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CONVERGENCE OF CONJUGATE DIRECTION AND QUASI-NEWTON METHODS ON SINGULAR PROBLEMS: THE FINITE-DIMENSIONAL CASE*

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Abstract

The convergence properties of the gradient, conjugate gradient, Davidon-Fletcher-Powell, and Powell's method for the singular, finite-dimensional quadratic minimization problem are developed. It is shown that for all of the methods, except the gradient method, that the minimum is obtained in at most m iterates, where m is the dimension of the range of the Hessian matrix, as opposed to $n > m$ iterates for nonsingular problems. A class of associated nonsingular quadratic problems is defined to show that the gradient method has slower convergence on singular problems than on corresppondíng nonsingular approximations to the singular problems while the conjugate direction methods have more rapid convergence. This implies that slow convergence attributed to singular problems is actually a property of the gradient method as opposed to the singularity of the problem.

1. Introduction

There is widespread belief that singular optimal control problems are more difficult to compute than nonsingular problems[1]. There is good reason for this since many researchers have experienced the slow convergence of the gradient method on a singular problem and/or the special preparations necessary to apply a Newton-type method (both shooting and function space types) to a singular problem. In fact, Johansen[2] studied the rate of convergence of the gradient method on the singular problem and verified theoretically the poor convergence characteristics noted in practice.

In Ref. 3 a recently developed class of accelerated function-space gradient methods, known as function-space quasi-Newton methods, was shown to converge certain singular optimal control problems much more accurately than the standard gradient method. Defects in the methods with regard to storage were also eliminated and a relatively large, realistic Space Shuttle trajectory optimization problem was solved with the methods[4]. Thus the major remaining problems associated with the methods involve theoretical questions of convergence and rate of convergence, especially on singular problems. For example, was the improved convergence reported in Ref. 3 problem dependent or applicable to more general classes of problems?

The goal of this paper is to present the results of the first part of such a theoretical study, namely the convergence of a number of algorithms on the finite-dimensional singular problem. In addition to these results being useful in their own right, they also indicate an approach to the infinite-dimensional (or optimal control) problem which will be reported in a subsequent paper.

The convergence of the: gradient, conjugate gradient (C G),[5, 6] and Davidon-Fletcher-Powell (DFP),[7, 8] and Powell's[9] methods will be analyzed herein. For nonsingular quadratic optimization problems, convergence questions have been investigated by many authors with the following results: (i) Linear convergence for the gradient method in both finite-dimensional and function spaces[10], (ii) Finite-step convergence for both the C G and the DFP methods in finite-dimensional space[6, 8], (iii) A rate of convergence for the C G method[10, 11] and a convergence proof for the function-space DFP method[12, 13].

To date few papers have been concerned with the case of singular quadratic optimization problems. A convergence proof for a general system of m linear algebraic equations in m unknowns is implicit in Ref. 14, and as shown in Ref. 15 the necessary and sufficient condition for a very general class of iterative schemes to converge is that the linear system be positive semidefinite. Nashed and Kammerer[16,17,18] present convergence proofs for gradient and conjugate gradient methods applied to singular linear operator equations, but no such results exist for the application of Quasi-Newton methods[19] to the singular case.

In Section 2 the singular quadratic optimization problem and algorithms are presented along with the existence conditions for the problem. The main convergence theorem is presented in Section 3 along with examples to illustrate its properties. In Section 4 an example is thoroughly analyzed to demonstrate that defects attributed to the singular problem are actually due to a defect in the gradient method, and that conjugate direction methods actually have improved convergence properties on singular problems.

2. Problem Formulation and Algorithms

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Consider the problem of determining a minimum of an unconstrained function f, where f has continuous partial derivative of, at least, second order. Convergence and rate of convergence analyses are restricted to the neighborhood of the minimum, and thus are actually terminal convergence properties. Thus, a quadratic approximation of the problem is employed for such analyses, and thus we shall consider the problem of determining an element $x^* \epsilon R^n$ which minimizes the quadratic function

$$f(x) = \frac{1}{2} <x, Q x> + <x, w> + f_o \qquad (2.1)$$

where $x, w \epsilon R^n$, $f_o \epsilon R$, $<x,w> = x^T w$ denotes the inner produce in R^n and Q can be assumed, without lost of generality, to be an n x n symmetric matrix. The gradient of f(x) at the element x, denoted by $g(x) \epsilon R^n$, is

$$g(x) \equiv \frac{df(x)}{dx} = Q x + w \qquad (2.2)$$

If Q is positive definite, then the minimum solution always exists, i.e., $x^* = -Q^{-1} w$. For a general quadratic function f, we need the following property.

Property 2.1: Problem (2.1) has a minimum solution $\bar{x}$ if and only if

(i) Q is positive semidefinite (denoted by $Q \geq 0$) (2.3)

(ii) w belongs to the range of Q, (denoted by $w \epsilon R(Q)$) (2.4)

Proof: Since f is twice differentiable, if $\bar{x}$ is a minimum element, then $g(\bar{x}) = Q \bar{x} + w = 0$ and $<x, \frac{d^2 f(\bar{x})}{dx^2} x> \geq 0, x \epsilon R^n$. But $Q \bar{x} \epsilon R(Q)$ $g(\bar{x}) = 0$ implies that $w = -Q\bar{x} \epsilon R(Q)$. Also, since $\frac{d^2 f}{dx^2} = Q$, $<x, \frac{d^2 f(\bar{x})}{dx^2} x> \geq 0$ implies that $<x, Q x> \geq 0$, that is, Q is positive semidefinite. Now, suppose $w \epsilon R(Q)$, there exist an element $\bar{x}$ such that $Q \bar{x} + w = 0$ and $f(\bar{x}) = \frac{1}{2} <\bar{x}, w> + f_o$. Let x be any element in R^n, then $x = \bar{x} + y$ where $y = x - \bar{x} \epsilon R^n$. After some calculations, $f(x) = f(\bar{x} + y) = \frac{1}{2} <y, Q y> + f(\bar{x})$, or $f(x) - f(\bar{x}) = \frac{1}{2} <y, Q y>$. Since Q is positive semidefinite, we obtain $f(x) \geq f(\bar{x})$, i.e., $\bar{x}$ is a minimum solution of Problem (2.1).

Remark 2.1 If $Q = Q^T \geq 0$ and $w \epsilon R(Q)$, there exist infinitely many minimum solutions of f(x). Actually, if x^* is a minimum solution of f(x), then $\bar{x} = x^* + X_N$, for any $X_N \epsilon N(Q)$ (the null space of Q), are also minimum solutions of f(x), that is, $f(\bar{x}) = f(x^*)$.

Remark 2.2. In the process of proving Property 2.1, we see that once an element $\bar{x}$ such that $g(\bar{x}) = Q \bar{x} + w = 0$ is determined, then $\bar{x}$ is a minimum solution of f(x).

The four iterative methods of interest here: the gradient, CG, DFP, and Powell's methods, will now be summarized. In general, the first three iterative schemes mentioned above attempt to generate a sequence $\{x_i\}$ which eventually converges to a minimizing element x^*, they all involve the iteration rule

$$x_{i+1} = x_i + \alpha_i S_i \qquad (2.5)$$

An initial element $x_o \epsilon R^n$ is chosen arbitrarily. At each step a direction S_i is schoen (the way this is done will define the method used) and a step size is determined such that

$$f(x_i + \alpha_i S_i) \leq f(x_i + \lambda S_i) \text{ for all } \lambda$$

This leads to the condition.

$$<g_{i+1}, S_i> = 0, \quad (g_{i+1} \equiv g(x_{i+1})) \qquad (2.6)$$

which, for the quadratic function in (2.1) gives

$$\alpha_i = - \frac{<S_i, g_i>}{<S_i, Q S_i>} \qquad (2.7)$$

In the gradient method

$$S_i = -g_i \quad \text{for all } i$$

In both the CG and the DFP methods, the members of the sequence $\{S_i\}$ are chosen to be Q - conjugate, i.e., they satisfy

$$<S_i, Q S_j> = 0 \qquad i \neq j$$

In the CG method, S_i is taken as

$$S_i = -g_i + \frac{<g_i, g_i>}{<g_{i-1}, g_{i-1}>} S_{i-1} \text{ with } S_o = -g_o$$

In the DFP method

$$S_i = -H_i g_i$$

$$\text{where } H_i = H_{i-1} + \frac{P_{i-1}><P_{i-1}}{<P_{i-1}, y_{i-1}>} - \frac{H_{i-1}y_{i-1}><H_{i-1}y_{i-1}}{<H_{i-1}y_{i-1}, y_{i-1}>}$$

$$P_{i-1} = x_i - x_{i-1} = \alpha_{i-1} S_{i-1}$$

$$y_{i-1} = g_i - g_{i-1} = \alpha_{i-1} Q S_{i-1}$$

The dyadic notation (><) is defined as (on R^n)

$$a >< b \equiv a b^T$$

and the following property is then easily verified

$$(a >< b) c = a < b, c > \quad a, b, c \epsilon R^n$$

The initial matrix H_0 is chosen to be any positive definite symmetric matrix.

In Powell's method, the directions of search are generated by the following four steps: Denote the starting point by x_o

(i) Initially choose $d_1, d_2, \ldots, d_n$ in the direction of n coordinates, that is $d_i = e_i$ where $e_i = (0, \ldots, 0, 1, 0, \ldots, 0)^T$

(ii) Given $d_1, d_2, \ldots, d_n$, find t_i^* so that f $(x_{i-1} + t_i^* d_i)$ is minimized. Define $x_i = x_{i-1} + t_i^* d_i$ $i = 1, \ldots, n$

(iii) Generate a new direction d by $d = x_n - x_o$ and replace $d_1, \ldots, d_n$ by $d_2, \ldots, d$. Rename the latter as $d_1, d_2, \ldots, d_n$

(iv) Minimize $f(x_n + t\, d_n)$ and replace x_o by $x_n + t^* d_n$ where t^* is the minimizing t. Take this point as x_o of the next iteration, and go to (ii).

It can be shown that the search directions generated in Powell's method at every iteration are mutually Q-conjugate for a quadratic function (see, for instance, Ref. 20, p. 158). This property holds for Q positive semidefinite also as long as $d \neq 0$. We will show later that if $d = 0$ during some iteration, then the initial element x_o for that iteration is indeed a minimum solution.

We shall now investigate the behavior of these algorithms on the singular quadratic problem (2.1) subject to (2.3), (2.4).

3. The Main Convergence Theorem

Before proving the general convergence theorem, the following properties are required.

Property 3.1: Let Q be a n x n symmetric positive semidefinite matrix (i.e., $Q^T = Q \geq 0$), let R (Q), N (Q) be the range of Q and the null space of Q, respectively, and m be the rank of Q. Then,

(i) $R(Q) = [N(Q)]^{\perp}$, $R^n = R(Q) \oplus N(Q)$

(ii) $< x, Q\, x > = 0 \quad x \in N(Q)$

Proof: Part (i) can be found in any elementary matrix book, so we need only prove (ii). If $x \in N(Q)$, clearly $Q\,x = 0$ and $< x, Q\,x > = 0$. Now, since $Q \geq 0$, $Q^{1/2}$ exists and $Q^{1/2} \geq 0$. Then $< x, Q\,x > = 0$ can be written as $< Q^{1/2} x, Q^{1/2} x > = 0$, which implies $Q^{1/2} x = 0$. Then $Q^{1/2}(Q^{1/2} x) = Q\,x = 0$, and $x \in N(Q)$ as desired.

Property 3.2: Let $Q = Q^T \geq 0$, and $\{d_1, d_2, \ldots, d_n\}$ be a nonzero Q-conjugate set of elements in the range of Q. If $\bar{x}$ minimizes problems (2.1), subject to (2.4) for all $x \in R(Q)$, then $g(\bar{x}) = 0$. i.e., $\bar{x}$ is a minimum solution of f (x).

Proof: First note that this property is trivial if $R(Q) = R^n$, but requires proof when Rank $(Q) < n$. Since $\{d_1, d_2, \ldots, d_m\}$ are Q-conjugate and nonzero, they are also independent. Then, since Rank (Q) = m, $\{d_1, d_2, \ldots, d_m\}$ form a basis for R (Q). For any $x \in R(Q)$, $\exists\, c_1, c_2, \ldots, c_m \ni x = \sum_{i=1}^{m} c_i d_i$, and implies

$$\frac{df(x)}{dc_i}\Big|_{x=\bar{x}} = \frac{df}{dx}^T \frac{dx}{dc_i}\Big|_{x=\bar{x}} = < g(x), d_i > \Big|_{x=\bar{x}} = 0,$$

$$i = 1, \ldots, m \tag{3.1}$$

or, $< g(\bar{x}), d_i > = 0 \quad i = 1, 2, \ldots, m$
It implies that, $< g(\bar{x}), x > = 0 \;\; \forall\, x \in R(Q)$
Therefore,

$$g(\bar{x}) \in [R(Q)]^{\perp} = N(Q) \tag{3.2}$$

By (2.4), $w \in R(Q)$ and $Q\,\bar{x} \in R(Q)$, which imply

$$g(\bar{x}) = Q\,\bar{x} + w \in R(Q) \tag{3.3}$$

Combining (3.2) and (3.3)

$$g(\bar{x}) \in R(Q) \cap N(Q) = \{0\},$$

i.e., $g(\bar{x}) = 0$, which completes the proof.

Theorem 1: Consider the problem (2.1) subject to (2.3) and (2.4). Let $\{x_i\}$ be a sequence of vectors in R^n generated by either the C G, DFP or Powell's method. Then, the sequence converges to a minimum vector $\bar{x}_o$ in at most m iterates, where $\bar{x}_o$ depends on the initial guess x_o and m is the rank of Q.

Proof: The details of the proof are presented in Appendix A. It is shown there that condition (ii) of property 3.1 guarantees that all iterates of the algorithms are well-defined, and property 3.2 leads to the finite m-step convergence result.

Remark 3.1: From the proof of the above theorem, the finite m-step convergence result holds for any algorithms which generates conjugate directions and employs an exact linear search. For example, all of Broyden's Quasi-Newton[19] and Huang's[21] methods possess this property.

Remark 3.2: Usually the minimum solution $\bar{x}_o$ depends on the initial estimate x_o. Actually, if we let $S = \{ x \mid x$ is a minimum solution of $f(x)\}$, then S is a non-empty closed convex set, hence there exists $x^* \in S$ such that $\|x^*\| \leq \|x\|$ for all $x \in S$, where $\|\cdot\|$ denotes the Euclidean norm in R^n. Nashed[16] showed that the sequence $\{x_o, x_1, \ldots, x_i, \ldots\}$ generated by the gradient method converges to $\bar{x}_o = x^* + (I-P)\,x_o$ where P is the projection matrix from R^n to R (Q). That is, if $x_o = x^R + x^N$ where $x^R \in R(Q)$ and $x^N \in N(Q)$, then $\bar{x}_o = x^* + x^N_o$. Now, if $H_o = I$ in the DFP method the search directions S_i in both the DFP and CG methods are linear combination of $g_o, g_1, \ldots, g_i$. By the same procedures as stated in Ref. 16 we can prove that the sequence $\{x_o, x_1, \ldots\}$ generated by the DFP and CG methods (with $H_o = I$) converges to $\bar{x}_o = x^* + (I - P) x_o$ where x^* is the unique minimum norm solution. Therefore, if we are interested in obtaining the minimum norm solution x^* by DFP or CG methods, the simplest way is to choose $x_o = 0$ as the initial estimate.

Remark 3.3: For a nonsingular quadratic function $f(x) = \frac{1}{2} < x, Ax > + < x, w > + f_o$ i.e., $A = A^T > 0$, the DFP method guarantees $H_k > 0$ for $0 \leq k \leq n$ and $H_n = A^{-1}$ if the sequence $\{x_i\}$ converges in exactly n iterations. For the singular case, $Q = Q^T \geq 0$ and Q^{-1} does not exist, but it is of interest to characterize the behavior of H_k in this case. The results are as follows:

Property 3.3: If $\{x_i\}$ converges at the ℓ^{th} iterate($\ell \leq m$) for the DFP method applied to a singular problem, then

(i) $H_k > 0 \qquad 0 < k \leq \ell$

(ii) $H_k Q p_i = p_i \quad 0 \leq i < k \leq \ell$

(iii) If $\ell = m$, $H_m Q x = x$ for $x \in R(Q)$.

Proof: If $x_\ell = \bar{x}_o$, the minimum solution of $f(x)$, then $g_i \neq 0$ for $i = 0, 1, \ldots, \ell-1$, and hence $p_i \neq 0$, $y_i \neq 0$, $i = 0, 1, \ldots, \ell-1$, which imply Properties (i) and (ii) carry over directly from the nonsingular case (e.g., Ref. 20, pp. 134-138). To prove (iii), observe from (ii) that

$$H_m Q \, p_i = p_i \qquad i = 0, 1, \ldots, m-1$$

But $\{p_o, p_1, \ldots, p_{m-1}\}$ are nonzero Q-conjugate vectors, hence they form a basis for R(Q). Therefore, for any $x \in R(Q)$, there exist constants $c_o, c_1, \ldots, c_{m-1}$ such that $x = \sum_{i=0}^{m-1} c_i p_i$, and, as desired,

$$H_m Q x = \sum_{i=0}^{m-1} c_i H_m Q p_i = \sum_{i=0}^{m-1} c_i p_i = x.$$

This means that $H_m Q$ plays the role of an identity matrix in the range of Q, or, $P = H_m Q$ is a projection matrix from R^n to R(Q). Therefore, as explained in Remark 3.2, $\bar{x}_o = x^* + (I - P) x_o$, or, $\bar{x}_o = x^* + (I - H_m Q) x_o$ if the DFP method converges at the m^{th} step with $H_o = I$.

Remark 3.4: The sequence $\{x_i\}$ generated by the gradient method for the singular problem converges linearly to $\bar{x}_o$ (by employing the results in Ref. 16).

Remark 3.5: Myers[22] showed that, for nonsingular quadratic problems in R^n, the search directions generated by the DFP method and the CG method are scalar multiples of each other, provided the initial step is in the direction of steepest descent. This is true also for the singular quadratic problem. In fact, Hestenes and Stiefel[6] showed that the search direction S_i of the CG method can be formed as

$$S_i = - < g_i, g_i > \sum_{j=0}^{i} \frac{g_j}{< g_j, g_j >}, \tag{3.4}$$

and Horwitz and Sarachik[12] showed that the search direction S_i of the DFP method can be written as

$$S_i = - < H_i g_i, H_i g_i > \sum_{j=0}^{i} \frac{H_o g_j}{< g_j, H_o g_j >} \tag{3.5}$$

Equations (3.4) and (3.5) are true for the singular quadratic case as long as $g_j \neq 0$, $j = 0, 1, 2, \ldots, i$. Therefore, from (3.4) and (3.5), we see that the CG and the DFP methods generate the same search directions S_i for the singular quadratic problems (provided $H_o = I$ and the same initial x_o is employed). Example: consider the minimization of:

$$f(x) = \frac{1}{2} < x, \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} x > + < x, B > + f_o \quad x, B \in R^3, \ f_o$$

real. First note that $Q = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} = Q^T$ with eigenvalues 0, 1, 2, which implies $Q = Q^T \geq 0$ with Rank $(Q) = 2$, and

$$R(Q) = \left\{ y \in R^3 \middle| y = Qx = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} x^1 \\ x^2 \\ x^3 \end{bmatrix} = \begin{bmatrix} x^1 + x^3 \\ x^2 \\ x^1 + x^3 \end{bmatrix} = \begin{bmatrix} a \\ b \\ a \end{bmatrix}, \ a, b \in R \right\}$$

By Property 2.1, B must belong to R(Q) to insure a minimum exists, i.e., B must be of the form $[\, a \ b \ a \,]^T$. For simplicity, let $B = [\, 0 \ 0 \ 0 \,]^T$, and $f_o = 0$. Then

$$f(x) = \frac{1}{2} < x, \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} x > = \frac{1}{2} (x^1 + x^3)^2 + \frac{1}{2} (x^2)^2$$

$$g(x) = Q x = \begin{bmatrix} x^1 + x^3 \\ x^2 \\ x^1 + x^3 \end{bmatrix}$$

By inspection, the set S of minima is given by

$$S = \{ x \mid x = \begin{bmatrix} a \\ 0 \\ -a \end{bmatrix}, \ a \in R \}$$

Clearly, the minimum norm solution $x^* \in S$ is $x^* = [\, 0 \ 0 \ 0 \,]^T$. Now, consider the application of the gradient, CG, DFP and Powell methods, with the same initial guess $x_o = [\, 1 \ 1 \ 1 \,]^T$, to this problem.

(i) Gradient Method: after straightforward calculations:

$$x_o = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \quad x_1 = \frac{1}{17} \begin{bmatrix} -1 \\ 8 \\ -1 \end{bmatrix}$$
$$g_o = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix}, \quad g_1 = \frac{1}{17} \begin{bmatrix} -2 \\ 8 \\ -2 \end{bmatrix} \tag{3.6}$$

and
$$x_{2n} = \left(\frac{4}{85}\right)^n x_o, \quad x_{2n+1} = \left(\frac{4}{85}\right)^n x_1$$
$$g_{2n} = \left(\frac{4}{85}\right)^n g_o, \quad g_{2n+1} = \left(\frac{4}{85}\right)^n g_1 \tag{3.7}$$

Thus, $x_k \to x^*$ and $g_k \to 0$ as $k \to \infty$, but $g_n \neq 0$ for any finite number n.

(ii) CG Method: Since the first iteration is a gradient step, the same x_o, x_1, g_o, g_1 as stated in (3.6) result and thus the search directions are

$$S_o = -g_o = \begin{bmatrix} -2 \\ -1 \\ -2 \end{bmatrix}, \quad S_1 = \frac{18}{(17)^2} \begin{bmatrix} -1 \\ 8 \\ -1 \end{bmatrix}, \tag{3.8}$$

which implies

$$x_2 = 0, \quad g_2 = 0.$$

the CG method converges in 2 iterations. (Note again that Rank $(Q) = 2$.)

(iii) DFP method: with $H_o = I_3$, it follows that x_o, x_1, g_o, g_1 are the same as in (3.6), and the search directions are

$$S_o = \frac{-9}{17}\begin{bmatrix}2\\1\\2\end{bmatrix}, \quad S_1 = \frac{2}{33}\begin{bmatrix}-1\\8\\-1\end{bmatrix}, \tag{3.9}$$

which implies

$$x_2 = 0, \quad g_2 = 0.$$

Since the DFP method converges in 2 iterations, it is of interest to display the properties of H_2, where

$$H_2 = \begin{bmatrix}\frac{3}{4} & 0 & -\frac{1}{4}\\ 0 & 1 & 0\\ -\frac{1}{4} & 0 & \frac{3}{4}\end{bmatrix}.$$

Then,

$$P = H_2 Q = \begin{bmatrix}\frac{1}{2} & 0 & \frac{1}{2}\\ 0 & 1 & 0\\ \frac{1}{2} & 0 & \frac{1}{2}\end{bmatrix}$$ is the projection matrix

on $R(Q)$, i.e., $Px = x$, for all $x \in R(Q)$ and

$Py = 0$ for all $y \in N(Q) = \{z \mid z = \begin{bmatrix}a\\0\\-a\end{bmatrix}, a \in R\}$

Note also that $T = I_3 - P = \begin{bmatrix}\frac{1}{2} & & -\frac{1}{2}\\ 0 & 0 & 0\\ -\frac{1}{2} & 0 & \frac{1}{2}\end{bmatrix}$ is the projection matrix on $N(Q)$. In this example, the initial guess $x_o = [\,1\,1\,1\,]^T$, $Tx_o = 0$, and therefore, $x_2 = x^* = 0$ in both the CG and DFP methods. Again, this result agrees with Remark 3.2. For an arbitrary $x_o = [\,a\ b\ c\,]^T$, $Tx = \begin{bmatrix}a-c\\0\\c-a\end{bmatrix}$, the CG and DFP method will converge in at most 2 steps to

$$\bar{x}_o = x^* + Tx_o = 0 + \frac{1}{2}\begin{bmatrix}a-c\\0\\c-a\end{bmatrix}.$$

(iv) Powell's Method: with $x_o = [\,1\,1\,1\,]^T$, the first iteration is (see the description of the algorithms in Section 2 for the notation definition):

$$x_1 = \begin{bmatrix}-1\\1\\1\end{bmatrix}, \quad x_2 = x_3 = \begin{bmatrix}-1\\0\\1\end{bmatrix}$$

Therefore, the first conjugate direction is $d = x_3 - x_o = [\,-2\ -1\ 0\,]^T$. The second iteration results in

$$x_o = x_1 = x_2 = x_3 = [\,-1\ 0\ 1\,]^T$$

Hence, the second conjugate direction is $d = 0$, and Powell's method converges at the second iteration to $\bar{x} = [\,-1\ 0\ 1\,]^T$. Note that $\bar{x} \in N(Q)$ and $g(\bar{x}) = 0$.

In the following we will consider the application of conjugate direction methods to the least squares solutions of linear algebraic equations. First we need the following definitions.

Definition 3.1: A vector $u \in R^n$ is a <u>least squares solution</u> of the linear algebraic equations

$$Ax = b \tag{3.10}$$

where $x \in R^n$, $b \in R^m$ and A is an $m \times n$ matrix with rank $(A) = k$, $k \leq \min\{m, n\}$ if

$$\|Au - b\| \leq \|Ax - b\| \text{ for all } x \in R^n.$$

The vector x^* is the <u>least squares solution of minimum norm of (3.10)</u> if x^* is a least squares solution of (3.10) and $\|x^*\| \leq \|u\|$ holds for all least squares solutions u of (3.10).

Definition 3.2: The generalized inverse A^+ of A is the linear extension of $\{A \mid N(A)^\perp\}^{-1}$ so that its domain of definition $D(A)$ is $R(A) \oplus R(A)^\perp = R^n$ and its null space is $R(A)^\perp = N(A^T)$, where $N(A)$ and $R(A)$ are the null space of A and Range of A, respectively, $N(A)^\perp$ is the orthogonal complement of $N(A)$, and $A \mid N(A)^\perp$ is the restriction of A to $N(A)^\perp$.

The following important results has been established by many researchers (see, e.g., [23]).

Property 3.4: If A is a bounded linear transformation with closed range mapping X into Y then the least squares solution of minimum norm (LSSMN) x^* of the linear operator equation $Ax = y$, $y \in Y$ is given by $x^* = A^+ y$.

The linear operator A defined in (3.10) is clearly a bounded linear transformation with $R(A)$ closed. Property 3.4 implies that the LSSMN, x^*, of (3.10) is given by $x^* = A^+ b$.

There are many papers concerned with least squares solutions of linear algebraic equations. Some of them present iterative methods to obtain a least squares solution $\bar{x} = A^+b + (I - A^+A)x_o$, where x_o is the initial estimate[24, 25]. Others describe iterative methods to compute the generalized inverse of a matrix[26, 27]. The conjugate *direction methods should be powerful methods for* determining least squares solutions of linear algebraic equations because of the following properties.

Property 3.5: Consider $J(x) = \frac{1}{2} \langle Ax - b, Ax - b \rangle$ or, equivalently, $J(x) = \frac{1}{2}\langle x, Qx\rangle + \langle x, \tilde{b}\rangle + \langle b, b\rangle$ where $Q = A^T A$ and $\tilde{b} = -A^T b$. Then,

(i) $Q = Q^T \geq 0$

(ii) $\tilde{b} \in R(Q)$

Proof: The proof of (i) is straightforward. To prove (ii), since $[R(A)]^\perp = N(A^T)$ and $R^m = R(A) \oplus N(A^T)$, $b \in R^m$ implies that $b = b_r + b_n$, where $b_r \in R(A)$ and $b_r \in N(A^T)$, and

$$\tilde{b} = -A^T b = -A^T(b_r + b_r) = -(A^T b_r + A^T b_n) = -A^T b_r$$

But $b_r \in R(A)$, which implies that there exists an x such that $b_r = Ax$, and then

$$\tilde{b} = -A^T b_r = -A^T A x = Q(-x) \in R(Q).$$

Property 3.6: $\bar{x}$ is a solution of (3.10) if and only if $\bar{x}$ is a least squares solution of (3.10) and $J(\bar{x}) = 0$.

Proof: It is well known that $Ax = b$ has solutions if and only if $b \in R(A)$. In general, $\bar{x}$ is a least squares solutionf of $Ax = b$ if and only if

$Q\bar{x} + \tilde{b} = 0$, or, $A^TA\bar{x} - A^Tb_r = 0$, since $A^Tb_n = 0$,

which implies

$$A^T(A\bar{x} - b_r) = 0.$$

Now, $A\bar{x} - b_r \in R(A)$, $Ax - b_r \neq 0$ implies that $A^T(Ax - b_r) \neq 0$ hence $A\bar{x} - \tilde{b}_r = 0$. That is, $\bar{x} = \bar{x}_r + \bar{x}_n$ where $\bar{x}_r$ is the minimum norm solution of $Ax - b_r = 0$ and $\bar{x}_n \in N(A)$. With this $\bar{x}$, we have

$$J(\bar{x}) = \frac{1}{2} < \bar{x}, Q\bar{x} > + < \bar{x}, \tilde{b} > + < b, b >$$

$$= \frac{1}{2} < \bar{x}, Q\bar{x} + \tilde{b} > + < \bar{x}, \tilde{b} > + < b, b >$$

$$= - < A(\bar{x}_r + \bar{x}_n), b > + < b, b >$$

$$= - < (A\bar{x}_r - b_r) - b_n, b_r + b_n > = < b_n, b_n >$$

Therefore $J(\bar{x}) = 0$ if and only if $b_n = 0$, or $b = b_r \in R(A)$.

Property 3.5 along with Theorem 1 and Remark 3.2 guarantee that the sequence $\{x_o, x_1, \ldots\}$ generated by either the CG or DFP method applied to the least squares problem of (3.10) converges in at most $k = \text{Rank}(A)$ steps to a least squares solutions $\bar{x}_o = A^+b + (I - A^+A)x_o$, provided the initial step each takes is in the direction of steepest descent. If $x_o = 0$, clearly the LSSMN $x^* = A^+b$. If also $J(x^{*o}) = 0$, then x^* is the minimum norm solution of $Ax = b$ by Property [3.6] .

4. Comparison of Conjugate Direction and Gradient Methods

Consider the singular problem (2.1) subject to (2.3) and (2.4), i.e.,

$$f(x) = \frac{1}{2} < x, Qx > + < x, w > + f_o$$

(SQP) where $x \in R^n$, $f_o \in R$

with $Q = Q^T \geq 0$, $w \in R(Q)$

Define the associated nonsingular quadratic problems (ANSQP) as

$$f_\eta(x) = \frac{1}{2} < x, Q_\eta x > + < x, w > + f_o$$

(ANSQP) where $Q_\eta = Q + \frac{1}{\eta} I$ for $\eta > 0$

and $x \in R^n$, $f_o \in R(O)$

The reason for introducing the ANSQP is to study the behavior of algorithms as a problem tends to singularity. There is widespread belief that singular problems are more difficult because Newton's method is not applicable and the gradient method typically exhibits very slow convergence. The goal of this section is to quantify such ideas, and to study the rate of convergence of the gradient and conjugate direction methods as a function of the degree of singularity. The following property is straightforward and presented without proof.

Property 4.1:

(i) (ANSQP) approaches (SQP) as $\eta \to \infty$.

(ii) Any eigenvector Z_i of Q in (SQP) with corresponding eigenvalue $\lambda_i \geq 0$, $i = 1, 2, \ldots, n$, is also an eigenvector of Q_η in (ANSQP) with corresponding eigenvalue $\beta_i = \lambda_i + \frac{1}{\eta}$.

The suitability of conjugate direction methods for singular problems is verified by the following property.

Property 4.2: If the sequence $\{\bar{x}_i\}$, generated by any one of conjugate direction methods applied to the (ANSQP), converges in $k \leq n$ steps, then the sequence $\{x_i\}$, generated by the same method applied to the (SQP) with the same initial estimate x_o, converges in at most k steps.

Proof: See Appendix B. (It is interesting to note that the proof in Appendix B involves a lemma which states that all conjugate direction methods will converge in at most k steps for quadratic problems if the Hessian matrix ($Q \geq 0$) has k distinct nonzero eigenvalues; this result is interesting in its own right).

Property 4.2 shows that the convergence of any conjugate direction method applied to the (SQP) is never slower (worse) than the result of the same method applied to the (ANSQP). However, the gradient method behaves in exactly the opposite way. Indeed, it has been shown[2] that the rate of convergence of the residual error for the gradient method will be slow whenever the spread of eigenvalues for the second-variation operator is large. Furthermore, when the second-variation operator is singular, the asymptotic rate of convergence of the residual error will be zero. This result holds for the gradient method in finite-dimensional space, also. Let us consider again the example presented in Section 3 to illustrate the above results.

Example: Minimize: $f(x) = \frac{1}{2} < x, \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} x >$ (4.1)

with $x_o = [\ 1, 1, 1\ ]^T$

$$x_1 = \frac{1}{17} [\ -1, 8, -1]^T$$

and, for $n = 1, 2, \ldots$

$$x_{2n} = \left(\frac{4}{85}\right)^n x_o, \quad x_{2n+1} = \left(\frac{4}{85}\right)^n x_1$$

clearly $x_k \to x^* = 0$ as $k \to \infty$

The ratio of linear convergence, θ, is defined as

$$\theta = \lim_{k\to\infty} \text{Sup.} \frac{||x_{k+1} - x^*||}{||x_k - x^*||} \quad (4.2)$$

It is straightforward to determine θ_s, the ratio of linear convergence of the gradient method applied to the (SQP), and

$$\theta_s = 0.2762 \qquad (4.3)$$

the (ANSQP) of (4.1) is given by

$$f_\eta(x) = \frac{1}{2} < x, \; \theta_\eta \; x > \qquad (4.4)$$

$$\text{where } Q_\eta = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} + \frac{1}{\eta} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \eta > 0$$

with the same $x_o = [\,1\,1\,1\,]^T$, the gradient method applied to the (ANSQP) (4.4) generates the sequence $\{x_i(\eta)\}$ with

$$x_1(\eta) = \frac{\eta}{17\eta^3 + 27\eta^2 + 15\eta + 3} [-(\eta+1)^2, 2(2\eta+1)^2, -(\eta+1)^2]^T$$

and for $n = 1, 2, \ldots$

$$x_{2n}(\eta) = [F(\eta)]^n x_o, \; x_{2n+1}(\eta) = [F(\eta)]^n x_1 \qquad (4.5)$$

$$\text{where } F(\eta) = \frac{2\eta^2(\eta+1)(2\eta+1)}{(17\eta^3 + 27\eta^2 + 15\eta + 3)(5\eta + 3)}$$

$$\text{Since } \frac{dF(\eta)}{d\eta} = \frac{234\eta^6 + 808\eta^5 + 1284\eta^4 + 864\eta^3 + 282\eta^2 + 36\eta}{(85\eta^4 + 186\eta^3 + 156\eta^2 + 60\eta + 9)^2},$$

$$\frac{dF(\eta)}{d\eta} > 0 \quad \text{for } \eta > 0.$$

That is, $F(\eta)$ is a strictly increasing function of positive η, or,

$$0 < F(\eta_1) < F(\eta_2) < 1 \quad \text{for } 0 < \eta_1 < \eta_2 \qquad (4.6)$$

$$\text{Clearly, } \lim_{\eta \to \infty} F(\eta) = \frac{4}{85} \qquad (4.7)$$

and

$$\lim_{\eta \to \infty} x_k(\eta) = x^*(\eta) = 0 \quad \text{for any } \eta > 0 \qquad (4.8)$$

Now, define $h(\eta)$ as

$$h^2(\eta) = \frac{F^2(\eta)}{||x_1(\eta)||^2}$$

It can be shown, by the same procedure for $F(\eta)$, that for $0 < \eta_1 < \eta_2$,

$$0 < ||\,x_1(\eta_1)\,|| < ||\,x_1(\eta_2)\,|| \qquad (4.9)$$

$$0 < ||\,h(\eta_1)\,|| < ||\,h(\eta_2)\,|| \qquad (4.10)$$

$$\text{and } \lim_{\eta \to \infty} ||x_1(\eta)||^2 = \frac{66}{289} = ||\,x_1\,||^2 \qquad (4.11)$$

Define $\theta(\eta)$, the ratio of linear convergence of the gradient method applied to the (ANSQP) (4.4)

$$\theta(\eta) = \lim_{k \to \infty} \text{Sup.} \frac{||\,x_{k+1}(\eta) - x^*(\eta)\,||}{||\,x_k(\eta) - x^*(\eta)\,||}$$

Straightforward application of conditions (4.5) to (4.11) imply that, for $0 < \eta_1 < \eta_2$,

$$0 < \theta(\eta_1) < \theta(\eta_2)$$

and,

$$\lim_{\eta \to \infty} \theta(\eta) = \theta_s \qquad (4.12)$$

The results in (4.12) show that, as $\eta > 0$ increases to infinity, i.e., the (ANSQP) approaches the (SQP), the ratio of linear convergence $\theta(\eta)$ of the gradient method applied to the (ANSQP) strictly increases to θ_s, the ratio of linear convergence of the method applied to the (SQP). In nonmathematical terms, this implies that as the problem becomes more singular, the performance of the gradient method deteriorates, whereas the performance of conjugate direction methods improves. This indicates that difficulties attributed to singular problems are actually due to defects in the two main classical methods: the gradient method (as the above analysis shows) and Newton's method, which is not applicable to the SQP in its standard form.

5. Concluding Remarks

In finite-dimensional space conjugate direction methods determine the inherent lower-dimensionality of the SQP, and converge in at most m steps, where m is the rank of the n x n Hessian matrix Q. Furthermore, the rate of convergence on the SQP is better than or equal to the rate of the same conjugate direction method applied to associated nonsingular quadratic problems. The gradient method has exactly opposite properties. This shows explicitly that the slow convergence of the gradient algorithm applied to a singular quadratic problem is due to the method and not the problem.

Similar properties hold for the conjugate gradient and quasi-Newton methods applied to singular quadratic optimal control problems, and these results are in preparation.

Appendix A. Proof of Theorem 1

First consider the CG and the DFP methods. Given x_o, if $g(x_o) = 0$, x_o is a minimum. Thus, assume $g(x_o) \neq 0$, since $g(x_o) \in R(Q)$ (by Property 3.1 (ii)), $<g_o, Qg_o> > 0$. In the CG method, $S_o = -g_o$, so we have $<S_o, Q\,S_o> > 0$. In the DFP method, $S_o = -H_o g_o$, where H_o is any positive definite matrix, and thus $<S_o, Q\,S_o> = <H_o g_o, Q\,H_o g_o> \geq 0$. If $<H_o g_o, Q\,H_o g_o> = 0$, then $H_o g_o \in N(Q)$. i.e., $<H_o g_o, x> = 0$ for all $x \in R(Q)$. But, with $x = g_o$, $H_o > 0$ implies $g_o = 0$, contradicting the assumption $g_o \neq 0$. Hence we conclude that in both the CG and the DFP methods

$$< S_o, Q\,S_o > > 0 \qquad \text{if } g_o \neq 0$$

This condition insures that the algorithms are well-defined from one iterate to another, i.e., the linear search requires

$$<g_1, S_o> = 0 \text{ and } \alpha_o = -\frac{<S_o, g_o>}{<S_o, QS_o>} > 0.$$

Now, consider $g_1 = g(x_1)$; if $g_1 = 0$ we are done, so assume $g_1 \neq 0$. In the CG method:

$$S_1 = -g_1 + \frac{<g_1, g_1>}{<g_o, g_o>} S_o$$

In the DFP method:

$$-S_1 = H_1 g_1 = H_o g_o + \frac{<p_o, g_1> P_o}{<p_o, y_o>} - \frac{<H_o y_o, g_1> H_o y_o}{<H_o y_o, y_o>}$$

By the construction of the CG and the DFP methods, we have

$$<S_o, Q S_1> = 0$$

Note that in the CG method, S_1 is the linear combination of g_o, g_1 with $g_o \neq 0$, $g_1 \neq 0, g_o, g_i \in R(Q)$ and $<g_o, g_1> = 0$. This implies that $S_1 \neq 0$ and belongs to $R(Q)$, hence

$$<S_1, Q S_1'> > 0$$

In the DFP method, it has been proved that $\{H_k\}$ is a sequence of positive definite symmetric matrices if $H_o = H_o^T > 0$ for the nonsingular case. This result can be carried over directly to the singular case as long as $g_k \neq 0$, i.e., the sequence $\{H_o, H_1, \ldots, H_k\}$ of matrices is a finite sequence of positive definite symmetric matrics if $H_o = H_o^T > 0$ and $g_i \neq 0$ for $i = 0, 1, 2, \ldots, k$. Now, with $H_1 > 0$ and $g_1 \neq 0 \in R(Q)$, by condition (ii) of Property 3.1 we obtain $<S_1, Q S_1> = <H_1 g_1, Q H_1 g_1> > 0$.

We now proceed by introduction. Suppose after k iterations with $g_k \neq 0$, we have following properties

$<S_i, Q S_j> = 0 \qquad i \neq j,\ 0 \leq i, j < k$ (A.1)

$<S_i, Q S_i> > 0 \qquad i \leq k$ (A.2)

$<g_k, S_i> = 0 \qquad i < k$ (A.3)

The condition (A.2) allows the k+1 iteration to be well-defined. Assume $g_{k+1} \neq 0$; we shall show that (A.1) - (A.3) hold for k+1. Note that (A.1) is true by the construction of the CG and DFP methods, and (A.3) has been proved in Ref. 20 and can be carried over to the singular case as long as $g_{k+1} \neq 0$. Therefore, we need only prove (A.2). The Q-conjugate direction S_{k+1} of the CG method is

$$S_{k+1} = -g_{k+1} + \frac{<g_{k+1}, g_{k+1}>}{<g_k, g_k>} S_k$$

It is easy to show that

$$S_{k+1} = -g_{k+1} - \sum_{i=0}^{k} \frac{<g_{k+1}, g_{k+1}>}{<g_i, g_i>} g_i,$$

i.e., S_{k+1} is a linear combination of $\{g_o, g_1, \ldots, g_{k+1}\}$. It is well known that (see, e.g., Ref. 20)

$$<g_i, g_j> = 0 \quad i \neq j,\ 0 \leq i, j \leq k+1$$

Again, these results are true for the singular case as long as $g_i \neq 0, i = 0, 1, \ldots, k+1$. Therefore, $S_{k+1} \neq 0$ and $S_{k+1} \in R(Q)$. This implies (by Property 3.1(ii)) that, for the CG method,

$$<S_{k+1}, Q S_{k+1}> > 0$$

In the DFP method $-S_{k+1} = H_{k+1} g_{k+1}$, and we know that $H_{k+1} = H_{k+1}^T > 0$, and $<S_{k+1}, Q S_{k+1}> = <H_{k+1} g_{k+1}, Q H_{k+1} g_{k+1}>$. If $<S_{k+1}, Q S_{k+1}> = 0$, then $S_{k+1} = H_{k+1} g_{k+1} \in N(Q)$, i.e., $<H_{k+1} g_{k+1}, x> = 0$ for all $x \in R(Q)$. For the necessary contradiction, again pick $x = g_{k+1} \in R(Q)$. Then, $<H_{k+1} g_{k+1}, g_{k+1}> = 0$, or $g_{k+1} = 0$, which contradicts the assumption $g_{k+1} \neq 0$. Therefore, (A.2) is true for k+1.

Consider the iteration number $k = m-1$, where m is the rank of Q. If $g_m = 0$, we are done; if $g_m \neq 0$, from (A.3) we have $<g_m, S_i> = 0$ $(i = 0, 1, \ldots, m-1)$. This means that x^m minimizes f(x) over the subspace spaned by $\{S_o, S_1, \ldots, S_{m-1}\}$, a basis of $R(Q)$. Let $x_m = \overline{x}_m + z$ where $\overline{x}_m \in R^m(Q)$ Since $f(x_m) = f(\overline{x}_m + z) = f(\overline{x}_m)$, it follows that $\overline{x}_m \in R^m(Q)$ minimizes f(x) for all $x \in R(Q)$. From property 3.2 we conclude that $g_m = g(x_m) = g(\overline{x}_m + z) = g(\overline{x}_m) = 0$, i.e., the CG and the DFP methods converge in at most m steps.

For Powell's method, the proof is as follows. Given x_o, the method generates a Q-conjugate direction $d = x_n - x_o$; the directions $d_1, \ldots, d_n$ are replaced by $d_2, \ldots, d_n$, d, and then defined as $d_1, \ldots, d_n$. Suppose after k iterations that the last k directions of $\{d_1, d_2, \ldots, d_n\}$ are nonzero Q-conjugate vectors, i.e., $d_{n-k+1}, d_{n-k+2}, \ldots, d_n$. The starting point x_o for the $(k+1)^{th}$ iteration is the minimum of f(x) in the subspace spanned by these Q-conjugate directions. If, on the (k+1)th iteration the new direction $d = x_n - x_o = 0$, then (as will be shown) the starting point x_o at this iteration is a minimum of f(x), i.e., $g(x_o) = 0$.

First note that x_i is determined by $x_i = x_{i-1} + t_i^* d_i$ where t_i^* is chosen such that $f(x_{i-1} + t_i^* d_i) = \min f(x_{i-1} + t d_i)$, $t \in R$. Therefore $t_i^* = 0$, i.e., $x_i = x_{i+1}$, can happen if and only if $<g(x_{i-1}), d_i> = 0$. This implies that

(i) $g(x_{i-1}) = 0$, (ii) $d_i \in N(Q)$, (iii) $d_i \in R(Q)$ and $d_i \perp g(x_{i-1})$.

If (i) is true, then x_{i-1} is a minimum. Thus, assume $g(x_{i-1}) \neq 0$. Note that (ii) and (iii) are mutually exclusive. Equation (ii) shows that the renamed directions $\{d_1, d_2, \ldots, d_n\}$ for the next iteration at least span the range of Q. (Recall that the initial $d_1, d_2, \ldots, d_n$ form a basis for R^n). On the other hand, if (iii) is true, we have $g(x_j) \perp d_i$ for $j \geq i-1$ but the renamed directions $\{d_1, d_2, \ldots, d_n\}$ for the next iteration may or may not span the range of Q. Now, let $\{e_1, e_2, \ldots, e_m\}$ be a basis of $R(Q)$, such that $e_1 = d_i$. Then, $g^m(x_j) \perp d_i$ for $j > i-1$ and the renamed directions $\{d_1, \ldots, d_n\}$ for the next iteration span the same subspace as spanned by $\{e_2, e_3, \ldots, e_m\}$. It follows that if at the (k+1)th iteration the new direction $d = x_n - x_o$ is a zero vector, then the nth vector x_n minimizes f(x) over the space spanned by $\{d_1, d_2, \ldots, d_n\}$, which either contains the range of Q or contains some part of the range of Q, say $\{e_j, e_{j+1}, \ldots, e_m\}$ with $g(x_n) \perp e_i$ for $1 \leq i < j$ (where $\{e_1, e_2, \ldots, e_m\}$ form a basis for the range of Q). Both situations lead to the same condition that $g(x_n) \perp R(Q)$, i.e., $g(x_n) \in N(Q)$. Since $g(x_n) = Q x_n + w \in R(Q)$, then $g(x_n) = 0$ and $x_n = x_o$ is a minimum solutions of $f(x)$. Thus, we have proved that if $d = x_n - x_o = 0$ at the (k+1)th iteration, $k + 1 \leq m$, then the x_o of that iteration is a minimum solution.

Now suppose that after m iterations m Q - conjugate directions have been generated, i.e., $d_{n-m+1}, d_{n-m+2}, \ldots, d_n$ are nonzero Q-conjugate directions. Then, the starting point x_o for the (m+1)th iteration is the minimum of $f(x)$ in the subspace spanned by the m Q-conjugate vectors. Now, for each d_i, there exist unique p_i and z_i with $p_i \in R(Q)$ and $z_i \in N(Q)$ such that

$$d_i = p_i + z_i \qquad \text{for } i = n-m+1, \ldots, n$$

and,

$$\langle d_i, Q d_j \rangle = \langle p_i + z_i, Q(p_j + z_j) \rangle$$

$$= \langle p_i, Qp_j \rangle + \langle z_i, Qp_j \rangle = \langle p_i, Qp_j \rangle.$$

since $\langle d_i, Q d_j \rangle = 0 \qquad i \neq j, n-m+1 \leq i, j \leq n$

and $\langle d_j, Q d_j \rangle > 0 \qquad n+m+1 \leq j \leq n$

we have $\langle p_i, Q p_j \rangle = 0 \qquad i \neq j,\ n-m+1 \leq i, j \leq n$

and $\langle p_j, Q p_j \rangle > 0 \qquad n-m+1 \leq j \leq n$

That is, $\{p_{n-m+1}, p_{n-m+2}, \ldots, p_n\}$ are nonzero Q-conjugate directions in $R(Q)$. Therefore, the starting point x_o for the (m+1)th iteration is a minimum of $f(x)$ on the subspace spanned by $\{d_{n-m+1}, \ldots, d_n\}$ which contains $\{p_{n-m+1}, \ldots, p_n\}$ Q-conjugate directions in R(Q). This means that, by Property 3.2, $g(x_o) = 0$, and x_o is a minimum solution of $f(x)$ in R^n.

Appendix B Proof of Property 4.2

From Theorem 1 in Section 3, there is nothing to prove if $k \geq m$, where m is the rank of Q. Hence, assume $k < m$. It was shown in Ref. 28 that for the DFP method applied to non-singular quadratic problems, or, in our case, to the (ANSQP), the gradient at $\bar{x}_{i+1}$, denoted by $\bar{g}_{i+1} = \bar{g}(\bar{x}_{i+1}) = Q_\eta \bar{x}_{i+1} + w$, is the orthogonal projection of $\bar{g}_o = g(\bar{x}_o) = Q_\eta \bar{x}_o + w$ onto the orthogonal complement of the span of $Q_\eta \bar{S}_o, Q_\eta \bar{S}_1, \ldots, Q_\eta \bar{S}_i$ and the vectors $Q_\eta \bar{S}_o, Q_\eta \bar{S}_i$ span the same subspace as the vectors $Q_\eta \bar{g}_o, Q_\eta^2 \bar{g}_o, \ldots, Q_\eta^i \bar{g}_o$. These properties are also true for the DFP method applied to the (SQP) as long as $g_i \neq 0$, that is, the gradient of the (SQP) at x_{i+1}, denoted by $g_{i+1} = g(x_{i+1}) = Q x_{i+1} + w$, is the orthogonal direction projection of $g_o = g(x_o) = Q x_o + w$ onto the orthogonal complement of the span of $Q S_o, Q S_1, \ldots, Q S_i$ which has the same span as by the vectors $Qg_o, Q^2 g_o, \ldots, Q^{i+1} g_o$.

Lemma B.1: For a nonsingular quadratic minimization problem $f(x) = \frac{1}{2}\langle x, A x\rangle + \langle x, w\rangle + f_o$, $x \in R^n$ with $A = A^T > 0$, if A has k distinct positive eigenvalues $\lambda_1, \lambda, \ldots, \lambda$ with multiplicities $r_1, r_2, \ldots, r_k$, respectively, and $\sum_{i=1}^{k} r_i = n$, then the DFP method converges in at most k steps.

Proof: Let $z_1^{(i)}, z_2^{(i)}, \ldots, z_{r_i}^{(i)}$ be eigenvectors of A corresponding to the same eigenvalue λ_i for $i = 1, 2, \ldots, k$. Then clearly $\{z_1^{(i)}, z_2^{(i)}, \ldots, z_{r_i}^{(i)}\}_{i=1}^{k}$ form a basis in R^n. Given x_o, $g_o = A x_o + w$, and there exist unique $c_j^{(i)}$ such that

$$g_o = \sum_{i=1}^{k} \sum_{j=1}^{r_i} c_j^{(i)} z_j^{(i)} \equiv \sum_{i=1}^{k} y^{(i)}, \tag{B.1}$$

Note that: $Ay_i = \lambda_i y_i (i=1, \ldots, k), \langle y_i, y_j \rangle = 0 (i \neq j)$ (B.2)

Now, if $c_1^{(i)} = c_2^{(i)} = \ldots = c_{r_i}^{(i)} = 0$ for some i, then we have, from (B.1), $y^{(i)} = 0$ for that index i. Therefore, g_o is the sum of $y^{(1)}, y^{(2)}, \ldots, y^{(k)}$ and some of the $y^{(i)}$ may be zero-vectors. Assume that g_o is the sum of ℓ nonzero vectors and rename them as $w^{(1)}, w^{(2)}, \ldots, w^{(\ell)}$ where $\ell \leq k$. Recall that $Aw^{(i)} = \zeta_i w^{(i)}$ $(i = 1, \ldots, \ell)$ where $\zeta_1, \zeta_2, \ldots, \zeta_\ell$ are distinct eigenvalues of A selected from $\lambda_1, \lambda_2, \ldots, \lambda_k$. Clearly $\langle w^{(i)}, w^{(j)} \rangle = 0$ for $i \neq j$. From the above, for any finite integer $j > 0$, $A^j g_o = (\zeta_1)^j w^{(1)} + (\zeta_2)^j w^{(2)} + \ldots + (\zeta_\ell)^j w^{(\ell)}$ since $\zeta_1, \zeta_2, \ldots, \zeta_\ell$ are distinct positive real numbers, the matrix $B = [b_{ij}]$, defined by $b_{ij} = (\zeta_j)^i$ $(1 \leq i, j \leq \ell)$, is a nonsingular Vandermonde matrix. This leads to the results that $g_o, Ag_o, \ldots, A^{(\ell-1)} g_o$ are nonzero linear independent vectors, and span $\{g_o, Ag_o, \ldots, A^{(\ell-1)} g_o\}$ = span $\{w^{(1)}, w^{(2)}, \ldots, w^{(\ell)}\}$ since $\{w^{(1)}, \ldots, w^{(\ell)}\}$ are linearly independent and $g_o = \sum_{i=1}^{\ell} w^{(i)}$. Since $A^\ell g_o = \sum_{i=1}^{\ell} (\zeta_i)^\ell w^{(i)}$ is contained in the span of $\{w^{(1)}, \ldots, w^{(\ell)}\}$, then it is also contained in the span of $\{g_o, Ag_o, \ldots, A^{(\ell-1)} g_o\}$, i.e.,

$$A^\ell g_o = \sum_{i=0}^{\ell} \alpha_i A^i g_o \tag{B.3}$$

Since $\zeta_1, \zeta_2, \ldots, \zeta_\ell$ are distinct positive real numbers, then $\alpha_o, \alpha_1, \ldots, \alpha_{\ell-1}$ in (B.3) are all nonzero numbers. Therefore, from (B.3)

$$g_o = \sum_{i=1}^{\ell-1} \frac{\alpha_i}{\alpha_o} A^i g_o - \alpha_o A^\ell g_o = \sum_{i=1}^{\ell} \beta_i A^i g_o \tag{B.4}$$

But, as previously mentioned

span $\{Ag_o, A^2 g_o, \ldots, A^\ell g_o\}$ = span $\{AS_o, AS_1, \ldots, AS_\ell\}$; which implies $g_o = \sum_{i=0}^{\ell-1} \nu_i AS_i$ $(\ell \leq k)$, and

then from (B.4) $g_\ell = \sum_{i=0}^{\ell-1} \nu_i AS_i - g_o = 0$ $(\ell \leq k)$. This implies that the DFP method converges in exactly ℓ steps with $\ell \leq k$.

With Lemma B.1 it is easy to prove Property 4.2 . Now, assume that the DFP method applied to the (ANSQP) converges at $k < m$ steps, where m is the rank of Q. From the arguments of Lemma B.1, we can write $\bar{g}_o = \sum_{i=1}^{k} w_i$, where w_i is a nonzero eigenvector of Q_η corresponding to the eigenvalue ζ_i with $\zeta_i \neq \zeta_j$ for $i \neq j$. But, $\bar{g}_o = Q_\eta x_o + w = Qx_o + w + \frac{1}{\eta} x_o = g_o + \frac{1}{\eta} x_o, g_o \in R(Q)$ and $Qw_i = \lambda_i w_i$ $(i = 1, \ldots, k)$ (where $\lambda_i = \zeta_i - \frac{1}{\eta} \geq 0$), we conclude that $g_o = \sum_{i=1}^{k} c_i w_i$. Also from the above and the fact that $\zeta_1, \zeta_2, \ldots, \zeta_k$ are distinct positive real values, at most only one of the λ_i may become zero and the rest of the λ_i are distinct positive values. If $\lambda_j = \zeta_j - \frac{1}{\eta} = 0$ for a specific index j, then $Qw_j = 0$ and the corresponding coefficient c_j must be zero. Let us denote $z_i = c_i w_i$, collect the nonzero vectors z_i, and rename the index order to form $g_o = \sum_{i=1}^{r} z_i$ $(r \leq k)$, where z_i are the eigenvectors of Q corresponding to the distinct reordered eigenvalues λ_i. Using the same arguments as in Lemma B.1 and the fact that span $\{Qg_o, Q^2 g_o, \ldots, Q^r g_o\}$ = span $\{QS_o, QS_1, \ldots, QS_{r-1}\}$ We get $g_o = \sum_{i=0}^{r-1} \alpha_i QS_i$ $(r \leq k)$, or

$g_r = \sum_{i=0}^{r-1} \alpha_i QS_i - g_o = 0$, and, thus, the DFP method applied to the (SOP) converges in r steps, $r \leq k$.

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