Linear Algebra

Positive Definite Matrix

Source: Introduction to linear algebra by Gilbert Strang

This section concentrates on ***symmetric matrices that have positive eigenvalues***. If symmetry makes a matrix important, this extra property (*all* $\lambda > 0$) makes it special. When we say special, we don't mean rare. Symmetric matrices with positive eigenvalues enter all kinds of applications of linear algebra. They are called ***positive definite***.

The first problem is to recognize these matrices. You may say, just find the eigenvalues and test $\lambda > 0$. That is exactly what we want to avoid. Calculating eigenvalues is work. When the λ's are needed, we can compute them. But if we just want to know that they are positive, there are faster ways. Here are the two goals of this section:

Start with 2 by 2. When does $A = \begin{bmatrix} a & b \\ b & c \end{bmatrix}$ ***have*** $\lambda_1 > 0$ ***and*** $\lambda_2 > 0$?

6L ***The eigenvalues of A are positive if and only if*** $a > 0$ ***and*** $ac - b^2 > 0$.

$A = \begin{bmatrix} 4 & 5 \\ 5 & 7 \end{bmatrix}$ has $a = 4$ and $ac - b^2 = 28 - 25 = 3$. So A has positive eigenvalues. The test is failed by $\begin{bmatrix} 4 & 5 \\ 5 & 6 \end{bmatrix}$ and also failed by $\begin{bmatrix} -1 & 0 \\ 0 & -7 \end{bmatrix}$. One failure is because the determinant is $24 - 25 < 0$. The other failure is because $a = -1$. The determinant of $+7$ is not enough to pass, because the test has *two parts*: the 1 by 1 determinant a and the 2 by 2 determinant.

Proof of the 2 by 2 tests: If $\lambda_1 > 0$ and $\lambda_2 > 0$, then their product $\lambda_1\lambda_2$ and sum $\lambda_1 + \lambda_2$ are positive. Their product is the determinant so $ac - b^2 > 0$. Their sum is the trace so $a + c > 0$. Then a and c are both positive (if one were not positive then $ac - b^2 > 0$ would have failed).

6M ***The eigenvalues of $A = A^T$ are positive if and only if the pivots are positive:***

$$a > 0 \qquad \text{and} \qquad \frac{ac - b^2}{a} > 0.$$

Example 1 This matrix has $a = 1$ (positive). But $ac - b^2 = 3 - 2^2$ is negative:

$$\begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix} \quad \text{has a negative determinant and pivot. So a } \textbf{negative eigenvalue}.$$

The pivots are 1 and -1. The eigenvalues also multiply to give -1. One eigenvalue is negative (we don't want its formula, which has a square root, just its sign).

Definition The matrix A is ***positive definite*** if $\boldsymbol{x}^{\mathrm{T}} A \boldsymbol{x} > 0$ for every nonzero vector:

$$\boldsymbol{x}^{\mathrm{T}} A \boldsymbol{x} = \begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} a & b \\ b & c \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = ax^2 + 2bxy + cy^2 > 0.$$

$\boldsymbol{x}^{\mathrm{T}} A \boldsymbol{x}$ is a number (1 by 1 matrix). The four entries a, b, b, c give the four parts of $\boldsymbol{x}^{\mathrm{T}} A \boldsymbol{x}$. From a and c come the pure squares ax^2 and cy^2. From b and b off the diagonal come the cross terms bxy and byx (the same). Adding those four parts gives $\boldsymbol{x}^{\mathrm{T}} A \boldsymbol{x}$:

$$f(x, y) = \boldsymbol{x}^{\mathrm{T}} A \boldsymbol{x} = ax^2 + 2bxy + cy^2 \quad \text{is “second degree.”}$$

$$\frac{\partial f}{\partial x} = 2ax + 2by \qquad \frac{\partial f}{\partial y} = 2bx + 2cy \quad \text{and} \quad \begin{bmatrix} \dfrac{\partial^2 f}{\partial x^2} & \dfrac{\partial^2 f}{\partial y \partial x} \\ \dfrac{\partial^2 f}{\partial x \partial y} & \dfrac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 2a & 2b \\ 2b & 2c \end{bmatrix} = 2A.$$

For a two-variable function $f(x, y)$, the *matrix of second derivatives* holds the key. One number is not enough to decide minimum versus maximum (versus saddle point). ***The function*** $f = \boldsymbol{x}^{\mathrm{T}} A\boldsymbol{x}$ ***has a minimum at*** $x = y = 0$ ***if and only if*** A ***is positive definite***. The statement "A is a positive definite matrix" is the 2 by 2 version of "a is a positive number".

Example 2 This matrix A is positive definite. We test by pivots or determinants:

$$A = \begin{bmatrix} 1 & 2 \\ 2 & 7 \end{bmatrix} \quad \text{has positive pivots and determinants (1 and 3).}$$

More directly, $\boldsymbol{x}^{\mathrm{T}} A\boldsymbol{x} = x^2 + 4xy + 7y^2$ is positive because it is a **sum of squares**:

$$\text{Rewrite} \quad x^2 + 4xy + 7y^2 \quad \text{as} \quad (x + 2y)^2 + 3y^2.$$

The pivots 1 and 3 multiply those squares. This is no accident! By the algebra of "completing the square," this always happens. So when the pivots are positive, the quadratic function $f(x, y) = \boldsymbol{x}^{\mathrm{T}} A\boldsymbol{x}$ is guaranteed to be positive: a sum of squares.

6N When a 2 by 2 symmetric matrix has one of these four properties, it has them all:

1. Both of the eigenvalues are positive.

2. The 1 by 1 and 2 by 2 determinants are positive: $a > 0$ and $ac - b^2 > 0$.

3. The pivots are positive: $a > 0$ and $(ac - b^2)/a > 0$.

4. The function $x^{\mathrm{T}}Ax = ax^2 + 2bxy + cy^2$ is positive except at $(0, 0)$.

Note We deal only with symmetric matrices. The cross derivative $\partial^2 f/\partial x \partial y$ always equals $\partial^2 f/\partial y \partial x$. For $f(x, y, z)$ the nine second derivatives fill a symmetric 3 by 3 matrix. It is positive definite when the three pivots (and the three eigenvalues, and the three determinants) are positive. **When the first derivatives $\partial f/\partial x$ and $\partial f/\partial y$ are zero and the second derivative matrix is positive definite, we have found a local minimum.**

Example 3 Is $f(x, y) = x^2 + 8xy + 3y^2$ everywhere positive—except at $(0, 0)$?

Solution The second derivatives are $f_{xx} = 2$ and $f_{xy} = f_{yx} = 8$ and $f_{yy} = 6$, all positive. But the test is not positive derivatives. We look for positive *definiteness*. The answer is *no*, this function is not always positive. By trial and error we locate a point $x = 1$, $y = -1$ where $f(1, -1) = 1 - 8 + 3 = -4$. Better to do linear algebra, and apply the exact tests to the matrix that produced $f(x, y)$:

$$x^2 + 8xy + 3y^2 = \begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} 1 & 4 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}.$$

The matrix has $ac - b^2 = 3 - 16$. The pivots are 1 and -13. The eigenvalues are _____ (we don't need them). The matrix is not positive definite.

Example 4 For which numbers c is $x^2 + 8xy + cy^2$ always positive (or zero)?

Solution The matrix is $A = \left[\begin{smallmatrix} 1 & 4 \\ 4 & c \end{smallmatrix}\right]$. Again $a = 1$ passes the first test. The second test has $ac - b^2 = c - 16$. For a positive definite matrix we need $c > 16$.

Example 5 When A is positive definite, write $f(x, y)$ as a sum of two squares.

Solution This is called "completing the square." The part $ax^2 + 2bxy$ is correct in the first square $a\left(x + \frac{b}{a}y\right)^2$. But that ends with a final $a\left(\frac{b}{a}y\right)^2$. To stay even, this added amount b^2y^2/a has to be subtracted off from cy^2 at the end:

Completing the Square
$$ax^2 + 2bxy + cy^2 = a\left(x + \frac{b}{a}y\right)^2 + \left(\frac{ac - b^2}{a}\right)y^2. \qquad (1)$$

After that gentle touch of algebra, the situation is clearer. The two squares (never negative) are multiplied by numbers that could be positive or negative. *Those numbers a and $(ac - b^2)/a$ are the pivots!* So positive pivots give a sum of squares and a positive definite matrix. Think back to the pivots and multipliers in LDL^{T}:

$$A = \begin{bmatrix} a & b \\ b & c \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ b/a & 1 \end{bmatrix} \begin{bmatrix} a & \\ & (ac - b^2)/a \end{bmatrix} \begin{bmatrix} 1 & b/a \\ 0 & 1 \end{bmatrix}. \qquad (2)$$

To complete the square, we started with a and b. *Elimination does exactly the same.* It starts with the first column. Inside $\left(x + \frac{b}{a}y\right)^2$ are the numbers 1 and $\frac{b}{a}$ from L.

Every positive definite symmetric matrix factors into $A = LDL^T$ with positive pivots in D. The "Cholesky factorization" is $A = (L\sqrt{D})(L\sqrt{D})^T$.

6O When a symmetric matrix has one of these four properties, it has them all:

1. All n ***eigenvalues*** are positive.
2. All n ***upper left determinants*** are positive.
3. All n ***pivots*** are positive.
4. $x^T A x$ is positive except at $x = 0$. The matrix A is ***positive definite***.

Example 6 Test these matrices A and A^* for positive definiteness:

$$A = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} \quad \text{and} \quad A^* = \begin{bmatrix} 2 & -1 & b \\ -1 & 2 & -1 \\ b & -1 & 2 \end{bmatrix}.$$

Solution This A is an old friend (or enemy). Its pivots are 2 and $\frac{3}{2}$ and $\frac{4}{3}$, all positive. Its upper left determinants are 2 and 3 and 4, all positive. Its eigenvalues are $2 - \sqrt{2}$ and 2 and $2 + \sqrt{2}$, all positive. That completes tests **1**, **2**, and **3**.

We can write $\boldsymbol{x}^{\mathrm{T}} A \boldsymbol{x}$ as a sum of *three* squares (since $n = 3$). The pivots 2, $\frac{3}{2}$, $\frac{4}{3}$ appear outside the squares. The multipliers $-\frac{1}{2}$ and $-\frac{2}{3}$ in L are inside the squares:

$$\begin{aligned} \boldsymbol{x}^{\mathrm{T}} A \boldsymbol{x} &= 2(x_1^2 - x_1 x_2 + x_2^2 - x_2 x_3 + x_3^2) \\ &= 2\left(x_1 - \tfrac{1}{2}x_2\right)^2 + \tfrac{3}{2}\left(x_2 - \tfrac{2}{3}x_3\right)^2 + \tfrac{4}{3}(x_3)^2 > 0. \qquad \textbf{This is positive.} \end{aligned}$$

Go to the second matrix A^*. *The determinant test is easiest.* The 1 by 1 determinant is 2, the 2 by 2 determinant is 3. The 3 by 3 determinant comes from the whole A^*:

$$\det A^* = 4 + 2b - 2b^2 = (1 + b)(4 - 2b) \quad \text{must be positive.}$$

At $b = -1$ and $b = 2$ we get $\det A^* = 0$. In those cases A^* is positive *semi*definite (no inverse, zero eigenvalue, $\boldsymbol{x}^{\mathrm{T}} A^* \boldsymbol{x} \geq 0$). *Between $b = -1$ and $b = 2$ the matrix is positive definite.* The corner entry $b = 0$ in the first matrix A was safely between.