What Is a Symmetric Positive Definite Matrix?

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July 21, 2020

A real $n \times n$ matrix A is symmetric positive definite if it is symmetric (A is equal to its transpose, A^T) and

$$x^T A x > 0 \quad \text{for all nonzero vectors } x.$$

By making particular choices of x in this definition we can derive the inequalities

$$\begin{aligned} a_{ii} &> 0 && \text{for all } i, \\ a_{ij} &< \sqrt{a_{ii} a_{jj}} && \text{for all } i \neq j. \end{aligned}$$

Satisfying these inequalities is not sufficient for positive definiteness. For example, the matrix

$$A = \begin{bmatrix} 1 & 3/4 & 0 \\ 3/4 & 1 & 3/4 \\ 0 & 3/4 & 1 \end{bmatrix}$$

satisfies all the inequalities but $x^T A x < 0$ for $x = [1, \ -\sqrt{2}, \ 1]^T$.

A sufficient condition for a symmetric matrix to be positive definite is that it has positive diagonal elements and is diagonally dominant, that is, $a_{ii} > \sum_{j \neq i} |a_{ij}|$ for all i.

The definition requires the positivity of the quadratic form $x^T A x$. Sometimes this condition can be confirmed from the definition of A. For example, if $A = B^T B$ and B has linearly independent columns then $x^T A x = (Bx)^T Bx > 0$ for $x \neq 0$. Generally, though, this condition is not easy to check.

Two equivalent conditions to A being symmetric positive definite are
- every leading principal minor $\det(A_k)$, where the submatrix $A_k = A(1\colon k, 1\colon k)$ comprises the intersection of rows and columns 1 to k, is positive,
- the eigenvalues of A are all positive.

The first condition implies, in particular, that $\det(A) > 0$, which also follows from the second condition since the determinant is the product of the eigenvalues.

Here are some other important properties of symmetric positive definite matrices.
- A^{-1} is positive definite.
- A has a unique symmetric positive definite square root X, where a square root is a matrix X such that $X^2 = A$.
- A has a unique Cholesky factorization $A = R^T R$, where R is upper triangular with positive diagonal elements.

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Sources of positive definite matrices include statistics, since nonsingular correlation matrices and covariance matrices are symmetric positive definite, and finite element and finite difference discretizations of differential equations.

Examples of symmetric positive definite matrices, of which we display only the 4×4 instances, are the Hilbert matrix

$$H_4 = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} \\ \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{7} \end{bmatrix},$$

the Pascal matrix

$$P_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 \\ 1 & 3 & 6 & 10 \\ 1 & 4 & 10 & 20 \end{bmatrix},$$

and minus the second difference matrix, which is the tridiagonal matrix

$$S_4 = \begin{bmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & -1 & 2 & -1 \\ & & -1 & 2 \end{bmatrix}.$$

All three of these matrices have the property that a_{ij} is non-decreasing along the diagonals. However, if A is positive definite then so is $P^T AP$ for any permutation matrix P, so any symmetric reordering of the row or columns is possible without changing the definiteness.

A 4×4 symmetric positive definite matrix that was often used as a test matrix in the early days of digital computing is the Wilson matrix

$$W = \begin{bmatrix} 5 & 7 & 6 & 5 \\ 7 & 10 & 8 & 7 \\ 6 & 8 & 10 & 9 \\ 5 & 7 & 9 & 10 \end{bmatrix}.$$

What is the best way to test numerically whether a symmetric matrix is positive definite? Computing the eigenvalues and checking their positivity is reliable, but slow. The fastest method is to attempt to compute a Cholesky factorization and declare the matrix positivite definite if the factorization succeeds. This is a reliable test even in floating-point arithmetic. If the matrix is not positive definite the factorization typically breaks down in the early stages so and gives a quick negative answer.

Symmetric block matrices

$$C = \begin{bmatrix} A & X \\ X^T & B \end{bmatrix}$$

often appear in applications. If A is nonsingular then we can write

$$\begin{bmatrix} A & X \\ X^T & B \end{bmatrix} = \begin{bmatrix} I & 0 \\ X^T A^{-1} & I \end{bmatrix} \begin{bmatrix} A & 0 \\ 0 & B - X^T A^{-1} X \end{bmatrix} \begin{bmatrix} I & A^{-1} X \\ 0 & I \end{bmatrix},$$

which shows that C is congruent to a block diagonal matrix, which is positive definite when its diagonal blocks are. It follows that C is positive definite if and only if both A and $B - X^T A^{-1} X$ are positive definite. The matrix $B - X^T A^{-1} X$ is called the Schur complement of A in C.

We mention two determinantal inequalities. If the block matrix C above is positive definite then $\det(C) \leq \det(A) \det(B)$ (Fischer's inequality). Applying this inequality recursively gives Hadamard's inequality for a symmetric positive definite A:

$$\det(A) \leq a_{11} a_{22} \ldots a_{nn},$$

with equality if and only if A is diagonal.

Finally, we note that if $x^T A x \geq 0$ for all $x \neq 0$, so that the quadratic form is allowed to be zero, then the symmetric matrix A is called symmetric positive semidefinite. Some, but not all, of the properties above generalize in a natural way. An important difference is that semidefinitness is equivalent to all principal minors, of which there are 2^{n-1}, being nonnegative; it is not enough to check the n leading principal minors. Consider, as an example, the matrix

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

which has leading principal minors 1, 0, and 0 and a negative eigenvalue.

A complex $n \times n$ matrix A is Hermitian positive definite if it is Hermitian (A is equal to its conjugate transpose, A^*) and $x^* A x > 0$ for all nonzero vectors x. Everything we have said above generalizes to the complex case.

References

This is a minimal set of references, which contain further useful references within.

- Rajendra Bhatia, Positive Definite Matrices, Princeton University Press, Princeton, NJ, USA, 2007.
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- Roger A. Horn and Charles R. Johnson, Matrix Analysis, second edition, Cambridge University Press, 2013. My review of the second edition.

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