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Authors: The instructions of the Editor/Associate Editor should have been followed, including both structural modifications (e.g. we splitted the former section of Conclusions) and minor suggestions.

Answer to the First Referee

Authors: All this Reviewer's comments should have been included, following her/his indications. In addition, an English native speaker has contributed with proofreading.

Answer to the Second Referee

Authors: All the accurate Reviewer's modifications should have been implemented, following her/his indications. Furthermore, we also did our best to revise the entire paper, on the basis of the specific comments of this Reviewer. This has led to some additional small changes, including punctuation, with respect to the previous version of the paper.

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Conjugate Direction Methods and Polarity

for Quadratic Hypersurfaces

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Abstract We use some results from polarity theory to recast several geometric properties of Conjugate Gradient-based methods, for the solution of nonsingular symmetric linear systems. This approach allows us to pursue three main theoretical objectives. First, we can provide a novel geometric perspective on the generation of conjugate directions, in the context of positive definite systems. Second, we can extend the above geometric perspective to treat the generation of conjugate directions for handling indefinite linear systems. Third,

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by exploiting the geometric insight suggested by polarity theory, we can easily study the possible degeneracy (pivot breakdown) of Conjugate Gradient-based methods on indefinite linear systems. In particular, we prove that the degeneracy of the standard Conjugate Gradient on nonsingular indefinite linear systems can occur only once in the execution of the Conjugate Gradient.

Keywords Polarity in homogeneous coordinates · Quadratic hypersurfaces · Conjugate Gradient method · Indefinite linear systems

Mathematics Subject Classification (2010) 90C30 · 65K99 · 51N15

1 Introduction

In this paper, we consider methods based on the generation of conjugate directions, namely Conjugate Gradient (CG) methods for the solution of linear systems [1–3], within the framework of polarity theory. The fact of introducing this perspective as polarity may provide a geometric framework to describe the properties of CG-based methods [4], i.e. a different viewpoint from the algorithmic usually considered in the literature. This perspective also motivates the extension of the use of CG-based methods for solving indefinite linear systems and, possibly, for the search of stationary points of polynomial functions. In addition, it allows us to recast Planar-CG methods [4–7], for solving indefinite linear systems (the relevant analysis is not included in the current paper). Finally, we conjecture that this perspective may suggest a possible geometric insight for the Quasi-Newton updates, given the relation between CG

1 and BFGS (Broyden-Fletcher-Goldfarb-Shanno) or L-BFGS (Limited memory
2 Broyden-Fletcher-Goldfarb-Shanno) methods [3].
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6 To the best of the authors' knowledge, the use of polarity to detail CG-
7 based methods was just hinted by Hestenes and Stiefel in [1], but since then
8 little can be found in the literature. Indeed, most of the literature studies the
9 algebraic formalization of CG-based methods, to exploit and improve their
10 computational performance. As an example, in [8] we can read that "*At that*
11 *time [1952] it [the CG] was derived from the theory of polarity. Nowadays one*
12 *prefers to see it as a method which permits the transformation of a matrix in*
13 *tridiagonal form*".
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23 Although the algorithmic perspective defines a line of research of great im-
24 portance for CG-based methods, it is beyond the scope of the present work.
25 Here, we focus on the theoretic characteristics of these methods that justify
26 their use as iterative solvers for linear systems [9], in particular within large
27 scale optimization problems. In this context, CG-based methods are imple-
28 mented to solve either positive definite or indefinite linear systems, whose
29 approximate solutions define *gradient-related* directions that ensure the global
30 convergence of the optimization algorithms, along with their fast convergence
31 to stationary points.
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42 Truncated Newton algorithms (see [9,10]), used to solve large scale min-
43 imization problems for a real objective function, often implement CG-based
44 methods. Specifically, these methods are a fast choice to approximately solve
45 Newton's equation at the h -th outer iteration, as it reduces to a linear sys-
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1 tem. As an example, in [11, 12] CG-based methods are used to yield superlinear
2 convergence to an optimal solution of large scale unconstrained minimization
3 problems. Within truncated Newton algorithms CG-based methods are also
4 used to compute *negative curvature directions* for the objective function [13–
5 15]. These directions turn out to be useful in proving the convergence of the
6 algorithm to stationary points, along with the satisfaction of second order
7 optimality conditions.
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10 Sequential Quadratic Programming procedures [9], used to solve constrained
11 minimization problems, may also adopt CG-based methods. In this case, at
12 the current iteration h , CG-based methods are called to solve a (possibly)
13 indefinite linear system.
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15 CG-based methods have been recently proposed also to deflate conjugacy
16 loss [16], and to generate efficient preconditioners for Newton's equation in
17 different contexts [17, 18].
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19 In this paper, initially, we show how the main characteristics of the CG in
20 \mathbb{R}^n have a counterpart in homogeneous coordinates. Then, we show that po-
21 larity justifies the application of CG-based methods to the solution of linear
22 systems, both in the positive definite and indefinite case. Finally, we observe
23 that fundamental theorems of polarity theory, such as the Reciprocity Theo-
24 rem and the Section Theorem (see [19] or the early work [20]), apply to general
25 nonquadratic hypersurfaces. This last observation might possibly suggest fur-
26 ther guidelines to study the geometry underlying the Nonlinear CG-based
27 methods and BFGS. In addition, by Proposition 8.3 we are going to see the
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1 dramatic impact of CG premature stop in the indefinite case, when proving
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3 global convergence properties (see also [11]).
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6 The rest of the paper is organized as follows. In Section 2, we provide an
7 introduction to polarity theory. In Section 3, we detail the main concepts of
8 polarity theory in homogeneous coordinates, for quadratic hypersurfaces. In
9 Sections 4–6, we analyze the relation between polarity for quadratic hypersur-
10 faces and the solution of symmetric linear systems, both in the case where the
11 Hessian matrix of the quadratic hypersurface is positive definite and indefi-
12 nite. Then, in Section 7, we focus on a basic tool (namely *polar hyperplanes*)
13 used to describe the relation between polarity and the CG. We prove that
14 polar hyperplanes are generalizations of tangent hyperplanes to algebraic hy-
15 persurfaces. We show that the CG implicitly handles polar hyperplanes, and
16 in particular that the latter hyperplanes coincide with tangent hyperplanes,
17 when we consider finite points on specific quadratic hypersurfaces. Section 8
18 contains advances on polarity applied to study the CG. Finally, in Section 9 we
19 propose some perspectives for possible further investigation, and in Section 10
20 we draw some conclusions.
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37 We use the following notation throughout this paper. $\|\cdot\|$ is the Euclidean
38 norm. \mathbb{R}^n is the n -dimensional Cartesian space and \mathbb{P}^n is the associated ho-
39 mogeneous coordinates projective space (in which each point is indicated as
40 $(x_1 : x_2 : \dots : x_n : x_0)$). Given the vector $x \in \mathbb{R}^n$ and the scalar $x_0 \in \mathbb{R}$, for
41 brevity and with a little abuse of notation we might indicate with $(x, x_0)^T$ a
42 vector in \mathbb{P}^n . $\dim(S)$ is the dimension of the subspace S of \mathbb{R}^n . $A \succ 0$ denotes
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1 that the matrix A is symmetric positive definite and $Ker(A)$ is the null space
 2 of matrix A . Lowercase Greek letters refer to hyperplanes, either in Cartesian
 3 coordinates or homogeneous coordinates. Finally, we use terms like *hyperplane*
 4 and *linear manifold* as synonyms. When a hyperplane includes the origin we
 5 may remark the fact that it represents a *linear subspace*.
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11 **2 Introduction to Polarity Theory**

12 This section is devoted to detail aspects of projective geometry in \mathbb{R}^n , with
 13 a specific attention to study algebraic hypersurfaces in homogeneous coordi-
 14 nates. Within this last class of geometric entities, quadratics have attractive
 15 properties which play a key role in this work, in order to exploit iterative meth-
 16 ods for the solution of symmetric linear systems (see also [19–21] for further
 17 references).
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33 2.1 Homogeneous Coordinates in \mathbb{R}^n

34 Cartesian coordinates $(y_1, \dots, y_n) \in \mathbb{R}^n$ define a one-to-one map between real
 35 n -tuples and finite points in \mathbb{R}^n . In order to handle a simple algebra, including
 36 both points with finite coordinates and points at infinity, the *homogeneous*
 37 *coordinates* $(x_1 : \dots : x_n : x_0)$ can be introduced, so that
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$$45 \quad y_i = \frac{x_i}{x_0}, \quad i = 1, \dots, n, \quad (1)$$

46 where $x_i \in \mathbb{R}$, $i = 0, \dots, n$, are $n + 1$ finite values.
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Proposition 2.1 Let us consider the relation ' \sim ' on the set $\mathbb{R}^{n+1} \setminus \{0\}$, as defined by

$$(x_1, \dots, x_n, x_0) \sim (\hat{x}_1, \dots, \hat{x}_n, \hat{x}_0)$$

iff

$$(\hat{x}_1, \dots, \hat{x}_n, \hat{x}_0) = \rho(x_1, \dots, x_n, x_0)$$

for some real value $\rho \neq 0$. Then, ' \sim ' is an equivalence relation and the point

$(x_1 : \dots : x_n : x_0) \in \mathbb{P}^n$ represents the equivalence class

$$\{\rho(x_1, \dots, x_n, x_0) : \rho \in \mathbb{R} \setminus \{0\}\}.$$

In other words, the homogeneous coordinates define the projective space \mathbb{P}^n as a one-to-one map between points (possibly at infinity) in \mathbb{R}^n and points $(\rho x_1 : \dots : \rho x_n : \rho x_0)$ in \mathbb{P}^n , where $\rho \neq 0$, provided that $(x_1, \dots, x_n, x_0) \neq 0$.

2.2 Basics on Polarity for Algebraic Hypersurfaces

Let $\varphi(x_1, \dots, x_n, x_0)$ be a homogeneous polynomial of degree $r \in \mathbb{N}$, then we say that the locus of points of \mathbb{P}^n satisfying

$$\mathcal{F} : \{(x, x_0)^T \in \mathbb{P}^n : \varphi(x_1, \dots, x_n, x_0) = 0\} \quad (2)$$

is an *algebraic hypersurface* of order r .

Definition 2.1 Given the algebraic hypersurface (2) of order $r \geq 1$, in homogeneous coordinates, consider the point (*pole*) $P = (\bar{x}_1 : \dots : \bar{x}_n : \bar{x}_0) \in \mathbb{P}^n$.

Then, the equation

$$\sum_{i=0}^n \frac{\partial \varphi(x_1, \dots, x_n, x_0)}{\partial x_i} \bar{x}_i = 0 \quad (3)$$

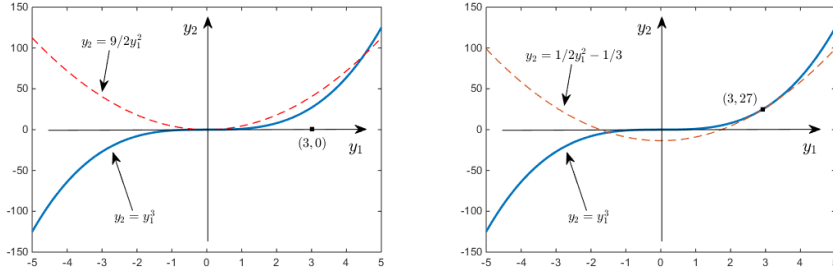


Fig. 1 The (blue) continuous line represents the hypersurface with equation $\varphi(x_1, x_2, x_0) = x_1^3 - x_2x_0^2 = 0$, while the (red) dashed line is its polar hypersurface (3), in Cartesian coordinates. (*left*) The pole $(\bar{x}, 1)^T \in \mathbb{P}^2$, where $\bar{x} = (3, 0)^T \in \mathbb{R}^2$, does not belong to the hypersurface; (*right*) the pole $(\bar{w}, 1)^T \in \mathbb{P}^2$, where $\bar{w} = (3, 27)^T \in \mathbb{R}^2$, belongs to the hypersurface.

represents an algebraic hypersurface of order $r - 1$, which is said to be the *first polar* (or *polar*) of the point P with respect to the hypersurface (2), in homogeneous coordinates.

Figure 1 helps to detail the geometry behind (2) (blue continuous line) and (3) (red dashed line), being $\varphi(x_1, x_2, x_0) = x_1^3 - x_2x_0^2 = 0$. In particular, Figure 1 (*left*) describes the case in which the pole $(\bar{x}, 1)^T \in \mathbb{P}^2$, where $\bar{x} = (3, 0)^T \in \mathbb{R}^2$, is not a point of \mathcal{F} , while in Figure 1 (*right*) the point $(\bar{w}, 1)^T \in \mathbb{P}^2$, where $\bar{w} = (3, 27)^T \in \mathbb{R}^2$, belongs to \mathcal{F} .

We immediately realize that in case $\varphi(x_1, \dots, x_n, x_0) = 0$ is a quadratic hypersurface (i.e. $r = 2$ and $\partial\varphi(x_1, \dots, x_n, x_0)/\partial x_i$ is linear) then we have from (3)

$$\sum_{i=0}^n \frac{\partial\varphi(x_1, \dots, x_n, x_0)}{\partial x_i} \cdot \bar{x}_i = \sum_{i=0}^n \frac{\partial\varphi(x_1, \dots, x_n, x_0)}{\partial x_i} \Big|_{x_i=\bar{x}_i} \cdot x_i = 0. \quad (4)$$

Using a standard taxonomy, the algebraic hypersurface (2) is often addressed as the 0-th *polar* (of any point in \mathbb{P}^n , with respect to itself), while the first polar of the point $P \in \mathbb{P}^n$ with respect to (2), when $r = 2$, is often called the *polar hyperplane* of P .

We report here two of the essential results for polarity, where we focus on (quadratic) hypersurfaces of order $r = 2$.

Theorem 2.1 [Reciprocity Theorem] *Consider the algebraic hypersurface (2) of order $r = 2$ and the points $P, Q \in \mathbb{P}^n$. If the polar hyperplane of P with respect to (2) passes through Q , then the polar hyperplane of Q with respect to (2) passes through P .*

Theorem 2.2 [Section Theorem] *Consider the algebraic hypersurface (2) of order $r \geq 1$. Let V_d be a linear space of dimension $d \leq n$, such that $\bar{\mathcal{F}} = \mathcal{F} \cap V_d$ and $\bar{\mathcal{F}} \neq V_d$. For every point $P \in V_d$, the section by V_d of the first polar of P (with respect to (2)) coincides with the first polar of P with respect to $\bar{\mathcal{F}}$.*

An example of the geometry behind the Reciprocity Theorem is detailed in Figure 2 (left), where for simplicity $n = 2$ and hyperplanes are represented by lines: the point P is the pole of ℓ'_2 with respect to \mathcal{F} , while the dashed lines by P admit as poles their intersections with the line ℓ'_2 .

The definition of polarity, along with the fact that the gradient of φ in (2) is well-defined, implies that, if a finite point P satisfies (2) and $r = 2$, then the polar (i.e. the polar hyperplane) of P with respect to (2) coincides with the *tangent hyperplane* of (2) in P . On the other hand, Theorem 2.2 allows the definition of polar hyperplane also for points at infinity, where the tangent

hyperplane (in Cartesian coordinates) does not exist. In this regard, the next (simplified) definition and the subsequent result (whose proof can be found in [19]) clarify the taxonomy of points.

Definition 2.2 Given the algebraic hypersurface (2) of order $r \geq 1$ and a point $P \in \mathbb{P}^n$ in homogeneous coordinates, we say that P is *self-conjugate with respect to (2)*, if P belongs to its first polar with respect to (2).

In particular, it follows that, if the point P is self-conjugate and $r = 2$, then its polar hyperplane coincides with the tangent hyperplane of $\varphi(x_1, \dots, x_n, x_0) = 0$ in P . Moreover, we have the following result.

Proposition 2.2 *Given the algebraic hypersurface (2) and a point $P \in \mathbb{P}^n$, P is self-conjugate if and only if P satisfies (2), i.e. P belongs to the algebraic hypersurface (2).*

3 Polarity and the Geometry Behind Conjugacy

In this section, we study some basics of polarity for *quadratic hypersurfaces* [19, 21], in the homogeneous coordinates projective space \mathbb{P}^n . Given a symmetric matrix $A = \{a_{ij}\} \in \mathbb{R}^{n \times n}$, a vector $b = (b_1, \dots, b_n)^T \in \mathbb{R}^n$, and a scalar $c \in \mathbb{R}$, we consider the reference symmetric linear system

$$Ay = b, \tag{5}$$

and as a reference quadratic functional

$$g(y) = \frac{1}{2}y^T Ay - b^T y + c. \tag{6}$$

Initially, we associate a quadratic hypersurface \mathcal{F} to g , in the corresponding \mathbb{P}^n homogeneous coordinates projective space. To this end, we observe that g can be associated to the functional $f : \mathbb{P}^n \rightarrow \mathbb{R}$ in homogeneous coordinates defined, for $x_0 \neq 0$, by

$$f(x_1, \dots, x_n, x_0) = g\left(\frac{x}{x_0}\right) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n a_{ij} \left(\frac{x_i}{x_0}\right) \left(\frac{x_j}{x_0}\right) - \sum_{i=1}^n b_i \left(\frac{x_i}{x_0}\right) + c, \quad (7)$$

where $x = (x_1, \dots, x_n)^T$. In turn, the functional $f(x_1, \dots, x_n, x_0)$ can be associated with the quadratic hypersurface

$$\begin{aligned} \mathcal{F} &:= \{(x, x_0)^T \in \mathbb{P}^n : f(x, x_0)x_0^2 = 0\} \\ &\equiv \{(x, x_0)^T \in \mathbb{P}^n : x^T A x - 2x_0 b^T x + 2cx_0^2 = 0\}. \end{aligned} \quad (8)$$

Hereinafter, the symbol \mathcal{F} will always indicate the quadratic hypersurface in (8). Moreover, the next assumption will hold throughout the paper with the exception of a few highlighted results.

Assumption 3.1 *Given the nonsingular symmetric matrix $A \in \mathbb{R}^{n \times n}$, the vector $b \in \mathbb{R}^n$ and the scalar c in (8), the next two equivalent conditions hold:*

– *matrix*

$$\begin{pmatrix} A & -b \\ -b^T & 2c \end{pmatrix} \in \mathbb{R}^{(n+1) \times (n+1)}$$

is nonsingular;

– *we have $2c - b^T A^{-1} b \neq 0$.*

Under Assumption 3.1, \mathcal{F} in (8) has a finite centre and is nondegenerate, so that polarity identifies a *one-to-one* correspondence between points and

1 hyperplanes in the space of homogeneous coordinates [22] (see also Figure 4).
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 3 Indeed, invoking the duality principle, we can consider the projective space \mathbb{P}^n
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 5 and the dual space $(\mathbb{P}^n)^*$ of hyperplanes corresponding to points in \mathbb{P}^n (using
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 7 the dual map in Definition 2.1, which associates the hyperplane of equation (3)
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 9 to the point P). Then, if Assumption 3.1 holds, the dual map is nondegenerate,
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 11 and the set of all the dual hyperplanes of the points of \mathcal{F} in (8) coincides with
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 13 its closure (i.e. the dual variety of \mathcal{F} – see also [23]).
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16 We note that the transformation $y = x/x_0$ makes the *hyperplane at infinity*
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 18 $x_0 = 0$ (in homogeneous coordinates) correspond to the locus of all the points
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 20 at infinity of \mathbb{R}^n . Then, we can use the hypersurface \mathcal{F} to study the proper-
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 22 ties of g at points at infinity. To this end, we introduce some definitions and
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 24 propositions concerning \mathcal{F} that will prove to be useful for a complete analysis.
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27
 28 **Definition 3.1** Given \mathcal{F} and the points $(x^*, x_0^*)^T, (\bar{x}, \bar{x}_0)^T \in \mathbb{P}^n$:

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 30 – $(\bar{x}, \bar{x}_0)^T$ is the **pole** of the hyperplane $\bar{\pi}$ if $\bar{\pi}$ is the first polar hyperplane
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 32 of $(\bar{x}, \bar{x}_0)^T$ with respect to \mathcal{F} ;
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 34 – the pole $(x^*, x_0^*)^T$ of the hyperplane $x_0 = 0$ is the **centre** of \mathcal{F} ;
- 35
 36 – the hyperplanes through the centre $(x^*, x_0^*)^T$ of \mathcal{F} are the **diametral hy-**
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 38 **perplanes** of \mathcal{F} ;
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 40 – the lines through the centre $(x^*, x_0^*)^T$ of \mathcal{F} are the **diameters** of \mathcal{F} .
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45 Let us stress that a finite centre for \mathcal{F} can be defined only in case Assump-
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 47 tion 3.1 holds. We also observe that, by the *Reciprocity Theorem* (Theo-
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 49 rem 2.1), the diametral hyperplanes of \mathcal{F} are polar hyperplanes of points at
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infinity, i.e. the pole of a diametral hyperplane is a point at infinity whose coordinates satisfy the equation $x_0 = 0$.

Definition 3.2 Two diametral hyperplanes π_1 and π_2 of \mathcal{F} are **conjugate**, if π_i contains the pole of π_j , for $i, j \in \{1, 2\}$, $i \neq j$.

Definitions 3.1 and 3.2 imply that, if π_1 and π_2 are conjugate diametral hyperplanes, then the pole of π_1 is one of the points at infinity of π_2 and vice versa.

Figure 2 (*left*) presents the simple geometry behind polarity for quadratic hypersurfaces. The point P is the pole of the hyperplane (i.e. line, since $n = 2$) ℓ'_2 . In particular, ℓ'_2 is obtained joining the tangency points of lines from P to \mathcal{F} . With a similar construction the point at infinity $(d_1, 0)^T$ of ℓ_1 represents also the pole of ℓ_2 , being parallel the tangent lines from $(d_1, 0)^T$ to \mathcal{F} .

As a consequence, ℓ_1 contains the pole of ℓ_2 . A similar analysis also holds for Figure 2 (*right*), in the indefinite case. It can be noticed that the vector d_1 is parallel to ℓ_1 and that, as $n = 2$, the line ℓ_2 may be also seen as a diametral hyperplane whose pole is $(d_1, 0)^T$.

Definition 3.3 Given \mathcal{F} :

- two diameters ℓ_1 and ℓ_2 of \mathcal{F} are **conjugate** if the point at infinity $(d_i, 0)^T \in \mathbb{P}^n$ of ℓ_i , $i \in \{1, 2\}$, is the pole of a (diametral) hyperplane which contains ℓ_j , $j \in \{1, 2\}$, for $i \neq j$. Two lines ℓ_1 and ℓ_2 are conjugate, if they are respectively parallel to conjugate diameters.
- a **diametral hyperplane** π_1 is **conjugate** to the diameter ℓ_2 if any line contained in π_1 is conjugate to ℓ_2 . A hyperplane π_1 is conjugate to the line

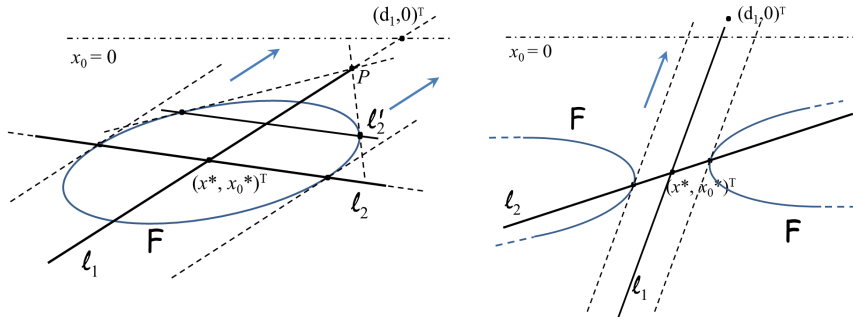


Fig. 2 Conjugate lines ℓ_1 and ℓ_2 with respect to the quadratic hypersurface \mathcal{F} in (8), characterized by a positive definite matrix A (*left*) and an indefinite matrix A (*right*).

ℓ_2 if π_1 and ℓ_2 are respectively parallel to a diametral hyperplane and a diameter that are conjugate.

We point out that Definition 3.3 may sound unusual. In the literature (see, e.g., [19]), lines ℓ_1 and ℓ_2 are addressed as conjugate if the polar hyperplanes of *all the points* (not just of the point at infinity) of ℓ_1 include lines parallel to ℓ_2 and vice versa. However, this latter definition and Definition 3.3 are equivalent. Indeed, let π_3 be the polar hyperplane of the point at infinity of the diameter ℓ_1 (see Figure 3). Simple geometric considerations prove that ℓ_1 and ℓ_2 are conjugate according to Definition 3.3 (i.e. $\ell_2 \in \pi_3$). Hence, all the points on the line ℓ_1 are the poles of hyperplanes parallel to π_3 . This fact is represented in Figure 3, where a 3-dimensional quartic \mathcal{F} and the polar hyperplanes of three points of ℓ_1 are depicted. There, π_1 is the polar hyperplane of the point P_1 of tangency between \mathcal{F} and π_1 ; π_2 is the polar hyperplane of a generic point $P_2 \in \ell_1$; π_3 is the polar hyperplane of $(d_1, 0)^T$, i.e. the point at infinity of ℓ_1 . As the three hyperplanes π_1 , π_2 and π_3 are parallel, π_1 and π_2 certainly include

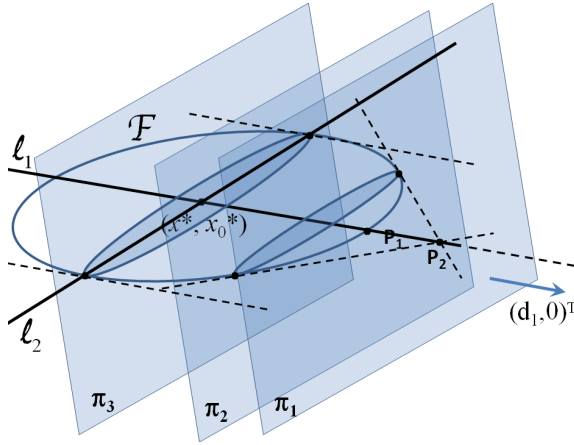


Fig. 3 Polar hyperplanes of points on the line ℓ_1 , with respect to \mathcal{F} . π_3 is the polar hyperplane of $(d_1, 0)^T$, π_2 is the polar hyperplane of P_2 and π_1 is the polar hyperplane of P_1 .

lines parallel to $\ell_2 \in \pi_3$. Finally, we highlight that the results in Figure 3 (which refer to $n = 3$), can be similarly obtained when $n = 2$, as in Figure 2 (left).

4 Basic Practical Consequences of Conjugacy

In this section, we show that the geometric concept of conjugacy of lines has an immediate algebraic counterpart, involving the directional cosines of the lines. This fact will be useful to address some properties of CG-based methods in Sections 5–7.

Proposition 4.1 *Two lines ℓ_1 and ℓ_2 are conjugate with respect to \mathcal{F} if and only if*

$$d_1^T A d_2 = 0, \tag{9}$$

where $(d_1, 0)^T$ and $(d_2, 0)^T$ are points at infinity of respectively ℓ_1 and ℓ_2 .

Proof The polar hyperplane of $(d_1, 0)^T \in \ell_1$, with respect to \mathcal{F} , is given by the diametral hyperplane whose points $(x, x_0)^T \in \mathbb{P}^n$ satisfy

$$2(Ax - bx_0)^T d_1 = 0 \quad (10)$$

(see relation (4)). Thus, by Definition 3.3, the line ℓ_2 is conjugate to ℓ_1 if and only if the point at infinity $(d_2, 0)^T$ satisfies (10), i.e. (9) holds. \square

The above proposition highlights how the geometric concept of conjugacy between lines ℓ_1 and ℓ_2 simply depends on the matrix A in (8), regardless of the choice of the vector b and the scalar c in \mathcal{F} . The algebraic counterpart (9) of the geometric concept of conjugacy has also an additional equivalent characterization. Indeed, in case $A \succ 0$ relation (9) shows that the conjugacy between ℓ_1 and ℓ_2 is equivalent to impose the orthogonality condition $\langle d_1, d_2 \rangle_A = 0$, being $\langle \cdot, \cdot \rangle_A$ the inner product induced by A . As a consequence, in case $A = I_n$ then the conjugacy between ℓ_1 and ℓ_2 reduces to the orthogonality condition $d_1^T d_2 = 0$.

Definition 4.1 Two vectors $d_1 \in \mathbb{R}^n$ and $d_2 \in \mathbb{R}^n$ are **conjugate vectors** with respect to \mathcal{F} , if (9) holds.

We highlight that the proof of the next proposition indicates a simple but relevant property: namely, given a direction $d \in \mathbb{R}^n$, the vector Ad is orthogonal to any direction conjugate to d . We will use this fact later on in the paper (Proposition 6.2).

Proposition 4.2 Consider a line $\hat{\ell}$ with point at infinity $(\hat{d}, 0)^T$. Then, a hyperplane π is conjugate to $\hat{\ell}$, with respect to \mathcal{F} , if and only if any line contained in π is conjugate to $\hat{\ell}$. Moreover, π is parallel to the polar hyperplane of $(\hat{d}, 0)^T$.

Proof The first part of the proposition trivially follows from Definition 3.3.

To prove the second part of the proposition, consider the polar hyperplane of $(\hat{d}, 0)^T$, i.e. the hyperplane whose points $(x, x_0)^T \in \mathbb{P}^n$ satisfy $(Ax - bx_0)^T \hat{d} = 0$. Let ℓ be a generic line in this hyperplane. Then ℓ can be expressed as the locus of the points $(\bar{x}, \bar{x}_0)^T + \lambda(d, 0)^T$ for all $\lambda \in \mathbb{R}$, where $(\bar{x}, \bar{x}_0)^T$ is a point of ℓ and $(d, 0)^T$ is the point at infinity of ℓ . As ℓ is in the polar hyperplane of $(\hat{d}, 0)^T$, then

$$[A(\bar{x} + \lambda d) - b\bar{x}_0]^T \hat{d} = 0 \iff (A\bar{x} - b\bar{x}_0)^T \hat{d} + \lambda(Ad)^T \hat{d} = 0, \quad \forall \lambda \in \mathbb{R},$$

and hence $\lambda(Ad)^T \hat{d} = 0$, because $(\bar{x}, \bar{x}_0)^T \in \pi$. Consequently, ℓ is conjugate to $\hat{\ell}$ by Proposition 4.1. \square

In the next proposition, we state the relation between the centre of \mathcal{F} and the solution of the symmetric linear system $Ay = b$.

Proposition 4.3 [Equivalence of centre] Consider the quadratic hypersurface \mathcal{F} with centre $(x^*, x_0^*)^T$ and let Assumption 3.1 hold. Then $x_0^* = 1/(4c - 2b^T A^{-1}b)$ and the vector $v^* = (x^*/x_0^*)$ is the unique solution of the linear system $Ay = b$.

Proof We first observe that, by definition the hyperplane $x_0 = 0$ is the polar of $(x^*, x_0^*)^T$ with respect to \mathcal{F} . Thus, by (4) we have that the hyperplane

$$\sum_{i=0}^n \frac{\partial \varphi(x_1, \dots, x_n, x_0)}{\partial x_i} \Big|_{x_i=x_i^*} \cdot x_i = 0$$

must coincide with $x_0 = 0$, i.e.,

$$\left. \frac{\partial \varphi(x_1, \dots, x_n, x_0)}{\partial x_i} \right|_{x_i = x_i^*} = \begin{cases} 0 & \text{for } i = 1, \dots, n, \\ 1 & \text{for } i = 0. \end{cases} \quad (11)$$

Recalling that by (8) we have $\varphi(x_1, \dots, x_n, x_0) = x^T A x - 2x_0 b^T x + 2c x_0^2$, we obtain that (11) is equivalent to

$$\begin{pmatrix} 2A & -2b \\ -2b^T & 4c \end{pmatrix} \begin{pmatrix} x^* \\ x_0^* \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (12)$$

By Assumption 3.1 the coefficient matrix in (12) is nonsingular. Hence, it admits a unique solution $(x^*, x_0^*)^T$ with $x_0^* = 1/(4c - 2b^T A^{-1}b)$ by Rouché-Capelli Theorem.

Finally, the first n equations of (12) imply $Ax^* = bx_0^*$, that is $(x^*/x_0^*) = A^{-1}b$. Hence, $v^* = x^*/x_0^*$ is the unique solution of $Ay = b$. \square

Let us here briefly comment the hypotheses in Proposition 4.3. The non-singularity of matrix A implies that the coefficient matrix in (12) has rank greater than or equal to n . Hence, hypersurface \mathcal{F} is irreducible [19], i.e. it contains at most a double point and cannot degenerate into a pair of hyperplanes. However, this hypothesis alone would not prevent \mathcal{F} from being a cone or a cylinder (see Figure 4). The additional hypothesis $c \neq 1/2b^T A^{-1}b$ in Assumption 3.1 implies $x_0^* \neq 0$, and hence ensures that the centre of \mathcal{F} is not a point at infinity. This fact, along with the non-singularity of A guarantees that \mathcal{F} can be only an ellipsoid or a hyperboloid or a paraboloid.

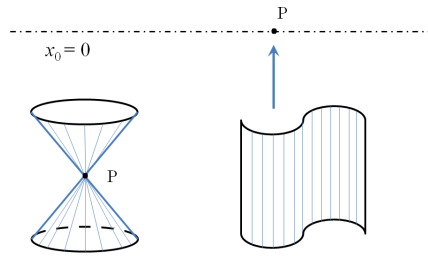


Fig. 4 Degenerate quadratic hypersurface \mathcal{F} in (8) (*cone* or *cylinder*), when the coefficient matrix A in (12) has full rank n and exactly one double point P exists (i.e. $c = 1/2b^T A^{-1}b$).

5 A Basis of Conjugate Directions: the Positive Definite Case

In this section, we report some additional results that hold as long as the matrix A in the hypersurface \mathcal{F} , defined in (8), is positive definite. In the spirit of this paper, the proofs of these results will rely on geometric properties suggested by polarity, instead of invoking algebraic arguments.

Proposition 5.1 [Existence of n conjugate lines, case $A \succ 0$] *Consider the quadratic hypersurface \mathcal{F} and let Assumption 3.1 hold, with $A \succ 0$. Then, there exist n conjugate lines ℓ_j , $j = 1, \dots, n$, with respect to \mathcal{F} . These lines are also linearly independent.*

Proof Note that by Assumption 3.1 and since $A \succ 0$, then \mathcal{F} is a real hyperellipsoid which does not include points at infinity. Then, in the proof we consider a simplified expression of \mathcal{F} . Indeed, under the nonsingular linear transformation

$$\begin{pmatrix} x \\ x_0 \end{pmatrix} = \begin{pmatrix} I_n & A^{-1}b \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \hat{x} \\ \hat{x}_0 \end{pmatrix}, \quad (13)$$

we can transform \mathcal{F} into

$$\hat{\mathcal{F}} := \{(\hat{x}, \hat{x}_0)^T \in \mathbb{P}^n : (\hat{x} + A^{-1}b \cdot \hat{x}_0)^T A(\hat{x} + A^{-1}b \cdot \hat{x}_0) - 2\hat{x}_0 b^T (\hat{x} + A^{-1}b \cdot \hat{x}_0) + 2c\hat{x}_0^2 = 0\},$$

i.e. we obtain the simplified expression

$$\hat{\mathcal{F}} = \left\{ (\hat{x}, \hat{x}_0)^T \in \mathbb{P}^n : \begin{aligned} &\hat{f}(\hat{x}_1, \dots, \hat{x}_n, \hat{x}_0) = 0, \\ &\hat{f}(\hat{x}_1, \dots, \hat{x}_n, \hat{x}_0) = \hat{x}^T A \hat{x} + (2c - b^T A^{-1}b)\hat{x}_0^2 \end{aligned} \right\}, \quad (14)$$

whose centre $(\hat{x}^*, \hat{x}_0^*)^T$ is

$$\hat{x}^* = 0 \quad \hat{x}_0^* = \frac{1}{4c - 2b^T A^{-1}b}. \quad (15)$$

Now we carry on the proof by induction and we first compute the n lines $\hat{\ell}_j$, with $j = 1, \dots, n$. Then, by the inverse transformation of (13) we will obtain the conjugate lines ℓ_j , with $j = 1, \dots, n$.

Base case. Consider the line $\hat{\ell}_1$, with point at infinity $(\hat{d}_1, 0)^T$, and let $\hat{\pi}_1$ be the polar hyperplane of $(\hat{d}_1, 0)^T$ with respect to $\hat{\mathcal{F}}$. In case $n = 1$ the proof is over. Otherwise, we recursively define the remaining $n - 1$ conjugate lines $\hat{\ell}_j$, with $j = 2, \dots, n$. To this end, the hyperplane $\hat{\pi}_1$ is an $(n - 1)$ -dimensional hyperplane and includes the point $(0, \hat{x}_0)^T$, being $\hat{x}_0 \neq 0$.

Indeed, by (4) and since $(\hat{x}^*, \hat{x}_0^*)^T \equiv (0, 1/(4c - 2b^T A^{-1}b))^T$, we have

$$\hat{\pi}_1 := \left\{ (\hat{x}, \hat{x}_0)^T \in \mathbb{P}^n : \sum_{i=0}^n \frac{\partial \hat{f}(\hat{x}_1, \dots, \hat{x}_n, \hat{x}_0)}{\partial \hat{x}_i} \Big|_{(\hat{d}_1, 0)^T} \hat{x}_i = 0 \right\},$$

which is equivalent to

$$\hat{\pi}_1 = \{(\hat{x}, \hat{x}_0)^T \in \mathbb{P}^n : \hat{d}_1^T A \hat{x} = 0\}. \quad (16)$$

Then, we show that $(\hat{d}_1, 0)^T \notin \hat{\pi}_1$. Since the (symmetric) matrix A is not singular, it easily follows from (15) that $(\hat{d}_1, 0)^T \notin \hat{\pi}_1$. Moreover, Proposition 4.2 implies that $\hat{\ell}_1$ is conjugate to any line contained in $\hat{\pi}_1$.

Induction step. For $i = 1, \dots, j-1$, we denote by $\hat{\pi}_i$, the $(n-1)$ -dimensional polar hyperplane of $(\hat{d}_i, 0)^T$ with respect to $\hat{\mathcal{F}}$, i.e. $\hat{\pi}_i = \{(\hat{x}, \hat{x}_0)^T \in \mathbb{P}^n : \hat{d}_i^T A \hat{x} = 0\}$. Also, we denote by $\hat{\Pi}_{j-1}$ the following $[n - (j - 1)]$ -dimensional hyperplane

$$\hat{\Pi}_{j-1} = \bigcap_{i=1}^{j-1} \hat{\pi}_i.$$

Then, we introduce $\hat{\ell}_j$ as an arbitrary line in $\hat{\Pi}_{j-1}$, being $(\hat{d}_j, 0)^T$ its point at infinity and $\hat{\pi}_j$ the polar hyperplane of $(\hat{d}_j, 0)^T$.

We observe that also $\hat{\pi}_j$ is a $(n-1)$ -dimensional diametral hyperplane of $\hat{\mathcal{F}}$, since $(\hat{d}_j, 0)^T$ is a point at infinity. As a consequence, we can deduce that $(\hat{d}_j, 0)^T \notin \hat{\pi}_j$ by repeating for $\hat{\pi}_j$ the same reasoning which yielded (16). We also observe that the *Section Theorem 2.2* guarantees that the intersection $\hat{\pi}_j \cap \hat{\Pi}_{j-1}$ is a $(n-j)$ -dimensional hyperplane which is conjugate to both $\hat{\ell}_j$ and all the lines $\hat{\ell}_i$, for $i = 1, \dots, j-1$. Finally, we note that the line $\hat{\ell}_j$ cannot be obtained as a linear combination of the lines contained in $\hat{\pi}_j$, since $(\hat{d}_j, 0)^T \notin \hat{\pi}_j$.

The arguments above prove that we can iterate the recursion step $n-1$ times, i.e. for $j = 2, 3, \dots, n$, so that $n-1 = \dim(\hat{\Pi}_1) > \dim(\hat{\Pi}_2) > \dots > \dim(\hat{\Pi}_{n-1}) = 0$, and the conjugate lines $\hat{\ell}_1, \dots, \hat{\ell}_n$ are linearly independent.

Thus, using backwards the transformation (13), we obtain n lines ℓ_j , $j =$

1, ..., n, with points at infinity $\{(d_j, 0)^T\}$, satisfying

$$\begin{pmatrix} d_j \\ 0 \end{pmatrix} = \begin{pmatrix} I_n & A^{-1}b \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \hat{d}_j \\ 0 \end{pmatrix}, \quad j = 1, \dots, n.$$

The latter equalities yield $d_j \equiv \hat{d}_j$, $j = 1, \dots, n$, which implies that also ℓ_1, \dots, ℓ_n are conjugate and linearly independent. \square

As a natural consequence, we can use the above proposition to easily provide an alternative proof of the following well-known result from the literature: the solution of the positive definite linear system $Ay = b$ can be computed starting from any point $\bar{y} \in \mathbb{R}^n$, provided that up to n conjugate directions are given.

6 A Basis of Conjugate Directions: the Indefinite Case

In this section, we extend the results presented in the previous section to the case of matrix A indefinite. These contents may appear a step away from the case, where the CG can be applied and is well-posed. However, as we already pointed out, in several optimization frameworks the CG is applied to solve indefinite linear systems accepting the risk of possible failures. In this context, we explain why an extension to the projective space of homogeneous coordinates is mandatory, in order to describe possible CG failures in the indefinite case. Indeed, we show that using finite points in \mathbb{R}^n , as those usually generated by the CG, does not allow to grasp CG possible degeneracy.

To this end, we first denote by \mathcal{C}_∞ the intersection between the hyperplane at infinity $x_0 = 0$ and the hypersurface \mathcal{F} , i.e.

$$\mathcal{C}_\infty := \{(x, 0)^T \in \mathbb{P}^n : x^T A x = 0\}. \quad (17)$$

Then, we introduce the following definitions.

Definition 6.1 The **asymptotic cone** of the hypersurface \mathcal{F} , with finite centre, is the set of all the lines connecting the centre of \mathcal{F} and any point of \mathcal{C}_∞ .

An immediate consequence of the above definition is that, if the centre $(x^*, x_0^*)^T$ of \mathcal{F} is finite, in Cartesian coordinates the equation of the asymptotic cone of \mathcal{F} is given by

$$\frac{1}{2} \left(y - \frac{x^*}{x_0^*} \right)^T A \left(y - \frac{x^*}{x_0^*} \right) = 0. \quad (18)$$

Indeed, we note that equation (18) is homogeneous in $(y - x^*/x_0^*)$, so that it is a cone, and that the line $\ell = \{y \in \mathbb{R}^n : x^*/x_0^* + \lambda d, \lambda \in \mathbb{R}\}$ belongs to the asymptotic cone of \mathcal{F} if and only if $d^T A d = 0$.

Definition 6.2 A direction $d \in \mathbb{R}^n \setminus \{0\}$ is **auto-conjugate** with respect to the hypersurface \mathcal{F} with finite centre, if the point at infinity $(d, 0)^T$ belongs to the asymptotic cone of \mathcal{F} , i.e. $d^T A d = 0$.

The taxonomy in Definition 6.2 aims at avoiding confusion with *self-conjugate* points, introduced in Definition 2.2. A relation exists between the two concepts as, by Definition 2.2, the polar hyperplane π of the point $(d, 0)^T$, such that $d^T A d = 0$, is tangent to \mathcal{F} in $(d, 0)^T$, inasmuch as $(d, 0)^T$ also

1 belongs to \mathcal{F} . Figure 5 (*left*) illustrates the latter fact: the dashed lines are
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 3 auto-conjugate (with respect to \mathcal{F}) and are tangent to \mathcal{F} in points at infinity.
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 5 These points are self-conjugate with respect to \mathcal{F} .
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 9 Relation (18) and Definition 6.2 indicate that the hypersurface \mathcal{C}_∞ is what
 10 really matters in order to identify the asymptotic cone of \mathcal{F} . In this section,
 11 we see that the possible degeneracy of the CG in the indefinite case only deals
 12 with the points (at infinity) in \mathcal{C}_∞ . In Section 7, we will prove that when the
 13 auto-conjugate direction $d \in \mathbb{R}^n \setminus \{0\}$ is computed by the CG in Cartesian
 14 coordinates, then equivalently the point $(d, 0)^T \in \mathbb{P}^n$ is indirectly generated
 15 in homogeneous coordinates. For this point at infinity, we will prove that the
 16 polar hyperplane is defined while no tangent hyperplane exists.
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27 Definitions 6.1 and 6.2 imply that if $A \succ 0$ the quadratic hypersurface \mathcal{F}
 28 has no real (as opposed to ‘complex’) auto-conjugate directions, since $\mathcal{C}_\infty = \emptyset$.
 29 On the other hand, if A is indefinite, auto-conjugate directions may exist.
 30 For example, Figure 5 (*left*) shows the projection of the hypersurface $\mathcal{F} =$
 31 $\{(x, x_0)^T \in \mathbb{P}^2 : 4x_1^2 - 3x_2^2 - x_0^2 = 0\}$ in the Cartesian space \mathbb{R}^2 . Figure 5 (*right*)
 32 shows the corresponding intersection between \mathcal{F} and the hyperplane at infinity,
 33 i.e. $\mathcal{C}_\infty = \{(x, 0)^T \in \mathbb{P}^2 : 4x_1^2 - 3x_2^2 = 0\}$, in the homogeneous coordinate
 34 projective space \mathbb{P}^2 . In this latter context, $d_1 = (\sqrt{3}, 2)^T$ and $d_2 = (\sqrt{3}, -2)^T$
 35 are the two auto-conjugate directions in \mathbb{R}^2 .
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47 In the next proposition, conditions such that \mathcal{F} admits auto-conjugate
 48 directions are given, which is a relevant result when investigating CG-based
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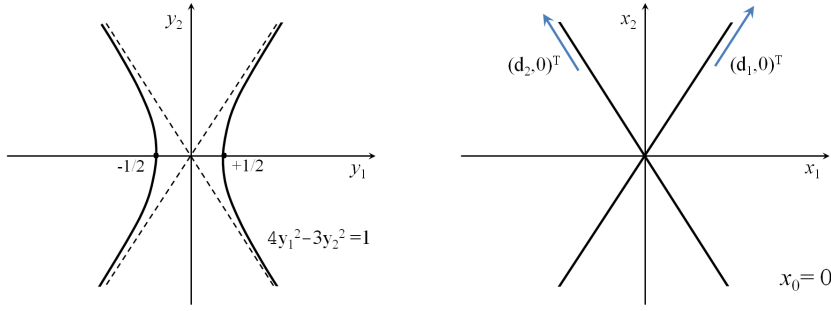


Fig. 5 (left) The quadratic hypersurface $\mathcal{F} = \{(x, x_0)^T \in \mathbb{P}^2 : 4x_1^2 - 3x_2^2 - x_0^2 = 0\}$ (in Cartesian coordinates), and (right) the intersection between \mathcal{F} and the hyperplane at infinity, i.e. the hypersurface $\mathcal{C}_\infty = \{(x, 0)^T \in \mathbb{P}^2 : 4x_1^2 - 3x_2^2 = 0\}$ (in homogeneous coordinates).

methods in the indefinite case. We also remark that the Assumption 3.1 is unnecessary to prove both the next proposition and the subsequent corollary.

Proposition 6.1 [Conjugate and auto-conjugate directions] Consider

the quadratic hypersurface \mathcal{F} with finite centre and A indefinite. Then:

1. if A is nonsingular, the asymptotic cone of \mathcal{F} cannot contain pairs of directions that are both conjugate and auto-conjugate;
2. if A is singular, the asymptotic cone of \mathcal{F} may possibly contain an infinite number of directions that are both conjugate and auto-conjugate.

Proof We preliminarily note that if two conjugate directions d_1 and d_2 are auto-conjugate with respect to \mathcal{F} , then any of their linear combination $\alpha d_1 + \beta d_2$ is also auto-conjugate with respect to \mathcal{F} . Indeed, if $d_1^T A d_2 = 0$ and $d_1^T A d_1 = d_2^T A d_2 = 0$, then for any $\alpha, \beta \in \mathbb{R}$ we have

$$(\alpha d_1 + \beta d_2)^T A (\alpha d_1 + \beta d_2) = \alpha^2 d_1^T A d_1 + \beta^2 d_2^T A d_2 + 2\alpha\beta d_1^T A d_2 = 0. \quad (19)$$

1 The above fact implies that if the conjugate directions d_1 and d_2 are auto-
 2 conjugate with respect to \mathcal{F} , then \mathcal{C}_∞ in (17) must also include the linear
 3 manifold $\text{span}\{d_1, d_2\}$. Using a similar argument, we can prove that, if *any*
 4 manifold $\text{span}\{d_1, d_2\}$. Using a similar argument, we can prove that, if *any*
 5 two conjugate directions d_1 and d_2 are auto-conjugate with respect to \mathcal{F} ,
 6 then any pair of directions linear combinations of d_1 and d_2 are conjugate
 7 with respect to \mathcal{F} .
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10 We also observe that \mathcal{C}_∞ is the set of the auto-conjugate directions with
 11 respect to \mathcal{F} , and that \mathcal{C}_∞ includes a linear manifold only if A is singular.
 12 This latter fact is trivially verifiable, as an example, by observing that if A is
 13 nonsingular, then \mathcal{C}_∞ is a regular hypersurface and each point in \mathcal{C}_∞ corre-
 14 sponds to a different gradient vector. On the contrary, when A is singular all
 15 the points $z = w + n$, where $w \in \mathcal{C}_\infty$ and $n \in \text{Ker}(A)$, belong to \mathcal{C}_∞ and have
 16 the same gradient $2Aw$.
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30 Given the above observation, we can derive those two cases considered in
 31 the problem statement: Case 1. A is nonsingular, so that \mathcal{C}_∞ cannot include a
 32 hyperplane (i.e., \mathcal{C}_∞ cannot degenerate into the product of two hyperplanes).
 33 Thus, if the directions d_1 and d_2 are auto-conjugate with respect to \mathcal{F} , then
 34 they cannot be conjugate as $\text{span}\{d_1, d_2\} \not\subseteq \mathcal{C}_\infty$.
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40 Case 2. A is singular, \mathcal{C}_∞ includes at least a linear manifold π , possibly of
 41 dimension 1. So, by definition of \mathcal{C}_∞ , given a pair of conjugate directions d_1
 42 and d_2 on π , they are also auto-conjugate with respect to \mathcal{F} . Finally, if a pair
 43 of conjugate directions d_1 and d_2 on π exists, then any linear combination of
 44 d_1 and d_2 belongs to π by (19). □
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1 An example of the latter result is provided by the hypersurface $\mathcal{F} =$
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 3 $\{(x, x_0)^T \in \mathbb{P}^2 : 4x_1^2 - 3x_2^2 - x_0^2 = 0\}$ in Figure 5, where
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$$5 \quad A = \begin{pmatrix} 4 & 0 \\ 0 & -3 \end{pmatrix}.$$

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 10 The two directions in \mathbb{R}^2 $d_1 = (\sqrt{3}, 2)^T$ and $d_2 = (\sqrt{3}, -2)^T$, though auto-
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 12 conjugate, are not conjugate, being $d_1^T A d_2 = 24 \neq 0$.
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Though it is beyond the purposes of this paper, the following result can be used in order to justify that some CG-based methods from the literature (namely Planar-CG methods [4-7]) for indefinite linear systems are well-posed.

Corollary 6.1 *Consider the quadratic hypersurface \mathcal{F} with finite centre and A indefinite nonsingular. Consider also two directions $d_1, d_2 \in \mathbb{R}^n$. If $(d_1, 0)^T$ and/or $(d_2, 0)^T$ belong to the asymptotic cone of \mathcal{F} and d_1 is not conjugate to d_2 , then*

$$(d_1^T A d_1)(d_2^T A d_2) - (d_1^T A d_2)^2 \neq 0.$$

Proof The result follows immediately from Proposition 6.1 and Definitions 6.1 - 6.2, as $(d_1^T A d_1)(d_2^T A d_2) = 0$ and $d_1^T A d_2 \neq 0$. \square

We conclude this section with a result similar to the one stated in Proposition 5.1, but referred to the case of matrix A indefinite and nonsingular. Once again, the proof is entirely based on geometric properties suggested by polarity.

Proposition 6.2 [Existence of $n - 1$ conjugate lines, case A indefinite] *Consider the quadratic hypersurface \mathcal{F} with A indefinite and let Assump-*

tion 3.1 hold. Then, there exist n linearly independent lines ℓ_i , $i = 1, \dots, n$, such that at least $n - 1$ of these lines are also conjugate with respect to \mathcal{F} .

Proof Preliminarily, we note that by Proposition 4.3 the centre $(x^*, x_0^*)^T$ of \mathcal{F} is finite. Hence, similarly to Proposition 5.1, we can apply without loss of generality the linear transformation in (13) to \mathcal{F} , in order to obtain the simplified hypersurface $\hat{\mathcal{F}}$ in (14), with centre $(\hat{x}^*, \hat{x}_0^*)^T$ in (15). Then, we carry on the proof by induction, recursively defining the lines $\hat{\ell}_i$, $i = 1, \dots, n$. In the end, we compute the lines ℓ_i , $i = 1, \dots, n$, from $\hat{\ell}_i$, $i = 1, \dots, n$.

Base case. Consider the line $\hat{\ell}_1$ with point at infinity $(\hat{d}_1, 0)^T$, and the corresponding polar hyperplane $\hat{\pi}_1$ (which includes the centre of $\hat{\mathcal{F}}$). In case $n = 1$ the proof is over. Otherwise, if $\hat{\ell}_1$ is not in the asymptotic cone of $\hat{\mathcal{F}}$ the proof proceeds by construction as the proof of Proposition 5.1, until possibly a line $\hat{\ell}_i$, $1 \leq i \leq n$, in the asymptotic cone of $\hat{\mathcal{F}}$ is detected. In case the latter line does not exist, then the directions $\hat{\ell}_1, \dots, \hat{\ell}_n$ are linearly independent and also conjugate. Finally, the proposition is proved using again the transformation (13) and retrieving the vectors d_1, \dots, d_n as in Proposition 5.1, i.e. computing ℓ_1, \dots, ℓ_n .

Induction step. Let $\hat{\ell}_i$ be a line in the asymptotic cone of $\hat{\mathcal{F}}$, being $(\hat{d}_i, 0)^T$ its point at infinity. The polar hyperplane $\hat{\pi}_i$ of $(\hat{d}_i, 0)^T$ is

$$\hat{\pi}_i := \left\{ (\hat{x}, \hat{x}_0)^T \in \mathbb{P}^n : (2A\hat{x})^T \hat{d}_i + 2(2c - b^T A^{-1}b)\hat{x}_0 \cdot 0 = 0 \right\},$$

i.e. (similarly to (16))

$$\hat{\pi}_i := \left\{ (\hat{x}, \hat{x}_0)^T \in \mathbb{P}^n : \hat{d}_i^T A \hat{x} = 0 \right\}. \quad (20)$$

As $\hat{\ell}_i$ is in the asymptotic cone of $\hat{\mathcal{F}}$, then $\hat{d}_i^T A \hat{d}_i = 0$ and $(\hat{d}_i, 0)^T \in \hat{\pi}_i$. Let now $\hat{d}_{i+1} \in \mathbb{R}^n$ be any vector satisfying the following properties:

- \hat{d}_i and \hat{d}_{i+1} are linearly independent but not conjugate;
- \hat{d}_{i+1} is conjugate to $\hat{d}_1, \dots, \hat{d}_{i-1}$ (i.e. \hat{d}_{i+1} is orthogonal to $A\hat{d}_1, \dots, A\hat{d}_{i-1}$, being $\hat{d}_{i+1}^T A \hat{d}_j = 0$, $j = 1, \dots, i-1$).

Recalling Proposition 6.1 and that $i < n$, we prove that such a vector surely exists and does not belong to $\hat{\pi}_i$ (since otherwise by (20) \hat{d}_i and \hat{d}_{i+1} would be conjugate). Indeed, it suffices to set

$$\hat{d}_{i+1} = \beta_{i,0} A \hat{d}_i + \sum_{j=1}^i \beta_{i,j} \hat{d}_j, \quad \beta_{i,0} \neq 0, \quad (21)$$

observing that $A \hat{d}_i$ is orthogonal to \hat{d}_i (see also the comment to Proposition 4.2), with $\hat{d}_j^T A \hat{d}_j \neq 0$, $j = 1, \dots, i-1$, and compute $\{\beta_{i,j}\}$ such that

$$\hat{d}_{i+1}^T A \hat{d}_j = 0, \quad j = 1, \dots, i-1, \quad \text{i.e.} \quad \beta_{i,j} = -\beta_{i,0} \frac{(A \hat{d}_i)^T (A \hat{d}_j)}{\hat{d}_j^T A \hat{d}_j}. \quad (22)$$

The computation of $\beta_{i,j}$ in (22) is well-posed since $\hat{d}_1, \dots, \hat{d}_{i-1}$ are not in the asymptotic cone of $\hat{\mathcal{F}}$. Thus, (21)–(22) yield the conjugacy of \hat{d}_{i+1} with $\hat{d}_1, \dots, \hat{d}_{i-1}$. Moreover, since $(A \hat{d}_i)^T \hat{d}_j = 0$, $j = 1, \dots, i$, by (21) $\hat{d}_{i+1}^T A \hat{d}_i = \beta_{i,0} \|A \hat{d}_i\|^2 \neq 0$, proving that \hat{d}_{i+1} and \hat{d}_i are linearly independent but not conjugate.

The proof proceeds by following the guidelines of the proof of Proposition 5.1. We can thus compute the polar hyperplane $\hat{\pi}_{i+1}$ of the point $(\hat{d}_{i+1}, 0)^T$, with respect to $\hat{\mathcal{F}}$, which includes the point $(0, \hat{x}_0)^T$, being $\hat{x}_0 \neq 0$. Indeed, since $(\hat{x}^*, \hat{x}_0^*)^T \equiv (0, 1/(4c - 2b^T A^{-1}b))^T$ then $\hat{\pi}_{i+1} = \{(\hat{x}, \hat{x}_0)^T \in \mathbb{P}^n : \hat{d}_{i+1}^T A \hat{x} = 0\}$. By the *Section Theorem 2.2* the intersection of $\hat{\pi}_{i+1}$ and $\hat{\pi}_i$

provides a $(n - 2)$ -dimensional hyperplane which is conjugate to $\hat{d}_1, \dots, \hat{d}_{i-1}$.

Finally, by this proposition hypotheses and Proposition 6.1, there cannot be two conjugate lines in the asymptotic cone of $\hat{\mathcal{F}}$. Thus, we can generate the remaining $\hat{d}_{i+2}, \hat{d}_{i+3}, \dots, \hat{d}_n$ directions as in Proposition 5.1.

On the overall, the $n - 1$ directions $\hat{d}_1, \dots, \hat{d}_i, \hat{d}_{i+2}, \dots, \hat{d}_n$ are conjugate by construction, and by (21)–(22) the n directions $\hat{d}_1, \dots, \hat{d}_n$ are linearly independent.

Finally, using again the nonsingular transformation (13), as for Proposition 5.1 we can obtain the lines $\ell_i, i = 1, \dots, n$, with points at infinity $\{(d_i, 0)^T\}$, such that $d_i = \hat{d}_i, i = 1, \dots, n$, which completes the proof. \square

Remark 6.1 Proposition 6.1 and Proposition 6.2 substantially ensure that even in case the matrix A is indefinite, though nonsingular, at least $(n - 1)$ conjugate directions exist. Among these directions no more than one can be auto-conjugate. The latter simple conclusion is noteworthy, since one of the most used methods in the literature which generates conjugate directions (namely the CG method), may fail in the indefinite case, because it can iteratively yield auto-conjugate lines. The item 1. in Proposition 6.1 ensures that the latter fact can occur at most once during the execution of the CG method, even in case A is indefinite.

To better comment the last remark, the following considerations have been formulated. To the best of the authors' knowledge, the literature of the CG method based on the use of algebraic arguments has not given any results yet on the frequency of possible CG degeneracies in the nonsingular indefinite case. Such a fact is not surprising, since in the literature the main focus is often on

1 the CG performance in practice, exploiting the current iteration rather than
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3 analyzing the whole CG method within a general framework. On the contrary,
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5 Proposition 6.1 states that a geometric standpoint behind the CG indicates at
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7 most one possible degeneracy among all the iterations it can possibly perform.
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9 This also suggests another remarkable result, which will be more evident after
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11 introducing the CG in Table 1. Indeed, let the solution of a sequence of linear
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13 systems be sought (which is a typical problem from constrained numerical
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15 optimization), where the nonsingular matrix A remains unchanged and the
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17 recursion of the CG method is applied starting from a given (arbitrary) initial
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19 point $y_0 = \bar{y} \in \mathbb{R}^n$. Then, in case a degeneracy occurs when solving the h -th
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21 linear system of the sequence, we can slightly perturb the point \bar{y} so that by
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23 Proposition 6.1 in none of the remaining linear systems the CG experiences a
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25 degeneracy.
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38 The above remark also justifies the frequent use of the CG-based meth-
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40 ods, on large indefinite linear systems, like those arising in optimization frame-
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42 works. In these cases, in order to provide gradient-related directions, a fast
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44 approximate solution of the linear system is often required. Here, CG-based
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46 methods, may be preferred to more sophisticated and well-posed, but more
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48 computationally burdensome, techniques.
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7 Polar and Tangent Hyperplanes: from Homogeneous to Cartesian Coordinates

In this section, we recast specific aspects of the standard CG method from the perspective of polarity theory. Specifically, we consider the case in which the CG method is used for solving the linear system $Ay = b$ in the Cartesian space \mathbb{R}^n , when $A \succ 0$. Our aim is to show that in this situation polarity theory gives an easy geometric interpretation of the steps of the CG. This interpretation turns out to be useful also in providing a general theoretical framework, when the matrix A is indefinite, and then the CG is not well-posed.

Throughout this section, as previously done we consider the linear system $Ay = b$ and the quadratic hypersurface \mathcal{F} in \mathbb{P}^n (see (8)), but also the associated quadratic functionals $g(y)$ in \mathbb{R}^n and $f(x, x_0)$ in \mathbb{R}^{n+1} , as respectively defined in relations (6) and (7).

Table 1 reports the standard CG method. We can note that, when $A \succ 0$, the standard CG method solves the linear system $Ay = b$ by computing a sequence of points y_k , $k = 1, \dots, m$, $m \leq n$, along with a sequence of m linearly independent conjugate vectors $\{p_k\}$. The method iteratively generates these vectors by imposing that at each Step k the condition $p_k^T A p_j = 0$, for $j < k$, is satisfied. A similar result holds for the generalized class of CG-based methods proposed in [16].

The next three results show that the polar hyperplane of a point in homogeneous coordinates has an equivalent counterpart in Cartesian coordinates. In particular, note that Lemma 7.1 and Corollary 7.1 refer to the polar hyper-

The standard Conjugate Gradient method

Input: $y_0 \in \mathbb{R}^n$.

Step 0: Set $k = 0$, $r_0 = b - Ay_0$.

If $r_0 = 0$, then STOP. Else, set $p_0 = r_0$; $k = k + 1$.

Set $p_{-1} = 0$ and $\beta_{-1} = 0$.

Step k : Compute $\alpha_{k-1} = r_{k-1}^T p_{k-1} / p_{k-1}^T A p_{k-1}$,

$y_k = y_{k-1} + \alpha_{k-1} p_{k-1}$, $r_k = r_{k-1} - \alpha_{k-1} A p_{k-1}$.

If $r_k = 0$, then STOP. Else, set

- $\beta_{k-1} = \|r_k\|^2 / \|r_{k-1}\|^2$, $p_k = r_k + \beta_{k-1} p_{k-1}$, $k = k + 1$,

- (or equivalently set $p_k = -\alpha_{k-1} A p_{k-1} + (1 + \beta_{k-1}) p_{k-1} - \beta_{k-2} p_{k-2}$)

Go to **Step k** .

Output: $\{p_k\}$ and $\{y_k\}$.

Table 1 The standard CG method for solving the linear system $Ay = b$ [24].

plane of a finite point, whereas Corollary 7.2 refers to the polar hyperplane of a point at infinity.

Lemma 7.1 [Equivalence with Polar Hyperplane 1] *Consider the quadratic hypersurface \mathcal{F} in (8), the quadratic functional $g(y)$ in (6), and relation $y = x/x_0$ between Cartesian coordinates $y \in \mathbb{R}^n$ and homogeneous coordinates $(x, x_0)^T \in \mathbb{P}^n$. Let $(x^*, x_0^*)^T$ be the centre of \mathcal{F} . Then, the first polar π of a finite point $P = (\bar{x}, \bar{x}_0)^T \neq (x^*, x_0^*)^T$, $\bar{x}_0 \neq 0$, with respect to \mathcal{F} has the following expression in Cartesian coordinates*

$$\pi := \left\{ y \in \mathbb{R}^n : 2g(\bar{y}) + \sum_{i=1}^n \frac{\partial g(\bar{y}_1, \dots, \bar{y}_n)}{\partial y_i} (y_i - \bar{y}_i) = 0 \right\}. \quad (23)$$

Proof First note that $x_0 = 0$ cannot be the polar hyperplane of P , since $P \neq (x^*, x_0^*)^T$. Hence, hereinafter, together with $\bar{x}_0 \neq 0$, we can assume that

$x_0 \neq 0$ and consider finite points.

The following relations hold given $y = x/x_0$ and the chain rule:

$$\begin{aligned} \frac{\partial f(x_1, \dots, x_n, x_0)}{\partial x_i} &= \frac{\partial g(y_1, \dots, y_n)}{\partial y_i} \cdot \frac{\partial y_i}{\partial x_i} \\ &= \frac{\partial g(y_1, \dots, y_n)}{\partial y_i} \cdot \left(\frac{1}{x_0} \right), \quad i = 1, \dots, n. \end{aligned} \quad (24)$$

Then, using equation (4) and relation

$$\frac{\partial f(x, x_0)}{\partial x_0} = -\nabla_x f(x, x_0)^T \left(\frac{x}{x_0} \right),$$

we can write the first polar of the point $(\bar{x}, \bar{x}_0)^T$ as:

$$\begin{aligned} &\left\{ (x, x_0)^T \in \mathbb{P}^n : \sum_{i=0}^n \frac{\partial [2f(\bar{x}, \bar{x}_0) \bar{x}_0^2]}{\partial x_i} x_i = 0 \right\} \equiv \\ &\left\{ (x, x_0)^T \in \mathbb{P}^n : \right. \\ &\quad \left. 2 \left[\frac{\partial f(\bar{x}, \bar{x}_0)}{\partial x_0} \bar{x}_0^2 + f(\bar{x}, \bar{x}_0) \cdot 2\bar{x}_0 \right] x_0 + 2 \sum_{i=1}^n \frac{\partial f(\bar{x}, \bar{x}_0)}{\partial x_i} \bar{x}_0^2 x_i = 0 \right\} \equiv \\ &\left\{ (x, x_0)^T \in \mathbb{P}^n : \right. \\ &\quad \left. 2 \left[-\nabla_x f(\bar{x}, \bar{x}_0)^T \bar{x} \bar{x}_0 + g(\bar{y}) \cdot 2\bar{x}_0 \right] x_0 + 2\bar{x}_0^2 \nabla_x f(\bar{x}, \bar{x}_0)^T x = 0 \right\}, \end{aligned}$$

so that dividing by $2\bar{x}_0 x_0 \neq 0$ and using (24) we obtain for π the expression

$$\left\{ (x, x_0)^T \in \mathbb{P}^n : -\nabla g(\bar{y})^T \bar{y} + 2g(\bar{y}) + \nabla g(\bar{y})^T y = 0 \right\}. \quad (25)$$

Finally, we note that (25) (in homogeneous coordinates) becomes (23) in Cartesian coordinates as $y = x/x_0$. \square

The polar hyperplane (23) is a generalization of the tangent hyperplane to an algebraic hypersurface. The result is formally detailed in the next corollary.

Corollary 7.1 *Consider the quadratic hypersurface \mathcal{F} in (8), the quadratic functional $g(y)$ in (6), and relation $y = x/x_0$ between Cartesian coordinates $y \in \mathbb{R}^n$ and homogeneous coordinates $(x, x_0)^T \in \mathbb{P}^n$.*

1. Let $(x^*, x_0^*)^T \in \mathbb{P}^n$ be the centre of \mathcal{F} . The first polar π in (23) of a finite point $P \equiv (\bar{x}, \bar{x}_0)^T \neq (x^*, x_0^*)^T$, when expressed in Cartesian coordinates, coincides with the tangent hyperplane to $g(y) = 0$ at $\bar{y} = \bar{x}/\bar{x}_0$, if and only if $g(\bar{y}) = 0$;
2. Let A be nonsingular and $c \neq 1/2b^T A^{-1}b$, then the set π in (23) is nonempty if and only if $A\bar{y} \neq b$;
3. Let A be nonsingular and $c = 1/2b^T A^{-1}b$, then the set π in (23) is nonempty.

Proof As regards point 1., observe that if $g(\bar{y}) = 0$ then the tangent hyperplane to $g(y) = 0$ at \bar{y} is unique, having the expression $\nabla g(\bar{y})^T (y - \bar{y}) = 0$. The latter equation coincides with (23) if and only if $g(\bar{y}) = 0$. As regards point 2., for the sufficient condition, by (6) and (23) we have

$$\begin{aligned} \pi &:= \{y \in \mathbb{R}^n : \bar{y}^T A\bar{y} - 2b^T \bar{y} + 2c + (A\bar{y} - b)^T (y - \bar{y}) = 0\} \quad (26) \\ &\equiv \{y \in \mathbb{R}^n : (2c - b^T \bar{y}) + (A\bar{y} - b)^T y = 0\}. \end{aligned}$$

Thus, if $A\bar{y} \neq b$ then the point

$$y = \frac{b^T \bar{y} - 2c}{\|A\bar{y} - b\|^2} (A\bar{y} - b) \quad (27)$$

belongs to π , so that π is nonempty. Conversely, for the necessary condition, let π be nonempty and assume by contradiction $A\bar{y} = b$. Then, (26) would imply that the relation $0 = 2c - b^T \bar{y} = 2c - b^T A^{-1}b$ holds for any $y \in \mathbb{R}^n \setminus \{0\}$, in contradiction with the assumption $c \neq 1/2b^T A^{-1}b$.

As regards point 3., we distinguish between the two cases: $A\bar{y} = b$ and $A\bar{y} \neq b$.

In the first case $\pi \equiv \mathbb{R}^n$. In the second case, again the vector in (27) belongs to π . □

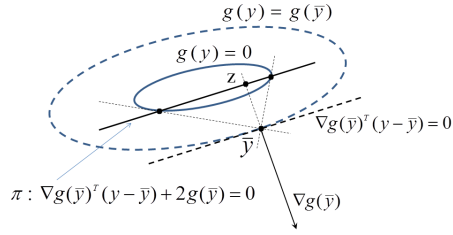


Fig. 6 The geometry, in Cartesian coordinates, behind the polar hyperplane π in (23). \bar{y} is the pole of π , while the point z is given by $z = \bar{y} - 2g(\bar{y})/\|\nabla g(\bar{y})\|^2 \nabla g(\bar{y})$.

The Figure 6 depicts (in Cartesian coordinates) the geometry behind the first polar π in (23). Here consider the hypersurface $g(y) = 0$, along with the tangent hyperplane $\nabla g(\bar{y})^T (y - \bar{y}) = 0$ to $g(y) = g(\bar{y})$ at \bar{y} . Then, observe that π is parallel to the latter hyperplane and contains the point $z = \bar{y} - 2g(\bar{y})/\|\nabla g(\bar{y})\|^2 \nabla g(\bar{y})$.

The next corollary defines the first polar of points at infinity, and will represent an essential tool to study the possible CG degeneracy in the indefinite case.

Corollary 7.2 [Equivalence with Polar Hyperplane 2] *Consider the quadratic hypersurface \mathcal{F} in (8), the quadratic functional $g(y)$ in (6), and relation $y = x/x_0$ between Cartesian coordinates $y \in \mathbb{R}^n$ and homogeneous coordinates $(x, x_0)^T \in \mathbb{P}^n$. Let $(x^*, x_0^*)^T$ be the centre of \mathcal{F} . Then, the first polar π of the point at infinity $(\bar{p}, 0)^T$, $\bar{p} \in \mathbb{R}^n$, with respect to \mathcal{F} , has the following expression in Cartesian coordinates*

$$\pi := \{y \in \mathbb{R}^n : \nabla g(y)^T \bar{p} = 0\}. \quad (28)$$

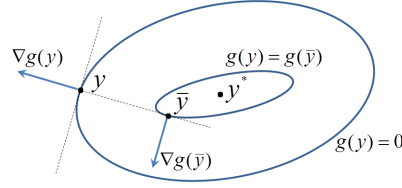


Fig. 7 A graphical description in \mathbb{R}^n of the general iteration of the CG, for $A \succ 0$ and $n = 2$.

If A is nonsingular, then the hyperplane π is nonempty.

Proof The proof follows immediately from Definition 2.1 and (24). \square

We now observe that, for $\bar{y} \in \mathbb{R}^n$ such that $g(\bar{y}) = 0$, the equation that describes the polar hyperplane π both in (23) and in (28) is equivalent to the Ritz–Galerkin condition

$$\nabla g(\bar{y})^T (y - \bar{y}) = 0, \tag{29}$$

imposed by the standard CG–based methods at point $\bar{y} \in \mathbb{R}^n$ [2]. Indeed, in Table 1, at Step k , the coefficient α_{k-1} is chosen by imposing the Ritz–Galerkin condition $0 = r_k^T r_{k-1} = r_k^T p_{k-1}$, i.e. $\nabla g(y_k)^T (y_k - y_{k-1}) = 0$. Then, given β_k , the new conjugate direction p_k is determined using r_k and p_{k-1} . As an example with $n = 2$, consider Figure 7. The ellipsoids in \mathbb{R}^n represent level sets of the function $g(y)$ in (6). Starting from the point y the standard CG method finds the new point \bar{y} , by setting $\bar{\alpha}$ along the direction $-\nabla g(y)$ so that (29) is satisfied. Finally, note that (28) may easily reduce to (23) after setting $\bar{y} = \bar{x}/\bar{x}_0$ in (28), with $\bar{x} = \bar{p}$ and $\bar{x}_0 \rightarrow 0$.

8 CG-based Methods and Polarity Theory: Advances

In this section, we further analyze the relation between polarity theory for the quadratic functional $g(y)$ in (6) and the CG method, in order to get some advances.

For the ease of notation and without loss of generality, in the current and in the following section we assume to have first performed the change of variables

$$y = \hat{y} - \tilde{y}, \quad \tilde{y} = -A^{-1}b, \quad (30)$$

and hence (6) becomes

$$\hat{g}(\hat{y}) = \frac{1}{2}\hat{y}^T A \hat{y} + \left(c - \frac{1}{2}b^T A^{-1}b \right). \quad (31)$$

Then, in (30) we re-denominate \hat{y} and \hat{g} as y and g , respectively. This allows us to address the linear system $Ay = 0$, in place of (5).

As long as A is nonsingular, the linear transformation (30) leaves unchanged the Hessian matrix, and the quadratic functional $g(y)$ in (6) becomes

$$g(y) = \frac{1}{2}y^T A y + \xi, \quad \xi \in \mathbb{R}. \quad (32)$$

Then, if $A \succ 0$, $y^* = 0$ is trivially the optimal solution of the linear system $Ay = 0$ and coincides also with the ratio x^*/x_0^* , being $(x^*, x_0^*)^T \equiv (0, -1/(4\gamma))^T$ the centre of the family (see Proposition 4.3, with $c = -\gamma$ and $b = 0$) of quadratic hypersurfaces (ellipsoids)

$$\frac{1}{2}y^T A y = \gamma, \quad \gamma \geq 0. \quad (33)$$

In homogeneous coordinates, the hypersurfaces (33) are described by the following quadratic homogeneous functions

$$\mathcal{F}_\gamma := \left\{ (x, x_0)^T \in \mathbb{P}^n : \frac{1}{2}x^T Ax - \gamma x_0^2 = 0 \right\}. \quad (34)$$

In this section:

- we prove that the standard CG method generates at any iteration k a hyperplane in \mathbb{R}^n that is equivalent to a diametral hyperplane of \mathcal{F}_γ , for some $\gamma > 0$, in \mathbb{P}^n . In particular, we show that the resulting diametral hyperplane has the point at infinity $(p_k, 0)^T$ as a pole, being p_k the conjugate direction generated at the iteration k (see Table 1);
- we show that all the directions $\{p_k\}$, generated by the standard CG method in \mathbb{R}^n , are parallel to lines contained in polar hyperplanes with respect to different quadratic hypersurfaces \mathcal{F}_γ , for some $\gamma > 0$, in \mathbb{P}^n ;
- we give evidence that the standard CG method generates at each iteration a pair hyperplane–point in \mathbb{R}^n . This pair hyperplane–point corresponds to a pair polar hyperplane–pole in \mathbb{P}^n , and the pole is a finite self–conjugate point as in Definition 2.2;
- we provide a geometric motivation for the fact that, if A is indefinite non-singular in (34), the standard CG method may fail to provide at current iteration a diametral hyperplane of \mathcal{F}_γ , for some $\gamma > 0$, in \mathbb{P}^n .

Proposition 8.1 [CG – Polar Hyperplane 1] *Let the standard CG method perform m steps to solve the linear system $Ay = 0$, with $A \succ 0$. Then, for every*

$k < m$ the linear manifold

$$y_{k+1} + \text{span}\{p_1, \dots, p_{k-1}, p_{k+1}, \dots, p_m\}$$

represents in Cartesian coordinates a diametral hyperplane of the homogeneous hypersurface \mathcal{F}_γ in (34), for any $\gamma > 0$. This diametral hyperplane is the polar hyperplane of the pole $(p_k, 0)^T$, with respect to \mathcal{F}_γ , and can be written as

$$\pi_{k+1} = \{y \in \mathbb{R}^n : (Ap_k)^T y = 0\}.$$

Proof We observe that, at the $(k+1)$ -th iteration, the standard CG method detects the minimum point y_{k+1} of $g(y)$ along the line $y = y_k + \alpha p_k$, where p_k is a suitable search direction and $\alpha \in \mathbb{R}$ (see Table 1 or, for $n = 3$, Figure 8). In particular, the method determines the steplength α_k by solving the unconstrained problem

$$\min_{\alpha} g(y_k + \alpha p_k).$$

Hence, we have $\nabla g(y_k + \alpha_k p_k)^T p_k = 0$, or equivalently

$$0 = \nabla g(y_{k+1})^T p_k = (Ay_{k+1})^T p_k. \quad (35)$$

On the other hand, for any $\gamma > 0$, the polar hyperplane π_{k+1} of $(p_k, 0)^T$ with respect to the hypersurface \mathcal{F}_γ can be rewritten in Cartesian coordinates as

$$\pi_{k+1} := \{y \in \mathbb{R}^n : p_k^T A y = 0\}, \quad (36)$$

by Corollary 7.2. In fact, explicitly computing the polar (diametral) hyperplane of the point $(p_k, 0)^T$, with respect to \mathcal{F}_γ , we obtain

$$\begin{aligned} \{(x, x_0)^T \in \mathbb{P}^n : (Ap_k)^T x + (-2\gamma \cdot 0)x_0 = 0\} &\equiv \\ \{(x, x_0)^T \in \mathbb{P}^n : (Ap_k)^T x = 0\}, \end{aligned}$$

1 which indeed yields (36) in Cartesian coordinates. Thus, by the *Reciprocity*
 2
 3 *Theorem* the latter hyperplane contains the centre $(x^*, x_0^*)^T \equiv (0, -1/(4\gamma))^T$
 4
 5 of \mathcal{F}_γ . Hence, π_{k+1} in (36) contains $x^*/x_0^* = 0$ and is equivalently a diametral
 6
 7 hyperplane (in Cartesian coordinates) of \mathcal{F}_γ . Furthermore, the ellipsoid $g(y) =$
 8
 9 γ , for any $\gamma > 0$, intersects the hyperplane π_{k+1} into an $(n - 2)$ -dimensional
 10
 11 ellipsoid (see also the contours of the shaded areas in Figure 8, where G_2
 12
 13 represents an ellipse).

14
 15 It remains to show that the manifold $y_{k+1} + \text{span}\{p_1, \dots, p_{k-1}, p_{k+1}, \dots, p_m\}$
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 17 satisfies equation (36). Indeed, by simple substitution in (36) and recalling (35)
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 19 we have
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$$\begin{aligned} (Ap_k)^T [y_{k+1} + \text{span}\{p_1, \dots, p_{k-1}, p_{k+1}, \dots, p_m\}] = \\ (Ap_k)^T [\text{span}\{p_1, \dots, p_{k-1}, p_{k+1}, \dots, p_m\}] = 0, \end{aligned}$$

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 23 where the last equality follows from the conjugacy among the m vectors
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 25 $\{p_1, \dots, p_m\}$, generated by the CG. □
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 29 **Proposition 8.2 [CG – Polar Hyperplane 2]** *Let the standard CG method*
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 31 *perform m steps to solve the linear system $Ay = 0$, with $A \succ 0$. Then, at*
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 33 *Step k , $k < m$, the standard CG method generates a hyperplane in Cartesian*
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 35 *coordinates equivalent to the polar hyperplane of the point y_k , with respect to*
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 37 *the quadratic hypersurface \mathcal{F}_{γ_k} , $\gamma_k = 1/2y_k^T Ay_k$. This hyperplane has equation*
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$$\tilde{\pi}_k := \{y \in \mathbb{R}^n : (Ay_k)^T (y - y_k) = 0\} \quad (37)$$

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 49 and contains the line $y_{k-1} + \alpha p_{k-1}$, $\alpha \in \mathbb{R}$.
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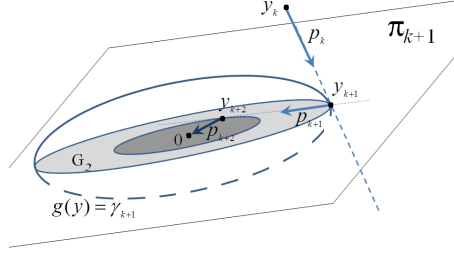


Fig. 8 A detail of the geometry of the $(k+1)$ -th CG iteration: the hyperplane π_{k+1} (which includes the *span* of the directions p_{k+1} and p_{k+2}) is conjugate to direction p_k , with respect to $g(y) = \gamma_{k+1}$, $\gamma_{k+1} = 1/2y_{k+1}^T Ay_{k+1}$.

Proof Let us consider Step k in Table 1 (for $n = 3$, see Figure 9). From point y_{k-1} , the standard CG method moves along p_{k-1} and determines the new point y_k on a hyperplane $\tilde{\pi}_k$, which is tangent to $g(y) = 1/2y_k^T Ay_k$ at y_k . Thus, the hyperplane $\tilde{\pi}_k$ has equation in Cartesian coordinates

$$(Ay_k)^T(y - y_k) = 0. \quad (38)$$

Since $y_k \in \tilde{\pi}_k$ is finite, Definition 2.2 guarantees that $\tilde{\pi}_k$ represents (in Cartesian coordinates) the polar hyperplane of the pole $(x_k, x_{0k})^T$, where $y_k = x_k/x_{0k}$, $x_{0k} \neq 0$, with respect to \mathcal{F}_{γ_k} , and $\gamma_k = 1/2y_k^T Ay_k$. Indeed, as

$$\mathcal{F}_{\gamma_k} := \left\{ (x, x_0)^T \in \mathbb{P}^n : \frac{1}{2}x^T Ax - \gamma_k x_0^2 = 0, \quad \gamma_k = \frac{1}{2}y_k^T Ay_k \right\}, \quad (39)$$

the polar hyperplane of the pole $(x_k, x_{0k})^T$ is given by

$$(Ax_k)^T x - 2\gamma_k x_{k0} x_0 = 0. \quad (40)$$

As for $x_{0k} \neq 0$, $x_0 \neq 0$, $y = x/x_0$, then the equivalence between (38) and (40) holds. When $y = y_{k-1} + \alpha p_{k-1}$, $\alpha \in \mathbb{R}$, the equation (38) yields

$$(Ay_k)^T p_{k-1} = 0, \quad (41)$$

showing that $\tilde{\pi}_k$ contains the line $y_{k-1} + \alpha p_{k-1}$, $\alpha \in \mathbb{R}$, which completes the proof. \square

8.1 CG Iterations and CG Failure: a Geometric Viewpoint

Here we preliminarily show how the CG iterations can be rewritten in terms of polarity; then, we present a geometric motivation of the CG failure when A is indefinite. To this end, we recall that $y^* = 0$ is a solution of $Ay = 0$, by (30)–(31) and therein comments. Hence, unless the standard CG method has reached the very last iteration, the direction p_k computed at Step k has the extremes which are both nonzero.

In the following, we consider the polar hyperplane π_k (see also Figure 9) of $(p_{k-1}, 0)^T$, with respect to \mathcal{F}_{γ_k} , both written in homogeneous coordinates

$$\begin{aligned} \pi_k &:= \{(x, x_0)^T \in \mathbb{P}^n : (Ap_{k-1})^T x - 2\gamma_k \cdot 0 \cdot x_0 = 0\} \\ &\equiv \{(x, x_0)^T \in \mathbb{P}^n : (Ap_{k-1})^T x = 0\}, \end{aligned}$$

and in Cartesian coordinates (see also Corollary 7.2)

$$\pi_k := \{y \in \mathbb{R}^n : (Ap_{k-1})^T y = 0\}. \quad (42)$$

The representation of π_k in Cartesian coordinates allows one to conclude that π_k includes the origin. The representation of π_k in homogeneous coordinates

allows to use Proposition 4.2, showing that π_k has the pole $(p_{k-1}, 0)^T$, with respect to \mathcal{F}_{γ_k} , and contains all the directions conjugate to the vector p_{k-1} .

We also consider in homogeneous coordinates the manifold $V_d \subset \mathbb{P}^n$

$$V_d := \{(x, x_0)^T \in \mathbb{P}^n : a^T x = 0, a \in \mathbb{R}^n \setminus \{0\}\},$$

and the quadratic hypersurface

$$\bar{\mathcal{F}} := \mathcal{F}_{\gamma_k} \cap V_d = \begin{cases} x^T A x - 2\gamma_k x_0^2 = 0 \\ a^T x = 0. \end{cases}$$

We note that the polar hyperplane of $(x_k, x_{k0})^T \in \bar{\mathcal{F}}$ with respect to \mathcal{F}_{γ_k} has equation $(Ax_k)^T x - 2\gamma_k x_{k0} x_0 = 0$, and the intersection ℓ between the latter hyperplane and the manifold V_d is given by

$$\ell := \begin{cases} (Ax_k)^T x - 2\gamma_k x_{k0} x_0 = 0 \\ a^T x = 0. \end{cases}$$

The *Section Theorem* guarantees that ℓ also coincides with the polar hyperplane of $(x_k, x_{k0})^T$ with respect to $\bar{\mathcal{F}}$. Thus, the point $(x_k, x_{k0})^T \in \bar{\mathcal{F}}$ satisfies

$$\begin{cases} x_k^T A x_k - 2\gamma_k x_{k0}^2 = 0 \\ (Ax_k)^T x - 2\gamma_k x_{k0} x_0 = 0 \Big|_{(x,x_0)^T = (x_k, x_{k0})^T} \\ a^T x_k = 0. \end{cases} \quad (43)$$

In order to understand how the above concepts are of interest for the standard CG method, let us consider again Figure 9. The hyperplane π_k contains

1 the centre of $g(y) = \gamma_k$ and is therefore both a diametral hyperplane in \mathbb{R}^n
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 3 and a subspace. Then consider the linear manifold ℓ , i.e. the intersection be-
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 5 tween π_k (polar hyperplane of $(p_{k-1}, 0)^T$) and the tangent hyperplane $\tilde{\pi}_k$ to
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 7 $g(y) = 1/2y_k^T Ay_k$ at $y_k = x_k/x_{k0}$. Now, ℓ is equivalent in \mathbb{R}^n to the polar
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 9 hyperplane of the point y_k with respect to the hypersurface Γ_k (contour of the
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 11 shaded area in Figure 9), which is the intersection between $g(y) = \gamma_k$ and π_k ,
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 14 i.e.

$$15 \quad \Gamma_k : \begin{cases} g(y) = \gamma_k, & \text{where } \gamma_k = \frac{1}{2}y_k^T Ay_k, \\ y \in \pi_k. \end{cases} \quad (44)$$

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 23 The above observation implies that the k -th iteration of the standard CG
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 25 method can be simply analyzed in terms of the linear manifold ℓ and the
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 27 $(n - 1)$ -dimensional hyperplane π_k (which is sketched also in Figure 10). It
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 29 also implies that
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$$31 \quad \pi_k := y_k + \text{span}\{p_1, \dots, p_{k-2}, p_k, \dots, p_m\},$$

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 36 being $p_1, \dots, p_{k-2}, p_k, \dots, p_m$ conjugate to p_{k-1} . In particular, note that at
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 38 Step k the standard CG method computes the residual r_k orthogonal to $\tilde{\pi}_k$
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 40 (and hence also orthogonal to ℓ), and defines a vector p_k linearly independent
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 42 from p_1, \dots, p_{k-1} and belonging to π_k .
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 45 These facts allow to focus, at Step k of the standard CG method, only on
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 47 π_k , Γ_k and ℓ . I.e., Step k of the standard CG method can be rewritten only
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 49 in terms of π_k , Γ_k and ℓ , as in Figure 10, without any explicit reference to
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directions p_1, \dots, p_{k-1} . In Figure 10 one can see the conjugate directions p_k and p_{k+1} generated at both the k -th and the $(k+1)$ -th iteration.

As a general achievement, we can equivalently conclude that the $(k+1)$ -th iteration of the standard CG method can be described by limiting the analysis to the hyperplane π_k in (42) and the hypersurface Γ_k in (44). This is partially summarized in the next corollary to Propositions 8.1 and 8.2.

Corollary 8.1 *Let the standard CG method perform m steps to solve the linear system $Ay = 0$, with $A \succ 0$. Then, at Step k , $k \leq m$, the polar hyperplane of $(p_{k-1}, 0)^T$, with respect to $g(y) = \gamma_k$, includes the point y_k , and is conjugate to p_{k-1} .*

Proof First observe that Proposition 8.1 implies that the polar hyperplane π_k of $(p_{k-1}, 0)^T$, with respect to $g(y) = \gamma_k$, satisfies $(Ap_{k-1})^T y = 0$. Recall that this last equation defines the locus of all the conjugate directions to p_{k-1} . Then, π_k coincides with $z + \text{span}\{p_1, \dots, p_{k-2}, p_k, \dots, p_m\}$, where z is such that $(Ap_{k-1})^T z = 0$. Consequently, the proof follows immediately from the proof of Propositions 8.1 and 8.2, since (41) imposes

$$(Ap_{k-1})^T y_k = (Ay_k)^T p_{k-1} = 0,$$

which implies that $y_k \in \pi_k$. □

The next proposition proposes a geometric insight of the standard CG method failure (also addressed as *pivot breakdown* in the literature [2]), in case the matrix A is indefinite. In particular, it turns out to be useful in explaining

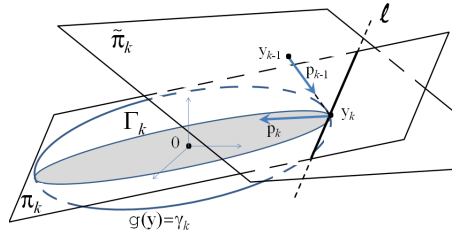


Fig. 9 An application (in Cartesian coordinates) of *Section Theorem*, within the k -th CG iteration: we have $y_{k-1} \in \tilde{\pi}_k$. The direction p_{k-1} is conjugate to the hyperplane π_k ; $\tilde{\pi}_k$ represents in Cartesian coordinates the polar hyperplane of y_k with respect to $g(y) = \gamma_k$.

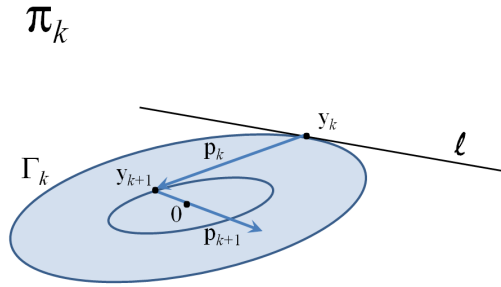


Fig. 10 The $(k + 1)$ -th iteration of the CG reduces to analyze the $(n - 1)$ -dimensional hyperplane π_k of Figure 9.

why the method may fail to generate a further search direction, when a line in the asymptotic cone (see Definition 6.1) of \mathcal{F}_γ is detected.

Proposition 8.3 [CG – Failure] *Let the standard CG method solve the linear system $Ay = 0$, with A indefinite nonsingular. Suppose that at Step k the CG computes the vector p_k satisfying $p_k^T A p_k = 0$, i.e. the point at infinity $(p_k, 0)^T$ belongs to the asymptotic cone of \mathcal{F}_γ in (34), for some $\gamma > 0$. Then,*

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(i) the point $(p_k, 0)^T$ belongs to its polar hyperplane with respect to \mathcal{F}_γ and is self-conjugate with respect to \mathcal{F}_γ ;

(ii) p_k belongs to the span of all the directions conjugate to p_k .

Proof We prove (i) by observing that the intersection between the asymptotic cone of \mathcal{F}_γ in (34) and the hyperplane at infinity $x_0 = 0$ is given by $\{(x, 0)^T \in \mathbb{P}^n : x^T A x = 0\}$. Then, by the hypotheses, $(p_k, 0)^T$ is also a point of \mathcal{F}_γ . Proposition 2.2 and Definition 2.2 guarantee that $(p_k, 0)^T$ is self-conjugate with respect to \mathcal{F}_γ , and it satisfies the equation of its polar hyperplane $\pi_{k+1} = \{(x, x_0)^T \in \mathbb{P}^n : (A p_k)^T x - 2\gamma \cdot 0 \cdot x_0 = 0\}$ since

$$(A p_k)^T p_k = p_k^T A p_k = 0.$$

As regards (ii), we observe that π_{k+1} is the locus of all the points $(d, 0)^T \in \mathbb{P}^n$ such that d and p_k are conjugate as in (4). Hence p_k is in the span of its conjugate directions. \square

Let us remark that, if the point $(p_k, 0)^T$ satisfies the equation of the asymptotic cone of the quadratic hypersurface \mathcal{F}_γ , then nevertheless p_k might be appealing as a direction along which to search the centre of the hypersurface. Unfortunately, the standard CG method gets stuck if this direction is generated, since it is unable to compute a suitable finite steplength along it. In addition, we highlight that item (i) in the previous proposition does not imply also that the point $(x_k, x_{0k})^T$, with $y_k = x_k/x_{0k}$, is in the asymptotic cone of \mathcal{F}_γ . Indeed (i) in general implies the situation depicted in Figure 11 (*left*), where $(p_k, 0)^T \in \mathcal{C}_\infty$, but the point y_k does not satisfy equation (18). Figure 11 (*right*) gives a graphical representation of item (ii) of Proposition 8.3. In the

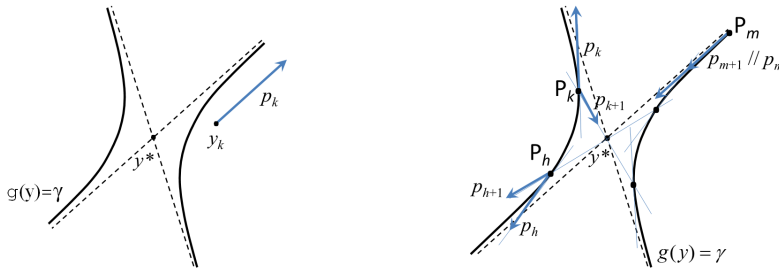


Fig. 11 A failure of the standard CG method when the matrix A is indefinite, in Cartesian coordinates. (left) The point $(p_k, 0)^T$ in homogeneous coordinates belongs to the asymptotic cone of \mathcal{F}_γ , for any γ . (right) When the current direction p_m generated at Step m of the CG approaches the asymptotic cone of \mathcal{F}_γ (i.e. $p_m^T A p_m \approx 0$), for some γ , then the angle between p_m and p_{m+1} tends to zero.

case that Step m provides a direction p_m in the asymptotic cone of \mathcal{F}_γ (i.e. $p_m^T A p_m = 0$), then a direction p_{m+1} can not be generated since it would be parallel to p_m , unlike p_{h+1} or p_{k+1} at points (respectively) P_k and P_h .

Finally, Proposition 8.3 may have a dramatic impact in optimization frameworks. Indeed, we recall that whenever $A \succ 0$, the standard CG method iteratively computes *gradient-related* directions with respect to the functional $g(y)$. Specifically, at Step k , the following condition holds $\nabla g(y_k)^T p_k \leq -\varepsilon_1 \|\nabla g(y_k)\|^2$ with $\varepsilon_1 > 0$, and $\|p_k\|$ is bounded as long as $\nabla g(y_k) \neq 0$. As a consequence, p_k can be used within linesearch procedures of Armijo-type or Wolfe-type (see for instance [9]), in order to guarantee global convergence properties. Differently, if A is indefinite and at Step k we have $p_k^T A p_k \approx 0$, then the standard CG method stops prematurely and p_{k+1} is no more generated, which claims

1 for some adjustments in the optimization framework, in order to preserve con-
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4 vergence properties (see e.g. [11]).
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7 **9 Perspectives**

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10 In this brief section, we suggest items which can represent issues of interest
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12 for further research, where polarity may possibly play a key role. Since our
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14 analysis in the previous sections follows a different perspective, with respect
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16 to the current literature on CG-based methods, we conjecture that our hints
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18 here can give the opportunity for novel discussions and investigations on well-
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20 known topics.
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23 – It may be worth exploring the possibility that the properties of polarity in
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25 Sections 3 – 7 can lead to possible extensions of the Nonlinear Conjugate
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27 Gradient (NCG) method (see [9]). In this regard there is the chance that in
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29 the nonlinear case, not only the pairs polar hyperplane–point may play a
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31 keynote role, but also the so called h -th polars [19] of points (with $h > 1$)
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33 may be helpful. The h -th polar of an algebraic hypersurface can capture in
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35 fact h -order information, which is unavailable in case the analysis includes
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37 only polar hyperplanes.
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- 40 – Polarity perspective may also provide some contribution in the definition
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42 of possibly inexact linesearch procedures for NCG methods. Indeed, the
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44 results of Lemma 7.1 suggest that in Cartesian coordinates the polar hy-
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46 perplane of a point not only includes first order information (i.e. the gra-
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48 dent of the function at the current iterate), but also information on the
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1 function value at that point. More specific linesearch procedures may rely
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3 on this latter information.
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- 5 – The proof of Proposition 8.3 guarantees that if in (8) the matrix A is indef-
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7 inite, then the polar hyperplane of a point at infinity P in the asymptotic
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9 cone is well-defined. On the contrary, we can not formally define at the lat-
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11 ter point the tangent hyperplane in Cartesian coordinates. This suggests
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13 that a possible failure of the CG, in case A is indefinite, might be possibly
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15 recovered by suitably alternating homogeneous coordinates and Cartesian
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17 coordinates in CG iterations. Indeed, by Proposition 8.3 a CG failure oc-
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19 curs in case at Step k we have $p_k^T A p_k = 0$, i.e. p_k is auto-conjugate with
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21 respect to the quadratic hypersurface. Thus, from the definition of asymp-
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23 totic cone, p_k is in principle still a possible search direction, in order to
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25 detect the centre of the hypersurface, by computing a suitable steplength.
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27 Of course, since possibly y_k in Table 1 does not satisfy equation (18), in
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29 general in Cartesian coordinates the line $y_k + \lambda p_k$, $\lambda \in \mathbb{R}$, does not in-
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31 clude the centre y^* of \mathcal{F} . Unfortunately, the CG is unable to compute
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33 a finite steplength along p_k (see also Figure 11), so that it stops prema-
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35 turely. Nevertheless, an *ad hoc* inexact linesearch procedure along p_k could
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37 be conceived.
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- 40
41 – The case when the CG detects a *nearly* auto-conjugate direction p_k (i.e.,
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43 such that $p_k^T A p_k \approx 0$ but $p_k^T A p_k \neq 0$) represents another intriguing sce-
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45 nario to theoretically investigate from a geometric standpoint. In fact, the
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latter case makes the CG well-posed but possibly numerically unstable (see e.g. [25]).

- Finally, it is worth considering the role of polarity theory also to study stationary points of cubic functions. They have recently gained the attention of the optimization community, due to their role within regularization problems (see the seminal paper [26]).

10 Conclusions

In this paper, we have investigated the role of polarity in homogeneous coordinates for quadratic hypersurfaces, in order to provide general tools for CG-based methods, from a geometric perspective. We have presented both the analytical properties and the geometric insight revealed by polarity, justifying the fact that in CG-based methods n -dimensional vectors are typically introduced, without recurring to homogeneous coordinates. Our use of polarity in homogeneous coordinates has not required the quadratic hypersurface in (8) to be an hyperellipsoid (i.e. $A \succ 0$). This allowed us to prove additional general results, to treat indefinite linear systems. Moreover, we showed to what extent the premature stop of the CG, in the indefinite case, is likely to be a very rare event.

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