Numerical experiments with CG-DESCENT for solving 14 applications of unconstrained optimization

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This technical report presents the numerical performances of CG-DESCENT [19] for solving a number of 14 applications of unconstrained optimization. The following applications are considered in this numerical experiment:

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:

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			

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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: $k_1 = 31{,}24 \quad k_2 = 0{,}272 \quad k_3 = 303{,}03 \quad r_1 = 2{,}062 \quad r_2 = 0{,}02$.

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

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

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 $y_i, i = 1,...,13$ 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 $a_i, b_i,\ \ i=1,\ldots,7$ 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]

$$\begin{aligned}
f(x)=&\left(x_1x_2+x_1-3x_5\right)^2+\\
&\left(2x_1x_2+x_1+2R_{10}x_2^2+x_2x_3^2+R_7x_2x_3+R_9x_2x_4+R_8x_2-Rx_5\right)^2+\\
&\left(2x_2x_3^2+R_7x_2x_3+2R_5x_3^2+R_6x_3-8x_5\right)^2+\\
&\left(R_9x_2x_4+2x_4^2-4Rx_5\right)^2+\\
&\left(x_1x_2+x_1+R_{10}x_2^2+x_2x_3^2+R_7x_2x_3+R_9x_2x_4+R_8x_2+R_5x_3^2+R_6x_3+x_4^2-1\right)^2
\end{aligned}$$

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]

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

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

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

$$\left(x_1x_5(x_5^2-3x_7^2)+x_3x_7(x_7^2-3x_5^2)+x_2x_6(x_6^2-3x_8^2)+x_4x_8(x_8^2-3x_6^2)-s_E\right)^2+$$
$$\left(x_3x_5(x_5^2-3x_7^2)-x_1x_7(x_7^2-3x_5^2)+x_4x_6(x_6^2-3x_8^2)-x_2x_8(x_8^2-3x_6^2)-s_F\right)^2$$

where:

$s_{mx}=0{,}485$ $\quad s_A=-0{,}0581$ $\quad s_C=0{,}105$ $\quad s_E=0{,}167$

$s_{my}=-0{,}0019$ $\quad s_B=0{,}015$ $\quad s_D=0{,}0406$ $\quad s_F=-0{,}399$.

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]

$$\begin{aligned}f(x)=&(x_2+2x_6+x_9+2x_{10}-10^{-5})^2+\\&(x_3+x_8-3\cdot10^{-5})^2+\\&(x_1+x_3+2x_5+2x_8+x_9+x_{10}-5\cdot10^{-5})^2+\\&(x_4+2x_7-10^{-5})^2+\\&(0.5140437\cdot10^{-7}x_5-x_1^2)^2+\\&(0.1006932\cdot10^{-6}x_6-2x_2^2)^2+\\&(0.7816278\cdot10^{-15}x_7-x_4^2)^2+\\&(0.1496236\cdot10^{-6}x_8-x_1x_3)^2+\\&(0.6194411\cdot10^{-7}x_9-x_1x_2)^2+\\&(0.2089296\cdot10^{-14}x_{10}-x_1x_2^2)^2.\end{aligned}$$

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

$$\begin{aligned} a_k &= (1 - x_1 x_2) x_3 \left\{ \exp\left[x_5 (g_{1k} - g_{3k} x_7 \cdot 10^{-3} - g_{5k} x_8 \cdot 10^{-3}) \right] - 1 \right\} \\ &\quad + g_{4k} x_2 - g_{5k}, \quad k = 1, \ldots, 4, \\ b_k &= (1 - x_1 x_2) x_4 \left\{ \exp\left[x_6 (g_{1k} - g_{2k} - g_{3k} x_7 \cdot 10^{-3} - g_{4k} x_9 \cdot 10^{-3}) \right] - 1 \right\} \\ &\quad + g_{4k} - g_{5k} x_1, \quad k = 1, \ldots, 4, \end{aligned}$$

$$g = \begin{bmatrix} 0.4850 & 0.7520 & 0.8690 & 0.9820 \\ 0.3690 & 1.2540 & 0.7030 & 1.4550 \\ 5.2095 & 10.0677 & 22.9274 & 20.2153 \\ 23.3037 & 101.7790 & 111.4610 & 191.2670 \\ 28.5132 & 111.8467 & 134.3884 & 211.4823 \end{bmatrix},$$

Solution of these applications, given by CG-DESCENT, are as follows:

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

Line Search with Appproximate Wolfe conditions

   1  CG_DESCENT Algorithm. Function: 1. Weber Function (Andrei, U71)

        n     iter    nfunc    ngrad  time(c)              f                  gnorm         s
-------------------------------------------------------------------------------------------------
        2      130      526      493        0     -0.2644531414650E+03   0.4360555021096E+00 4

      1      0.9000000000000E+02
      2      0.1100000000000E+02

                                  f(x0) = -0.3747313737140E+02
                                  f(x*) = -0.2644531414650E+03

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   2  CG_DESCENT Algorithm. Function: 2. Enzyme reaction  (Andrei, U79) (A)

        n     iter    nfunc    ngrad  time(c)              f                  gnorm         s
-------------------------------------------------------------------------------------------------
        4       87      183      118        0      0.3075057506207E-03   0.9351232549738E-06 0

      1      0.1927935781610E+00
      2      0.1915622536017E+00
      3      0.1231043441257E+00
      4      0.1361907911046E+00

                                  f(x0) =  0.5313172272109E-02
                                  f(x*) =  0.3075057506207E-03

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   3  CG_DESCENT Algorithm. Function: 3. Solution of a chemical reactor (A)

        n     iter    nfunc    ngrad  time(c)              f                  gnorm         s
```

```
-----------------------------------------------------------------------------------------------
        6      242      531      368        0      0.1546034033470E-11   0.8328999653862E-06 0

      1      0.1030426052817E+01
      2      0.1020285145007E+01
      3     -0.6085275430773E-01
      4     -0.1003023286520E-03
      5      0.1001051855002E+01
      6     -0.9516200559670E-03

                                  f(x0) =  0.1961733675060E+08
                                  f(x*) =  0.1546034033470E-11

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   4  CG_DESCENT Algorithm. Function: 4. Robot kinematics problem (A)

        n     iter    nfunc    ngrad  time(c)               f                   gnorm         s
-----------------------------------------------------------------------------------------------
        8       13       79       67        0      0.1045002080991E-04   0.2937120722379E-02 6

      1      0.1624947122889E+00
      2     -0.9864083470059E+00
      3     -0.9461693964057E+00
      4     -0.3222724562702E+00
      5     -0.9985473660099E+00
      6      0.5718849742519E-01
      7      0.4089103596085E+00
      8     -0.9123489935322E+00

                                  f(x0) =  0.1069004717719E-01
                                  f(x*) =  0.1045002080991E-04

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   5  CG_DESCENT Algorithm. Function: 5. Solar Spectroscopy (A)

        n     iter    nfunc    ngrad  time(c)               f                   gnorm         s
-----------------------------------------------------------------------------------------------
        4       34       73       50        0      0.6872367741557E+01   0.3753421634575E-06 0

      1      0.1535174717598E+01
      2     -0.1011388878511E+01
      3     -0.1155997176102E+01
      4      0.3618353391853E+01

                                  f(x0) =  0.3214000000000E+02
                                  f(x*) =  0.6872367741557E+01

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   6  CG_DESCENT Algorithm. Function: 6. Estimation of parameters (A)

        n     iter    nfunc    ngrad  time(c)               f                   gnorm         s
-----------------------------------------------------------------------------------------------
        4      638     1436     1036        0      0.3194075831746E-01   0.9984546877919E-06 0

      1      0.2716632389555E+01
      2      0.1343554437416E+03
      3      0.1528569798352E+04
      4      0.2905915355136E+02

                                  f(x0) =  0.2905300235663E+01
                                  f(x*) =  0.3194075831746E-01

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   7  CG_DESCENT Algorithm. Function: 7. Propan combustion in air (A)

        n     iter    nfunc    ngrad  time(c)               f                   gnorm         s
-----------------------------------------------------------------------------------------------
        5     9001    18039    11664        1      0.1327993904766E-03   0.3013599273355E-03 2

      1      0.2095625903599E-01
      2      0.4711582566884E+01
      3      0.1733909882699E+00
      4      0.8556104729056E+00
```

```
     5      0.3660495418761E-01

                                  f(x0) =  0.3312269269234E+08
                                  f(x*) =  0.1327993904766E-03

   <><><>
```

```
                                f(x*) =  0.1279714516413E-09

   <><><>
```

Table 1

Performances of CG-DESCENT

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)
TOTAL	17773	37199	13.00 centeseconds			

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

Line Search with Appproximate Wolfe conditions

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