Convergence of Gradient-Type Methods on Singular Parameter Optimization Problems

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The convergence properties of the gradient, conjugate gradient, and Davidon-Fletcher-Powell methods 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 corresponding 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.

I. 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 (CG), and Davidon-Fletcher-Powell (DFP) methods will be analyzed herein. For nonsingular quadratic optimization problems, convergence questions have been investigated by many authors with the following results: 1) linear convergence for the gradient method in both finite-dimensional and function space,[5] 2) finite-step convergence for both the CG and the DFP methods in finite-dimensional space,[6,7] 3) A rate of convergence for the CG method[5,8] and a convergence proof for the function-space DFP method.[9]

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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. 10, and as shown in Ref. 11 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[12-14] 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 to the singular case.

In Sec. II the singular quadratic optimization problem and algorithms are presented along with the existence conditions for the problem. The main convergence theorem is presented in Sec. III along with examples to illustrate its properties. In Sec. IV 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.

II. Problem Formulation and Algorithms

Consider the problem of determining a minimum of an unconstrained function f, where f has continuous partial derivatives of, at least, second order. Convergence and rate of convergence analyses are restricted to the neighborhood of the minimum, and 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

$$f(x) = \tfrac{1}{2} <x,Qx> + <x,w> + f_0 \tag{1}$$

where x, $w \;\epsilon\; R^n, f_0 \epsilon R$, $<x, w> = x^T w$ denotes the inner product in R^n and Q can be assumed, without loss of generality, to be an $n \times n$ symmetric matrix. The gradient of $f(x)$ at the element x, denoted by $g(x) \epsilon R^n$, is

$$g(x) \equiv \mathrm{d}f(x)/\mathrm{d}x = Qx + w \tag{2}$$

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 proprty:

Property 1: Eq. (1) has a minimum solution $\bar{x}$ if and only if

$$Q \text{ is positive semidefinite (denoted by } Q \geq 0) \tag{3}$$

$$w \text{ belongs to the range of [denoted by } w \epsilon R(Q)] \tag{4}$$

Proof: Since f is twice differentiable, if $\bar{x}$ is a minimum element, then $g(\bar{x})=Q\bar{x}+w=0$ and $<x, d^2f(\bar{x})/dx^2x> \geq 0$, $x \epsilon R^n$. But $Q\bar{x}\epsilon R(Q)$, $g(\bar{x})=0$ implies that $w=-Q\bar{x}\epsilon R(Q)$. Also, since $d^2f/dx^2=Q$, $<x, d^2f(\bar{x})/dx^2x> \geq 0$ implies that $<x, Qx> \geq 0$, i.e., Q is positive semidefinite. Now, suppose $w \epsilon R(Q)$. There exists an element x such that $Q\bar{x}+w=0$ and $f(\bar{x})=\frac{1}{2}<\bar{x},w>+f_0$. Let x be any element in R^n, then $x=\bar{x}+y$ where $y=x-\bar{x}\epsilon R^n$. After some calculations, $f(x)=f(\bar{x}+y)=\frac{1}{2}<y,Qy>+f(\bar{x})$, or $f(x)-f(\bar{x})=\frac{1}{2}<y,Qy>$. Since Q is positive semidefinite, we obtain $f(x) \geq f(\bar{x})$, i.e, $\bar{x}$ is a minimum solution of Problem 1.

Remark 1: If $Q=Q^T \geq 0$ and $w \epsilon R(Q)$, there may 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 $f(x)$, i.e., $f(\bar{x})=f(x^*)$.

Remark 2: In the process of proving Property (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 three iterative methods of interest here, the gradient, CG, and DFP methods, will now be summarized. In general, the iterative schemes metioned above attempt to generate a sequence $\{x_i\}$ which eventually converges to a minimizing element x^*, and they all involve the iteration rule

$$x_{i+1}=x_i+\alpha_i s_i \tag{5}$$

An initial element $x_0 \epsilon R^n$ is chosen arbitrarily. At each step a direction s_i is chosen (the way this is done will define the method used) and a step size is determined such that

$$f(x_i+\alpha_i s_i) \leq f(x_i+\lambda s_i) \quad \text{for all } \lambda \tag{6}$$

This leads to the condition

$$<g_{i+1}, s_i> =0, \qquad (g_{i+1} \equiv g(x_{i+1})) \tag{7}$$

which, for the quadratic function in Eq. (1), gives

$$\alpha_i = -<s_i, g_i>/<s_i, Qs_i> \tag{8}$$

In the gradient method $s_i=-g_i$ 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

$$<s_i, Qs_j> =0 \qquad i \neq j$$

In the CG method, s_i is taken as

$$s_i=-g_i+\frac{<g_i, g_i>}{<g_{i-1}, g_{i-1}>}s_{i-1} \text{with } s_0=-g_0$$

In the DFP method $s_i=-H_i g_i$ where

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

$$p_{i-1}=x_i-x_{i-1}=\alpha_{i-1}s_{i-1}$$

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

The dyadic notation $(><)$ is defined as (on R^n) $a><b \equiv ab^T$ and the following property is then easily verified:

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

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

A more general class of algorithms, which possess the uniqueness of search directions property and include the CG and DFP algorithms, will now be defined.

Definition 1: The *conjugate direction algorithms* employ Eqs. (5) and (6) to determine the update element x_{i+1} and stepsize α_i, respectively, where the search direction s_i satisfies

$$<g_i, s_i> \neq 0 \tag{9}$$

and

$$<s_i, Qs_j> =0, \quad i \neq j. \tag{10}$$

It has been shown in Ref. 15 that, for the nonsingular case, conjugate direction algorithms have both the descent property and the quadratic convergence property, i.e., they are stable and converge a quadratic function in a finite number of steps. The finite-step convergence result will be extended to the singular quadratic problem, Eq. (1), subject to Eqs. (3) and (4) in the next section.

III. The Main Convergence Theorem

Before proving the general convergence theorem, the following property is required.

Property 2: Let Q be a $n \times n$ 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,

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

b) $<x,Qx> =0$ if and only if $x \epsilon N(Q)$

where $[N(Q)]^{\perp}$ is the orthogonal complement of $N(Q)$.

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

Theorem 1: Consider problem (1) subject to Eqs. (3) and (4). Let $\{x_i\}$ be a sequence of vectors in R^n generated by a conjugate direction algorithm. Then the sequence converges to a minimum vector $\bar{x}_0$ in at most m iterates, where m is the rank of Q and $\bar{x}_0$ depends on the initial guess x_0.

Proof: The details of this proof are presented in Appendix A.

Remark 3: The finite m-step convergence property in Theorem 1 has been shown for the CG, DFP, and Powell's methods in particular in Ref. 16. Note that the CG and DFP methods belong to the class of conjugate direction algorithms but Powell's method does not necessarily belong since a gradient is assumed to exist in Eq. (9).

Remark 4: Usually the minimum solution $\bar{x}_0$ depends on the initial estimate x_0. Actually, if we let $S=\{x | x$ is a minimum solution of $f(x)\}$, then S is a nonempty closed convex set. Hence there exists $x^* \epsilon S$ such that $\|x^*\| \leq \|x\|$ for all $x \epsilon S$, where $\|\cdot\|$ denotes the Euclidean norm in R^n. Nashed[12] shows that the sequence $\{x_0,x_1,\ldots,x_i,\ldots\}$ generated by the gradient method converges to $\bar{x}_0=x^*+(I-P)x_0$ where P is the projection matrix from R^n to $R(Q)$. That is, if $x_0=x_0^r+x_0^n$ where $x_0^r \epsilon R(Q)$ and $x_0^n \epsilon N(Q)$, then $\bar{x}_0=x^r+x_0^n$. Now, if $H_0=I$ in the DFP method the search directions s_i in both the DFP and CG methods are linear combinations of $g_0,g_1,\ldots,g_i$. By the same procedures as stated in Ref. 12 we can prove that the sequence $\{x_0,x_1,\ldots\}$ generated by the DFP and CG methods (with $H_0=I$) converges to $\bar{x}_0=x^*+(I-P)x_0$ 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 $x_0=0$ as the initial estimate.

Remark 5: For a nonsingular quadratic function $f(x)=\frac{1}{2}<x, Ax>+<x, w>+f_0$, 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: If $\{x_i\}$ converges at the ℓth iterate ($\ell \leq m$) for the DFP method applied to a singular problem, then

a) $H_k > 0 \qquad 0 < k \leq \ell$

b) $H_k Q p_i = p_i \qquad 0 \leq i < k \leq \ell$

c) If $\ell = m$, then $H_m Q x = x$ for $x \epsilon R(Q)$.

Proof: If $x_\ell = \bar{x}_0$, 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 a) and b) carry over directly from the nonsingular case (e.g., Ref. 15, pp. 134-138). To prove c), observe from b) that

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

But $\{p_0, p_1, \ldots, p_{m-1}\}$ are nonzero Q-conjugate vectors. Hence they form a basis for $R(Q)$. Therefore, for any $x \epsilon R(Q)$, there exist constants $c_0, c_1, \ldots, c_{m-1}$ such that

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

and

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

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 4, $\bar{x}_0 = x^* + (I - P)x_0$, or, $\bar{x}_0 = x^* + (I - H_m Q)x_0$ if the DFP method converges at the mth step with $H_0 = I$.

Remark 6: The sequence $\{x_i\}$ generated by the gradient method for the singular problem converges linearly to $\bar{x}_0$ (by employing the results in Ref. 12).

Remark 7: Myers[17] shows 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] show that the search direction s_i of the CG method can be formed as

$$s_i = -\langle g_i, g_i \rangle \sum_{j=0}^{i} \frac{g_j}{\langle g_j, g_j \rangle} \tag{11}$$

and Horwitz and Sarachik[9] show that the search direction s_i of the DFP method can be written as

$$s_i = -\langle H_i g_i, H_i g_i \rangle \sum_{j=0}^{i} \frac{H_0 g_j}{\langle g_j, H_0 g_j \rangle} \tag{12}$$

Equations (11) and (12) are true for the singular quadratic case as long as $g_j \neq 0$, $j = 0, 1, 2, \ldots, i$. Therefore, from Eqs. (11) and (12), we see that the CG and the DFP methods generate the same search directions s_i for the singular quadratic problem (provided $H_0 = I$ and the same initial x_0 is employed).

Example: Consider the minimization of

$$f(x) = \frac{1}{2} \left\langle x, \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} x \right\rangle + \langle x, B \rangle + f_0 \qquad x, B \epsilon R^3, f_0 \epsilon R$$

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

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

By Property 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 $f_0 = 0$. Then

$$f(x) = \frac{1}{2} \left\langle x, \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} x \right\rangle = \frac{1}{2} (x^1 + x^3)^2 + \frac{1}{2} (x^2)^2$$

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

By inspection, the set S of minima is given by

$$S = \left\{ x \,|\, x = \begin{bmatrix} a \\ 0 \\ -a \end{bmatrix}, \; a \epsilon R \right\}$$

Clearly, the minimum norm solution $x^* \epsilon S$ is $x^* = [0\ 0\ 0]^T$. Now, consider the application of the gradient, CG, and DFP methods, with the same initial guess $x_0 = [1\ 1\ 1]^T$, to this problem.

a) Gradient Method: After straightforward calculations:

$$x_0 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \; x_1 = \frac{1}{17} \begin{bmatrix} -1 \\ 8 \\ -1 \end{bmatrix} \tag{13a}$$

$$g_0 = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix}, \; g_1 = \frac{1}{17} \begin{bmatrix} -2 \\ 8 \\ -2 \end{bmatrix} \tag{13b}$$

and

$$x_{2n} = \left(\frac{4}{85}\right)^n x_0, \; x_{2n+1} = \left(\frac{4}{85}\right)^n x_1 \tag{14a}$$

$$g_{2n} = \left(\frac{4}{85}\right)^n g_0, \; g_{2n+1} = \left(\frac{4}{85}\right)^n g_1 \tag{14b}$$

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

b) CG Method: Since the first iteration is a gradient step, the same x_0, x_1, g_0, g_1 as stated in Eq. (13) result and thus the search directions are

$$s_0 = -g_0 = \begin{bmatrix} -2 \\ -1 \\ -2 \end{bmatrix}, \; s_1 = \frac{18}{(17)^2} \begin{bmatrix} -1 \\ 8 \\ -1 \end{bmatrix} \tag{15}$$

which implies $x_2=0$, $g_2=0$. The CG method converges in 2 iterations. [Note again that Rank$(Q)=2$.]

c) DFP method: With $H_0=I_3$, it follows that x_0, x_1, g_0, g_1 are the same as in Eq. (13) and the search directions are

$$s_0=\frac{-9}{17}\begin{bmatrix}2\\1\\2\end{bmatrix},\ s_1=\frac{2}{33}\begin{bmatrix}-1\\8\\-1\end{bmatrix} \tag{16}$$

which implies $x_2=0$, $g_2=0$. 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,

$$P=H_2Q=\begin{bmatrix}\frac{1}{2} & 0 & \frac{1}{2}\\ 0 & 1 & 0\\ \frac{1}{2} & 0 & \frac{1}{2}\end{bmatrix}$$

is the projection matrix on $R(Q)$, i.e., $Px=x$, for all $x\epsilon R(Q)$ and

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

Note also that

$$T=I_3-P=\begin{bmatrix}\frac{1}{2} & 0 & -\frac{1}{2}\\ 0 & 0 & 0\\ -\frac{1}{2} & 0 & \frac{1}{2}\end{bmatrix}$$

is the projection matrix on $N(Q)$. In this example, the initial guess $x_0=[1\ 1\ 1]^T$, $Tx_0=0$, and therefore, $x_2=x^*=0$ in both the CG and DFP methods. Again, this result agrees with Remark 4. For an arbitrary

$$x_0=[a\,b\,c]^T,\ Tx=\begin{bmatrix}a-c\\0\\c-a\end{bmatrix};$$

the CG and DFP methods will converge in at most 2 steps to

$$\bar{x}_0=x^*+Tx_0=0+\frac{1}{2}\begin{bmatrix}a-c\\0\\c-a\end{bmatrix}$$

In Ref. 16 this example is also analyzed for Powell's method, and shown to converge at the second iterate, also. In the following, we will consider the application of conjugate direction methods to the least squares solution of linear algebraic equations since this class of problems can be defined as a singular quadratic optimization problem. First, we need the following definitions.

Definition 2: A vector $u\epsilon R^n$ is a least squares solution of the linear algebraic equations

$$Ax=b \tag{17}$$

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

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

The vector x^* is the *least squares solution of minimum norm of Eq. (17)* if x^* is a least squares solution of Eq. (17) and $\|x^*\|\leq\|u\|$ holds for all least squares solutions u of Eq. (17).

Definition 3: The generalized inverse A^+ of A is the linear extension of $[A\,|N(A)^\perp]^{-1}$ 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 $A\,|N(A)$ is the restriction of A to $N(A)$.

The following important results have been established by many researchers.[18]

Property 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 $Ax=y$, $y\epsilon Y$ is given by $x^*=A^+y$.

The linear operator A defined in Eq. (17) is clearly a bounded linear transformation with $R(A)$ closed. Property 4 implies that the LSSMN, x^*, of Eq. (17) 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 $\bar{x}=A^+b+(I-A^+A)x_0$, where x_0 is the initial estimate. Others describe iterative methods to compute the generalized inverse of a matrix. The conjugate direction methods should be powerful methods for determining least squares solutions of linear algebraic equations because of the following properties.

Property 5: Consider $J(x)=\frac{1}{2}<Ax-b,\ Ax-b>$ or, equivalently, $J(x)=\frac{1}{2}<x,\ Qx>+<x,\ \tilde{b}>+<b,b>$ where $Q=A^TA$ and $\tilde{b}=-A^Tb$. Then: a) $Q=Q^T\geq 0$, and b) $\tilde{b}\epsilon R(Q)$.

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

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

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

$$\tilde{b}=-A^Tb_r=-A^T-Ax=Q(-x)\epsilon R(Q)$$

Property 6: $\bar{x}$ is a solution of Eq. (17) if and only if $\bar{x}$ is a least squares solution of Eq. (17) and $J(\bar{x})=0$.

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

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

which implies

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

Now, $A\bar{x}-b_r\epsilon R(A)$, $Ax-b_r\neq 0$ and thus $A\bar{x}-b_r=0$. 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 $\bar{x}_n\epsilon N(A)$. With this $\bar{x}$, we have

$$\begin{aligned}J(\bar{x})&=\tfrac{1}{2}<\bar{x},\ Q\bar{x}>+<\bar{x},\ \tilde{b}>+<b,b>\\&=\tfrac{1}{2}<\bar{x},\ Q\bar{x}+\tilde{b}>+<\bar{x},\tilde{b}>+<b,b>\\&=-<A(\bar{x}_r+\bar{x}_n),\ b>+<b,b>\\&=-<(A\bar{x}_r-b_r)-b_n,\ b_r+b_n>=<b_n,\ b_n>\end{aligned}$$

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

Property 5: Along with Theorem 1 and Remark 4 guarantee that the sequence $\{x_0, x_1, \ldots\}$ generated by either the CG or DFP method applied to the least squares problem of Eq. (17) converges in at most $k = \text{Rank}(A)$ steps to a least squares solution $\bar{x}_0 = A^+ b + (I - A^+ A) x_0$, provided the initial step each takes is in the direction of steepest descent. If $x_0 = 0$, clearly the LSSMN $x^* = A^+ b$. If also $J(x^*) = 0$, then x^* is the minimum norm solution of $Ax = b$ by Property 6.

IV. Comparison of Conjugate Direction and Gradient Methods

Consider the singular problem, Eq. (1), subject to Eqs. (3) and (4), i.e.,

$$f(x) = \tfrac{1}{2} \langle x, Qx \rangle + \langle x, w \rangle + f_0 \quad \text{(SQP)}$$

where $x \epsilon R^n$, $f_0 \epsilon R$ with $Q = Q^T \geq 0$, $w \epsilon R(Q)$. Define the *associated nonsingular quadratic problem* (ANSQP) as

$$f_\eta(x) = \tfrac{1}{2} \langle x, Q_\eta x \rangle + \langle x, w \rangle + f_0 \quad \text{(ANSQP)}$$

where $Q_\eta = Q + 1/\eta \, I$ for $\eta > 0$

and $x \epsilon R^n$, $w \epsilon R(Q)$

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 7: a)(ANSQP) approaches (SQP) as $\eta \to \infty$; and b) 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 the (ANSQP) with corresponding eigenvalue $\beta_i = \lambda_i + 1/\eta$.

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

Property 8: If the sequence $\{\bar{x}_i\}$, generated by any one of conjugate direction methods applied to the (ANSQP), converges in $k < n$ steps, then the sequence $\{x_i\}$, generated by the same method applied to the (SQP) with the same initial estimate x_0, converges in at most k steps.

Proof: It has been shown in Theorem 2 of Ref. 19 that if $J(x)$ is a quadratic function with nondefinite matrix A (either nonsingular or singular matrix), then the DFP method with $H_0 = I$ and initial guess x_0 converges (or diverges to the value $-\infty$) to a stationary point of $J(x)$ after exactly ℓ iterations where ℓ is the number of distinct nonzero eigenvalues of A whose eigenvectors are not orthogonal to the gradient of $J(x)$ at x_0. Now, if the DFP method applied to the (ANSQP) converges in k steps, then by employing the above result, the gradient of $f_\eta(x)$, denoted by $\bar{g}(x_0)$, can be written as

$$\bar{g}(x_0) = Q_\eta x_0 + w = \sum_{i=1}^{k} a_i z_i \tag{18}$$

where $a_i \neq 0$ and z_i is an eigenvector of Q_η corresponding to the positive eigenvalue β_i for $i = 1, 2, \ldots, k$, and $\beta_i \neq \beta_j$ if $i \neq j$. Now, since

$$\begin{aligned} \bar{g}(x_0) &= Q_\eta x_0 + w = Q x_0 + w + (1/\eta) x_0 \\ &= g(x_0) + (1/\eta)\, x_0 \end{aligned} \tag{19}$$

Equations (18) and (19) imply that $g(x_0)$ is a linear combination of z_i, $1 \leq i \leq k$. Furthermore, part b) of Property 7 implies that z_i is an eigenvector of A with corresponding eigenvalue $\lambda_i = \beta_i - 1/\eta$ for $1 \leq i \leq k$, and $\lambda_i \neq \lambda_j$ if $i \neq j$. Therefore, the result of Ref. 19 implies again that the DFP method applied to the (SQP) with the same x_0 and $H_0 = I$ converges in k (or $k-1$) steps. This result can be generalized to the case of H_0 being any positive definite symmetric matrix (e.g., Ref. 16, Appendix B).

Property 8 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. A similar result holds for the gradient method in finite-dimensional space, also. Let us consider again the example presented in Sec. III to illustrate the above results.

Example:

$$\text{Minimize: } f(x) = \frac{1}{2} \left\langle x, \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} x \right\rangle \tag{20}$$

with $x_0 = [1, 1, 1]^T$, $x_1 = \dfrac{1}{17} [-1, 8, -1]^T$

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

$$x_{2n} = \left(\frac{4}{85}\right)^n x_0, \quad x_{2n+1} = \left(\frac{4}{85}\right)^n x_1.$$

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

The ratio of linear convergence, θ, is defined as

$$\theta = \lim_{k \to \infty} \sup . \frac{\| x_{k+1} - x^* \|}{\| x_k - x^* \|} \tag{21}$$

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

$$\theta_s = 0.2762 \tag{22}$$

The (ANSQP) of Eq. (20) is given by

$$f_\eta(x) = \tfrac{1}{2} x, Q_\eta x \rangle \tag{23}$$

where

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

With the same $x_0 = [1 \; 1 \; 1]^T$, the gradient method applied to the (ANSQP) [Eq. (23)] generates the sequence $\{x_i(\eta)\}$ with

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

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

$$x_{2n}(\eta) = [F(\eta)]^n x_0, \quad x_{2n+1}(\eta) = [F(\eta)]^n x_1 \tag{24}$$

where

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

Since

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

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

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

$$0<F(\eta_1)<F(\eta_2)<1 \quad \text{for} \quad 0<\eta_1<\eta_2 \tag{25}$$

Clearly, $$\lim_{\eta\to\infty} F(\eta)=\frac{4}{85} \tag{26}$$

and

$$\lim_{\eta\to\infty} x_k(\eta)=x^*(\eta)=0 \text{ for any } \eta>0 \tag{27}$$

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 $0<\eta_1<\eta_2$,

$$0<\|x_1(\eta_1)\|<\|x_1(\eta_2\| \tag{28}$$

$$0<|h(\eta_1)|<|h(\eta_2)| \tag{29}$$

and

$$\lim_{\eta\to\infty}\|x_1(\eta)\|^2=\frac{66}{289}=\|x_1\|^2 \tag{30}$$

Define $\theta(\eta)$, the ratio of linear convergence of the gradient method applied to the (ANSQP) [Eq. (23)]

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

Straightforward application of conditions (24) to (30) imply that, for $0<\eta_1<\eta_2$,

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

and,

$$\lim_{\eta\to\infty}\theta(\eta)=\theta_s \tag{31}$$

The result in Eq. (31) shows 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.

V. 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 $n\times n$ 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.

Appendix A: Proof of Theorem 1

Recall that a conjugate direction algorithm generates a sequence $\{x_i\}$ with the update formula

$$x_{i+1}=x_i+\alpha_i s_i, \quad x_0 \quad \text{initial guess} \tag{A1}$$

where the step size α_i is determined by

$$f(x_i+\alpha_i s_i)\le f(x_i+\lambda s_i) \tag{A2}$$

for all λ and the nonzero search direction s_i satisfies

$$<g_i, s_i>\neq 0 \tag{A3}$$

and

$$<s_i, Qs_j>=0, \quad i\neq j \tag{A4}$$

At the ith iteration, (A2) implies that

$$<g_{i+1}, s_i>=0 \tag{A5}$$

and

$$\alpha_i=-<g_i, s_i>/<s_i,Qs_i> \tag{A6}$$

Note that $<s_i, Qs_i>\neq 0$ is guaranteed by (A3) and part (b) of Property 2. Now, since

$$g(x)=Qx+w \tag{A7}$$

the gradient g_{i+1} can be related to the gradient g_i by

$$g_{i+1}=g_i+\alpha_i Qs_i, \tag{A8}$$

and the process can be repeated to imply

$$g_k=g_j+\sum_{i=j}^{k-1}\alpha_i Qs_i\,(k>j) \tag{A9}$$

If the transpose of (A9) is postmultiplied by s_j and (A6) is employed for α_j, then

$$<g_k,s_j> = \sum_{i=j+1}^{k-1}\alpha_i<s_i,Qs_j>, \; k-2\ge j\ge 0 \tag{A10}$$

$$<g_k, s_j>=0, \qquad k-2\ge j\ge 0 \tag{A11}$$

Since (A5) implies

$$<g_k, s_{k-1}>=0 \tag{A12}$$

(A11) and (A12) can be rewritten as

$$<g_k, s_j>=0, \qquad k-1\ge j\ge 0 \tag{A13}$$

and (A4) implies

$$R^n=R(Q)\oplus N(Q)$$

Then, each element x in R^n can be decomposed uniquely as

$$x=x^r+x^n$$

where $x^r\epsilon R(Q)$ and $x^n\epsilon N(Q)$, and in particular

$$s_i=s_i^r+s_i^n \tag{A14}$$

Substitution of (A14) into (A3), (A4) and (A13) implies

$$<g_i, s_i^r>\neq 0 \tag{A14a}$$

$$<s_i^r, Qs_j^r>=0, \quad i\neq j \tag{A15}$$

$$<g_k, s_j^r> = 0, \quad k-1 \geq j \geq 0 \tag{A16}$$

respectively, since $g_i \epsilon R(Q)$. It follows that

$$<s_i^r, Qs_i^r> > 0 \tag{A17}$$

for, if

$$<s_i^r, Qs_i^r> = 0$$

then part b) of Property 2 implies that $s_i^r \epsilon N(Q)$, and thus

$$<g_i, s_i^r> = 0,$$

which is contradictory to (A14a). Therefore, conditions (A15) and (A17) imply that $\{s_i^r\}$ is a set of nonzero Q-conjugate elements in $R(Q)$. Now, consider (A16) with $k=m$, i.e.,

$$<g_m, s_j^r> = 0 \qquad m-1 \geq j \geq 0 \tag{A18}$$

Since $\{s_0^r, s_1^r, \ldots, s_{m-1}^r\}$ is a linearly independent set of vectors in $R(Q)$, and the rank of Q is m, then $\{s_0^r, s_1^r, \ldots, s_{m-1}^r\}$ forms a basis in $R(Q)$. this implies that the gradient vector g_m which satisfies (A18) must be in the null space of Q, i.e,

$$g_m \epsilon N(Q). \tag{A19}$$

But

$$g_m = Qx_m + w \epsilon R(Q) \tag{A20}$$

and thus

$$g_m \epsilon N(Q) \cap R(Q) = \{0\}$$

i.e.,

$$g_m = Qx_m + w = 0$$

and the sequence $\{x_i\}$ converges in a maximum of m iterates.

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