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Riccardo Cambini – Claudio Sodini

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Via Cosimo Ridolfi, 10 – 56124 PISA – Tel. Segr. Amm. 050 2216231 Segr. Stud. 050 2216317 Fax 050 2216375
Cod. Fisc. 80003670504 - P. IVA 00286820501 - Web http://statmat.ec.unipi.it/ - E-mail: dipstat@ec.unipi.it

A solution algorithm for a class of box constrained quadratic programming problems

Riccardo Cambini - Claudio Sodini *
Dept. of Statistics and Applied Mathematics, University of Pisa
Via Cosimo Ridolfi 10, 56124 Pisa, ITALY
E-mail: cambric@ec.unipi.it, csodini@ec.unipi.it

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Abstract

The aim of this paper is to suggest an algorithm to solve a box constrained quadratic problem where the objective function is given by the sum of a quadratic strictly convex separable function and the square of an affine function multiplied by a real parameter. Depending on the value of the real parameter, the problem might be convex or not. The problem can be easily transformed in a simpler equivalent one, which can be solved in a linear number of steps. Within the algorithm, some global optimality conditions are used as stopping criteria even in the case of a nonconvex objective function. The results of a deep numerical test of the algorithm are also provided.

Keywords Quadratic programming, optimal level solutions, d.c. optimization.
AMS - 2000 Math. Subj. Class. 90C20, 90C26, 90C31.
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1 Introduction

In [1, 3, 4] particular box constrained minimum problems having the following objective function have been studied:

$$\frac{1}{2}y^T Dy + c^T y + \frac{1}{2}k\left(h^T y + h_0\right)^2$$

where D is an $n \times n$ positive diagonal matrix, k is a nonnegative parameter, $c, h, y \in \Re^n$ and $h_0 \in \Re$. It is worth noticing that problems of this kind are a variation of the tax programming model studied in [5] (see also [1]).

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The aim of this paper is to study this class of problems and propose, in an unifying approach, an algorithm which solves the problems for any fixed value of $k \in \Re$ (see Section 5). It is worth noticing that for $k < 0$ small enough the quadratic objective function is not convex.

We will show that this problem can be trivially transformed in a simpler form (see Section 2), having an objective function of the following kind:

$$\frac{1}{2}x^T x + c^T x + \frac{1}{2}k\left(h^T x + h_0\right)^2$$

where $x, c, h \in \Re^n$, $h > 0$, and $k, h_0 \in \Re$.

For this subclass of problems we provide an algorithm which finds the optimal solution in no more that $2n-1$ iterations. Since each iteration requires $O(n)$ elementary arithmetic operations, the computational complexity of the algorithm is $O(n^2)$.

In order to improve the algorithm itself, in Section 3 several initialization subprocedures have been proposed aimed to reduce the feasible region to be examined, and some optimality conditions have been stated providing further stopping criteria.

The proposed algorithm has been deeply tested in Section 4 by implementing it in a symbolic calculus environment (Maple 9.5 by Maplesoft), pointing out both the linear number of iterations and the quadratic CPU time required to solve the problem.

2 Solution algorithm for the basic problem

The aim of this section is to state a solution algorithm for the following box constrained problem:

$$P : \begin{cases} \min f(x) = \frac{1}{2}x^T x + c^T x + \frac{1}{2}k\left(h^T x + h_0\right)^2 \\ x \in B = \{x \in \Re^n : l \leqq x \leqq u\} \end{cases}$$

where $h > 0$ and $l < u$.

First of all, it is worth noticing that depending on the value of k the problem can be convex or not.

Theorem 2.1 *Consider problem P and define the following negative value:*

$$k_0 = -\frac{1}{h^T h} \tag{2.1}$$

Then function f is convex if and only if

$$k \geq k_0 \tag{2.2}$$

while for $k < k_0$ function f is neither convex nor concave.

Proof Note that f is convex if and only if $I + khh^T$ is positive semidefinite, that is to say if and only if its eigenvalues are nonnegative. It can be seen that $1 + kh^T h$ is eigenvalue of $I + khh^T$ with h corresponding eigenvector since:

$$(I + khh^T)h = h + khh^T h = (1 + kh^T h)h$$

Note also that $I + khh^T$ has $n - 1$ eigenvalues equal to 1, with eigenvectors belonging to the set $h^\perp = \{v \in \Re^n : h^T v = 0\}$ since:

$$(I + khh^T)v = v + khh^T v = v \quad \forall v \in h^\perp$$

As a consequence, all the eigenvalues of $I + khh^T$ are nonnegative if and only if $1 + kh^T h \geq 0$ and the result is proved since $h > 0$. □

2.1 Optimal level solutions approach

In this subsection we show how problem P can be solved by means of the optimal level solution approach (see [2]).

With this aim, for any $\xi \in \Re$ let us define the following strictly convex parametric subproblem, which is obtained just by adding the constraint $h^T x + h_0 = \xi$:

$$P_\xi : \begin{cases} \min f(x) = \frac{1}{2}x^T x + c^T x + \frac{1}{2}k\xi^2 \\ x \in B_\xi = \{x \in \Re^n : l \leq x \leq u, \ h^T x + h_0 = \xi\} \end{cases}$$

Note that the feasible region B_ξ is no more given by box constraints.

The parameter ξ is said to be a feasible level if the set B_ξ is nonempty. Clearly, since the feasible region B of problem P is compact, the linear function $h^T x + h_0$ attains both minimum and maximum values; since $h > 0$ these minimum and maximum values are $\xi_{min} = h^T l + h_0$ and $\xi_{max} = h^T u + h_0$, respectively. As a consequence, the set of feasible levels is given by the interval $[\xi_{min}, \xi_{max}]$.

An optimal solution of problem P_ξ is called an optimal level solution [?, ?, ?]. For any given $\xi \in \Re$, the optimal solution for problem P_ξ can be computed by means of any solution algorithm for strictly convex quadratic problems.

For the sake of completeness, let us now briefly recall the optimal level solution approach (see for example [?]). It is trivial that the optimal solution of problem P is also an optimal level solution and that, in particular, it is the optimal level solution with the smallest value; the idea of this approach is then to scan all the feasible levels, studying the corresponding optimal level solutions, until the minimizer of the problem is reached.

Starting from an incumbent optimal level solution, this can be done by means of a sensitivity analysis on the parameter ξ, which allows us to move in the various steps through several optimal level solutions until the optimal solution is found.

Let x' be the optimal solution of problem $P_{\xi'}$, where $h^T x' + h_0 = \xi'$. Since $P_{\xi'}$ is a strictly convex problem, x' is the unique optimal solution if and only if the following Karush-Kuhn-Tucker conditions hold:

$$\left\{ \begin{array}{cl} x + c = \lambda h + \alpha - \beta & \\ h^T x + h_0 = \xi, & \\ l \leqq x \leqq u & \textit{feasibility} \\ \alpha \geqq 0,\ \beta \geqq 0, & \textit{optimality} \\ \alpha^T (x - l) = 0,\ \beta^T (u - x) = 0 & \textit{complementarity} \\ \lambda \in \Re,\ \alpha, \beta \in \Re^n & \end{array} \right. \tag{2.3}$$

These Karush-Kuhn-Tucker conditions can be rewritten in the following componentwise way:

$$\left\{ \begin{array}{ll} \alpha_i = 0,\ \beta_i = 0,\ \lambda = \frac{1}{h_i}(x_i + c_i) & \forall i \text{ such that } l_i < x_i < u_i \\ \beta_i = 0,\ \alpha_i = l_i + c_i - \lambda h_i \geq 0 & \forall i \text{ such that } x_i = l_i \\ \alpha_i = 0,\ \beta_i = \lambda h_i - u_i - c_i \geq 0 & \forall i \text{ such that } x_i = u_i \\ h^T x = \xi\ ,\ l \leqq x \leqq u & \end{array} \right.$$

Let $(x', \lambda', \alpha', \beta')$ be a solution of such an optimality conditions system and let us define the following sets of indices:

- $L = \{i :\ l_i = x'_i < u_i\}$,
- $U = \{i :\ l_i < x'_i = u_i\}$.

Note that since $h > 0$ it follows:

$$\left\{ \begin{array}{ll} \lambda = \frac{1}{h_i}(x_i + c_i) & \forall i \notin L \cup U \\ \lambda \leq \frac{1}{h_i}(l_i + c_i) & \forall i \in L \\ \lambda \geq \frac{1}{h_i}(u_i + c_i) & \forall i \in U \end{array} \right.$$

Given the optimal level solution x' for problem $P_{\xi'}$ the multipliers $\lambda', \alpha', \beta'$ can then be computed as follows. First, we have to determine the value of λ' as described below:

$$\lambda' = \left\{ \begin{array}{ll} \frac{x'_i + c_i}{h_i},\ i \notin L \cup U & \text{if } \{1, \ldots, n\} \setminus (L \cup U) \neq \emptyset \\ \min_{i \in L} \left\{ \frac{l_i + c_i}{h_i} \right\} & \text{if } x' \neq u \text{ and } L \cup U = \{1, \ldots, n\} \\ \max_{i \in U} \left\{ \frac{u_i + c_i}{h_i} \right\} & \text{if } x' = u \end{array} \right. \tag{2.4}$$

Then, α' and β' can be obtained as follows:

$$\alpha'_i = \left\{ \begin{array}{ll} 0 & \forall i \text{ such that } x'_i \neq l_i \\ x'_i + c_i - \lambda' h_i & \forall i \text{ such that } x'_i = l_i \end{array} \right. \tag{2.5}$$

$$\beta'_i = \left\{ \begin{array}{ll} 0 & \forall i \text{ such that } x'_i \neq u_i \\ \lambda' h_i - x'_i - c_i & \forall i \text{ such that } x'_i = u_i \end{array} \right. \tag{2.6}$$

In the light of the optimal level solution parametrical approach we now have to study the solution of problem $P_{\xi'+\theta}$, with $\theta > 0$. Since the Karush-Kuhn-Tucker system is linear whenever the complementarity conditions are implicitly handled, then the solution of the optimality conditions regarding to $P_{\xi'+\theta}$ are given by:

$$x'(\theta) = x' + \theta\Delta_x \ , \ \lambda'(\theta) = \lambda' + \theta\Delta_\lambda \tag{2.7}$$

$$\alpha'(\theta) = \alpha' + \theta\Delta_\alpha \ , \ \beta'(\theta) = \beta' + \theta\Delta_\beta \tag{2.8}$$

Since x', λ', α' and β' are known, we are left to compute $\Delta_x, \Delta_\lambda, \Delta_\alpha, \Delta_\beta$.

From (2.7) and (2.8) we obtain the following Karush-Kuhn-Tucker conditions corresponding to $P_{\xi'+\theta}$:

$$(x' + \theta\Delta_x) + c = (\lambda' + \theta\Delta_\lambda)h + (\alpha' + \theta\Delta_\alpha) - (\beta' + \theta\Delta_\beta)$$
$$h^T(x' + \theta\Delta_x) + h_0 = \xi' + \theta$$

as well as the following complementarity conditions which hold for all indices $i = 1, \ldots, n$ and for all $\theta > 0$ small enough:

$$(\alpha'_i + \theta\Delta_{\alpha_i})(x'_i - l_i + \theta\Delta_{x_i}) = 0$$
$$(\beta'_i + \theta\Delta_{\beta_i})(u_i - x'_i - \theta\Delta_{x_i}) = 0$$

From the Karush-Kuhn-Tucker conditions of $P_{\xi'}$ we then obtain:

$$\Delta_x = \Delta_\lambda h + \Delta_\alpha - \Delta_\beta \quad , \quad h^T\Delta_x = 1 \tag{2.9}$$

while, in particular, from the complementarity conditions of $P_{\xi'}$ we have that for all indices $i = 1, \ldots, n$ and for all $\theta > 0$ small enough:

$$\Delta_{\alpha_i}(x'_i - l_i) + \alpha'_i\Delta_{x_i} + \theta\Delta_{\alpha_i}\Delta_{x_i} = 0$$
$$\Delta_{\beta_i}(u_i - x'_i) - \beta'_i\Delta_{x_i} - \theta\Delta_{\beta_i}\Delta_{x_i} = 0$$

which yields:

$$\Delta_{\alpha_i}\Delta_{x_i} = 0 \quad , \quad \Delta_{\beta_i}\Delta_{x_i} = 0 \tag{2.10}$$

$$\Delta_{\alpha_i}(x'_i - l_i) + \alpha'_i\Delta_{x_i} = 0 \quad , \quad \Delta_{\beta_i}(u_i - x'_i) - \beta'_i\Delta_{x_i} = 0 \tag{2.11}$$

We are now able to prove the following preliminary lemma.

Lemma 2.1 *The following properties hold for all indices $i = 1, \ldots, n$:*

i) it is $\Delta_\lambda = \frac{1}{\sum_{i:\Delta_{x_i}\neq 0} h_i^2} > 0$;

ii) if $\Delta_{x_i} \neq 0$ then $\Delta_{x_i} = \Delta_\lambda h_i > 0$ and $\Delta_{\alpha_i} = \Delta_{\beta_i} = 0$;

iii) if $\Delta_{x_i} = 0$ then either $x'_i = l_i$ or $x'_i = u_i$;

iv) if $\Delta_{x_i} = 0$ *and* $x'_i = l_i$ *then* $\Delta_{\beta_i} = 0$ *and* $\Delta_{\alpha_i} = -\Delta_\lambda h_i < 0$;

v) if $\Delta_{x_i} = 0$ *and* $x'_i = u_i$ *then* $\Delta_{\alpha_i} = 0$ *and* $\Delta_{\beta_i} = \Delta_\lambda h_i > 0$.

Proof i),ii) If $\Delta_{x_i} \neq 0$ then from (2.10) we have that $\Delta_{\alpha_i} = \Delta_{\beta_i} = 0$, as a consequence from (2.9) it yields $\Delta_{x_i} = \Delta_\lambda h_i$. From (2.9) it then follows:

$$1 = h^T \Delta_x = \sum_{i=1,\dots,n} h_i \Delta_{x_i} = \sum_{i:\Delta_{x_i}\neq 0} h_i \Delta_{x_i} = \Delta_\lambda \sum_{i:\Delta_{x_i}\neq 0} h_i^2$$

so that, being $h > 0$, it is $\Delta_\lambda = \frac{1}{\sum_{i:\Delta_{x_i}\neq 0} h_i^2} > 0$ and hence $\Delta_{x_i} = \Delta_\lambda h_i > 0$.

iii) Let $\Delta_{x_i} = 0$ and assume by contradiction that $x'_i \in]l_i, u_i[$. From (2.11) it follows $\Delta_{\alpha_i} = \Delta_{\beta_i} = 0$ so that from (2.9) we get $0 = \Delta_\lambda h_i > 0$ which is a contradiction.

iv),v) Follow directly from (2.11) and (2.9). □

We are now able to fully determine the values of $\Delta_x, \Delta_\lambda, \Delta_\alpha, \Delta_\beta$. With this aim, the following further sets of indices are needed:

- $L^+ = \{i : x'_i = l_i \text{ and } \alpha'_i > 0\}$,
- $M = \{i : x'_i \neq u_i \text{ and } \alpha'_i = 0\}$.

Note that the following partition of the indices $\{1, \dots, n\}$ is obtained:

$$L^+ \cup M \cup U = \{1, \dots, n\}$$

Theorem 2.2 *For all indices* $i = 1, \dots, n$ *it is:*

$$\Delta_\lambda = \frac{1}{\sum_{i\in M} h_i^2} > 0 \tag{2.12}$$

$$\Delta_{x_i} = \begin{cases} 0 & \text{if } i \notin M \\ \Delta_\lambda h_i > 0 & \text{if } i \in M \end{cases} \tag{2.13}$$

$$\Delta_{\alpha_i} = \begin{cases} 0 & \text{if } i \notin L^+ \\ -\Delta_\lambda h_i < 0 & \text{if } i \in L^+ \end{cases} \tag{2.14}$$

$$\Delta_{\beta_i} = \begin{cases} 0 & \text{if } i \notin U \\ \Delta_\lambda h_i > 0 & \text{if } i \in U \end{cases} \tag{2.15}$$

Proof Taking into account that $\theta > 0$, $l \leqq (x' + \theta\Delta_x) \leqq u$ and $(\alpha' + \theta\Delta_\alpha) \geqq 0$, just notice that from Lemma 2.1 the following properties yield:

- for all $i \in M$ (hence $\beta_i = 0$) it is:

$$\Delta_{\alpha_i} = \Delta_{\beta_i} = 0 \quad , \quad \Delta_{x_i} = \Delta_\lambda h_i$$

- for all $i \in L^+$ (hence $\beta_i = 0$) it is:

$$\Delta_{x_i} = \Delta_{\beta_i} = 0 \quad , \quad \Delta_{\alpha_i} = -\Delta_\lambda h_i$$

- for all $i \in U$ (hence $\alpha_i = 0$) it is:

$$\Delta_{x_i} = \Delta_{\alpha_i} = 0 \quad , \quad \Delta_{\beta_i} = \Delta_\lambda h_i$$

□

The following important monotonicity properties follow straightforward from the previous theorem:

i) since $\Delta_x \geq 0$ then $x'(\theta)$ is componentwise nondecreasing,

ii) since $\Delta_\alpha \leq 0$ then $\alpha'(\theta)$ is componentwise nonincreasing,

iii) since $\Delta_\beta \geq 0$ then $\beta'(\theta)$ is componentwise nondecreasing.

Finally, we are able to determine the values of θ which guarantee both the optimality and the feasibility of $x'(\theta)$. From the feasibility conditions $l \leqq x' + \theta\Delta_x \leqq u$ and (2.13) we have

$$\theta \leq \hat{F} = \begin{cases} \min_{i \in M} \left\{ \frac{u_i - x'_i}{\Delta_{x_i}} \right\} & \text{if } M \neq \emptyset \\ 0 & \text{if } M = \emptyset \end{cases}$$

while from the optimality conditions $\alpha' + \theta\Delta_\alpha \geqq 0$ and (2.14) we have

$$\theta \leq \hat{O} = \begin{cases} \min_{i \in L^+} \left\{ \frac{-\alpha'_i}{\Delta_{\alpha_i}} \right\} & \text{if } L^+ \neq \emptyset \\ +\infty & \text{if } L^+ = \emptyset \end{cases}$$

As a consequence, $x'(\theta)$ is an optimal level solution for all θ such that:

$$0 \leq \theta \leq \min \left\{ \hat{F}, \hat{O} \right\}$$

Set $z' = \frac{1}{2}x'^T x' + c^T x'$ and $z(\theta) = \frac{1}{2}x'(\theta)^T x'(\theta) + c^T x'(\theta) + \frac{1}{2}k\,(\xi' + \theta)^2$. By means of simple calculations we obtain $\Delta_x^T \Delta_x = \Delta_\lambda$ and $\Delta_x^T(\alpha' - \beta') = 0$ so that an explicit formula for the function $z(\theta)$ can be stated:

$$z(\theta) = \frac{1}{2}(\Delta_\lambda + k)\theta^2 + (\lambda' + k\xi')\theta + z' + \frac{1}{2}k\xi'^2 \tag{2.16}$$

As a consequence, we have that $\frac{dz}{d\theta}(\theta) = (\Delta_\lambda + k)\theta + (\lambda' + k\xi')$ and hence:

If $\lambda' + k\xi' > 0$ [$\lambda' + k\xi' < 0$] then $z(\theta)$ is locally increasing [decreasing] at $\theta = 0$.

Level optimality can be helpful also in studying local optimality, since a minimum point in a segment of optimal level solutions is a local minimizer of the problem. This fundamental property, together with (2.16), allows to prove the following conditions.

Theorem 2.3 *Let x' be an optimal solution of problem $P_{\xi'}$. The following properties hold:*

i) if $\lambda' + k\xi' \geq 0$ and $\Delta_\lambda + k \geq 0$ then x' is a minimizer for $f(x)$ on the region

$$\left\{x \in B : \ \xi' \leq h^T x + h_0 \leq \xi' + \hat{O}\right\};$$

ii) if $\lambda' + k\xi' < 0$, $\Delta_\lambda + k > 0$ and $\theta' = -\frac{\lambda' + k\xi'}{\Delta_\lambda + k} \leq \min\left\{\hat{F}, \hat{O}\right\}$ with $\theta' \neq \hat{O}$ then $x'(\theta') = x' + \theta'\Delta_x$ is a local minimizer for problem P.

2.2 Solution algorithm

In order to find a global minimum it would be necessary to solve problem P_ξ for all the feasible levels (obviously, if $f(x)$ is convex we can stop as soon as a local minimizer is reached). In this subsection we will show that this can be done by means of a finite number of iterations, using the results obtained so far.

The algorithm starts from a certain minimal level and then scans all the greater ones looking for the optimal solution.

Initialization

1) Compute the values $\xi_{min} := h^T l + h_0$ and $\xi_{max} := h^T u + h_0$;

2) Determine an interval of feasible levels $[\xi_{start}, \xi_{end}] \subseteq [\xi_{min}, \xi_{max}]$ which contains an optimal solution and which are going to be visited;

3) Determine the optimal level solution x_{start} of problem $P_{\xi_{start}}$ and the starting incumbent optimal (level) solution x^*.

□

Note that a trivial initialization for steps 2) and 3) above is the following:

$$\xi_{start} := \xi_{min} \ , \quad \xi_{end} := \xi_{max} \ , \quad x_{start} := l$$
$$\text{if } f(u) < f(l) \text{ then } x^* := u \text{ else } x^* := l \text{ end if}$$

More effective initializations will be studied in subsection 3.1.

The optimal solution can now be searched iteratively by means of the following algorithms.

2.2.1 Convex case $k \geq k_0$

First note that when $f(x)$ is a convex function, that is to say that $k \geq k_0$, then $\Delta_\lambda + k \geq \Delta_\lambda + k_0 \geq 0$.

Algorithm-CX

1) $\xi' := \xi_{start}$; $x' := x_{start}$; $UB := f(x^*)$; local:= $false$;

2) While not local and $\xi' < \xi_{end}$ do

   2a) With respect to ξ' and x' determine λ', α', β', Δ_x, Δ_λ, Δ_α, Δ_β, $\hat{F}$, $\hat{O}$; $\theta_m := \min\{\hat{F}, \hat{O}\}$;

   2b) If $\lambda' + k\xi' \geq 0$ then local:= $true$
   else if $\Delta_\lambda + k = 0$ then $\xi' := \xi' + \theta_m$; $x' := x' + \theta_m \Delta_x$; $\overline{x} := x'$;
   else begin
   - Let $\theta_1 := -(\lambda' + k\xi')/(\Delta_\lambda + k)$;
   - If $\theta_1 < \theta_m$ then $\overline{x} := x' + \theta_1 \Delta_x$; local:= $true$;
   else $\xi' := \xi' + \theta_m$; $x' := x' + \theta_m \Delta_x$; $\overline{x} := x'$;
   - If $f(\overline{x}) < UB$ then $x^* := \overline{x}$ and $UB := f(\overline{x})$;

   end

3) x^* is the optimal solution for problem P.

□

This procedure looks for the minimizer by visiting segments of optimal level solutions where the objective function is decreasing. The procedure stops when the region has been fully scanned or a local minimizer (which is also global for the convexity of the objective function) is found.

2.2.2 Nonconvex case $k < k_0$

Let us notice that in this nonconvex case the functions $z(\theta)$ might be convex or not, depending on the value of $\Delta_\lambda + k$, so that all the feasible levels are to be examined (explicitly or implicitly).

Algorithm-NC

1) $\xi' := \xi_{start}$; $x' := x_{start}$; $UB := f(x^*)$; *stop*:= $false$;

2) While not *stop* and $\xi' < \xi_{end}$ do

   2a) With respect to ξ' and x' determine λ', α', β', Δ_x, Δ_λ, Δ_α, Δ_β, $\hat{F}$, $\hat{O}$; $\theta_m := \min\{\hat{F}, \hat{O}\}$;

   2b) Determine the best optimal level solution $\overline{x}$ for the levels $\xi \in [\xi', \xi' + \theta_m]$ and check the variable *stop*;

2c) If $f(\overline{x}) < UB$ then $x^* := \overline{x}$ and $UB := f(\overline{x})$;

2d) $\xi' := \xi' + \theta_m$ and $x' := x' + \theta_m \Delta_x$;

3) x^* is the optimal solution for problem P.

□

Note that in all the iterations the variable UB gives an upper bound for the optimal value with respect to the levels $\xi > \xi'$, while x^* is the best optimal level solution with respect to the levels $\xi \leq \xi'$.

It remains to show how to implement step *2b)* in the previous procedure. With this aim, first note that for all $\theta \in [0, \hat{O}]$, the value $z(\theta)$ is a lower bound for the parametric problem $P_{\xi'+\theta}$; in fact if $\theta \leq \hat{F}$ then $x'(\theta)$ is an optimal level solution, otherwise (if $\theta > \hat{F}$) $x'(\theta)$ is unfeasible for $P_{\xi'+\theta}$ but is an optimal solution of a problem with the same objective function as $P_{\xi'+\theta}$ and a feasible region containing $B_{\xi'+\theta}$.

Moving Steps 2b)

One of the following exhaustive cases occurs:

1) ($\Delta_\lambda + k > 0$ and $\lambda' + k\xi' < 0$), that is $z(\theta)$ is strictly convex and locally decreasing at $\theta = 0$. Let $\theta_1 := -(\lambda' + k\xi')/(\Delta_\lambda + k)$; two subcases have to be considered:

   1a) $\theta_1 \leq \theta_m$: $\overline{x} := x' + \theta_1 \Delta_x$; if $\xi' + \hat{O} > \xi_{end}$ then *stop* := *true*;

   1b) $\theta_1 > \theta_m$: $\overline{x} := x' + \theta_m \Delta_x$;

2) ($\Delta_\lambda + k \geq 0$ and $\lambda' + k\xi' \geq 0$), that is $z(\theta)$ is convex and locally nondecreasing at $\theta = 0$. Then $\overline{x} := x'$; if $\xi' + \hat{O} > \xi_{end}$ then *stop* := *true*;

3) ($\Delta_\lambda + k = 0$ and $\lambda' + k\xi' < 0$) or ($\Delta_\lambda + k < 0$ and $\lambda' + k\xi' \leq 0$), that is $z(\theta)$ is concave and locally decreasing at $\theta = 0$. Then $\overline{x} := x' + \theta_m \Delta_x$;

4) ($\Delta_\lambda + k < 0$ and $\lambda' + k\xi' > 0$), that is $z(\theta)$ is strictly concave and locally increasing at $\theta = 0$. Let θ_r be the positive root of the second order equation $z(\theta) = UB$, that is:

$$\theta_r = \frac{-(\lambda' + k\xi') + \sqrt{(\lambda' + k\xi')^2 - 2(\Delta_\lambda + k)(z' + \frac{1}{2}k\xi'^2 - UB)}}{(\Delta_\lambda + k)};$$

   three subcases have to be considered:

   4a) $\hat{O} \leq \theta_r$: $\overline{x} := x'$; if $\xi' + \hat{O} > \xi_{end}$ then *stop* := *true*;

   4b) $\hat{F} \leq \theta_r < \hat{O}$: $\overline{x} := x'$; if $\xi' + \theta_r > \xi_{end}$ then *stop* := *true*;

   4c) $\theta_r < \theta_m$: $\overline{x} := x' + \theta_m \Delta_x$;

□

The previously described Moving Steps 2b) use some global optimality conditions which allow us to implicitly examine some of the feasible levels thus reducing the number of the iterations needed to solve the problem.

2.2.3 Correctness and finiteness

The correctness of the proposed procedures follows directly since all the optimal level solutions are examined, either explicitly or implicitly.

As regards to the finiteness of the procedures, it is worth noticing that the optimal solution is found in no more that $2n-1$ iterations. In fact, in every iteration of the while cycle at least one of the two following situations occurs:

- at least one of the variables x_i, having the lower bound l_i as current value, is incremented;
- at least one of the variables x_i, having a current value lower than the upper bound u_i, is incremented up to its upper bound.

As a consequence, since the optimal level solutions $x'(\theta)$ are componentwise nondecreasing (as it has been pointed out by Theorem 2.2) and since the problem has n variables $x_1, \ldots, x_n$, no more than $2(n-1)$ iterations of the while cycle are needed to scan $n-1$ variables, then just one more iteration may be needed to complete the algorithm moving the last variable to its upper bound (it is not possible for this last considered variable to lose the level optimality before the feasibility, that is to have $\hat{O} < \hat{F}$).

In other words, we have just pointed out that these problems are solved in $O(n)$ iterations. With respect to the time spent to find the optimal solutions, in each of the $O(n)$ iterations a linear number of additions and multiplications are needed to compute the required scalar products, hence the total number of additions and multiplications is $O(n^2)$ and this will provide a quadratic behaviour to the CPU solution time.

3 Algorithm enhancements for the basic problem

Enhancements for the algorithm studied so far regarding both the initialization and the stop criteria can be obtained by analyzing the following unconstrained parametric problem:

$$\begin{cases} \min\ f(x) = \frac{1}{2}x^T x + c^T x + \frac{1}{2}k\xi^2 \\ \quad h^T x + h_0 = \xi \end{cases} \tag{3.1}$$

which differs from P_ξ problem only in the absence of the box constraints.

Lemma 3.1 *Let $\xi_h = h_0 - h^T c$. Then the quadratic problem (3.1) attains the unconstrained minimum at*

$$x(\xi) = -k_0(\xi - \xi_h)h - c$$

with minimum value

$$\phi(\xi) = \frac{1}{2}\xi^2 (k - k_0) + \xi k_0 \xi_h - \frac{1}{2} k_0 \xi_h^2 - \frac{1}{2} c^T c.$$

Proof The minimum point of the strictly convex problem verifies the following necessary and sufficient optimality condition:

$$\begin{cases} x + c = \lambda h \\ h^T x + h_0 = \xi \end{cases}$$

Hence $x(\xi) = \lambda(\xi)h - c$ and, by means of simple calculations, we have:

$$\begin{aligned} \lambda(\xi) &= -k_0(\xi - \xi_h) \\ x(\xi) &= -k_0(\xi - \xi_h)h - c \\ \phi(\xi) &= \frac{1}{2}x(\xi)^T x(\xi) + c^T x(\xi) + \frac{1}{2}k\xi^2 = \\ &= \frac{1}{2}\lambda(\xi)^2 h^T h - \frac{1}{2}c^T c + \frac{1}{2}k\xi^2 = \\ &= \frac{1}{2}\xi^2 (k - k_0) + \xi k_0 \xi_h - \frac{1}{2}k_0 \xi_h^2 - \frac{1}{2}c^T c. \end{aligned}$$

□

It is worth noticing that, since $k_0 < 0$ and $h > 0$, the optimal solutions $x(\xi)$ of problem (3.1) are componentwise strictly monotone with respect to the level ξ. By means of simple calculations, we obtain the corresponding first derivative:

$$\phi'(\xi) = \xi (k - k_0) + k_0 \xi_h$$

which allow us to study the behavior of the unconstrained minimum level values. Note that:

$$\text{if } k \neq k_0 \text{ then } \phi'(\xi) = 0 \text{ for } \xi_0 = \tfrac{-k_0 \xi_h}{k - k_0} = \xi_h - \tfrac{k \xi_h}{k - k_0}.$$

3.1 Initialization enhancements

Let us recall that in the initialization process described in subsection 2.2 we have to determine the interval of feasible levels $[\xi_{start}, \xi_{end}] \subseteq [\xi_{min}, \xi_{max}]$ which are going to be visited by the solution algorithm. The aim of this subsection is to determine initializations more efficient than the following trivial one:

$$\xi_{start} := \xi_{min}\ , \quad \xi_{end} := \xi_{max}\ , \quad x_{start} := l$$
$$\text{if } f(u) < f(l) \text{ then } x^* := u \text{ else } x^* := l \text{ end if}$$

that is to say, to determine intervals $[\xi_{start}, \xi_{end}]$ smaller than $[\xi_{min}, \xi_{max}]$.

With this aim, let us now consider the intersection between the unconstrained minima line $x(\xi) = -k_0(\xi - \xi_h)h - c$ and the feasible region B. Such an intersection, which provides a segment of optimal level solutions, exists if for all $i \in \{1, \ldots, n\}$ it is:

$$l_i \leq -k_0(\xi - \xi_h)h_i - c_i \leq u_i$$

that is, by means of simple calculations,

$$-\frac{1}{k_0} \cdot \max_{i=1,\ldots,n} \left\{ \frac{l_i + c_i}{h_i} \right\} + \xi_h \leq \xi \leq -\frac{1}{k_0} \cdot \min_{i=1,\ldots,n} \left\{ \frac{u_i + c_i}{h_i} \right\} + \xi_h \tag{3.2}$$

As a consequence, the intersection exists when:

$$\max_{i=1,\ldots,n} \left\{ \frac{l_i + c_i}{h_i} \right\} \leq \min_{i=1,\ldots,n} \left\{ \frac{u_i + c_i}{h_i} \right\} \tag{3.3}$$

The initialization process can now be described by using the following notations:

$$\mu_1 = \max_{i=1,\ldots,n} \left\{ \frac{l_i + c_i}{h_i} \right\} \qquad \mu_2 = \min_{i=1,\ldots,n} \left\{ \frac{u_i + c_i}{h_i} \right\}$$

$$\xi_1 = -\frac{1}{k_0} \cdot \mu_1 + \xi_h \qquad \xi_2 = -\frac{1}{k_0} \cdot \mu_2 + \xi_h$$

so that for Lemma 3.1 it is:

$$x(\xi_1) = \mu_1 h - c\,, \quad x(\xi_2) = \mu_2 h - c$$

Case $\mu_1 > \mu_2$

There is no intersection between the line of unconstrained minima and the feasible region, hence we have to visit the whole interval $[\xi_{min}, \xi_{max}]$:

$$\xi_{start} := \xi_{min}\,, \quad \xi_{end} := \xi_{max}\,, \quad x_{start} := l$$
$$\text{if } f(u) < f(l) \text{ then } x^* := u \text{ else } x^* := l \text{ end if}$$

Case $\mu_1 \leq \mu_2$

First observe that the points $x(\xi) = -k_0(\xi - \xi_h)h - c$, with $\xi \in [\xi_1, \xi_2]$, are feasible optimal level solutions. As a consequence, the problems P_ξ are solved for all $\xi \in [\xi_1, \xi_2]$ and hence the minimum of problem P for $h^T x + h_0 = \xi \in [\xi_1, \xi_2]$ can be obtained just looking for the minimum of $\phi(\xi)$ with $\xi \in [\xi_1, \xi_2]$, that is:

$$\min_{x \in B,\ h^T x + h_0 \in [\xi_1, \xi_2]} \{f(x)\} = \min_{\xi \in [\xi_1, \xi_2]} \{\phi(\xi)\}$$

The behaviour of $\phi(\xi)$ suggests how to implicitly study problems P_ξ even for some $\xi \notin [\xi_1, \xi_2]$. With this aim the following exhaustive cases must be considered.

Subcase $k > k_0$
Noticing that $\phi(\xi)$ is a convex parabola with vertex in ξ_0, the following possibilities occur:

i) if $\xi_0 > \xi_2$ then $x(\xi_2) = \mu_2 h - c$ is the best incumbent solution for all $\xi \leq \xi_2$ and for all $\xi \geq 2\xi_0 - \xi_2$. As a consequence, the initialization is:

$$\xi_{start} := \xi_2 \ , \ \xi_{end} := \min\{\xi_{max}, 2\xi_0 - \xi_2\} \ , \ x_{start} := \mu_2 h - c$$
$$\text{if } f(u) < f(x_{start}) \text{ then } x^* := u \text{ else } x^* := x_{start} \text{ end if}$$

ii) if $\xi_1 \leq \xi_0 \leq \xi_2$ then the problem is solved since the global uncostrained minimum $x(\xi_0)$ is feasible.

iii) if $\xi_0 < \xi_1$ then $x(\xi_1) = \mu_1 h - c$ is the best incumbent solution for all $\xi \geq \xi_1$ and for all $\xi \leq 2\xi_0 - \xi_1$. As a consequence, the initialization is:

$$\xi_{start} := \xi_{min} \ , \quad \xi_{end} := \xi_1 \ , \quad x_{start} := l$$
$$\text{if } f(\mu_1 h - c) < f(x_{start}) \text{ then } x^* := \mu_1 h - c \text{ else } x^* := x_{start} \text{ end if}$$

Subcase $k = k_0$
Noticing that $\phi(\xi)$ is a linear function which results to be decreasing if $\xi_h > 0$, increasing if $\xi_h < 0$, constant if $\xi_h = 0$. The following possibilities occur:

i) if $\xi_h > 0$ then $x(\xi_2)$ is the best incumbent solution for all $\xi \leq \xi_2$. As a consequence, the initialization is:

$$\xi_{start} := \xi_2 \ , \quad \xi_{end} := \xi_{max} \ , \quad x_{start} := \mu_2 h - c$$
$$\text{if } f(u) < f(x_{start}) \text{ then } x^* := u \text{ else } x^* := x_{start} \text{ end if}$$

ii) if $\xi_h = 0$ then the problem is solved since the global uncostrained minima $x(\xi)$ with $\xi \in [\xi_1, \xi_2]$ are feasible.

iii) if $\xi_h < 0$ then $x(\xi_1)$ is the best incumbent solution for all $\xi \geq \xi_1$. As a consequence, the initialization is:

$$\xi_{start} := \xi_{min} \ , \quad \xi_{end} := \xi_1 \ , \quad x_{start} := l$$
$$\text{if } f(\mu_1 h - c) < f(x_{start}) \text{ then } x^* := \mu_1 h - c \text{ else } x^* := x_{start} \text{ end if}$$

Subcase $k < k_0$
Noticing that $\phi(\xi)$ is a concave parabola with vertex in ξ_0, the following possibilities occur:

i) if $\xi_0 \geq \frac{\xi_1+\xi_2}{2}$ then $x(\xi_1)$ is the best incumbent solution for all $\xi \in [\xi_1, 2\xi_0 - \xi_1]$. As a consequence, problems P_ξ can be studied only for

$$\begin{cases} \xi \in [\xi_{min}, \xi_1] & \text{if } \xi_{max} \leq 2\xi_0 - \xi_1 \\ \xi \in [\xi_{min}, \xi_1] \cup [2\xi_0 - \xi_1, \xi_{max}] & \text{if } \xi_{max} > 2\xi_0 - \xi_1 \end{cases}$$

ii) if $\xi_0 < \frac{\xi_1+\xi_2}{2}$ then $x(\xi_2)$ is the best incumbent solution for all $\xi \in [2\xi_0 - \xi_2, \xi_2]$. As a consequence, problems P_ξ can be studied only for

$$\begin{cases} \xi \in [\xi_2, \xi_{max}] & \text{if } \xi_{min} \geq 2\xi_0 - \xi_2 \\ \xi \in [\xi_{min}, 2\xi_0 - \xi_2] \cup [\xi_2, \xi_{max}] & \text{if } \xi_{min} < 2\xi_0 - \xi_2 \end{cases}$$

In the initialization, we then have to choose the incumbent optimal (level) solution among vectors l, u, $x(\xi_1)$ and $x(\xi_2)$, that is:

$$x^* := arg \min_{x \in \{l, u, x(\xi_1), x(\xi_2)\}} \{f(x)\}$$

The other initialization values can be obtained as follows:

- if $\xi_0 \geq \frac{\xi_1+\xi_2}{2}$ and $\xi_{max} \leq 2\xi_0 - \xi_1$ then:

$$\xi_{start} := \xi_{min} \ , \quad \xi_{end} := \xi_1 \ , \quad x_{start} := l$$

- if $\xi_0 < \frac{\xi_1+\xi_2}{2}$ and $\xi_{min} \geq 2\xi_0 - \xi_2$ then:

$$\xi_{start} := \xi_2 \ , \quad \xi_{end} := \xi_{max} \ , \quad x_{start} := \mu_2 h - c$$

- otherwise, we can use the following settings

$$\xi_{start} := \xi_{min} \ , \quad \xi_{end} := \xi_{max} \ , \quad x_{start} := l$$

  taking into account that whenever $\xi' \geq \min\{\xi_1, 2\xi_0 - \xi_2\}$ and $\xi' < \xi_2$ it is possible to skip directly to $\xi' := \xi_2$ with $x' := \mu_2 h - c$.

Remark 3.1 In order to avoid the need of solving problem $P_{(2\xi_0 - \xi_1)}$, in the case $\xi_0 > \frac{\xi_1+\xi_2}{2}$ with $\xi_{max} > 2\xi_0 - \xi_1$ we suggest to skip to the level $\xi_2 < 2\xi_0 - \xi_1$ for which the optimal level solution $x(\xi_2) = \mu_2 h - c$ is *a priori* known.

As we have pointed out, a nontrivial initialization can be used whenever the intersection between the box and the line of unconstrained minima is nonempty, condition which is verified if and only if $\mu_1 \leq \mu_2$. It is then worth studying, in a computational light, how often such an intersection exists, that is to say how often the nontrivial initialization can be used. We considered 25 different classes of problems grouped with respect to the

n	2	3	4	5	6	7	8	9	10-12	13-16	> 16
%	61.25	35.81	20.07	10.98	5.94	3.24	1.65	0.98	0.1-0.5	0.01-0.1	< 0.01

Table 1: Occurrences of non trivial initialization

number of variables; these classes cover dimensions from 2 to 100 variables. By means of a symbolic calculus software (Maple^{TM} in an Apple^{TM} MacOSX environment) 10,000 problems have been randomly generated for each class of problems in order to see how often the condition $\mu_1 \leq \mu_2$ is verified. The obtained results are summarized in Table 1.

It can be easily seen that the possibility of using the nontrivial initialization is fastly decreasing with respect to the number of the variables (61% for 2 variables, less than 0.1% for more than 12 variables). In the next section we will show that the nontrivial initialization (when it can be used) may strongly reduce the number of iterations needed to solve the problem (hence also the time needed to find the solution). As a consequence, taking into account that the initialization process is done only once, it is always worth implementing the nontrivial initialization.

3.2 Stopping criteria

The study of the unconstrained minima line $x(\xi)$ allow us to propose the following stopping criteria which can be useful in improving the solution algorithm.

Theorem 3.1 *Consider problem P and let $x^* \in B$ and $\xi' \in [\xi_{min}, \xi_{max}]$ be such that $f(x^*) \leq \phi(\xi')$. If one of the following conditions holds:*

i) $k \leq k_0$ *and* $\phi(\xi_{max}) \geq f(x^*)$,

ii) $k > k_0$ *and* $\xi'(k - k_0) + k_0\xi_h \geq 0$,

then $f(x^*) \leq f(x)$ $\forall x \in B$ *such that* $h^T x + h_0 \geq \xi'$.

Proof *i)* Noticing that function $\phi(\xi)$ is concave for $k \leq k_0$ we get

$$\phi(\xi) \geq \min\{\phi(\xi'), \phi(\xi_{max})\} \geq f(x^*) \quad \forall \xi \in [\xi', \xi_{max}]$$

hence the result is proved since $f(x) \geq \phi(h^T x + h_0)$ $\forall x \in B$.

ii) Noticing that $\phi'(\xi') \geq 0$ and that function $\phi(\xi)$ is strictly convex for $k > k_0$ we get

$$\phi(\xi) \geq \phi(\xi') \geq f(x^*) \quad \forall \xi \geq \xi'$$

and the result is proved. □

Note that the previous stopping criterium *ii)* is already implicitly implemented in Algorithm-CX by means of the use of the flag "local". The stopping criterium *i)* can be implemented in Algorithm-NC by improving line 2) as follows:

2) While not *stop* and $\xi' < \xi_{end}$ and $UB > \min\{\phi(\xi'), \phi(\xi_{end})\}$ do

4 Computational results

In the light of the previous sections, we have fully implemented the solution algorithm by means of a symbolic calculus software (Maple^{TM} in an Apple^{TM} MacOSX environment). The following different implementations of the solution algorithm have been tested:

C_T) convex problems with the trivial initialization,

C_N) convex problems with the nontrivial initialization,

N_T) nonconvex problems with the trivial initialization,

N_{N_1}) nonconvex problems with the nontrivial initialization but without the stopping criteria proposed in section 3.2,

N_{N_2}) nonconvex problems with the nontrivial initialization and with the stopping criteria proposed in section 3.2.

The computational results confirm the $O(n)$ theoretical number of iterations and the $O(n^2)$ theoretical number of seconds needed to find the optimal solution (see Section 2.2.3).

As a first test, we examined problems having a number of variable from 2 to 10. In order to see the impact of the nontrivial initialization, each class of problems has been tested with 1,000 randomly created problems solved with all of the five previously described implementations. The obtained results, that are the average number of iterations and the average number of seconds needed to obtain the optimal solution, are summarized in Table 2 and graphically represented in Figure 1.

The linear behaviour of the number of iterations is confirmed. When the problems have few variables, that is from 2 to 5 variables, the number of iterations required to solve them is so small that the initialization process affects the total CPU time (5 different "lines" can be distinguished). When the number of variables is greater than 8 the initialization steps have a slight weight and it seems that just 3 "lines" are present.

Finally, we examined problems of bigger dimensions, that is having a number of variable from 20 to 200. In this case, from a computational point of view, there are no concrete differences between the trivial and the nontrivial initializations (see Table 1), hence we did not tested the C_T and the N_T implementations. Each class of problems has been tested with 250 randomly created problems; the obtained results, that are the average number

n	Average number of iterations					Average CPU time (seconds)				
	C_T	C_N	N_T	N_{N_1}	N_{N_2}	C_T	C_N	N_T	N_{N_1}	N_{N_2}
2	1.813	0.985	2.605	1.501	1.289	0.436	0.355	0.686	0.688	0.741
3	2.745	2.034	4.448	3.629	2.371	0.555	0.483	0.981	0.958	0.857
4	3.803	3.264	6.401	5.748	3.357	0.694	0.633	1.295	1.261	0.986
5	4.842	4.542	8.442	8.098	4.680	0.823	0.797	1.633	1.611	1.201
6	5.760	5.544	10.380	10.172	5.671	0.956	0.929	1.963	1.955	1.373
7	6.820	6.680	12.343	12.215	6.529	1.094	1.078	2.297	2.286	1.531
8	7.865	7.785	14.445	14.410	7.754	1.238	1.232	2.673	2.671	1.776
9	8.582	8.528	16.429	16.397	9.240	1.346	1.344	3.019	3.021	2.061
10	9.693	9.663	18.421	18.404	10.297	1.508	1.502	3.387	3.381	2.290

Table 2: Computational results : from 2 to 10 variables

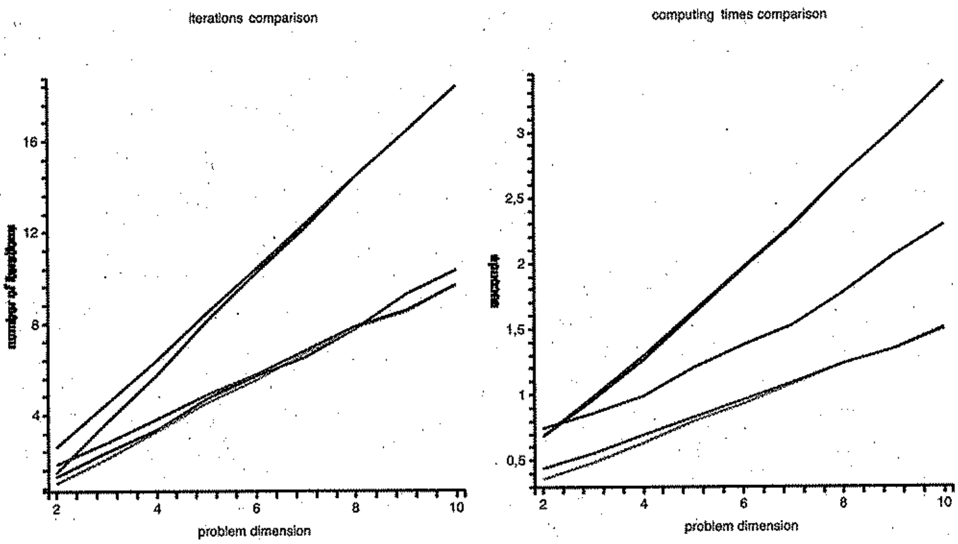

Figure 1: Iterations/seconds for 2-10 variables

n	Number of iterations			CPU time (seconds)		
	C_N	N_{N_1}	N_{N_2}	C_N	N_{N_1}	N_{N_2}
20	19.724	38.392	20.748	2.9102	6.9150	4.3912
30	29.790	58.368	31.460	4.6247	11.183	6.9793
50	49.062	98.440	55.302	8.6599	21.444	13.794
75	74.960	148.29	75.386	15.269	37.383	21.703
100	100.30	198.30	105.01	23.361	56.948	34.677
150	149.39	297.94	158.00	43.584	106.42	64.306
200	199.83	397.86	208.04	70.513	170.42	101.50

Table 3: Computational results : from 20 to 200 variables

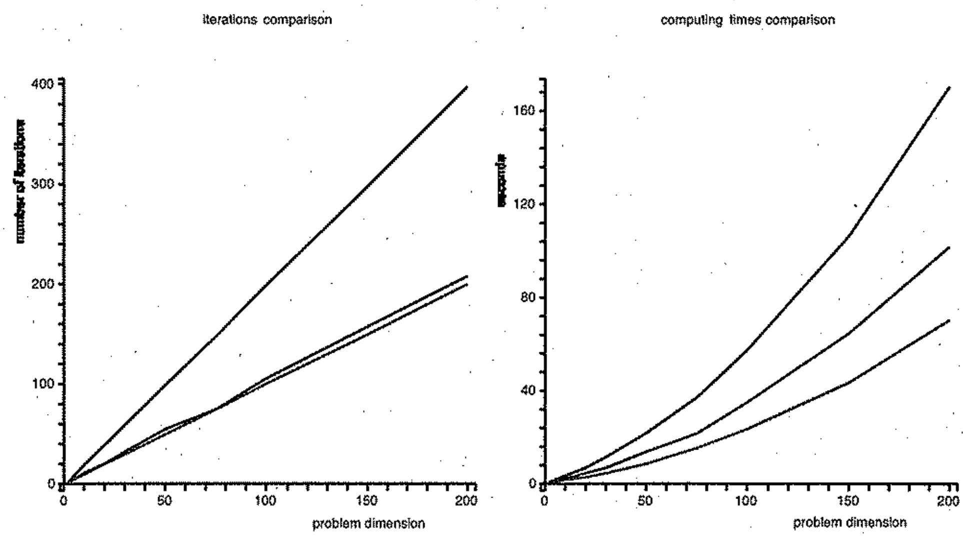

Figure 2: Iterations/seconds for 20-200 variables

of iterations and the average number of seconds needed to obtain the optimal solution, are summarized in Table 3 and graphically represented in Figure 2.

As regards the number of iterations, they results to have a linear behaviour with respect to the number of variables. Convex problems are solved in about n iterations, that is with the half of the maximum number of iterations which may be necessary to solve the problem. Nonconvex problems are solved in N_{N_2}) implementation with a number of iteration very close to the one needed by convex problems of the same dimension. On the other hand, nonconvex problems are solved in N_{N_1}) implementation with a number of iteration very close to the maximum value $2n - 1$. As regards the CPU times spent in solving the problems, they results to have a quadratic behaviour with respect to the number of variables. In this case, the times related to C_N) and N_{N_2}) differs since the iterations implemented in N_{N_2})

are more complex than the ones in C_N).

5 A more general problem

The aim of this section is to show how problem P allow us to study also the following more general one

$$P_G : \begin{cases} \min g(y) = \frac{1}{2}y^T D y + \bar{c}^T y + \frac{1}{2}k\left(\bar{h}^T y + h_0\right)^2 \\ y \in \bar{B} = \{y \in \Re^m : \bar{l} \leq y \leq \bar{u}\} \end{cases}$$

where $\bar{B}$ is a box constrained region, $D = \text{diag}(d_1, \ldots, d_n) \in \Re^{m \times m}$ is a positive definite diagonal matrix, $\bar{c}, \bar{h}, \bar{l}, \bar{u} \in \Re^m$ with $\bar{l} \leq \bar{u}$, $k, h_0 \in \Re$.

In [1, 3, 4] problem P_G has been studied assuming k as a nonnegative parameter, proposing $O(n^2)$ solution algorithms; obviously, since k is nonnegative the corresponding subproblem is convex. in this section we show that problem P_G can be solved in $O(n)$ iterations for any value of $k \in \Re$, hence even in the nonconvex case.

In the rest of the section we will describe how problem P_G can be transformed in an equivalent one of the form P reducing, if possible, the number of the variables.

5.1 Reducing the feasible region

Let us introduce the following sets of indices:

$$I_0 = \{i : \bar{h}_i = 0\}, \quad I_+ = \{i : \bar{h}_i > 0\}, \quad I_- = \{i : \bar{h}_i < 0\}$$

It is worth noticing that some variables can be fixed *a priori* to their optimal value, thus reducing the feasible region and the complexity of the problem.

Let us first consider the variables y_i such that $i \in I_0$. The objective function of problem P_G can be rewritten as follows:

$$\begin{aligned} g(y) &= \sum_{i \in I_0} \left(\frac{1}{2}d_i y_i^2 + \bar{c}_i y_i\right) + \\ &+ \sum_{i \in I_+ \cup I_-} \left(\frac{1}{2}d_i y_i^2 + \bar{c}_i y_i\right) + \frac{1}{2}k\left(\sum_{i \in I_+ \cup I_-} \bar{h}_i y_i + h_0\right)^2 \end{aligned}$$

As a consequence we have that:

$$\begin{aligned} \min_{y \in \bar{B}} \{g(y)\} &= \min_{y \in \bar{B}} \left\{\sum_{i \in I_0} \left(\frac{1}{2}d_i y_i^2 + \bar{c}_i y_i\right)\right\} + \\ &+ \min_{y \in \bar{B}} \left\{\sum_{i \in I_+ \cup I_-} \left(\frac{1}{2}d_i y_i^2 + \bar{c}_i y_i\right) + \frac{1}{2}k\left(\sum_{i \in I_+ \cup I_-} \bar{h}_i y_i + h_0\right)^2\right\} \end{aligned}$$

In is now worth noticing that the subproblem

$$\min_{y\in\bar{B}}\left\{\sum_{i\in I_0}\left(\frac{1}{2}d_i y_i^2+\bar{c}_i y_i\right)\right\}$$

can be solved explicitly. In fact the derivative of $\frac{1}{2}d_i y_i^2+\bar{c}_i y_i$ is $d_i y_i+\bar{c}_i$ which vanishes in $\tilde{y}_i=-\frac{\bar{c}_i}{d_i}$. As a consequence the minimum of $\frac{1}{2}d_i y_i^2+\bar{c}_i y_i$ is reached for the following values $\bar{y}_i$:

$$\bar{y}_i=\begin{cases}\bar{l}_i & \text{if } \tilde{y}_i\le\bar{l}_i\\ \bar{u}_i & \text{if } \tilde{y}_i\ge\bar{u}_i\\ \tilde{y}_i & \text{if } \bar{l}_i<\tilde{y}_i<\bar{u}_i\end{cases}$$

An interesting result can be stated also for the variables y_i such that $i\in I_+\cup I_-$. With this aim, denoting with e_i the i-th vector of the canonical basis of $\Re^m$, notice that:

$$\begin{aligned}\frac{\partial g}{\partial y_i}(y) &= \nabla g(y)^T e_i=\left[Dy+\bar{c}+k\left(\bar{h}^T y+h_0\right)\bar{h}\right]^T e_i=\\ &= y_i d_i+\bar{c}_i+k\bar{h}_i\left(\bar{h}^T y+h_0\right)=\\ &= (\bar{c}_i+k\bar{h}_i h_0)+k\bar{h}_i\sum_{j\neq i}\bar{h}_j y_j+\left(d_i+k\bar{h}_i^2\right)y_i\end{aligned}$$

Hence in the boxed feasible region we have:

$$\min_{y\in\bar{B}}\left\{\frac{\partial g}{\partial y_i}(y)\right\}=\frac{\partial g}{\partial y_i}(y') \quad\text{and}\quad \max_{y\in\bar{B}}\left\{\frac{\partial g}{\partial y_i}(y)\right\}=\frac{\partial g}{\partial y_i}(y'')$$

where

$$y'_j=\begin{cases}\bar{l}_j & \text{if } j\neq i \text{ and } k\bar{h}_i\bar{h}_j\ge 0\\ \bar{u}_j & \text{if } j\neq i \text{ and } k\bar{h}_i\bar{h}_j<0\\ \bar{l}_i & \text{if } j=i \text{ and } d_i+k\bar{h}_i^2\ge 0\\ \bar{u}_i & \text{if } j=i \text{ and } d_i+k\bar{h}_i^2<0\end{cases} \tag{5.1}$$

and

$$y''_j=\begin{cases}\bar{u}_j & \text{if } j\neq i \text{ and } k\bar{h}_i\bar{h}_j\ge 0\\ \bar{l}_j & \text{if } j\neq i \text{ and } k\bar{h}_i\bar{h}_j<0\\ \bar{u}_i & \text{if } j=i \text{ and } d_i+k\bar{h}_i^2\ge 0\\ \bar{l}_i & \text{if } j=i \text{ and } d_i+k\bar{h}_i^2<0\end{cases} \tag{5.2}$$

It is now clear that:

- if $\min_{y\in\bar{B}}\left\{\frac{\partial g}{\partial y_i}(y)\right\}\ge 0$ then $g(y)$ is always increasing in the feasible region with respect to variable y_i and hence the optimal value will be reached for the value $\bar{y}_i=\bar{l}_i$,

- if $\max_{y\in\bar{B}}\left\{\frac{\partial g}{\partial y_i}(y)\right\} \leq 0$ then $g(y)$ is always decreasing in the feasible region with respect to variable y_i and hence the optimal value will be reached for the value $\bar{y}_i = \bar{u}_i$.

Summarizing the results stated in this subsection, we can say that the feasible region can be reduced, without affecting the optimal solutions of the problem, by simply applying the following steps.

Box Reduction Steps

- for all $i \in I_0$ such that $\bar{l}_i < \bar{u}_i$ do
  $\tilde{y}_i := -\frac{c_i}{d_i}$;
  if $\tilde{y}_i \leq \bar{l}_i$ then $\bar{u}_i := \bar{l}_i$;
  else if $\tilde{y}_i \geq \bar{u}_i$ then $\bar{l}_i := \bar{u}_i$;
  else $\bar{l}_i := \tilde{y}_i$; $\bar{u}_i := \tilde{y}_i$
  end if;
  end if;
  end do;

- *found* := *true*;
  while *found* do
  found := *false*;
  for all $i \in I_+ \cup I_-$ such that $\bar{l}_i < \bar{u}_i$ while not *found* do
  compute y' and y'' as in (5.1) and (5.2);
  if $\frac{\partial g}{\partial y_i}(y') \cdot \frac{\partial g}{\partial y_i}(y'') \geq 0$
  then *found* := *true*;
  if $\frac{\partial g}{\partial y_i}(y') \geq 0$ then $\bar{u}_i := \bar{l}_i$ else $\bar{l}_i := \bar{u}_i$ end if;
  end if;
  end do;
  end do.

□

Remark 5.1 Note that at the end of the previous steps the following implication holds regarding to the components y_i:

$$\bar{l}_i < \bar{u}_i \quad \Rightarrow \quad i \in I_+ \cup I_- \text{ and } \min_{y\in\bar{B}}\left\{\frac{\partial g}{\partial y_i}(y)\right\} < 0 < \max_{y\in\bar{B}}\left\{\frac{\partial g}{\partial y_i}(y)\right\}$$

Note also that the external "while" cycle in the second step previously described can be repeated at most a number of times equal to $m - card(I_0)$, so that the complexity of the second step is equal to $O([m - card(I_0)]^2)$. Obviously, the complexity of the first step is equal to $O(card(I_0))$.

5.2 Converting the reduced subproblem

We are then left to solve the problem just with respect to the variables y_i such that $\bar{l}_i < \bar{u}_i$.

In order to transform problem P_G in the form P we use the following variable transformation:

$$x_i = \begin{cases} y_i\sqrt{d_i} & i \in I_+ \\ -y_i\sqrt{d_i} & i \in I_- \end{cases} \tag{5.3}$$

As a consequence we get:

$$l_i = \begin{cases} \bar{l}_i\sqrt{d_i} & i \in I_+ \\ -\bar{u}_i\sqrt{d_i} & i \in I_- \end{cases} \qquad u_i = \begin{cases} \bar{u}_i\sqrt{d_i} & i \in I_+ \\ -\bar{l}_i\sqrt{d_i} & i \in I_- \end{cases} \tag{5.4}$$

$$c_i = \begin{cases} \bar{c}_i\frac{1}{\sqrt{d_i}} & i \in I_+ \\ -\bar{c}_i\frac{1}{\sqrt{d_i}} & i \in I_- \end{cases} \qquad h_i = \begin{cases} \bar{h}_i\frac{1}{\sqrt{d_i}} & i \in I_+ \\ -\bar{h}_i\frac{1}{\sqrt{d_i}} & i \in I_- \end{cases} \tag{5.5}$$

It is worth noticing that $h > 0$ and that we have transformed problem P_G into the equivalent one P having a number of variables which is lower or equal than the cardinality of $I_+ \cup I_-$.

Appendix - Algorithm Implementation

In this appendix we provide the Maple code related to the algorithm implementation used in the numerical tests.

```
> ########  PROCEDURA RISOLUTIVA   #########
>
> soluzione := proc(n,c,k,h,h0,l,u,inibanale,usaphi)
>
>    local k0,ximin,ximax,xistart,xiend,xstart,xstar,mu1,mu2,xip,xp,
>          xih,xi0,xi1,xi2,Xxi1,Xxi2,skip,convex,inizializzazionebanale,
>          lambdap,alphap,betap,Deltalambda,Deltax,Deltaalpha,Deltabeta,
>          FF,OO,thetam,
>          f,calcolaparametri,casoconvesso,casononconvesso,st,UB,iter,
>          xb,fxb,theta1,thetar,val1,val2,locale,stopcrit;
>
> ## procedura valore funzione obiettivo
> f:=proc(x)
>  evalm((1/2)*evalm(x)&*evalm(x)+evalm(c)&*evalm(x)
>        +(1/2)*k*(evalm(h)&*evalm(x)+h0)^2);
> end proc;
>
> ## procedura per il calcolo dei parametri dell'algoritmo
> calcolaparametri := proc(xp)
```

```
> local L,U,M,N,Lp,i,j;
> L:={};U:={};N:={};
> for i from 1 to n do
>   if xp[i]=l[i] then L:=L union {i}
>     elif xp[i]=u[i] then U:=U union {i}
>     else N:=N union {i}
>   end if;
> end do;
> if nops(N)>0 then j:=N[1]; lambdap:=(xp[j]+c[j])/h[j]
>    elif nops(L)=0 then lambdap:=max(seq((u[j]+c[j])/h[j],j=1..n))
>    else lambdap:=min(seq((l[L[j]]+c[L[j]])/h[L[j]],j=1..nops(L)))
> end if;
> alphap:=vector(n);
> betap:=vector(n);
> for i from 1 to n do
>   if xp[i]=l[i] then alphap[i]:=xp[i]+c[i]-lambdap*h[i]
>                 else alphap[i]:=0
>   end if;
>   if xp[i]=u[i] then betap[i]:=lambdap*h[i] -xp[i]-c[i]
>                 else betap[i]:=0
>   end if;
> end do;
> #%#  print("lambdap=",lambdap,"alphap=",alphap,"betap=",betap);
> Lp:={};M:=N;
> for i from 1 to nops(L) do
>  if alphap[L[i]]>0 then Lp:=Lp union {L[i]}
>                      else M:=M union {L[i]}
>  end if;
> end do;
> if nops(M)=0 then print("attenzione insieme di indici M vuoto") end if;
> Deltalambda:=1/add(h[M[i]]^2,i=1..nops(M));
> Deltax:=vector(n,0);
> Deltaalpha:=vector(n,0);
> Deltabeta:=vector(n,0);
> if nops(M)>0 then
>   for i from 1 to nops(M) do
>     Deltax[M[i]]:=Deltalambda*h[M[i]]
>   end do;
> end if;
> if nops(Lp)>0 then
>   for i from 1 to nops(Lp) do
>     Deltaalpha[Lp[i]]:=-Deltalambda*h[Lp[i]]
>   end do;
> end if;
> if nops(U)>0 then
>   for i from 1 to nops(U) do
>     Deltabeta[U[i]]:=Deltalambda*h[U[i]]
>   end do;
> end if;
```

```
> #%# print("Deltalambda=",Deltalambda,"Deltax=",Deltax,
> #%#       "Deltaalpha=",Deltaalpha,"Deltabeta=",Deltabeta);
> if nops(M)=0 then FF:=0
>       else FF:=min(seq((u[M[i]]-xp[M[i]])/Deltax[M[i]],i=1..nops(M)))
> end if;
> if nops(Lp)=0 then OO:=infinity
>       else OO:=min(seq(-alphap[Lp[i]]/Deltaalpha[Lp[i]],i=1..nops(Lp)))
> end if;
> thetam:=eval(min(FF,OO));
> #%# print("FF=",FF,"OO=",OO,"thetam=",thetam);
> end proc:
>
> #### inizializzazione banale
> inizializzazionebanale := proc()
> #%#    print("Inizializzazione banale");
>    xistart:=evalm(ximin);
>    xiend:=evalm(ximax);
>    xstart:=evalm(l);
>    if f(u)<f(l) then xstar:=evalm(u) else xstar:=evalm(l) end if;
> end proc:
>
> ## procedura per il caso convesso
> casoconvesso := proc()
> #%#   print("caso convesso");
> if inibanale then inizializzazionebanale()
>    else mu1:=max(seq((l[i]+c[i])/h[i],i=1..n));
>         mu2:=min(seq((u[i]+c[i])/h[i],i=1..n));
>         if mu1>mu2 then inizializzazionebanale()
>            else
> #%#  print("mu1=",mu1,"mu2=",mu2,"Inizializzazione non banale");
>                 xih:=evalm(h0-evalm(h)&*evalm(c));
>                 xi1:=xih-mu1/k0;
>                 xi2:=xih-mu2/k0;
>                 Xxi1:=evalm(mu1*h-c);
>                 Xxi2:=evalm(mu2*h-c);
>                 if k>k0 then
>                    xi0:=(-k0*xih)/(k-k0);
>                    if xi0>xi2
>                       then xistart:=evalm(xi2);
>                            xiend:=min(ximax,2*xi0-xi2);
>                            xstart:=evalm(Xxi2);
>                            if f(u)<f(xstart)
>                               then xstar:=evalm(u)
>                               else xstar:=evalm(xstart)
>                            end if;
>                       elif xi0<xi1
>                            then xistart:=evalm(ximin);
>                                 xiend:=xi1;
>                                 xstart:=evalm(l);
```

```
>                                 if f(Xxi1)<f(xstart)
>                                    then xstar:=evalm(Xxi1)
>                                    else xstar:=evalm(xstart)
>                                 end if;
>                       else xistart:=evalm(xi0);
>                            xiend:=evalm(xi0);
>                            xstart:=evalm(-k0*(xi0-xih)*h-c);
>                            xstar:=evalm(xstart);
>                    end if;
>                 else if xih>0
>                         then xistart:=evalm(xi2);
>                              xiend:=evalm(ximax);
>                              xstart:=evalm(Xxi2);
>                              if f(u)<f(xstart)
>                                 then xstar:=evalm(u)
>                                 else xstar:=evalm(xstart)
>                              end if;
>                         elif xih<0
>                              then xistart:=evalm(ximin);
>                                   xiend:=evalm(xi1);
>                                   xstart:=evalm(l);
>                                   if f(Xxi1)<f(xstart)
>                                      then xstar:=evalm(Xxi1)
>                                      else xstar:=evalm(xstart)
>                                   end if;
>                         else xistart:=evalm(xi1);
>                              xiend:=evalm(xi1);
>                              xstart:=evalm(Xxi1);
>                              xstar:=evalm(xstart);
>                      end if;
>                 end if;
>         end if;
> end if;
> #%#   print("ximin=",ximin,"xistart",xistart,
> #%#         "xiend=",xiend,"ximax=",ximax);
> #%#   print("xstar=",xstar,"xstart=",xstart);
>    xip:=evalm(xistart);
>    xp:=evalm(xstart);
>    UB:=f(xstar);
>    iter:=0;
> locale:=false;
> while not(locale) and xip<xiend do
>   iter:=iter+1;
> #%# print("iterazione n. ",iter);
>   calcolaparametri(xp);
>   if lambdap+k*xip>=0 then locale:=true;
>       else if Deltalambda+k=0 then xp:=evalm(xp+thetam*Deltax);
>                                    xip:=evalm(evalm(h)&*evalm(xp)+h0);
>                                    xb:=evalm(xp)
```

```
>                  else theta1:=-(lambdap+k*xip)/(Deltalambda+k);
>                       if theta1<thetam then xb:=evalm(xp+theta1*Deltax);
>                                             locale:=true
>                           else xp:=evalm(xp+thetam*Deltax);
>                                xip:=evalm(evalm(h)&*evalm(xp)+h0);
>                                xb:=evalm(xp)
>                       end if;
>            end if;
>            fxb:=f(xb);
>            if fxb<UB then xstar:=evalm(xb); UB:=fxb end if;
>   end if;
> #%# print("xstar=",xstar,"UB=",evalf(UB),"xp=",xp,"xip=",xip);
> end do;
> #%# if locale then print("trovato ottimo locale") end if;
> #%# print("numero di iterazioni eseguite : ",iter);
> #%# print("soluzione ottima : ",xstar);
> #%# print("valore ottimo : ",UB);
> end proc:
>
> ## procedura per il caso non convesso
> casononconvesso := proc()
> local phi,phiend;
> phi:=proc(xi)
>  evalm((1/2)*xi^2*(k-k0)+xi*k0*xih-(1/2)*k0*xih^2
>        -(1/2)*evalm(c)&*evalm(c));
> end proc;
> #%# print("caso non convesso");
> xih:=evalm(h0-evalm(h)&*evalm(c));
> if inibanale then inizializzazionebanale(); skip:=false
>    else mu1:=max(seq((l[i]+c[i])/h[i],i=1..n));
>         mu2:=min(seq((u[i]+c[i])/h[i],i=1..n));
>         if mu1>mu2 then inizializzazionebanale(); skip:=false
>            else xi0:=(-k0*xih)/(k-k0);
> #%#     print("mu1=",mu1,"mu2=",mu2,"Inizializzazione non banale");
>                 xi1:=xih-mu1/k0;
>                 xi2:=xih-mu2/k0;
>                 Xxi1:=evalm(mu1*h-c);
>                 Xxi2:=evalm(mu2*h-c);
>                 if f(u)<f(l)
>                    then xstar:=evalm(u)
>                    else xstar:=evalm(l)
>                 end if;
>                 if f(Xxi1)<f(xstar) then xstar:=evalm(Xxi1) end if;
>                 if f(Xxi2)<f(xstar) then xstar:=evalm(Xxi2) end if;
>                 if xi0>=(xi1+xi2)/2 and ximax<=2*xi0-xi1
>                    then xistart:=evalm(ximin);
>                         xiend:=evalm(xi1);
>                         xstart:=evalm(l);
>                         skip:=false
```

```
>                       elif xi0<(xi1+xi2)/2 and ximin>=2*xi0-xi2
>                           then xistart:=evalm(xi2);
>                                xiend:=evalm(ximax);
>                                xstart:=evalm(Xxi2);
>                                skip:=false
>                       else xistart:=evalm(ximin);
>                            xiend:=evalm(ximax);
>                            xstart:=evalm(1);
>                            skip:=true
>                   end if
>           end if;
> end if;
> #%#   print("ximin=",ximin,"xistart",xistart,
> #%#         "xiend=",xiend,"ximax=",ximax);
> #%#   print("xstar=",xstar,"xstart=",xstart);
>    xip:=evalm(xistart);
>    xp:=evalm(xstart);
>    UB:=f(xstar);
>    iter:=0;
> if usaphi
>    then phiend:=phi(xiend);
>         stopcrit:=evalb(UB<=min(phi(xip),phiend));
> #%#         print("phiend=",evalf(phiend),"phi(xip)=",evalf(phi(xip)));
> #%#         if stopcrit
> #%#            then print("verificata la condizione di stop furba")
> #%#         end if;
>    else stopcrit:=false
> end if;
> while not(stopcrit) and xip<xiend do
> iter:=iter+1;
> #%# print("iterazione n. ",iter);
> calcolaparametri(xp);
> val1:=Deltalambda+k;
> val2:=lambdap+k*xip;
> #%# print("Deltalambda+k=",val1,"lambdap+k*xip",val2);
> if val1>0 and val2<0
>       then theta1:=-val2/val1;
> #%#           print("caso 1)"); print("theta1=",theta1);
>          if theta1>thetam then xb:=evalm(xp+thetam*Deltax)
>             else xb:=evalm(xp+theta1*Deltax);
>                  if xip+OO>xiend then stopcrit:=true end if;
>          end if;
>   elif  val1>=0 and val2>=0
>       then xb:=evalm(xp);
> #%#           print("caso 2)");
>          if xip+OO>xiend then stopcrit:=true end if;
>   elif  (val1=0 and val2<0) or (val1<0 and val2<=0)
>       then
> #%#            print("caso 3)");
```

```
>            xb:=evalm(xp+thetam*Deltax)
>    elif  val1<0 and val2>0
>        then
> #%#    print("caso 4)");
> thetar:=(-val2+sqrt(evalm(val2^2-2*val1*((1/2)*evalm(xp)&*evalm(xp)
>          +evalm(c)&*evalm(xp)+(1/2)*k*xip^2-UB))))/val1;
> #%#            print("thetar=",thetar);
>            if 00<=evalf(thetar) then xb:=evalm(xp);
>                                 if xip+00>xiend
>                                        then stopcrit:=true
>                                 end if;
>              elif FF<=evalf(thetar) and thetar<00 then xb:=evalm(xp);
>                                               if xip+thetar>xiend
>                                                       then stopcrit:=true
>                                               end if;
>              elif evalf(thetar)<thetam then xb:=evalm(xp+thetam*Deltax);
>              else print("errore nel caso 4)");
>            end if;
> else print("errore casi esaustivi");
> end if;
>     fxb:=f(xb);
>     if fxb<UB then xstar:=evalm(xb); UB:=fxb end if;
>     xp:=evalm(xp+thetam*Deltax); xip:=evalm(evalm(h)&*evalm(xp)+h0);
> #%#   print("xstar=",xstar,"UB=",evalf(UB),"xp=",xp,"xip=",xip);
>     if skip then
>        if xip>=min(xi1,2*xi0-xi2) then
>              skip:=false;
>              if xip<xi2
>                 then
> #%#     print("Eseguito salto da xi1 a xi2","xp=",xp,"xip=",xip);
>                      xip:=evalm(xi2);xp:=evalm(Xxi2)
>              end if;
>        end if;
>     end if;
>     if usaphi then
> #%#   print("phiend=",evalf(phiend),"phi(xip)=",evalf(phi(xip)));
>                 if UB<=min(phi(xip),phiend)
>                    then
> #%#   print("verificata la condizione di stop furba");
>                        break
>                 end if
>     end if;
> end do;
> #%# if stopcrit then print("utilizzato criterio di stop") end if;
> #%# print("numero di iterazioni eseguite : ",iter);
> #%# print("soluzione ottima : ",xstar);
> #%# print("valore ottimo : ",UB);
> end proc:
>
```

```
> ######    corpo principale della procedura      #######
>     st:= time():
>     ximin:=evalm(evalm(h)&*evalm(l)+h0);
>     ximax:=evalm(evalm(h)&*evalm(u)+h0);
>     k0:=-1/evalm(evalm(h)&*evalm(h));
>     convex:=evalb(k>=k0);
>     if convex then casoconvesso()
>               else casononconvesso()
>     end if;
>     [convex,[n,iter,time() - st]];
> end proc:
```

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- ☐ n. 38 I.Emke - Poulopoulos - V.Gozàlves Pèrez - Odo Barsotti - Laura Lecchini, International migration to northern Mediterranean countries the cases of Greece, Spain and Italy.
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- ☐ n. 40 Riccardo Cambini, Un problema di programmazione quadratica nella costituzione di capitale.
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- ☐ n. 47 Odo Barsotti - Laura Lecchini, Les parcours migratoires en fonction de la nationalité. Le cas de l'Italie.
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- ☐ n. 49 Alberto Cambini - Laura Martein, Tangent cones in optimization.
- ☐ n. 50 Alberto Cambini - Laura Martein, Optimality conditions in vector and scalar optimization: a unified approach.

Anno: 1992

- ☐ n. 51 Gilberto Ghilardi, Elementi di uno schema di campionamento areale per alcune rilevazioni ufficiali in Italia.
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- ☐ n. 53 Laura Lecchini - Odo Barsotti, Le rôle des immigrés extra- communautaires dans le marché du travail

- n. 54 Riccardo Cambini, Alcune condizioni di ottimalità relative ad un insieme stellato.
- n. 55 Gilberto Ghilardi, Uno schema di campionamento areale per le rilevazionninsulle famiglie in Italia.
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- n. 62 Vincenzo Bruno, Dell'elasticità in economia e dell'incertezza statistica.
- n. 63 Laura Martein, Alcune classi di funzioni concave generalizzate nell'ottimizzazione vettoriale
- n. 64 Anna Marchi, On the relationships between bicriteria problems and non-linear programming problems.
- n. 65 Giovanni Boletto, Considerazioni metodologiche sul concetto di elasticità prefissata.
- n. 66 Laura Martein, Soluzione efficienti e condizioni di ottimalità nell'otti-mizzazione vettoriale.

Anno: 1993

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- n. 70 Anna Marchi - Claudio Sodini, An algorithm for a non-differentiable non -linear fractional programming problem.
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- n. 74 Riccardo Cambini, Alcune nuove classi di funzioni concavo-generalizzate.

Anno: 1994

- n. 75 Alberto Cambini - Anna Marchi - Laura Martein, On nonlinear scalarization in vector optimization.
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- n. 77 Gilberto Ghilardi, Indici statistici della congiuntura.
- n. 78 Riccardo Cambini, Condizioni di efficienza locale nella ottimizzazione vettoriale.
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- n. 85 Vasile Preda - I.M.Stancu-Minasian, On duality for multiobjective mathematical programming of n-set.
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Anno: 1995

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- n. 90 Riccardo Cambini, Funzioni scalari affini generalizzate.
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- n. 92 Marco Bottai - Maria Caputo - Laura Lecchini, The "OLIVAR" survey.Methodology and quality.
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Anno: 1996

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- n. 110 Luciano Fanti - Piero Manfredi, Un modello "classico" di ciclo con crescita ed offerta di lavoro endogena.
- n. 111 Anna Marchi, On the connecttedness of the efficient frontier : sets without local maxima.

- ☐ **n. 112** Riccardo Cambini, Generalized concavity for bicriteria functions.
- ☐ **n. 113** Vincenzo Bruno, Variazioni dinamiche (1971-1981-1991)dei fenomeni demografici dei comuni (urbani e rurali) della Lombardia, in relazione ad alcune caratteristiche di mobilità territoriale.

Anno: **1997**

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Anno: **1998**

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- ☐ **n. 129** Emilio Barucci - Fausto Gozzi - Andrej Swiech, Incentive compatibility constraints and dynamic programming in continuous time.

Anno: **1999**

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- ☐ **n. 132** Alessandro Valentini, Proiezioni demografiche multiregionali a due sessi, con immigrazioni internazionali e vincoli di consistenza.
- ☐ **n. 133** Fabio Antonelli - Emilio Barucci - Maria Elvira Mancino, Backward-forward stochastic differential utility: existence, consumption and equilibrium analysis.
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- ☐ **n. 148** Francesco Billari - Piero Manfredi - Alberto Bonaguidi - Alessandro Valentini, Transition into adulthoold: its macro-demographic consequences in a multistatew stable population framework
- ☐ **n. 149** Francesco Billari - Piero Manfredi - Alessandro Valentini, Becoming Adult and its Macro-Demographic Impact: Multistate Stable Population Theory and an Application to Italy
- ☐ **n. 150** Alessandro Valentini, Le previsioni demografiche in presenza di immigrazioni: confronto tra modelli alternativi e loro utilizzo empirico ai fini della valutazione dell'equilibrio nel sistema pensionistico
- ☐ **n. 151** Emilio Barucci - Roberto Monte, Diffusion processes for asset prices under bounded rationality
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Anno: **2000**

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- ☐**n. 169** A. Marchi, Theorems of the Alternative by way of Separation Theorems
- ☐**n. 170** Emilio Barucci - Maria Elvira Mancino, Asset Pricing and Diversification with Partally Exchangeable random Variables
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- ☐**n. 179** E. Barucci - M.E. Mancini - Roberto Renò, Volatility Estimation via Fourier Analysis
- ☐**n. 180** Riccardo Cambini, Minimum Principle Type Optimality Conditions
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- ☐**n. 184** F.Antonelli, E.Barucci, M.E.Mancino, Asset Pricing with a Backward-Forward Stochastic Differential Utility
- ☐**n. 185** Riccardo Cambini - Laura Carosi, Coercivity Concepts and Recession Functions in Constrained Problems
- ☐**n. 186** John R. Williams, Piero Manfredi, The pre-vaccination dynamics of measles in Italy: estimating levels of under-reporting of measles cases
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- ☐**n. 188** Laura Carosi, Johannes Jahn, Laura Martein, On The Connections between Semidefinite Optimization and Vector Optimization
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- ☐**n. 190** Riccardo Cambini - Claudio Sodini, A finite Algorithm for a Particular d.c. Quadratic Programming Problem.
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- ☐**n. 196** M.Bottai, M.Bottai, N. Salvati, M.Toigo, Le proiezioni demografiche con il programma Nostradamus. (Applicazione all'area pisana)
- ☐**n. 197** A. Lemmi - B. Cheli - B. Mazzolli, La misura della povertà multidimensionale: aspetti metodologici e analisi della realtà italiana alla metà degli anni '90
- ☐**n. 198** C.R. Bector - Riccardo Cambini, Generalized B-invex vector valued functions
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Anno: **2001**

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- ☐**n. 207** Michele Longo, The competitive choice of innovation adoption: A finite-fuel singular stochastic control problem.
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- ☐**n. 209** Riccardo Cambini - Claudio Sodini, A Finite Algorithm for a Class of Non Linear Multiplicative Programs.
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- ☐**n. 212** Riccardo Cambini, Necessary Optimality Conditions in Vector Optimization.
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- n. 216 Luciano Fanti - Piero Manfredi, Population, unemployment and economic growth cycles: a further explanatory perspective
- n. 217 J.R.Williams,P.Manfredi,S.Salmaso,M.Ciofi, Heterogeneity in regional notification patterns and its impact on aggregate national case notification data: the example of measles in Italy.
- n. 218 Anna Marchi, On the connectedness of the efficient frontier: sets without local efficient maxima
- n. 219 Laura Lecchini - Odo Barsotti, Les disparités territoriales au Maroc au travers d'une optique de genre.

Anno: **2002**

- n. 220 Gilberto Ghilardi - Nicola Orsini, Sull'uso dei modelli statistici lineari nella valutazione dei sistemi formativi.
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- n. 222 E. Barucci - C. Impenna - R. Renò, The Italian Overnight Market: microstructure effects, the martingale hypothesis and the payment system.
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- n. 225 Andrea Mercatanti, Effetto dell'uso di carte Bancomat e carte di Credito sulla liquidità familiare: una valutazione empirica
- n. 226 Piero Manfredi - John R. Williams, Population decline and population waves: their impact upon epidemic patterns and morbidity rates for childhood infectious diseases. Measles in Italy as an example.
- n. 227 Piero Manfredi - Marta Ciofi degli Atti, La geografia pre-vaccinale del morbillo in Italia. I. Comportamenti di contatto e sforzi necessari all'eliminazione: predizioni dal modello base delle malattie prevenibili da vaccino.
- n. 228 I.M.Stancu-Minasian, Optimality Conditions and Duality in Fractional Programming Involving Semilocally Preinvex and Related
- n. 229 Nicola Salvati, Un software applicativo per un'analisi di dati sui marchi genetici (Genetic Markers)
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- n. 234 Riccardo Cambini and Claudio Sodini, Decomposition methods for nonconvex quadratic programs
- n. 235 R.Cambini and L. Carosi and S.Schaible, Duality in fractional optimization problems with set constraints
- n. 236 Anna Marchi, On the mix-efficient points

Anno: **2003**

- n. 237 Emanuele Vannucci, The valuation of unit linked policies with minimal return guarantees under symmetric and asymmetric information hypoteses
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- n. 239 Bruno Cheli, Errata Corrige del Manuale delle Impronte Ecologiche (2002) ed alcuni utili chiarimenti
- n. 240 Alessandra Petrucci-Nicola Salvati-Monica Pratesi, Stimatore Combinato r Correlazione Spaziale nella Stima per Piccole Aree
- n. 241 Riccardo Cambini - Laura Carosi, Mixed Type Duality for Multiobjective Optimization Problems with set constraints
- n. 242 O.Barsotti, L.Lecchini, F.Benassi, Foreigners from central and eastern European countries in Italy: current and future perspectives of eu enlargement
- n. 243 A. Cambini - L. Martein - S. Schaible, Pseudoconvexity under the Charnes-Cooper transformation
- n. 244 Eugene M. Cleur, Piero Manfredi, and John R. William, The pre-and post-Vaccination regional dynamics of measles in Italy: Insights from time series analysis

Anno: **2004**

- n. 245 Emilio Barucci - Jury Falini, Determinants of Corporate Governance in Italy: Path dependence or convergence?
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Anno: **2005**

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