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# Black-box optimization under constraints: simple selection algorithms and heuristic criteria \*

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## Abstract

This report was done during the Semaine d'Études Mathématiques et Entreprises (SEME) at the Institut de recherche mathématique de Rennes (IRMAR). The subject, proposed by the research centers Cenario and IRT Saint Exupéry, is about the characterization of optimization problems which can only be tested under a black-box procedure. We propose some selection criteria in order to categorize such problems.

## 1 Introduction

Optimization constitutes a large area of research in the context of modern applied mathematics, through its unique connection with over fields of mathematics such as linear algebra [O'L00], algebraic geometry [BPT13], topology [SM13], numerical analysis [All07], partial differential equations [Tr0], probability [Ste97] or statistics [Rus94], as well as its numerous applications in the contexts of classical mechanics [Bro88], civil engineering [HK03], molecular modeling [FT15], economics and finance [Dor69, Mal89, RW97], and so on.

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*MSC codes.* 49-01, 62-01, 65-01

In the mathematical formalism, an **optimization problem** aims to find (or at least estimate) a minimum  $x^*$  of a continuous function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  defined on the whole space  $\mathbb{R}^n$  with  $n \in \mathbb{N}^*$ , namely

$$x^* = \min_{x \in \mathbb{R}^n} f(x),$$

under the following constraints:

- some **bounded constraints**

$$l_i \leq x_i \leq u_i$$

for  $i = 1, \dots, n$  and  $l = (l_1, \dots, l_n)$ ,  $u = (u_1, \dots, u_n) \in \mathbb{R}^n$ ,

- some **inequality constraints**

$$g_j(x) \leq 0$$

for  $g_j : \mathbb{R}^n \rightarrow \mathbb{R}$  with  $j = 1, \dots, p$  and  $p \in \mathbb{N}$ ,

- some **equality constraints**

$$h_k(x) \leq 0$$

for  $h_k : \mathbb{R}^n \rightarrow \mathbb{R}$  with  $k = 1, \dots, q$  and  $q \in \mathbb{N}$ .

In the following, we will assume that the variable  $x$  satisfies some bounded constraints in each directions of the space  $\mathbb{R}^n$ , and we will denote

$$\Omega = \{x \in \mathbb{R}^n \mid \forall i \in \llbracket 1, n \rrbracket, l_i \leq x_i \leq u_i\}.$$

Inequality and equality constraints then generate a subset of  $\Omega$ , called **feasible set**,

$$\mathcal{C} = \{x \in \Omega \mid g(x) \leq 0 \text{ and } h(x) = 0\}.$$

As  $\Omega$  defines a compact subset of  $\mathbb{R}^n$ , the continuous function  $f$  well admits a global minimum  $x^*$  on the feasible set  $\mathcal{C}$ . Note that the unicity of the global minimum  $x^*$  is not guaranteed under such little assumptions, and would require additional properties such as convexity of the function  $f$  and the feasible set  $\mathcal{C}$ . We refer to the book [BV04] for an introduction to convex optimization.

In the literature, as  $\mathcal{C} \neq \mathbb{R}^n$ , our problem takes place in the field of *constrained optimization*, as opposed to *unconstrained optimization* which focuses on the minimization of the objective function on the whole space  $\mathbb{R}^n$  (see [NW06] for a presentation of the most popular techniques to solve this type of problem). At this stage, we can also mention the field of *combinatorial optimization* [CCPS98], which deals with discrete functions or/and discrete feasible sets (contrary to *continuous optimization*), and *stochastic optimization* [SDR21], when the function  $f$  depends on some random variables (otherwise we say that we have a *deterministic optimization* problem).

In our setting, the objective function  $f$  and the constraint  $g$  and  $h$  are unknown, and can only be tested under a **black-box procedure**: we assume that we can only generates random points on the feasible set  $\mathcal{C}$  and the graph of  $f$

$$\mathcal{G}_f = f(\Omega) = \{y \in \Omega \mid \exists x \in \Omega, y = f(x)\},$$

and that we can test if a random point  $x \in \Omega$  belongs to one of those sets or not. Note that generating random data points in a subset of  $\mathbb{R}^n$  is an area of research on its own, and is covered

by a large literature (see for instance [DHS13] and references within). Another important feature of statistical learning is about corrupted data, where samples are perturbed by typically Gaussian noise or outliers [BL94], hence efficient optimization algorithms in this black-box setting obviously have to be robust with respect to noisy data.

Finding relevant and computable criteria in the context of black-box optimization, as well as finding efficient methods in order to estimate these criteria, has been an important topic of *statistical optimization* in the past few years, in particular with the recent development of data analysis and machine learning, and the large demand coming from the industrial world. A particular focus has been made on the implementation of criteria based on the objective function [Mal21], but we can also cite [MOE15] for some criteria on the feasible set.

This report presents the results obtained during the *Semaine d'Etude Mathématiques et Entreprises* (SEME), organized by the *Agence pour les Mathématiques en Interaction avec l'Entreprise* (AMIES) and the *Centre Henri Lesbesgue*, which took place in Rennes from 2 to 6 May 2022. Our subject, called "Characterization of Optimization Problems", was proposed by Paul Beaucaire from the applied research center Cenearo and Benoît Pauwels from the technological research institute IRT Saint Exupéry. Note that the majority of the authors have never worked into the field of statistical optimization before this week, so a reader familiar with the topics of this paper may find our approach a bit naive, however, we hope we may have tackled some rather simple but still interesting discussions and opened some meaningful perspectives.

This note is outlined as follows. Section 2 presents a criterion based on the Hessian matrix of the cost function. In Section 3, we propose criterion based on the nature of the feasible set. Perspectives about our criteria are given in Section 4.

## 2 Condition number of the Hessian matrix criterion

The Hessian matrix of the cost function that we aim to minimize is rich of valuable information that can help us in the choice of a convenient algorithm to solve our optimization problem. In particular, the conditioning of the Hessian matrix can tell us whether it is judicious or not to choose a first or a second order optimization method. In fact, ill-conditioned Hessian matrix affects directly the numerical performance of first and second order optimization methods. In this case the contours of the basins of the cost function tend to be *ellipsoids* which imposes some difficulties on the convergence of the descent direction in a first order method towards a local minimum, for example, the descent gradient (since it has to follow a *zigzag* path towards the local minimum). On the other hand, for a second order optimization method, the computation of the descent direction is based on solving a linear system by taking the inverse of the Hessian matrix, hence ill-conditioned Hessian matrix remains its inversion numerically unstable, to see this we can simply take the SVD decomposition of the Hessian matrix  $U\Sigma V^t$ , if the Hessian is ill-conditioned the smallest singular value is tend to be *close* to zero, then its inverse that appears in the inversion of the Hessian matrix  $U\Sigma^{-1}V^t$  will blow up.

Hereafter, we present a simple test that can describe the conditioning of the Hessian matrix of the cost function. Based on this criterion one can decide if it is gainful to apply one determinist order one or two optimization algorithm. Roughly speaking, this could be the case when the objective

function tends to have a few number of points such that the Hessian matrix is ill-conditioned. More concretely, this is the case when the set of points of ill-conditioned Hessian matrix is not of large volume. In the opposite case, i.e., the test shows that the aforementioned set is of large volume, thus this can be a sign to move for instance to one of the stochastic search optimization algorithm that does not rely necessarily on the derivatives of the objective function, and this to avoid the weak numerical performance of first or second optimization method expected according to this test.

- Randomly sample  $k$  points in the search space according to an uniform distribution
- At each point construct a neighborhood that contains  $N$  random points according to a uniform distribution
- Set  $i_j = 0$  for  $j \in \{1, \dots, k\}$
- For each neighborhood, i.e., for each  $j \in \{1, \dots, k\}$  compute at each point the SVD of the Hessian matrix. If the ratio of the largest singular value over the smallest singular value is higher than a threshold  $\alpha$  (for example  $10^6$ ) then  $i_j = i_j + 1$
- Return  $I = (i_1, \dots, i_k)$ , the mean and the standard deviation given by the  $k$  set.

### 3 Geometry and topology of the feasible set

It is readily intuitive that the geometry and topology of the feasible set  $\mathcal{C}$  directly depend on the nature of the constraints: bound and inequality constraints generate **thick** subsets, namely sets of non-null volume with respect to the underlying Lebesgue measure  $d\lambda$  of the  $n$ -dimensional box  $\Omega$ , whereas equality constraints  $h_k$  generate **thin** subsets, whose implicit dimension  $d_k < n$ . From a black-box point of view, it is crucial to effectively estimate the underlying dimension  $d$  of the feasible set  $\mathcal{C}$ , in order to apply the most effective algorithm to estimate  $x^*$ .

A classical procedure in order to estimate the volume of a subset of  $\Omega$  is the **Monte Carlo method**: we generate a number of random samples  $X_1, \dots, X_N \in \Omega$  with  $N \in \mathbb{N}^*$ , and we compute the estimator

$$V_N = \frac{1}{N} \sum_{i=1}^N \mathbb{1}_{\{X_i \in \mathcal{C}\}},$$

which is an approximation of the volume  $V = \text{Vol}(\mathcal{C})$  with respect to the measure  $d\lambda$  from the law of large numbers. The Monte Carlo method is for instance used in order to estimate the transcendent number  $\pi$ , by simulation random points in a 2-dimensional box and calculating the ratio between the number points that lied inside the centered circle of radius 1 and the total number of generated points. This method is considered as pretty efficient, as it does not depend on the dimension  $n$ , and it converges in  $\mathcal{O}(N^{-1/2})$  from the Central Limit Theorem. Note that this simple Monte Carlo procedure can be improve for better efficiency, and we refer to the recent survey [LMB<sup>+</sup>20] for discussions on different refinements of the Monte Carlo method.

In our setting, we fix an infinitesimal threshold  $\varepsilon_V > 0$ , we perform a Monte Carlo procedure on the feasible set  $\mathcal{C}$  with a large number  $N$  of samples, and we infer:

- if  $V_N \geq \varepsilon_V$ , we consider that  $\mathcal{C}$  is a thick set, and we are then interested in determining some of its topological properties (see Section 3.1), such as connectedness, convexity, ect...

- if  $V_N < \varepsilon_V$ , then we consider that  $\mathcal{C}$  is a thin set, and we seek some of its geometrical properties such as its underlying dimension, if it fits an affine subset of  $\Omega$ , or more generally if it can be approximated by an algebraic curve or surface via a regression procedure (see Section 3.2).

### 3.1 Topology of a thick feasible subset

In this section we are interested in the study of the connected components of the feasible set  $\mathcal{C}$ . Some iterative optimization algorithms require to stay in the feasible set at each iteration which makes jumps from one connected component to another less likely and, therefore, restricts the exploration to a few components. Thus, it appears that, a lot of connected components for  $\mathcal{C}$  will result in inefficiency for some of those optimization algorithms.

Suppose that  $\mathcal{C}$  has a finite number of connected components denoted by  $C_1 \dots, C_k$ . From the previous discussion, it seems that estimating the number of connected components  $k$  is relevant. Another interesting quantity to look at could be the following:

$$p := \frac{\sum_{i=1}^k V_i^2}{\left(\sum_{i=1}^k V_i\right)^2}$$

where  $V_i$  is the volume of the component  $C_i$  (in the sense of the Lebesgue measure). It is important that the feasible set has a positive volume in order to make sense of the quantity  $p$ . Intuitively,  $p$  corresponds to the probability that an iterative algorithm initiates on the component containing the global minimum of the objective function. Indeed, if we suppose that the global minimum  $x^*$  and the starting point  $x_0$  of the algorithm are i.i.d random variables with uniform distribution on  $\mathcal{C}$ , then  $p$  is exactly the probability that  $x^*$  and  $x_0$  belongs to the same connected component. A small value for  $p$  implies that iterative algorithms restricted to the feasible set are less likely to find the global minimum.

**Description of the algorithm.** In this paragraph we describe an algorithm that estimates both  $k$  and  $p$ . The algorithm starts by taking  $N$  i.i.d points  $X_1, \dots, X_N$  uniformly in  $\mathcal{C}$ , where  $N$  is a parameter of the algorithm to choose. To do so, one can simply take i.i.d points uniformly in a big box containing  $\mathcal{C}$ , keep the points in  $\mathcal{C}$  and reject the points outside of  $\mathcal{C}$  until  $N$  points fall in  $\mathcal{C}$ . Then, for each pair of points  $(X_i, X_j)$  with  $i < j$  we test if  $X_i$  and  $X_j$  are *strongly connected*, meaning that the two following conditions are satisfied:

1. The distance between  $X_i$  and  $X_j$  is smaller than  $\gamma N^{-1/d}$  where  $d$  is the dimension of the problem and  $\gamma$  is a parameter of the algorithm. (In our implementation we took the euclidean distance but, one could take any distance, for instance, the distance associated with the  $L^\infty$  norm which is easy to handle in a program).
2. All the points  $tX_i + (1-t)X_j$  for  $t = 0, \frac{1}{K}, \frac{2}{K}, \dots, 1$  belongs to  $\mathcal{C}$  where  $K$  is another parameter of the algorithm.

Intuitively, two points  $X_i$  and  $X_j$  are strongly connected if they are close and the segment  $[X_i, X_j]$  "almost" belongs to  $\mathcal{C}$ . If two points are strongly connected the algorithm considers that they are in the same connected component. Of course the converse is false: two points could be in the same connected component without being strongly connected. This is why the algorithm determines

the transitive closure of this relation. To do so, the algorithm performs a depth first search on the underlying graph where the nodes are the points  $X_1, \dots, X_N$  and edges are drawn between points that are strongly connected. In the end, the algorithm returns the connected component of this graph which approximates the sets of points that are in the same connected component of  $\mathcal{C}$ . Counting the proportion of points in each component, one can determine  $V_1, \dots, V_k$  and therefore, deduce the quantity  $p$ . See Figure 1 for a visualisation.

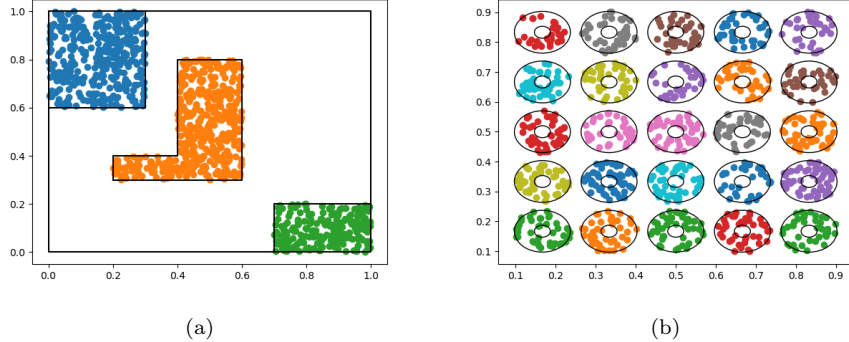


Figure 1: Application of our algorithm for two feasible sets in dimension 2. Here  $N = 1000$ ,  $K = 10$  and  $\gamma = \sqrt{10}$ . Points that share the same colour are considered to be in the same connected component by the algorithm. (a) The feasible set is composed of 2 rectangles and a L shape box, the algorithm finds the 3 components and computes  $p = 0.35$  (the real value being  $p = 0.36$ ). (b) The feasible set is composed of 25 rings, the algorithm finds the 25 components and computes  $p = 0.041$  (the real value being  $p = 0.4$ ).

**Complexity of the algorithm.** Here we discuss the complexity of the algorithm we presented. First, the rejection sampling is of complexity  $O(NV^{-1})$  where  $V = V_1 + \dots + V_k$  is the total volume of  $\mathcal{C}$ . Then, computing the adjacency matrix for the strongly connected relation is in  $O(N^2 + KN)$ . If, as a definition of strongly connected, we took only the second condition, the complexity would be  $O(KN^2)$ . Finally, the depth first search has a linear complexity  $O(N)$ .

**Extension to thin feasible sets.** Our method heavily relies on the fact that the feasible set  $\mathcal{C}$  has a positive volume. If it is not the case, then the rejection sampling won't work, because the probability that a point falls in  $\mathcal{C}$  is 0. However the study of connected components stay relevant even if the feasible set is thin. To circumvent this difficulty, one could relax the constraints in order to obtain a thick set. There are two drawbacks to this technique: first, even with a relaxation, the volume of the feasible set could stay really small and the complexity of the rejection sampling could be really high. Second, the algorithm will obviously be less precise since the relaxation will probably modify the number and the shape of the connected component. Another solution would be to be able to generate random points on the feasible set. This is not always possible, especially if the analytic form of the constraints is unknown (which is our case here). However, if the only constraint is of the type  $h(x) = 0$  with  $h$  continuous such that both  $h^{-1}(]-\infty, 0])$  and  $h^{-1}(]0, +\infty[)$  have positive volume, then it is possible to generate random points on the feasible set  $h^{-1}(\{0\})$ . To

do so, one could generate two random points  $X_1$  and  $X_2$  such that  $h(X_1) < 0$  and  $h(X_2) > 0$  with a rejection sampling method. Then, with Newton's method, one could find a zero of the function  $H : t \in [0, 1] \mapsto h(tX_2 + (1-t)X_1)$ . If the derivative of  $H$  is unknown, a simple discretisation of the derivative could be considered. The zero of  $H$ , will then be our random generated point on the feasible set. It should be noticed that the law of that random point has no reason to be uniform on the feasible set. But this does not necessarily imply that our algorithm will fail.

## 3.2 Geometry of a thin feasible subset

### 3.2.1 Affine subspace : Principal Component Analysis (PCA)

We first assume that  $\mathcal{C}$  is an affine subset of  $\Omega$ , in the sense that there exist  $d + 1$  vectors  $v_0, v_1, \dots, v_d \in \Omega$  such that

$$\mathcal{C} = \left\{ y \in \Omega \mid \exists (\alpha_1, \dots, \alpha_d) \in \mathbb{R}^d, y = v_0 + \sum_{i=1}^d \alpha_i v_i \right\}, \quad (1)$$

with the obvious inequality  $d < n$ . In order to obtain the dimension  $d$  of  $\mathcal{C}$ , as well as the vectors  $(v_i)_{1 \leq i \leq d}$ , we compute from  $N$  random samples  $X = X_1, \dots, X_N \in \mathcal{C}$  the empirical covariance matrix

$$C = \text{Cov}(X, X) = \frac{1}{N-1} \sum_{i=1}^N (X_i - \bar{X})(X_i - \bar{X})^T,$$

where  $\bar{X}$  denotes the sample mean

$$\bar{X} = \frac{1}{N} \sum_{i=1}^N X_i.$$

This matrix is a real symmetric matrix of dimension  $n$ , namely  $C \in \mathcal{S}_n(\mathbb{R})$ , and we denote by  $\lambda_1, \dots, \lambda_n$  its real positive eigenvalues sorted in decreasing order

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n, \quad (2)$$

and  $v_1, \dots, v_n$  the associated eigenvectors.

The idea of the PCA method is to determine an orthogonal linear change of basis in order to reduce the dimension of the problem by projecting the data onto the first relevant components. Mathematically speaking, it is a direct consequence of standard linear algebra theory: as the covariance matrix  $C \in \mathcal{S}_n(\mathbb{R})$ , there exists a diagonal matrix  $D = \text{diag}(\lambda_1, \dots, \lambda_n)$  satisfying (2) and an orthogonal matrix  $P \in \mathcal{O}_n(\mathbb{R})$  that can be written

$$P = \left( \begin{array}{c|c|c} v_1 & \dots & v_n \end{array} \right),$$

such that  $C = PDP^{-1}$ . In practice, we then have to fix an infinitesimal threshold  $\varepsilon_\lambda > 0$  (typically  $\varepsilon_\lambda \sim 10^{-15}$ ), so that the PCA method determines that eigenvectors associated to eigenvalues smaller



than the threshold  $\varepsilon_\lambda$  do not constitute relevant directions for the sample data. In our setting, that induces the existence of an integer  $d_N < n$  such that

$$\varepsilon_\lambda \geq \lambda_{d_N+1} \geq \dots \geq \lambda_n,$$

and we can consider that the feasible set is an affine space generated by the eigenvectors associated to the first  $d_N$  eigenvalues, namely  $\mathcal{C}$  is of the form (1). Note that this method also works if  $\mathcal{C}$  is a substantial enough subset of an affine space. At the contrary, this method is considered to fail if it sends back the value  $d_N = n$ , as we have already assume that  $\mathcal{C}$  generates no volume with respect to  $d\lambda$  on  $\Omega$ . It is also pretty robust to small perturbation of the data samples, and the threshold  $\varepsilon_\lambda$  can be adapted with respect to the supposed noise of the data.

In our test,  $N = 100$  data samples  $X_1, \dots, X_N \in \Omega = [0, 1]^3$  are generated on a random plane. We obtain a covariance matrix

$$C = \begin{pmatrix} 0.072471 & 0.016504 & 0.033138 \\ 0.016504 & 0.085320 & 0.036600 \\ 0.033138 & 0.036600 & 0.025502 \end{pmatrix},$$

which have the following eigenvalues  $\lambda_1 = 0, 12168$ ,  $\lambda_2 = 0, 061614$  and  $\lambda_3 = 4, 3514 \cdot 10^{-18}$ , associated with the eigenvectors

$$v_1 = \begin{pmatrix} -0.543298 \\ -0.705192 \\ -0.455556 \end{pmatrix}, v_2 = \begin{pmatrix} -0.770248 \\ 0.634557 \\ -0.063683 \end{pmatrix}, \text{ and } v_3 = \begin{pmatrix} -0.333985 \\ -0.316292 \\ 0.887927 \end{pmatrix}.$$

The PCA method then determines that the third eigenvalue is below the eigenvalue threshold, namely  $\lambda_3 < \varepsilon_\lambda = 10^{-15}$ , so our algorithm establishes that the data samples are not correlated under the direction  $v_3$ , and that we can estimate the set

$$\mathcal{C} = \{y \in \Omega \mid \exists \alpha_1, \alpha_2 \in \mathbb{R}, y = \alpha_1 v_1 + \alpha_2 v_2\}.$$

The algorithm also obviously estimate than the underlying dimension of the feasible set is  $d_N = 2$ . Figure 2 represents our simulation described above.

Some interesting generalization of the PCA method can be performed in the case where  $\mathcal{C}$  is an union of affine subspaces of  $\Omega$ : these methods are called *Generalized Principal Component Analysis* (GPCA), and we refer to [VMS16, MYDF08] for an introduction to these methods in the case of high-dimensional data. Note that these methods can be pretty robust to noisy data and outliers.

### 3.2.2 Algebraic variety: Multivariate Polynomial Regression (MPR)

Feasible set  $\mathcal{C}$  being an affine subspace of  $\Omega$  is of course a pretty strong assumption on the constraint  $h$ . A lighter assumption would naturally consists in  $h$  being a polynomial function on  $\Omega$ , which can be written  $h \in \mathbb{R}[x_1, \dots, x_n]$ , so that the constraint  $h = 0$  generates a feasible set contained in an algebraic variety

$$\mathcal{C} = \{x = (x_1, \dots, x_n) \in \Omega \mid h(x_1, \dots, x_n) = 0\}.$$

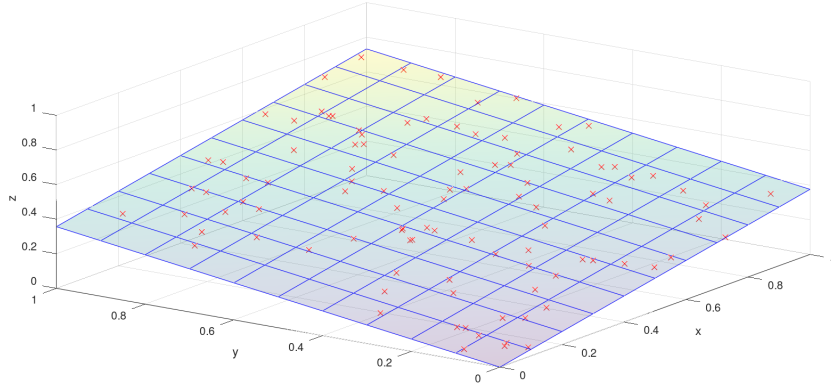


Figure 2: PCA method applied for data samples generated on a random plane of  $[0, 1]^3$ .

We restrain our attention in the case where  $h$  is of degree 1 with respect to at least one of the variable  $x_i$  with  $1 \leq i \leq n$ , so there exists a polynomial  $P \in \mathbb{R}[x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n]$  such that

$$h(x_1, \dots, x_n) = 0 \Leftrightarrow x_i = P(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n).$$

The Multivariate Polynomial Regression is then a surface fitting algorithm based on the minimisation of the standard Mean-Square Error (MSE). Note that, denoting

$$P(x_1, \dots, x_n) = \sum_{j \in \mathcal{J}} c_j x_1^{j_1} \dots x_n^{j_n}$$

with  $c_j \in \mathbb{R}$  for all  $j \in \mathcal{J}$  and

$$\mathcal{J} = \{j = (j_1, \dots, j_n) \in \mathbb{N}^n \mid j_i = 0 \text{ and } |j| := j_1 + \dots + j_n \leq \deg(P)\},$$

the dimension of the curve then corresponds to the quantity

$$d = \sup \{|j| \in \mathbb{N} \mid j \in \mathcal{J} \text{ and } c_j \neq 0\}.$$

In our test, in dimension  $n = 3$ ,  $N = 100$  data samples  $X_1, \dots, X_N \in \Omega = [0, 1]^3$  are randomly generated on a cubic curve

$$\mathcal{C} = \left\{ (x, y, z) \in \Omega \mid z = \frac{1}{8}(x + y)^3 \right\} \subset \Omega.$$

The aim of the MPR procedure is then to determine the algebraic equation

$$z = P(x, y) = \frac{1}{8}x^3 + \frac{3}{8}x^2y + \frac{3}{8}xy^2 + \frac{1}{8}y^3$$

by finding its coefficient in the basis  $(1, x, y, x^2, xy, y^2, x^3, x^2y, xy^2, y^3)$ . In practice, denoting  $X_i = (x_i, y_i, z_i)$  for  $1 \leq i \leq N$ , the algorithm solves the linear equation

$$Ac = z,$$

where  $A$  is the  $N \times 10$  Vandermonde matrix

$$A = \begin{pmatrix} 1 & x_1 & y_1 & x_1^2 & x_1 y_1 & y_1^2 & x_1^3 & x_1^2 y_1 & x_1 y_1^2 & y_1^3 \\ 1 & x_2 & y_2 & x_2^2 & x_2 y_2 & y_2^2 & x_2^3 & x_2^2 y_2 & x_2 y_2^2 & y_2^3 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_N & y_N & x_N^2 & x_N y_N & y_N^2 & x_N^3 & x_N^2 y_N & x_N y_N^2 & y_N^3 \end{pmatrix},$$

and

$$z = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_N \end{pmatrix}.$$

Note that the number of samples  $N$  is usually larger than the number of coefficients of the polynomial  $c$ , leading to an over-determined system, so the inverse matrix  $A^{-1}$  is to be understood in the least square sense, such that it is the unique matrix in  $\mathcal{M}_{10,N}(\mathbb{R})$  such that

$$AA^{-1} = \text{Id}_{N,N} \quad \text{and} \quad A^{-1}A = \text{Id}_{10,10}.$$

It is pretty straightforward to see that  $c$  minimizes the MSE, namely

$$c = \min_{c \in \mathbb{R}^{10}} \sum_{i=1}^N (Ac - z)^2$$

where the square notation as to be understand pointwisely. In our simulations, the algorithm do not manage to fit the samples  $X_1, \dots, X_N$  in the case of an approximation by a polynomial of degree 2 in the 6-dimensional basis  $(1, x, y, x^2, xy, y^2)$  (cf Figure 3), as it send back the polynomial

$$P^{(2)}(x, y) = 0.061575 - 0.333735x - 0.270596y + 0.386687x^2 + 0.747629xy + 0.329421y^2,$$

but manages to fit the data with a polynomial of degree 3 (cf Figure 4), sending back the polynomial

$$P^{(3)}(x, y) = 0.125x^3 + 0.375x^2y + 0.375xy^2 + 0.125y^3.$$

When dealing with polynomial regression, one have to care about overfitting phenomenon, *ie* that increasing too much the polynomial degree would exhibits some oscillatory and unnatural behavior between and outside the data sample points.

## 4 Perspectives

- We proposed to investigate the conditioning of the Hessian matrix of the objective function at points in the feasible set by proposing a test that computes the condition number of this matrix via SVD computation. A natural extension is to render this test more efficient in term of complexity and to propose more precised method than the random one to choose the points on which we look at the conditioning of the Hessian matrix. This can be done using for instance methods based on statistics and probabilistic analysis which can make the choice of the points more representative and then yields a more accurate study for the

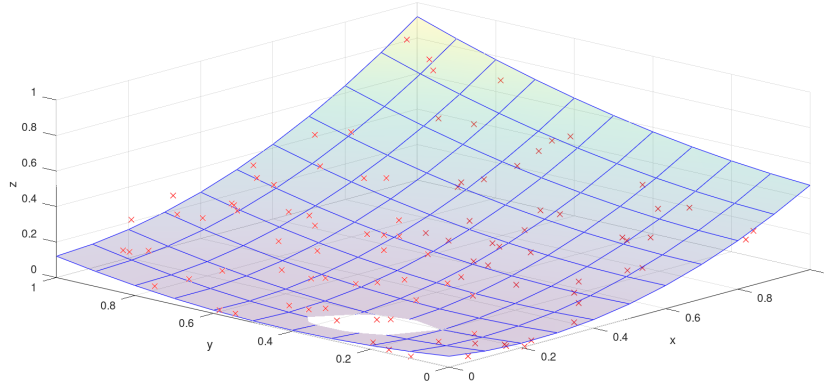


Figure 3: MPR method applied for data samples generated on a degree 3 surface of  $[0, 1]^3$  by a polynomial of degree 2.

conditioning of the Hessian matrix. Another important point to investigate is to study the Hessian matrix of the functions that appear in the equality and inequality constraints. This able us to understand for instance the curvature of the constraint set and then to have an idea on how much the geometry of this set is complicated. This can offer a valuable criterion that helps us in the selection algorithm process.

- A natural perspective of our work would be to implement a method which fits any algebraic curve from a number of sample data points. In fact, in optimization problems, natural constraints can appear under the form of sphere

$$\mathcal{S} = \{(x, y, z) \in \Omega \mid x^2 + y^2 + z^2 = 1\},$$

or more generally as ellipsoid, cylinder, circular paraboloid and so on. We can briefly mention some works which goes into this direction. In [HOZM08, GG20], the authors tackle the case of conics in  $\mathbb{R}^2$  in the case of noisy data, taking advantages of their algebraic classification. In a more general setting, [BKSW18] constitutes a pretty complete overview to this problem, but lack some precise convergence estimate with respect to  $N$ . For an introduction to precise statistical convergence rate, we refer to the preprint [AS21] and references within. We can howver mention that in the case of  $k$ -times smooth manifold [AL19], the authors E. Aamari and C. Levrard have shown a convergence rate in  $\mathcal{O}(N^{-k/d})$  in the case of noiseless data, where  $d$  is the intrinsic dimension of  $\mathcal{C}$  and  $N$  is the number of samples, and also give a lower bound in the framework of orthogonal noise models. The case of estimating singular varieties however seems to currently remain an open problem to the best of the authors knowledge.

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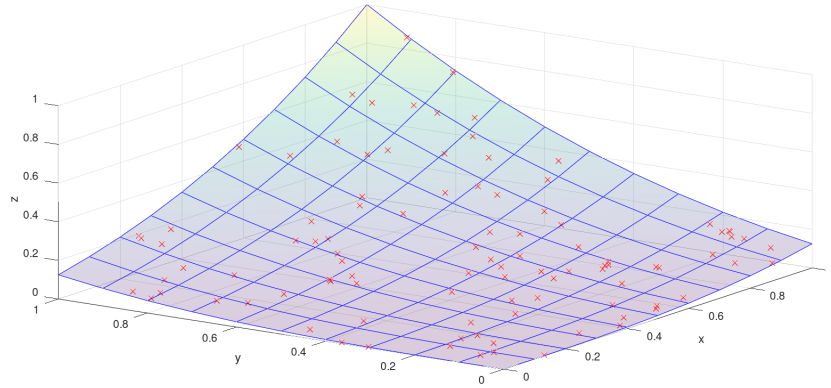


Figure 4: MPR method applied for data samples generated on a degree 3 surface of  $[0, 1]^3$  by a polynomial of degree 3.

## References

- [AL19] Eddie Aamari and Clément Levrard. Nonasymptotic rates for manifold, tangent space and curvature estimation. *Ann. Statist.*, 47(1):177–204, 2019.
- [All07] Grégoire Allaire. *Numerical analysis and optimization*. Numerical Mathematics and Scientific Computation. Oxford University Press, Oxford, 2007. An introduction to mathematical modelling and numerical simulation, Translated from the French by Alan Craig.
- [AS21] Yariv Aizenbud and Barak Sober. Non-parametric estimation of manifolds from noisy data, 2021.
- [BKSW18] Paul Breiding, Sara Kališnik, Bernd Sturmfels, and Madeleine Weinstein. Learning algebraic varieties from samples. *Rev. Mat. Complut.*, 31(3):545–593, 2018.
- [BL94] Vic Barnett and Toby Lewis. *Outliers in statistical data*. Wiley Series in Probability and Mathematical Statistics: Applied Probability and Statistics. John Wiley & Sons, Ltd., Chichester, third edition, 1994.
- [BPT13] Grigoriy Blekherman, Pablo A. Parrilo, and Rekha R. Thomas, editors. *Semidefinite optimization and convex algebraic geometry*, volume 13 of *MOS-SIAM Series on Optimization*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA; Mathematical Optimization Society, Philadelphia, PA, 2013.
- [Bro88] Pierre Brousse. *Optimization in mechanics: problems and methods*, volume 34 of *North-Holland Series in Applied Mathematics and Mechanics*. North-Holland Publishing Co., Amsterdam, 1988.
- [BV04] Stephen Boyd and Lieven Vandenberghe. *Convex optimization*. Cambridge University Press, Cambridge, 2004.

- [CCPS98] William J. Cook, William H. Cunningham, William R. Pulleyblank, and Alexander Schrijver. *Combinatorial optimization*. Wiley-Interscience Series in Discrete Mathematics and Optimization. John Wiley & Sons, Inc., New York, 1998. A Wiley-Interscience Publication.
- [DHS13] Persi Diaconis, Susan Holmes, and Mehrdad Shahshahani. Sampling from a manifold. In *Advances in modern statistical theory and applications: a Festschrift in honor of Morris L. Eaton*, volume 10 of *Inst. Math. Stat. (IMS) Collect.*, pages 102–125. Inst. Math. Statist., Beachwood, OH, 2013.
- [Dor69] Robert Dorfman. An economic interpretation of optimal control theory. *The American Economic Review*, 59(5):817–831, 1969.
- [FT15] Gero Friesecke and Florian Theil. *Molecular Geometry Optimization, Models*, pages 951–957. Springer Berlin Heidelberg, Berlin, Heidelberg, 2015.
- [GG20] Subharup Guha and Sujit K. Ghosh. Probabilistic detection and estimation of conic sections from noisy data. *J. Comput. Graph. Statist.*, 29(3):513–522, 2020.
- [HK03] M. Herty and A. Klar. Modeling, simulation, and optimization of traffic flow networks. *SIAM J. Sci. Comput.*, 25(3):1066–1087, 2003.
- [HOZM08] Matthew Harker, Paul O’Leary, and Paul Zsombor-Murray. Direct type-specific conic fitting and eigenvalue bias correction. 26(3):372–381, mar 2008.
- [LMB<sup>+</sup>20] David Luengo, Luca Martino, Mónica Bugallo, Víctor Elvira, and Simo Särkkä. A survey of monte carlo methods for parameter estimation. *EURASIP Journal on Advances in Signal Processing*, 2020, 05 2020.
- [Mal89] A. G. Malliaris. *Stochastic Optimal Control*, pages 246–251. Palgrave Macmillan UK, London, 1989.
- [Mal21] Katherine Mary Malan. A survey of advances in landscape analysis for optimisation. *Algorithms (Basel)*, 14(2):Paper No. 40, 16, 2021.
- [MOE15] Katherine M. Malan, Johannes F. Oberholzer, and Andries P. Engelbrecht. Characterising constrained continuous optimisation problems. In *2015 IEEE Congress on Evolutionary Computation (CEC)*, pages 1351–1358, 2015.
- [MYDF08] Yi Ma, Allen Y. Yang, Harm Derksen, and Robert Fossum. Estimation of subspace arrangements with applications in modeling and segmenting mixed data. *SIAM Rev.*, 50(3):413–458, 2008.
- [NW06] Jorge Nocedal and Stephen J. Wright. *Numerical optimization*. Springer Series in Operations Research and Financial Engineering. Springer, New York, second edition, 2006.
- [O’L00] Dianne P. O’Leary. Symbiosis between linear algebra and optimization. volume 123, pages 447–465. 2000. Numerical analysis 2000, Vol. III. Linear algebra.
- [Rus94] Jagdish S. Rustagi. *Optimization techniques in statistics*. Statistical Modeling and Decision Science. Academic Press, Inc., Boston, MA, 1994.

- [RW97] Julio J. Rotemberg and Michael Woodford. An optimization-based econometric framework for the evaluation of monetary policy. *NBER Macroeconomics Annual*, 12:297–346, 1997.
- [SDR21] Alexander Shapiro, Darinka Dentcheva, and Andrzej Ruszczyński. *Lectures on stochastic programming—modeling and theory*, volume 28 of *MOS-SIAM Series on Optimization*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA; Mathematical Optimization Society, Philadelphia, PA, [2021] ©2021. Third edition [of 2562798].
- [SM13] Ole Sigmund and Kurt Maute. Topology optimization approaches. *Struct. Multidiscip. Optim.*, 48(6):1031–1055, 2013.
- [Ste97] J. Michael Steele. *Probability theory and combinatorial optimization*, volume 69 of *CBMS-NSF Regional Conference Series in Applied Mathematics*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1997.
- [Tr0] Fredi Tröltzsch. *Optimal control of partial differential equations*, volume 112 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, 2010. Theory, methods and applications, Translated from the 2005 German original by Jürgen Sprekels.
- [VMS16] René Vidal, Yi Ma, and S. Shankar Sastry. *Generalized principal component analysis*, volume 40 of *Interdisciplinary Applied Mathematics*. Springer, New York, 2016.