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## 2 **Projection under pairwise distance control**

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### 6 **ARTICLE HISTORY**

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### 8 **ABSTRACT**

9 Visualization of high dimensional and possibly complex data onto a low-dimensional  
10 space is often difficult. Several projection methods have been already proposed to  
11 display such high-dimensional structures on a lower-dimensional space, but the infor-  
12 mation lost is not always considered. Here, a new projection paradigm is presented  
13 to describe a non-linear projection method that takes into account the projection  
14 quality of each projected point in the reduced space, this quality being directly avail-  
15 able at the scale of this reduced space. More specifically, this novel method allows  
16 for a straightforward visualization of data in  $\mathbb{R}^2$  with a simple reading of the ap-  
17 proximation quality, and thus provides a novel variant of dimensionality reduction.

### 18 **KEYWORDS**

19 Data visualization; dimensionality reduction; multidimensional scaling; principal  
20 component analysis; kernel principal component analysis.

## 21 **1. Introduction**

22 Several domains in science use data with large numbers of variables in their studies  
23 such as in biology (Cheung 2012, Golub *et al.* 1999), chemistry (Svante *et al.* 1984),  
24 geography (Van der Hilst *et al.* 2007) and finance (Jagannathan and Ma 2003). These  
25 data can be viewed as a large matrix and extracting results from this type of matrix

26 is often difficult and complicated. In such cases, it is desirable to reduce the number  
27 of dimensions of data by conserving as much information as possible from the given  
28 initial matrix.

29 Different types of multivariate data analysis methods have been developed to study  
30 these data such as dimensionality reduction, variable selection, cluster analysis and  
31 other methods. Typically, dimensionality reduction is used to summarize the data  
32 with variable selection used to choose the pertinent variables from the set of candidate  
33 variables and cluster analysis used to group the objects or variables. In our study, we  
34 focus on dimensionality reduction. Dimensionality reduction techniques can be used in  
35 different ways, to solely lower the dimensionality to prepare data for other treatments  
36 or for data visualization to provide a simple interpretation of the data in  $\mathbb{R}^2$  or  $\mathbb{R}^3$ .

37 Due to the difficulties faced by high dimensional data, many methods for data  
38 dimensionality reduction and data visualization have been proposed (Chan 2006;  
39 Chinchilli and Sen 1987; Dempster 1971; Keim and Kriegel 1996; Mardia *et al.*  
40 1979). Some of the most common methods include principal component analysis (PCA)  
41 (Jackson 1991), multidimensional scaling (MDS) (Togerson 1958), scatter plot matrix  
42 (Cleveland and McGill 1988), parallel coordinates (Inselberg 1985) and Sammon's  
43 mapping (Sammon 1969). Scatter plot matrix and parallel coordinates methods are  
44 widely used to visualize multidimensional data sets. An issue with PCA and MDS is  
45 that as the number of dimensions grows, important multi-dimensional relationships  
46 might not be visualized. Moreover, the quality of projection usually assessed by the  
47 percentage of variance (PCA case) that is conserved or by the stress factor (MDS  
48 case) is a global projection quality measure and does not give information about local  
49 quality.

50 In some projection methods such as PCA, a local measure is defined to indicate  
51 the projection quality of each projected point taken individually. This local measure is  
52 evaluated by the squared cosine of the angle between the principal space and the vector  
53 of the point (Jolliffe 1986). A good representation in the projected space is hinted by  
54 high squared cosine values. This measure is useful in cases of linear projection, which  
55 happens in PCA, but cannot be applied in the case of nonlinear projection. Moreover,  
56 linear dimensionality reduction misses important nonlinear structure in the data which

57 does not allow to give powerful results in case of nonlinear configurations. Therefore,  
58 many methods have been developed to perform nonlinear projections by nonlinearizing  
59 a linear dimensionality reduction or by using manifold learning methods.

60 The nonlinearization of linear dimensionality reduction is applied to extract nonlinear  
61 principal components. Kernel PCA is one of the most popular methods in this domain,  
62 which integrates a kernel function to determine principal components in different high-  
63 dimensional space (Schölkopf 1998). Manifold learning methods are an approach to  
64 construct a matrix using the neighborhood information and take a spectral decom-  
65 position to find a nonlinear embedding (like Locally Linear Embedding LLE, Isomap  
66 algorithm etc) (Lee and Verleysen 2007, Tenenbaum *et al.* 2000, Roweis and Saul  
67 2000).

68 In this paper, we propose a new nonlinear projection method that projects the  
69 points into a reduced space by using the pairwise distance between pairs of points and  
70 by taking into account the projection quality of each point taken individually. Nonlin-  
71 ear projection methods cited in the previous paragraph project the points in a feature  
72 space which makes the distances between the projected points hard to be interpreted.  
73 In our method, the distances between projected points are related to the initial dis-  
74 tances between points, offering a way to easily interpret the distances observed in the  
75 projection plane. This projection leads to a representation of the points as circles with  
76 a different radius associated to each point. Henceforth, this method will be referred to  
77 as “Projection under pairwise distance control”. Furthermore, visualization of data in  
78 a reduced space is not the only objective of this method. It can serve as a dimension-  
79 ality reduction method to reduce the number of variables by minimizing the sum of  
80 the radii and to then determine the number of variables that can be kept.

81 The main contribution of this study is to provide a simple data visualization in  $\mathbb{R}^2$   
82 with a straightforward interpretation and to provide a new variant of dimensionality  
83 reduction. Firstly, the new projection method is presented in Section 2. In Section 3,  
84 the algorithms used in solving the optimization problems related to this method are  
85 then illustrated. In Section 4 the application of this method to various real data sets  
86 is shown. Finally, the conclusions are drawn in Section 5.

87 **2. Projection under pairwise distance control**

88 Let us consider  $n$  points given by their pairwise distances denoted by  $d_{ij}$  for  $i, j \in$   
89  $\{1, \dots, n\}$ . The objective is to project these points using distances into a reduced  
90 space  $\mathbb{R}^q$  by introducing additional variables, called hereafter radii, that indicate the  
91 extent to which the projection of each point is accurate. The local quality is then given  
92 by the values of the radii. A good projection quality of point  $i$  is indicated by a small  
93 radius value denoted by  $r_i$ . It is important to note that both units of  $d_{ij}$ 's and  $r_i$ 's are  
94 identical, thus allowing for a direct comparison.

95 Before presenting our method, an overview of principal component analysis, Kernel  
96 PCA and multidimensional scaling is given to highlight the significance of our method.

97 **2.1. Overview of certain existing methods: PCA, KPCA and MDS**

98 ***Principal Component Analysis (PCA)***

99 The PCA method is the most used linear projection technique for data visualization  
100 and dimensionality reduction. PCA can be stated as an optimization problem involving  
101 the squared Euclidean distances (Mardia *et al.* 1979). This optimization problem is  
102 the following:

$$\mathcal{P}_{\text{PCA}} : \begin{cases} \min_{A \in \mathcal{M}_{p \times q}} \sum_{1 \leq i < j \leq n} |d_{ij}^2 - \|Ay_i - Ay_j\|^2| \\ \text{s.t. } \text{rank}(A) = m \\ AA^T = I_p, \end{cases}$$

103 where  $y_i \in \mathbb{R}^p$  is the original coordinates vector of point  $i$ ,  $d_{ij}^2$  is the squared distance  
104 for couple  $(i, j)$  given by  $\|y_i - y_j\|^2$  and  $A$  is the projection matrix of dimension  $p \times q$   
105 with  $q$  being the reduced space dimension. By its nature, PCA cannot take into account  
106 nonlinear structures, as it describes the data in terms of a linear subspace. To deal  
107 with nonlinearity, Kernel PCA, the reproducing kernel Hilbert space variant of PCA,  
108 can be used.

109 **Kernel PCA (KPCA)**

110 The idea behind KPCA is to perform PCA in a feature space denoted by  $\mathcal{F}$ , obtained  
 111 by a nonlinear mapping of data from its original space into the feature space  $\mathcal{F}$ , where  
 112 the low-dimensional latent structure is hopefully easier to discover (Schölkopf 1998).  
 113 The mapping function noted  $\Phi$  is considered as:

$$\begin{aligned} \Phi : \mathbb{R}^p &\rightarrow \mathcal{F} \\ Y &\rightarrow \Phi(Y) . \end{aligned}$$

115 The original data  $y_i$  is represented in the feature space as a function  $\Phi(y_i) = k(y_i, \cdot)$ ,  
 116 where  $k(\cdot, \cdot)$  is a positive kernel. Similar to PCA, KPCA is based on finding the first  
 117  $q$  eigenvectors corresponding to the  $q$  largest eigenvalues  $\lambda_i$  of the Gram matrix  $K =$   
 118  $(k_{ij})_{ij \in 1, \dots, n}$ , where  $k_{ij} = k(y_i, y_j) = \langle \Phi(y_i), \Phi(y_j) \rangle$  is a chosen positive kernel. Letting  
 119  $V_v$ , for  $v = 1, \dots, q$ , the eigenvectors in the feature space and  $P_{\Phi(y_i)}$  the projection  
 120 of  $\Phi(y_i)$  onto the subspace  $V_1, \dots, V_q$ . The KPCA problem can be represented as a  
 121 minimization problem with the following error:

$$\mathcal{E}_{\text{KPCA}} : \|\Phi(y) - P_{\Phi(y)}\|_2^2 ,$$

122 where  $P_{\Phi(y)} = \sum_{v=1}^q \langle \Phi(y), V_v \rangle V_v$ .

123 Furthermore, the most well-known and used measure applied to evaluate the pro-  
 124 jection quality of points for PCA and KPCA is the squared cosine value. Squared  
 125 cosine values cannot be interpreted at the same time as the distances in the projection  
 126 because the cosine values do not have a specific unit. More precisely, the visualization  
 127 of the projection in the reduced space using PCA and KPCA cannot simply be inter-  
 128 preted in terms of original distances between the points. Indeed, in PCA, the cosine  
 129 values do not provide a quantitative assessment of the error made when considering  
 130 the distances between the projected points, even less in KPCA where the projected  
 131 points are in the feature space so the term “distances” is not related to the distances  
 132 between the points in the original space.

133 **Multidimensional Scaling (MDS)**

134 As with PCA, Multidimensional scaling (MDS) consists of finding a new data config-  
 135 uration in a reduced space. The main difference between these two methods is that  
 136 the input data in MDS is in the form of a similarity or dissimilarity matrix, called  
 137 “proximity”, representing the proximity between pairs of objects. MDS are developed  
 138 where the proximities behave like distances or not respectively (Borg and Groenen  
 139 2005, Shepard 1962). The key idea of MDS is to perform dimensionality reduction in  
 140 a way to approximate high-dimensional distances denoted by  $\delta_{ij}$  the low-dimensional  
 141 distances  $d_{ij}$ , where  $d_{ij}$  is equal to the distance between  $x_i$  and  $x_j$ , the coordinates of  
 142  $i$  and  $j$  in the reduced space. In his original paper on MDS (Kruskal 1964), Kruskal  
 143 proposed the least-squares loss function denoted by “Stress” as follows

$$\text{Stress} = \sqrt{\frac{\sum_{1 \leq i < j \leq n} (d_{ij} - \|x_i - x_j\|)^2}{\sum_{1 \leq i < j \leq n} d_{ij}^2}}.$$

144 By minimizing the Stress function, we find the best configuration of  $(x_1, \dots, x_n) \in \mathbb{R}^q$   
 145 such that the distances fit to the initial distances.

146 If we consider  $n$  variables as  $r_1, \dots, r_n \in \mathbb{R}^+$ , the sum of which bounds the stress  
 147 function, the optimization problem  $\mathcal{P}_{\text{MDS}}$  can be equivalently rewritten as:

$$\mathcal{P}_{\text{MDS}} : \begin{cases} \min_{x_1, \dots, x_n \in \mathbb{R}^q, r_1, \dots, r_n \in \mathbb{R}^+} \sum_{i=1}^n r_i \\ \text{s.t.} \quad \sum_{i=1}^n r_i \geq \frac{1}{n-1} \sqrt{\frac{\sum_{1 \leq i < j \leq n} (d_{ij} - \|x_i - x_j\|)^2}{\sum_{1 \leq i < j \leq n} d_{ij}^2}}. \end{cases}$$

148 Note that the optimal solution of the MDS problem may not be unique (Kruskal and  
 149 Wish 1978).

150 A criterion to determine the local projection quality has been proposed by Born  
 151 and Groenen called Stress-per-point (*SPP*) (Borg and Groenen 2005). The *SPP* of

152 point  $i$  is given by:

$$SPP_i = \frac{\sum_{j=1, j \neq i}^n (d_{ij} - \|x_i - x_j\|)^2}{\sum_{j=1, j \neq i}^n d_{ij}^2},$$

153 with  $Stress = \frac{\sum_{1 \leq i < j \leq n}^n (d_{ij} - \|x_i - x_j\|)^2}{\sum_{1 \leq i < j \leq n}^n d_{ij}^2}$ .

154 Again, this is difficult to interpret directly on the projection as a distance error because  
155 the projected points are not in the same metric as the initial data.

156 However, we can observe that the constraint on  $\sum_{i=1}^n r_i$  can be modified to have a  
157 stronger control on each  $d_{ij}$  in the following way:  $|d_{ij} - \|x_i - x_j\|| \leq r_i + r_j$  where  $x_i$   
158 and  $x_j$  are the projected coordinates of points  $i$  and  $j$ .

159 Therefore, our objective is to propose a new nonlinear projection method that indi-  
160 vidually controls the projection of points and provides a graphical representation in  
161 the same metric as the original space with an error associated to each point.

## 162 **2.2. Our proposal: Projection under pairwise distance control method**

163 Let  $x_1, \dots, x_n$  be the coordinates of the projected points in  $\mathbb{R}^p$  and  $\|x_i - x_j\|$  the  
164 distance between two projected points  $(i, j)$ . Radii are introduced in this paper to  
165 assess how far  $\|x_i - x_j\|$  is from the given distance  $d_{ij}$ . Indeed, for the couple  $(i, j)$ , we  
166 are aiming for a  $\|x_i - x_j\|$  value close to  $d_{ij}$ , which should imply a small radius  $(r_i, r_j)$ .  
167 Figure 1 depicts this idea: for each point  $i \in \{1, \dots, n\}$ , the projection of  $i$  belongs to  
168 a sphere with center  $x_i$  and radius  $r_i$  such that for each couple  $(i, j) \in \{1, \dots, n\}$  we  
169 have  $\|x_i - x_j\| - (r_i + r_j) \leq d_{ij} \leq \|x_i - x_j\| + r_i + r_j$ .

170 **Radii for uncertainty metric:** The idea presented above can be expressed by  
171 finding the value of radii that satisfy these two constraints:

- 172 •  $\sum_{i=1}^n r_i$  is minimal.
- 173 •  $d_{ij} \in [\|x_i - x_j\| - r_i - r_j; \|x_i - x_j\| + r_i + r_j]$ , for  $1 \leq i < j \leq n$ .

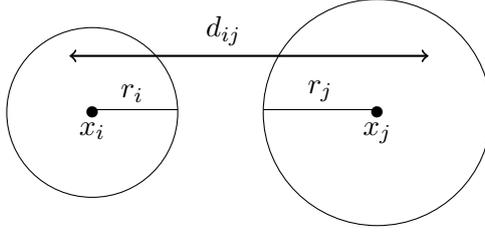


Figure 1.. Example of radii for bounding of the original distance  $d_{ij}$

174 The projection under pairwise distance control problem can be written as the following  
 175 optimization problem:

$$\mathcal{P}_{r,x} : \begin{cases} \min_{r_1, \dots, r_n \in \mathbb{R}^+, x_1, \dots, x_n \in \mathbb{R}^q} \sum_{i=1}^n r_i \\ \text{s.t. } |d_{ij} - \|x_i - x_j\|| \leq r_i + r_j, \text{ for } 1 \leq i < j \leq n \end{cases}$$

176 **Linear optimization program using fixed coordinates  $(x_1, x_2, \dots, x_n)$ :** Of  
 177 course, by fixing the coordinates vectors  $x_i$  for all  $i \in \{1, \dots, n\}$  using principal com-  
 178 ponent analysis or any other projection method, the optimization problem can easily  
 179 be solved in  $(r_1, \dots, r_n)$  using linear programming. This problem can be written as  
 180 follows:

$$\mathcal{P}_r : \begin{cases} \min_{r_1, \dots, r_n \in \mathbb{R}^+} \sum_{i=1}^n r_i \\ \text{s.t. } |d_{ij} - \|x_i - x_j\|| \leq r_i + r_j, \text{ for } 1 \leq i < j \leq n \end{cases}$$

181 It should be noted that a solution for problem  $\mathcal{P}_r$  always exists. Indeed, to satisfy the  
 182 constraints it is sufficient to increase all  $r_i$ . Thus, for any method producing points in  
 183 a reduced space as PCA for instance, we can compute the radii as a post-processing  
 184 to assess the local quality of the projected points.

185  **$\mathcal{P}_{r,x}$  is a non-convex optimization problem:** For any dimension  $p$ , even with  
 186  $p = 1$ , note that the optimization problem  $\mathcal{P}_{r,x}$  is not convex. Indeed, to easily illus-  
 187 trate this fact, we take the function  $g(x, y) = |d - \|x - y\||$  considering two solutions  
 188  $(x_1, y_1) = (0, 2)$  and  $(x_2, y_2) = (3, 1)$  with  $d$  equal to 2. Thus, we have  $g(x_1, y_1) = 0$  and

189  $g(x_2, y_2) = 0$  but  $g\left(\frac{x_1 + x_2}{2}, \frac{y_2 + y_2}{2}\right) = \left|d - \left\|\frac{x_1 + x_2}{2} - \frac{y_1 + y_2}{2}\right\|\right| = |2 - 0| = 2$   
190 which is larger than  $\frac{g(x_1, x_2) + g(y_1, y_2)}{2} = 0$  proving non convexity associated to this  
191 sample design.

192 Many methods available in the literature propose different ways to solve such opti-  
193 mization problems. Examples include: trust-region-reflective (Conn *et al.* 2000), which  
194 chooses and computes an approximation of the objective function, and then chooses  
195 and modifies the trust region and finally solves the trust-region subproblem; sequential  
196 quadratic programming (SQP) which solves the optimization problem by addressing  
197 a sequence of quadratic programming problems where the Lagrangian function is ap-  
198 proximated by a quadratic function and the constraints are approximated by a linear  
199 hyper-space (Boggs and Tolle 1995); the active-set method, which is composed of  
200 two phases, wherein for the first phase (the feasibility phase) the objective function is  
201 ignored while a feasible point is found for the constraints, and in the second phase (the  
202 optimality phase) the objective function is minimized while feasibility is maintained  
203 (Wong 2011, Cristofari *et al.* 2007). The choice of optimization method to use to  
204 achieve optimality of the optimization problem is essential and depends on many fac-  
205 tors such as the type of problem, desired quality of solution, time limit and availability  
206 of the algorithm implementation etc. In fact, all of the methods cited above can be  
207 used in optimizing problem  $\mathcal{P}_{r,x}$  which is a constrained optimization problem having  
208 inequality constraints and they are all available in MATLAB using the function “fmi-  
209 con” for constrained nonlinear optimization problems. Having small radii is the main  
210 constraint in our optimization problem, thus the objective is to obtain good solution  
211 within a reasonable and practical timeframe. Therefore, a method that balances time  
212 and quality of the solution is required.

213 **Another strategy of use: Dimensionality reduction** One of the main objectives  
214 of high-dimensional data studies is to choose, from a large number of variables, those  
215 that are important for understanding the underlying studied phenomena. In addition  
216 to visualization, our aim can thus be to reduce the dimension rather than to visualize  
217 data in  $\mathbb{R}^2$ . Therefore, the proposed method can serve to reduce the number of variables  
218 by taking into account the value of  $\sum_{i=1}^n r_i$ . Indeed, by solving the problem  $\mathcal{P}_{r,x}$  using

219 different dimension values, we can choose the dimension with respect to the local  
 220 projection quality promoted in this study.

221 **2.3. A toy example for illustrating our method**

222 Let us apply the proposed projection method to a simple example by taking a tetrahe-  
 223 dron with all pairwise distances equal to 1. For problem  $\mathcal{P}_r$ , the coordinates of points  
 224  $x_i$  for  $i = 1, \dots, 4$  are obtained using multidimensional scaling. The optimization was  
 225 carried out using the MATLAB software with the optimization toolbox for linear and  
 226 nonlinear optimization problem used for problems  $\mathcal{P}_r$  and  $\mathcal{P}_{r,x}$ , respectively. The value  
 227 of  $\sum_{i=1}^4 r_i$  is equal to 0.7935 for problem  $\mathcal{P}_r$  and 0.4226 for  $\mathcal{P}_{r,x}$ . It is clear that prob-  
 228 lem  $\mathcal{P}_{r,x}$  gives better solutions than problem  $\mathcal{P}_r$  with smaller radii, which indicates  
 better projection quality of points.

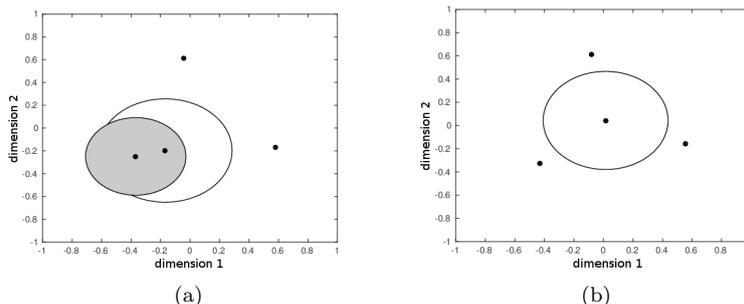


Figure 2.. Projected points after solving problem  $\mathcal{P}_r$  and problem  $\mathcal{P}_{r,x}$ . The x-axis and y-axis are dimension 1 and dimension 2, respectively. (a) and (b) show the projection obtained from the solution of problem  $\mathcal{P}_r$  using MDS and of problem  $\mathcal{P}_{r,x}$ , respectively.

229

230 This result is shown in Figure 2, which depicts the solution obtained using  $\mathcal{P}_r$  and  $\mathcal{P}_{r,x}$ .  
 231 In Figures 2a and 2b, the circles with different radii indicate the quality of projection  
 232 for each point. The circle color is related to the radius value, the shades of gray lie  
 233 between white and black, the smaller the radius, the darker the circle. The points that  
 234 have circles with small radii are also considered as projected points. Note that the  
 235 points represented as points and not as circles are very well projected, having radii  
 236 almost equal to zero.

237 In Figure 2b, just one circle appears indicating that the projection quality using prob-  
 238 lem  $\mathcal{P}_{r,x}$  is better than when using problem  $\mathcal{P}_r$ . In Figure 2a, half of the points are

239 well projected whereas the other half have large radii, indicating that they are not well  
 240 projected. Moreover, it is worth noting that the three outer points all have radii equal  
 241 to 0, which indicates that they are all perfectly placed with respect to one another.  
 242 In Figure 2b, the distances between the three points that are very well projected  
 243 are equal to the distances between these points in their original space ( $d_{kl} = \|x_k -$   
 244  $x_l\|$  where  $k$  and  $l$  are two very well projected points) whereas the distances from  
 245 the badly projected points to the perfectly projected points are not yet conserved.  
 246 Therefore, using the proposed method, we have succeeded in conserving half of the  
 247 original distances in the new projection plane and the other half have been changed  
 248 to fit the new configuration. If we now apply the proposed method to the distances  
 249 obtained by MDS to find the radius of each projected point (Figure 2a), it can be noted  
 250 that one distance is conserved as the original distance and the other five distances  
 251 are changed which indicates that the proposed method projects the points well by  
 252 conserving the distances between the points as much as possible.

253 It is also important to note that, in general, our method is not only a nonlinear  
 254 projection method with local quality measure, but it can act as a new tool to give  
 255 the local quality of projection for the classical projection methods using the radii by  
 256 solving problem  $\mathcal{P}_r$ . It can be used outside our method as post-processing of classical  
 257 methods.

#### 258 **2.4. Connection with existing methods**

259 Multidimensional fitting (MDF) (Berge *et al.* 2010) is a method that modifies the  
 260 coordinates of a set of points in order to make the distances calculated on the modified  
 261 coordinates similar to a given set of distances on the same set of points. The so-called  
 262 “target matrix”, the matrix that contains the point coordinates and “reference matrix”  
 263 is the matrix that contains the given distances.

264 Let us take  $X = \{x_1 | \dots | x_n\}$ , the target matrix of coordinates and  $D = \{d_{ij}\}$ , the  
 265 reference matrix of distances. The objective function of the MDF problem is given by:

$$\sum_{1 \leq i < j \leq n} |d_{ij} - \|x_i - x_j\||.$$

266 **Proposition 2.1.** *Problem  $\mathcal{P}_{r,x}$  is bounded from below by  $\frac{1}{n-1} \sum_{1 \leq i < j \leq n} |d_{ij} - \|x_i - x_j\||$*   
 267 *where  $x_1, \dots, x_n$  is the optimum for the associated MDF problem.*

268 **Proof.** By summing all the constraints of problem  $\mathcal{P}_{r,x}$ , we obtain:

$$\sum_{1 \leq i < j \leq n} |d_{ij} - \|x_i - x_j\|| \leq \sum_{1 \leq i < j \leq n} (r_i + r_j) = (n-1) \sum_{i=1}^n r_i.$$

269 So,  $\sum_{i=1}^n r_i \geq \frac{1}{n-1} \sum_{1 \leq i < j \leq n} |d_{ij} - \|x_i - x_j\||$ , which concludes the proof.  $\square$

### 270 3. Optimization tools for performing the proposed method

271 Problem  $\mathcal{P}_{r,x}$  can be solved using different initialization points for the coordinate  
 272 matrix  $X$ . In this section, we first discuss the different initialization points of the  
 273 proposed optimization problem and then propose two algorithms to be used in our  
 274 optimization.

#### 275 3.1. Initialization point for problem $\mathcal{P}_{r,x}$

276 Different solutions of problem  $\mathcal{P}_{r,x}$  can be obtained using different initial values of  
 277 matrix  $X$ . We have considered three possibilities:

278 **1- Initial point using a known projection method** The first possibility is to  
 279 use the matrix obtained by PCA or another projection method. The choice of method  
 280 must be based on the type of data. In this application, we use PCA for quantitative  
 281 data and MDS for categorical and functional data.

282 **2- Initial point using squared distances** The optimization problem  $\mathcal{P}_{r,x}$  can be  
 283 changed by taking the squared distances between points instead of the distances.

284 Rewriting  $r_i^2$  as  $R_i$ , the problem is changed into

$$\mathcal{P}_{R,x} : \begin{cases} \min_{R_1, \dots, R_n \in \mathbb{R}^+, x_1, \dots, x_n \in \mathbb{R}^k} \sum_{i=1}^n R_i \\ \text{s.t. } |d_{ij}^2 - \|x_i - x_j\|^2| \leq R_i + R_j, \text{ for } 1 \leq i < j \leq n. \end{cases}$$

285 This transformation is interesting because if the constraints of problem  $\mathcal{P}_{R,x}$  are sat-  
286 isfied, the constraints of problem  $\mathcal{P}_{r,x}$  will also be satisfied. Indeed,

$$|d_{ij}^2 - \|x_i - x_j\|^2| \leq R_i + R_j = r_i^2 + r_j^2.$$

If without loss of generality,  $d_{ij} \geq \|x_i - x_j\|$ , we obtain:

$$\begin{aligned} (d_{ij} - \|x_i - x_j\|)(d_{ij} + \|x_i - x_j\|) &\leq r_i^2 + r_j^2 \leq (r_i + r_j)^2 \Rightarrow \\ |d_{ij} - \|x_i - x_j\||^2 &\leq (r_i + r_j)^2 \Rightarrow |d_{ij} - \|x_i - x_j\|| \leq (r_i + r_j). \end{aligned}$$

287 In this way problem  $\mathcal{P}_{R,x}$  can serve as an initial step in solving problem  $\mathcal{P}_{r,x}$ .

288 **3- Initial point using an improved solution of problem  $\mathcal{P}_r$ .** This strategy is  
289 more involved. First, we need two properties that provide a way to improve the opti-  
290 mization results of problem  $\mathcal{P}_{r,x}$ .

**Proposition 3.1.** *Let us consider a point  $x_i$  such that for an index  $j$ , the following inequality is saturated:*

$$|d_{ij} - \|x_i - x_j\|| \leq r_i + r_j,$$

291 *and the other inequalities involving  $i$  are not saturated. The corresponding solution*  
292 *can then be improved by moving  $x_i$  along the line  $x_j - x_i$  in order to decrease  $r_i$  and*  
293  *$|d_{ij} - \|x_i - x_j\||$ .*

294 Another manner to improve the resolution of problem  $\mathcal{P}_{r,x}$  is to perform a scale  
295 change by multiplying the coordinates  $x_i$ , for  $i = 1, \dots, n$ , by a constant  $a \in \mathbb{R}$ . Thus,

296 the new optimization problem is given by:

$$\mathcal{P}_{r,a} : \begin{cases} \min_{r_1, \dots, r_n, a \in \mathbb{R}^+} \sum_{i=1}^n r_i \\ \text{s.t. } \|d_{ij} - a\|x_i - x_j\| \leq r_i + r_j. \end{cases}$$

297 **Proposition 3.2.** *Let  $r_1, \dots, r_n; x_1, \dots, x_n$  be a feasible solution of  $\mathcal{P}_{r,x}$ , if  $\exists a$  such*  
 298 *that  $\eta(a) < \sum_{i=1}^n r_i$  with  $\eta(a) = \sum_{1 \leq i < j \leq n} \|d_{ij} - a\|x_i - x_j\|$ , then  $\exists \tilde{r}_1, \dots, \tilde{r}_n$  a solution*  
 299 *of  $\mathcal{P}_{r,a}$  such that  $\sum_{i=1}^n \tilde{r}_i < \sum_{i=1}^n r_i$ .*

300 The new initial point called  $X_{imp}$ , is the improved solution given by using these two  
 301 properties as follows:

- 302 • Firstly, improving the solution of problem  $\mathcal{P}_r$  by solving problem  $\mathcal{P}_{r,a}$  and using  
 303 proposition 3.2.
- 304 • Secondly, improving the solution of problem  $\mathcal{P}_{r,a}$  using proposition 3.1.

### 305 3.2. A deterministic strategy: Algorithm 1

306 As discussed, three possibilities of coordinate matrix  $X$  can be used as the initial point:

- 307 1- Coordinates given by PCA or MDS:  $X_{\mathcal{P}_{PCA/MDS}}$  is the coordinate matrix obtained  
 308 by applying PCA or MDS and  $r_{\mathcal{P}_r}$  is a vector that contains the radius of each  
 309 point obtained by solving  $\mathcal{P}_r$ .
- 310 2- Coordinates given by squared distances:  $X_{\mathcal{P}_{R,x}}$  is the coordinate matrix obtained  
 311 by solving problem  $\mathcal{P}_{R,x}$  and  $R_{\mathcal{P}_{R,x}} = r_{\mathcal{P}_{R,x}}^2$  is a vector that contains the squared  
 312 radius for each point obtained by solving the subsequent  $\mathcal{P}_{R,x}$  problem.
- 313 3- Coordinates given by improving the solution of problem  $\mathcal{P}_r$ :  $X_{imp}$  is the coordi-  
 314 nate matrix obtained by improving the previous solution using Proposition 3.1  
 315 and  $r_{imp}$  is a vector that contains the radius of each point obtained after each  
 316 iteration of solving problem  $\mathcal{P}_{r,a}$

317 Finding these matrices requires solving the following optimization problems:  $\mathcal{P}_r$ ,  
 318  $\mathcal{P}_{R,x}$  and  $\mathcal{P}_{r,a}$ . Problems  $\mathcal{P}_r$  and  $\mathcal{P}_{r,a}$  are both constrained linear optimization problems

319 that can be solved using interior-point or simplex algorithms, which are the most  
320 widely used algorithms for linear programming. The interior-point algorithm uses a  
321 primal-dual predictor-corrector algorithm and the simplex algorithm uses a systematic  
322 procedure for generating and testing candidate vertex solutions to a linear program  
323 (Murty 1983). On the contrary, problem  $\mathcal{P}_{R,x}$  is a nonlinear optimization problem  
324 that can be solved using one of the nonlinear optimization algorithms cited in Section  
325 2.2. All these algorithms are available in MATLAB using the optimization toolbox  
326 and can be used for the corresponding problem.

327 To find the best solution of problem  $\mathcal{P}_{r,x}$ , we solve it with the three different initial-  
328 ization matrices described above. For this task, we define Algorithm 1 that gives the  
329 best solution using the different coordinate matrices. This algorithm consists of two  
330 steps, an initialization step and an optimization step. The initialization step offers  
331 three different coordinate matrices to be used in the optimization step as an initial  
332 point to quickly reach the best solution. During the optimization step, problem  $\mathcal{P}_{r,x}$   
333 is solved using one of the nonlinear optimization algorithms mentioned in Section 2.2,  
334 starting each time with one matrix of the three initial matrices already found.  
335 Thus, for Algorithm 1, described below, the three different initialization matrices are  
336 tried and then the best one is chosen that gives the minimum value of  $\sum_{i=1}^n r_i$ .

---

**Algorithm 1**

---

Input:  $D$ : distance matrix,  $N$ : number of iterations.

**Initialization step**

Project the points using PCA or MDS.

Solve  $\mathcal{P}_r$  using a linear optimization method. Obtained solution:  $(X_{\mathcal{P}_{\text{PCA/MDS}}}, r_{\mathcal{P}_r})$ .

Solve  $\mathcal{P}_{R,x}$  using a nonlinear optimization method and starting from the solution of  
 $\mathcal{P}_r$  obtained at the previous step. Obtained solution:  $(X_{\mathcal{P}_{R,x}}, R_{\mathcal{P}_{R,x}})$ .

$X_{imp} \leftarrow X_{\mathcal{P}_{R,x}}$ .

**for**  $t = 1$  to  $N$  **do**

    Solve  $\mathcal{P}_{r,a}$  starting from  $X_{imp}$  using a linear optimization method.

    Improve the solution of  $\mathcal{P}_{r,a}$ . Obtained solution:  $(X_{imp}, r_{imp})$ .

**end for**

**Optimization step**

Optimize  $\mathcal{P}_{r,x}$  using a nonlinear optimization method and starting from  $X_{\mathcal{P}_{\text{PCA/MDS}}}$ ,  
 $X_{\mathcal{P}_{R,x}}$  and  $X_{imp}$ .

Choose the minimal solution obtained by these three different starting points.

---

337 **3.3. A stochastic strategy: Algorithm 2**

338 Problem  $\mathcal{P}_{r,x}$  is a hard problem, thus it is natural to resort to stochastic optimization  
 339 methods. In the present case, we resort to the Metropolis-Hastings algorithm (Jo-  
 340 hansen and Evers 2007) which allows us to build a Markov chain with the desired  
 341 stationary distribution. The challenging parts are the choice of the proposal distri-  
 342 bution and the necessity to solve the problem  $\mathcal{P}_r$  at each iteration. Specifically, the  
 343 Metropolis-Hastings algorithm requires:

344 1- A *target distribution*:

345 The target distribution is related to the objective function of problem  $\mathcal{P}_{r,x}$   
 346 and is given by:

347 
$$\pi(x) \propto \exp\left(\frac{-E(x)}{T}\right),$$

where  $E$  is a function in  $\mathbb{R}$  given by:

$$E(x) = \sum_{i=1}^n r_i, \text{ where } \{r_1, \dots, r_n\} \text{ is the solution of problem } \mathcal{P}_r \text{ with fixed } x.$$

348 The variable  $T$  is the temperature parameter, to be fixed according to the value  
 349 range of  $E$ .

350 2- A *proposal distribution*:

351 The choice of the proposal distribution is very important to obtain mean-  
 352 ingful results. It should be chosen in such a way that the proposal distribution  
 353 approaches the target distribution. The proposal distribution  $q(X \rightarrow \cdot)$  is con-  
 354 structed as follows, giving priority to the selection of points involved in saturated  
 355 constraints:

356 

- o For each point  $i$ , choose a point  $j^{(i)}$  with probability equal to:

$$P_{j^{(i)}} = \frac{\lambda \exp(-\lambda(r_i + r_{j^{(i)}} - |d_{ij^{(i)}} - \|x_i - x_{j^{(i)}}\||))}{\sum_{k=1, k \neq i}^n \lambda \exp(-\lambda(r_i + r_k - |d_{ik} - \|x_i - x_k\||))}.$$

357 

- o Choose a constant  $c_{ij^{(i)}}$  using Gaussian distribution  $\mathcal{N}_k(0, \sigma)$ .

358 

- o Generate a matrix  $X^*$  by moving each vector  $x_i$  of matrix  $X^{t-1}$  as follows:

359

360

– If  $d_{ij^{(i)}} - \|x_i - x_{j^{(i)}}\| > 0$  then  $x_i^* = x_i + |c_{ij^{(i)}}|L_{ij^{(i)}}$ .

361

– else  $x_i^* = x_i - |c_{ij^{(i)}}|L_{ij^{(i)}}$ ,

362

where  $L_{ij^{(i)}} = \frac{x_i - x_{j^{(i)}}}{\|x_i - x_{j^{(i)}}\|}$ .

363

3- A linear optimization problem:

364

For the matrix  $X$  generated at each iteration, we solve the linear optimization

365

problem  $\mathcal{P}_r$  and we choose finally the matrix  $X$  and the vector of radii which

366

give the smallest value of  $\sum_{i=1}^n r_i$ .

367

Algorithm 1 and Algorithm 2 are both implemented in MATLAB and a code for

368

each algorithm can be provided by the authors upon request.

369

#### 4. Numerical applications

370

The projection method presented has been applied to different types of real data sets

371

and also to a simulated data set to illustrate its practical interest.

372

##### 4.1. Experimental setup

373

In practice, we have tested the proposed method on different simulated and real data

374

sets by solving the optimization problem  $\mathcal{P}_{r,x}$  using Algorithm 1 in addition to the

375

proposed Metropolis-Hastings algorithm (Algorithm 2). A distance matrix is required

376

each time. For quantitative data, the Euclidean distance between points  $y_i \in \mathbb{R}^p$ ,

377

for  $i = 1, \dots, n$ , is computed by the known formula  $d_{ij} = \sqrt{\sum_{k=1}^p (y_{ik} - y_{jk})^2}$ . For

378

categorical data, the distance between two points  $(i, j)$  is given through the Eskin

379

similarity measure (Boriah *et al.* 2008) computed by the formula  $p_{ij} = \sum_{t=1}^Q w_t p_{ij}^t$

380

where  $p_{ij}^t = \begin{cases} 1 & \text{if } i^t = j^t \\ \frac{n_t^2}{n_t^2 + 2} & \text{else} \end{cases}$ ,  $p_{ij}^t$  is the per-attribute Eskin similarity between

381

two values for the categorical attribute indexed by  $t$ ,  $w_t$  is the weight associated to

382

the attribute  $t$  called  $w_t$  which is defined by:  $w_t = \frac{1}{Q}$ ,  $Q$  is the number of attributes

383

and  $n_t$  is the number of values taken by each attribute. Then, the distances can be

384 obtained by the standard transformation formula (Du Toit *et al.* 1986) converting  
 385 similarities to distances:  $d_{ij} = \sqrt{s_{ii} - 2s_{ij} + s_{jj}}$ .

386 In addition, to compute the distances between curves of functional data, we have cho-  
 387 sen a measure of proximity similar to that studied by Ieva *et al.* (2012). In their  
 388 paper, the authors develop a proper classification designed to distinguish the grouping  
 389 structures by using a functional k-means clustering procedure with three sorts of dis-  
 390 tances. For our work we chose one of these three proximity measures as their results  
 391 are similar. The proximity measure chosen between two curves  $F_i$  and  $F_j$  is the follow-  
 392 ing:  $d_0(F_i, F_j) = \sqrt{\int_{\mathcal{T}} (F_i(t) - F_j(t))^2 dt}$ . This measure is calculated using the function  
 393 *metric.lp()* of the *fda.usc* package for the **R** software (Febrero-Bande and Oviedo de  
 394 la Fuente 2011).

395 For problems  $\mathcal{P}_r$  and  $\mathcal{P}_{r,a}$ , we first applied PCA for quantitative data and MDS for  
 396 categorical and functional data; a linear programming package, called “linprog” which  
 397 solves linear programming problems, was then used to solve the optimization problems  
 398 with an interior-point algorithm. Problems  $\mathcal{P}_{r,x}$  and  $\mathcal{P}_{R,x}$  are nonlinear optimization  
 399 problems; therefore, we used a nonlinear programming package, called “fmincon” which  
 400 finds minimum of constrained nonlinear multi-variable function, to solve them. The  
 401 algorithms cited in Section 2.2 can be used here, but we recommend to use the active-  
 402 set algorithm. Algorithm 2 can provide a good solution if the parameters  $\lambda$ ,  $\sigma$  and  
 403  $T$  are chosen adequately. For instance,  $\lambda$  should be such that the points belonging  
 404 to unsaturated constraints are chosen with small probabilities. Therefore, we took it  
 405 equal to 100. For the other parameters  $\sigma$  and  $T$ , we took their values in the range  
 406 from 0.01 to 100. The choice of these numbers is taken after trying different values of  
 407  $\sigma$  and  $T$  in order to have the best solution that gives a minimal value of  $\sum_{i=1}^n r_i$ .

408 Moreover, the visualization of the projection of each point  $i$  in  $\mathbb{R}^2$  is represented  
 409 as a circle having  $x_i$  as the center and  $r_i$  as the radius in a two-dimensional space,  
 410 where the horizontal and vertical axes correspond to the first and the second dimension  
 411 associated to the projection in  $\mathbb{R}^2$ , respectively. The projected point belongs to this  
 412 circle and this is the specificity of our method. For each data set, the circles obtained  
 413 for each point after solving the optimization problem  $\mathcal{P}_{r,x}$  are shown. To compare the

414 projection quality of our representation with that obtained by PCA and KPCA, we  
 415 used the squared cosine values as projection quality, and for MDS, the Stress-per-  
 416 point (*SPP*) (Borg and Groenen 2005). Indeed, for PCA and KPCA, we plotted  
 417 the projected points indexed by their squared cosine values and for MDS, we used  
 418 the smacof package in R to compute the stress-per-point and to plot the bubble plot  
 419 represented the stress-per-point.

#### 420 4.2. A simulation study

421 To evaluate the performance of projection under pairwise distance control method,  
 422 we conducted a simulation study. We generated 100 random samples of  $y_i$  from a 5-  
 423 dimensional multivariate normal distribution with mean  $\mathbf{0}$  and covariance matrix  $I$ ,  
 424 the identity matrix, and we calculated the Euclidean distances between pairs  $(y_i, y_j)$   
 425 for  $1 \leq i < j \leq n$ . The projection result was compared with those obtained by KPCA.

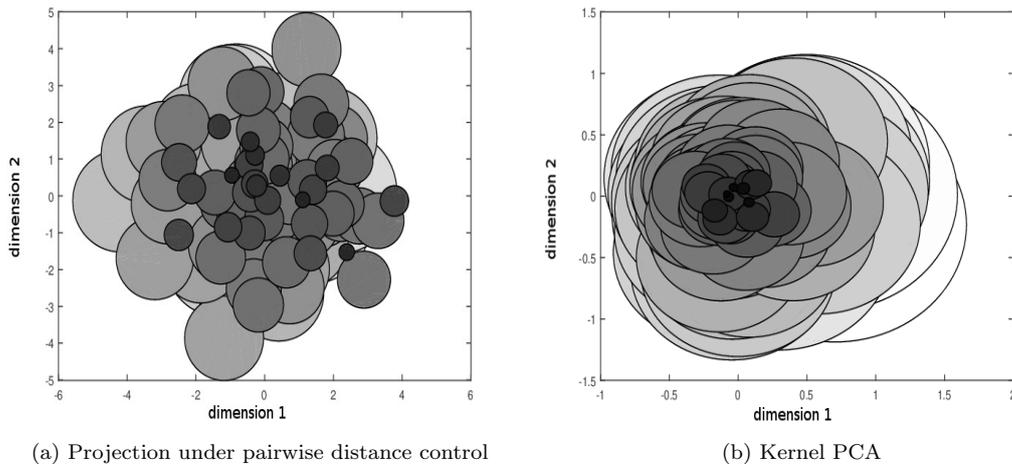


Figure 3.. Projection of the simulated data using the proposed method (a) and Kernel PCA (b). The points that have circles with small radii are considered as well projected points.

426

427 Figure 3 shows the results of the projection of the simulated data using the proposed  
 428 method and KPCA. By comparing Figure 3a and Figure 3b, it can be shown that  
 429 the projection quality of points using KPCA is somehow dependent on the position  
 430 of the points in the reduced space. Indeed, the projection is likely to give better local

431 projection quality if the projected point is located near to the center  $(0, 0)$ . On the  
432 contrary, this is less visible for the proposed method.  
433 This simulated data illustrates the originality and the efficiency of the proposed  
434 method in giving a good local projection quality.

### 435 **4.3. Introducing the real data sets**

436 Four real data sets were used and divided into three categories:

- 437 • Quantitative data: Iris and car data sets.
- 438 • Categorical data: Soybean data set.
- 439 • Functional data: Coffee data set.

440 The Iris data set (Anderson 1935) is a famous data set and is presented to show that  
441 the projection works as expected. This data set contains 3 classes of 50 instances each,  
442 where each class refers to a species of Irises. The four variables studied in this data  
443 set are: sepal length, sepal width, petal length and petal width (in *cm*). The car data  
444 set (Saporta 2006) is a data set studied in the book by Saporta (Table 17.1, page  
445 428). This data set describes 18 cars according to various variables (cylinders, power,  
446 length, width, weight and speed).

447 The soybean data set (Stepp 1984) from *UCI Machine Learning Repository* charac-  
448 terizes 47 soybean disease case histories defined over 35 attributes. Each observation is  
449 identified by one of the 4 diseases: Diaporthe Stem Canker (D1), Charcoal Rot (D2),  
450 Rhizoctonia Root Rot (D3) and Phytophthora Rot (D4).

451 The coffee data set is a time series data set used in chemometrics to classify food  
452 types. It is a functional data set where 56 samples of coffee are available with 286  
453 timestamps for each sample (as a result of spectroscopic analysis). This kind of time  
454 series is common in many applications in food safety and quality assurance and was  
455 taken from the *UCR time Series Classification and Clustering* website (Chen *et al.*  
456 2015). *Coffea Arabica* and *Coffea Canephora* variant *Robusta* are the two species of  
457 coffee bean that have acquired a worldwide economic importance, and many methods  
458 have been developed to discriminate between these two species by chemical analysis  
459 (Briandet *et al.* 1996).

460 **4.4. Results from the real data sets**

461 *4.4.1. Data visualization in  $\mathbb{R}^2$*

462 The optimization results for these four data sets are given in Table 1. For each data,  
 463 the sum of radii  $\sum_{i=1}^n r_i$  obtained using Algorithm 1 and Algorithm 2 is provided.

Table 1.. Solution of problem  $\mathcal{P}_{r,x}$  for data sets using Algorithm 1 and Algorithm 2.

	$\sum_{i=1}^n r_i$	
	Algorithm 1	Algorithm 2
Iris	16.19	17.2
Cars	3.27	3.35
Soybean	3.98	3.93
Coffee	21.68	21.97

464 Based on Table 1, the solutions of Algorithm 2 for the different data sets are shown  
 465 to be very close to those obtained using Algorithm 1. Thus, the radii obtained are  
 466 estimated to be close to the solution of Algorithm 1. Moreover, it is interesting to  
 467 note here that the number of iterations  $N$  in Algorithm 1 has an important role  
 468 in finding the minimal value of  $\sum_{i=1}^n r_i$  for problem  $\mathcal{P}_{r,a}$  and then for problem  $\mathcal{P}_{r,x}$   
 469 and also to reduce the computing time. In fact, the important decrease in the value of  
 470  $\sum_{i=1}^n r_i$  occurred in the first 500 iterations through of 1000 iterations, and then a small  
 471 decrease occurred after 500 iterations. This small decrease in value of  $\sum_{i=1}^n r_i$  after 500  
 472 iterations shows that a size of 500 iterations can be a good choice for the Algorithm  
 473 1 since all the studied data sets are concerned. Indeed, this result can be observed for  
 474 all data sets presented in our application with approximately 500 iterations.

475 **Iris data set:** Figure 4 depicts the result of projection under pairwise distance control  
 476 for the Iris data set. In the projection of the Iris data set shown in Figure 4, it is  
 477 interesting to note that two areas are well separated. This corresponds to the well-  
 478 known fact that Iris versicolor and virginica are close whereas the species Iris setosa  
 479 are more distant.

480 Referring to the original data, the Iris data set contains three classes corresponding

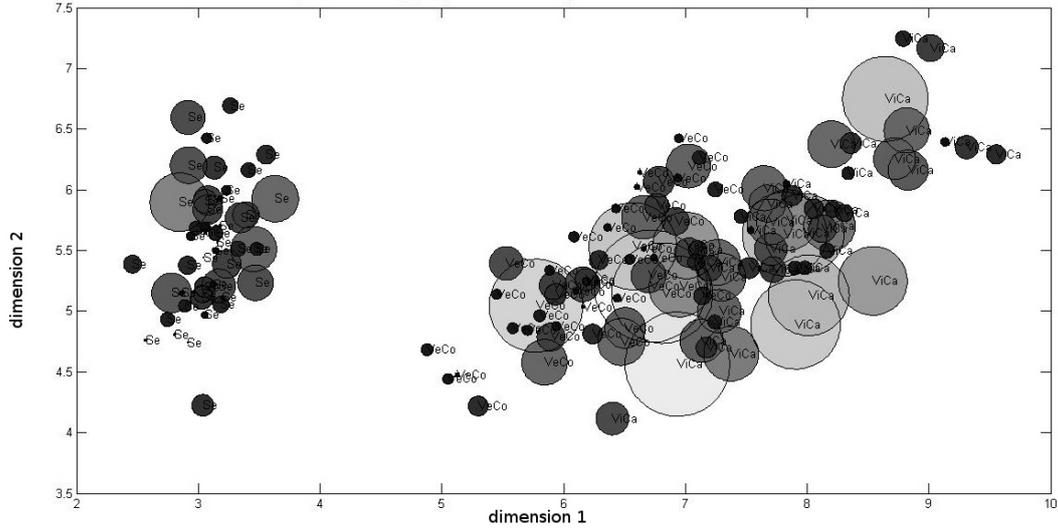


Figure 4.. Projection of the Iris data set using projection under pairwise distance control method. Two well separated groups can be observed. The points that have circles with small radii are considered as well projected points.

481 to the three types of Iris plants and one class is linearly separable from the other two  
 482 classes. This result clearly appears in our projection.

483 Moreover, we have compared the local projection quality of PCA, KPCA and MDS  
 484 with the local projection quality obtained using projection under pairwise distance  
 485 control. By comparing the projection of PCA with the projection of our method for  
 486 the Iris data set given respectively in Figures 5 and 4, we can say that our method  
 487 projected the points without giving any importance to any group. Figure 5 depicts a  
 488 group with small values of the quality measure and another group with high values  
 489 of quality measure, whereas the radii obtained by projection under pairwise distance  
 490 control method are distributed in an equivalent way.

491 For KPCA, we plotted the squared cosine values as circles to make the representation  
 492 clearer, especially for the Iris data set as the Iris setosa species are projected next to  
 493 each other. From Figure 6a, we can conclude that in each category, the points that  
 494 have close quality values are located side by side.

495 Furthermore, by comparing the proposed projection method with the one obtained by  
 496 MDS, it can be concluded that, as is the case when using PCA, the points in Figure  
 497 6b are projected by giving more importance to the Iris setosa group. Indeed, almost  
 498 all the red circles (indicating a very good projection) are assigned to the Iris setosa

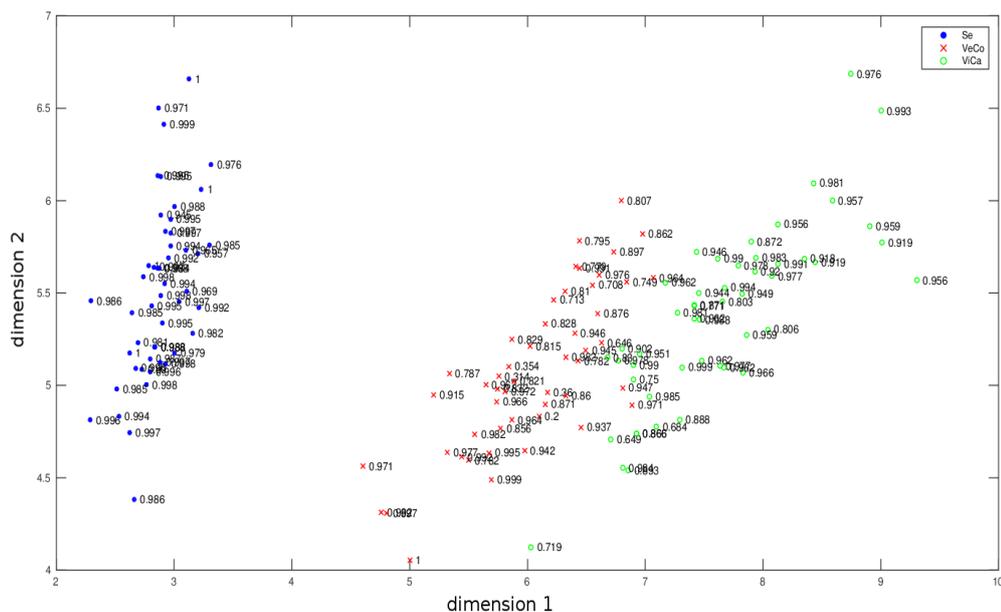


Figure 5.. Projection of the Iris data set using PCA. The values of local projection quality are given for each instance. The values of projection quality for Iris setosa species (Se) vary between 0.97 and 1 indicating then a very good projection quality whereas for Iris versicolor (VeCo) and Iris virginica (ViCa) species, the values of projection quality vary between 0.2 and 0.99 indicating a very large variability in the projection quality.

499 species. Moreover, the comparison of the position of points in the reduced space in  
 500 terms of distance between points cannot be viewed in this classical method as the  
 501 points in the reduced space are not in a metric compatible to the initial distances,  
 502 whereas in our method we have conserved the metric of the initial distances.

503 **Cars data set:** The projection of points using projection under pairwise distance  
 504 control for the car data set is shown in Figure 7. The expensive cars, the “Audi 100”,  
 505 “Alfetta-1.66”, “Datsun-200L” and “Renault 30” are well-separated from the low-  
 506 standard cars, the “Lada-1300”, “Toyota Corolla”, “Citroen GS Club” and “Simca  
 507 1300”. Moreover, we can assert that the projected points obtained using projection  
 508 under pairwise distance control are well separated as there are no circle intersections.  
 509 By comparing our projection with the projection obtained using PCA presented in  
 510 Figure 8, it can be shown that in the projection of PCA, there is a group with small

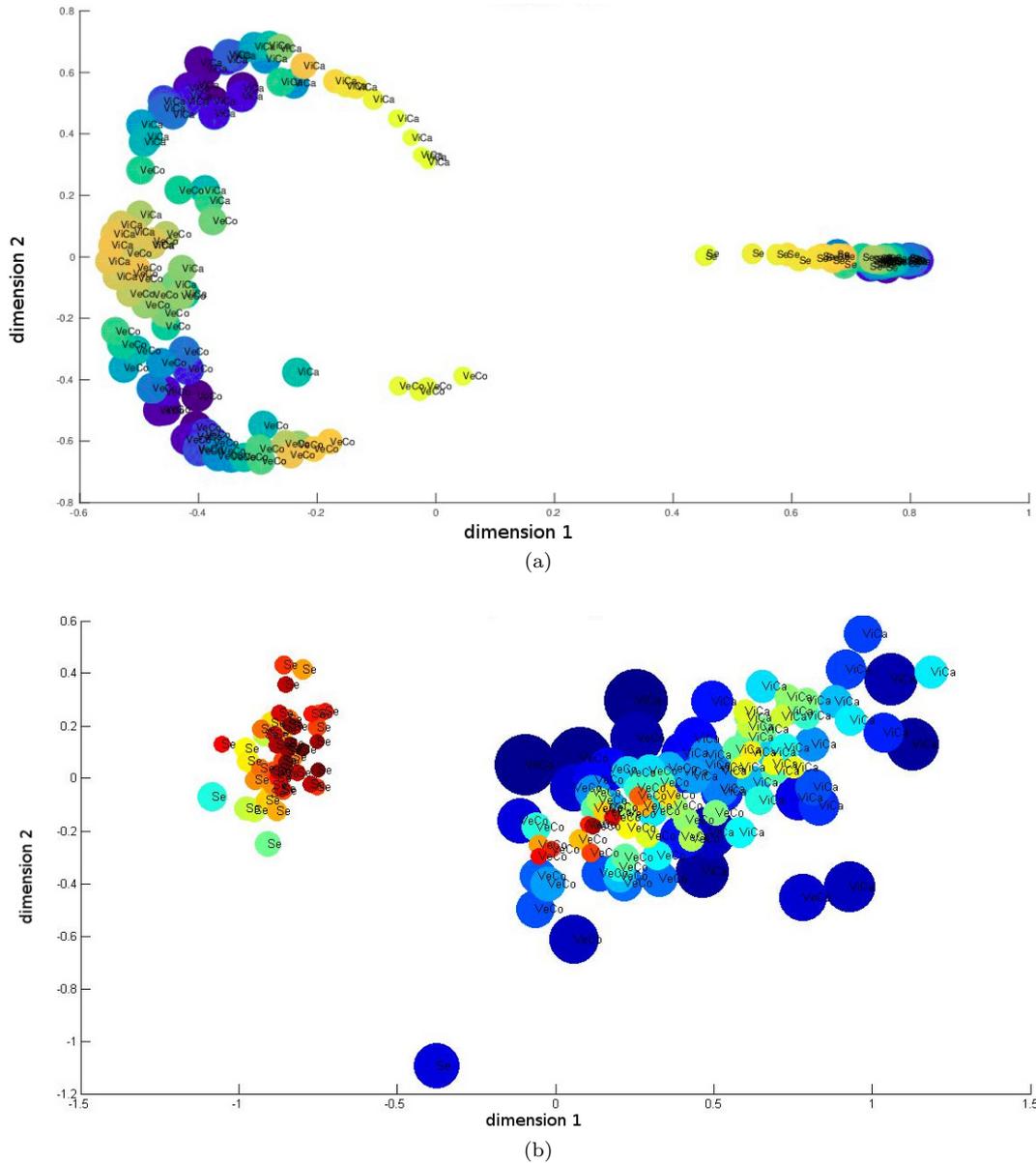


Figure 6.. Projection of the Iris data set using KPCA (a) and MDS (b). The color convention is as follows: the darker the red color of a particular disk, the better the projection. Inversely, the darker the blue color of a particular disk, the worse the projection.

511 values of the quality measure located at the center, which corresponds to the cars:  
 512 Lanca-Beta, Mazda, Fiat, Simcs and Rancho, and a group with high values of quality  
 513 measure located far from the center.

514 Regarding KPCA, we can see in Figure 9a that the points with navy circles are almost  
 515 all located almost around the same y-axis coordinates and the same applies for the

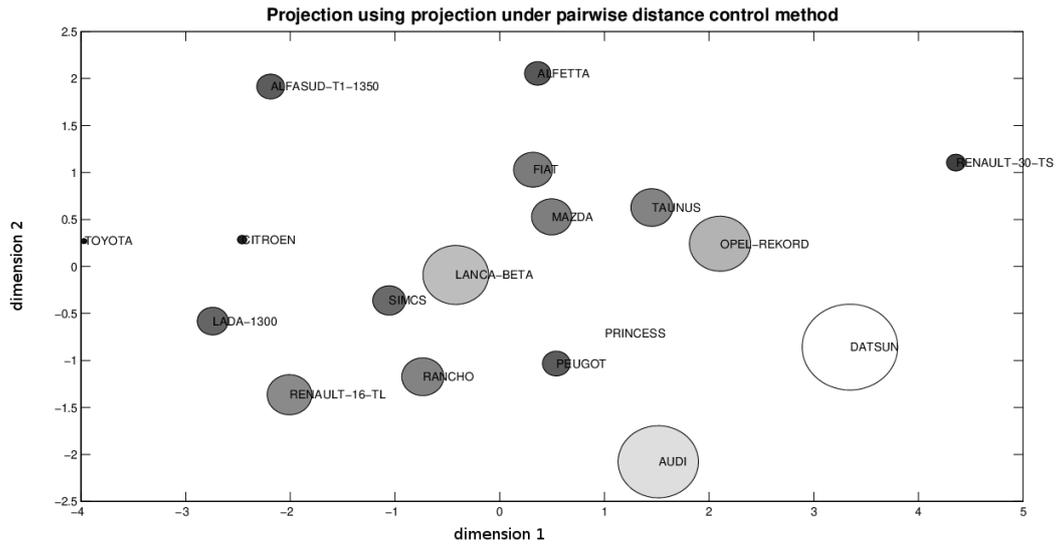


Figure 7.. Projection of the car data set using projection under pairwise distance control.

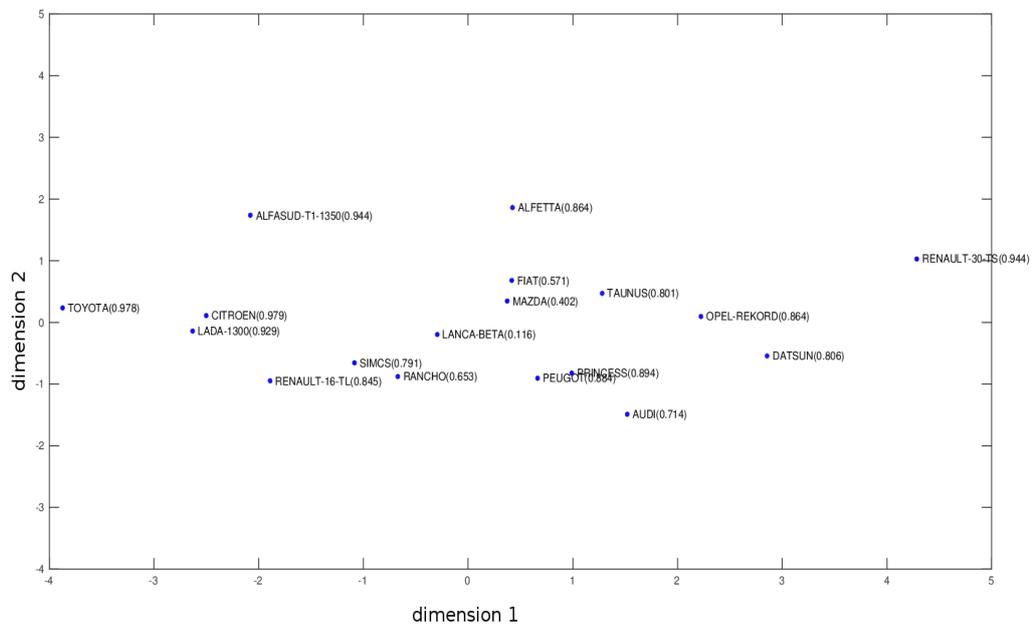


Figure 8.. Projection of the cars data set using PCA. The values of local projection quality are given for each car.

516 red circles. So the local quality for KPCA is dependent on the position of the points.  
 517 It can also be noticed that the cars Princess, Mazda, Fiat and Peugeot located in  
 518 the same area with small circles. Therefore, the only conclusion that we arrive at

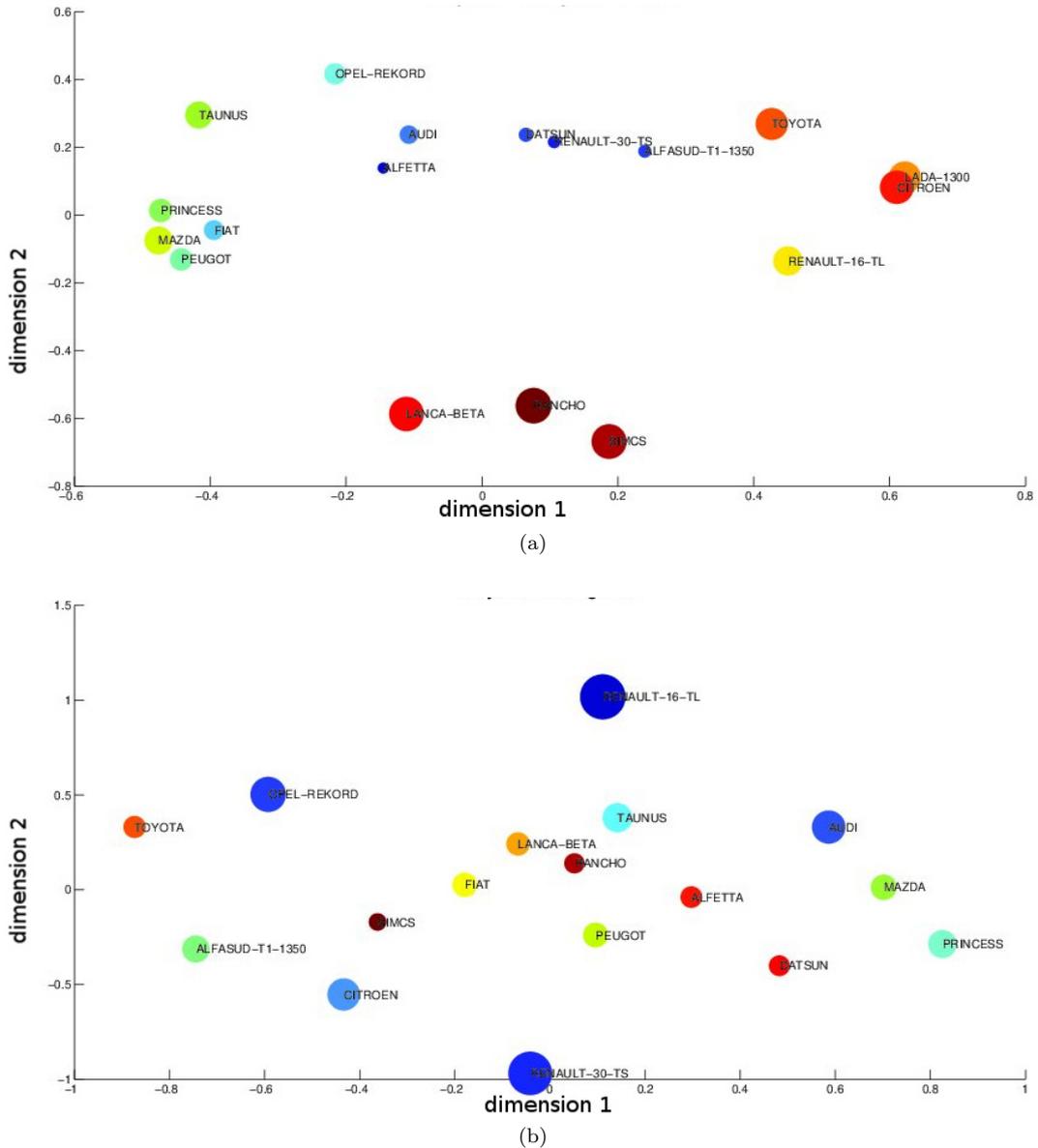


Figure 9.. Projection of the car data set using KPCA (a) and MDS (b).

519 is in relation to the size of the circles and to the quality of the projected points.  
 520 However, it is not possible to conclude anything about the closeness of these 4 points  
 521 as the distances here are in the feature space and are not related to the original space.  
 522 In Figure 7, we can however conclude that the two cars, the Mazda and Fiat, are  
 523 well projected in the reduced space, and they have similar characteristics as these  
 524 two cars are close. The same conclusion can be made for the Peugeot and Princess  
 525 cars. From this, it is possible to conclude that there is a large difference between the  
 526 two cars, the “Toyota” and “Renault 3” as the distance between these two cars is

527 significant. Conversely, the distance between the “Lada1300” and “Citroen” is small,  
528 thus indicating the closeness of these two cars. Note that these two cars are very well  
529 projected, resulting in a very good interpretation of the distance between them.

530 Therefore, radii are meaningful in our method and give an interpretation about the  
531 distances between points whereas the distances between the projected points using  
532 PCA, KPCA and MDS are not interpretable. This is a particular strength of our  
533 method. Projection under pairwise distance control suggests an absolute interpretation  
534 whereas the other methods provide a relative one.

535 For the qualitative and functional data sets and using MDS, recall the definition of  
536 the Gram matrix called  $B$  which is equal to  $X'X$  where  $X$  is the coordinate matrix in  
537 the reduced space. Thus, it is necessary to verify that the matrix  $B$  obtained by the  
538 MDS method is semi-definite positive to use the squared cosine as the quality measure  
539 because the starting point of optimization is obtained from MDS. After this, in case  
540 of positiveness of matrix  $B$ , the quality measure can be calculated.

541 **Soybean data set:** In the projection of the soybean data set, four classes are shown  
542 in Figure 10 and each class contains the disease number of the class. The whole set of  
543 points can however be divided in two large classes. Indeed, it is clear that Class 2 is  
544 well separated from the other classes as there is no intersection between the circles of  
545 Class 2 and the circles of other classes. Moreover, Class 1 can be considered as well  
546 separated class from Classes 3 and 4 if the largest circle  $D_3$  is not taken into account.  
547 Classes 3 and 4 are not well separated at all, as there are different intersections between  
548 the circles of these two classes. This result is shown in Stepp (1984) which labels the  
549 first two classes as “normal” and the latter two classes as “irrelevant”. A comparison  
550 of results from projection under pairwise distance control with PCA and KPCA is not  
551 possible for this data set because the matrix  $B$  is not semi-definite positive. Regarding  
552 Figure 11, it is clear that Class 4 exhibits the worst projection quality, whereas Classes  
553 1 and 2 show better projection quality. Therefore, it is possible to draw the same  
554 conclusion for the Iris and car data sets when using MDS as a projection method, the  
555 projection quality of points is dependent on the class of the points.

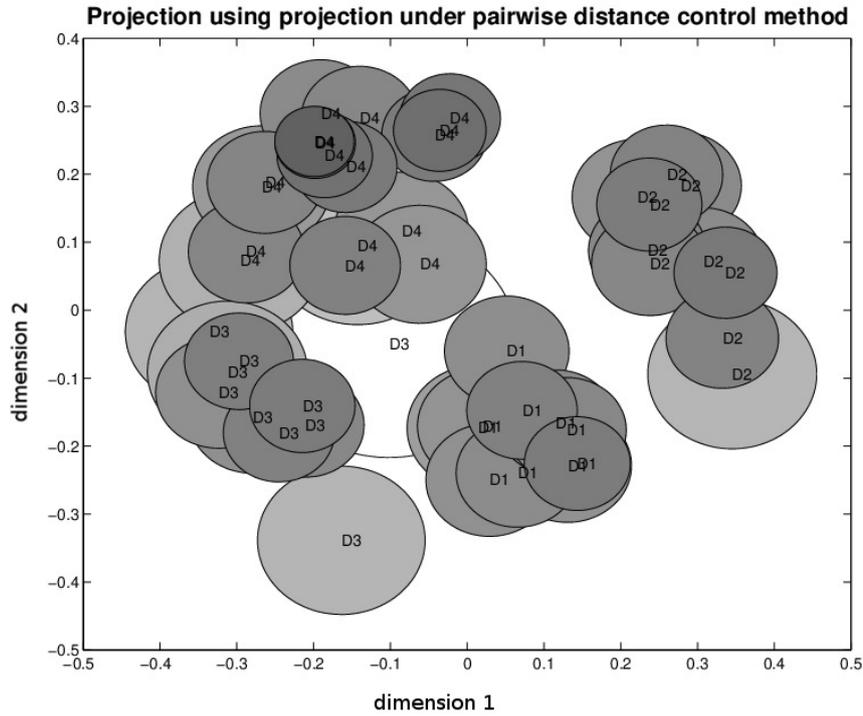


Figure 10.. Projection under pairwise distance control for the soybean data set. Four groups are presented, indexed by D1, D2, D3 and D4.

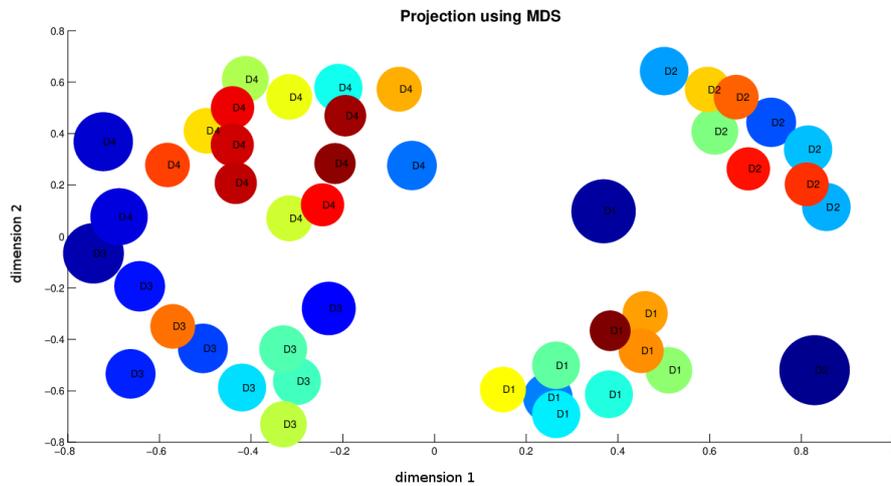


Figure 11.. MDS for the soybean data set. Four groups are presented, indexed by D1, D2, D3 and D4.

556 **Coffee data set:** The coffee data set has been studied in several articles (Briandet  
 557 *et al.* 1996, Bagnall *et al.* 2012) and different classification methods have shown the  
 558 different groups contained in this data set. The grouping structure obtained can be

559 clearly seen in Figures 12 and 13

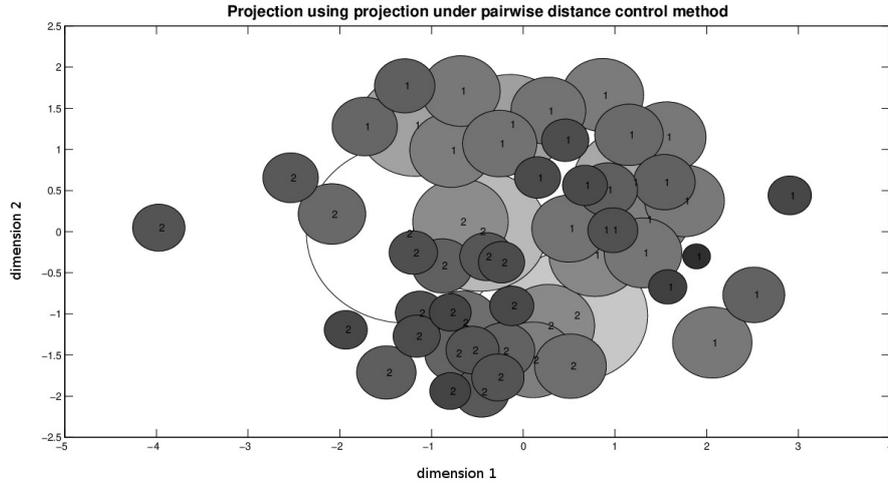
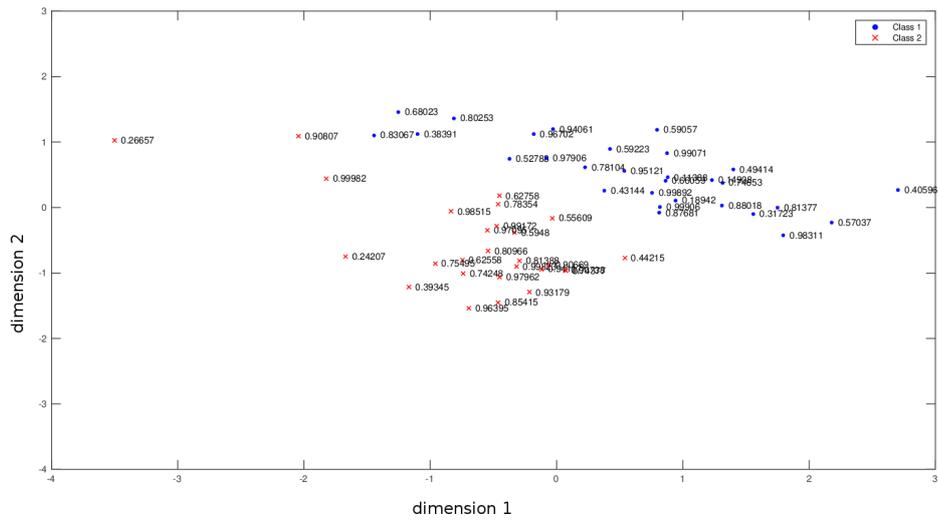


Figure 12.. Projection of the coffee data set using projection under pairwise distance control. Two clusters, indexed 1 and 2, indicate the Arabica and Robusta classes respectively.

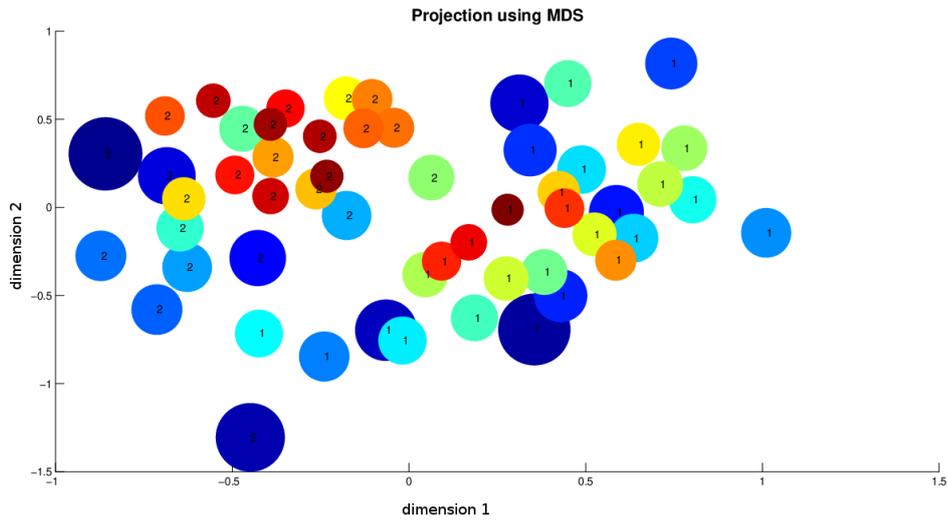
560 In Figure 12, we show that we have succeeded in differentiating the Arabica from  
561 Robusta coffee. These two classes are clearly presented, the first class indexed by  
562 number 1, corresponding to Arabica coffee, and the second one indexed by number 2,  
563 corresponding to Robusta coffee. These classes are not well separated in comparison  
564 with the results of quantitative data, since there are many intersections. Therefore,  
565 the representation of the points as circles and not as simple points provides more  
566 information about the real point classes and shows the points that are at risk of being  
567 misplaced in a particular class.

568 Figures 13a and 13b show the projection quality using PCA and MDS respectively.  
569 As all the eigenvalues of matrix  $B$  are positive, we can compute the quality measure  
570 given by PCA. Comparing the projection quality of PCA and projection under pairwise  
571 distance control provided by Figures 13a and 12, respectively, it can be seen that the  
572 quality of projection of the set of points is quite steady.

573 Additionally, Algorithm 2 was applied to these data sets. The trace plots of the  
574 optimization problem  $\mathcal{P}_{r,x}$  are shown in Figure 14 after 5000 iterations. It is important  
575 to note that the value of the sum of radii  $\sum_{i=1}^n r_i$  decreases rapidly in the first iterations  
576 and stays roughly constant after 1000 iterations for the different data sets, with the



(a)



(b)

Figure 13.. Projection of coffee data set using PCA and MDS.

577 exception of the car data sets. Thus, we can decrease the number of iterations from  
 578 5000 to almost 2000, or even 1000, in order to reduce the speed time.

579 Finally, the computer speed time of the proposed method is compared with that  
 580 using the classical methods. Table 2 shows the computer speed time for the four data  
 581 sets using PCA, KPCA, MDS, Algorithm 1 and Algorithm 2. It is clear that our  
 582 method takes more time than the existing methods. However, Algorithms 1 and 2 are  
 583 expected to significantly increased by using the C++ programming language (instead

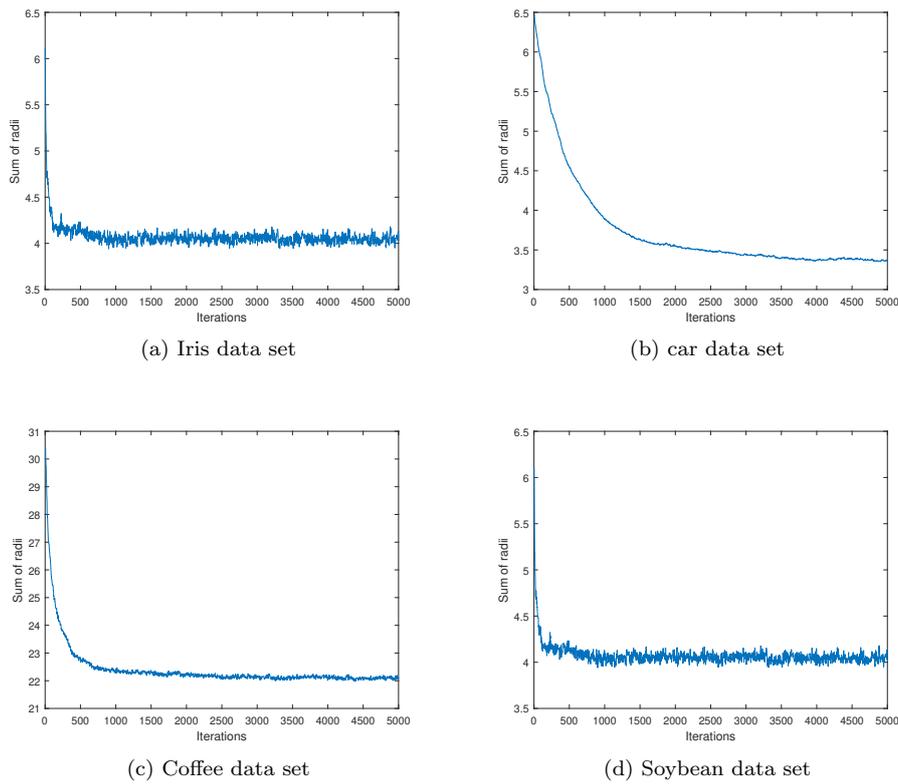


Figure 14.. Trace plots of Metropolis Hastings for different data sets. The x-axis corresponds to the iteration number and the y-axis to the value of  $\sum_{i=1}^n r_i$ .

584 of MATLAB currently) to produce more efficient code. In addition, by comparing the  
 585 computer speed time of the two algorithms and by referring to Table 1, the solu-  
 586 tions obtained using Algorithm 1 and Algorithm 2 are very close, which indicates that  
 587 Algorithm 2 can be used instead of Algorithm 1 to obtain a better solution faster (be-  
 588 tween two and four times faster). Thus, Algorithm 2 (Metropolis Hastings algorithm)  
 is recommended for use as it takes less time.

Table 2.. Computer speed time (in seconds) using different methods for the four data sets

Computer speed time (sec.)					
	PCA	KPCA	MDS	Algo 1	Algo 2
Iris	3.61	5.21	5.54	1124	600
Cars	2.70	4.17	4.62	671	300
Soybean	–	–	2.65	2036	698
Coffee	3.68	–	3.18	1968	589

590 4.4.2. Dimensionality reduction results

591 Our method can also be directly used to reduce the dimensionality of data (possibly  
 592 using it beyond visualization in  $\mathbb{R}^2$ ). This only requires solving problem  $\mathcal{P}_{r,x}$  using  
 593 different dimension values. In Figure 15, the values of  $\sum_{i=1}^n r_i$  were plotted as a guide  
 594 for choosing the reduced number of variables. This figure shows the values of  $\sum_{i=1}^n r_i$   
 595 for the different data sets using different dimensions. It is clear that the value of  $\sum_{i=1}^n r_i$   
 596 decreases when the dimension increases. Indeed, the sum of radii  $\sum_{i=1}^n r_i$  decreased  
 597 rapidly in low dimensions and then decreased slowly when the dimension increases.

598 The main problem, which is widely posed in dimensionality reduction methods, is  
 599 the determination of the number of components that need to be kept. Many meth-  
 600 ods have been discussed in the literature (Besse 1992; Jolliffe 1986) to determine  
 601 the dimension of the reduced space, relying on different strategies related to a good  
 602 explanation or a good prediction. Thus, with our method the choice of the reduced  
 603 space dimension is related to the local projection quality of points and how much the  
 604 user is interested in the projection quality of points.

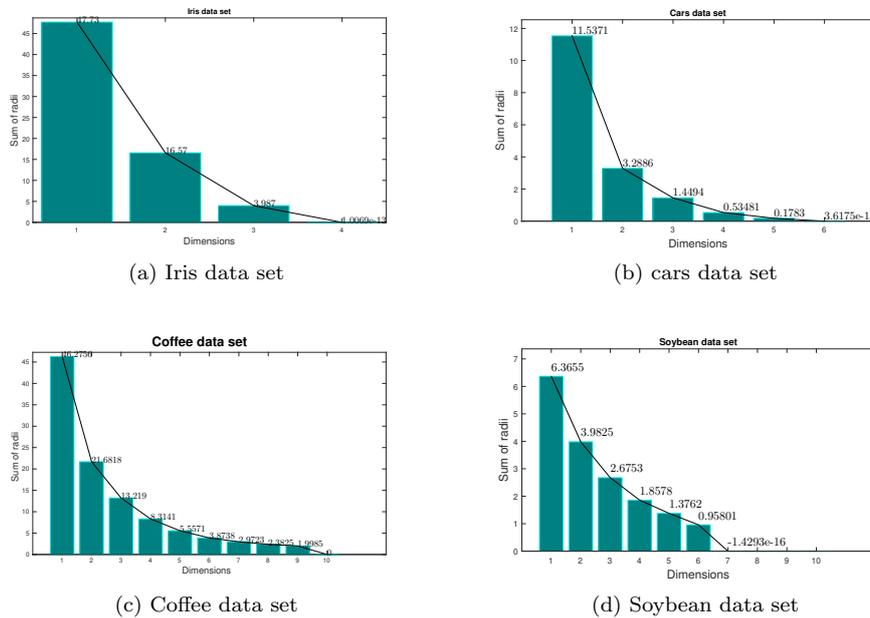


Figure 15.. Scree plots of  $\sum_{i=1}^n r_i$  for different dimensions for the four data sets.

605 Regarding the quantitative data sets (Iris and car), if the main objective of the  
 606 user is to obtain a very good projection quality, then a choice of three components

607 against four for Iris data set, and six for the car data set can be a good choice, as the  
608 value of  $\sum_{i=1}^n r_i$  is small and there is not a large difference between this value and  
609 the values for higher dimensions. For the coffee data set, a dimensionality reduction  
610 from 56 sample time series down to 6 simple extracted features is considered as a good  
611 choice. As for the soybean data set, a reduced space dimension equal to 4 dimensions  
612 can be considered as an appropriate reduced space.

613 A comparison of our results with the existing results shows a coherence between  
614 them. For the Iris data set, Chiu (1996) and Liu and Setiono (1995) concluded  
615 that the number of variables could be reduced to 2 as the petal length and petal  
616 width variables are the most important variables from all the variables. For the car  
617 data set, Saporta (2006) (Table 7.4.1 page 178) noticed that the conservation of two  
618 dimensions led to the explanation of 88% of inertia, where the inertia term reflects  
619 the importance of a component. Therefore, these results seem very similar to our  
620 results, with the important decrease located between dimensions 1 and 2. The other  
621 reductions are negligible for these two data sets. A selection of variables was studied on  
622 time series coffee data set by Andrews and McNicholas (2014). Using several analysis  
623 methods, the number of selected variables ranged between 2 and 13. This result is also  
624 seen using our method, a number of reduced variables taken between 2 and 9 gives a  
625 good projection. Regarding the soybean data set, Dela Cruz shows in his paper Dela  
626 Cruz (2015) that the 35 attributes can be reduced to 15. With our method, we have  
627 succeeded in reducing the attributes to 6 by having a very good projection of points.  
628 Hence, the results presented confirm that the dimension nonlinearly can be reduced  
629 while assessing a reasonable number of dimensions at the same time.

## 630 5. Conclusion

631 The purpose of this paper was to outline a new nonlinear projection method based  
632 on a new local measure of projection quality. Of course, in some projection methods,  
633 a local measure is given but this measure cannot be applied unless in cases of linear  
634 projections, and even then it is not efficiency for graphical representation.

635 The quality of projection is given here by additional variables called radii, which enable

636 bound on the original distances to be obtained. We have also shown that the idea can  
637 be written as an optimization problem in order to minimize the sum of the radii  
638 under some constraints. As the solution of this problem cannot be obtained exactly,  
639 we developed a stochastic optimization method.

640 This method has several advantages. Firstly, it is a nonlinear projection method that  
641 takes into account the projection quality of each point individually. Secondly, the  
642 distances between projected points are related to the initial distances between points  
643 offering a way to easily interpret the distances observed in the projection plane. The  
644 projection quality of each point can even then be used outside our method, as a post-  
645 processing of PCA or MDS for example. Finally, it appears to be efficient in terms of  
646 dimensionality reduction for the selection of the dimension of the reduced space based  
647 on the local quality of projection.

648 As perspectives, a lower bound for the optimization problem is needed and this radii  
649 approach could also be applied to other methods.

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# Appendix

## 748 Proof of proposition 3.1

Let us consider a point  $x_i$  such that for an index  $j$ , the following inequality is saturated:

$$|d_{ij} - \|x_i - x_j\|| \leq r_i + r_j,$$

749 and the other inequalities involving  $i$  are not saturated. Then, the corresponding solu-  
 750 tion can be improved by moving  $x_i$  along the line  $x_j - x_i$  in order to decrease  $r_i$  and  
 751  $|d_{ij} - \|x_i - x_j\||$ .

752 **Proof.** The above condition means that  $x_i$  is rewritten as  $x_i + a(x_j - x_i)$  with  $a \in \mathbb{R}$   
 753 and we look for  $a$  such that  $|d_{ij} - \|x_i + a(x_j - x_i) - x_j\|| < r_i + r_j$ . In particular  $a \leq 0$   
 754 if  $d_{ij} - \|x_i - x_j\| \geq 0$  and is otherwise  $> 0$ . Let us now consider the other inequalities  
 755 corresponding to index pairs  $(i, k)$  with  $k \neq j$ . For each of them,  $\exists a \in [a'_k, a''_k]$  with  
 756  $a'_k < 0$  and  $a''_k > 0$  such that

$$|d_{ij} - \|x_i + a(x_j - x_i) - x_j\|| \leq r_i + r_j,$$

757 as these constraints are unsaturated. Finally, taking  $a$  different from 0 in  $[a', a'']$  with  
 758  $a' = \max_k a'_k$  and  $a'' = \min_k a''_k$ , all constraints involving  $i$  get unsaturated so that  $r_i$   
 759 can be decreased, thereby decreasing the objective function. Depending on whether  $a$   
 760 must be negative or positive, we take  $a = a'$  or  $a = a''$  respectively.

762 **Proof of proposition 3.2**

763 Let  $r_1, \dots, r_n; x_1, \dots, x_n$  be a feasible solution of  $\mathcal{P}_{r,x}$ , if  $\exists a$  such that  $\eta(a) < \sum_{i=1}^n r_i$

764 with  $\eta(a) = \sum_{1 \leq i < j \leq n} |d_{ij} - a \|x_i - x_j\||$ , then  $\exists \tilde{r}_1, \dots, \tilde{r}_n$  a solution of  $\mathcal{P}_{r,a}$  such that

765 
$$\sum_{i=1}^n \tilde{r}_i < \sum_{i=1}^n r_i.$$

766 **Proof.** Let us consider  $r_1, \dots, r_n; x_1, \dots, x_n$  a feasible solution of problem  $\mathcal{P}_{r,x}$  and

767  $a, \tilde{r}_1, \tilde{r}_2, \dots, \tilde{r}_n$  a solution of  $\mathcal{P}_{r,a}$  where  $a$  is kept constant. For the solution of  $\mathcal{P}_{r,a}$ , for

768 each point  $i$ , we have a certain saturated constraint associated to point  $k$  denoted by

769  $C_{ik(i)}$ , otherwise we can easily saturate it using proposition 3.1. Thus, we have:

$$\begin{aligned} |d_{i1} - a \|x_i - x_1\|| &\leq \tilde{r}_i + \tilde{r}_1 \\ &\vdots \\ |d_{ik(i)} - a \|x_i - x_{k(i)}\|| &= \tilde{r}_i + \tilde{r}_{k(i)} \\ &\vdots \\ |d_{ij} - a \|x_i - x_j\|| &\leq \tilde{r}_i + \tilde{r}_j \\ &\vdots \\ |d_{in} - a \|x_i - x_n\|| &\leq \tilde{r}_i + \tilde{r}_n. \end{aligned}$$

770 Then,  $|d_{ik(i)} - a \|x_i - x_{k(i)}\|| = \tilde{r}_i + \tilde{r}_{k(i)} \geq \tilde{r}_i$ . By summing for all points  $i$ , for  $i =$

771  $1, \dots, n$ , we obtain:

$$\sum_{i=1}^n |d_{ik(i)} - a \|x_i - x_{k(i)}\|| \geq \sum_{i=1}^n \tilde{r}_i.$$

772 Thus,  $\sum_{1 \leq i < j \leq n} |d_{ij} - a \|x_i - x_j\|| \geq \sum_{i=1}^n |d_{ik(i)} - a \|x_i - x_{k(i)}\|| \geq \sum_{i=1}^n \tilde{r}_i.$

773 Note  $\eta(a) = \sum_{1 \leq i < j \leq n} |d_{ij} - a \|x_i - x_j\||$ , then if  $\eta(a) < \sum_{i=1}^n r_i$  there is a solution of  $\mathcal{P}_{r,a}$

774 such that  $\sum_{i=1}^n \tilde{r}_i < \sum_{i=1}^n r_i.$  □