_j$ to $\mathcal{H}_{j'}$ if the same assignment (i, j') has occurred in the previous l iterations, therefore is in $\mathcal{T}$, unless the current distance d_{ij} is smaller that d_{ij}^T, i.e., the value when the pair was added to $\mathcal{T}$.

All remaining points are reassigned in the regular way, that is only if there is an $\mathcal{H}_{j'}$ which is a better fit than the current j.

Finally an M-RLP program is solved: given the classification function $c(\cdot)$ resulting from the optimization we correct the misclassification errors, if any, and reassign the points according to the discrimination bounds. This works in exactly the same way as the error removal phase in 3-PAMF.

At each iteration the solution $\mathbf{s}_t$ is stored if it improves the best solution found. Once we have reached a local optimum, this is to say that the pa-

rameter α_t has reached 0 and the current solution is stable, i.e., all points are assigned to their closest $\mathcal{H}_j$, the procedure halts. Moreover, even with $\alpha_t > 0$, the search stops if the current objective value v has already been found a maximum number of times ζ in the previous p iterations. This is done with a finite list $\mathcal{O}$ of length p that contains the old objective values. If the index i has reached ζ solutions with identical values, we stop the search as we consider the randomization unable to move the algorithm out of a local minimum.

3.2.2 Adaptive Metaheuristic

A single run of the above procedure, although we expect it to be an improvement over a single 3-PAMF thanks to its additional features, may still give very variable results starting from different initial points and be easily trapped in a local minimum. Even in this case, we embed the local search in a randomized framework, a metaheuristic that adjusts adaptively the value of the control parameter α_t and, once in a while, restarts the search from scratch generating a random solution.

ADAPTIVE P-R METAHEURISTIC

$\alpha_0 \leftarrow \eta$, $r \leftarrow 0$, $s_b \leftarrow s_0$
repeat
  if $r > \xi$ *//restart*
    Generate a new random solution s_0
    $\alpha_0 \leftarrow \eta$, $r \leftarrow 0$, $s_b \leftarrow s_0$, $\xi \leftarrow 0$
  $\mathbf{s}_b \leftarrow$ POINT-REASSIGNMENT LOCAL SEARCH(α_0, s_b)
  if $\mathbf{s}_b$ improves $\tilde{\mathbf{s}}$
    $\tilde{\mathbf{s}} \leftarrow \mathbf{s}_b$
    $\alpha_0 \leftarrow \beta$
    $r \leftarrow 0$
  else
    $\alpha_0 \leftarrow \min\{\eta, \alpha_0\nu\}$
    $r \leftarrow r + 1$
until time limit is reached

The update of α_0 depends on the value found by the local search. If the new solution is better than the current best, α_0 is set to an initial value β. If the objective value is not lower, then α_0 is set to a higher value $\min\{\eta, \alpha_0\nu\}$, where η is an upper bound on the value of the parameter, usually 1. The idea is refining a good solution when α is small and driven to zero by the parameter ρ in the local search. Viceversa, a large α_0 introduces a large amount of variability, that is what we want when the solution appears to be far from optimal. The occasional random restart is made necessary by the fact that the parameter α_t, even with large values, is not always enough to guarantee sufficient diversification. A restart takes place after a number ξ of non-improving solutions obtained by the local search.

3.2.3 APR Variant

The considerations made for the variants of 3-PAMF are valid for the Adaptive-Point Reassignment heuristic. The core of the algorithm is similar to 3-PAMF, therefore even in APR we can choose to replace the ℓ_1-norm Parameter Update with an approximate ℓ_2 version. We expect the approximate ℓ_2-norm update to be faster but generally less effective in finding good solutions.

Chapter 4

Computational results

In the first section we describe the generation of instances for the problem of k-PAMF. We then discuss the implementation of the proposed exact and heuristic methods. For each approach we show computational experiments on artificially generated and real-world instances.

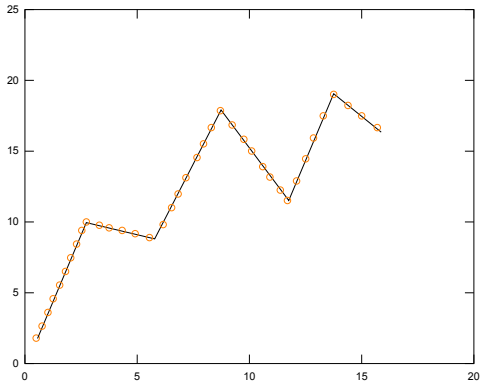
4.1 Instances

The instances that we have generated in order to test the effectiveness of our approaches are of three different kinds: *wave*, *semi-random* and *noncontinuous regression*. The generation process was implemented in C++ and iterated with a Python script.

4.1.1 Wave

Instances of the type *wave* contain points which are spread on piecewise linear continuous functions on $\mathbb{R}^2$ with no noise. The optimal objective value for these instances is 0, as a piecewise linear model should be able to fit perfectly the data. These instances have the advantage that they can be easily visualized and we immediate know, looking at the objective value of an optimization, whether the optimum has been reached – that being 0. *Wave* instances are constructed from a progressively increasing x-value and an associated y-value which grows according to a fixed slope. We start with

$t = 0$ and a random w. When a number $\lceil m/k \rceil$ of points has been generated, the value w is changed to $rand(0, 1)(-1)^t$ and t is incremented.



(a)

Figure 4.1: Example of a *wave* instance.

4.1.2 Semi-random

The second type of test sets, *semi-random* (*s-r* for short), is made of points that are generated with a given variability over random hyperplanes. The hyperplanes can intersect, so in some cases a piecewise linear function might fit badly the data. *Semi-random* instances are built by generating k random hyperplanes. Then, a number m of point is generated on the domain $\mathcal{D}$. Each of them is assigned to a random $\mathcal{H}_j$, and their y_i value is computed according to the hyperplane j with an additional Gaussian noise ε with zero mean and a given variance.

4.1.3 Noncontinuous regression

The instances of type *noncontinuous regression* (*nc-r*) contain sets of points that have been built explicitly from noncontinuous piecewise linear models in $\mathbb{R}^n$. The data are perturbed with Gaussian noise. To build an instance we first generate k distinct points that we call *centroids*. Such points are the representative of k subdomains of $\mathcal{D}$, and are obviously piecewise-linearly separable: the definition regions are computed with a modified M-RLP for-

mulation which looks for a maximal margin separation between the k centroids. Once we have a partition of $\mathcal{D}$ in k subdomains, we assign a random hyperplane to each of them. The algorithm then generates a large number of random points in $\mathcal{D}$, and for each of them computes the observed values y_i using the corresponding linear submodel. The procedure stops when a total number of m points has been generated. Even in this case an additional Gaussian noise is added to the y-value, and, in addition, the algorithm optionally adds a fraction of misclassified points. One thing to notice is that we do not fix the number of points belonging to the submodels, so that a cluster could be much more populated than another, although we do not accept instances with empty submodels.

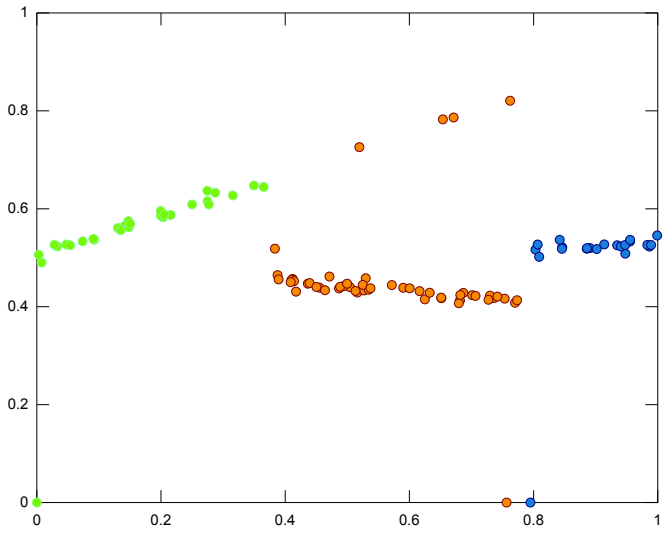


Figure 4.2: A *nc-r* dataset.

4.2 Exact formulations

We describe the implementation and the computational results for the exact methods we have proposed.

4.2.1 Implementation of symmetry breaking techniques

The Extended Formulation for the partitioning orbitope and the MZ symmetry breaking inequalities can be added to a formulation that includes partitioning constraints in a straightforward way.

On the other hand, the exponentially many SCIs cannot be added directly to the model, and require the solution of a separation algorithm for the generation of violated cuts. In order to be effective the algorithm needs a Branch and Cut framework that supports it, as we need to solve the separation problem for every node of the branching tree. The construction of the model and the separation algorithm were implemented in C++ and embedded in CPLEX/Concert: at each node, within a `Cut Callback` we produce and add to the global cut pool only the Shifted Column Inequalities that are violated by the current solution $\mathbf{x}^*$. CPLEX treats the cuts as *lazy constraints*, that are constraints not specified in the constraint matrix of the MIP problem, but that must be not be violated in a final solution.

4.2.2 Symmetry detection in CPLEX

ILOG-CPLEX offers some symmetry breaking features that are automatically executed by the solver. The parameter `IloCPLEX::Symmetry` allows the user to choose the amount of effort put during the preprocessing phase to reduce symmetry in the MIP model. By default, CPLEX attempts to find the best setting for the problem it is evaluating. However, it seems that in our case the solver is not always able to automatically detect symmetry. In fact, even if we explicitly turn off the symmetry reduction by setting the parameter to 0, CPLEX often does not show any change in the solution process: the runs appear to be identical, and the number of iterations and nodes generated in the search tree is the same.

We have therefore attempted to manually raise the parameter to the highest level, which is 5, that corresponds to the most aggressive symmetry-breaking reductions. It is not clear if it is *always* useful to force the most aggressive strategy for symmetry-reduction. However, for the comparisons that follow, we set `IloCPLEX::Symmetry` to the maximum value. In fact we have noticed that the most aggressive CPLEX symmetry-breaking reduction usually appears to be greatly effective in reducing the solution time especially on large instances, and we would like to compare the techniques that we have introduced with the best possible performance offered by CPLEX.

It should be noticed that CPLEX symmetry reduction is automatically turned off by the solver when using Cut Callbacks.

4.2.3 Choice of big-M

CPLEX has an internal integrality tolerance `EpsInt` which is chosen by CPLEX depending on the problem. In our case, the default tolerance is 10^{-5}, which requires a rather large value of M in order to have correct results and avoid inconsistencies caused by rounding errors. For example, if a constant M such as 10^5 has to be multiplied by a variable that is considered to be 0, due to the integrality tolerance the variable may in fact have a value in $\pm 10^{-5}$. The result of the product could be potentially influential – while it should be 0 instead. Indeed, for high value of M we have experienced numerical issues and inconsistent or suboptimal results.

The best results were obtained by setting $M = 1000$ and raising the integrality tolerance to 10^{-8}. The drawback of setting a smaller integrality tolerance is that CPLEX generally requires more time in reaching the optimum.

4.2.4 Remarks about notation

The *basic* exact formulation for k-PALM used in the experiments is the one described in Equation (2.32). When this formulation is solved by default CPLEX techniques with the most aggressive symmetry-breaking parameter (`IloCPLEX::Symmetry`=5) we use the notation `CPLEX`.

The formulation can be amended by symmetry-breaking constraints or reformulated without big-M as described in Chapter 2. In case of MZ inequalities, the notation `MZ` is used. When violated cuts are added by the SCI separation algorithm we use the notation `SCI`. The Extended Formulation is identified by `Ext`. In Table 4.1 we summarize the settings for the different methods and the notation that is used in the tables. The cuts that are

	Formulation	Cutting Planes	CPLEX `Symmetry`
`CPLEX`	Basic [Eq. (2.32)]	Cplex Cuts	Max (5)
`MZ`	Basic + MZ ineq.	Cplex Cuts	Default (-1)
`SCI`	Basic	Cplex Cuts + SCI	Disabled (0)
`Ext`	Extended	Cplex Cuts	Default (-1)

Table 4.1: Summary of the settings for the exact methods.

by default added by CPLEX in k-PAMF instances typically are Gomory or Mixed Integer Rounding cuts.

4.2.5 Exact formulations on *wave* instances

On *wave* instances the exact formulation of k-PAMF can be solved with all the exact methods. MZ symmetry breaking inequalities do not give particularly brilliant results: the technique is able on average to beat CPLEX with the standard k-PAMF formulation (indicated by CPLEX in tables), but it achieves a lower runtime only 5 times over 15.

On the other hand the approach with Shifted Column Inequalities manages to achieve the minimum much faster: on larger instances the SCI method reaches the optimum in as low as 5% of the time needed by the standard technique (instance with m=85).

Even the Extended Formulation proves to be effective, although to a minor extent. On smaller instances the basic formulation (`CPLEX`) and the Extendend Formulation (`Ext`) still have an edge over `SCI`, probably suggesting that the cuts are effective mostly if the search tree is not too small.

m	Time to opt (s) CPLEX	MZ	SCI	Ext	Nodes generated CPLEX	MZ	SCI
25	0.87	0.87	1.22	0.37	210	328	688
30	0.52	1.71	1.13	0.79	211	628	653
35	1.26	5.46	1.9	1.77	192	1872	904
40	0.92	1.37	1.61	2.45	216	194	605
45	8	5.08	1.19	5.38	579	913	324
50	1.54	2.81	5.05	8.51	471	403	873
55	8.09	3.63	1.87	3.19	753	366	376
60	2.6	10.27	4.61	6.72	557	3340	592
65	13.39	29.48	2.61	2.07	671	8458	601
70	12.81	2.29	1.97	11.27	813	220	146
75	17.59	56.42	2.86	12.26	879	14291	486
80	14.01	19.52	4.84	21.95	1910	2702	1272
85	255.38	136.26	14.83	75.16	7930	43446	3858
90	26.45	121.08	11.07	13.85	732	18585	2300
95	123.4	23.53	6.77	38.87	2355	2594	1010

Table 4.2: Comparison of the exact methods on *wave* instances ($n = 2$ and $k = 3$).

4.2.6 Exact formulations on *semi-random* instances

On *semi-random* instances we have performed experiments with higher dimensions and number of submodels. We expect that raising n will make the exact formulation substantially harder. Increasing k even more so, since it goes directly to increase the number of binary variables, that are $m \times k$. On large instances indeed an optimal solution could not be obtained.

When the chosen number k of submodels grows the problem indeed proves very hard. What can be observed from the results (Table 4.3) is, again, the good efficiency displayed by `SCI` and the Extended formulation: both approaches outperform `CPLEX` on all instances. The nodes generated by `SCI` are often not fewer than those visited by `CPLEX`, nevertheless, the runtime is typically smaller.

			Time (s)			Nodes generated	
m	n	k	CPLEX	SCI	Ext	CPLEX	SCI
20	2	2	0.47	0.29	0.23	408	203
20	2	3	9.68	5.38	7.69	2728	4474
20	2	5	315.5	425.67	142.34	160979	132198
20	3	2	1.8	1.24	0.65	1713	541
20	3	3	58.8	53.06	159.43	19799	46141
20	5	2	12.62	3.62	6.73	6730	2854
20	5	3	1717.27	842.86	2580	340242	583846
20	5	5	1.41	0.98	4.4	237	50
30	2	2	2.13	0.65	0.67	887	306
30	2	3	146.85	22.61	48.78	32061	15635
30	3	2	7.2	4.22	4.64	6513	2693
30	3	3	1010.19	425.86	1360.9	130079	250362
30	5	2	217.36	31.81	114.34	49026	24509
40	2	2	2.24	1.28	3.36	1479	969
40	2	3	157.98	68.7	38.86	92274	26462
40	3	2	49.54	6.05	13.03	9185	4185
40	3	3	9872.2	3435.12	2338.68	732085	1541586
40	5	2	1789.74	146.46	1214.95	201023	120523

Table 4.3: Time to optimum on *semi-random* instances for the exact methods.

4.2.7 Exact formulations on *nc-r* instances

Also on *noncontinuous regression* instances the symmetry-breaking methods that we propose appear to be effective in speeding up considerably the solution process. However in one case ($m = 100$) `CPLEX` finds the minimum in a fraction of the time required by `SCI` and `Ext`. On the biggest instance the improvement given by the Extended Formulation is drastic: it requires a runtime of less than an hour, while the basic formulation requires 7 hours (6 hours with SCIs).

Notice that using CPLEX with no symmetry-breaking we experienced much larger runtimes on all instances, and we do not include them here.

It is surprising that the Extended Formulation in more than one case is more efficient than SCIs, while we would typically expect the cutting planes technique to perform better.

m	Optimal value	Time (s) CPLEX	Time (s) SCI	Time (s) Ext	Nodes CPLEX	Nodes SCI	Nodes Ext
20	0.2510	0.39	0.85	0.98	402	948	1386
30	0.8356	5.02	6	3.92	3567	6667	4103
40	1.2727	28.82	24.25	26.56	21865	23851	27120
50	1.9706	185.01	96.71	33.72	23000	77213	25110
60	2.0129	185.63	190.38	144.19	24042	99447	63745
70	2.2537	1225.67	528.03	1119.14	132255	225588	250794
80	3.62043	2124.15	2083.79	2461.03	849052	5358054	479063
100	2.4895	1354.9	12090.6	5739.5	60602	2721730	714559
150	3.99114	26059.1	23148.3	3439.2	484712	2924244	1325152

Table 4.4: Time to optimum on *nc-r* ($n = 2$, $k = 3$) instances for the exact methods.

4.2.8 Implementation of CBC procedure

The iterative approach that is described in Section 2.3.2 is sufficient to find an exact optimal solution. However it is best used for decomposition and cut generation in a more general Branch and Cut context. Hopefully the B&C scheme will generate violated cuts not only when we have an integer solution of the master, but also at each node of the branching tree. Indeed practice has confirmed that, using CBC within ILOG-CPLEX, the solver is able to produce a number of other cuts, such as $\{0, \frac{1}{2}\}$ cuts.

The procedure has been implemented within Concert. The Master ILP problem is solved via B&C. At each integer solution in the search tree, an `Incumbent Callback` builds the Slave problem and verifies if it is infeasible. In that case, it rejects the solution and a `CutCallback` is called. The modified Slave dual problem is then used to find a number of violated cuts. The generation of cuts works as described in Section 2.3.3. The ability to produce several IIS efficiently is crucial when applied to the generation of CB cuts: for our purpose the proposed IIS search has proved to be more efficient than the default algorithm provided by CPLEX with the function `IloCPLEX::refineConflict()`.

The results have been positive in the sense that the approach succeeds in removing the need of the big-M coefficients. In fact, CBC even helped in the decision of the right value of big-M to use in the previous formulation:

since the optimality of CBC solutions is guaranteed, to have an *optimality check* on what has been found using big-M it is enough to compare the value with the optimum from CBC. It highlighted the fact that with M values lower than 1000 the MILP formulation sometimes fails in achieving the true minimum, stressing once again the difficulties in big-M formulations.

Computationally speaking, the runtime of the algorithm is unfortunately much larger than what we have using B&C with the classic big-M formulation (see Table 4.5). While in [CF06] and [BR09] two problems efficiently solved by means of CBC are reported, our experiments have showed that in k-PAMF Combinatorial Benders' Cuts alone do not appear to be sufficiently strong to guarantee a fast convergence. The approach is not competitive timewise with the big-M formulation, showing that in this case only *nogoods* constraints might not be enough.

4.2.9 Combining CBC and SCI

The CBC procedure appears to be relatively fast in finding good solutions, but it has troubles in certificating their optimality. It would be crucial to add other cuts that help the search process. On k-PAMF, we have showed that it can be done with symmetry-breaking constraints. We therefore combine the CBC mechanism with the SCI-cuts generation that we have previously discussed. Hence we generate optimality and feasibility Combinatorial Benders' Cuts whenever we have a feasible integer solution, while we add Shifted Column Inequalities at each B&C node.

The additional cuts seem to be effective, and they do help in speeding up the solution. Table 4.5 displays the results on a set of small-size instances that show how SCI cuts typically succeed in consistently reducing the runtime. However, although CBC have the major advantage of removing the need for big-M terms, on k-PAMF the algorithm is still not competitive with the big-M formulation, the runtimes still being around an order of magnitude larger.

The key in order to have a better performance for CBC would probably be the identification of other families of cuts that work well on the problem.

Dataset			Optimal	Time to opt (s)			
m	n	k	value	CBC	CBC-SCI	SCI	CPLEX
20	2	2	23.38	4.56	2.4	0.29	0.47
20	2	3	26.28	355.58	33.11	5.38	9.68
20	3	2	15.88	42.83	12.78	1.24	1.8
30	2	2	27.87	7.7	3.79	0.65	2.13
30	2	3	40.88	3387	347.45	22.61	146.85
30	3	2	25.38	431.35	51.9	4.22	7.2

Table 4.5: Comparing the time of CBC, CBC-SCI, SCI and CPLEX on small-size instances (s-r). CBC and CBC-SCI use the CBC decomposition method. CPLEX and SCI solve the big-M formulation.

4.3 Heuristics

4.3.1 Implementation

All variants of the heuristic algorithms described in this work have been implemented in C++ within an object-oriented framework. Most of the mathematical structures (vectors, matrices) and high-level operations (inner product, matrix-vector product, LS minimization) were provided by the Linear Algebra library LAPACK 2.5.3 accessed by the C++ wrapper LAPACK++. ILOG-CPLEX was called for the solution of the LP and MILP problems. The parameters used for APR in the experiments are: $\eta = 1, \rho = 0.6, \nu = 1/0.95$, $\zeta = 5$, $\xi = 10$.

4.3.2 3-PAMF vs classic approach

As we have described in Chapter 1, the novelty of the proposed approach is the fact that we attempt to partition and fit the discrete data and simultaneously partition the continuous domain.

In Table 4.6 we report the results on a number of instances where we compare the solutions of 3-PAMF with those obtained by a method which follows the classical two-phase approach for k-PAMF (as described in Section 1.1). It is an adaptation of k-PC where we just modify the objective function to suit the ℓ_1-norm of k-PAMF. At a later stage, we use an M-RLP phase to determine the definition domains of the submodels. We call this

algorithm kPC-RLP .

m	n	k	Best solution 3-PAMF	Best solution kPC-RLP	Diff (%)	Overall time (s) 3-PAMF	Overall time (s) kPC-RLP	Inner it. (avg) 3-PAMF	Inner it. (avg) kPC-RLP
20	2	3	**33.64**	34.27 (9.9)	1.8	3.82	7.184	2.73	5.05
20	2	5	**32.41**	32.66 (6.3)	0.7	4.25	7.628	2.45	4.82
20	3	2	15.88	15.88 (8.0)	0.0	4.03	3.478	2.89	3.19
20	3	3	**20.69**	31.15 (9.0)	33.6	3.92	6.34	2.27	4.36
20	3	5	**4.97**	19.28 (2.0)	74.2	5.58	6.662	2.89	3.98
20	5	2	**6.25**	7.64 (5.0)	18.3	4.27	3.764	2.98	3.44
20	5	3	**2.95**	6.26 (1.8)	52.8	5.83	4.88	3.22	3.42
20	5	5	**0.00027**	2.70 (0.0)	100.0	6.68	6.742	2.69	3.24
30	2	3	55.93	**51.91** (11.1)	-7.2	3.87	8.254	2.56	5.98
30	2	5	**56.60**	60.64 (11.6)	6.7	5.83	9.078	2.94	4.76
30	3	2	**25.39**	25.67 (18.2)	1.1	3.83	3.59	2.78	3.11
30	3	3	**46.76**	49.64 (12.7)	5.8	4.45	5.944	2.73	4.22
30	3	5	**48.36**	49.79 (3.8)	2.9	5.70	9.376	2.49	4.56
30	5	2	**31.92**	40.04 (24.7)	20.3	4.88	4.568	3.23	3.92
30	5	3	**20.45**	28.08 (5.9)	27.2	6.33	6.418	3.34	4.29
30	5	5	**2.30**	21.62 (1.7)	89.3	9.43	9.196	3.2	4.04
40	2	3	**59.74**	61.79 (21.3)	3.3	5.07	7.676	3.14	5.22
40	2	5	**73.60**	73.81 (15.9)	0.3	5.40	9.494	2.99	5.04
40	3	2	**57.65**	62.94 (41.5)	8.4	3.60	6.044	2.42	5.15
40	3	3	61.82	**61.02** (19.4)	-1.3	5.76	8.638	3.14	5.66
40	3	5	**38.79**	60.51 (9.3)	35.9	4.78	10.71	1.91	5.28
40	5	2	**47.44**	48.94 (21.0)	3.0	4.89	6.09	3.13	5.08
40	5	3	**32.91**	42.78 (13.6)	23.1	6.56	7.888	3.22	4.93
40	5	5	**48.38**	74.02 (7.1)	34.6	5.77	12.42	1.78	5.25

Table 4.6: Comparison of 3-PAMF and kPC-RLP on a *s-r* testbed

3-PAMF outperforms kPC-RLP on all instances but two. The improvement is relevant: the solutions found by 3-PAMF have an objective value which can be even an order of magnitude smaller than the ones found by kPC-RLP, and on average are more than 20% smaller. Somehow surprising, 3-PAMF also seems to be faster than BM-RLP: this can be explained observing the lower average number of iterations required to converge for a single run of 3-PAMF, that balance the higher number of LP problems to be solved w.r.t. to kPC-RLP. In 3-PAMF convergence is faster most likely due to the fact that, having more constraints, it falls more easily in local minima. In brackets we report also the objective value of the k-PC runs before

the second phase (the M-RLP phase): the values are very small compared to what is obtained after the classification phase, indicating that k-PC finds solutions that fit well the discrete data but are often not well suited to induce a domain partition.

4.3.3 Heuristics on *wave* instances

On *wave* instances the two heuristics 3-PAMF and APR are able to find the global optimum (that is 0) in most cases (Table 4.2). On 1 instance however both algorithms have troubles in identifying the true piecewise model, that presents two consecutive linear models which are almost coplanar. The time limit for APR and 3-PAMF on these instances is set to just 50 seconds.

Dataset			Time	Optimal	Best solution		Time to Best	
m	n	k	(s)	value	APR	3-PAMF	APR	3-PAMF
25	2	3	50	0	0.000	0.000	7.30	2.13
30	2	3	50	0	0.000	0.000	6.91	16.83
35	2	3	50	0	0.000	0.000	9.62	12.19
40	2	3	50	0	0.000	0.000	7.84	16.23
45	2	3	50	0	0.001	0.001	8.09	18.61
50	2	3	50	0	0.000	0.000	2.64	0.23
55	2	3	50	0	0.000	0.000	8.54	0.32
60	2	3	50	0	0.001	0.001	9.89	0.46
65	2	3	50	0	0.000	0.000	3.27	0.25
70	2	3	50	0	0.000	0.000	2.93	1.12
75	2	3	50	0	0.000	0.000	8.26	1.57
80	2	3	50	0	0.002	0.002	46.9	1.73
85	2	3	50	0	0.001	0.001	3.15	1.32
90	2	3	50	0	1.008	1.008	3.04	0.16
95	2	3	50	0	0.003	0.003	3.25	1.34

Table 4.7: Comparison of APR-ℓ_1 and 3-PAMF-ℓ_1 with a time limit of 50 seconds.

4.3.4 Heuristics on *semi-random* instances

Almost on all *semi-random* instances the solutions found by APR have an objective value that is better or equal to the best solution found by 3-PAMF, although in two cases 3-PAMF is able to achieve a slightly better optimum (Table 4.8). In Table 4.9 we report a comparison with the results obtained with exact formulations: on seven instances APR finds the true optimum. The gap between the best objective value of APR and the global minimum is always lower than 10% of the optimal value.

m	n	k	Best solution 3-PAMF	Best solution APR
30	2	2	27.87	**27.87**
30	2	3	50.95	**45.30**
30	2	5	51.85	**44.70**
30	3	2	**25.39**	**25.39**
30	3	3	40.04	**33.00**
30	3	5	38.74	**23.04**
30	5	2	**31.50**	**31.50**
30	5	3	**17.73**	18.22
30	5	5	**1.26**	1.65
40	2	2	**51.82**	**51.82**
40	2	3	57.00	**53.80**
40	2	5	67.79	**43.55**
40	3	2	**57.65**	**57.65**
40	3	3	45.87	**45.51**
40	3	5	31.84	**21.86**
40	5	2	44.26	**44.16**
40	5	3	28.85	**22.19**
40	5	5	17.32	**14.84**
500	2	2	34.70	**29.47**
500	2	3	68.63	**64.34**
500	2	5	62.65	**59.05**
750	2	2	51.83	**47.37**
750	2	3	103.55	**97.48**
750	2	5	97.58	**87.33**
1000	2	2	**72.60**	**72.60**
1000	2	3	138.65	**129.20**
1000	2	5	130.36	**124.83**
500	5	2	117.18	**113.28**
500	5	3	66.55	**61.03**
500	5	5	99.14	**88.92**
750	5	2	175.46	**174.60**
750	5	3	99.06	**93.45**
750	5	5	151.88	**143.82**
1000	5	2	237.45	**236.66**
1000	5	3	134.90	**124.68**
1000	5	5	208.72	**201.87**

Table 4.8: Objective values of the best solution obtained with the heuristics on *semi-random* instances. The time limit was set to 120 seconds for each instance.

Dataset			Exact formulations		3-PAMF			APR		
			Opt	Min time	Best	Gap	Time	Best	Gap	Time
m	n	k	Value	to opt	sol	(%)	to best	sol	(%)	to best
20	2	2	23.38	0.23	24.77	5.93	69.50	24.77	5.93	25.24
20	2	3	26.29	5.38	27.79	5.73	105.68	26.29	0.00*	6.39
20	2	5	16.30	142.34	29.81	82.83	83.88	17.82	9.31	4.97
20	3	2	15.88	0.65	15.88	0.00*	47.99	15.88	0.00*	0.04
20	3	3	16.79	53.06	17.59	4.79	107.77	18.47	10.04	93.46
20	5	2	5.87	3.62	6.25	6.42	2.57	6.25	6.42	1.85
20	5	5	0.00	0.10	0.00	0.00*	79.54	0.00	0.00*	34.36
30	2	2	27.87	0.65	27.87	0.00*	37.90	27.87	0.00*	96.22
30	2	3	40.88	22.50	50.95	24.63	20.06	45.30	10.82	9.61
30	3	2	25.39	4.22	25.39	0.00*	0.76	25.39	0.00*	10.94
30	3	3	30.19	425.90	40.04	32.63	95.84	33.00	9.31	20.10
30	5	2	31.36	31.80	31.50	0.43	20.89	31.50	0.43	21.89
40	2	2	51.82	1.30	51.82	0.00*	23.31	51.82	0.00*	27.28
40	2	3	50.51	38.90	57.00	12.83	34.21	53.80	6.50	19.46
40	3	2	57.65	6.10	57.65	0.00*	3.05	57.65	0.00*	6.63
40	3	3	41.98	2339.00	45.87	9.27	24.38	45.51	8.41	110.47
40	5	2	41.25	146.50	44.26	7.29	19.88	44.16	7.03	30.62

Table 4.9: Comparison of the optimal results on *s-r* with the best solutions found by the heuristics in 120 seconds. In seven cases (*) APR finds the global minimum.

4.3.5 Heuristics on *nc-r* instances

Small and large-size *nc-r* instances were solved with our heuristic algorithms. On small-size instances (Table 4.10) APR and 3-PAMF are executed with a time limit of 120 seconds, and in this time APR finds solutions which are within 10% gap of the optimum value in all but 1 case, where the gap is almost 20%. On medium-size instances (Table 4.11) the time limit for the two algorithms was set to 1000 seconds. APR has the better results, with substantially better solutions. The objective values obtained with APR compare favorably to the true minimum (or, in case where it was not found, to the best value attained by the exact formulation). Large-size instances (with time limits ranging from 20 minutes to 35) confirm again that APR appears to find better solutions than 3-PAMF (Table 4.12). Notice that on large-size instances the exact methods are unable to find solutions in a short

time improving those obtained with the heuristics. In Table 4.13 we report a comparison of the average gap of 3-PAMF and APR with respect to the true optimum, and the ratios between the time required by the heuristics and the time taken by the fastest exact method on each instance. APR has an average gap that is below 9%, and we believe this value could be further improved by raising the time limit. The time required by the heuristics to find the best solutions are on average 11% of the time for the best exact formulation.

		Exact formulations		3-PAMF			APR		
Dataset		Opt	Min time	Best	Gap	Time	Best	Gap	Time
m	k	Value	to opt	sol	(%)	to best	sol	(%)	to best
30	3	**0.84**	3.92	1.327	36.98	48.3	0.84	0.00	7.85
40	3	**1.27**	24.25	1.457	12.64	31.3	1.296	1.80	2.73
50	3	**1.97**	33.72	2.13	7.68	8.9	2.21	10.67	29.83
60	3	**2.01**	144.19	3.74	46.2	57.5	2.49	19.47	48.57
70	3	**2.25**	528.03	2.462	8.44	13.5	2.461	8.437	13.8
80	3	**3.62**	2084	4.236	14.53	29.2	3.95	8.30	16.60
90	3	**3.44**	5058.04	3.65	5.80	30.5	3.66	6.00	64.9

Table 4.10: Results on small *nc-r* instances ($n = 2$) by heuristic methods compared to the optimal solution. Time limit of 120 seconds.

		Exact formulations		3-PAMF			APR		
Dataset		Opt	Min time	Best	Gap	Time	Best	Gap	Time
m	k	Value	to opt	sol	(%)	to best	sol	(%)	to best
100	3	**2.49**	1355	3.00	17.13	156.15	2.85	12.52	332.09
150	3	**3.99**	3439	7.89	49.41	126.92	4.40	9.29	864.86
250	3	**6.69***	18622	8.57	21.97	319.99	7.65	12.57	703.52
500	3	-	-	15.72	-	540.51	14.99	-	339.2

Table 4.11: Results on medium *nc-r* instances ($n = 2$) by heuristic methods compared to the optimal solution. Time limit of 1000 seconds. The solution with (*) represents the best feasible solution obtained with the exact formulation but is not proved to be optimal.

Dataset			Time	Best solution		Diff	Time to Best	
m	n	k	Limit (s)	3-PAMF	APR	(%)	3-PAMF	APR
750	2	3	1200	29.23	23.80	18.57	891.8	1057.44
1000	2	3	1200	38.87	26.50	31.80	1148.4	483.17
2000	2	3	1200	164.46	114.45	30.41	8.1	275.76
5000	2	3	1800	192.73	190.21	1.30	476.0	1140.93
10000	5	5	2000	602.60	545.934	9.40	1674.3	1068.33

Table 4.12: Results on big *nc-r* instances by heuristics.

	Gap (%)		Ratio time to best / min time to opt	
m	3-PAMF	APR	3-PAMF	APR
30	36.984	0.000	12.321	2.003
40	12.641	1.800	1.291	0.069
50	7.682	10.670	0.264	0.885
60	46.210	19.476	0.399	0.337
70	8.444	8.438	0.026	0.026
80	14.533	8.304	0.014	0.008
90	5.804	6.003	0.006	0.013
100	17.133	12.518	0.115	0.245
150	49.406	9.290	0.037	0.251
250	21.967	12.572	0.017	0.043
Average:	22.080	8.907	0.110	0.111

Table 4.13: In the first columns, a comparison of the gaps between the objective values found by the heuristics and the true optimum. In the rightmost columns, the ratio between the time required to obtain the best solution with the heuristics and the time required by the fastest exact method on each instance.

4.4 Comparison of heuristic variants

As we have mentioned discussing the heuristic algorithms, a number of variants of the original method have been proposed. We report the tests obtained with the variants.

4.4.1 3-PAMF variants

Selective Parameter Update

With Selective Parameter Update (section 3.1.6) we do not expect the objective value to decrease, but we believe that the estimated model will be more accurate. In other words, not accounting for outliers when we update the hyperplane parameters, we expect the piecewise to approximate better the real function. We perform an experiment on *nc-r* instances with 5% of misclassified points, hence non linearly-separable classes.

	Objective value	
m	3-PAMF	3-PAMF-SPU
40	1.332	1.3448
50	2.20757	2.21235
60	3.19725	2.52758
70	2.01934	2.02339
80	3.10233	3.16652
90	4.44525	2.19392
100	2.38837	2.39205

Table 4.14: Results obtained by 3-PAMF and 3-PAMF-SPU on a set of artificial *nc-r* instances with $n = 2$, $k = 3$ and 100 runs of Multistart.

We can observe that typically the objective value of 3-PAMF-SPU is slightly higher, meaning that it fits worse the data in the set, although in two cases SPU obtains in fact a substantial better solutions. Let us now consider the sum of the Euclidean distances between the vectors $[\hat{\mathbf{w}}_j^T, \hat{\gamma}_j]$ computed by the algorithm and the actual parameters $[\mathbf{w}_j^T, \gamma_j]$ used in the data generation process, where by Euclidean distance we mean the square root of the sum of the squared differences.

m	3-PAMF	3-PAMF-SPU	Diff (%)
40	0.655	0.652	0.33
50	0.717	0.715	0.37
60	1.51	0.18	87.90
70	0.708	0.707	0.06
80	0.58	0.51	11.93
90	0.32	0.08	74.53
100	0.048	0.045	5.11

Table 4.15: Sum of the Euclidean distances between the *estimated* hyperplanes parameters and the *true* parameters.

Although the overall objective value on the data points can be worse with SPU, on these instances 3-PAMF-SPU always gives predictions that are closer to the actual value of the parameters used to generate the data. In conclusion, it appears to be able to better approximate the real parameters.

2-norm Parameter Update

In 3-PAMF it is possible to replace the exact ℓ_1-norm Parameter Update with the approximate ℓ_2-norm Update. We expect to have a faster method with the latter - we call the modified algorithm 3-PAMF-ℓ_2, while we indicate the method with the exact move as 3-PAMF-ℓ_1.

A first example is given by the following test on a real-world instance. We consider the UCI dataset BCW [UCI], that contains 699 vectors with dimension $n = 9$. We want to approximate a piecewise *constant* function whose output value can assume only the value 2 or 4. On such a simple function it is straight forward to be convinced about the advantage given by the exact ℓ_1-update over an approximation of it.

Algorithm	Best Value	3-PAMF it.(avg)	Meta-it.
3-PAMF-ℓ_2	96.43	3.8	10
3-PAMF-ℓ_1	40	3.4	10

The result given by the 3-PAMF-ℓ_2 is much worse than what is found

by 3-PAMF-ℓ_1. Another impressive difference is found in the parameters of approximation function which is computed by the two algorithms:

	$w_{1,1}$	$w_{1,2}$	$w_{1,3}$	$w_{1,4}$	$w_{1,5}$	$w_{1,6}$	$w_{1,7}$	$w_{1,8}$	$w_{1,9}$	γ_1
True	0	0	0	0	0	0	0	0	0	-4
3-PAMF-ℓ_2	0.02	0.01	0.01	0.01	-0.01	0.02	0.02	0.002	0.01	-3.36
3-PAMF-ℓ_1	0	0	0	0	0	0	0	0	0	-4
	$w_{2,1}$	$w_{2,2}$	$w_{2,3}$	$w_{2,4}$	$w_{2,5}$	$w_{2,6}$	$w_{2,7}$	$w_{2,8}$	$w_{2,9}$	γ_2
True	0	0	0	0	0	0	0	0	0	-2
3-PAMF-ℓ_2	0.003	0.07	0.03	0.07	-0.01	0.07	0.01	0.06	0.01	-1.64
3-PAMF-ℓ_1	0	0	0	0	0	0	0	0	0	-2

3-PAMF-ℓ_1 manages to find the *true* value of $(\mathbf{w}_j, \gamma_j)$, while the 2-norm parameter update is much less accurate.

A more extensive set of tests on artificially generated dataset follows. On the same amount of multistart iterations the results confirm the superiority of the ℓ_1 update (Table 4.16). On the other hand, comparing the results on a test where the *runtime* is fixed (Table 4.17) we can observe that the larger number of iterations carried out by 3-PAMF-ℓ_2 balances the drawback of the approximate update, giving solutions which are not far from those of the original version, although still worse on average.

The tests that we have run indicate that the approximate ℓ_2-norm Parameter Update is indeed faster, in spite of a generally worse quality of the solutions.

m	n	k	MS	Best sol 3-PAMF-ℓ_1	Best sol 3-PAMF-ℓ_2	Diff (%)	Overall time (s) 3-PAMF-ℓ_1	Overall time (s) 3-PAMF-ℓ_2
20	2	2	100	**26.65**	27.61	3.5	3.256	1.408
20	2	3	100	**33.64**	34.67	3.0	3.82	1.60
20	2	5	100	**32.41**	34.50	6.0	4.25	1.47
20	3	2	100	**15.88**	17.66	10.1	4.03	1.41
20	3	3	100	**20.69**	20.98	1.4	3.92	1.44
20	3	5	100	**4.97**	10.78	53.9	5.58	1.62
20	5	2	100	**6.25**	8.59	27.3	4.27	1.56
20	5	3	100	2.95	**2.71**	-8.2	5.83	1.74
20	5	5	100	0.00	0.00	0.0	6.68	1.84
30	2	2	100	**28.52**	31.50	9.4	3.44	1.32
30	2	3	100	55.93	**55.75**	-0.3	3.87	1.35
30	2	5	100	56.60	**53.38**	-5.7	5.83	1.64
30	3	2	100	**25.39**	28.53	11.0	3.83	1.31
30	3	3	100	**46.76**	50.18	6.8	4.45	1.56
30	3	5	100	**48.36**	49.75	2.8	5.70	1.85
30	5	2	100	**31.92**	34.71	8.0	4.88	2.09
30	5	3	100	**20.45**	29.65	31.0	6.33	1.84
30	5	5	100	**2.30**	4.06	43.2	9.43	2.65
40	2	2	100	**57.93**	60.94	4.9	3.15	1.40
40	2	3	100	**59.74**	63.57	6.0	5.07	1.86
40	2	5	100	**73.60**	74.19	0.8	5.40	2.44
40	3	2	100	**57.65**	59.49	3.1	3.60	1.72
40	3	3	100	61.82	**59.93**	-3.0	5.76	2.09
40	3	5	100	**38.79**	43.82	11.5	4.78	2.07
40	5	2	100	**47.44**	51.35	7.6	4.89	1.85
40	5	3	100	**32.91**	39.83	17.4	6.56	2.44
40	5	5	100	**48.38**	62.59	22.7	5.77	2.15

Table 4.16: Comparison of 3-PAMF-ℓ_1 and 3-PAMF-ℓ_2 with the same number of multistarts.

Dataset			Time	Best solution		Diff	MS It.	
m	n	k	Limit (s)	3-PAMF-ℓ_1	3-PAMF-ℓ_2	(%)	3-PAMF-ℓ_1	3-PAMF-ℓ_2
20	2	2	10	**26.65**	27.61	3.6	123	200
20	2	3	10	33.64	**33.57**	-0.2	112	182
20	2	5	10	**32.41**	34.50	6.0	97	193
20	3	2	10	**15.88**	17.66	10.1	99	197
20	3	3	10	**20.69**	20.92	1.1	110	217
20	3	5	10	**4.97**	5.99	17.0	76	250
20	5	2	10	**6.25**	7.27	14.0	99	308
20	5	3	10	2.95	**2.71**	-8.2	81	308
20	5	5	10	0.0003	0.0003	9.9	73	340
30	2	2	10	**28.52**	31.50	9.4	139	419
30	2	3	10	55.75	55.75	0.0	147	426
30	2	5	10	56.60	**53.38**	-5.7	102	261
30	3	2	10	**25.39**	28.53	11.0	115	317
30	3	3	10	46.76	**45.01**	-3.8	92	246
30	3	5	10	**48.36**	48.84	1.0	80	218
30	5	2	10	**31.92**	34.71	8.0	81	209
30	5	3	10	**25.43**	26.15	2.7	66	188
30	5	5	10	**2.30**	5.37	57.1	45	161
40	2	2	10	**52.64**	54.25	3.0	126	289
40	2	3	10	**59.74**	63.57	6.0	82	200
40	2	5	10	**73.60**	73.96	0.5	78	173
40	3	2	10	**57.65**	59.49	3.1	111	242
40	3	3	10	61.82	**55.42**	-10.3	59	191
40	3	5	10	**38.79**	43.25	10.3	96	239
40	5	2	10	**47.44**	51.09	7.1	115	212
40	5	3	10	34.44	**32.98**	-4.2	87	163
40	5	5	10	**48.38**	49.51	2.3	106	225

Table 4.17: Comparison of 3-PAMF-ℓ_1 and 3-PAMF-ℓ_2 with the same time limit.

4.4.2 APR Variants

In Table 4.18 we report an example of results obtained by the two variants of APR on small instances with a time limit of 10 seconds each. The ℓ_2-norm update is faster, and therefore the algorithm manages to complete a higher number of iterations in the given timespan - in fact always more than twice the iterations of APR-ℓ_1. Nevertheless, the solutions are often worse than those of the algorithm with exact ℓ_1-update.

			Best solution		Overall iterations	
m	n	k	APR-ℓ_1	APR-ℓ_2	APR-ℓ_1	APR-ℓ_2
20	2	2	**24.77**	25.54	776	1844
20	2	3	**26.29**	28.86	703	1707
20	2	5	17.82	**15.71**	640	1483
20	3	2	**15.88**	17.66	667	1813
20	3	3	**17.74**	20.27	555	1656
20	3	5	**2.21**	2.34	453	1481
20	5	2	**6.27**	8.44	654	1771
20	5	3	3.43	**2.51**	518	1628
20	5	5	0.00	0.00	358	1411
30	2	2	**28.52**	32.93	700	1737
30	2	3	**46.12**	49.87	704	1555
30	2	5	**44.70**	48.07	538	1301
30	3	2	**25.67**	28.78	678	1712
30	3	3	**33.00**	46.68	611	1515
30	3	5	**30.70**	36.48	470	1229
30	5	2	**32.36**	34.61	625	1648
30	5	3	**18.22**	22.50	477	1461
30	5	5	2.28	**1.44**	306	975
40	2	2	**51.82**	54.25	740	1638
40	2	3	**58.48**	62.27	592	1517
40	2	5	**48.85**	49.50	488	1019
40	3	2	**57.65**	59.49	634	1605
40	3	3	**45.87**	68.51	618	1390
40	3	5	30.16	**27.83**	374	807
40	5	2	**45.75**	47.76	615	1551
40	5	3	**22.1874**	33.02	484	1310
40	5	5	**14.84**	21.30	299	785

Table 4.18: Comparison of APR-ℓ_1 and APR-ℓ_2 on a 10 seconds run on *s-r*.

4.5 UCI Machine Learning Instances

We report the results on two real-world instances freely available at the UCI Machine Learning Repository [UCI].

4.5.1 WPBC

The Wisconsin Prognostic Breast Cancer or *wpbc* is a dataset that contains real medical data. Each of the 198 vectors in $\mathbb{R}^{32}$ represents follow-up data for one breast cancer patient. The first 30 features are computed from a digitized image of a fine needle aspirate (FNA) of a breast mass. They describe characteristics of the cell nuclei present in the image, e.g. their radius, perimeter, area, symmetry. The dataset has been used for classification or prediction. In the second case, that is what we are interested in, the aim is predicting the Time To Recur. Originally the prediction has been performed by Mangasarian using Recurrence Surface Approximation, that is an *ad-hoc* linear programming model which predicts the values in the dataset with an estimated mean error of 16.5 months [BM94]. Our best result with $k = 2$ and APR is an average error, on both recurrent and non-recurrent cases, of 16.78 months. Using an exact method, with the extended formulation, we are able to find a feasible solution in short time (< 50 seconds) that gives an error of of less than 16 months, while if we continue the optimization with a time limit of 2 hours the algorithm yields a solution with an average error of 14.6 months.

4.5.2 Machine-CPU

The *machine* instance [UCI] contains data describing the CPU performance (an integer value) of 209 machines. The value is defined in terms of 9 attributes, such as cycle time, maximum main memory, cache memory. While all other features are integer valued, the first feature is *categorical*, i.e., it can assume only a finite number of values, that are in this case 30 vendor names (HP, IBM, Siemens, etc.). To use our methods we have translated them into numerical values assigning a distinct integer value to each category. The

observed value to be estimated is the published Relative CPU Performance. The estimated values computed in [KA88] with a linear regression method are available, so we can compare our results with them. We choose $k = 2$, which seems to be the best guess based on a few preliminary experiments on the dataset.

The overall approximation error obtained by APR is well below the previous result on the dataset. It is positive that a fast heuristic technique in this case easily beats an exact method, although linear. While the mean error was more than 24 units in [KA88], our piecewise model cuts it down to 19, that is an average error of slightly more than 29% from the actual values, a 22% improvement.

	Overall error	Mean error	Avg. diff.
[KA88]	5085	24.33	33.9%
APR-ℓ_1	3960	18.95	29.27%

Chapter 5

Concluding remarks

In this work we have addressed *k-Piecewise Affine Model Fitting* (k-PAMF), a problem that has recently been attracting growing attention in number of fields. k-PAMF is typically tackled with a two-phase approach: first the data points are partitioned and the submodels are fitted on them, then the subdomains of the linear submodels are determined. In this work we propose a single-phase approach: we describe a single mixed-integer linear programming formulation that is able to provide an optimal solution for k-PAMF. Since solving instances of small size is already hard, we have refined the formulation by focusing on two crucial aspects: symmetries and modelling of implications.

Column symmetry has been removed by means of symmetry-breaking constraints. Among them, the Shifted Column Inequalities (SCI) proved to be the best. We have implemented a dynamic programming separation algorithm proposed in [KP08] that allowed us to add to the model only the SCI cuts that are violated at a certain node of the B&C tree. An extended formulation that avoids the generation of SCIs has also been implemented and tested with good results. Our implementation of symmetry-breaking methods typically outperforms CPLEX antisymmetry techniques on k-PAMF.

Furthermore, we attempted to get rid of big-Ms in the refined formulation with a decomposition method based on *Combinatorial Benders' Cuts*. The approach seems promising as it removes numerical instabilities introduced

by the big-Ms, although it is still not computationally competitive with the original formulation.

In the second part of the work we have proposed two heuristics inspired by algorithms for k-HC. Both algorithms are based on a local search embedded into a randomized metaheuristic. On the basis of computational tests the Adaptive Point Reassignment heuristic (APR) achieves considerably better results. We have also considered and compared some variants of the two heuristics.

Extensive computational experiments on several randomly generated and real-world instances show that the exact formulations are a good choice to obtain optimal results for small-size instances, while APR provides good solutions even on large-size instances within a short amount of time.

There are several possible future developments. First the formulation can be further refined to be more efficient even on large-scale instances. The work on symmetry-breaking can be extended with the so-called Orbitopal Fixing [KPP07], a recent technique related to SCIs that borrows ideas typical of constraint programming. The work on Combinatorial Benders' Cuts could be extended by taking the IIS of the Slave problems as a cutting-plane generation technique rather than using a pure decomposition approach, that turns out to be not very efficient on this problem. Another step that may be useful in practice is using *ad-hoc* primal heuristics in the nodes of the B&C search tree. A variant of the Adaptive Point Reassignment heuristic could also be devised by replacing the costly MRLP with the more computationally attractive k-RLP.

Appendix A

SCI separation algorithm

We describe in details the separation algorithm [KP08] that was used in Branch and Cut to generate violated cuts based on Shifted Column Inequalities. The notation introduced in Section 2.2.2 is followed.

Given a solution $\mathbf{x}^* \in \mathbb{R}^{\mathcal{I}_{m,k}}$ we first build in linear time the matrix β that contains the value $\mathbf{x}^*(B(i,j))$ of each bar $B(i,j)$.

```
1  foreach i ∈ [m], j = min{i, k}  //inizialization
2        β(i, j) ← x*_ij
3  foreach i ∈ [m]
4        for j = min{i, k} − 1 to j = 1
5              β(i, j) ← x*_ij + β(i, j + 1)
```

The algorithm then needs a matrix $w \in \mathbb{R}^{m \times k}$ that contains the value $x(\mathcal{S})$ of the minimal shifting for each $\langle \eta, j \rangle \in \mathcal{I}_{m,k}$. The weight of a Shifted Column is computed top-down via Dynamic Programming. The crucial idea of the algorithm is that for each element (i,j) we can choose whether or not to *shift* diagonally the corresponding column $col(i,j)$. The choice is based on the weight of the two distinct cases, which are computed for each (i,j) in constant time thanks to the *memoization* of the previous entries. Since we are looking for a minimal weight shifting, the algorithm selects the case with lower value.

```
1  foreach j ∈ [k]  //inizialization of upper row
2      ω⟨1, j⟩ ← min{x*_⟨i,ℓ⟩ | ℓ ≤ j}
3  foreach η ∈ [m]  //inizialization of leftmost column
4      ω⟨η, 1⟩ ← ω⟨η − 1, 1⟩ + x*_⟨η,1⟩
5  for η = 2 . . . m
6      for j = 2 . . . k
7          ω1 ← ω⟨η, j − 1⟩ //shifting
8          ω2 ← ω⟨η − 1, j⟩ + x*_⟨η,j⟩ //no shifting
9          ω⟨η, j⟩ ← min{ω1, ω2}
10         if ω1 < ω2
11             τ⟨η, j⟩ ← 0
12         else
13             τ⟨η, j⟩ ← 1
```

The support structure $\tau \in \{0,1\}^{m \times k}$ is used for the reconstruction of the minimal Shifted Columns. Now just by comparing the values in ω with the values of the respective *bars* $\mathcal{B}$ in β it is possible to identify the SCIs which are violated in $O(mk)$ time.

```
1  ViolatedCuts ← ∅
2  for η = 2 . . . m
3      for j = 2 . . . k
4          if ω⟨η, j⟩ ≤ β(i, j) − ε
5              S(i, j) ← BuildMinimalSC(⟨η, j⟩)
6              add {x(B(i, j)) − x(S(i, j)) ≤ 0} to ViolatedCuts
```

BuildMinimalSC can be described for convenience in a recursive way, although in practice it has been implemented as an iterative procedure.

```
1  BuildMinimalSC⟨η, j⟩
2  if τ⟨η, j⟩ = 0
3      S⟨η, j⟩ ← BuildMinimalSC(⟨η, j − 1⟩) //shifting
4  else
5      S⟨η, j⟩ ← BuildMinimalSC(⟨η − 1, j⟩) ∪ {⟨η, j⟩} //no shifting
6  return S⟨η, j⟩
```

The construction of the data structures is done in $O(mk)$, while the reconstruction of a Shifted Column in $O(m)$. Then, to have a violated cut the algorithm takes an overall linear time with respect to the dimension $m \times k$.

Appendix B

Code

We report here a part of the C++ code that shows the implementation of the SCI separation algorithm and the 3-PAMF heuristic.

SCI cuts generation

The implementation in C++ follows the pseudo code illustrated in Appendix A. It makes use of the data structures provided by CPLEX/Concert, that include `IloExpr`, `IloNumVar` and `IloRange` for the handling of numerical expressions and linear constraints with numerical variables.

```
/// minimal weight SCI computation and construction

IloNumArray icses(getEnv());
double beta[M][K];
double omega[M][K]; //in "diagonal" coordinates <n,j>=(n+j,j)
int tau[M][K];

getValues(icses,vars); //get variable values
//build beta
for(int i=0;i<M;i++){
  if(i<K){
    beta[i][i]=icses[i*K+i];
    for(int j=i-1;j>=0;j--)
      beta[i][j]=icses[i*K+j]+beta[i][j+1];
    }
```

```
  else{
    beta[i][K-1]=icses[i*K+K-1];
    for(int j=K-2;j>=0;j--)
      beta[i][j]=icses[i*K+j]+beta[i][j+1];
      }
    }
double minx=IloInfinity;
//build omega
for(int j=0;j<K;j++){
  if(icses[0*K+j]<minx)
    minx=icses[0*K+j];
  omega[0][j]=minx;
  }
for(int eta=1;eta<M;eta++)
      omega[eta][0]=omega[eta-1][0]+icses[eta*K+0];

for(int eta=1;eta<M;eta++)
  for(int j=1;j<K && eta+j<M;j++){
    double omega1= omega[eta][j-1];
    double omega2= omega[eta-1][j]+icses[(eta+j)*K+j];

    if(omega1<=omega2){
      omega[eta][j]=omega1;
      tau[eta][j]=1;}
    else{
      omega[eta][j]=omega2;
      tau[eta][j]=2;}
    }

for(int eta=1;eta<M;eta++)
  for(int j=1;j<K && eta+j<M;j++)
    if(omega[eta][j-1]<beta[eta+j][j]){
        //compute the shifted colum (given eta and j-1)
      IloExpr shiftedColumn(getEnv());
      int _eta=eta;
      int _j=j-1;
      bool finished=false;
      while(!finished){
        if(_eta>0 && _j>0){
```

```
            if(tau[_eta][_j]==1)
              _j--;
            else{
              shiftedColumn+=vars[(_eta+_j)*K+_j];
              _eta--;
            }
          }else{
            if(_eta==0){
              shiftedColumn+=vars[(_eta+_j)*K+_j];
              finished=true;}
            else{
              for(int i=_eta;i>=0;i--)
                shiftedColumn+=vars[i];
              finished=true;
            }
          }
        }

        IloExpr bar(getEnv());
        for(int jj=j;jj<K && jj<(eta+j);jj++)
            bar+=vars[(eta+j)*K + jj];
        if(getValue(bar-shiftedColumn)>eps){
          try { //add a violated cut
            add(bar-shiftedColumn<=0);
            }
            catch (...) {throw;}
        }
        bar.end();
        shiftedColumn.end();
    }
```

3-PAMF

We show the code implementing the basic version of the heuristic 3-PAMF. The procedure calls other methods that compute the ℓ_1-norm distances, re-assign the points and perform an RLP step.

```
double algorithm::3PAMF_solve(Problem_instance & pi){
  const int k = pi.K();
```

```
double init_time = pi.chrono.elapsed_time();
pi.randomly_populate_clusters();
pi.update_distances();
plain_combinatorial_reassignment(pi);
double last_obj = 1e300;
double obj = pi.solution_measure();

int iteration = 0;
while (obj < last_obj && pi.chrono.elapsed_time() < pi.ops.
    max_time){
  last_obj = obj;

  for (int j = 0; j < k; j++)
    recalculate_l1_norm_affine_submodel_parameters(pi, j);
  pi.update_distances();
  plain_combinatorial_reassignment(pi);
  reassign_with_RLP(pi);

  obj = pi.solution_measure();
  iteration++;
} // end of the iterations

obj = pi.solution_measure();
return obj;
```

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