

## Objective Functions

When a new method for unconstrained minimization of a function of several variables is devised, it is customary for its author to give numerical results which are obtained by applying the method to a selection of well known objective functions. These functions have been constructed in such a way as to present various computational difficulties. The following is a list of some of the more frequently used test functions, together with an initial estimate  $\mathbf{x}^{(0)}$  of the minimizer  $\mathbf{x}^*$ , and a brief description, where appropriate, of the computational difficulties presented by the optimization problem. Problems 1 and 8–12 are used to illustrate the behaviour of the methods for the least squares problem which is described in Chapter 7.

### 1. Rosenbrock (1960)

$$f(\mathbf{x}) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$

$$\mathbf{x}^{(0)} = [-1.2, 1.0]^T \quad \mathbf{x}^* = [1, 1]^T \quad f(\mathbf{x}^*) = 0$$

This is a steep-sided sharply curving valley, the bottom of which follows the parabolic curve  $x_2 = x_1^2$ . A descent method must in general take very short steps in order to negotiate the sharp bend near  $[0, 0]^T$  and must therefore provide new search directions  $\mathbf{p}$  very frequently.

### 2. Wood's function, quoted by Colville (1968)

$$f(\mathbf{x}) = 100(x_1^2 - x_2)^2 + (x_1 - 1)^2 + (x_3 - 1)^2 + 90(x_3^2 - x_4)^2$$

$$+ 10.1\{(x_2 - 1)^2 + (x_4 - 1)^2\} + 19.8(x_2 - 1)(x_4 - 1)$$

$$\mathbf{x}^{(0)} = [-3, -1, -3, -1]^T \quad \mathbf{x}^* = [1, 1, 1, 1]^T \quad f(\mathbf{x}^*) = 0$$

This objective function has a saddle point near  $[-1, 1, -1, 1]^T$  and the sequences  $\{\mathbf{x}^{(k)}\}$  generated by most methods tend, at least initially, to stay near this point.

### 3. Miele and Cantrell (1969b)

$$f(\mathbf{x}) = (\exp(x_1) - x_2)^4 + 100(x_2 - x_3)^6 + \{\tan(x_3 - x_4)\}^4 + x_1^8$$

$$\mathbf{x}^{(0)} = [1, 2, 2, 2]^T \quad \mathbf{x}^* = [0, 1, 1, 1]^T \quad f(\mathbf{x}^*) = 0$$

This is a severely nonlinear function in all variables.

### 4. Powell (1962)

$$f(\mathbf{x}) = (x_1 + 10x_2)^2 + 5(x_3 - x_4)^2 + (x_2 - 2x_3)^4 + 10(x_1 - x_4)^4$$

$$\mathbf{x}^{(0)} = [3, -1, 0, 1]^T \quad \mathbf{x}^* = [0, 0, 0, 0]^T \quad f(\mathbf{x}^*) = 0$$

For this problem the Hessian matrix of  $f$  at  $\mathbf{x}^*$  is singular

### 5. Fletcher and Powell (1963)

$$f(\mathbf{x}) = 100\{(x_3 - 10\theta)^2 + (r - 1)^2\} + x_3^2$$

where

$$r = |(x_1^2 + x_2^2)^{1/2}|$$

and

$$\theta = \begin{cases} \frac{1}{2\pi} \tan^{-1} \left( \frac{x_2}{x_1} \right) & (x_1 > 0) \\ \frac{1}{2\pi} \tan^{-1} \left( \frac{x_2}{x_1} \right) + \frac{1}{2} & (x_1 < 0) \end{cases}$$

$$\mathbf{x}^{(0)} = [-1, 0, 0]^T \quad \mathbf{x}^* = [1, 0, 0]^T \quad f(\mathbf{x}^*) = 0$$

This is a steep-sided valley which follows a helical path. It presents the same kind of difficulties as Problem 1.

### 6. Dixon (1973b)

$$f(\mathbf{x}) = (1 - x_1)^2 + (1 - x_{10})^2 + \sum_{i=1}^9 (x_i^2 - x_{i+1})^2$$

$$\mathbf{x}^{(0)} = [-2, \dots, -2]^T \quad \mathbf{x}^* = [1, \dots, 1]^T \quad f(\mathbf{x}^*) = 0$$

This objective function has 10 variables and provides some indication of the behaviour of optimization methods as the number of variables increases.

### 7. Powell (1966)

$$f(\mathbf{x}) = x_1^4 + x_1 x_2 + (1 + x_2)^2$$

$$\mathbf{x}^{(0)} = [0, 0]^T$$

For this problem,

$$\min_{\alpha} f(\mathbf{x}^{(0)} - \alpha \mathbf{G}^{(0)-1} \mathbf{g}^{(0)}) = f(\mathbf{x}^{(0)})$$

so that no progress can be made beyond  $\mathbf{x}^{(0)}$  by using Newton's method together with an exact line search.

### 8. Hartley (1961)

$$S(\mathbf{x}) = \sum_{i=1}^m \{Y(t_i; \mathbf{x}) - y_i\}^2$$

where

$$Y(t_i; \mathbf{x}) = x_1 + x_2 \exp(t_i x_3)$$

and the  $t_i$  and the  $y_i$  are given in the following table.

| $i$ | $t_i$ | $y_i$ |
|-----|-------|-------|
| 1   | -5    | 127   |
| 2   | -3    | 151   |
| 3   | 1     | 421   |
| 4   | 3     | 460   |
| 5   | 5     | 426   |
| 6   | -1    | 379   |

For this problem,  $m = 6, n = 3$  and

$$\mathbf{x}^{(0)} = [580, -180, -0.16]^T \quad S^{(0)} \approx 0.3 \times 10^5$$

$$\mathbf{x}^* = [523.3, -157.0, -0.1994]^T \quad S^* \approx 0.13 \times 10^5$$

This is a least squares problem in which  $S^*$  is non-zero.

9. Meyer and Roth (1972)

$$S(\mathbf{x}) = \sum_{i=1}^m \{Y(t_i; \mathbf{x}) - y_i\}^2$$

in which

$$Y(t_i; \mathbf{x}) = \frac{x_1 x_3 t_{1i}}{(1 + x_1 t_{1i} + x_2 t_{2i})}$$

and the  $t_i$  and the  $y_i$  are given in the following table.

| $i$ | $t_{1i}$ | $t_{2i}$ | $y_i$ |
|-----|----------|----------|-------|
| 1   | 1.0      | 1.0      | 0.126 |
| 2   | 2.0      | 1.0      | 0.219 |
| 3   | 1.0      | 2.0      | 0.076 |
| 4   | 2.0      | 2.0      | 0.126 |
| 5   | 0.1      | 0.0      | 0.186 |

For this problem,  $m = 5, n = 3$  and

$$\mathbf{x}^{(0)} = [10.39, 48.83, 0.74]^T \quad S^{(0)} \approx 0.365 \times 10^{-1}$$

$$\mathbf{x}^* = [3.13, 15.16, 0.78]^T \quad S^* \approx 0.4 \times 10^{-4}$$

This least squares problem was originally presented by Box and Hunter (1965). As in Problem 8,  $S^*$  is non-zero.

10. Meyer and Roth (1972)

$$S(\mathbf{x}) = \sum_{i=1}^m \{Y(t_i; \mathbf{x}) - y_i\}^2$$

where

$$Y(t_i; \mathbf{x}) = x_1 \exp \left\{ \frac{x_2}{(t_i + x_3)} \right\}$$

and the  $t_i$  and the  $y_i$  are given in the following table.

| $i$ | $t_i$ | $y_i$  |
|-----|-------|--------|
| 1   | 50    | 34 780 |
| 2   | 55    | 28 610 |
| 3   | 60    | 23 650 |
| 4   | 65    | 19 630 |
| 5   | 70    | 16 370 |
| 6   | 75    | 13 720 |
| 7   | 80    | 11 540 |
| 8   | 85    | 9 744  |
| 9   | 90    | 8 261  |
| 10  | 95    | 7 030  |
| 11  | 100   | 6 005  |
| 12  | 105   | 5 147  |
| 13  | 110   | 4 427  |
| 14  | 115   | 3 820  |
| 15  | 120   | 3 307  |
| 16  | 125   | 2 872  |

For this problem,  $m = 16, n = 3$  and

$$\mathbf{x}^{(0)} = [0.02, 4000, 250]^T \quad S^{(0)} \approx 0.17 \times 10^{10}$$

$$\mathbf{x}^* = [0.0056, 6181.4, 345.2]^T \quad S^* \approx 88$$

The data for this least squares problem give the resistance of a thermistor as a function of temperature. The problem defeats many least squares fitting procedures.

11. Pereyra (1967)

$$S(\mathbf{x}) = \sum_{i=1}^m \{Y(t_i; \mathbf{x}) - y_i\}^2$$

where

$$Y(t_i; \mathbf{x}) = x_2 \sin(t_i x_1) + x_3$$

The data are obtained from

$$y_i = \sin t_i \quad (i = 1, \dots, 13)$$

where the values of the  $t_i$  are given in the following table.

| $i$ | $t_i$ | $i$ | $t_i$ |
|-----|-------|-----|-------|
| 1   | 0.105 | 7   | 1.1   |
| 2   | 0.25  | 8   | 1.25  |
| 3   | 0.4   | 9   | 1.35  |
| 4   | 0.55  | 10  | 1.45  |
| 5   | 0.7   | 11  | 1.55  |
| 6   | 0.9   | 12  | 1.57  |
|     |       | 13  | 1.6   |



For this problem,  $m = 13$ ,  $n = 3$ , and

$$\mathbf{x}^{(0)} = [0.9, 0.9, 0.1]^T \quad S^{(0)} \approx 0.16 \times 10^{-1}$$

$$\mathbf{x}^* = [1.0, 1.0, 0.0]^T \quad S^* = 0.0$$

12. Meyer and Roth (1972)

$$S(\mathbf{x}) = \sum_{i=1}^m \{Y(t_i; \mathbf{x}) - y_i\}^2$$

where

$$Y(t_i; \mathbf{x}) = x_3 \{\exp(-x_1 t_{1i}) + \exp(-x_2 t_{2i})\}$$

The values of  $y_i$  are computed from  $Y(t_i; \mathbf{x}^*)$  with the values of  $t_{1i}$  and  $t_{2i}$  given in the following table.

| $i$ | $t_{1i}$ | $t_{2i}$ |
|-----|----------|----------|
| 1   | 0.0      | 0.0      |
| 2   | 0.6      | 0.4      |
| 3   | 0.6      | 1.0      |
| 4   | 1.4      | 1.4      |
| 5   | 2.6      | 1.4      |
| 6   | 3.2      | 1.6      |
| 7   | 0.8      | 2.0      |
| 8   | 1.6      | 2.2      |
| 9   | 2.6      | 2.2      |
| 10  | 4.0      | 2.2      |
| 11  | 1.2      | 2.6      |
| 12  | 2.0      | 2.6      |
| 13  | 4.6      | 2.8      |
| 14  | 3.2      | 3.0      |
| 15  | 1.6      | 3.2      |
| 16  | 4.2      | 3.4      |
| 17  | 2.0      | 3.8      |
| 18  | 3.2      | 3.8      |
| 19  | 2.8      | 4.2      |
| 20  | 4.2      | 4.2      |
| 21  | 5.4      | 4.4      |
| 22  | 5.6      | 4.8      |
| 23  | 3.2      | 5.0      |

For this problem,  $m = 23$ ,  $n = 3$  and

$$\mathbf{x}^{(0)} = [12.0, 1.0, 25.0]^T \quad S^{(0)} \approx 216.0$$

$$\mathbf{x}^* = [14.3, 1.5, 20.1]^T \quad S^* = 0.0$$

The double exponential formula is notoriously difficult to fit to a set of data.

## APPENDIX C

# The Cholesky Decomposition of a Symmetric Positive Definite Matrix

In this appendix we prove Theorem 3.4.1 which for convenience is restated.

*Theorem 3.4.1*

If  $\mathbf{A}$  is an  $n \times n$  symmetric positive definite matrix, then there exists a lower triangular matrix  $\mathbf{L}$  such that  $\mathbf{A} = \mathbf{L}\mathbf{L}^T$ .

*Proof*

The theorem is trivially true for  $n = 1$  because a  $1 \times 1$  positive definite matrix is equivalent to a positive real number, which certainly has a square root.

Let  $\mathbf{A}_i$  be the  $i \times i$  principal minor matrix of  $\mathbf{A}$  (i.e. the matrix formed from the first  $i$  rows and the first  $i$  columns of  $\mathbf{A}$ ). Since  $\mathbf{A}$  is positive definite,  $\mathbf{x}^T \mathbf{A} \mathbf{x} > 0$  ( $\forall \mathbf{x} \neq \mathbf{0}$ ). In particular,  $\mathbf{x}_i^T \mathbf{A} \mathbf{x}_i > 0$ , where  $\mathbf{x}_i$  is given by

$$\mathbf{x}_i = [x_{1i}, \dots, x_{ii}, 0, \dots, 0]^T$$

in which the first  $i$  elements  $x_{ji}$  ( $j = 1, \dots, i$ ) of  $\mathbf{x}_i$  are non-zero.

Now  $\mathbf{A}$  may be partitioned according to

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_i & \mathbf{P}_i \\ \mathbf{Q}_i & \mathbf{R}_i \end{bmatrix}$$

where  $\mathbf{P}_i$ ,  $\mathbf{Q}_i$ , and  $\mathbf{R}_i$  are  $i \times (n-i)$ ,  $(n-i) \times i$ , and  $(n-i) \times (n-i)$  matrices respectively, and  $1 \leq i \leq n-1$ . So

$$\mathbf{x}_i^T \mathbf{A} \mathbf{x}_i = \mathbf{y}_i^T \mathbf{A}_i \mathbf{y}_i$$

where

$$\mathbf{y}_i = [x_{1i}, \dots, x_{ii}]^T$$

Hence

$$\mathbf{y}_i^T \mathbf{A}_i \mathbf{y}_i > 0 \quad (\forall \mathbf{y}_i \neq \mathbf{0})$$

and so  $\mathbf{A}_i$  is positive definite. Clearly this holds for  $i = 1, \dots, n$  so all principal minor matrices  $\mathbf{A}_i$  of a positive definite matrix  $\mathbf{A}$  are themselves positive definite.

Suppose that there is a lower triangular matrix  $\mathbf{L}_{i-1}$  such that

$$\mathbf{A}_{i-1} = \mathbf{L}_{i-1} \mathbf{L}_{i-1}^T \quad (\text{C.1})$$

for some  $i \geq 2$ . We shall show that this implies the existence of a lower triangular matrix  $\mathbf{L}_i$  such that

$$\mathbf{A}_i = \mathbf{L}_i \mathbf{L}_i^T \quad (\text{C.2})$$



## A Criterion for the Convergence of a Sequence in a Compact Set of $\{R^n, \|\cdot\|\}$

In the proof of Theorem 7.7.2 it is stated that if the sequence  $\{x^{(k)}\}$  has only one limit point then we are entitled to assert that  $\{x^{(k)}\}$  is convergent. This is a consequence of a theorem which, it would appear, is seldom proved in textbooks of analysis, although often quoted in various forms.

### Theorem J.1

If 1.  $\{R^n, \|\cdot\|\}$  is a normed linear space;  
 2.  $S \subset R^n$  is compact;  
 3.  $\{x^{(k)}\}$  is a sequence in  $S$ ;  
 4.  $x^*$  is the unique limit point of  $\{x^{(k)}\}$ ,  
 then  $\{x^{(k)}\}$  converges to  $x^*$  as  $k \rightarrow \infty$ .

### Proof

Suppose that the sequence  $\{x^{(k)}\}$  does not converge to  $x^*$ . Then there is a subsequence  $\{x^{(k_i)}\}$  of  $\{x^{(k)}\}$  and a real number  $\epsilon > 0$  such that

$$\|x^{(k_i)} - x^*\| > \epsilon \quad (\forall i)$$

Therefore no subsequence of  $\{x^{(k_i)}\}$  converges to  $x^*$ . Therefore by Hypothesis 4, no subsequence of  $\{x^{(k_i)}\}$  converges. But by Hypothesis 3,  $\{x^{(k_i)}\}$  lies in  $S$ , and so by Hypothesis 2 and Definition 1.3.6,  $\{x^{(k_i)}\}$  must contain a subsequence  $\{x^{(k_j)}\}$  which is convergent in  $S$ . Also, since  $\{x^{(k_j)}\}$  is a subsequence of  $\{x^{(k)}\}$ , then  $\{x^{(k_j)}\}$  must converge to  $x^*$  by Hypothesis 4. This contradicts the fact that no subsequence of  $\{x^{(k_i)}\}$  converges to  $x^*$ . Therefore  $\{x^{(k)}\}$  converges to  $x^*$ .  $\square$

For a far more sophisticated treatment of the convergence of descent methods and, in particular, of the ideas presented in Section 7.7 the reader should consult Chapter 14 of the book by Ortega and Rheinboldt (1970).

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