

QUADRATIC FORMS AND DEFINITE MATRICES

1. DEFINITION AND CLASSIFICATION OF QUADRATIC FORMS

1.1. Definition of a quadratic form. Let A denote an $n \times n$ symmetric matrix with real entries and let x denote an $n \times 1$ column vector. Then $Q = x'Ax$ is said to be a *quadratic form*. Note that

$$\begin{aligned}
 Q = x'Ax &= (x_1 \dots x_n) \begin{pmatrix} a_{11} & \cdots & a_{1n} \\ & \ddots & \\ a_{n1} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \\
 &= (x_1, x_2, \dots, x_n) \begin{pmatrix} \sum a_{1i}x_i \\ \vdots \\ \sum a_{ni}x_i \end{pmatrix} \\
 &= a_{11}x_1^2 + a_{12}x_1x_2 + \dots + a_{1n}x_1x_n \\
 &\quad + a_{21}x_2x_1 + a_{22}x_2^2 + \dots + a_{2n}x_2x_n \\
 &\quad + \dots \\
 &\quad + \dots \\
 &\quad + \dots \\
 &\quad + a_{n1}x_nx_1 + a_{n2}x_nx_2 + \dots + a_{nn}x_n^2 \\
 &= \sum_{i \leq j} a_{ij}x_i x_j
 \end{aligned} \tag{1}$$

For example, consider the matrix

$$A = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$$

and the vector x . Q is given by

$$\begin{aligned}
 Q = x'Ax &= [x_1 \ x_2] \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\
 &= [x_1 + 2x_2 \ 2x_1 + x_2] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\
 &= x_1^2 + 2x_1x_2 + 2x_1x_2 + x_2^2 \\
 &= x_1^2 + 4x_1x_2 + x_2^2
 \end{aligned}$$

1.2. Classification of the quadratic form $Q = x'Ax$: A quadratic form is said to be:

- a:** negative definite: $Q < 0$ when $x \neq 0$
- b:** negative semidefinite: $Q \leq 0$ for all x and $Q = 0$ for some $x \neq 0$
- c:** positive definite: $Q > 0$ when $x \neq 0$
- d:** positive semidefinite: $Q \geq 0$ for all x and $Q = 0$ for some $x \neq 0$
- e:** indefinite: $Q > 0$ for some x and $Q < 0$ for some other x

Consider as an example the 3x3 diagonal matrix D below and a general 3 element vector x.

$$D = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{bmatrix}$$

The general quadratic form is given by

$$\begin{aligned} Q &= x'Ax = [x_1 \ x_2 \ x_3] \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \\ &= [x_1 \ 2x_2 \ 4x_3] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \\ &= x_1^2 + 2x_2^2 + 4x_3^2 \end{aligned}$$

Note that for any real vector $x \neq 0$, that Q will be positive, because the square of any number is positive, the coefficients of the squared terms are positive and the sum of positive numbers is always positive. Also consider the following matrix.

$$E = \begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$

The general quadratic form is given by

$$\begin{aligned} Q &= x'Ax = [x_1 \ x_2 \ x_3] \begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 0 \\ 0 & 0 & -2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \\ &= [-2x_1 + x_2 \ x_1 - 2x_2 - 2x_3] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \\ &= -2x_1^2 + x_1x_2 + x_1x_2 - 2x_2^2 - 2x_3^2 \\ &= -2x_1^2 + 2x_1x_2 - 2x_2^2 - 2x_3^2 \\ &= -2[x_1^2 - x_1x_2] - 2x_2^2 - 2x_3^2 \\ &= -2x_1^2 - 2[x_2^2 - x_1x_2] - 2x_3^2 \end{aligned}$$

Note that independent of the value of x_3 , this will be negative if x_1 and x_2 are of opposite sign or equal to one another. Now consider the case where $|x_1| > |x_2|$. Write Q as

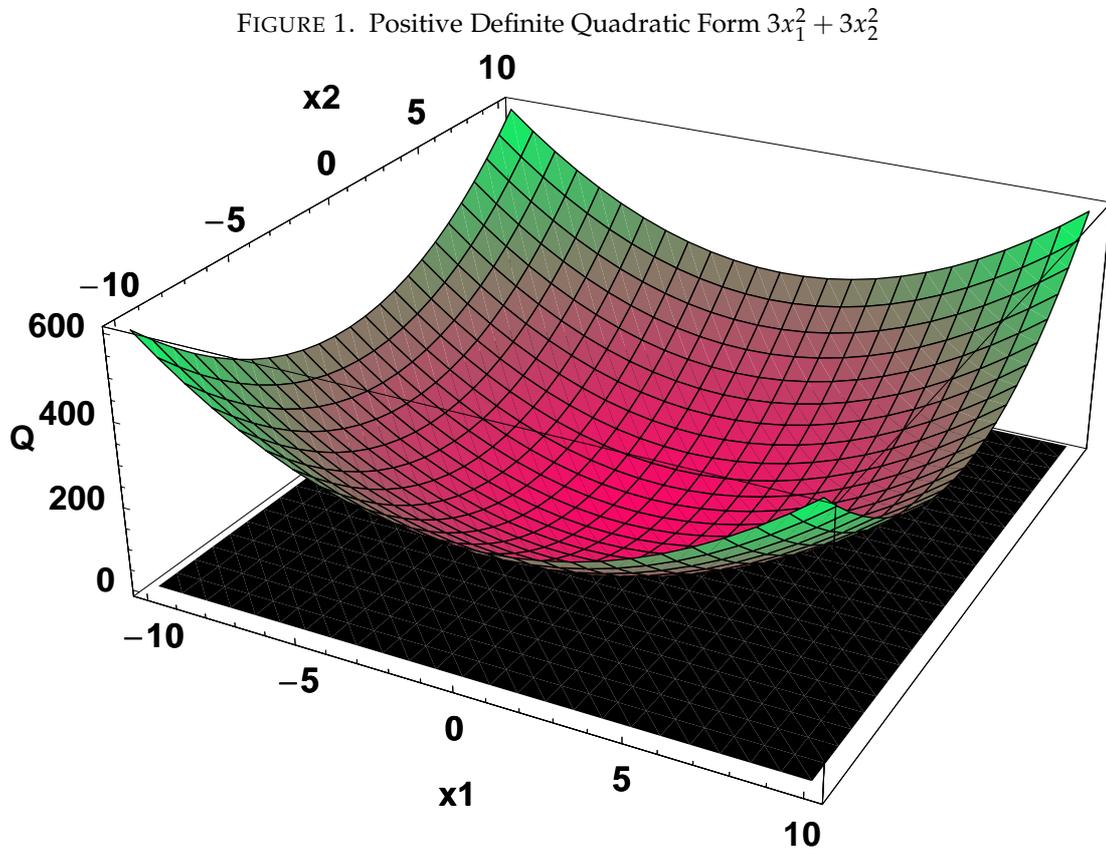
$$Q = -2x_1^2 + 2x_1x_2 - 2x_2^2 - 2x_3^2$$

The first, third, and fourth terms are clearly negative. But with $|x_1| > |x_2|$, $|2x_1^2| > |2x_1x_2|$ so that the first term is more negative than the second term is positive, and so the whole expression is negative. Now consider the case where $|x_1| < |x_2|$. Write Q as

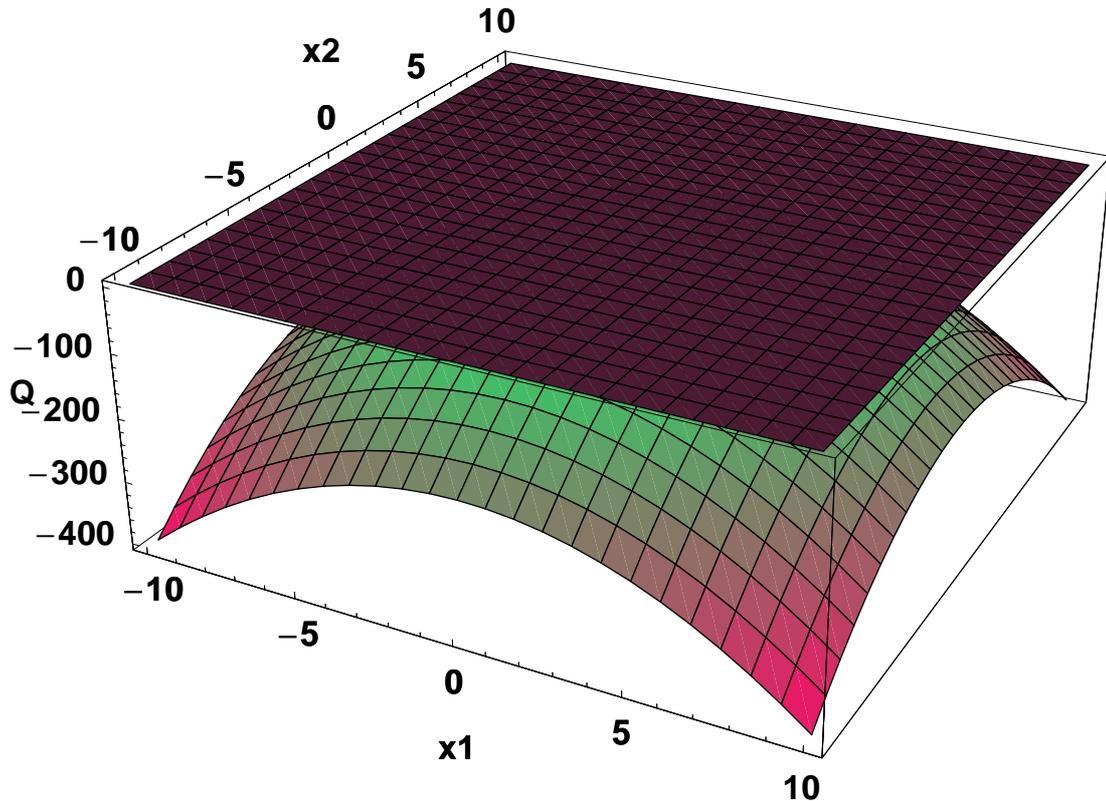
$$Q = -2x_1^2 + 2x_1x_2 - 2x_2^2 - 2x_3^2$$

The first, third, and fourth terms are clearly negative. But with $|x_1| < |x_2|$, $|2x_2^2| > |2x_1x_2|$ so that the third term is more negative than the second term is positive, and so the whole expression is negative. Thus this quadratic form is negative definite for any and all real values of $x \neq 0$.

1.3. **Graphical analysis.** When x has only two elements, we can graphically represent Q in 3 dimensions. A positive definite quadratic form will always be positive except at the point where $x = 0$. This gives a nice graphical representation where the plane at $x = 0$ bounds the function from below. Figure 1 shows a positive definite quadratic form.



Similarly, a negative definite quadratic form is bounded above by the plane $x = 0$. Figure 2 shows a negative definite quadratic form.

FIGURE 2. Negative Definite Quadratic Form $-2x_1^2 - 2x_2^2$ 

A positive semi-definite quadratic form is bounded below by the plane $x = 0$ but will touch the plane at more than the single point $(0,0)$, it will touch the plane along a line. Figure 3 shows a positive semi-definite quadratic form.

A negative semi-definite quadratic form is bounded above by the plane $x = 0$ but will touch the plane at more than the single point $(0,0)$. It will touch the plane along a line. Figure 4 shows a negative-definite quadratic form.

An indefinite quadratic form will not lie completely above or below the plane but will lie above for some values of x and below for other values of x . Figure 5 shows an indefinite quadratic form.

1.4. Note on symmetry. The matrix associated with a quadratic form B need not be symmetric. However, no loss of generality is obtained by assuming B is symmetric. We can always take definite and semidefinite matrices to be symmetric since they are defined by a quadratic form. Specifically consider a nonsymmetric matrix B and define A as $\frac{1}{2}(B + B')$, A is now symmetric and $x'Ax = x'Bx$.

2. DEFINITE AND SEMIDEFINITE MATRICES

2.1. Definitions of definite and semi-definite matrices. Let A be a square matrix of order n and let x be an n element vector. Then A is said to be positive semidefinite iff for all vectors x

FIGURE 3. Positive Semi-Definite Quadratic Form $2x_1^2 + 4x_1x_2 + 2x_2^2$

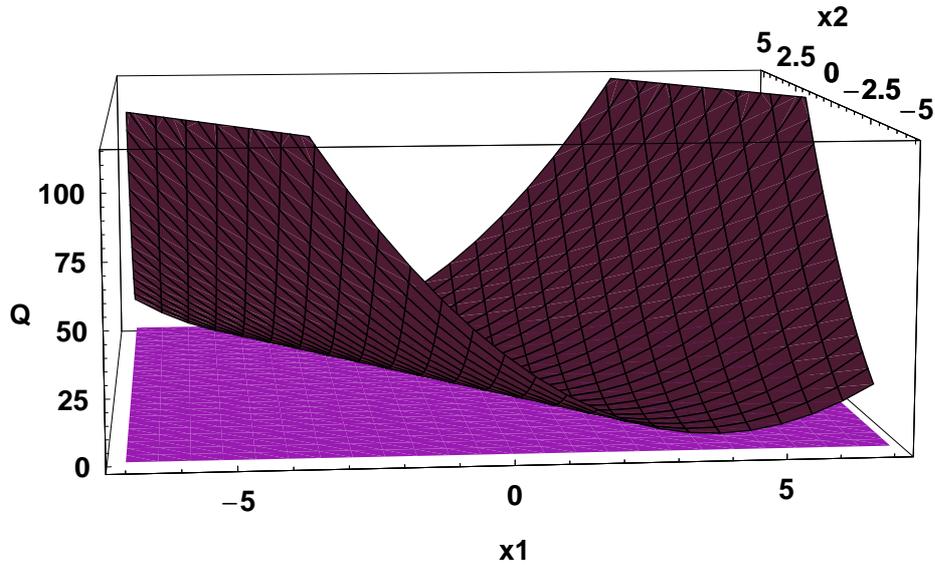
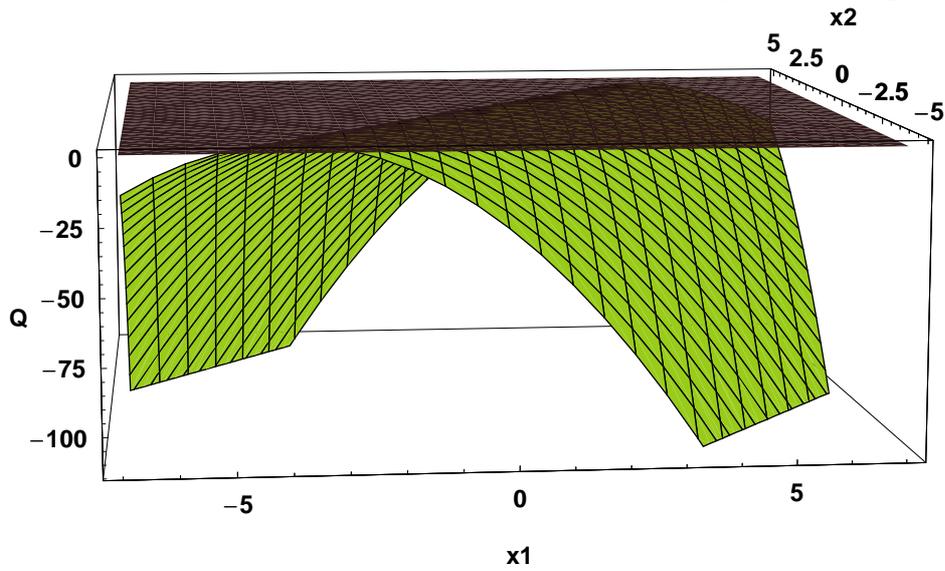


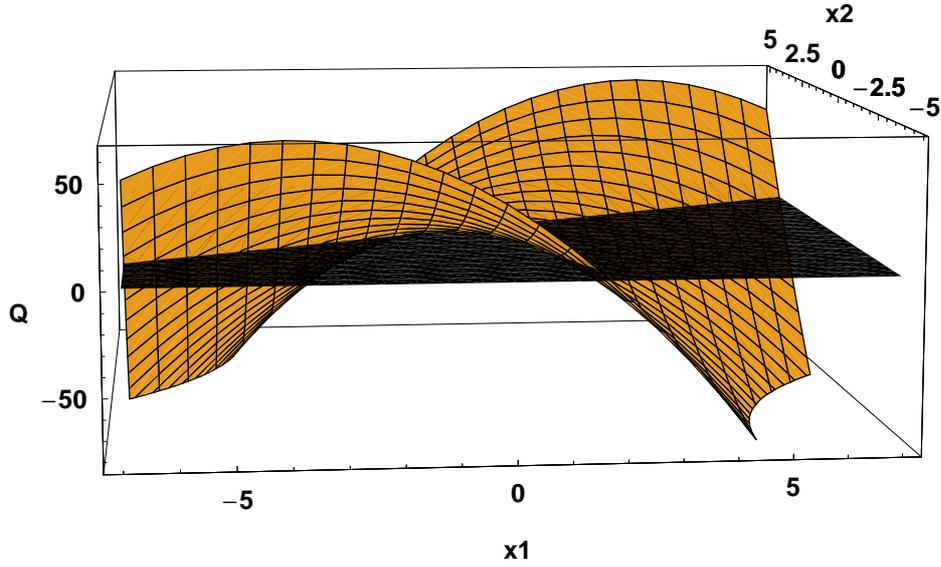
FIGURE 4. Negative Semi-Definite Quadratic Form $-2x_1^2 + 4x_1x_2 - 2x_2^2$



$$x'Ax \geq 0 \tag{2}$$

The matrix A is said to be positive definite if for non zero x

$$x'Ax > 0 \tag{3}$$

FIGURE 5. Indefinite Quadratic Form $-2x_1^2 + 4x_1x_2 + 2x_2^2$ 

Let A be a square matrix of order n . Then A is said to be negative (semi)definite iff $-A$ is positive (semi)definite.

2.2. Diagonal elements of positive definite matrices.

Theorem 1. Let A be a positive definite matrix of order m . Then

$$a_{ii} > 0, i = 1, 2, \dots, m.$$

If A is only positive semidefinite then

$$a_{ii} \geq 0, i = 1, 2, \dots, m.$$

Proof. Let e_i be the m -element vector all of whose elements are zeros save the i th, which is unity. For example if $m = 5$ and $i = 2$ then $e_2 = [0, 1, 0, 0, 0]$. If A is positive definite, because e_i is not the null vector, we must have

$$e_i' A e_i > 0, i = 1, 2, \dots, m. \quad (4)$$

But

$$e_i' A e_i = a_{ii}, i = 1, 2, \dots, m. \quad (5)$$

If A is positive semidefinite but *not* positive definite then repeating the argument above we find

$$a_{ii} = e_i' A e_i \geq 0, i = 1, 2, \dots, m. \quad (6)$$

2.3. Factoring positive definite matrices (Cholesky factorization).

Theorem 2. Let A be a positive definite matrix of order n . Then there exists a lower triangular matrix T such that

$$A = TT' \quad (7)$$

Proof. Define T as follows

$$T = \begin{bmatrix} t_{11} & 0 & 0 & \cdots & 0 \\ t_{21} & t_{22} & 0 & \cdots & 0 \\ t_{31} & t_{32} & t_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ t_{n1} & t_{n2} & t_{n3} & \cdots & t_{nn} \end{bmatrix} \quad (8)$$

Now define TT'

$$\begin{aligned} TT' &= \begin{bmatrix} t_{11} & 0 & 0 & \cdots & 0 \\ t_{21} & t_{22} & 0 & \cdots & 0 \\ t_{31} & t_{32} & t_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ t_{n1} & t_{n2} & t_{n3} & \cdots & t_{nn} \end{bmatrix} \begin{bmatrix} t_{11} & t_{21} & t_{31} & \cdots & t_{n1} \\ 0 & t_{22} & t_{32} & \cdots & t_{n2} \\ 0 & 0 & t_{33} & \cdots & t_{n3} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & t_{nn} \end{bmatrix} \\ &= \begin{bmatrix} t_{11}^2 & t_{11}t_{21} & t_{11}t_{31} & \cdots & t_{11}t_{n1} \\ t_{21}t_{11} & t_{21}^2 + t_{22}^2 & t_{21}t_{31} + t_{22}t_{32} & \cdots & t_{21}t_{n1} + t_{22}t_{n2} \\ t_{31}t_{11} & t_{31}t_{21} + t_{32}t_{22} & t_{31}^2 + t_{32}^2 + t_{33}^2 & \cdots & t_{31}t_{n1} + t_{32}t_{n2} + t_{33}t_{n3} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ t_{n1}t_{11} & t_{n1}t_{21} + t_{n2}t_{22} & t_{n1}t_{31} + t_{n2}t_{32} + t_{n3}t_{33} & \cdots & \sum_{i=1}^n t_{ni}^2 \end{bmatrix} \end{aligned} \quad (9)$$

Now define $A = TT'$ and compare like elements

$$\begin{aligned} A &= TT' \\ \Rightarrow \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} &= \begin{bmatrix} t_{11}^2 & t_{11}t_{21} & t_{11}t_{31} & \cdots & t_{11}t_{n1} \\ t_{21}t_{11} & t_{21}^2 + t_{22}^2 & t_{21}t_{31} + t_{22}t_{32} & \cdots & t_{21}t_{n1} + t_{22}t_{n2} \\ t_{31}t_{11} & t_{31}t_{21} + t_{32}t_{22} & t_{31}^2 + t_{32}^2 + t_{33}^2 & \cdots & t_{31}t_{n1} + t_{32}t_{n2} + t_{33}t_{n3} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ t_{n1}t_{11} & t_{n1}t_{21} + t_{n2}t_{22} & t_{n1}t_{31} + t_{n2}t_{32} + t_{n3}t_{33} & \cdots & \sum_{i=1}^n t_{ni}^2 \end{bmatrix} \end{aligned} \quad (10)$$

Solve the system now for each t_{ij} as functions of the a_{ij} . The system is obviously recursive because we can solve first for t_{11} , then t_{21} , etc. A schematic algorithm is given below.

$$\begin{aligned}
t_{11} &= \pm\sqrt{a_{11}}, t_{21} = \frac{a_{12}}{t_{11}}, t_{31} = \frac{a_{13}}{t_{11}}, \dots, t_{n1} = \frac{a_{1n}}{t_{11}} \\
t_{22} &= \pm\sqrt{a_{22} - \frac{a_{12}^2}{a_{11}}}, t_{32} = \frac{a_{23} - t_{21}t_{31}}{t_{22}}, \dots, t_{n2} = \frac{a_{2n} - t_{21}t_{n1}}{t_{22}} \\
t_{33} &= \pm\sqrt{a_{33} - t_{31}^2 - t_{32}^2} = \pm\sqrt{a_{33} - \frac{a_{13}^2}{a_{11}} - \left(\frac{a_{23} - t_{21}t_{31}}{t_{22}}\right)^2} \\
t_{43} &= \frac{a_{34} - t_{31}t_{41} - t_{32}t_{42}}{t_{33}}, \dots, t_{n3} = \frac{a_{3n} - t_{31}t_{n1} - t_{32}t_{n2}}{t_{33}}
\end{aligned} \tag{11}$$

This matrix is not unique because the square roots involve two roots. The standard procedure is to make the diagonal elements positive. Consider the following matrix as an example

$$F = \begin{bmatrix} 4 & 2 & 0 \\ 2 & 9 & 0 \\ 0 & 0 & 2 \end{bmatrix}.$$

We can factor it into the following matrix T

$$T = \begin{bmatrix} 2 & 0 & 0 \\ 1 & 2\sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \end{bmatrix}$$

and its transpose T' . Then $TT' = F$.

$$TT' = \begin{bmatrix} 2 & 0 & 0 \\ 1 & 2\sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \end{bmatrix} \begin{bmatrix} 2 & 1 & 0 \\ 0 & 2\sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \end{bmatrix} = \begin{bmatrix} 4 & 2 & 0 \\ 2 & 9 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

2.4. Characteristic roots of positive definite matrices.

Theorem 3. Let A be a symmetric matrix of order n . Let $\lambda_i, i=1, \dots, n$ be its characteristic roots. Then if A is positive definite, $\lambda_i > 0$, for all i .

Proof. Because A is symmetric, choose an orthonormal set of eigenvectors Q . Clearly $Q'AQ = \Lambda$, where Λ is a diagonal matrix with the eigenvalues of A on the diagonal. Now consider any one of the rows of Q' . This is one of the eigenvectors of A . Denote it by q'_i . Then clearly

$$q'_i A q_i = \lambda_i > 0 \tag{12}$$

2.5. Nonsingularity of positive definite matrices.

Theorem 4. Let A be a symmetric matrix of order n . If A is positive definite then $r(A) = n$.

Proof. Because A is symmetric, choose an orthonormal set of eigenvectors Q . Clearly $Q'AQ = \Lambda$, where Λ is a diagonal matrix with the eigenvalues of A on the diagonal. Because Q is orthogonal its inverse is its transpose and we also obtain that $AQ = Q\Lambda$. Now because A is positive definite, all the characteristic roots on the diagonal of Λ are positive. Thus the inverse of Λ is just a matrix with the reciprocal of each characteristic root on its diagonal. Thus Λ is invertible. Because $Q\Lambda$ is the product of two invertible matrices, it is invertible. Thus AQ is invertible, and because Q is invertible, this means A is invertible and of full rank. See Dhrymes [1, Proposition 2.61] or Horn and Johnson [4].

Theorem 5. *If A in the above theorem is merely positive semidefinite then $r(A) < n$.*

Proof. Because A is positive semidefinite, we know that $\lambda_i \geq 0, i = 1, 2, \dots, n$. The proof is based on showing that at least one of the roots is zero. We can diagonalize A as

$$Q' A Q = \Lambda. \tag{13}$$

Consequently, for any vector y ,

$$y' Q' A Q y = \sum_{i=1}^n \lambda_i y_i^2. \tag{14}$$

Now, if x is *any nonnull* vector, by the semidefiniteness of A we have

$$0 \leq x' A x = x' Q Q' A Q Q' x = x' Q \Lambda Q' x = \sum_{i=1}^n \lambda_i y_i^2, \tag{15}$$

where now we set

$$y = Q' x. \tag{16}$$

Because x is nonnull then y is also nonnull, because Q is orthogonal and thus non-singular.

If none of the λ_i is zero, 15 implies that for *any* nonnull x

$$x' A x > 0, \tag{17}$$

thus showing A to be positive definite. Consequently, at least one of the $\lambda_i, i = 1, 2, \dots, n$, must be zero and there must exist at least one nonnull x such that

$$x' A x = \sum_{i=1}^n \lambda_i y_i^2 = 0. \tag{18}$$

But this shows that

$$r(A) < n. \tag{19}$$

2.6. Factoring symmetric positive definite matrices.

Theorem 6. *Let A be a symmetric matrix, of order m . Then A is positive definite if and only if there exists a matrix S of dimension $n \times m$ and rank m ($n \geq m$) such that*

$$A = S' S.$$

It is positive semidefinite if and only if

$$r(S) < m.$$

Proof. (Dhrymes [1, Proposition 2.61] or Horn and Johnson [4]). If A is positive (semi)definite then, as in the proof of theorem 56, we have the representation

$$A = Q \Lambda Q'.$$

Here Q is an orthonormal set of eigenvectors and Λ is a diagonal matrix with the eigenvalues of A on the diagonal. Taking

$$S = \Lambda^{1/2} Q'$$

we have

$$A = S'S.$$

If A is positive definite, Λ is nonsingular and thus

$$r(S) = m.$$

If A is merely positive semidefinite then $r(\Lambda) < m$ and hence

$$r(S) < m.$$

This proves the first part of the theorem.

On the other hand suppose

$$A = S'S \tag{20}$$

and S is $n \times m$ matrix ($n \geq m$) of rank m . Let x be any nonnull vector and note

$$x'Ax = xS'Sx. \tag{21}$$

The right side of the equation above is a sum of squares and thus is zero if and only if

$$Sx = 0. \tag{22}$$

If the rank of S is m , equation 22 can be satisfied only with *null* x . Hence A is positive definite. So for any x

$$x'Ax = x'S'Sx \geq 0,$$

and if S is of rank less than m , there exists at least one nonnull x such that

$$Sx = 0.$$

Consequently, there exists at least one nonnull x such that

$$x'Ax = 0.$$

which shows that A is positive semidefinite but *not* positive definite.

2.7. Using naturally ordered principal minors to test for positive definiteness.

2.7.1. *Definition of naturally ordered (leading) principal minors.* The naturally ordered principal minors of a matrix A are defined as determinants of the matrices

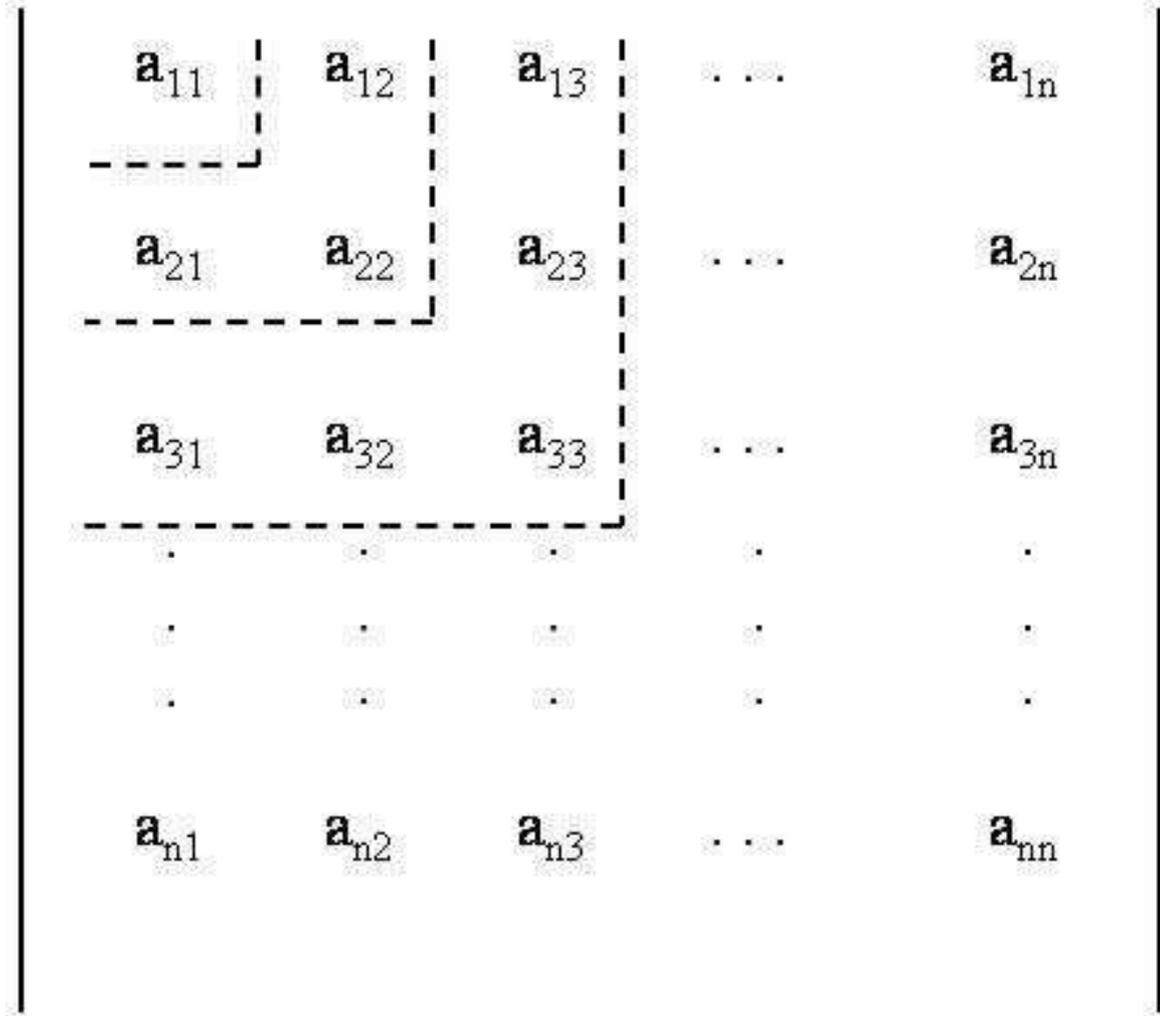
$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & & \vdots \\ a_{k1} & a_{k2} & \cdots & a_{kk} \end{bmatrix} \quad k = 1, 2, \dots, n. \tag{23}$$

A principal minor is the minor of a principal submatrix of A where a principal submatrix is a matrix formed from a square matrix A by taking a subset consisting of n rows and column elements from the same numbered columns. The natural ordering considers only those principal minors that fall along the main diagonal. Specifically for a matrix A , the naturally ordered principal minors are

$$a_{11}, \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}, \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}, \dots, \begin{vmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{vmatrix} \quad (24)$$

or schematically

FIGURE 6. Naturally Ordered Principle Minors of a Matrix



Theorem 7. Let A be a symmetric matrix of order m . Then A is positive definite iff its naturally ordered principal minors are all positive.

For a proof, see Gantmacher [2, p. 306] or Hadley [3, p. 260-262].

As an example consider the matrix $G1$.

$$G1 = \begin{bmatrix} 4 & 2 & 0 \\ 2 & 9 & 0 \\ 0 & 0 & 2 \end{bmatrix}.$$

Element $a_{11} = 4 > 0$. Now consider the first naturally occurring principal 2x2 submatrix

$$\begin{vmatrix} 4 & 2 \\ 2 & 9 \end{vmatrix} = 36 - 4 = 32 > 0.$$

Now consider the determinant of the entire matrix

$$\begin{vmatrix} 4 & 2 & 0 \\ 2 & 9 & 0 \\ 0 & 0 & 2 \end{vmatrix} = (4)(9)(2) + (2)(0)(0) + (2)(0)(0) - (9)(0)(0) - (2)(2)(2) - (4)(0)(0) = \\ = 72 + 0 + 0 - 0 - 8 - 0 = 64 > 0$$

This matrix is then positive definite.

2.8. Characteristic roots of positive semi-definite matrices. Let A be a symmetric matrix of order n . Let $\lambda_i, i=1, \dots, n$ be its characteristic roots. If A is positive semi-definite then

$$\lambda_i \geq 0 \quad i = 1, 2, \dots, n \text{ and at least one } \lambda_i = 0.$$

2.9. Using principal minors to test for positive definiteness and positive semidefiniteness.

2.9.1. Definition of principal minors. A principal minor of order r is defined as the determinant of a principal submatrix. A principal submatrix is defined as follows. If A is a matrix of order n , and we wipe out r of the rows and the corresponding r columns as well, the resulting $(n-r) \times (n-r)$ submatrix is called a principal submatrix of A . The determinant of this matrix is called a principal minor of A . Another way to write a principal minor of order p is

$$A \begin{pmatrix} i_1, i_2, i_3, \dots, i_p \\ i_1, i_2, i_3, \dots, i_p \end{pmatrix} = \begin{vmatrix} a_{i_1 i_1} & a_{i_1 i_2} & \cdots & a_{i_1 i_p} \\ a_{i_2 i_1} & a_{i_2 i_2} & \cdots & a_{i_2 i_p} \\ \vdots & \vdots & \ddots & \vdots \\ a_{i_p i_1} & a_{i_p i_2} & \cdots & a_{i_p i_p} \end{vmatrix} \quad (25)$$

Note: A matrix of order m has

$$\binom{m}{p}$$

principal minors of order p where

$$\binom{m}{p} = \frac{m!}{p!(m-p)!}.$$

For example a 4x4 matrix has 1 principal minor of order 4, (the matrix itself), 4 principal minors of order 3, 6 principle minors of order 2, and 4 principle minors of order 1 for a total of 15 principal minors.

As an example, consider the following matrix of order 3 which has 1 principal minor of order 3, 3 principal minors of order 2,

$$\binom{3}{2} = \frac{3!}{2!(3-2)!} = \frac{(3)(2)}{(1)(2)(1)(1)} = \frac{6}{2} = 3$$

and 3 principle minors of order 1 for a total of 7 principal minors.

$$G = \begin{bmatrix} 4 & 2 & 0 \\ 2 & 9 & 0 \\ 0 & 0 & 2 \end{bmatrix} .$$

$$\text{Order 3} \quad \left| \begin{array}{ccc} 4 & 2 & 0 \\ 2 & 9 & 0 \\ 0 & 0 & 2 \end{array} \right| .$$

$$\text{Order 2} \quad \left| \begin{array}{cc} 4 & 2 \\ 2 & 9 \end{array} \right| \quad \left| \begin{array}{cc} 4 & 0 \\ 0 & 2 \end{array} \right| \quad \left| \begin{array}{cc} 9 & 0 \\ 0 & 2 \end{array} \right|$$

$$\text{Order 1} \quad 4 \quad 2 \quad 9$$

Now consider the general 4x4 matrix A and some of its principal minors

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \quad A \binom{1 \ 2 \ 4}{1 \ 2 \ 4} = \begin{vmatrix} a_{11} & a_{12} & a_{14} \\ a_{21} & a_{22} & a_{24} \\ a_{41} & a_{42} & a_{44} \end{vmatrix} \quad (26)$$

$$A \binom{1 \ 3}{1 \ 3} = \begin{vmatrix} a_{11} & a_{13} \\ a_{31} & a_{33} \end{vmatrix} \quad A \binom{2 \ 4}{2 \ 4} = \begin{vmatrix} a_{22} & a_{24} \\ a_{42} & a_{44} \end{vmatrix} \quad A \binom{3}{3} = a_{33}$$

2.9.2. A test for for positive definiteness and positive semidefiniteness using principle minors.

Theorem 8. A matrix A is positive semidefinite iff all the principal minors of A are non-negative.

For a proof see Gantmacher [2, p. 307].

As an example consider the matrix G2.

$$G2 = \begin{bmatrix} 2 & 0 & 2 \\ 0 & 4 & 4 \\ 2 & 4 & 6 \end{bmatrix} .$$

The diagonal elements are all positive so the 1x1 test is passed. Now consider the principal 2x2 minors

$$\left| \begin{array}{cc} 2 & 0 \\ 0 & 4 \end{array} \right| = 8 - 0 = 8 > 0 \quad \left| \begin{array}{cc} 2 & 2 \\ 2 & 6 \end{array} \right| = 12 - 4 = 8 > 0 \quad \left| \begin{array}{cc} 4 & 4 \\ 4 & 6 \end{array} \right| = 24 - 16 = 8 > 0$$

These are all positive and so we pass the 2x2 test. Now consider the determinant of the entire matrix

$$\begin{vmatrix} 2 & 0 & 2 \\ 0 & 4 & 4 \\ 2 & 4 & 6 \end{vmatrix} = (2)(4)(6) + (0)(4)(2) + (2)(4)(0) - (2)(4)(2) - (4)(4)(2) - (6)(0)(0) = \\ = 48 + 0 + 0 - 16 - 32 - 0 = 0$$

This determinant is zero and so the matrix is positive semidefinite but not positive definite.

2.9.3. *Some characteristics of negative semidefinite matrices.* The results on positive definite and positive semidefinite matrices have counterparts for negative definite and semidefinite matrices.

- a:** A negative semidefinite matrix is negative definite only if it is non-singular.
b: Let A be a negative definite matrix of order m . Then

$$a_{ii} < 0 \quad i = 1, \dots, m$$

- c:** If A is only negative semidefinite then

$$a_{ii} \leq 0 \quad i = 1, \dots, m.$$

- d:** Let A be a symmetric matrix of order m . Then A is negative definite iff its naturally ordered (leading) principal minors alternate in sign starting with a negative number.

The naturally ordered principle minors of a matrix A are defined as determinants of matrices

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{k1} & a_{k2} & \cdots & a_{kk} \end{bmatrix} \quad k = 1, 2, \dots, m. \quad (27)$$

As an example consider the matrix

$$E = \begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$

Element $a_{11} = -2 < 0$. Now consider the first naturally occurring principal 2x2 submatrix

$$\begin{vmatrix} -2 & 1 \\ 1 & -2 \end{vmatrix} = 4 - 1 = 3 > 0.$$

Now consider the determinant of the entire matrix

$$\begin{vmatrix} -2 & 1 & 0 \\ 1 & -2 & 0 \\ 0 & 0 & -2 \end{vmatrix} = (-2)(-2)(-2) + (1)(0)(0) + (1)(0)(0) - (-2)(0)(0) - (-2)(0)(0) - (-2)(1)(1) \\ = -8 + 0 + 0 - 0 - 0 + 2 = -6 < 0$$

This matrix is then negative definite.

- e:** Let A be a symmetric matrix of order m . A is negative semidefinite iff the following inequalities hold:

$$(-1)^p A \begin{pmatrix} i_1 & i_2 & \cdots & i_p \\ i_1 & i_2 & \cdots & i_p \end{pmatrix} \geq 0 \quad (28) \\ [1 \leq i_1 \leq i_2 \leq \cdots \leq i_p \leq m, p = 1, 2, \dots, m]$$

Here $A(i_1, i_2, \dots, i_p)$ is the determinant of the submatrix of A with p rows and columns of A , i.e., it is a principle minor of A .

$$A(i_1, i_2, \dots, i_p) = \begin{vmatrix} a_{i_1 i_1} & a_{i_1 i_2} & \cdots \\ a_{i_2 i_1} & a_{i_2 i_2} & \cdots \\ \vdots & \vdots & \ddots \\ a_{i_p i_1} & a_{i_p i_2} & \cdots \end{vmatrix} \quad (29)$$

For a 3x3 matrix this means that all the diagonal elements are non-positive, all 2x2 principal minors are non-negative and the determinant of the matrix is non-positive. Consider as an example the matrix G_3

$$G_3 = \begin{bmatrix} -2 & 1 & -1 \\ 1 & -2 & -1 \\ -1 & -1 & -2 \end{bmatrix}.$$

The diagonal elements are all negative so the 1x1 test is passed. Now consider the principal 2x2 minors

$$\begin{vmatrix} -2 & 1 \\ 1 & -2 \end{vmatrix} = 4 - 1 = 3 > 0 \quad \begin{vmatrix} -2 & -1 \\ -1 & -2 \end{vmatrix} = 4 - 1 = 3 > 0 \quad \begin{vmatrix} -2 & -1 \\ -1 & -2 \end{vmatrix} = 4 - 1 = 3 > 0 .$$

These are all positive and so we pass the 2x2 test. Now consider the determinant of the entire matrix

$$\begin{aligned} |G_3| &= \begin{vmatrix} -2 & 1 & -1 \\ 1 & -2 & -1 \\ -1 & -1 & -2 \end{vmatrix} \\ &= [(-2)(-2)(-2)] + [(1)(-1)(-1)] + [(1)(-1)(-1)] \\ &\quad - [(-1)(-2)(-1)] - [(-1)(-1)(-2)] - [(1)(1)(-2)] \\ &= -8 + 1 + 1 - (-2) - (-2) - (-2) = 0 \end{aligned}$$

This determinant is zero and so the matrix is negative semidefinite but not negative definite.

f: Characteristic roots of negative definite matrices.

Let A be a symmetric matrix of order m and let $\lambda_i, i = 1, \dots, m$ be its real characteristic roots. If A is negative definite then

$$\lambda_i < 0 \quad i = 1, 2, \dots, m$$

g: Characteristic roots of negative semi-definite matrices.

Let A be a symmetric matrix of order m and let $\lambda_i, i = 1, \dots, m$ be its real characteristic roots. If A is negative semi-definite then

$$\lambda_i \leq 0 \quad i = 1, 2, \dots, m \text{ and at least one } \lambda_i = 0.$$

2.10. Example problems. Determine whether the following matrices are positive definite, positive semidefinite, negative definite, negative semidefinite, or indefinite.

$$A = \begin{pmatrix} -2 & 0 & -1 \\ 0 & -2 & -1 \\ -2 & -4 & -3 \end{pmatrix}$$

$$B = \begin{pmatrix} -2 & 4 & -1 \\ 4 & -2 & -1 \\ -1 & -1 & -2 \end{pmatrix}$$

$$C = \begin{pmatrix} 2 & 1 & -1 \\ 1 & 4 & -2 \\ -1 & -2 & 4 \end{pmatrix}$$

$$D = \begin{pmatrix} 2 & -1 & 3 \\ -1 & 5 & 3 \\ 3 & 3 & 9 \end{pmatrix}$$

$$E = \begin{pmatrix} -2 & 1 & -1 \\ 1 & -3 & -2 \\ -1 & -2 & -5 \end{pmatrix}$$

3. SECOND ORDER CONDITIONS FOR OPTIMIZATION PROBLEMS AND DEFINITENESS CONDITIONS ON MATRICES

3.1. Restatement of second order conditions for optimization problems with 2 variables.

Theorem 9. Suppose that $f(x_1, x_2)$ and its first and second partial derivatives are continuous throughout a disk centered at (a, b) and that $\frac{\partial f}{\partial x_1}(a, b) = \frac{\partial f}{\partial x_2}(a, b) = 0$. Then

a: f has a **local maximum** at (a, b) if $\frac{\partial^2 f}{\partial x_1^2}(a, b) < 0$ and $\frac{\partial^2 f}{\partial x_1^2} \frac{\partial^2 f}{\partial x_2^2} - \left[\frac{\partial^2 f}{\partial x_1 \partial x_2} \right]^2 > 0$ at (a, b) . We can also write this as $f_{11} < 0$ and $f_{11} f_{22} - f_{12}^2 > 0$ at (a, b) .

b: f has a **local minimum** at (a, b) if $\frac{\partial^2 f}{\partial x_1^2}(a, b) > 0$ and $\frac{\partial^2 f}{\partial x_1^2} \frac{\partial^2 f}{\partial x_2^2} - \left[\frac{\partial^2 f}{\partial x_1 \partial x_2} \right]^2 > 0$ at (a, b) . We can also write this as $f_{11} > 0$ and $f_{11} f_{22} - f_{12}^2 > 0$ at (a, b) .

c: f has a **saddle point** at (a, b) if $\frac{\partial^2 f}{\partial x_1^2} \frac{\partial^2 f}{\partial x_2^2} - \left[\frac{\partial^2 f}{\partial x_1 \partial x_2} \right]^2 < 0$ at (a, b) . We can also write this as $f_{11} f_{22} - f_{12}^2 < 0$ at (a, b) .

d: The **test is inconclusive** at (a, b) if $\frac{\partial^2 f}{\partial x_1^2} \frac{\partial^2 f}{\partial x_2^2} - \left[\frac{\partial^2 f}{\partial x_1 \partial x_2} \right]^2 = 0$ at (a, b) . If this case we must find some other way to determine the behavior of f at (a, b) .

The expression $\frac{\partial^2 f}{\partial x_1^2} \frac{\partial^2 f}{\partial x_2^2} - \left[\frac{\partial^2 f}{\partial x_1 \partial x_2} \right]^2$ is called the **discriminant** of f .

3.2. Expressing the second order conditions in terms of the definiteness of the Hessian of the objective function.

3.2.1. *Second order conditions for a local maximum.* The Hessian of a function f is the $n \times n$ matrix of second order partial derivatives, that is

$$|H| = \begin{vmatrix} f_{11} & f_{12} & \cdots & f_{1n} \\ f_{21} & f_{22} & \cdots & f_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ f_{n1} & f_{n2} & \cdots & f_{nn} \end{vmatrix} \quad (30)$$

We can write the discriminant condition as the determinant of the Hessian of the objective function f when there are just 2 variables in the function as

$$\frac{\partial^2 f}{\partial x_1^2} \frac{\partial^2 f}{\partial x_2^2} - \left[\frac{\partial^2 f}{\partial x_1 \partial x_2} \right]^2 = \begin{vmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \end{vmatrix} = |H| \quad (31)$$

The second order condition for a local maximum is then that

$$f_{11} < 0 \text{ and } \begin{vmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \end{vmatrix} > 0$$

which is just the condition that H is negative definite.

3.2.2. *Second order conditions for a local minimum.* The second order condition for a local minimum is that

$$f_{11} > 0 \text{ and } \begin{vmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \end{vmatrix} > 0$$

which is just the condition that H is positive definite.

3.2.3. *Extension of condition on Hessian to more than two variables.* The second order conditions, for local maxima and minima based on the sign of f_{11} and the discriminant written in terms of whether the Hessian of the objective function is positive or negative, extend to problems involving objective functions with more than 2 variables.

4. CONVEXITY AND CONCAVITY AND DEFINITENESS CONDITIONS ON HESSIAN MATRICES

4.1. **Definition of concavity.** Let S be a nonempty convex set in R^n . The function $f: S \rightarrow R^1$ is said to be concave on S if $f(\lambda x_1 + (1-\lambda)x_2) \geq \lambda f(x_1) + (1-\lambda)f(x_2)$ for each $x_1, x_2 \in S$ and for each $\lambda \in [0, 1]$. The function f is said to be strictly concave if the above inequality holds as a strict inequality for each distinct $x_1, x_2 \in S$ and for each $\lambda \in (0, 1)$.

4.2. Characterizations of concave functions.

- a: The function f is continuous on the interior of S .
- b: The function f is concave on S if and only if the set $\{(x, y): x \in S, y \leq f(x)\}$ is convex. This set is called the hypograph of f . It is a subset of R^2 . Thus concavity of f is equivalent to convexity of its hypograph.
- c: The set $\{x \in S, f(x) \geq \alpha\}$ is convex for every real α .
- d: A differentiable function f is concave on S if and only if

$$f(x) \leq f(\bar{x}) + f'(\bar{x})(x - \bar{x}) \text{ for each distinct } x, \bar{x} \in S.$$

This implies that tangent line is above the graph.

- e: A twice differentiable function f is concave iff the Hessian $H(x)$ is negative semidefinite for each $x \in S$.

- f:** Let f be twice differentiable. Then if the Hessian $H(x)$ is negative definite for each $x \in S$, f is strictly concave. Further if f is strictly concave, then the Hessian $H(x)$ is negative semidefinite for each $x \in S$.
- g:** Every local maximum of f over a convex set $W \subseteq S$ is a global maximum.
- h:** If $f'(\bar{x}) = 0$ for a concave function then, \bar{x} is the global maximum of f over S .

4.3. Definition of convexity. Let S be a nonempty convex set in R^n . The function $f: S \rightarrow R^1$ is said to be convex on S if $f(\lambda x_1 + (1 - \lambda)x_2) \leq \lambda f(x_1) + (1 - \lambda)f(x_2)$ for each $x_1, x_2 \in S$ and for each $\lambda \in [0, 1]$. The function f is said to be strictly convex if the above inequality holds as a strict inequality for each distinct $x_1, x_2 \in S$ and for each $\lambda \in (0, 1)$.

4.4. Characteristics of convex functions.

- a:** The function f is continuous on the interior of S .
- b:** The function f is convex on S if and only if the set $\{(x, y): x \in S, y \geq f(x)\}$ is convex. This set is called the epigraph of f . It is a subset of R^2 . Thus concavity of f is equivalent to convexity of its epigraph.
- c:** The set $\{x \in S, f(x) \leq \alpha\}$ is convex for every real α .
- d:** A differentiable function f is convex on S if and only if

$$f(x) \geq f(\bar{x}) + f'(\bar{x})(x - \bar{x}) \text{ for each distinct } x, \bar{x} \in S.$$

This implies that tangent line is below the graph.

- e:** A twice differentiable function f is convex iff the Hessian $H(x)$ is positive semidefinite for each $x \in S$.
- f:** Let f be twice differentiable. Then if the Hessian $H(x)$ is positive definite for each $x \in S$, f is strictly concave. Further if f is strictly concave, then the Hessian $H(x)$ is positive semidefinite for each $x \in S$.
- g:** Every local minimum of f over a convex set $W \subseteq S$ is a global minimum.
- h:** If $f'(\bar{x}) = 0$ for a convex function then, \bar{x} is the global minimum of f over S .

5. LINEAR CONSTRAINTS AND BORDERED MATRICES

5.1. Definition of a quadratic form with linear constraints. Let the quadratic form be given by

$$Q = x'Ax = (x_1 \dots x_n) \begin{pmatrix} a_{11} & \dots & a_{1n} \\ & \ddots & \\ a_{n1} & \dots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_n \end{pmatrix} \quad (32)$$

with a set of m linear constraints represented by

$$x'B = 0$$

$$(x_1 \ x_2 \ \dots \ x_n) \begin{pmatrix} b_{11} & b_{12} & \dots & b_{1m} \\ b_{21} & b_{22} & \dots & b_{2m} \\ \vdots & \vdots & & \\ b_{n1} & b_{n2} & \dots & b_{nm} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad (33)$$

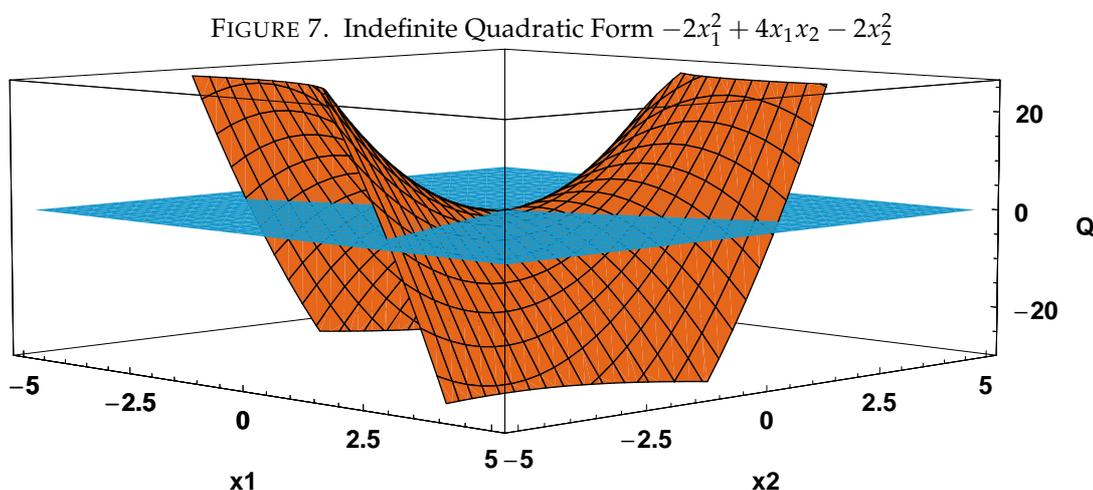
5.2. **Graphical analysis.** Consider the indefinite matrix A given by

$$A = \begin{bmatrix} -2 & 2 \\ 2 & 2 \end{bmatrix} \tag{34}$$

The quadratic form is given by

$$\begin{aligned} Q &= x'Ax = [x_1 \ x_2] \begin{bmatrix} -2 & 2 \\ 2 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\ &= [-2x_1 + 2x_2 \ 2x_1 + 2x_2] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\ &= -2x_1^2 + 2x_1x_2 + 2x_1x_2 + 2x_2^2 \\ &= -2x_1^2 + 4x_1x_2 + 2x_2^2 \\ &= 4x_2^2 - (\sqrt{2}x_1 - \sqrt{2}x_2)^2 \end{aligned} \tag{35}$$

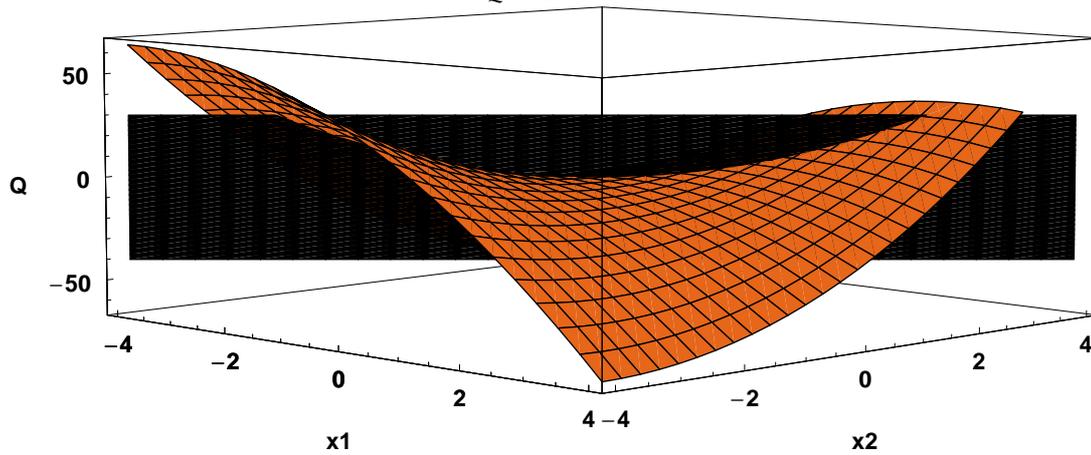
The graph in 3 dimensions is contained in figure 7.



where it is clear that Q takes both positive and negative values.

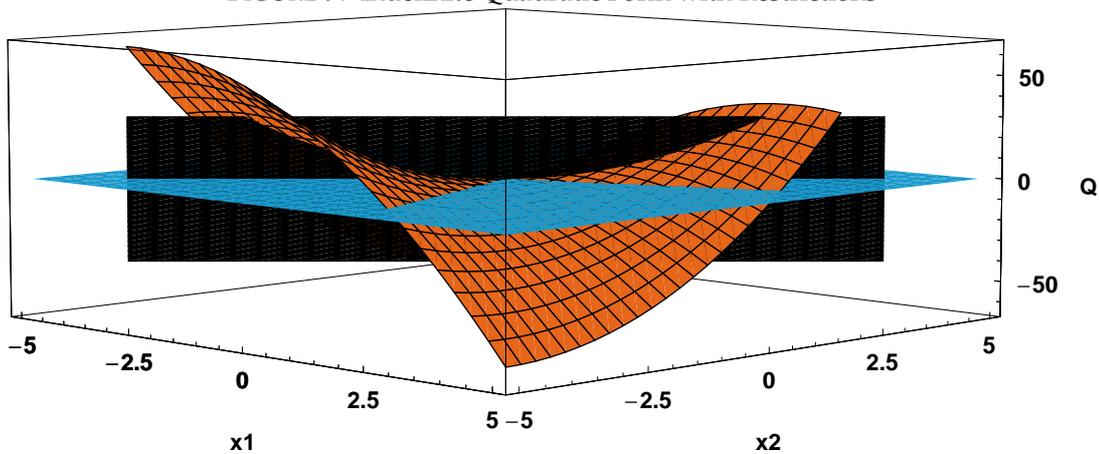
If we restrict our attention to values of x_1 and x_2 where $x_1 = x_2$ or a matrix $b = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$ then the function will be positive for all values of $x \neq 0$ as is obvious from the last line of equation 35. To see this more clearly, draw a vertical plane through the graph above along the $x_1 = x_2$ line in figure 8.

FIGURE 8. Indefinite Quadratic Form with Restrictions



If we combine figure 8 with the plane dividing the positive and negative orthants, the positive definiteness of the quadratic form subject to the constraint is even more obvious as shown in figure 9.

FIGURE 9. Indefinite Quadratic Form with Restrictions



Now along the set of points where $x_1 = x_2$, the function is always positive except where $x_1 = x_2 = 0$. So this function is positive definite subject to the constraint that $x_1 = x_2$.

5.3. Definition of a bordered matrix with constraints. Define the bordered matrix H_B as follows

$$H_B = \left(\begin{array}{cccc|cccc} a_{11} & a_{12} & \cdots & a_{1n} & b_{11} & b_{12} & \cdots & b_{1m} \\ a_{21} & a_{22} & \cdots & a_{2n} & b_{21} & b_{22} & \cdots & b_{2m} \\ \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} & b_{n1} & b_{n2} & \cdots & b_{nm} \\ \hline & & & & \vdots & & & \\ b_{11} & b_{21} & \cdots & b_{n1} & 0 & 0 & \cdots & 0 \\ b_{12} & b_{22} & \cdots & b_{n2} & 0 & 0 & \cdots & 0 \\ \vdots & \vdots \\ b_{1m} & b_{2m} & \cdots & b_{nm} & 0 & 0 & \cdots & 0 \end{array} \right) \quad (36)$$

On the right of the A matrix we append the columns of the B matrix. If there are three constraints, then the matrix H_B will have $n + 3$ columns or in general $n+m$ columns. Below the A matrix we append the transpose of the B matrix, one row at a time as we add constraints. So if $m = 2$, then H_B will have $n+2$ rows. For the case of one linear constraint we obtain

$$H_B = \left(\begin{array}{cc|c} a_{11} & a_{12} & b_{11} \\ a_{21} & a_{22} & b_{21} \\ \hline b_{11} & b_{21} & 0 \end{array} \right) \quad (37)$$

5.4. Definiteness of a quadratic form subject to linear constraints.

5.4.1. *Constructing minors of H_B .* To determine the definiteness of the quadratic form in equation 32 subject to equation 33 construct the matrix H_B in equation 36. The definiteness is checked by analyzing the signs of the naturally order principal minors of H_B starting with the minor that has $m+1$ rows and columns of the matrix A along with the borders for those rows and columns. For example, if $m = 1$, then the first minor we check is

$$\left| \begin{array}{cc|c} a_{11} & a_{12} & b_{11} \\ a_{21} & a_{22} & b_{21} \\ \hline b_{11} & b_{21} & 0 \end{array} \right| \quad (38)$$

Then we check

$$\left| \begin{array}{ccc|c} a_{11} & a_{12} & a_{13} & b_{11} \\ a_{21} & a_{22} & a_{23} & b_{21} \\ a_{31} & a_{32} & a_{33} & b_{31} \\ \hline b_{11} & b_{21} & b_{31} & 0 \end{array} \right| \quad (39)$$

and so forth. In general we are checking the signs of minors with $p + m$ rows, where p goes from $m+1$ to n . The minors we check can be written as below when there are m constraints.

$$\begin{array}{cccc|cccc}
a_{11} & a_{12} & \cdots & a_{1p} & b_{11} & b_{12} & \cdots & b_{1m} \\
a_{21} & a_{22} & \cdots & a_{2p} & b_{21} & b_{22} & \cdots & b_{2m} \\
\vdots & \vdots \\
a_{p1} & a_{p2} & \cdots & a_{pp} & b_{p1} & b_{p2} & \cdots & b_{pm} \\
\hline
& & & & \vdots & & & \\
\hline
b_{11} & b_{21} & \cdots & b_{p1} & 0 & 0 & \cdots & 0 \\
b_{12} & b_{22} & \cdots & b_{p2} & 0 & 0 & \cdots & 0 \\
\vdots & \vdots \\
b_{1m} & b_{2m} & \cdots & b_{pm} & 0 & 0 & \cdots & 0
\end{array} \tag{40}$$

5.4.2. *Definiteness of a quadratic form subject to one linear constraint.* Construct the $(n+1) \times (n+1)$ matrix H_B as in 37 where the constraint equation is now given by

$$b_{11}x_1 + b_{21}x_2 + \cdots + b_{n1}x_n = 0 \tag{41}$$

Suppose that $b_1 \neq 0$. If the last n leading principal minors of H_B have the same sign, Q is positive definite on the constraint set.

If the last n leading principal minors alternate in sign, then Q is negative definite on the constraint (Simon [5, Section 16.3]).

5.4.3. *General condition for a matrix to be positive definite subject to a set of linear constraints.* If the determinant of H_B and these last $n-m$ leading principal minors all have the same sign as $(-1)^m$, then Q is **positive definite** on the constraint set $x'B = 0$. With one constraint, $m = 1$, so that the first minor is negative as are all subsequent ones.

5.4.4. *General condition for a matrix to be negative definite subject to a set of linear constraints.* If determinant of H_B has the same sign as $(-1)^p$ and if these last $n-m$ leading principal minors **alternate in sign**, then the quadratic form Q is **negative definite** on the constraint set $x'B = 0$. With one constraint, $m = 1$, and so p starts at 2, so that the first minor is positive, the second negative and so forth.

5.4.5. *If both of these conditions 5.4.3 and 5.4.4 are violated by **nonzero** leading principal minors, then Q is indefinite on the constraint set $x'B = 0$.*

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