Positive Definite Matrices (正定矩阵)

Lecture 27

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Minima, Maxima, and Saddle Points

Minimum Point, Positive Definiteness

Questions:

1. Given a matrix, how could you determine the signs of the eigenvalues?
2. What test can guarantee that all of the eigenvalues of a matrix are positive?
3. How to find a minimum point efficiently? This arises throughout science and engineering and every problem of optimization. The mathematical problem is to move the second derivative test $F'' > 0$ into n dimensions.

Examples

Here are two examples:

$$F(x,y) = 7 + 2(x+y)^2 - y\sin y - x^3$$
$$f(x,y) = 2x^2 + 4xy + y^2$$

Does either $F(x,y)$ or $f(x,y)$ have a minimum at the point $x = y = 0$?

Remark 1

The zero-order terms $F(0,0) = 7$ and $f(0,0) = 0$ have no effect on the answer. They simply raise or lower the graphs of F and f.

The linear terms of F give a necessary condition:

To have any chance of a minimum, the first derivatives must vanish at $x = y = 0$:

$$\frac{\partial F}{\partial x} = 4(x+y) - 3x^2 = 0 \quad \text{and}$$
$$\frac{\partial F}{\partial y} = 4(x+y) - y\cos y - \sin y = 0$$

Remark 2

The linear terms of f give a necessary condition:

To have any chance of a minimum, the first derivatives must vanish at $x = y = 0$:

$$\frac{\partial f}{\partial x} = 4(x+y) = 0 \quad \text{and}$$
$$\frac{\partial f}{\partial y} = 4x - 2y = 0. \quad \textit{All zero.}$$

Thus $(x,y) = (0,0)$ is a stationary point for both functions. The surface $z = F(x,y)$ is tangent to the horizontal plane $z = 7$, and the surface $z = f(x,y)$ is tangent to the plane $z = 0$. The question is whether the graphs go above those planes or not, as we move away from the tangency point $x = y = 0$.

Remark 3

The second derivatives at $(0,0)$ are decisive:

$$\frac{\partial^2 F}{\partial x^2} = 4 - 6x = 4 \qquad \frac{\partial^2 f}{\partial x^2} = 4$$

$$\frac{\partial^2 F}{\partial x \partial y} = \frac{\partial^2 F}{\partial y \partial x} = 4 \qquad \frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x} = 4$$

$$\frac{\partial^2 F}{\partial y^2} = 4 + y\sin y - 2\cos y = 2 \qquad \frac{\partial^2 f}{\partial y^2} = 2.$$

These second derivatives $4,4,2$ contain the answer. Since they are the same for F and f, they must contain the same answer. The two functions behave in exactly the same way near the origin. F has a minimum if and only if f has a minimum. We are going to show that those functions don't!

Remark 4

For $F(x,y)$:

(a) The higher-degree terms in F have no effect on the question of a local minimum, but they can prevent it from being a global minimum.

(b) In our example the term $-x^3$ must sooner or later pull F toward $-\infty$.

For $f(x,y)$ with no higher terms, all the action is at $(0,0)$:

(a) Every quadratic form $f(x,y) = ax^2 + 2bxy + cy^2$ has a stationary point at the origin, where $\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y} = 0$.

(b) A local minimum would also be a global minimum.

(c) The surface $z = f(x,y)$ will then be shaped like a bowl, resting on the origin.

Positive Definiteness

(a) If the stationary point of F is at $x=\alpha, y=\beta$, the only change would be to use the second derivatives at (α,β):

$$f(x,y)=\frac{x^2}{2}\frac{\partial^2 F}{\partial x^2}(\alpha,\beta)+xy\frac{\partial^2 F}{\partial x\partial y}(\alpha,\beta)+\frac{y^2}{2}\frac{\partial^2 F}{\partial y^2}(\alpha,\beta)$$

(b) This $f(x,y)$ behaves near $(0,0)$ in the same way that $F(x,y)$ behaves near (α,β).

(c) The third derivatives are drawn into the problem when the second derivatives fail to give a definite decision. That happens when the quadratic part is singular.

(d) For a true minimum, f is allowed to vanish only at $x=0, y=0$. When $f(x,y)$ is strictly positive at all other points (the bowl goes up), it is called **positive definite**.

Figure 6.1

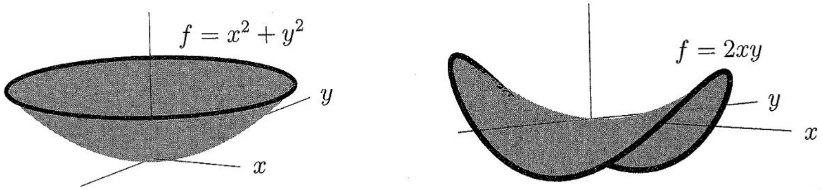

Figure 6.1: A bowl and a saddle: Definite $A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ and indefinite $A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$.

The problem comes down to this: For a function of two variables x and y, what is the correct replacement for the condition $\frac{\partial^2 F}{\partial x^2} > 0$? With only one variable, the sign of the second derivative decides between a minimum or a maximum. Now we have three derivatives: $F_{xx}, F_{xy} = F_{yx}, F_{yy}$. These three numbers must determine whether or not F has a minimum.

Examples

Example 1 $f(x,y)=x^2-10xy+y^2$. Here $a=1$ and $c=1$ are both positive. But f is not positive definite, because $f(1,1)=-8$. The conditions $a>0$ and $c>0$ ensure that $f(x,y)$ is positive on the x and y axes. But this function is negative on the line $x=y$, because $b=-10$ overwhelms a and c.

Example 2 In our original f the coefficient $2b=4$ was positive. Does this ensure a minimum? Again the answer is no; the sign of b is of no importance! Even though its second derivatives are positive, $2x^2+4xy+y^2$ is not positive definite. Neither F nor f has a minimum at $(0,0)$ because $f(1,-1)=2-4+1=-1$. It is the size of b, compared to a and c, that must be controlled.

General requirements

1. It is the size of b, compared to a and c, that must be controlled. We now want a necessary and sufficient condition for positive definiteness.
2. The simplest technique is to complete the square:

$$f(x,y) = ax^2 + 2bxy + cy^2 = a\left(x + \frac{b}{a}y\right)^2 + \left(c - \frac{b^2}{a}\right)y^2 \tag{1}$$

   The first term on the right is never negative, when the square is multiplied by $a > 0$. But this square term must then be positive. That term has coefficient $\frac{ac-b^2}{a}$.
3. The last requirement for positive definiteness is that this coefficient must be positive:

   If $ax^2 + 2bxy + cy^2$ stays positive, then necessarily $ac > b^2$.

Test for a minimum

The conditions $a > 0$ and $ac > b^2$ are just right. They guarantee $c > 0$. The right side of (1) is positive, and we have found a minimum.

Theorem

$ax^2 + 2bxy + cy^2$ is positive definite if and only if $a > 0$ and $ac > b^2$. Any $F(x,y)$ has a minimum at a point (α,β) where $\frac{\partial F}{\partial x}(\alpha,\beta) = \frac{\partial F}{\partial y}(\alpha,\beta) = 0$ with

$$\frac{\partial^2 F}{\partial x^2}(\alpha,\beta) > 0 \text{ and } \left[\frac{\partial^2 F}{\partial x^2}(\alpha,\beta)\right]\left[\frac{\partial^2 F}{\partial y^2}(\alpha,\beta)\right] > \left[\frac{\partial^2 F}{\partial x \partial y}(\alpha,\beta)\right]^2$$

Here

$$a = \frac{1}{2}\frac{\partial^2 F}{\partial x^2}(\alpha,\beta),\ b = \frac{1}{2}\frac{\partial^2 F}{\partial x \partial y}(\alpha,\beta),\ c = \frac{1}{2}\frac{\partial^2 F}{\partial y^2}(\alpha,\beta).$$

Test for a Maximum

Since f has a maximum whenever $-f$ has a minimum, we just reverse the signs of a, b, and c.

- This actually leaves $ac > b^2$ unchanged: The quadratic form is negative definite if and only if $a < 0$ and $ac > b^2$.
- The same change applies for a maximum of $F(x, y)$.

Singular case $ac = b^2$

(a) The second term in equation

$$f(x,y) = ax^2 + 2bxy + cy^2 = a\left(x + \frac{b}{a}y\right)^2 + \left(c - \frac{b^2}{a}\right)y^2$$

disappears to leave the first square–which is either positive semidefinite, when $a > 0$, or negative semidefinite, when $a < 0$.

(b) The prefix semi allows the possibility that f can equal zero, as it will at the point $x = b, y = -a$.

(c) The surface $z = f(x,y)$ degenerates from a bowl into a valley. For $f = (x+y)^2$, the valley runs along the line $x + y = 0$.

Saddle point

(a) In one dimension, $F(x)$ has a minimum or a maximum, or $F'' = 0$.

(b) In two dimensions, a very important possibility still remains: The combination $ac - b^2$ may be negative. This occurred in both examples, when b dominated a and c. It also occurs if a and c have opposite signs. Then two directions give opposite results–in one direction f increases, in the other it decreases.

(c) It is useful to consider two special cases:

$$f_1(x,y) = 2xy \quad \text{and} \quad f_2(x,y) = x^2 - y^2$$

Saddle points at $(0,0)$.

(d) The saddles $2xy$ and $x^2 - y^2$ are practically the same; if we turn one through 45° we get the other. They are also hard to draw.

Quadratic Forms

For any symmetric matrix A, the product $x^T Ax$ is a pure **quadratic form** $f(x_1, x_2, \cdots, x_n)$:

$$x^T Ax = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ . & . & . & . \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} x_i x_j$$

There are no higher-order terms or lower-order terms-only second-order. The function is zero at $x = (0, \cdots, 0)$, and its first derivatives are zero.

Examples

Example 3 $f = 2x^2 + 4xy + y^2$ and $A = \begin{bmatrix} 2 & 2 \\ 2 & 1 \end{bmatrix} \rightarrow$ saddle point.

Example 4 $f = 2xy$ and $A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \rightarrow$ saddle point.

Example 5 A is 3 by 3 for $2x_1^2 - 2x_1x_2 + 2x_2^2 - 2x_2x_3 + 2x_3^2$:

$$f = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

f has a minimum at $(0,0,0)$.

Test for positive definiteness

For function $F(x_1, x_2, \cdots, x_n)$: F has a minimum when the pure quadratic $x^T Ax$ is positive definite. These second-order terms control F near the stationary point:

$$F(x) = F(0) + x^T(\text{grad } F) + \frac{1}{2}x^T Ax + \text{higher order terms}$$

The next section contains the tests to decide whether $x^T Ax$ is positive (the bowl goes up from $x = 0$). Equivalently, the tests decide whether the matrix A is positive definite–which is the main goal of the chapter.

Homework Assignment 27

6.1: 1, 4, 5, 7, 11, 13, 17, 21, 22.