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A NOTE ON SEMIDEFINITE MATRICES

by

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ABSTRACT

It is of general interest to find criteria for a matrix to be positive (or negative)- semidefinite. The usual characterization of semidefinite matrices in terms of their principal minors can be rather laborious to implement practically. We present here an elementary proof of a known alternate characterization of a semidefinite matrix in terms of its null-space and of its largest characteristic value. An iterative procedure is also suggested which may be useful in deciding the semidefiniteness of a matrix.

A NOTE ON SEMIDEFINITE MATRICES

In what follows A will *always* represent a real, symmetric, $n \times n$ matrix. If, for each $x \in R^n$ (*) it is true that $xAx^T \geq 0$ (**) then we say that A is *positive-semidefinite*, denoted: *p.s.d.*; if $(xAx^T)(yAy^T) \geq 0$ for all $x, y \in R^n$ we say that A is *semidefinite*, denoted *s.d.*. We first prove the following:

THEOREM 1. The following are equivalent:

(i) A is s.d.

(ii) $(xAy^T)^2 \leq (xAx^T)(yAy^T)$, all $x, y \in R^n$

(iii) $x \in R^n$, $xAx^T = 0 \Longrightarrow xA^2x^T = 0$

(iv) $x \in R^n$, $xA^2x^T = 1 \Longrightarrow (xAx^T)^2 > 0$

(v) $x \in R^n$, $xAx^T = 0 \Longrightarrow xA = 0$

PROOF: We show (i) $\Rightarrow$ (ii) $\Rightarrow$ (iii) $\Rightarrow$ (iv) $\Rightarrow$ (v) $\Rightarrow$ (i).

(i) $\Rightarrow$ (ii)

Suppose A is s.d., let $x, y \in R^n$. Consider the real quadratic polynomial p defined by:

$$p(\lambda) = (x + \lambda y)A(x + \lambda y)^T =$$

$$= xAx^T + 2\lambda\, xAy^T + \lambda^2 yAy^T.$$

Since A is s.d., p does not change sign, i.e., its discriminant is non-positive, whence:

$$4(xAy^T)^2 - 4(xAx^T)(yAy^T) \leq 0 ,$$

(*) $R^n = \left\{ x \mid x = (x_1, \ldots, x_n) \text{ and } x_i \text{ is a real number for } i = i, \ldots, n \right\}$.

(**) If $x \in R^n$, x^T denotes the transpose of x.

giving the desired result.

(ii) $\Rightarrow$ (iii).

Suppose $x \in R^n$ and $xAx^T = 0$, then, from (ii), $(xAy^T)^2 \leq 0$, i.e., $xAy^T = 0$, for all $y \in R^n$. Thus $xA = 0$, but $xA^2x^T = (xA)(xA)^T = 0$.

(iii) $\Rightarrow$ (iv).

If $x \in R^n$ and $(xAx^T)^2 \leq 0$ then $xAx^T = 0$ and, by (iii), $xA^2x^T = 0$, contradicting $xA^2x^T = 1$.

(iv) $\Rightarrow$ (v).

If $x \in R^n$ and $xAx^T = 0$ then, by (iv), $xA^2x^T \leq 0$ (because if $xA^2x^T > 0$ then we could normalize x to get $xA^2x^T = 1$, $xAx^T = 0$). However, $xA^2x^T = (xA)(xA)^T$, and thus $xA^2x^T \geq 0$ with equality holding if and only if $xA = 0$.

(v) $\Rightarrow$ (i).

Suppose (i) is false, i.e., there exist $x, y \in R^n$ such that $xAx^T > 0$, $yAy^T < 0$. By suitable normalization [dividing x by $(xAx^T)^{1/2}$ and y by $(-yAy^T)^{1/2}$], we may assume that $xAx^T = 1$, $yAy^T = -1$. Now let:

$$(1) \quad \lambda = -xAy^T + [1 + (xAy^T)^2]^{1/2}$$

$$(2) \quad z = \lambda x + y .$$

We claim that $zA \neq 0$ and $zAz^T = 0$, thus contradicting (v). First, if $zA = 0$ then multiplying (2) by Ax^T and Ay^T we get:

$$0 = \lambda xAx^T + yAx^T = \lambda + xAy^T$$

$$0 = \lambda xAy^T + yAy^T = \lambda xAy^T - 1 ,$$

Combining the last two equations:

$$0 = \lambda xAy^T - 1 = (-xAy^T)(xAy^T) - 1 =$$
$$= -1-(xAy^T)^2 ,$$

a contradiction, thus $zA \neq 0$. However,

$$zAz^T = (\lambda x + y)A(\lambda x + y)^T =$$

$$= \lambda^2 xAx^T + 2\lambda xAy^T + yAy^T$$

$$= \lambda^2 + 2\lambda xAy^T - 1 ,$$

and λ was chosen to be precisely one of the two (real) roots of the preceding quadratic polynomial in λ. q. e. d.

Several comments are in order. Obviously, A is s. d. if and only if A is p. s. d. or -A is p. s. d. Condition (ii) of Theorem 1 is a generalization of the Cauchy-Schwartz inequality, namely:

$$(3) \quad (uv^T)^2 \leq (uu^T)(vv^T) \qquad \text{all } u, v \in R^n,$$

for if we take A to be the nxn identity matrix which is clearly p. s. d., we obtain (3) from (ii) - Theorem 1. Condition (v) - Theorem 1, or its obvious equivalents (iii) and (iv), states that if we consider xA, the image under the linear transformation A of a point x in R^n, then A cannot be perpendicular to x unless x is in the null-space of A. Alternately, (v) - Theorem 1 states that if x is <u>not</u> in the null-space of A then its image under A cannot be perpendicular to x.

We proceed next to obtain results which are, in a sense, "refinements" of conditions (ii) (see Lemma 1 below) and (iv) (see Theorem 2) of Theorem 1. Lemma 1 is a generalization of the well known fact, associated with the Cauchy-Schwartz inequality, stating that equality holds in (3) if and only if u, v are linearly dependent. We shall apply Lemma 1 in the proof of Theorem 3.

LEMMA 1

Let A be s.d.. If $x, y \in R^n$ then $(xAy^T)^2 = (xAx^T)(yAy^T)$ if and only if xA, yA are linearly dependent.

PROOF: If, say, $xA = \lambda yA$, where λ is a real number, then $xAy^T = \lambda yAy^T$ while $xAx^T = \lambda yAx^T = \lambda xAy^T = \lambda^2 yAy^T$. Whence it follows that $(xAy^T)^2 = \lambda^2(yAy^T)^2 = (xAx^T)(yAy^T)$.

On the other hand, suppose $(xAy^T)^2 = (xAx^T)(yAy^T)$. If $xAx^T = 0$ or $yAy^T = 0$ then, by (v) - Theorem 1, $xA = 0$ or $yA = 0$ and we certainly can conclude that xA, yA are linearly dependent. Otherwise, say, $xAx^T > 0$ and $yAy^T > 0$, consequently $xAy^T \neq 0$. Let $\rho = \text{signum}(xAy^T)$ and let:

$$\alpha = (yAy^T)^{1/2}$$

$$\beta = -\rho(xAx^T)^{1/2},$$

then $\alpha, \beta \neq 0$ and:

$$\begin{aligned}(\alpha x + \beta y)A(\alpha x + \beta y)^T &= \alpha^2 xAx^T + \beta^2 yAy^T + 2\alpha\beta xAy^T = \\ &= 2(xAx^T)(yAy^T) - 2\rho(xAy^T)(xAx^T)^{1/2}(yAy^T)^{1/2} = \\ &= 2(xAx^T)(yAy^T) - 2|xAy^T|(xAx^T)^{1/2}(yAy^T)^{1/2} = \\ &= 2(xAx^T)(yAy^T) - 2(xAx^T)(yAy^T) = 0 .\end{aligned}$$

Thus, $(\alpha x + \beta y)A(\alpha x + \beta y)^T = 0$ and, by (v) - Theorem 1, $0 = (\alpha x + \beta y)A = \alpha xA + \beta yA$. q.e.d.

The preceding lemma was motivated, in part, by an examination of (ii) - Theorem 1 in case A is the identity matrix, in that case (since the square of the identity is the identity), (iv) - Theorem 1 states: $x \in R^n$, $xx^T = 1$ implies $(xx^T)^2 > 0$, which is, of course, true. We notice, though, that $(xAx^T)^2$ has then a positive lower bound, namely 1. In general, this will be the case, i.e., a positive lower bound will exist for $(xAx^T)^2$ in (iv) - Theorem 1, whenever A is s.d.. Clearly, when A is identically zero any positive number will serve as a lower bound, because there is no $x \in R^n$ for which $xA^2x^T = 1$, thus we will exclude $A = 0$ in the next theorem:

THEOREM 2

Suppose A is p.s.d. and $A \neq 0$, then there exist a positive real number μ and an $x_0 \in R^n$ such that:

(4) $\quad x \in R^n,\ xA^2x^T = 1 \Rightarrow xAx^T \geq \mu$

(5) $\quad x_0A^2x_0^T = 1$ and $x_0Ax_0^T = \mu.$

PROOF: Let

$$X = \left\{ x \mid x \in R^n \text{ and } xA^2x^T = 1 \right\}$$

$$\mu = \inf_{x \in X} xAx^T .$$

Since A is p.s.d. and $A \neq 0$, μ is well defined and in fact $\mu \geq 0$ and satisfies (4). By definition of μ, there exists a sequence x_k such that

(6) $\quad x_k \in X$ for $k = 1, 2, \ldots$

(7) $\quad x_kAx_k^T$ converges to μ.

We consider two cases:

Case 1. The sequence x_k has a bounded subsequence. In this eventuality the x_k have a point of accumulation x_0, for which it must be true (by (6) and (7) and because X is closed) that $x_0 \in X$ and $x_0Ax_0^T = \mu$. Thus x_0 satisfies (5). That μ is positive then follows from (v) - Theorem 1. The two preceding facts, together with the remark above that μ satisfies 4, complete the proof.

Case 2. The sequence $\{x_k\}$ has no bounded subsequence, i.e., we may assume that $|x_k| = (x_k x_k^T)^{1/2} \to \infty$, and $|x_k| > 0$, $k = 1, 2, \ldots$.
We define another sequence $\{y_k\}$ by:

$$y_k = \frac{x_k}{|x_k|} .$$

Now, $y_k A y_k^T$ converge to zero, because $x_k A x_k^T$ converge to μ and also $y_k A^2 y_k^T$ converge to zero, because $x_k A^2 x_k = 1$ all k. However, $|y_k| = 1$, thus the y_k's have an accumulation point y, for which it must be true that $yAy^T = 0$. Thus $yA = 0$ by (v) - Theorem 1.

Next we observe that from the definition of y and the y_k's it follows that whenever y has a non-zero component then infinitely many x_k's have the same component non-zero, and in fact of the same sign. We may assume that an appropriate subsequence of x_k has been selected so that whenever y has a positive (negative) component then all the x_k's have the same component positive (negative). Now, if $\{\lambda_k\}$ is any sequence of real numbers then:

$$(x_k + \lambda_k y)A(x_k + \lambda_k y)^T = x_k A x_k^T$$

and

$$(x_k + \lambda_k y)A^2(x_k + \lambda_k y)^T = x_k A^2 x_k^T ,$$

because $yA = 0$. We can thus replace x_k by $x_k + \lambda_k y$, $k = 1, 2, \ldots$, and (6) and (7) will still hold. However, by an appropriate choice of λ_k we can reduce the number of non-zero components in each of the x_k's, eventually (repeating the above process, if necessary) we obtain a sequence $\{x_k\}$, satisfying (6)-(7) and which has an accumulation point, thus reducing it to case 1.

q.e.d.

As an immediate consequence of Theorem 2 we can "strengthen" (iv) - Theorem 1.

Corollary

If A is s.d. and $A \neq 0$ then

$$\text{minimum} \left\{ \left(xAx^T \right)^2 \middle| \; x \in R^n \text{ and } xA^2x^T = 1 \right\}$$

exists and is positive.

PROOF: As noted before, if A is s.d., then either A is p.s.d. or $-A$ is p.s.d., in either case the square of the μ in Theorem 2 is the required minimum and the x_0 of the same theorem is the required minimizing x.

The μ and x_0 of Theorem 2 are, as one might expect, intimately related to the characteristic values of A. This is brought forth in the next theorem.

THEOREM 3

Let A be p.s.d., $A \neq 0$. Let μ and x_0 be as in Theorem 2 and let λ_n be the largest characteristic value of A, then $\lambda_n = \mu^{-1}$ and x_0A is a characteristic vector of A corresponding to λ_n.

PROOF: Suppose λ is any characteristic value of A, i.e., there exists an $x \in R^n$, $x \neq 0$, such that $xA = \lambda x$, whence $xA^2x^T = \lambda xAx^T$. If $\lambda = 0$ then certainly $\lambda \leq \mu^{-1}$. Assuming $\lambda \neq 0$, it follows that $xA \neq 0$ (because $x \neq 0$) and thus, by (v) - Theorem 1, $xAx^T > 0$. Let $y = (xA^2x^T)^{-1/2}x$, then $yA^2y = 1$ and, by definition of μ, $yAy^T \geq \mu$. However $yAy^T = (xA^2x^T)^{-1}(xAx^T) = = \lambda^{-1}$, thus $\lambda \leq \mu^{-1}$. We have just demonstrated that $\lambda \leq \mu^{-1}$ for any characteristic value λ of A, thus $\lambda_n \leq \mu^{-1}$.

To complete the proof of this theorem it will suffice to show that there is a characteristic value λ of A such that $\lambda = \mu^{-1}$, and $(x_0A)A = \lambda(x_0A)$, x_0 being as in Theorem 2. Let $x = x_0$ be a minimizing x_0 in question. Since A and A^2 are p. s. d. (the square of any real symmetric matrix is p. s. d.), and $xA \neq 0$ ($xAx^T = x_0Ax_0^T = \mu > 0$), it follows that $xA^3x^T = (xA)A(xA)^T > 0$, and $xA^4x = (xA)A^2(xA)^T > 0$. Thus, if we define

$$(8) \qquad \rho = 2(xA^3x^T)(xA^4x^T)^{-1}$$

then ρ is positive. Next let

$$(9) \qquad y = x - \rho x A .$$

The motivation for the above definition of y is as follows: we know x minimizes a certain function, namely xAx, since we wish to derive from this fact some properties of x we examine how xAx will change in the direction of its gradient, namely $2xA$. As defined in (9), y is a translation from x precisely in the direction of that gradient, the particular value of ρ chosen is designed to keep y within the "feasibility" set, i. e., $yA^2y = 1$. We check next the last mentioned condition:

$$\begin{aligned} yA^2y^T &= (x - \rho xA)A^2(x - \rho xA)^T = \\ &= xA^2x^T - 2\rho xA^3x^T + \rho^2 xA^4x^T = \\ &= 1 - 2\rho\left[xA^3x^T - \frac{\rho}{2}(xA^4x^T)\right] \\ &= 1 - 2\rho\left[xA^3x^T - (xA^3x^T)(xA^4x^T)^{-1}(xA^4x^T)\right] \\ &= 1 . \end{aligned}$$

One can, incidentally, readily check that the particular value of ρ, as given in (8), is the only value of ρ (other than $\rho = 0$) which yields $yA^2y = 1$. Now, since $yA^2y^T = 1$, we must have, by definition of μ,

(10) $yAy^T - xAx^T \geq 0$.

However,

$$yAy^T - xAx^T = (x-\rho xA)A(x-\rho xA)^T - xAx^T =$$
$$= -2\rho xA^2x^T + \rho^2 xA^3x^T =$$
$$= 2\rho\left[\frac{\rho}{2}(xA^3x^T) - (xA^2x^T)\right] =$$
$$= 2\rho(xA^4x^T)^{-1}\left[(xA^3x^T)^2 - (xA^2x^T)(xA^4x^T)\right].$$

Thus, since $\rho > 0$, $(xA^4x^T)^{-1} > 0$ and because (10) holds, we have:

(11) $(xA^3x^T)^2 \geq (xA^2x^T)(xA^4x^T)$.

We now refer to inequality (3), which is a special case of (ii) - Theorem 1 with A being the identity, letting $u = xA$, $v = xA^2$ we get:

(12) $(xA^3x^T)^2 \leq (xA^2x^T)(xA^4x^T)$.

Combining (11) and (12), we get:

(13) $(xA^3x^T)^2 = (xA^2x^T)(xA^4x^T)$.

However, from Lemma 1, again with A being the identity matrix, we then know that xA, xA^2 are linearly dependent. Since $xA \neq 0$, it follows that there is a real number λ such that $xA^2 = \lambda xA$, multiplying by x^T: $1 = xA^2x^T = \lambda xAx^T$, and $\lambda = (xAx^T)^{-1} = \mu^{-1}$. q. e. d.

As a final general result, we specialize (ii) - Theorem 1, and Lemma 1, for the case where A is non-singular.

THEOREM 4

Let A be p. s. d. and non-singular then,

$$(14) \quad (uv^T)^2 \leq (uAu^T)(vA^{-1}v^T) \quad \text{all } u, v \in R^n$$

and equality holds above if and only if u, vA^{-1} are dependent.

PROOF: We first note that A^{-1} must be symmetric because $AA^{-1} = I$, thus $I^T = I = (AA^{-1})^T = (A^{-1})^T A^T = (A^{-1})^T A$. But the inverse is unique, thus $A^{-1} = (A^{-1})^T$. Next, let $u, v \in R^n$, we let

$$(15) \quad x = u, \; y = vA^{-1} .$$

One readily checks that:

$$xAy^T = uv^T, \; xAx^T = uAu^T, \; yAy^T = vA^{-1}v^T .$$

Thus the desired inequality (14) follows from (ii) - Theorem 1. Now if (14) is actually an equation, then from Lemma 1, using x, y as defined in (15), we get u, vA^{-1} are linearly dependent. The converse also follows readily.

q. e. d.

Note: The condition of equality in (14) is directly connected with characteristic vectors of A (and of course, those of A^{-1}), for suppose (14) is an equation and $u = v \neq 0$, then one sees immediately that $uA = \lambda u$ for some real number λ. The corresponding converse also holds in this case.

An iterative scheme, for deciding the definiteness of A, based on the proof of Theorem 3 might go as follows:

(a) By examining the diagonal elements of A we have decided that, if at all, A is p. s. d.

(b) We have an x such that $xA \neq 0$; if $xA^2x \leq 0$ then A is not p.s.d., if $xA^2x > 0$ normalize x so that $xA^2x = 1$ and proceed to (c)

(c) We have an x such that $xA \neq 0$, $xA^2x = 1$; perform the transformation given by (8) and (9). There are three cases:

Case 1. if $yAy^T > xAx^T$ then A is not p.s.d.

Case 2. if $yAy^T < xAx^T$ return to beginning of (c), using y as the new "test" vector.

Case 3. if $yAy^T = xAx^T$ we have isolated a characteristic vector of A, return to (b) using, as x, a vector independent of all characteristic vectors thus far obtained.

The preceding is, of course, "informal" in the sense that the iterative procedure described above has not been shown to coverge.

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