Modern Fortran routines for testing unconstrained optimization software with derivatives up to third-order*

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Abstract

In this report, we provide a user guide to the modern Fortran package implementation of the problems proposed by J. J. Moré, B. S. Garbow, and K. E. Hillstrom (*ACM Trans. Math. Softw.* 7, 14–41, 136–140, 1981). Furthermore, for each problem, the expressions of the objective function and its derivatives up to order three are given.

Key words: unconstrained minimization, third-order derivatives subroutines, testset.

1 User guide

2 Test problems and derivatives expressions

For each test problem, we show

(a) Number of variables and equations (from [1])

(b) Objective function expressions (from [1])

(c) Initial point (from [1])

(d) Local optimizer (from [1])

(e) First-order derivative expressions

(f) Second-order derivative expressions

(g) Third-order derivative expressions

Remark: Null derivatives are omitted. Only terms $h_{i,j}$ from any Hessian such that $i \leq j$ are showed. Similarly, only terms $t_{i,j,k}$ from any third-order derivative tensor such that $i \leq j \leq k$ are showed.

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2.1 Rosenbrock

(a) $n = 2, \quad m = 2$

(b) $f_1 = 10(x_2 - x_1^2)$
$f_2 = 1 - x_1$

(c) $x_0 = (-1.2, 1)^T$

(d) $f = 0$ at $(1, 1)^T$

(e) **First-order partial derivatives**

$$\frac{\partial f_1}{\partial x_1} = -20x_1$$

$$\frac{\partial f_2}{\partial x_1} = -1$$

(f) **Second-order partial derivatives**

$$\frac{\partial^2 f_1}{\partial x_1^2} = -20$$

2.2 Freudstein and Roth

(a) $n = 2, \quad m = 2$

(b) $f_1(x) = -13 + x_1 + ((5 - x_2)x_2 - 2)x_2$
$f_2(x) = -29 + x_1 + ((x_2 + 1)x_2 - 14)x_2$

(c) $x_0 = (0.5, -2)^T$

(d) $f = 0$ at $(5, 4)^T$
$f = 48.9842\ldots$ at $(11.41\ldots, -0,8968\ldots)^T$

(e) **First-order partial derivatives**

$$\frac{\partial f_1}{\partial x_1} = 1$$

$$\frac{\partial f_1}{\partial x_2} = (10 - 3x_2)x_2 - 2$$

$$\frac{\partial f_2}{\partial x_1} = 1$$

$$\frac{\partial f_2}{\partial x_2} = (3x_2 + 2)x_2 - 14$$

(f) **Second-order partial derivatives**

$$\frac{\partial^2 f_1}{\partial x_2^2} = 10 - 6x_2$$

$$\frac{\partial^2 f_2}{\partial x_2^2} = 6x_2 + 2$$

(g) **Third-order partial derivatives**

$$\frac{\partial^3 f_1}{\partial x_2^3} = -6$$

$$\frac{\partial^3 f_2}{\partial x_2^3} = 6$$

2.3 Powell badly scaled

(a) $n = 2, \quad m = 2$

(b) $f_1(x) = 10^4 x_1 x_2 - 1$
$f_2(x) = \mathrm{e}^{-x_1} + \mathrm{e}^{-x_2} - 1.0001$

(c) $x_0 = (0, 1)^T$

(d) $f = 0$ at $(1.098 \ldots 10^{-5}, 9.106 \ldots)^T$

(e) **First-order partial derivatives**

$$\frac{\partial f_1}{\partial x_1} = 10^4 x_2$$

$$\frac{\partial f_1}{\partial x_2} = 10^4 x_1$$

$$\frac{\partial f_2}{\partial x_1} = -\mathrm{e}^{-x_1}$$

$$\frac{\partial f_2}{\partial x_2} = -\mathrm{e}^{-x_2}$$

(f) **Second-order partial derivatives**

$$\frac{\partial^2 f_2}{\partial x_1^2} = \mathrm{e}^{-x_1}$$

$$\frac{\partial^2 f_1}{\partial x_1 \partial x_2} = 10^4$$

$$\frac{\partial^2 f_2}{\partial x_2^2} = \mathrm{e}^{-x_2}$$

(g) **Third-order partial derivatives**

$$\frac{\partial^3 f_2}{\partial x_1^3} = -\mathrm{e}^{-x_1}$$

$$\frac{\partial^3 f_2}{\partial x_2^3} = -\mathrm{e}^{-x_2}$$

2.4 Brown badly scaled

(a) $n = 2, \quad m = 3$

(b) $f_1(x) = x_1 - 10^6$

$f_2(x) = x_2 - 2 \times 10^{-6}$

$f_3(x) = x_1 x_2 - 2$

(c) $x_0 = (1, 1)^T$

(d) $f = 0$ at $(10^6, 2 \times 10^{-6})^T$

(e) **First-order partial derivatives**

$$\frac{\partial f_1}{\partial x_1} = 1$$

$$\frac{\partial f_2}{\partial x_2} = 1$$

$$\frac{\partial f_3}{\partial x_1} = x_2$$

$$\frac{\partial f_3}{\partial x_2} = x_1$$

(f) **Second-order partial derivatives**

$$\frac{\partial^2 f_3}{\partial x_1 \partial x_2} = 1$$

2.5 Beale

(a) $n = 2, \quad m = 3$

(b) $f_i = y_i - x_1(1 - x_2^i)$,
where $y_1 = 1{,}5, \quad y_2 = 2{,}25, \quad y_3 = 2{,}625$

(c) $x_0 = (1, 1)^T$

(d) $f = 0$ at $(3, 0.5)^T$

(e) **First-order partial derivatives**

$$\frac{\partial f_i}{\partial x_1} = x_2^i - 1$$

$$\frac{\partial f_i}{\partial x_2} = i x_1 x_2^{i-1}$$

(f) **Second-order partial derivatives**

$$\frac{\partial^2 f_i}{\partial x_1 \partial x_2} = i x_2^{i-1}$$

$$\frac{\partial^2 f_i}{\partial x_2^2} = i(i-1) x_1 x_2^{i-2}$$

(g) **Third-order partial derivatives**

$$\frac{\partial^3 f_i}{\partial x_1 \partial x_2^2} = i(i-1)x_2^{i-2}$$

$$\frac{\partial^3 f_i}{\partial x_2^3} = i(i-1)(i-2)x_1 x_2^{i-3}$$

2.6 Jennrich e Sampson

(a) $n = 2, \quad m \geq n$

(b) $f_i(x) = 2 + 2i - (\mathrm{e}^{ix_1} + \mathrm{e}^{ix_2})$

(c) $x_0 = (0.3, 0.4)^T$

(d) $f = 124.362\ldots$ at $x_1 = x_2 = 0.2578\ldots$ for $m = 10$

(e) **First-order partial derivatives**

(f) **Second-order partial derivatives**

(g) **Third-order partial derivatives**

2.7 Helical valley

(a) $n = 3, \quad m = 3$

(b) $f_1(x) = 10[x_3 - 10\theta(x_1, x_2)]$
$f_2(x) = 10[(x_1^2 + x_2^2)^{1/2} - 1]$
$f_3(x) = x_3$

where

$$\theta(x_1, x_2) = \begin{cases} \dfrac{1}{2\pi} \arctan\left(\dfrac{x_2}{x_1}\right), & \text{se } x_1 > 0 \\ \dfrac{1}{2\pi} \arctan\left(\dfrac{x_2}{x_1}\right) + 0.5, & \text{se } x_1 < 0 \end{cases}$$

(c) $x_0 = (-1, 0, 0)^T$

(d) $f = 0$ at $(1, 0, 0)^T$

(e) **First-order partial derivatives**

$$\frac{\partial \theta}{\partial x_1} = -\frac{x_2}{2\pi(x_1^2 + x_2^2)}$$
$$\frac{\partial \theta}{\partial x_2} = \frac{x_1}{2\pi(x_1^2 + x_2^2)}$$
$$\frac{\partial f_1}{\partial x_1} = \frac{50x_2}{\pi(x_1^2 + x_2^2)}$$
$$\frac{\partial f_1}{\partial x_2} = -\frac{50x_1}{\pi(x_1^2 + x_2^2)}$$
$$\frac{\partial f_1}{\partial x_3} = 10$$
$$\frac{\partial f_2}{\partial x_1} = \frac{10x_1}{(x_1^2 + x_2^2)^{1/2}}$$
$$\frac{\partial f_2}{\partial x_2} = \frac{10x_2}{(x_1^2 + x_2^2)^{1/2}}$$
$$\frac{\partial f_3}{\partial x_3} = 1$$

(f) **Second-order partial derivatives**

$$\frac{\partial^2 f_1}{\partial x_1^2} = -\frac{100x_1x_2}{\pi(x_1^2 + x_2^2)^2}$$
$$\frac{\partial^2 f_1}{\partial x_1 \partial x_2} = \frac{50(x_1^2 - x_2^2)}{\pi(x_1^2 + x_2^2)^2}$$
$$\frac{\partial^2 f_1}{\partial x_2^2} = \frac{100x_1x_2}{\pi(x_1^2 + x_2^2)^2}$$
$$\frac{\partial^2 f_2}{\partial x_1^2} = \frac{10x_2^2}{(x_1^2 + x_2^2)^{3/2}}$$
$$\frac{\partial^2 f_2}{\partial x_1 \partial x_2} = -\frac{10x_1x_2}{(x_1^2 + x_2^2)^{3/2}}$$
$$\frac{\partial^2 f_2}{\partial x_2^2} = \frac{10x_1^2}{(x_1^2 + x_2^2)^{3/2}}$$

(g) **Third-order partial derivatives**

$$\frac{\partial^3 f_1}{\partial x_1^3} = \frac{100(3x_1^2x_2 - x_2^3)}{\pi(x_1^2 + x_2^2)^3}$$
$$\frac{\partial^3 f_1}{\partial x_1^2 \partial x_2} = \frac{100(3x_1x_2^2 - x_1^3)}{\pi(x_1^2 + x_2^2)^3}$$
$$\frac{\partial^3 f_1}{\partial x_1 \partial x_2^2} = -\frac{100(3x_1^2x_2 - x_2^3)}{\pi(x_1^2 + x_2^2)^3}$$

$$\frac{\partial^3 f_1}{\partial x_2^3} = -\frac{100(3x_1x_2^2 - x_1^3)}{\pi(x_1^2 + x_2^2)^3}$$

$$\frac{\partial^3 f_2}{\partial x_1^3} = -\frac{30x_1x_2^2}{(x_1^2 + x_2^2)^{5/2}}$$

$$\frac{\partial^3 f_2}{\partial x_1^2 \partial x_2} = \frac{10(2x_1^2x_2 - x_2^3)}{(x_1^2 + x_2^2)^{5/2}}$$

$$\frac{\partial^3 f_2}{\partial x_1 \partial x_2^2} = \frac{10(2x_1x_2^2 - x_1^3)}{(x_1^2 + x_2^2)^{5/2}}$$

$$\frac{\partial^3 f_2}{\partial x_2^3} = -\frac{30x_1^2x_2}{(x_1^2 + x_2^2)^{5/2}}$$

2.8 Bard

(a) $n = 3, \quad m = 15$

(b) $f_i = y_i - \left(x_1 + \dfrac{u_i}{v_ix_2 + w_ix_3}\right)$

where $u_i = i, \quad v_i = 16 - i, \quad w_i = \min(u_i, v_i), \quad$ and

i	y_i	i	y_i	i	y_i
1	0,14	6	0,32	11	0,73
2	0,18	7	0,35	12	0,96
3	0,22	8	0,39	13	1,34
4	0,25	9	0,37	14	2,10
5	0,29	10	0,58	15	4,39

(c) $x_0 = (1, 1, 1)^T$

(d) $f = 8.21487\ldots 10^{-3}$

$f = 17.4286\ldots$ at $(0.8406\ldots, -\infty, -\infty)^T$

(e) **First-order partial derivatives**

$$\frac{\partial f_i}{\partial x_1} = -1$$

$$\frac{\partial f_i}{\partial x_2} = \frac{u_iv_i}{(v_ix_2 + w_ix_3)^2}$$

$$\frac{\partial f_i}{\partial x_3} = \frac{u_iw_i}{(v_ix_2 + w_ix_3)^2}$$

(f) **Second-order partial derivatives**

$$\frac{\partial^2 f_i}{\partial x_2^2} = -\frac{2u_iv_i^2}{(v_ix_2 + w_ix_3)^3}$$

$$\frac{\partial^2 f_i}{\partial x_2 \partial x_3} = -\frac{2u_iv_iw_i}{(v_ix_2 + w_ix_3)^3}$$

$$\frac{\partial^2 f_i}{\partial x_3^2} = -\frac{2u_iw_i^2}{(v_ix_2 + w_ix_3)^3}$$

(g) **Third-order partial derivatives**

$$\frac{\partial^3 f_i}{\partial x_2^3} = \frac{6u_i v_i^3}{(v_i x_2 + w_i x_3)^4}$$

$$\frac{\partial^3 f_i}{\partial x_2^2 \partial x_3} = \frac{6u_i v_i^2 w_i}{(v_i x_2 + w_i x_3)^4}$$

$$\frac{\partial^3 f_i}{\partial x_2 \partial x_3 \partial x_2} = \frac{6u_i v_i w_i^2}{(v_i x_2 + w_i x_3)^4}$$

$$\frac{\partial^3 f_i}{\partial x_3^3} = \frac{6u_i w_i^3}{(v_i x_2 + w_i x_3)^4}$$

2.9 Gaussian

(a) $n = 3, \quad m = 15$

(b) $f_i(x) = x_1 \mathrm{e}^{-x_2(t_i - x_3)^2/2} - y_i$,
where $t_i = (8 - i)/2$ and

i	y_i
$1, 15$	0,0009
$2, 14$	0,0044
$3, 13$	0,0175
$4, 12$	0,0540
$5, 11$	0,1295
$6, 10$	0,2420
$7, 9$	0,3521
8	0,3989

(c) $x_0 = (0.4, 1, 0)^T$

(d) $f = 1.12793\ldots 10^{-8}$

(e) **First-order partial derivatives**

$$\frac{\partial f_i}{\partial x_1} = \mathrm{e}^{-x_2(t_i - x_3)^2/2}$$

$$\frac{\partial f_i}{\partial x_2} = -\frac{x_1(t_i - x_3)^2}{2} \mathrm{e}^{-x_2(t_i - x_3)^2/2}$$

$$\frac{\partial f_i}{\partial x_3} = x_1 x_2 (t_i - x_3) \mathrm{e}^{-x_2(t_i - x_3)^2/2}$$

(f) **Second-order partial derivatives**

$$\frac{\partial^2 f_i}{\partial x_1 \partial x_2} = -\frac{(t_i - x_3)^2}{2} \mathrm{e}^{-x_2(t_i-x_3)^2/2}$$

$$\frac{\partial^2 f_i}{\partial x_1 \partial x_3} = x_2(t_i - x_3)\mathrm{e}^{-x_2(t_i-x_3)^2/2}$$

$$\frac{\partial^2 f_i}{\partial x_2^2} = \frac{x_1(t_i - x_3)^4}{4} \mathrm{e}^{-x_2(t_i-x_3)^2/2}$$

$$\frac{\partial^2 f_i}{\partial x_2 \partial x_3} = x_1(t_i - x_3)\mathrm{e}^{-x_2(t_i-x_3)^2/2} \left[-\frac{x_2(t_i - x_3)^2}{2} + 1\right]$$

$$\frac{\partial^2 f_i}{\partial x_3^2} = x_1 x_2 \mathrm{e}^{-x_2(t_i-x_3)^2/2} \left[x_2(t_i - x_3)^2 - 1\right]$$

(g) **Third-order partial derivatives**

$$\frac{\partial^3 f_i}{\partial x_1 \partial x_2^2} = \frac{(t_i - x_3)^4}{4} \mathrm{e}^{-x_2(t_i-x_3)^2/2}$$

$$\frac{\partial^3 f_i}{\partial x_1 \partial x_2 \partial x_3} = (t_i - x_3)\mathrm{e}^{-x_2(t_i-x_3)^2/2} \left[-\frac{x_2(t_i - x_3)^2}{2} + 1\right]$$

$$\frac{\partial^3 f_i}{\partial x_1 \partial x_3^2} = x_2 \mathrm{e}^{-x_2(t_i-x_3)^2/2} \left[x_2(t_i - x_3)^2 - 1\right]$$

$$\frac{\partial^3 f_i}{\partial x_1 \partial x_3^2} = -\frac{x_1(t_i - x_3)^6}{8} \mathrm{e}^{-x_2(t_i-x_3)^2/2}$$

$$\frac{\partial^3 f_i}{\partial x_2^2 \partial x_3} = x_1(t_i - x_3)^3 \mathrm{e}^{-x_2(t_i-x_3)^2/2} \left[\frac{x_2(t_i - x_3)^2}{4} - 1\right]$$

$$\frac{\partial^3 f_i}{\partial x_2 \partial x_3^2} = x_1 \mathrm{e}^{-x_2(t_i-x_3)^2/2} \left\{\frac{x_2(t_i - x_3)^2}{2} \left[5 - x_2(t_i - x_3)^2\right] - 1\right\}$$

$$\frac{\partial^3 f_i}{\partial x_3^3} = x_1 x_2^2 (t_i - x_3)\mathrm{e}^{-x_2(t_i-x_3)^2/2} \left[x_2(t_i - x_3)^2 - 3\right]$$

2.10 Meyer

(a) $n = 3, \quad m = 16$

(b) $f_i(x) = x_1 \mathrm{e}^{x_2/(t_i+x_3)} - y_i$,

where $t_i = 45 + 5i$ and

i	y_i	i	y_i
1	34780	9	8261
2	28610	10	7030
3	23650	11	6005
4	19630	12	5147
5	16370	13	4427
6	13720	14	3820
7	11540	15	3307
8	9744	16	2872

(c) $x_0 = (0.02, 4000, 250)^T$

(d) $f = 87.9458\ldots$

(e) **First-order partial derivatives**

$$\frac{\partial f_i}{\partial x_1} = \mathrm{e}^{x_2/(t_i+x_3)}$$
$$\frac{\partial f_i}{\partial x_2} = \frac{x_1}{t_i+x_3}\mathrm{e}^{x_2/(t_i+x_3)}$$
$$\frac{\partial f_i}{\partial x_3} = -\frac{x_1 x_2}{(t_i+x_3)^2}\mathrm{e}^{x_2/(t_i+x_3)}$$

(f) **Second-order partial derivatives**

$$\frac{\partial^2 f_i}{\partial x_1 \partial x_2} = \frac{1}{t_i+x_3}\mathrm{e}^{x_2/(t_i+x_3)}$$
$$\frac{\partial^2 f_i}{\partial x_1 \partial x_3} = -\frac{x_2}{(t_i+x_3)^2}\mathrm{e}^{x_2/(t_i+x_3)}$$
$$\frac{\partial^2 f_i}{\partial x_2^2} = \frac{x_1}{(t_i+x_3)^2}\mathrm{e}^{x_2/(t_i+x_3)}$$
$$\frac{\partial^2 f_i}{\partial x_2 \partial x_3} = -\frac{x_1}{(t_i+x_3)^2}\mathrm{e}^{x_2/(t_i+x_3)}\left[\frac{x_2}{t_i+x_3}+1\right]$$
$$\frac{\partial^2 f_i}{\partial x_3^2} = \frac{x_1 x_2}{(t_i+x_3)^3}\mathrm{e}^{x_2/(t_i+x_3)}\left[\frac{x_2}{t_i+x_3}+2\right]$$

(g) **Third-order partial derivatives**

$$\frac{\partial^3 f_i}{\partial x_1 \partial x_2^2} = \frac{1}{(t_i+x_3)^2}\mathrm{e}^{x_2/(t_i+x_3)}$$
$$\frac{\partial^3 f_i}{\partial x_1 \partial x_2 \partial x_3} = -\frac{1}{(t_i+x_3)^2}\mathrm{e}^{x_2/(t_i+x_3)}\left[\frac{x_2}{t_i+x_3}+1\right]$$
$$\frac{\partial^3 f_i}{\partial x_1 \partial x_3^2} = \frac{x_2}{(t_i+x_3)^3}\mathrm{e}^{x_2/(t_i+x_3)}\left[\frac{x_2}{t_i+x_3}+2\right]$$
$$\frac{\partial^3 f_i}{\partial x_2^3} = \frac{x_1}{(t_i+x_3)^3}\mathrm{e}^{x_2/(t_i+x_3)}$$
$$\frac{\partial^3 f_i}{\partial x_2^2 \partial x_3} = -\frac{x_1}{(t_i+x_3)^3}\mathrm{e}^{x_2/(t_i+x_3)}\left[\frac{x_2}{t_i+x_3}+2\right]$$
$$\frac{\partial^3 f_i}{\partial x_2 \partial x_3^2} = \frac{x_1}{(t_i+x_3)^3}\mathrm{e}^{x_2/(t_i+x_3)}\left[\left(\frac{x_2}{t_i+x_3}+2\right)^2-2\right]$$
$$\frac{\partial^3 f_i}{\partial x_3^3} = -\frac{x_1 x_2}{(t_i+x_3)^4}\mathrm{e}^{x_2/(t_i+x_3)}\left[\left(\frac{x_2}{t_i+x_3}+3\right)^2-3\right]$$