HYPERBOLIC PAIRS IN THE METHOD OF CONJUGATE GRADIENTS*

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1. Introduction. Let $X = E^n$, Euclidean n space, with the usual inner product $(\cdot, \cdot)$. Let A be a real symmetric $n \times n$ matrix. Given $b \in X$ we shall be concerned with solving the equation

$$(1) \qquad\qquad Ax = b$$

by a generalized method of conjugate gradients.

If A is positive definite, then, as is well known [1]–[4], the sequence $\{x_k\}$ resulting from the iterative process

$$(2a) \qquad\qquad x_{k+1} = x_k + \alpha_k p_k,$$

$$(2b) \qquad\qquad r_{k+1} = b - Ax_{k+1} = r_k - \alpha_k A p_k,$$

$$(2c) \qquad\qquad p_{k+1} = r_{k+1} - \beta_k p_k,$$

$$(2d) \qquad\qquad \alpha_k = (r_k, p_k)/(p_k, A p_k),$$

$$(2e) \qquad\qquad \beta_k = (r_{k+1}, A p_k)/(p_k, A p_k)$$

(starting from an arbitrary x_1 and $r_1 = b - Ax_1, p_1 = r_1$) converges to the solution of (1) in n steps or less. Theoretically, the process (2) can be carried out in such a manner that only one multiplication of A times a vector is required at each step, although in practice two such multiplications are often employed.

In many applications we are led to equations of the form (1) where A is nonsingular and symmetric but not positive definite. For example the problem of minimizing the quadratic form

$$\tfrac{1}{2}(x, Qx) - (c, x)$$

subject to the linear constraint

$$Dx = d,$$

where Q is a symmetric positive definite $n \times n$ matrix, c is an n-vector, D is an $m \times n$ matrix of rank m, and d is an m-vector, leads to the equation

$$\begin{bmatrix} Q & D' \\ D & 0 \end{bmatrix} \begin{bmatrix} x \\ \lambda \end{bmatrix} = \begin{bmatrix} c \\ d \end{bmatrix}$$

which has coefficient matrix of this type. In cases such as these, where the matrix A is nonsingular and symmetric but not positive definite, the procedure (2) may break down since $(p_k, A p_k)$ may vanish for some k.

The difficulties associated with the method in such cases can, of course, be rectified in a trivial way by applying the method to the equivalent equation

$$A^2 x = Ab;$$ (3)

but the resulting iterative process then requires a minimum of two multiplications by A at each step. In this paper we develop a modification of the standard method that cannot break down and which requires only one multiplication by A at each step. The method employed exploits the concept of a hyperbolic pair which is fundamental in the algebraic study of symmetric quadratic forms [5]. It should be noted that, although the revised algorithm developed here is very similar to the standard one, we cannot convert the problem to that of minimizing the quadratic form $(x, Ax) - 2(x, b)$, and hence convergence proofs cannot be based on this fact.

2. The algorithm. Let A be a real symmetric nonsingular $n \times n$ matrix. A nonzero vector $x \in X$ is said to be *singular* if $(x, Ax) = 0$. A pair of vectors $x, y \in X$ is said to be a *hyperbolic pair* if x and y are both singular and $(x, Ay) \neq 0$. The conjugate gradient method (2) breaks down if, at stage k, the direction vector p_k is singular. In the algorithm below singular directions, if generated at all, are generated as hyperbolic pairs.

The revised algorithm (starting from an arbitrary x_1, with $r_1 = b - Ax_1$, $p_1 = r_1$) is as follows.

Case A: p_k *is nonsingular.* Use (2a)–(2e).

Case B: p_k *is singular.*

$$p_{k+1} = Ap_k - \frac{(Ap_k, A^2 p_k)}{2(Ap_k, Ap_k)} p_k,$$ (4a)

$$x_{k+1} = x_k + a_k p_k,$$ (4b)

$$x_{k+2} = x_{k+1} + \alpha_{k+1} p_{k+1},$$ (4c)

$$r_{k+2} = b - Ax_{k+2},$$ (4d)

$$\alpha_k = \frac{(r_k, p_{k+1})}{(p_k, Ap_{k+1})},$$ (4e)

$$\alpha_{k+1} = \frac{(r_k, p_k)}{(p_k, Ap_{k+1})},$$ (4f)

$$p_{k+2} = r_{k+2} - \frac{(r_{k+2}, Ap_{k+1})}{(p_k, Ap_{k+1})} p_k.$$ (4g)

In this case p_k, p_{k+1} is a hyperbolic pair. Note that r_{k+1} is not explicitly defined in this case.

3. Proof of convergence. Throughout this section we use the notation $[x_1, x_2, \cdots, x_k]$ to denote the subspace of X generated by the vectors $x_1, x_2, \cdots, x_k$.

The revised algorithm of § 2 is constructed so that none of the required constants become infinite. We prove also that it cannot get "stuck" at any point which is not the solution.

LEMMA 1. *If p_k is nonsingular and $r_k \neq 0$, then $x_{k+1} \neq x_k$.*

Proof. The vector p_{k-1} may either be nonsingular or the second member of a hyperbolic pair. In the first case it follows from (2b), (2d) that $(r_k, p_{k-1}) = 0$ and then from (2c) that

$$(r_k, p_k) = (r_k, r_k) > 0.$$

In the second case it follows from (4b), (4c), (4d) that $(r_k, p_{k-2}) = 0$ and then from (4g) that

$$(r_k, p_k) = (r_k, r_k) > 0.$$

LEMMA 2. *If p_{k+1} is the second member of a hyperbolic pair and $r_k \neq 0$, then $x_{k+2} \neq x_{k+1}$.*

Proof. The vector p_{k-1} is either nonsingular or the second member of a hyperbolic pair. In the proof of Lemma 1 it was shown that in either case

$$(p_k, r_k) = (r_k, r_k) > 0.$$

LEMMA 3. *For every k, $[p_1, p_2, \cdots, p_k] = [r_1, Ar_1, \cdots, A^{k-1}r_1]$.*

Proof. It is clear from the construction of the iterative process that

$$[p_1, p_2, \cdots, p_k] \subset [r_1, Ar_1, \cdots, A^{k-1}r_1].$$

Since x_{k+1} has the form

$$(5) \qquad x_{k+1} = x_1 + \sum_{i=1}^{k} \alpha_i p_i,$$

it follows that

$$(6) \qquad r_{k+1} = r_1 - \sum_{i=1}^{k} \alpha_i A p_i.$$

If p_k is not the first member of a hyperbolic pair, it follows directly from Lemmas 1 and 2 that $\alpha_k \neq 0$; and hence if p_k contains a component of $A^{k-1}r_1$, r_{k+1} will contain a component of $A^k r_1$, and hence, finally from (2c) or 4(g), p_{k+1} contains a component of $A^k r_1$. On the other hand, if p_k is the first member of a hyperbolic pair, it is clear from (4a) that if p_k contains a component of $A^{k-1}r_1$, p_{k+1} will contain a component of $A^k r_1$.

THEOREM 1. *The following relations hold for the algorithm of § 2:*

$$(7) \qquad (p_i, Ap_j) = 0 \quad for \quad i \neq j \quad unless \ p_i, p_j \ is \ a \ hyperbolic \ pair;$$

$$(8) \qquad (r_j, p_i) = 0 \quad for \quad i < j.$$

Proof. The proof is by induction. Suppose the relations are true for $\{p_i\}, \{r_i\}$, $i = 1, \cdots, k$, and that p_{k-1}, p_k is not a hyperbolic pair.

Case A: p_k *is not singular.* From (2b),

$$(r_{k+1}, p_i) = (r_k, p_i) - \alpha_k (Ap_k, p_i).$$

For $i = k$ the two terms on the right cancel while for $i < k$ they are both zero.

Likewise from (2c),

$$(p_{k+1}, Ap_i) = (r_{k+1}, Ap_i) - \beta_k(p_k, Ap_i).$$

For $i = k$ the two terms on the right cancel, while for $i < k$, in view of (8), they are both zero.

Case B: p_k *is singular.* From (4a) we have $(p_{k+1}, Ap_{k+1}) = 0$ and (p_{k+1}, Ap_k) $= (Ap_k, Ap_k) > 0$; hence p_k, p_{k+1} is a hyperbolic pair. Furthermore, we have immediately from the induction hypotheses for $i < k$,

$$(p_{k+1}, Ap_i) = (Ap_k, Ap_i) = (p_k, AAp_i);$$

but from Lemma 3 it follows that $Ap_i \in [p_1, p_2, \cdots, p_{i+1}]$, and hence, again by the induction hypotheses and the singularity of p_k,

$$(p_{k+1}, Ap_i) = 0 \quad \text{for } i < k.$$

Now from (4b), (4c), (4d),

$$(r_{k+2}, p_i) = (r_k, p_i) - \frac{(r_k, p_{k+1})}{(p_k, Ap_{k+1})}(Ap_k, p_i)$$

$$- \frac{(r_k, p_k)}{(p_k, Ap_{k+1})}(Ap_{k+1}, p_i).$$

For $i = k + 1$ the first two terms on the right cancel while the third term vanishes. For $i = k$ the first and third term cancel while the second vanishes. And for $i < k$ all terms vanish.

Finally we have, from (4e),

$$(p_{k+2}, Ap_i) = (r_{k+2}, Ap_i) - \frac{(r_{k+2}, Ap_{k+1})}{(p_k, Ap_{k+1})}(p_k, Ap_i),$$

which by a similar analysis is seen to be zero for all $i \leqq k + 1$.

LEMMA 4. *In the algorithm of* § 2 *there holds*

$$(r_k, p_j) = (r_1, p_j) \quad \text{for } j \geqq k.$$

Proof. This follows from (6) and the A-orthogonality of the p_i's.

THEOREM 2. *The algorithm of* § 2 *converges to the unique solution* x *of* (1) *in* n *steps or less.*

Proof. Equation (1) is equivalent to

(9) $$A(x - x_1) = r_1,$$

and hence we must show that

(10) $$x_{n+1} - x_1 = \sum_{i=1}^{n} \alpha_i p_i$$

solves (9). It is clear from Lemma 3 that the solution does have a representation of form (10); it remains only to verify the coefficients α_i are correct. Any two vectors in the sequence $\{p_i\}$ are mutually A-orthogonal except, of course, two vectors that form a hyperbolic pair. Hence the coefficients in (10) can be found by forming the

inner product of both sides of (9) with p_k. If p_k is nonsingular this will determine α_k. If p_k is singular it will determine the coefficient of its hyperbolic partner. In view of Lemma 4 these coefficients are precisely those of the algorithm.

4. Computational experience. The procedure discussed above has been programmed in FORTRAN and applied to a variety of numerical examples. In the examples tested the entries of the A matrix were always integers between -100 and $+100$. A direction vector p_k was treated as singular if

$$\left| \frac{(p_k, Ap_k)}{(p_k, p_k)} \right| < 10^{-4}.$$

For problems having ten or less variables this procedure worked without difficulty. Problems with as many as one hundred variables were easily solved when double precision was employed.

An interesting example problem that was constructed to yield a sequence of hyperbolic pairs and was easily solved by the method of this paper is

$$A = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \end{bmatrix},$$

$$b = (1, 0, 0, 0, 0, 0, 0, 0)',$$

$$x_1 = (0, 0, 0, 0, 0, 0, 0, 0)'.$$

There is a number of difficult unsettled questions related to routine practical application of this method—such as how small (p_k, Ap_k) should be in order that p_k be treated as singular. Initial experience indicates, however, that the method can feasibly handle large problems.

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