

**Comparison of the modern conjugate gradient methods:
DESCON, CUBIC, CG-DESCENT (4.1)
for solving 14 small-scale applications of unconstrained optimization**

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This technical report presents a comparison of performances of modern conjugate gradient methods DESCN [19], CUBIC [20], CG-DESCENT version (4.1) [21] for solving a collection of 14 applications of unconstrained optimization.

DESCN is a conjugate gradient method for which the search direction satisfies both the sufficient descent and conjugacy conditions implementing a modified Wolfe line search (see Andrei,). CUBIC implements a conjugate gradient with subspace minimization based on regularization model of the minimizing function (see Andrei, 2020, Chapter 11, pp. 400-414). CG-DESCENT is a conjugate gradient method with sufficient descent condition (see Hager and Zhang, 2005).

The applications used in these numerical experiments are as follows:

1. Weber Function [1, pp. 58]

$$f(x) = 2\sqrt{(x_1 - 2)^2 + (x_2 - 42)^2} + 4\sqrt{(x_1 - 90)^2 + (x_2 - 11)^2} + 5\sqrt{(x_1 - 43)^2 + (x_2 - 88)^2}.$$

2. Enzyme reaction [1, pp. 62]

$$f(x) = \sum_{i=1}^{11} \left(y_i - \frac{x_1(u_i^2 + u_i x_2)}{u_i^2 + u_i x_3 + x_4} \right)^2,$$

where y_i and u_i have the following values:

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i	y_i	u_i	i	y_i	u_i
1	0.1957	4.000	7	0.0456	0.125
2	0.1947	2.000	8	0.0342	0.100
3	0.1735	1.000	9	0.0323	0.0833
4	0.1600	0.500	10	0.0235	0.0714
5	0.0844	0.250	11	0.0246	0.0625
6	0.0627	0.167			

3. Solution of a chemical reactor [2, pp. 1455-1481]

$$\begin{aligned}
f(x) = & (1 - x_1 - k_1 x_1 x_6 + r_1 x_4)^2 \\
& + (1 - x_2 - k_2 x_2 x_6 + r_2 x_5)^2 \\
& + (-x_3 + 2k_3 x_4 x_5)^2 \\
& + (k_1 x_1 x_6 - r_1 x_4 - k_3 x_4 x_5)^2 \\
& + (1,5(k_2 x_2 x_6 - r_2 x_5) - k_3 x_4 x_5)^2 \\
& + (1 - x_4 - x_5 - x_6)^2
\end{aligned}$$

where: $k_1 = 31,24$ $k_2 = 0,272$ $k_3 = 303,03$ $r_1 = 2,062$ $r_2 = 0,02$.

4. Robot kinematics problem [3, pp. 152-157], [4, pp. 101-103], [5, pp. 329-331]

$$\begin{aligned}
f(x) = & (4,731 \cdot 10^{-3} x_1 x_3 - 0,3578 x_2 x_3 - \\
& 0,1238 x_1 + x_7 - 1,637 \cdot 10^{-3} x_2 - 0,9338 x_4 - 0,3571)^2 \\
& +(0,2238 x_1 x_3 + 0,7623 x_2 x_3 \\
& + 0,2638 x_1 - x_7 - 0,07745 x_2 - 0,6734 x_4 - 0,6022)^2 \\
& +(x_6 x_8 + 0,3578 x_1 + 4,731 \cdot 10^{-3} x_2)^2 \\
& +(-0,7623 x_1 + 0,2238 x_2 + 0,3461)^2 \\
& +(x_1^2 + x_2^2 - 1)^2 \\
& +(x_3^2 + x_4^2 - 1)^2 \\
& +(x_5^2 + x_6^2 - 1)^2 \\
& +(x_7^2 + x_8^2 - 1)^2.
\end{aligned}$$

5. Solar Spectroscopy [1, p. 68]

$$f(x) = \sum_{i=1}^{13} \left(x_1 + x_2 \exp \left(-\frac{(i+x_3)^2}{x_4} \right) - y_i \right)^2,$$

where $y_i, i=1, \dots, 13$ are as in the below table

i	y_i	i	y_i
1	0.5	8	2.5
2	0.8	9	1.6

3	1	10	1.3
4	1.4	11	0.7
5	2	12	0.4
6	2.4	13	0.3
7	2.7		

6. Estimation of parameters [6, p. 430]

$$f(x) = \sum_{i=1}^7 \left(\frac{x_1^2 + a_i x_2^2 + a_i^2 x_3^2}{(1 + a_i x_4^2) b_i} - 1 \right)^2,$$

where the parameters a_i, b_i , $i = 1, \dots, 7$ have the following values:

i	a_i	b_i
1	0.0	7.391
2	0.000428	11.18
3	0.0010	16.44
4	0.00161	16.20
5	0.00209	22.20
6	0.00348	24.02
7	0.00525	31.32

7. Propan combustion in air [7, p. 143-151], [8, pp.18-19], [4, pp. 54-56], [5, p. 327]

$$\begin{aligned} f(x) = & (x_1 x_2 + x_1 - 3x_5)^2 + \\ & (2x_1 x_2 + x_1 + 2R_{10} x_2^2 + x_2 x_3^2 + R_7 x_2 x_3 + R_9 x_2 x_4 + R_8 x_2 - Rx_5)^2 + \\ & (2x_2 x_3^2 + R_7 x_2 x_3 + 2R_5 x_3^2 + R_6 x_3 - 8x_5)^2 + \\ & (R_9 x_2 x_4 + 2x_4^2 - 4Rx_5)^2 + \\ & (x_1 x_2 + x_1 + R_{10} x_2^2 + x_2 x_3^2 + R_7 x_2 x_3 + R_9 x_2 x_4 + R_8 x_2 + R_5 x_3^2 + R_6 x_3 + x_4^2 - 1)^2 \end{aligned}$$

where:

$$R_5 = 0.193 \quad R_6 = 0.4106217541E-3 \quad R_7 = 0.5451766686E-3$$

$$R_8 = 0.44975E-6 \quad R_9 = 0.3407354178E-4 \quad R_{10} = 0.9615E-6$$

$$R = 10$$

8. Gear train with minimum inertia [9], [10, Problem 328, p. 149]

$$f(x) = 0.1(12 + x_1^2 + (1 + x_2^2)/x_1^2 + (x_1^2 x_2^2 + 100)/x_1^4 x_2^4).$$

9. Human Heart Dipole. [1, p. 65], [8, p. 17], [4, pp. 51-54], [11, pp. 817-823]

$$\begin{aligned} f(x) = & (x_1 + x_2 - s_{mx})^2 + \\ & (x_3 + x_4 - s_{my})^2 + \end{aligned}$$

$$\begin{aligned}
& \left(x_1x_5 + x_2x_6 - x_3x_7 - x_4x_8 - s_A \right)^2 + \\
& \left(x_1x_7 + x_2x_8 + x_3x_5 + x_4x_6 - s_B \right)^2 + \\
& \left(x_1(x_5^2 - x_7^2) - 2x_3x_5x_7 + x_2(x_6^2 - x_8^2) - 2x_4x_6x_8 - s_C \right)^2 + \\
& \left(x_3(x_5^2 - x_7^2) + 2x_1x_5x_7 + x_4(x_6^2 - x_8^2) + 2x_2x_6x_8 - s_D \right)^2 + \\
& \left(x_1x_5(x_5^2 - 3x_7^2) + x_3x_7(x_7^2 - 3x_5^2) + x_2x_6(x_6^2 - 3x_8^2) + x_4x_8(x_8^2 - 3x_6^2) - s_E \right)^2 + \\
& \left(x_3x_5(x_5^2 - 3x_7^2) - x_1x_7(x_7^2 - 3x_5^2) + x_4x_6(x_6^2 - 3x_8^2) - x_2x_8(x_8^2 - 3x_6^2) - s_F \right)^2
\end{aligned}$$

where:

$$\begin{array}{llll}
s_{mx} = 0,485 & s_A = -0,0581 & s_C = 0,105 & s_E = 0,167 \\
s_{my} = -0,0019 & s_B = 0,015 & s_D = 0,0406 & s_F = -0,399 .
\end{array}$$

10. Neurophysiology [4, pp. 57-61], [12, pp. 915-930]

$$\begin{aligned}
f(x) = & (x_1^2 + x_3^2 - 1)^2 + (x_2^2 + x_4^2 - 1)^2 \\
& + (x_5x_3^3 + x_6x_4^3 - 1)^2 + (x_5x_1^3 + x_6x_2^3 - 2)^2 \\
& + (x_5x_1x_3^2 + x_6x_2x_4^2 - 1)^2 + (x_5x_3x_1^2 + x_6x_4x_2^2 - 4)^2 .
\end{aligned}$$

11. Combustion application [17], [18, pp. 61-63]

$$\begin{aligned}
f(x) = & (x_2 + 2x_6 + x_9 + 2x_{10} - 10^{-5})^2 + \\
& (x_3 + x_8 - 3 \cdot 10^{-5})^2 + \\
& (x_1 + x_3 + 2x_5 + 2x_8 + x_9 + x_{10} - 5 \cdot 10^{-5})^2 + \\
& (x_4 + 2x_7 - 10^{-5})^2 + \\
& (0.5140437 \cdot 10^{-7} x_5 - x_1^2)^2 + \\
& (0.1006932 \cdot 10^{-6} x_6 - 2x_2^2)^2 + \\
& (0.7816278 \cdot 10^{-15} x_7 - x_4^2)^2 + \\
& (0.1496236 \cdot 10^{-6} x_8 - x_1x_3)^2 + \\
& (0.6194411 \cdot 10^{-7} x_9 - x_1x_2)^2 + \\
& (0.2089296 \cdot 10^{-14} x_{10} - x_1x_2^2)^2 .
\end{aligned}$$

12. Thermistor [13, pp.722-723]

$$f(x) = \sum_{i=1}^{16} \left(y_i - x_1 \exp \left(\frac{x_2}{45 + 5i + x_3} \right) \right)^2$$

where

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

13. Optimal design of a Gear Train [14, pp. 95-105], [4, p. 79]

$$f(x) = \left(\frac{1}{6.931} - \frac{x_1 x_2}{x_3 x_4} \right)^2.$$

14. Circuit design [15, p. 501], [13, pp.243-244], [16, pp.367-370]

$$f(x) = (x_1 x_3 - x_2 x_4)^2 + \sum_{k=1}^4 (a_k^2 + b_k^2),$$

where

$$\begin{aligned} a_k &= (1 - x_1 x_2) x_3 \left\{ \exp \left[x_5 (g_{1k} - g_{3k} x_7 \cdot 10^{-3} - g_{5k} x_8 \cdot 10^{-3}) \right] - 1 \right\} \\ &\quad + g_{4k} x_2 - g_{5k}, \quad k = 1, \dots, 4, \\ b_k &= (1 - x_1 x_2) x_4 \left\{ \exp \left[x_6 (g_{1k} - g_{2k} - g_{3k} x_7 \cdot 10^{-3} - g_{4k} x_9 \cdot 10^{-3}) \right] - 1 \right\} \\ &\quad + g_{4k} - g_{5k} x_1, \quad k = 1, \dots, 4, \\ g &= \begin{bmatrix} 0.4850 & 0.7520 & 0.8690 & 0.9820 \\ 0.3690 & 1.2540 & 0.7030 & 1.4550 \\ 5.2095 & 10.0677 & 22.9274 & 20.2153 \\ 23.3037 & 101.7790 & 111.4610 & 191.2670 \\ 28.5132 & 111.8467 & 134.3884 & 211.4823 \end{bmatrix}, \end{aligned}$$

The performances of DESCON for solving these applications are illustrated in Table 1, where where n is the number of variables, $iter$ is the number of iterations to get a solution, $fgcnt$ is the number of function and its gradient evaluations, $time(c)$ is the time in centesconds, fx^* is the value of the minimizing function in optimal point and $gnorm$ is the infinite norm of the gradient.

Table 1
Performances of DESCON

n	iter	fgcnt	time(c)	fx*	gnorm	Name of Application
2	1878	10001	0	-0.2644531414650E+03	0.8208740831576E+00	1. Weber Function (Andrei, U71)
4	48	143	0	0.3075056038514E-03	0.6886760990097E-08	2. Enzyme reaction (Andrei, U79) (A)
6	85	264	0	0.9665994663683E-15	0.4231231612939E-07	3. Solution of a chemical reactor (A)
8	1843	10006	1	0.5463981044793E-05	0.1781782618260E-02	4. Robot kinematics problem (A)
4	12	38	0	0.8312307692553E+01	0.8585722387648E-07	5. Solar Spectroscopy (A)
4	46	150	0	0.3185717881375E-01	0.6936429307668E-08	6. Estimation of parameters (A)
5	724	2246	0	0.1224151943762E-06	0.8166044868424E-07	7. Propan combustion in air (A)
2	14	154	0	0.17511922131346E+01	0.7760986494009E-07	8. Gear train with minimum inertia (A)
8	1916	10002	1	0.1120571259805E-01	0.1686188462847E-03	9. Human Heart Dipole. Andrei U84, pp.65
6	93	632	1	0.4539057615171E+01	0.4484463269794E-07	10. Neurophysiology (A)
10	51	142	0	0.6898812079492E-10	0.8219103504792E-07	11. Combustion application (A)
3	1839	10005	10	0.1726024568705E+03	0.1334938231384E+02	12. Thermistor (A)
4	1842	10004	0	0.2387780742094E-02	0.8995056760928E-04	13. Optimal design of a Gear Train (A)
9	739	2166	2	0.1454860731888E-13	0.1554041459749E-06	14. Circuit design (A)
TOTAL	11130	55953	15.00	centesconds		

Date: --- Month: 6 Day: 3 Year: 2020

The performances of CUBIC are given in Table 2.

Table 2
Performances of CUBIC

n	iter	fgcnt	time(c)	fx	gnorm	Name of Applications
2	1288	5001	1	-0.2643790043149E+03	0.6876989703321E+00	1. Weber Function (Andrei, U71)
4	39	116	0	0.307505606090E-03	0.1140193575396E-06	2. Enzyme reaction (Andrei, U79) (A)
6	94	287	0	0.7468342084540E-15	0.4147895225729E-07	3. Solution of a chemical reactor (A)
8	333	5017	1	0.4829469121831E+00	0.4942442115598E+00	4. Robot kinematics problem (A)
4	10	31	0	0.8312307695614E+01	0.7104616347572E-06	5. Solar Spectroscopy (A)
4	30	96	0	0.3187570933023E-01	0.5862905229454E-06	6. Estimation of parameters (A)
5	555	1670	0	0.4799163454696E-05	0.1371052281519E-05	7. Propan combustion in air (A)
2	11	138	0	0.1751192330768E+01	0.9461910026439E-06	8. Gear train with minimum inertia (A)
8	940	5006	1	0.1199116073210E-01	0.8786818146807E-01	9. Human Heart Dipole. Andrei U84, pp.65
6	24	79	0	0.4539057615171E+01	0.3989872629134E-08	10. Neurophysiology (A)
10	50	139	0	0.4967405721874E-09	0.3630146049766E-06	11. Combustion application (A)
3	395	5003	6	0.1721497388951E+03	0.2361553857583E+01	12. Thermistor (A)
4	7	101	0	0.2322924674570E-04	0.7867065011382E-06	13. Optimal design of a Gear Train (A)
9	563	1639	3	0.8544333431670E-14	0.2890489586180E-06	14. Circuit design (A)
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TOTAL	4339	24323	12.00	centeseconds		

Date: --- Month: 6 Day: 3 Year: 2020

Tables 3 and 4 shows the performances of CG-DESCENT(w) (version 1.4) with Wolfe line search and of CG-DESCENT(aw) with approximate Wolfe line search, respectively.

Table 3
Performances of CG-DESCENT(w)

n	iter	fgcnt	time(c)	fx	gnorm	Name of Applications
2	130	526	0	-0.2644531414650E+03	0.4360555021096E+00	1. Weber Function (Andrei, U71)
4	87	183	0	0.3075057506207E-03	0.9351232549738E-06	2. Enzyme reaction (Andrei, U79) (A)
6	242	531	0	0.1546034033470E-11	0.8328999653862E-06	3. Solution of a chemical reactor (A)
8	13	79	0	0.1045002080991E-04	0.2937120722379E-02	4. Robot kinematics problem (A)
4	34	73	0	0.6872367741557E+01	0.3753421634575E-06	5. Solar Spectroscopy (A)
4	638	1436	0	0.3194075831746E-01	0.9984546877919E-06	6. Estimation of parameters (A)
5	9001	18039	2	0.1327993904766E-03	0.3013599273355E-03	7. Propan combustion in air (A)
2	14	86	0	0.1745268282541E+01	0.6851854457169E-01	8. Gear train with minimum inertia (A)
8	2	57	0	0.1790818193032E+00	0.3756017838954E-01	9. Human Heart Dipole. Andrei U84, pp.65
6	39	100	0	0.4539057615171E+01	0.3103946255578E-07	10. Neurophysiology (A)
10	55	114	0	0.1279714516413E-09	0.1142557208812E-06	11. Combustion application (A)
3	32	462	0	0.1721680788246E+03	0.2931072079241E+03	12. Thermistor (A)
4	1	56	0	0.1743310601795E-01	0.5889113990961E-03	13. Optimal design of a Gear Train (A)
9	7485	15457	12	0.2419744215211E-10	0.8313476443084E-06	14. Circuit design (A)
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TOTAL	17773	37199	14.00	centeseconds		

Date: --- Month: 6 Day: 4 Year: 2020

Line Search with Wolfe conditions

Table 4
Performances of CG-DESCENT(aw)

n	iter	fgcnt	time(c)	fx	gnorm	Name of Applications
2	130	526	0	-0.2644531414650E+03	0.4360555021096E+00	1. Weber Function (Andrei, U71)
4	87	183	0	0.3075057506207E-03	0.9351232549738E-06	2. Enzyme reaction (Andrei, U79) (A)
6	242	531	0	0.1546034033470E-11	0.8328999653862E-06	3. Solution of a chemical reactor (A)
8	13	79	0	0.1045002080991E-04	0.2937120722379E-02	4. Robot kinematics problem (A)
4	34	73	0	0.6872367741557E+01	0.3753421634575E-06	5. Solar Spectroscopy (A)
4	638	1436	0	0.3194075831746E-01	0.9984546877919E-06	6. Estimation of parameters (A)
5	9001	18039	1	0.1327993904766E-03	0.3013599273355E-03	7. Propan combustion in air (A)
2	14	86	0	0.1745268282541E+01	0.6851854457169E-01	8. Gear train with minimum inertia (A)
8	2	57	0	0.1790818193032E+00	0.3756017838954E-01	9. Human Heart Dipole. Andrei U84, pp.65
6	39	100	0	0.4539057615171E+01	0.3103946255578E-07	10. Neurophysiology (A)
10	55	114	0	0.1279714516413E-09	0.1142557208812E-06	11. Combustion application (A)
3	32	462	1	0.1721680788246E+03	0.2931072079241E+03	12. Thermistor (A)
4	1	56	0	0.1743310601795E-01	0.5889113990961E-03	13. Optimal design of a Gear Train (A)
9	7485	15457	11	0.2419744215211E-10	0.8313476443084E-06	14. Circuit design (A)
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TOTAL	17773	37199	13.00	centeseconds		

Date: --- Month: 6 Day: 4 Year: 2020

Line Search with Approximate Wolfe conditions

A synthesis of these numerical experiments is presented in Table 5.

Performances of DESCON, CUBIC and CG-DESCENT			
	iter	fgcnt	time
DESCON	11130	55953	15
CUBIC	4339	24323	12
CG-DESCENT(w)	17773	37199	14
CG-DESCENT(aw)	17773	37199	13

Even if they are using different principle, their performances for solving small-scale unconstrained optimization problems are similar.

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