Exercises

13.3.1 By multiplying out the brackets in the expression $(\lambda \mathbf{a} + \mu \mathbf{b})^T (\lambda \mathbf{a} + \mu \mathbf{b})$, prove L3

13.3.2 Show that, if \mathbf{a} and \mathbf{b} are n-vectors such that $\|\mathbf{a}\| = \|\mathbf{b}\| = 1$, then $-1 \le \mathbf{a}^T \mathbf{b} \le 1$. Give examples where n=2, $\|\mathbf{a}\|=\|\mathbf{b}\|=1$ and

$$(a) \ \mathbf{a}^T\mathbf{b} = 1; \quad (b) \ \mathbf{a}^T\mathbf{b} = -1; \quad (c) \ \mathbf{a}^T\mathbf{b} = 0; \quad (d) \ 0 < \mathbf{a}^T\mathbf{b} < 1.$$

13.3.3 Prove the following n-dimensional version of Pythagoras' theorem: if u and v are orthogonal n-vectors then

$$\|\mathbf{u} - \mathbf{v}\|^2 = \|\mathbf{u}\|^2 + \|\mathbf{v}\|^2.$$

13.3.4 Prove that the determinant of an orthogonal matrix is either 1 or -1. Show that both cases can occur.

13.3.5 In Exercise 11.2.7, you were asked to find the 2 × 2 matrix that describes anticlockwise rotation about the origin through 45 degrees. Verify that this is an orthogonal matrix.

13.3.6 Give an example of a 3×2 matrix U such that $U^TU = I_2$. Is it an orthogonal matrix?

13.3.7 Let

$$\mathbf{u} = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}, \ \mathbf{v} = \begin{bmatrix} 2 \\ 2 \\ -1 \end{bmatrix}, \ \mathbf{w} = \begin{bmatrix} 1 \\ 1 \\ 4 \end{bmatrix}.$$

Verify that any two of the three 3-vectors u, v, w are orthogonal. Find scalars λ, μ, ν such that $[\lambda \mathbf{u} \ \mu \mathbf{v} \ \nu \mathbf{w}]$ is an orthogonal matrix.

13.4 Quadratic forms and symmetric matrices

In Chapter 4 we defined a quadratic function to be a function of the form

$$f(x) = ax^2 + bx + c$$

where a,b,c are constants. A slight generalisation of this is the expression

$$q(x,y) = ax^2 + bxy + cy^2,$$

which is known as a quadratic form in the two variables x and y. Notice that q(x,y) reduces to f(x) if we set reduces to f(x) if we set y = 1.

By the rules of matrix multiplication, we may write

$$q(x,y) = \mathbf{z}^{\mathrm{T}} \mathbf{A} \mathbf{z} \tag{13.10}$$

13.4 QUADRATIC FORMS AND SYMMETRIC MATRICES where $\mathbf{z} = \begin{bmatrix} x \\ y \end{bmatrix}$, $\mathbf{A} = \begin{bmatrix} a & s \\ t & c \end{bmatrix}$ and s and t are any two numbers such that s+t=b. The expression $q(\mathbf{z})$ has the same meaning as q(x,y).

pression $q(\mathbf{z})$ has the condition that s=t, their common value must be b/2; then \mathbf{A} is lift we impose the condition that s=t, their common value must be b/2; then \mathbf{A} is If we impose the coefficients a,b,c of the quadratic form, as the matrix determined uniquely by the coefficients a,b,c of the quadratic form, as the matrix

$$\left[\begin{array}{cc} a & b/2 \\ b/2 & c \end{array}\right].$$

Imposing the condition that s=t is the same as requiring that A be its own transpose; Imposing the conditions and to be symmetric. Generally, a symmetric matrix of a matrix with this property is said to be symmetric. A such that AT. a matrix with the particular the identity matrix \mathbf{I} is defined to be an $n \times n$ matrix \mathbf{A} such that $\mathbf{A}^T = \mathbf{A}$. Notice that any diagonal order n is defined to be an $n \times n$ matrix \mathbf{I} in particular, the identity matrix \mathbf{I} is matrix is symmetric; in particular, the identity matrix I is symmetric.

We have shown that, given a quadratic form in two variables q(x,y), there is exactly one symmetric 2×2 matrix A satisfying (13.10). Now consider the general quadratic form in three variables:

variables.
$$q(x_1, x_2, x_3) = ax_1^2 + bx_2^2 + cx_3^2 + dx_1x_2 + ex_1x_3 + fx_2x_3,$$

where a,b,c,d,e,f are constants. Let $\mathbf{x}=[x_1 \ x_2 \ x_3]^\mathrm{T};$ then there is exactly one symmetric 3×3 matrix A such that $q(\mathbf{x}) = \mathbf{x}^T \mathbf{A} \mathbf{x}$, namely

$$\begin{bmatrix} a & d/2 & e/2 \\ d/2 & b & f/2 \\ e/2 & f/2 & c \end{bmatrix}.$$

All of this may be generalised. A quadratic form in n variables x_1, x_2, \ldots, x_n is defined to be an expression of the form

$$q(\mathbf{x}) = \mathbf{x}^{\mathrm{T}} \mathbf{A} \mathbf{x},$$

where $\mathbf{x} = [x_1 \ x_2 \ \dots \ x_n]^\mathrm{T}$ and \mathbf{A} is a symmetric $n \times n$ matrix. By requiring that \mathbf{A} be symmetric $\mathbf{x} = [x_1 \ x_2 \ \dots \ x_n]^\mathrm{T}$ A be symmetric, we ensure that A is uniquely determined by the coefficients of x_1^2 , x_1x_2 and so on when the quadratic form is written out in full; we have just shown this for the special cases n=2 and n=3, and it is true for all n. The relation between quadratic for quadratic forms and symmetric matrices is discussed in more detail in the appendix to this chapter. this chapter.

When we discussed quadratic functions in Chapter 4, we devoted some attention to the question wheel question whether a function f(x) was positive for all values of x. There is no direct analogue of this analogue of this property for quadratic forms, since q(0) = 0 for every quadratic form q(x). However, $q(\mathbf{x})$. However, given a quadratic form $q(\mathbf{x})$, we can ask whether $q(\mathbf{x}) > 0$ for every non-zero vector. non-zero vector \mathbf{x} ; if so, we say that $q(\mathbf{x})$ is a **positive definite** quadratic form.

Example 1 A quadratic form in n variables x_1, \ldots, x_n that is obviously positive definite

 $x_1^2 + x_2^2 + \ldots + x_n^2$

Recall that this is what we called $\|\mathbf{x}\|^2$ in the preceding section.

The quadratic form $q(\mathbf{x})$ is said to be **positive semidefinite** if $q(\mathbf{x}) \ge 0$ for every vector x. Every positive definite quadratic form is positive semidefinite. On the other vector x. Every positive definite of ther hand, it is easy to find quadratic forms which are positive semidefinite but not positive definite.

Example 2 Consider the quadratic form in three variables

$$q(x_1, x_2, x_3) = x_1^2 + x_2^2 + x_3^2 - 2x_2x_3.$$

This can be written as $x_1^2 + (x_2 - x_3)^2$ which, being a sum of squares, is nonnegative. Therefore $q(x_1, x_2, x_3)$ is positive semidefinite; it is not positive definite because q(0, 1, 1) = 0.

We say that a quadratic form q(x) is negative semidefinite if -q(x) is positive semidefinite; this happens if and only if $q(\mathbf{x}) \leq 0$ for every vector \mathbf{x} . Similarly, $q(\mathbf{x})$ is said to be negative definite if -q(x) is positive definite.

Many quadratic forms are neither positive semidefinite nor negative semidefinite.

Example 3 The quadratic form

$$q(x_1, x_2) = x_1^2 - x_2^2$$

is neither positive semidefinite nor negative semidefinite, since q(0,1) = -1 and q(1,0) = 1.

The terms positive definite, negative definite and so on are often applied to symmetric matrices as well as to the corresponding quadratic forms. Thus a symmetric matrix A is said to be positive definite if $x^TAx > 0$ whenever $x \neq 0$, positive semidefinite if $x^T A x \ge 0$ for all x and negative (semi)definite if -A is positive (semi)definite. For instance, the symmetric matrices associated with the quadratic forms of Examples 1, 2 and 3 are respectively

$$\mathbf{I}_n, \ \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{bmatrix} \ \text{and} \ \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

The first of these matrices is positive definite (for all n), the second is positive semidefinite but not not a serious inite but not positive definite and the third is neither positive semidefinite nor negative 13.4 QUADRATIC FORMS AND SYMMETRIC MATRICES

Testing quadratic forms Testing quadratic form, how do we test whether it is positive definite, negative definite given a quadratic form, how do we test whether it is positive definite, negative definite given a quadratic form, how do we test whether it is positive definite, negative definite. Given a quadratic form, a quad or whatever? We can be standard tests; these are most easily stated in terms of the as-More typically, we use the sociated symmetric matrix, but of course they translate immediately into results about sociated symmetric forms themselves. We begin with symmetric matrices of order sociated symmetric sociated symmetric matrices of order 2. the quadratic forms themselves. We begin with symmetric matrices of order 2.

- (a) A 2×2 symmetric matrix is positive definite if and only if its diagonal entries are both positive and its determinant is positive.
- (b) A 2×2 symmetric matrix is positive semidefinite if and only if its diagonal entries are both non-negative and its determinant is non-negative.
- (c) A 2×2 symmetric matrix is negative definite if and only if its diagonal entries are both negative and its determinant is positive,
- (d) A 2×2 symmetric matrix is negative semidefinite if and only if its diagonal entries are both non-positive and its determinant is non-negative.

Example 4 Let

$$\mathbf{A} = \begin{bmatrix} 2+t & 1 \\ 1 & 2-t \end{bmatrix}.$$

Then A is symmetric and det $A = 3 - t^2$. If $-\sqrt{3} < t < \sqrt{3}$, the determinant and both diagonal entries are positive: thus A is positive definite. If $t = \pm \sqrt{3}$, A is positive semidefinite but not positive definite. If $|t| > \sqrt{3}$, det A < 0, so A is neither positive semidefinite nor negative semidefinite.

Since $1 < \sqrt{3} < 2$, these results imply that the quadratic form

$$3x_1^2 + x_2^2 + 2x_1x_2$$

is positive definite, while the quadratic form $4x_1^2 + 2x_1x_2$ is neither positive semidefinite nor negative semidefinite.

We now discuss briefly why these tests for 2×2 symmetric matrices are valid. We focus on (a). Consider the symmetric matrix

$$\mathbf{A} = \left[\begin{array}{cc} a & s \\ s & c \end{array} \right]$$

and the associated quadratic form

$$q(x,y) = ax^2 + 2sxy + cy^2.$$

Then a=q(1,0) and c=q(0,1): for our matrix to be positive definite, we need these diagonal entries diagonal entries to be positive.

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To see the relevance of the determinant, consider the case where a=c=1. Then To see the relevance of the determinant, c = 1. Then $\det \mathbf{A} = 1 - s^2$. To verify (a) in this case, we need to show that q(x, y) > 0 for all (x, y) det $\mathbf{A} = 1 - s^2$. To verify only if $s^2 < 1$. In fact, other than (0,0) if and only if $s^2 < 1$. In fact,

if and only if
$$s$$

$$q(x,y) = x^2 + 2sxy + y^2 = (x+sy)^2 + (1-s^2)y^2$$

by completing the square. This is clearly positive if $s^2 < 1$ and at least one of x and y by completing the square x = 1 we can make q(x, y) non-positive by setting x = 1by completing the square. This is the proofs of (a)—(d) in the general case consists x = s, y = -1is not zero; while if $s^* \ge 1$ we can interest in the general case consist of y = -1. Thus (a) holds for this matrix. The proofs of (a)–(d) in the general case consist of y = -1. elaborate versions of the same argument.

Higher dimensions

To generalise the tests (a)-(d) to matrices of order n, we need some definitions.

A submatrix of a matrix A is a matrix obtained from A by deleting some (or none) of its rows and some (or none) of its columns. A principal submatrix of a square matrix A is a submatrix obtained using the rule that the kth row of A is deleted if and only if the kth column of A is deleted. A leading principal submatrix of a square matrix A is a submatrix obtained by deleting the last m rows and columns, for some m.

For example, if

$$\mathbf{A} = \begin{bmatrix} a & b & c \\ p & q & r \\ u & v & w \end{bmatrix},$$

then the principal submatrices of A are its three diagonal entries a, q, w (considered as 1×1 matrices), the three 2×2 matrices

$$\left[\begin{array}{cc} a & b \\ p & q \end{array} \right], \quad \left[\begin{array}{cc} a & c \\ u & w \end{array} \right], \quad \left[\begin{array}{cc} q & r \\ v & w \end{array} \right]$$

and A itself. The first, fourth and seventh of these matrices are the leading principal submatrices of A.

A minor of a square matrix A is the determinant of a square submatrix of A; a principal minor is the determinant of a principal submatrix and a leading principal minor is the determinant of a leading principal submatrix. In the 3 × 3 example just given, the leading principal minors of A are a, aq - bp and $\det A$; the other principal minors are q, w, aw - cu and qw - rv.

Tests (a) and (b) for 2×2 symmetric matrices generalise as follows:

- (a) An $n \times n$ symmetric matrix is positive definite if and only if its principal minors are all positive.
- (b) An $n \times n$ symmetric matrix is positive semidefinite if and only if its principal minors are all non-negative.

These tests are usually cumbersome to apply. A more convenient version of (a) 15 the following:

13.4 QUADRATIC FORMS AND SYMMETRIC MATRICES (a) An $n \times n$ symmetric matrix is positive definite if and only if its leading principal minors are all positive. minors are all positive.

For example, the 3×3 symmetric matrix

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$$\begin{bmatrix} f & 1 & 4 \\ 1 & g & 5 \\ 4 & 5 & h \end{bmatrix}$$

is positive definite if and only if the following three conditions are met: f > 0, fg > 1 is positive determinant of the matrix is positive. and the determinant of the matrix is positive.

d the determined in the following form:

(a") An $n \times n$ symmetric matrix is positive definite if and only if it can be reduced by Gaussian elimination, without row exchanges, to an upper trial An $n \times n$ symmetries are all positive whose diagonal entries are all positive.

By contrast, non-negativity of the leading principal minors does not guarantee that By contract, a symmetric matrix is positive semidefinite; for example, the 3×3 diagonal matrix a symmetric matrix with diagonal entries 1, 0, -1 has leading principal minors 1, 0, 0 but is not positive

It is possible to generalise rules (c) and (d) to $n \times n$ symmetric matrices. However, it is usually easier to test for negative definiteness or semidefiniteness by applying (a') or (b) to the matrix $-\mathbf{A}$.

Three propositions

We end this section with three general propositions about positive definite and semidefinite symmetric matrices. We give the proofs because they are good illustrations of the use of simple logical reasoning employing the algebra of inner products, but the reader may omit them without loss of continuity.

Proposition 1 Let A be a positive semidefinite symmetric matrix, x a vector. Then $x^{T}Ax > 0$ if and only if $Ax \neq 0$.

PROOF Let y = Ax. If $x^Ty > 0$, then obviously $y \neq 0$. Now suppose $y \neq 0$; we wish to show that $\mathbf{x}^T\mathbf{y} > 0$. Since A is symmetric, $\mathbf{y}^T = \mathbf{x}^T\mathbf{A}$; hence the expressions $y^T A x$ and $x^T A y$ are both equal to $y^T y$. Therefore, for every scalar λ ,

$$(\mathbf{x} - \lambda \mathbf{y})^{\mathrm{T}} \mathbf{A} (\mathbf{x} - \lambda \mathbf{y}) = \mathbf{x}^{\mathrm{T}} \mathbf{y} - 2\lambda \mathbf{y}^{\mathrm{T}} \mathbf{y} + \lambda^{2} \mathbf{y}^{\mathrm{T}} \mathbf{A} \mathbf{y}.$$

Since A is positive semidefinite, the left-hand side of this equation is non-negative. Thus

$$\mathbf{x}^T\mathbf{y} \geq \lambda(2\mathbf{y}^T\mathbf{y} - \lambda\mathbf{y}^T\mathbf{A}\mathbf{y})$$

for any real number λ . But since $\mathbf{y} \neq \mathbf{0}$, $\mathbf{y}^T \mathbf{y} > 0$. We may therefore choose λ to be positive. be positive but sufficiently small that $\lambda y^T A y < 2y^T y$. Hence $x^T y > 0$.

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Proposition 2 A symmetric matrix is positive definite if and only if it is positive semi. definite and invertible.

PROOF Let A be a positive semidefinite symmetric matrix. By Proposition 1, A is p_{0sj} . DEF Let A be a positive semidefinite of the proposition of the definite if and only if $Ax \neq 0$ for every non-zero n-vector x. The proposition tive definite if and only fact that a square matrix is invertible if and only if $Ax \neq 0$ for that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible if and only in the fact that a square matrix is invertible in the fact that a square matrix is invertible in the fact that th tive definite if and only if Ax 7 or square matrix is invertible if and only if it is now follows from the fact that a square matrix is invertible if and only if it is

Proposition 3 If A is a positive definite symmetric matrix, so is A^{-1} .

PROOF Let A be a positive definite symmetric matrix. By Proposition 2, A^{-1} exists and is invertible with inverse A; it remains to show that A^{-1} is symmetric and and is invertible with inverse $(A^{-1})^T = (A^T)^{-1}$ for any invertible matrix A; but in positive semidefinite. Now $(A^{-1})^T = (A^T)^{-1}$ for any invertible matrix A; but in positive semidentite. Not (A) is symmetric; hence $(\mathbf{A}^{-1})^{\mathrm{T}} = \mathbf{A}^{-1}$, as required, this case $(\mathbf{A}^{\mathrm{T}})^{-1} = \mathbf{A}^{-1}$ since A is symmetric; we wish to show that To complete the proof, let x be any vector; we wish to show that $\mathbf{x}^{\mathrm{T}} \mathbf{A}^{-1} \mathbf{x} \ge 0$. Let $\mathbf{w} = \mathbf{A}^{-1}\mathbf{x}$. Since \mathbf{A}^{-1} is symmetric, $\mathbf{w}^{\mathrm{T}} = \mathbf{x}^{\mathrm{T}}\mathbf{A}^{-1}$. Therefore

$$\mathbf{x}^{\mathrm{T}}\mathbf{A}^{-1}\mathbf{x} = \mathbf{w}^{\mathrm{T}}\mathbf{x} = \mathbf{w}^{\mathrm{T}}\mathbf{A}\mathbf{w},$$

which is non-negative because A is positive definite.

Exercises

- 13.4.1 Show that, if a is a 2-vector, then $\mathbf{a}\mathbf{a}^T$ is a 2×2 symmetric matrix. How do you think this result generalises?
- 13.4.2 A data set consists of n observations on two variables x_1 and x_2 ; the ith observation is denoted (x_{1i}, x_{2i}) . Let X be the $n \times 2$ matrix whose ith row is $[x_{1i} \ x_{2i}]^4$. Calculate the matrix X^TX, expressing its entries in ∑-notation, and verify that it is symmetric.
- 13.4.3 Prove that if A is a symmetric matrix, so is $B^{T}AB$.
- 13.4.4 Show directly from the definitions that the quadratic form

$$q(x_1, x_2, x_3) = x_1^2 + x_2^2 + x_3^2 - x_2 x_3$$

is positive definite. Write down the associated symmetric matrix.

13.4.5 Determine the symmetric matrix A such that, for every 2-vector x,

$$2x_1^2 + 3x_2^2 + 4x_1x_2 = \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}$$

Use the test given in the text to show that the matrix A is positive definite.

13.4.6 Determine the values of t for which the symmetric matrix $\begin{vmatrix} 2t & 2 \\ 2 & t \end{vmatrix}$ is

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- (a) positive definite; (a) positive semidefinite but not positive definite;

 (b) positive definite:
- (c) negative definite; (c) negative semidefinite but not negative definite;
 (d) negative semidefinite but not negative definite;
- (e) none of the above.

(d) negative serification (e) none of the above.

(e) none of the above.

[3.4.7 Determine the definiteness of the symmetric matrices

$$\begin{bmatrix}
3 & -1 & 1 \\
-1 & 1 & 2 \\
1 & 2 & 9
\end{bmatrix}, \begin{bmatrix}
3 & -1 & 1 \\
-1 & 1 & 2 \\
1 & 2 & 6
\end{bmatrix}, \begin{bmatrix}
-1 & 1 & 0 \\
1 & -2 & 1 \\
0 & 1 & -1
\end{bmatrix}.$$

13.4.8 Suppose C is an $n \times k$ matrix. Show that C^TC is a positive semidefinite symmetric specific. Show also that C^TC is positive definite if the columns of CSuppose C is all C^TC is positive definite if the columns of C are linearly matrix. Show also that C^TC is positive definite if the columns of C are linearly matrix. Show what restriction on n and k does this condition impose?

Problems on Chapter 13

13-1. Let G be the parallelogram in the xy-plane whose vertices have coordinates (0,0), (a, b), (c, a) and (a, bc) by enclosing G in a rectangle and subtracting the surrounding area.

13-2. (i) Let

$$\mathbf{A} = \begin{bmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} a_1 & a_2 \\ b_1 & b_2 \end{bmatrix}.$$

Suppose B is non-singular and A is singular. In Problem 12-3 you were asked to prove that any change in the (3,3) entry transforms A into an invertible matrix. Give another proof of the same result, by expanding det A

- (ii) Sketch a proof of the following proposition: any singular square matrix can be transformed into an invertible matrix by arbitrarily small changes to its diagonal entries.
 - [HINT] First prove the proposition for 2×2 matrices. Then use the argument of (i) to extend the proposition to 3×3 matrices. Finally, explain how the same logic may be used to prove the proposition for square matrices of
- (iii) Explain why the proposition of (ii) ceases to be true when the words 'singular' and 'invertible' are interchanged.

[This problem shows that invertible matrices can be considered as 'normal' square matrices and singular matrices as 'peculiar' ones. For this reason, it is common in applications to assume that square matrices are invertible unless one has a good reason to suppose otherwise.]

⁴This notation, which is standard in the statistical literature, departs from the usual one for matrices, in that the second subscript indicates the row and the first the column.

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13-3. This problem develops further the n-good input-output model of Problems 11-4. Notation is as in those problems.

Suppose each industry j uses as inputs not only the produced goods $1, \dots, n$ by also non-produced goods such as labour and raw materials; let the cost of such inputs, per unit of gross output of j, be c_j . Let p_j be the price of good j. Write down an expression for the cost of producing each unit of gross output of good j. Derive a system of linear equations which must hold if all industries $\frac{1}{2}$ break even (price equals average cost).

Let c be the vector with components c_1, \ldots, c_n and let p be the price vector, with components p_1, \ldots, p_n . What properties must the input-output matrix A have if, for every vector c with non-negative components, there is a corresponding vector p of non-negative prices such that all industries break even? How are these properties related to the answer to Problem 12–4?

13-4. This problem is concerned with the most popular of all econometric techniques, least-squares estimation.

Suppose you have a data set consisting of n observations on three variables y, x_1, x_2 ; the ith observation is denoted $[y_i \ x_{1i} \ x_{2i}]$. You wish to find a linear function of the form

$$y = b_1 x_1 + b_2 x_2$$

which fits the data as well as possible in the following sense: b_1 and b_2 are chosen so as to minimise the expression

$$Q(b_1, b_2) = \sum_{i=1}^{n} (y_i - b_1 x_{1i} - b_2 x_{2i})^2.$$

Let y be the n-vector whose ith component is y_i , X the $n \times 2$ matrix whose ith row is $[x_{1i} \ x_{2i}]^5$. Assume that the columns of X are linearly independent. Let b be the 2-vector $[b_1 \ b_2]^T$.

- (i) Show that $Q(\mathbf{b}) = (\mathbf{y} \mathbf{X}\mathbf{b})^{\mathrm{T}}(\mathbf{y} \mathbf{X}\mathbf{b})$.
- (ii) Suppose that b* is a 2-vector such that

$$\mathbf{X}^{\mathrm{T}}(\mathbf{y} - \mathbf{X}\mathbf{b}^{*}) = \mathbf{0}. \tag{*}$$

Using the result of Exercise 13.3.2, show that

$$Q(\mathbf{b}) = (\mathbf{y} - \mathbf{X}\mathbf{b}^*)^{\mathrm{T}}(\mathbf{y} - \mathbf{X}\mathbf{b}^*) + (\mathbf{b}^* - \mathbf{b})^{\mathrm{T}}\mathbf{X}^{\mathrm{T}}\mathbf{X}(\mathbf{b}^* - \mathbf{b}).$$

(iii) Since the columns of X are linearly independent, the symmetric 2×2 matrix X^TX is positive definite (Exercise 13.4.8) and therefore invertible (Proposition 2 of Section 13.4). Deduce that there is only one vector b* satisfying (*), and find an explicit expression for b*.

(iv) Show that $Q(\mathbf{b})$ is minimised when $\mathbf{b} = \mathbf{b}^*$.

[All of this generalises easily to the case where the data set consists of n observations on 1+k variables y,x_1,\ldots,x_k . In particular, the case of three variables y,x_1,x_2 , where the function to be fitted is of the form

$$y = b_1 x_1 + b_2 x_2 + b_3,$$

may be treated in this framework by letting k = 3, $x_{3i} = 1$ for all i.]

⁵We commented on this notation in an earlier footnote, in connection with Exercise 13.4.2.