# Software V2 

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Technical Report
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This Technical Report is the second version of the list of the software I have written and tested along the years. The software in this version of this paper is an improvement of the software I listed in the Technical Report from December 8, 2011, where I introduced some new software elaborated along the years. The programs and subroutines are organized on directories and subdirectories. In each directory I placed a number of programs I have elaborated in my research activity. Some other information concerning the algorithms or the results of the software is also included. The list of chapters and their contents is as follows:

|  | Support Programs |  |
| :--- | :--- | :--- |
| 1. | ENORM | Program for computing the Euclidian norm of a vector. <br> (This is a variant of function enorm from MINPACK1) |
| 2. | PERFORM | Program for Profile Performance Analysis. <br> There are three subroutines: <br> PERF2N for analysis of two algorithms (ALG1 versus ALG2) subject <br> to the number of iterations, of function evaluations and CPU time in <br> sense of Dolan and Morè. [See: Dolan, E.D., \& Moré, J.J., (2002). <br> Benchmarking optimization software with performance profiles. <br> Mathematical Programming, 91, 201-213.] |
| PERFNN for analysis of at least 20 algorithms subject to the number of <br> iterations, of function evaluations and CPU time in sense of Dolan and <br> Morè. [See: Dolan, E.D., \& Moré, J.J., (2002). Benchmarking <br> optimization software with performance profiles. Mathematical <br> Programming, 91, 201-213.] |  |  |


|  |  | PERLOG for performance analysis of two algorithms according to the index $r_{i}=-\frac{\log \left(a^{A}\right)}{\log \left(a^{B}\right)}$ <br> where $a^{A}$ and $a^{B}$ referes to the number of iterations, or the number of functions evaluartions, or the CPU time respectively corresponding to the algorithm A or B . <br> A complete description of these algorithms could be find in: <br> N. Andrei, Criticism of the Unconstrained Optimization Algorithms Reasoning, Editura Academiei Române, Bucureşti, 2009. <br> ISBN: 978-973-27-1669-4 (pp. 89-94) <br> December 30, 2004 |
| :---: | :---: | :---: |
| 3. | GRADIENT | Approximation of derivatives of a function using forward or central finite difference. <br> The step length is sqrt of epsilon machine. <br> April 1983 |
| 4. | JACOBIAN | Program for computation of the sparse Jacobian with minimization of the number of function evaluations. <br> The algorithm is described in the paper: <br> N. Andrei, $R P$ - a package for efficient calculation of sparse jacobian matrix for nonlinear systems of equations using finite differences. Technical Report, Bucharest, April 15, 1983. <br> (Please see the file: JACOBIAN.DOC) <br> April 15, 1983 |
| 5. | LS | A collection of subroutines for one-dimensional searching used in nonlinear optimization. <br> The following subroutines belong to this collection: <br> L1 Golden search <br> L2 Fibonacci search <br> L3 Quadratic interpolation of Powell technique <br> L4 Dichotomous search <br> April, 1990 |
| 6. | LINESEARCH | Line search: Backtracking versus Wolfe versus Moré - Thuente in context of Steepest Descent Method. <br> The purpose of this program is to see 3 line search subroutines (backtracking, Wolfe and Strong Wolfe) in some particular Fortran implementation. <br> - Subroutine BACK (backtracking) is authored by Andrei. <br> - Subroutine WOLFE (standard Wolfe conditions) is coauthored by Shanno and Phua with some additional modifications by Andrei. <br> - Subroutine MTLINES (strong Wolfe conditions) is coauthored by Moré and Thuente. <br> A description of these algorithms could be find in: <br> N. Andrei, Criticism of the Unconstrained Optimization Algorithms Reasoning, Editura Academiei Române, Bucureşti, 2009. <br> ISBN: 978-973-27-1669-4 (pp. 122-133) |


|  |  | August 30, 2006 |
| :---: | :---: | :---: |
| 7. | AORDER | Subroutine for setting the elements of an array in ascending order. The elements of the array may be positive or negative. <br> This subroutine is accompanied by an main program illustrating the calling of the subroutine. <br> Array to be ordered (increasingly) <br> $1 \quad 0.1000000000000 \mathrm{E}+02$ <br> $2 \quad 0.90000000000000 \mathrm{E}+01$ <br> $\begin{array}{cc}3 & 0.8000000000000 \mathrm{E}+01 \\ 4 & -\mathbf{0 . 6 0 0 0 0 0 0 0 0 0 0 0 0 E}+01\end{array}$ <br> $5 \quad 0.6000000000000 \mathrm{E}+01$ <br> $6 \quad 0.5000000000000 \mathrm{E}+01$ <br> $7 \quad 0.4000000000000 \mathrm{E}+01$ <br> $8 \quad 0.30000000000000 \mathrm{E}+01$ <br> $9 \quad 0.20000000000000 \mathrm{E}+01$ <br> $10 \quad 0.1000000000000 \mathrm{E}+01$ <br> Ordered array <br> $1-\mathbf{- 0 . 6 0 0 0 0 0 0 0 0 0 0 0 0 E}+01$ <br> $0.1000000000000 \mathrm{E}+01$ <br> $3 \quad 0.2000000000000 \mathrm{E}+01$ <br> $4 \quad 0.3000000000000 \mathrm{E}+01$ <br> $5 \quad 0.4000000000000 \mathrm{E}+01$ <br> $6 \quad 0.5000000000000 \mathrm{E}+01$ <br> $7 \quad 0.6000000000000 \mathrm{E}+01$ <br> $8 \quad 0.80000000000000 \mathrm{E}+01$ <br> $9 \quad 0.9000000000000 \mathrm{E}+01$ <br> $10 \quad 0.1000000000000 \mathrm{E}+02$ |
|  |  | August, 1995 |

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## Numerical Linear Algebra

1. $\quad$ SIMEQ $\quad$ Directory SIMEQ

## Simultaneous linear equations system solving

SIMEQ subroutine for solving linear algebraic systems of equations (the dense case). The matrix and its inverse are stored in ( NxN ) arrays.
SIMEQL subroutine for solving linear algebrais systems of equations (the dense case). In this case the matrix and its inverse are stored in onedimensional arrays on rows in natural order, i.e. [row1, row2, ... rowKC].
Both subroutines implements the Gauss method of ellimination with column pivoting to determine the solution vector and the inverse of the matrix.
Calling sequence:
CALL SIMEQ (A,RHS,KC,AINV,X,IERR)
CALL SIMEQL(A,RHS,KC,AINV,X,IERR)
where:
A $\quad=$ The array of the system's matrix.
RHS $=$ The right-hand-side of the system.
KC $=$ The order of the system (The number of variables).
AINV $=$ The array of the inverse of the matrix.
X $\quad=$ The solution vector of the system.
IERR = Return code with the following values:
0 if the matrix is singular,


|  |  | $\mathrm{X}=\mathrm{A}^{* *}(-\mathrm{T}) * \mathrm{~B}=\mathrm{B}^{*}\left(((\mathrm{QP}) * \mathrm{Tn})^{*} \ldots . . . . \mathrm{T} 1\right) .$ <br> RM02A is for insitu permutation of a vector according to a permutation vector. <br> The theory of Product Form of Inverse (PFI) factorization is described in: N. Andrei, Criticism of the linear programming algorithms reasoning. Romanian Academy Publishing House, Bucharest, 2011. ISBN: 978-973-27-2076-9 (pages: 1239-273) <br> December 4, 1995 |
| :---: | :---: | :---: |
| 4. | LU | Directory LU <br> Package for Solving Large-Scale Linear Algebraic Systems with LU Factorization and Markowitz Procedure for Pivots Selection <br> The calling sequence is as follows: $\begin{gathered} \text { LU ----- RF01A } \\ \text {--- RM01A, }, \\ ----- \text { RS01A } \end{gathered}$ <br> where: <br> LU Main program for solving linear algebraic systems of equations $\mathrm{Ax}=\mathrm{b}$ or $\mathrm{ATx}=\mathrm{b}$ using LU factorization of the matrix with Markowitz's pivot selection strategy. <br> RF01A Subroutine for LU factorization of the matrix A. <br> RS01A Subroutine for solving large-scale systems of linear equations computing: $\mathrm{A}^{* *}(-1) * \mathrm{~b}$ or $\mathrm{A}^{* *}(-\mathrm{T}) * \mathrm{~b}$, for a given vector b , using the LU factorization of the matrix A (given by RF01A subroutine), exploiting the sparsity in all cases. <br> RM01A Subroutine for sorting the non-zeros of a sparse matrix from arbitrary order to column order, but unordered within each column. <br> RM04A Subroutine for compressing the column / row array of U factor (from the LU factorization of a sparse matrix) in order to eliminate the spaces between columns / rows. <br> - The file LU.DOC contains a number of 15 examples of linear algebraic systems solved by LU package. <br> The theory of LU factorization is described in: <br> N. Andrei, Criticism of the linear programming algorithms reasoning. Romanian Academy Publishing House, Bucharest, 2011. <br> ISBN: 978-973-27-2076-9 (pages: 287-316) <br> May 3, 1995 |
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| Zero of nonlinear functions |  |  |
| 1. | ZERO1 | In sub-directory ZERO, directory: SOFT-ANDREI-TOTAL: <br> A simple algorithm for computing zero of a nonlinear function of a variable in a given interval $[a, b]$. |



|  | Solving Nonlinear Algebraic Systems F(x) = 0 |  |
| :---: | :---: | :---: |
| 1. | NEWTON | Newton method without line search. <br> The method is described in: <br> N. Andrei, Criticism of the Unconstrained Optimization Algorithms Reasoning, Academiei Publishing House, Bucharest, 2009, Chapter 6, (pages: 243-255). <br> The Newton system is solved by means of the LA05** package by J.K. Read with minor modifications by N. Andrei. <br> In directory NEWTON there are the following nonlinear algebraic systems: <br> 1) CANAL - Flow in a chanel problem, <br> 2) CAVITATE - Flow in a driven cavity problem, <br> 3) CIRCUIT - Circuit design problem, <br> 4) E1 - Calculul temperaturii stationare într-un reactor. <br> 5) E2 - Calculul fractiei de conversie a unei substante într-un reactor Chimic, <br> 6) PROPAN - Propan combustion in aer - Reduced Formulation, <br> 7) REACTOR - Stationar solution of a chemical reactor, <br> 8) ROBOT - Robot kinematics problem, <br> 9) SOLID - Solid Fuel Ignition. |
|  |  | June 1, 2006 |
| 2. | GRFLOW | Gradient Flow Algorithm for solving nonlinear algebraic systems $F(x)=0$, where $F(x)=\left[f_{1}(x), \ldots, f_{m}(x)\right]$. <br> The algorithm is as follows: $x_{k+1}=x_{k}+d_{k},$ <br> where $d_{k}$ is computed as solution ofthe following system of linear algebraic equations: $\left[I+h_{k} \theta\left(\nabla F\left(x_{k}\right)^{T} \nabla F\left(x_{k}\right)+\sum_{i=1}^{m} f_{i}\left(x_{k}\right) \nabla^{2} f_{i}\left(x_{k}\right)\right)\right] d_{k}=-h_{k} \nabla F\left(x_{k}\right)^{T} F(x)$ <br> If $f_{i}(x)$ are convex and positive for all $i=1, \ldots, m ; \operatorname{rank}(\nabla F(x))=n$; $\theta=1$ and $h_{k} \rightarrow \infty$, then the algorithm is quadratically convergent to a local solution of the system. <br> FLOW.FOR is the main program for the Gradient Flow Algorithm for solving $\mathrm{F}(\mathrm{x})=0$. Some variants of this Fortran program can be found in FLOWC.FOR and FLOWZ.FOR. <br> In directory ACAD there are the following problems (please see MINPACK-2 collection): <br> GFLOWS1 - Circuit design problem, |


|  |  | GFLOWS2 - Propan combustion problem, <br> GFLOWS3 - Stationar solution of a chemical reactor, <br> GFLOWS4 - Robot kinematics problem, <br> GFLOWS5 - Solid fuel ignition problem, <br> GFLOWS6 - Flow in a driven cavity problem, <br> GFLOWS7 - Flow in a chanel problem, <br> GFLOWS8 - Human heart dipole problem. <br> The mathematical description of these problems, as well as their solution can be studied in: <br> N. Andrei, Criticism of the Unconstrained Optimization Algorithms Reasoning, Academiei Publishing House, Bucharest, 2009, Chapter 6, (pages: 243-255). <br> The theoretical aspects of the gradient flow method are presented in: <br> N. Andrei, Criticism of the Unconstrained Optimization Algorithms Reasoning, Academiei Publishing House, Bucharest, 2009, Chapter 15. <br> The performances of the gradient flow method are shown in chapter 15 of this monography, (pages: 675-679). <br> Please, see the paper: Gradient Flow Algorithm for Systems of Nonlinear Equations, (ZEROF.PDF) (ZEROS.RTF). |
| :---: | :---: | :---: |
|  |  | April 4, 2004 |
| 3. | $\begin{aligned} & \hline \text { LEV- } \\ & \text { MARQ } \end{aligned}$ | Levenberg-Marquardt Algorithm for solving nonlinear algebraic systems $F(x)=0$. <br> This directory contains the following problems (please see MINPACK-2 collection): <br> LMS1 - Circuit design problem, <br> LMS2 - Propan combustion problem, <br> LM3 - Stationar solution of a chemical reactor, <br> LMS4 - Robot kinematics problem, <br> LMS5 - Solid fuel ignition problem, <br> LMS6 - Flow in a driven cavity problem, <br> LMS7 - Flow in a chanel problem, <br> A description of this algorithm together with the applications are presented in: N. Andrei, Criticism of the Unconstrained Optimization Algorithms Reasoning, Academiei Publishing House, Bucharest, 2009, Chapter 14.3 (pages: 636-655) |

## Linear programming

| 1. | $\begin{aligned} & \hline \text { AFFINE- } \\ & \text { SCALING } \end{aligned}$ | Main program Affine Scaling with Rows Partitioning for solving Linear Programming Problems: $\text { Min } c^{T} x \text { subject to } A x \leq b, x \geq 0$ <br> The program implements an algorithm described into the book: <br> N. Andrei, Programarea Matematică - Metode de punct interior, Editura Tehnică, 1999, chapter 5, section 5.4. (pages: 125-157) <br> The program uses two dimensional arrays and doesn't takes the advantage of sparsity of the matrix A. <br> May 21, 1998 |
| :---: | :---: | :---: |
| 2. | SPLIT | Splitting the dense columns of a Linear Programming Problem. <br> Please see: Chapter 15 of the book: <br> N. Andrei, "Criticism of the Linear Programming Algorithms Reasoning". Romanian Academy Publishing - Bucharest, Romania. 2010. (pages: 605-612) <br> June 9, 2010 |
| 3. | BCR | Balance Rows Reduction in linear programming. <br> The idea of this program is to eliminate the balance constraints, i.e. the constraints with zero RHS term. <br> The package has two main components. The first one eliminate the balance constraints and solve the reduced problem. The second one recover the solution from the solution of the reduced problem. <br> Please see: Chapter 16, Section 2, pp. 591-605 of the book: <br> N. Andrei, Criticism of the Linear Programming Algorithms Reasoning. Romanian Academy Publishing - Bucharest, 2011. (pages: 591-612) January 21, 1993 |
| 4. | ISLO | Interactive System for maintaing Linear Programming Problems. This is an interactive package for solving linear programming problems using PFI of the basis having the possibility to establish the optrimization conditions at the very beginning of the process. <br> January 12, 1995 |
| 5. | ASLO | Advanced System for Linear Optimization. <br> The LU factorization of the basis (subroutines LA05AD, LA05BD, LA05CD, LA05ED and MC20AD) is used to implement the primal simplex method. <br> The input of the problem is in MPS format. <br> December 16, 1992 |
| 6. | ASLONEW | Advanced System for Linear Optimization - New version. |
| 7. | CALP | A collection of Linear Programming Applications in ALLO Language. Se prezintă 10 prototupuri de modele de programare linară în limbajul ALLO, direct utilizate în context industrial. <br> See: N. Andrei, $O$ colecţie de aplicaţii de programare liniară in limbajul ALLO. Technical Report No.4/2007, September 3, 2007. (88 pagini cu CD) (see files: FRONT-RT3-2007.DOC \& RT3-2007.DOC in directory CALP) <br> Please, see the directory CALP in LINEAR-PROGRAMMING. Please, |


|  | see the Technical Report RT3-2007.doc. The mathematical models in <br> ALLO language are placed in the directory MODELS. |
| :--- | :--- | :--- |
| September 3, 2007 |  |

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|  | SAMO Technology <br> Advanced System for Linear Optimization |  |
| :---: | :---: | :---: |
| 1. | ALLO | Directory ALLO_LANGUAGE <br> ALLO is a mathematical programming language having the ability to write linear programming models. <br> It is fully algebraic, being notable for its syntax which is very simple but comprehensive, with a small number of reserved keywords. The compiler associated to ALLO language translate the model into the equivalent MPS form, directly admited by any professional linear optimizer. <br> The directory ALLO_LANGUAGE contains the following subdirectories: <br> - ALLO-source: <br> - Subdirectory ALLO contains three executable programs: ALLOPAS1 .EXE and ALLOPAS2.EXE for compiling an ALLO textsource and DSOLVER.EXE for solving the generated linear programming problem. - Subdirectories PAS1 and PAS2 contains Fortran and C programs which implement the ALLO compiler. The list of subroutines is described in LIST-OF-SUBROUTINES.DOC file. <br> - Subdirectory MODELE contains 11 prototypes of linear programming models in ALLO language. <br> -ALLO language is also described in ALLO.RTF file (17 pages, September 10, 2004) <br> - APPLIC: includes 25 prototypes of linear programming models in ALLO language. <br> - DOC: contains some files describing the ALLO language. <br> - ALLO language is explained in LANGALLO.RTF file (english version, 16 pages, September 10, 2004) <br> - The documents ALLO1.DOC and ALLO2.DOC present a collection of linear programming models including: allocation models, assembling models, desassembling, desassembling-assembling, transportation models, diet models, production modelswith optimal selection of technologies, systems with stocks, combined models of production with stocks, discrete production models. <br> - EXE: contains an old version of ALLO compiler (executables), SAMO executable, DSOLVER for solving a linear programming problem and HOPD which is HOPDM package by Gondzio. <br> The language ALLO is described in a number of papers as: |


|  |  | - N. Andrei, Gh. Borcan, ALLO: Algebraic Language for Linear Optimization. Technical Report, LSSO-2-95, Research Institute for Informatics, Bucharest, September 1995. <br> - N. Andrei, Gh. Borcan, ALLO - Limbaj algebric pentru optimizare liniară. Revista Română de Informatică şi Automatică, vol.8, nr. 3, 1998, pp.55-67. <br> - N. Andrei, Pachete de Programe, Modele şi Probleme de Test pentru Programarea Matematică, Editura MATRIXROM, București, 2001. <br> - N. Andrei, Critica Raţiunii Algoritmilor de Programare Liniară, Editura Academiei Române, Bucureşti, 2011. (pages: 815-830) <br> Martie 8, 2007 |
| :---: | :---: | :---: |
| 2. | SAMO | Directory INSTAL_SAMO <br> Advanced informatic technology for linear programming modeling and optimization. <br> SAMO - is an advanced informatic technology for linear programming modeling and optimization at an industrial level. SAMO permits conceptualization, elaboration, maintainance, modification and solving large-scale linear programming models. The system SAMO is based of the language ALLO which is a dialect of the natural language used by the user to conceptualize, to build up, to modify linear programming models in algebraic format, as well as on the ALLO compiler which translate the algebraic format of the model in MPS format. <br> SAMO uses a professional optimizer able to solve large-scale linear programming problems. <br> SAMO allows generation and solving of linear programming prototypes. SAMO is described in: <br> TR18.DOC file: SAMO - tehnologie informatică avansată pentru modelare şi optimizare. (Advanced informatioc technology for modeling and optimization.) Description of SAMO. Illustration of an ecran capture of this technology. (Martie 8, 2007) <br> SAMO.MSI is windows installer package. To install SAMO, the serial number is: CB48T H668K C9W64 <br> A description of SAMO, as well as some prototypes of industrial models in ALLO language, working under SAMO technology are presented in: <br> N. Andrei, Critica Raţiunii Algoritmilor de Programare Liniară, Editura Academiei Române, Bucureşti, 2011. (pages: 642-752) <br> N. Andrei, Pachete de Programe, Modele şi Probleme de Test pentru Programarea Matematică, Editura MATRIXROM, Bucureşti, 2001. (Lucrarea conţine 13 prototipuri de modele de programare liniară exprimate în limbajul ALLO.) |
|  |  | Martie 8, 2007 <br> New Version: June 8, 2011 |

## Unconstrained optimization

| Direct Search Methods |  |  |
| :---: | :---: | :---: |
| 1. | UNO | Directory UNO <br> UNCONSTRAINT OPTIMIZATION METHODS using <br> DIRECT SEARCHING TECHNIQUES <br> The following techniques are implemented: <br> - Hook-Jeeves - form searching, (HOOKJ.FOR <br> - Rosenbrook - rotation of coordinates, (ROSE.FOR) <br> - Powell - conjugate directions, (POWEL.FOR) <br> - Nelder-Mead - Simplex, (NELMED.FOR) <br> - Parallel with Axes Searching. (CPA.FOR) <br> These methods are implemented with different onedimensional optimization methods like: <br> L1 - golden section, <br> L2 - Fibonacci search, <br> L3 - Quadratic fitting of Powell, <br> L4 - Simple lambda $=1.0$. <br> The theory behind all these direct search methods is presented in: N. Andrei, Criticism of the Unconstrained Optimization Algorithms Reasoning, Academy Publishing House, Bucharest, 2009, Chapter 16. |
| 2. | FIBO | Directory FIBONACCI <br> O subrutină de calcul a minimului unei funcţii neliniare de o variabilă, pe un interval dat, bazată pe metoda de căutare directă Fibonacci. <br> The Fibonacci search method is presented in: fibonacci.doc file. Februarie 4, 1980 |
| 3. | MAXFUN | Directory MAXFUN <br> O subrutină de calcul a maximului unei funcţii neliniare de o variabilă, bazată pe metoda de interpolare pătratică Powell. <br> The maxfun search method is described in: maxfun.doc file. Septembrie 23, 1980 |
| 4. | PSO-UO | Directory PSO-UO <br> Particle Swarm Optimization for unconstrained optimization <br> In this directory I included three Fortran programs for minimizing the Rosenbrock function (extended and generalized) and the Wood function using the particle swarm optimization method. <br> May 21, 2014 |
| 5. | DEEPS | Directory DEEPS-TOTAL <br> This directory contains a number of 13 sub-directories as follows: DEEPS1 |



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minimum inertia, Human Heart Dipole, Neurophysiology, Combustion application, Circuit design, Termistor and Optimal design of a Gear Train. The performances of DEEPS8A is presented in Table 5 below.

Table 5. Performances of DEEPS for solving 16 unconstrained optimization applications

| Table 5. Performances of DEEPS for solving 16 unconstrained optimization applications |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $N r$. | $n$ | $N$ | $M$ | iter | $n f u n c$ | $c p u$ | $f\left(x^{*}\right)$ | $f\left(x_{0}\right)$ |
|  |  |  |  |  |  |  | $f(1473$ | 0.01 |
| 1. | 2 | 2 | 5 | 118 | -264.453135 | -37.473137 |  |  |
| 2. | 2 | 3 | 5 | 67 | 1318 | 0.0 | 9.56074405 | 78.594324 |
| 3. | 2 | 5 | 10 | 167 | 9160 | 0.0 | 8.74984910 | 78.602864 |
| 4. | 4 | 30 | 50 | 28 | 42903 | 0.02 | $0.308765 \mathrm{E}-03$ | $0.531317 \mathrm{E}-02$ |
| 5. | 6 | 50 | 100 | 1375 | 6989983 | 2.76 | $0.747292 \mathrm{E}-04$ | $0.196173 \mathrm{E}+08$ |
| 6. | 8 | 5 | 10 | 43 | 2459 | 0.0 | $0.182801 \mathrm{E}-07$ | 5.334258 |
| 7. | 4 | 5 | 10 | 4 | 233 | 0.0 | 8.3163822 | 9.958700 |
| 8. | 4 | 100 | 500 | 54 | 2705727 | 1.73 | $0.3185759-01$ | 2.905300 |
| 9. | 5 | 9900 | 100 | 10 | 10013014 | 4.83 | $0.2467602 \mathrm{E}-04$ | $0.331226 \mathrm{E}+08$ |
| 10. | 2 | 5 | 3 | 15 | 342 | 0.0 | 1.7441520 | 2563.3250 |
| 11. | 8 | 50 | 300 | 2404 | 36265585 | 26.67 | $0.996608 \mathrm{E}-04$ | 0.190569 |
| 12. | 6 | 1000 | 6 | 1044 | 7999853 | 3.87 | $0.854501 \mathrm{E}-04$ | 23.917600 |
| 13. | 10 | 3 | 10 | 25 | 856 | 0.0 | $0.406198 \mathrm{E}-08$ | 121.998899 |
| 14. | 9 | 50 | 50 | 3731 | 9654682 | 23.62 | $0.103618 \mathrm{E}-03$ | 2964.578187 |
| 15. | 3 | 100 | 500 | 15 | 752179 | 4.73 | 175.565438 | $0.233591 \mathrm{E}+10$ |
| 16. | 4 | 10 | 50 | 6 | 3090 | 0.0 | $0.3886716 \mathrm{E}-13$ | $0.737081 \mathrm{E}-03$ |
| Total |  |  |  |  |  |  |  |  |
| 9106 | 74442856 | 68.24 |  |  |  |  |  |  |

NELMEAD.FOR is designed to solve the above 16 applications by NelderMead method in implementation of R. Oneill and modified by John Burkard and Neculai Andrei. Table 16 below shows the performances of NelderMead method.

\left.| Table 6. Performances of Nelder-Mead for solving 16 applications |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| (FORTRAN77 version by R. ONeill |  |  |  |  |  |
| [73], modifications by John Burkardt) |  |  |  |  |  |$\right]$

The Technical Report R2020T9.DOC contains an Appendix with the mathematical expression of the applications considered in these numerical experiments.

## DEEPS10

A two level random search method for solving the Elastic Plastic Torsion from MINPACK2
This directory contains:
A1EPT.FOR - Fortran program for solving the Elastic Plastic Torsion application from MINPACK2 with 2500 variables
R2020T10.DOC - Technical Report with results of optimization by DEEPS.
Figures 1 and 2 show the solution of this application with 2500 variables





Total CPU time (centeseconds) $=1733441$ (4.5 hours)
Figure 1 shows the Dolan and More's performance profiles of these algorithms


Fig. 1. Performance profiles of DEEPS and NELMED for solving 120 problems

## DEEPS13

A two level random search method for unconstrained optimization.
This directory contains:
DEEPSPR.for (Fortran package)
FUNC120.TXT
NMPF.FOR (Fortran package of Nelder-Mead)




## $\rangle\rangle\rangle\rangle\rangle\rangle\rangle\rangle\rangle\rangle$

## Conjugate Gradient Methods

| 1. | $\begin{aligned} & \text { CGALL } \\ & \text { CGLOOP } \end{aligned}$ | Package implementing 23 Conjugate Gradient Algorithms. The package implements 80 unconstrained test function examples. <br> The following CG algorithms have been implemented: <br> 1) Hestenes - Stiefel, <br> 2) Fletcher - Reeves, <br> 3) Polak-Ribiere-Polyak, <br> 4) Polak-Ribiere-Polyak plus, <br> 5) CD - Conjugate Descent (Fletcher), <br> 6) Liu - Storey, <br> 7) Dai - Yuan, <br> 8) Dai-Liao, <br> 9) Dai - Liao plus, <br> 10) Andrei (SDC), (Please see the paper: N. Andrei, A Dai-Yuan conjugate gradient algorithm with sufficient descent and conjugacy conditions for unconstrained optimization. Applied Mathematics Letters, 21, (2008), pp.165-171.) <br> 11) hybrid Dai - Yuan, |
| :---: | :---: | :---: |


|  |  | 12) hybrid Dai - Yuan zero, <br> 13) Gilbert - Nocedal, <br> 14) Hu and Storey, <br> 15) Touat-Ahmed and Storey, <br> 16) Hybrid LS - CD, <br> 17) Birgin - Martinez (scaled Perry), <br> 18) Birgin - Martinez plus (scaled Perry), <br> 19) scaled Polak-Ribiere-Polyak, <br> 20) scaled Fletcher-Reeves, <br> 21) New cg from PRP: beta=(ytg+ -yty stg+/gtg)/yts (Please, see (8.3.130) in the BOOK. Please, see (5.5.40) in the CG-BOOK.), <br> 22) New cg from DY: beta $=y \operatorname{tg}+/ y t s-y t g+* s t g /(y t s * * 2)$ (Please, see (8.3.102) in the BOOK. Please, see (5.5.12) in the CG-BOOK.), <br> 23) New cg from DY: beta $=\max (0, \mathrm{ytg} / \mathrm{yts}) *(1-\mathrm{stg} / \mathrm{yts})$, <br> 24) New cg: Please see the paper: W07P26.pdf <br> Please see the books: <br> 1) (BOOK) N. Andrei, Critica Ratiunii Algoritmilor de Optimizare fără Restricţii. Editura Academiei Române, Bucureşti, 2009. <br> 2) (CG-BOOK) N. Andrei, Metode Avansate de Ggradient Conjugat pentru Optimizare fără Restricţii. Editura Academiei Oamenilor de Ştiinţă, Bucureşti, 2009. <br> The Fortran program CGLOOP.FOR implements the above 20 conjugate gradient algorithms using the loop unrolling of depth 5 . <br> Subdirectory APPLIC contains 7 applications from MINPACK-2. Please see OPISAPL.DOC file. |
| :---: | :---: | :---: |
|  |  | February 8, 2007 |
| 2. | CG- <br> ACCELERAT | This package implements a number of 24 conjugate gradient algorithms accelerated by means of a procedure presented in: <br> N. Andrei, Acceleration of conjugate gradient algorithms for unconstrained optimization. Applied Mathematics and Computation, vol. 213, Issue 2, 2009, pp. 361-369. <br> DOI information: 10.1016/j.amc.2009.03.020 <br> The package implements 80 unconstrained test function examples. <br> The following conjugate gradient algorithms have been implemented: <br> 1) Hestenes - Stiefel, <br> 2) Fletcher - Reeves, <br> 3) Polak-Ribiere-Polyak, <br> 4) Polak-Ribiere-Polyak plus , <br> 5) CD - Conjugate Descent (Fletcher), <br> 6) Liu - Storey, <br> 7) Dai - Yuan, <br> 8) Dai-Liao, <br> 9) Dai - Liao plus, <br> 10) Andrei (ACGSD/2) <br> (Please see the paper: <br> Andrei, N., A Dai-Yuan conjugate gradient algorithm with sufficient descent and conjugacy conditions for unconstrained optimization. <br> Applied Mathematics Letters, vol 21, 2008, pp. 165-171. |




Fig. 2. Solution of the application A2 - Pressure Distribution in a Journal Bearing. $n x=200, n y=200$


Fig. 3. Solution of the application A3 - Optimal Design with Composite Materials. $n x=200, n y=200$


|  |  | The norm of gradient $\\|g(k)\\|$ is: <br> $0.8335591087430 \mathrm{E}+05$ <br> $0.1770302860649 \mathrm{E}+05$ <br> $0.1290104898224 \mathrm{E}+03$ <br> $0.2202119533104 \mathrm{E}+04$ <br> $0.1128337396401 \mathrm{E}+03$ <br> $0.2510029662606 \mathrm{E}+04$ <br> $0.3112527173225 \mathrm{E}+04$ <br> $0.4760512089568 \mathrm{E}+03$ <br> $0.6871298669484 \mathrm{E}+02$ <br> $0.1197855311342 \mathrm{E}+05$ <br> $0.1207581561453 \mathrm{E}+05$ <br> $0.3458177452260 \mathrm{E}+02$ <br> $0.1034945886632 \mathrm{E}+03$ <br> $0.5609625857035 \mathrm{E}+03$ <br> $0.1078967162139 \mathrm{E}+04$ <br> $0.6620819548126 \mathrm{E}+03$ <br> $0.1787862322948 \mathrm{E}+02$ <br> $0.4539204111787 \mathrm{E}+03$ <br> $0.1067589106626 \mathrm{E}+04$ <br> $0.3678916480927 \mathrm{E}+03$ <br> $0.6861727730327 \mathrm{E}+01$ <br> $0.3594559195106 \mathrm{E}+03$ <br> $0.4227395335853 \mathrm{E}+03$ <br> $0.1523510891905 \mathrm{E}+02$ <br> $0.1749839153294 \mathrm{E}+01$ <br> $0.1539429121421 \mathrm{E}+03$ <br> $0.9512788103020 \mathrm{E}+02$ <br> $0.3761432997981 \mathrm{E}+02$ <br> $0.1934700602985 \mathrm{E}+00$ <br> $0.5261841571038 \mathrm{E}+01$ <br> $0.6658363856712 \mathrm{E}-01$ <br> 0.2459542556525E-02 <br> $0.9613587612598 \mathrm{E}-06$ <br> Observe that out 33 iterations only for the last two the norm of gradient is below $10^{-2}$ and $10^{-6}$ respectively. <br> March 30, 2009 |
| :---: | :---: | :---: |
| 3. | $\begin{aligned} & \hline \text { CCOMB } \\ & \text { NDOMB } \end{aligned}$ | The package includes two hybrid conjugate gradient algorithms as a convex combination of PRP and DY. <br> CCOMB is a Fortran package implementing a New Hybrid Conjugate Gradient Algorithm as a Convex Combination of PRP and DY conjugate gradient algorithms for unconstrained optimization in which the parameter theta is selected from the conjugacy condition. <br> The search direction in CCOMB algorithm is as follows: $\begin{gathered} d_{k+1}=-g_{k+1}+\beta_{k}^{\text {CCOMB }} s_{k}, \\ \beta_{k}^{\text {CCOMB }}=\left(1-\theta_{k}^{\text {CCOMB }}\right) \beta_{k}^{P R P}+\theta_{k}^{\text {CCOMB }} \beta_{k}^{D Y}, \\ \theta_{k}^{\text {CCOMB }}=\frac{\left(y_{k}^{T} g_{k+1}\right)\left(y_{k}^{T} s_{k}\right)-\left(y_{k}^{T} g_{k+1}\right)\left\\|g_{k}\right\\|^{2}}{\left(y_{k}^{T} g_{k+1}\right)\left(y_{k}^{T} s_{k}\right)-\left\\|g_{k+1}\right\\|^{2}\left\\|g_{k}\right\\|^{2}} . \end{gathered}$ <br> NDOMB is a Fortran package implementing a New Hybrid Conjugate Gradient Algorithm as a Convex Combination of PRP and DY |


|  |  | conjugate gradient algorithms for unconstrained optimization in which the parameter theta is selected from the Newton direction. The search direction in NDOMB algorithm is as follows: $\begin{aligned} & d_{k+1}=-g_{k+1}+\beta_{k}^{\text {NDOMB }} s_{k}, \\ & \beta_{k}^{\text {NDOMB }}=\left(1-\theta_{k}^{\text {NDOMB }}\right) \beta_{k}^{\text {PRP }}+\theta_{k}^{\text {NDOMB }} \beta_{k}^{D Y}, \\ & \theta_{k}^{\text {NDOMB }}=\frac{\left(y_{k}^{T} g_{k+1}-s_{k}^{T} g_{k+1}\right)\left\\|g_{k}\right\\|^{2}-\left(y_{k}^{T} g_{k+1}\right)\left(y_{k}^{T} s_{k}\right)}{\left\\|g_{k+1}\right\\|^{2}\left\\|g_{k}\right\\|^{2}-\left(y_{k}^{T} g_{k+1}\right)\left(y_{k}^{T} s_{k}\right)} . \end{aligned}$ <br> In both algorithms if $\theta_{k} \leq 0$, then set $\theta_{k}=0$, if $\theta_{k} \geq 1$, set $\theta_{k}=1$. <br> The CCOMB and NDOMB algorithms are detailed in the papers: <br> N. Andrei, "Hybrid conjugate gradient algorithm for unconstrained optimization". Journal of Optimization Theory and Applications, vol.41, (2009), pp.249-264. <br> N. Andrei, "New hybrid conjugate gradient algorithms for unconstrained optimization". C.A. Floudas and P.M. Pardalos, (Eds.) Encyclopedia of Optimization, second edition, 2009, Springer, pages: 2560-2571. <br> N. Andrei, "Performance profiles of conjugate gradient algorithms for unconstrained optimization". C.A. Floudas and P.M. Pardalos, (Eds.) Encyclopedia of Optimization, second edition, 2009, Springer, pages: 2938-2953. |
| :---: | :---: | :---: |
| 4. | CGSYS | CGSYS is a package dedicated to compute the minimizer of a differentiable function with a large number of variables. <br> The search direction of this algorithm is a linear combination of $-g_{k+1}$ and $s_{k}$, where the coefficients in this linear combination are computed in such a way that both the descent and the conjugacy conditions to be guaranteed at every iteration. <br> The search direction is computed as: $\begin{gathered} d_{k+1}=-\theta_{k} g_{k+1}+\beta_{k} s_{k}, \\ \theta_{k}=\frac{-\left(y_{k}^{T} s_{k}\right)\left\\|g_{k+1}\right\\|^{2} t+\left(s_{k}^{T} g_{k+1}\right)^{2} u}{\Delta_{k}}, \\ \beta_{k}=\frac{-\left(y_{k}^{T} g_{k+1}\right)\left\\|g_{k+1}\right\\|^{2} t+\left(s_{k}^{T} g_{k+1}\right)\left\\|g_{k+1}\right\\|^{2} u}{\Delta_{k}}, \\ \Delta_{k}=\left(y_{k}^{T} g_{k+1}\right)\left(s_{k}^{T} g_{k+1}\right)-\left\\|g_{k+1}\right\\|^{2}\left(y_{k}^{T} s_{k}\right) . \end{gathered}$ <br> The parameters $t$ and $u$ are set $t=7 / 8$ and $u=0.01$. <br> The algorithm is described in: <br> N. Andrei, An accelerated conjugate gradient algorithm with guaranteed descent and conjugacy conditions for unconstrained optimization. Technical Report, March 6, 2009. <br> (Please see the paper: cgsyspap.doc) |


|  |  | The subdirectory APPLIC contains 7 applications from MINPACK-II collection. |
| :---: | :---: | :---: |
|  |  | October 24, 2 |
| 5. | CGSECM | Conjugate gradient algorithm based on the equality of the Newton direction with the conjugate gradient direction and modified secant condition. <br> The algorithm depends on the scalar parameter $\delta$. <br> The search direction is as follows: $d_{k+1}=-g_{k+1}+\beta_{k} s_{k}$ <br> If $\delta=0$, then: $\beta_{k}=\max \left\{\frac{y_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}, 0\right\}-\frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}$ <br> If $\delta \neq 0$, then: $\begin{gathered} \beta_{k}=\max \left\{\frac{y_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}+\delta \eta}, 0\right\}-\left(1-\frac{\delta \eta}{\left\\|s_{k}\right\\|^{2}}\right) \frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}+\delta \eta} \\ \eta=6\left(f_{k}-f_{k+1}\right)+3\left(g_{k}+g_{k+1}\right)^{T} s_{k} \end{gathered}$ |
|  |  | February 12, 2008 |
| 6. | CGHSDY (HSDY9, HSDYNG, HSDYPLUS) | A hybrid conjugate gradient algorithm with convex combination of HS and DY and Newton direction. <br> There are three variants of hybrid conjugate gradient algorithms: <br> 1) HSDY9 algorithm: <br> The search direction is computed as follows: $\begin{gathered} d_{k+1}=-g_{k+1}+\beta_{k} s_{k}, \\ \theta_{k}=-\frac{s_{k}^{T} g_{k+1}+y_{k}^{T} g_{k+1}}{g_{k}^{T} g_{k+1}} \end{gathered}$ <br> If $0<\theta_{k}<1$, then $\beta_{k}=-\frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}$, <br> If $\theta_{k} \geq 1$, then $\beta_{k}=\frac{\left\\|g_{k+1}\right\\|^{2}}{y_{k}^{T} s_{k}}$,(DY) <br> If $\theta_{k} \leq 0$, then $\beta_{k}=\frac{y_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}$. (HS) <br> 2) HSDYNG algorithm <br> In this algorithm the parameter $\theta_{k}$ is computed in 6 different ways: <br> a) Hybrid CG with Newton and secant equation: $\theta_{k}=-\frac{s_{k}^{T} g_{k+1}}{g_{k}^{T} g_{k+1}}$ <br> b) Hybrid CG with Newton and spectral gradient: |



|  |  | Unconstrained Optimization, Numerical Algorithms, vol.47, no.2, February 2008, pp.143-156. <br> N. Andrei. Accelerated hybrid conjugate gradient algorithm with modified secant condition for unconstrained optimization. Numerical Algorithms, vol. 54 (2010), pp.23-46. <br> April 2, 2007 |
| :---: | :---: | :---: |
| 7. | CONGRAD <br> (AML5382, <br> PCONMIN, <br> MCONMIN) | Package for unconstrained minimization using the conjugate gradient algorithm of Shanno with Beale's restart procedure. <br> Prof. Shanno sent me a copy of the package on October 17, 1983. I modified it in some respects, including the possibility to work on a train of numerical experiments. <br> The algorithm is described in: <br> Shanno, D.F., (1978) Conjugate gradient methods with exact searches. Mathematics of Operations Research, vol.3, no.3, August 1978, pp.244-256. <br> The subdirectory MINPACK includes 7 applications from MINPACKII collection. <br> The package aml5382.for implements the conjugate gradient algorithm BFGS preconditioned, in variant given by Shanno, with a train of 80 unconstarined optimization test functions. This is a variant of the Shanno's package which I modified in some respects. The line search procedure is incorporated into the package. Another variant of this package is given by PCONMIN. <br> The package MCONGRAD, wich includes the subroutine CONGRAD uses the numerical derivatives facilities. The subroutine NUMGRAD is designed for numerical derivatives computation. |
| 8. | CONMINEX | November 26, 2001 <br> Another variant of the package for unconstrained minimization using the conjugate gradient algorithm by Shanno and Phua with Beale's restart procedure. <br> Mainly, this package is the same as CONGRAD. |
| 9. | CONMIN | March: 27, 2007 <br> Another variant of the package implementing the conjugate gradient by Shanno and Phua. <br> Subroutine CONMIN is described in the papers: <br> 1) Shanno, D.F., Conjugate gradient methods with inexact searches. Mathematics of Operations Research, vol. 3, No. 3, August 1978, pp. 244256. <br> 2) Shanno, D.F., On the convergence of a new conjugate gradient algorithm. <br> SIAM J. Numer. Anal., vol.15, No.6, December 1978, pp.1247-1257. <br> 3) Shanno, D.F., Phua, K.H., Algorithm 500. Minimization of unconstrained multivariate functions. <br> ACM TOMS, vol.2, No.1, March 1976, pp.87-94. <br> 4) Andrei, N., Criticism of the unconstrained optimization |


|  |  | algorithms reasoning. <br> Academy Publishing House, Bucharest 2009. <br> ISBN 978-973-27-1669-4 <br> (Chapter 8, pp.317-448.) <br> Remark: <br> Professor Shanno sent me the Fortran subrutine CONMIN in October 17, 1983. I modified it in some respects. <br> October 15, 2004 |
| :---: | :---: | :---: |
| 10. | DLDC | DLDC is a subroutine dedicated to compute the minimizer of a differentiable function with a large number of variables. <br> Mainly, this is a modification of the Dai-Liao conjugate gradient algorithm with guaranteed descent and conjugacy conditions. <br> The search direction is computed as: $d_{k+1}=-\theta_{k} g_{k+1}+\max \left\{\frac{y_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}, 0\right\} s_{k}-t_{k} \frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}} s_{k}$ <br> The parameters $\theta_{k}$ and $t_{k}$ are computed as solution of the following linear algebraic system: $\begin{aligned} & \theta_{k}\left(y_{k}^{T} g_{k+1}\right)+t_{k}\left(s_{k}^{T} g_{k+1}\right)=a_{k} \\ & \theta_{k}\left(y_{k}^{T} s_{k}\right)\left\\|g_{k+1}\right\\|^{2}+t_{k}\left(s_{k}^{T} g_{k+1}\right)^{2}=b_{k} \end{aligned}$ <br> where $\begin{aligned} & a_{k}=v\left(s_{k}^{T} g_{k+1}\right)+\left(y_{k}^{T} g_{k+1}\right) \\ & b_{k}=w\left(s_{k}^{T} y_{k}\right)\left\\|g_{k+1}\right\\|^{2}+\left(y_{k}^{T} g_{k+1}\right)\left(s_{k}^{T} g_{k+1}\right) \end{aligned}$ <br> The scalar parameters $w$ and $v$ are introduced in such a way that the algorithm to satisfies the sufficient descent condition and the conjugacy condition respectively. These parameters are assigned to the values: $w=\left(1+\left\\|s_{k}^{T} g_{k+1}\right\\|\right), v=0.1$. <br> The algorithm is described in: <br> N. Andrei, (2009) An accelerated modified Dai-Liao conjugate gradient algorithm with guaranteed descent and conjugacy conditions for unconstrained optimization. Technical Report, July 16, 2009. <br> (Please see the Technical Report: n41a09.doc) <br> N. Andrei, Another accelerated conjugate gradient algorithm with guaranteed descent and conjugacy conditions for large-scale unconstrained optimization. Technical Report, January 29, 2010. <br> (Please see the paper in DLDCNEW.DOC file) <br> The directory MINPACK includes 5 applications from MINPACK-II collection. |
| 11. | DLDN | DLDN is a subroutine dedicated to compute the minimizer of a differentiable function with a large number of variables. <br> Mainly, this is a variant of a modification of the Dai-Liao conjugate gradient algorithm with guaranteed descent and conjugacy conditions. The search direction is computed as: |


|  |  | $d_{k+1}=-\theta_{k} g_{k+1}+\max \left\{\frac{y_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}, 0\right\} s_{k}-t_{k} \frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}} s_{k},$ <br> The parameters $\theta_{k}$ and $t_{k}$ are computed as solution of the following linear algebraic system: $\begin{aligned} & \theta_{k}\left(y_{k}^{T} g_{k+1}\right)+t_{k}\left(s_{k}^{T} g_{k+1}\right)=a_{k}, \\ & \theta_{k}\left(y_{k}^{T} s_{k}\right)\left\\|g_{k+1}\right\\|^{2}+t_{k}\left(s_{k}^{T} g_{k+1}\right)^{2}=b_{k}, \end{aligned}$ <br> where $\begin{aligned} a_{k} & =v\left(s_{k}^{T} g_{k+1}\right)+\left(y_{k}^{T} g_{k+1}\right), \\ b_{k} & =w\left(s_{k}^{T} y_{k}\right)\left\\|g_{k+1}\right\\|^{2}+\left(y_{k}^{T} g_{k+1}\right)\left(s_{k}^{T} g_{k+1}\right) . \end{aligned}$ <br> The scalar parameters $w$ and $v$ are introduced in such a way that the algorithm to satisfies the sufficient descent condition and the conjugacy condition respectively. These parameters are assigned to the values: $w=7 / 8, v=0.1$. <br> The algorithm is not too much sensitive to the values of these parameters. |
| :---: | :---: | :---: |
|  |  | January 29, 2010 |
| 12. | DESCON | DESCON is a subroutine dedicated to compute the minimizer of a differentiable function with a large number of variables. <br> The search direction is computed as: $\begin{gathered} d_{k+1}=-\theta_{k} g_{k+1}+\beta_{k} s_{k}, \\ \beta_{k}=\frac{y_{k}^{T} g_{k+1}-t_{k} s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}, \end{gathered}$ <br> where $\theta_{k}$ and $t_{k}$ are scalar parameters which are computed as: $\begin{aligned} & t_{k}=\frac{b_{k}\left(y_{k}^{T} g_{k+1}\right)-a_{k}\left(y_{k}^{T} s_{k}\right)\left\\|g_{k+1}\right\\|^{2}}{\Delta_{k}}, \\ & \theta_{k}=\frac{a_{k}-t_{k}\left(s_{k}^{T} g_{k+1}\right)}{y_{k}^{T} g_{k+1}}, \\ & \bar{\Delta}_{k}=\left(y_{k}^{T} g_{k+1}\right)\left(s_{k}^{T} g_{k+1}\right)-\left\\|g_{k+1}\right\\|^{2}\left(y_{k}^{T} s_{k}\right), \\ & \Delta_{k}=\left(s_{k}^{T} g_{k+1}\right) \bar{\Delta}_{k}, \\ & a_{k}=v\left(s_{k}^{T} g_{k+1}\right)+y_{k}^{T} g_{k+1}, \\ & b_{k}=w\left\\|g_{k+1}\right\\|^{2}\left(y_{k}^{T} s_{k}\right)+\left(y_{k}^{T} g_{k+1}\right)\left(s_{k}^{T} g_{k+1}\right) . \end{aligned}$ <br> $v>0$ and $w>0$ are known scalar parameters. <br> The algorithm is described in: <br> - N. Andrei, An accelerated conjugate gradient algorithm with guaranteed descent and conjugacy conditions for large-scale unconstrained optimization. <br> ICI Technical Report, November 29, 2010. <br> Please see the Technical Report: R5A11.DOC file. <br> - N. Andrei, Another conjugate gradient algorithm with guaranteed |


|  |  | descent and conjugacy conditions for large-scale unconstrained optimization. Journal of Optimization Theory and Applications, vol. 159, Number 1, 2013, pp159-182. <br> Please, see the paper: JOTA-2013.pdf (paper published in JOTA) <br> - N. Andrei, Nonlinear Conjugate Gradient Methods for Unconstrained Optimization, vol. 158 Springer Optimization and Its Applications, Springer, 2020, (Chapter 7, pp.227-245) <br> A comprehensive numerical comparasions between DESCON and some other conjugate gradient algorithms are presented into the paper N. Andrei, A numerical study on efficiency and robustness of some conjugate gradient algorithms for large-scale unconstrained optimization. Technical Report, June 6, 2013. <br> (Please see the paper: ANpaper.doc.) <br> Fig. 1. Performance profile of DESCONa versus HS and versus PRP <br> Fig. 2. Performance profile of DESCONa versus DL $(t=1)$ and versus CG-DESCENT <br> The subdirectory MINPACK2 contains 5 applications from the MINPACK-2 Collection. |
| :---: | :---: | :---: |
| 13. | HS | This package implements the Hestenes and Stiefel (HS) conjugate gradient algorithm using loop unrollong of depth 5 . <br> The search direction is computed as: $\begin{gathered} d_{k+1}=-g_{k+1}+\beta_{k} s_{k}, \\ \beta_{k}=\frac{y_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}} . \end{gathered}$ <br> January 10, 2013 |
| 14. | hDY | The package implements the hybrid Day and Yuan conjugate gradient algorithm using loop unrolling of depth 5 . <br> The search direction is computed as: |


|  |  | $\begin{gathered} d_{k+1}=-g_{k+1}+\beta_{k} s_{k}, \\ \beta_{k}=\max \left\{-c \frac{\left\\|g_{k+1}\right\\|^{2}}{y_{k}^{T} s_{k}}, \min \left\{\alpha_{k} \frac{y_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}, \frac{\left\\|g_{k+1}\right\\|^{2}}{y_{k}^{T} s_{k}}\right\}\right\}, \end{gathered}$ <br> where $c=0.05263157$ and $\alpha_{k}$ is the step length computed by the Wolfe line search conditions. <br> March 29, 2013 |
| :---: | :---: | :---: |
| 15. | HYBRID, HYBRIDM, AHYBRIDM | A hybrid conjugate gradient algorithm with Convex combination of HS and DY and Newton direction with secant condition. <br> This subdirectory contains three packages: HYBRID, HYBRIDM, AHYBRIDM. <br> In HYBRID it is assumed that the pair $\left(s_{k}, y_{k}\right)$ satisfies the secant condition. <br> The search direction is as follows: $d_{k+1}=-g_{k+1}+\beta_{k}^{C} s_{k} .$ <br> A parameter $\theta_{k}$ is computed as: $\theta_{k}=\frac{s_{k}^{T} g_{k+1}}{g_{k}^{T} g_{k+1}}$ <br> If $0<\theta_{k}<1$, then $\beta_{k}^{C}=\left(1-\theta_{k}\right) \frac{g_{k+1}^{T} y_{k}}{y_{k}^{T} s_{k}}+\theta_{k} \frac{\left\\|g_{k+1}\right\\|^{2}}{y_{k}^{T} s_{k}} .$ <br> If $\theta_{k} \geq 1$, then $\beta_{k}^{C}=\beta_{k}^{D Y}=\frac{\left\\|g_{k+1}\right\\|^{2}}{y_{k}^{T} s_{k}}$. <br> If $\theta_{k} \leq 0$, then $\beta_{k}^{C}=\beta_{k}^{H S}=\frac{g_{k+1}^{T} y_{k}}{y_{k}^{T} s_{k}}$. <br> The theoretical developments of HYBRID algorithm are described into the paper: <br> N. Andrei, (2008) Another hybrid conjugate gradient algorithm for Unconstrained Optimization, Numerical Algorithms, vol.47, no.2, February 2008, pp.143-156. <br> HYBRIDM is an extension of the HYBRID package authored by N . Andrei. In HYBRIDM it is assumed that the pair $\left(s_{k}, y_{k}\right)$ satisfies the modified secant condition given by Zhang, Deng and Chen into the paper: J.Z. Zhang, N.Y. Deng and L.H. Chen, "New quasi-Newton equation and related methods for unconstrained optimization", JOTA, 102 (1999), p. 147-167. <br> AHYBRIDM is an acceleration of the HYBRIDM package. <br> The directory APPLIC contains 7 applications from MINPACK-II |




|  |  | $t_{k}=\frac{2}{s_{k}^{T} y_{k}}\left(f_{k}-f_{k+1}+s_{k}^{T} g_{k+1}\right)$ <br> and $t_{k}$ belongs to the interval $[0.01,100]$. <br> 6) $s_{k}^{T} B_{k+1} s_{k}$ is from the interpolation condition by Yuan. $s_{k}^{T} B_{k+1} s_{k}=2\left(f_{k}-f_{k+1}\right)+s_{k}^{T} g_{k+1}$ <br> 7) $s_{k}^{T} B_{k+1} s_{k}$ is from the Hermite interpolation condition. If the function $f$ is cubic along the line between $x_{k-1}$ and $x_{k}$ then by considering the Hermite interpolation we get: $s_{k}^{T} B_{k+1} s_{k}=4 s_{k}^{T} g_{k+1}+2 s_{k}^{T} g_{k}-6\left(f_{k+1}-f_{k}\right)$ <br> October 6, 2010 |
| :---: | :---: | :---: |
| 19. | PRP | Polak-Ribière-Polyak conjugate gradient algorithm. The search direction is computed like: $\begin{gathered} d_{k+1}=-g_{k+1}+\beta_{k} s_{k}, \\ \beta_{k}=\frac{y_{k}^{T} g_{k+1}}{g_{k}^{T} g_{k}} . \end{gathered}$ <br> January 15, 2013 |
| 20. | PRP-DC | Three-term Conjugate Gradient Algorithms in three variants: <br> 1) PRP Modified Method (Andrei) (PRPDC) <br> 2) Zhang, Zhou and Li (ZZL) <br> 3) Zhang, Xiao and Wei (ZXW) <br> The search direction in version PRPDC: $d_{k+1}=\frac{1}{\left\\|g_{k}\right\\|^{2}}\left[-\left(y_{k}^{T} s_{k}\right) g_{k+1}+\left(y_{k}^{T} g_{k+1}\right) s_{k}-\left(s_{k}^{T} g_{k+1}\right) y_{k}\right]$ <br> The search direction in version ZZL: $d_{k+1}=-g_{k+1}+\frac{y_{k}^{T} g_{k+1}}{\alpha_{k}\left\\|g_{k}\right\\|^{2}} s_{k}-\frac{s_{k}^{T} g_{k+1}}{\alpha_{k}\left\\|g_{k}\right\\|^{2}} y_{k}$ <br> The search direction in version ZXW: $d_{k+1}=-g_{k+1}+\frac{1}{y_{k}^{T} s_{k}}\left[\left(y_{k}^{T} g_{k+1}\right) s_{k}-\left(s_{k}^{T} g_{k+1}\right) y_{k}\right]$ <br> The algorithm PRP modified (PRP-DC) is described in the paper: N. Andrei, A modified Polak-Ribie`re-Polyak conjugate gradient algorithm for unconstrained optimization. Optimization, Vol. 60, No. 12, December 2011, 1457-1471. (Please se the paper: optimiz11.pdf) |
| 21. | ACGA | Another Nonlinear Conjugate Gradient Algorithm for Unconstrained Optimization. <br> The search direction in ACGA is computed as: |
|  |  | $\begin{gathered} d_{k+1}=-g_{k+1}+\beta_{k}^{A} s_{k}, \\ \beta_{k}^{A}=\frac{1}{y_{k}^{T} s_{k}}\left(y_{k}-\frac{g_{k+1}^{T} y_{k}}{y_{k}^{T} s_{k}} s_{k}\right)^{T} g_{k+1} . \end{gathered}$ <br> Please see the paper: <br> Andrei, N., (2009), Another Nonlinear Conjugate Gradient Algorithm for Unconstrained Optimization, Optimization Methods and Software, vol.24, No.1, February 2009, pp. 89-104. <br> July 31, 2008 |
| :---: | :---: | :---: |
| 22. | ACGHES | Accelerated conjugate gradient algorithm based on the equality of the Newton direction with the conjugate gradient direction and using the Hessian / vector product. <br> The search direction in this algorithm is computed as: $d_{k+1}=-g_{k+1}+\frac{s_{k}^{T} \nabla^{2} f\left(x_{k+1}\right) g_{k+1}-s_{k}^{T} g_{k+1}}{s_{k}^{T} \nabla^{2} f\left(x_{k+1}\right) s_{k}}$ <br> where the Hessian / vector product is computed using the finite difference: $\begin{gathered} \nabla^{2} f\left(x_{k+1}\right) s_{k}=\frac{\nabla f\left(x_{k+1}+\delta s_{k}\right)-\nabla f\left(x_{k+1}\right)}{\delta}, \\ \delta=\frac{2 \sqrt{\varepsilon_{m}}\left(1+\left\\|x_{k+1}\right\\| \sqrt{n}\right)}{\left\\|s_{k}\right\\|}, \end{gathered}$ <br> $\varepsilon_{m}$ is epsilon machine. <br> The algorithm is described in: <br> Andrei., N., (2009) Accelerated conjugate gradient algorithm with finite difference Hessian/vector product approximation for unconstrained optimization. Journal of Computational and Applied Mathematics, vol. 230, 2009, pp. 570-582. <br> Please see the paper jcam2009.pdf. <br> The directory MINPACK contains 7 applications from MINPACK-II collection: <br> ACGHES1.FOR - elastic-plastic torsion, <br> ACGHES2.FOR - pressure distribution in a journal bearing problem, <br> ACGBES3.FOR - optimal design with composite materials problem, <br> ACGHES4.FOR - Inhomogeneous Superconductors. GinzburgLandau (1-dimensional) problem, <br> ACGHES5.FOR - steady state combustion problem, <br> ACGHES6.FOR - Jones Clusters (Molecular Conformation) Problem, <br> ACGHES7.FOR - minimal surface area problem. |
|  |  | February 12, 2008 |
| 23. | ACGHESM | Accelerated conjugate gradient algorithm based on the equality of the Newton direction with the conjugate gradient direction and using the Hessian / Vector product. <br> The Hessian / vector product is computed by finite difference using 5 |
|  |  | different increments. The package is testing the numerical performances of this conjugate gradient algorithm subject to the values of increments for Hessian / vector product approximations. <br> The search direction in this algorithm is computed as: $d_{k+1}=-g_{k+1}+\frac{s_{k}^{T} \nabla^{2} f\left(x_{k+1}\right) g_{k+1}-s_{k}^{T} g_{k+1}}{s_{k}^{T} \nabla^{2} f\left(x_{k+1}\right) s_{k}}$ <br> where the Hessian / vector product is computed using the finite difference: $\nabla^{2} f\left(x_{k+1}\right) s_{k}=\frac{\nabla f\left(x_{k+1}+\delta s_{k}\right)-\nabla f\left(x_{k+1}\right)}{\delta}$ <br> where $\varepsilon_{m}$ is epsilon machine and $\delta$ is estimated by the following methods: <br> 1) Schlick-Fogelson (TNPACK) (SF) $\delta=\frac{2 \sqrt{\varepsilon_{m}}\left(1+\left\\|x_{k+1}\right\\| \sqrt{n}\right)}{\left\\|s_{k}\right\\|}$ <br> 2) Schlick-Fogelson (variant) (SFV) $\delta=\frac{2 \sqrt{\varepsilon_{m}}\left(1+\left\\|x_{k+1}\right\\|\right)}{\left\\|s_{k}\right\\|}$ <br> 3) Nash (Truncated-Newton) (NASH) $\delta=\sqrt{\varepsilon_{m}\left(1+\left\\|x_{k+1}\right\\|\right.}$ <br> 4) Dembo-Steihaug (DS) $\delta=\frac{\sqrt{\varepsilon_{m}}}{\left\\|s_{k}\right\\|}$ <br> 5) O'Leary (LEARY) $\delta=\frac{2 \sqrt{\varepsilon_{m}}\left(1+\left\\|x_{k+1}\right\\|\right)}{\left\\|s_{k}\right\\|^{2}} .$ <br> The algorithm is described in: <br> N. Andrei, Accelerated conjugate gradient algorithm with finite difference Hessian/vector product approximation for unconstrained optimization. Journal of Computational and Applied Mathematics, 230 (2009) 570-582. |
| :---: | :---: | :---: |
| 24. | ACGSEC | February 23, 2010 <br> This algorithm uses a hybrid approach by considering a convex combination of Hestenes and Stiefel (HS) and Dai and Yuan (DY) conjugate gradient algorithms. <br> ACGSEC is an accelerated conjugate gradient algorithm based on the equality of the Newton direction with the conjugate gradient direction and secant condition. <br> The search direction is computed as: $d_{k+1}=-g_{k+1}+\beta_{k} s_{k},$ |
|  |  | $\beta_{k}=\max \left\{\frac{y_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}, 0\right\}-\frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}} .$ <br> The algorithm is described in: <br> Andrei, N., (2010) Accelerated hybrid conjugate gradient algorithm with modified secant condition for unconstrained optimization. <br> Numerical Algorithms (2010) vol.54, pp.23-46. <br> (Please see the Technical Report n14a09.doc: „Accelerated hybrid conjugate gradient algorithm with modified secant condition for unconstrained optimization", February 23, 2009.) <br> February 22, 2008 |
| :---: | :---: | :---: |
| 25. | ACGMSEC | This algorithm uses a hybrid approach by considering a convex combination of Hestenes and Stiefel (HS) and Dai and Yuan (DY) conjugate gradient algorithms. <br> ACGMSEC is an accelerated conjugate gradient algorithm based on the equality of the Newton direction with the conjugate gradient direction and modified secant condition. <br> The search direction is computed as: $\begin{gathered} d_{k+1}=-g_{k+1}+\beta_{k} s_{k}, \\ \beta_{k}=\max \left\{\frac{y_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}+\delta \eta}, 0\right\}-\left(1-\frac{\delta \eta}{\left\\|s_{k}\right\\|^{2}}\right) \frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}+\delta \eta}, \\ \eta=6\left(f_{k}-f_{k+1}\right)+3\left(g_{k}+g_{k+1}\right)^{T} s_{k} . \end{gathered}$ <br> $\delta$ is a parameter. If $\delta=0$ we get the ACGSEC algorithm. <br> The algorithm is described in: <br> Andrei, N., (2010) Accelerated hybrid conjugate gradient algorithm with modified secant condition for unconstrained optimization. Numerical Algorithms (2010) vol.54, pp.23-46. <br> (Please see the Technical Report n14a09.doc: „Accelerated hybrid conjugate gradient algorithm with modified secant condition for unconstrained optimization", February 23, 2009.) <br> The directory MINPACK2 contains 7 applications from MINPACK-II collection. |
| 26. | $\begin{aligned} & \text { SCALCG } \\ & \text { ASCALCG } \end{aligned}$ | February 11, 2008 <br> Scaled Conjugate Gradient Algorithm BFGS Preconditioned with Powell restart. The package implements 80 unconstrained test function examples. <br> The search direction in this algorithm is computed as: $\begin{aligned} d_{k+1}= & -\theta_{k+1} g_{k+1}+\theta_{k+1} \frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}} y_{k}- \\ & {\left[\left(1+\theta_{k+1} \frac{\left\\|y_{k}\right\\|^{2}}{y_{k}^{T} s_{k}}\right) \frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}-\theta_{k+1} \frac{y_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}\right] s_{k} . } \end{aligned}$ |



|  |  | April, 5, 2013 |
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| 29. | TTSNC | This is a variant of an accelerated subspace minimization three-term conjugate gradient algorithm for unconstrained optimization in which the three-term search direction is equal to the Newton direction. <br> The search direction is computed as: $\begin{aligned} & d_{k+1}=-g_{k+1}+a_{k} s_{k}+b_{k} y_{k}, \\ & a_{k}=\frac{2\left(y_{k}^{T} g_{k+1}\right)}{y_{k}^{T} s_{k}}-\frac{\omega_{k}-\left(y_{k}^{T} g_{k+1}\right)}{y_{k}^{T} y_{k}}, \\ & b_{k}=\frac{1}{\left(y_{k}^{T} y_{k}\right)^{2}}\left[\left(y_{k}^{T} s_{k}\right)\left(\omega_{k}-y_{k}^{T} g_{k+1}\right)-\left(y_{k}^{T} g_{k+1}\right)\left(y_{k}^{T} y_{k}\right)\right] \\ & \omega_{k}=g_{k+1}^{T} y_{k}+\frac{\left(g_{k+1}^{T} y_{k}\right)\left(y_{k}^{T} y_{k}\right)}{y_{k}^{T} s_{k}}-\frac{\left(g_{k+1}^{T} s_{k}\right)\left(s_{k}^{T} y_{k}\right)}{s_{k}^{T} s_{k}} . \end{aligned}$ <br> TTSNC is very close to TTS. The three-term conjugate gradient algorithm TTS is obtained as the minimization of the quadratic approximation model of function $f$ in a subspace spanned by $-g_{k+1}, s_{k}$ and $y_{k}$. In this algorithm the searching direction is computed as above, where the parameters $a_{k}$ and $b_{k}$ are determined as: $\begin{gathered} a_{k}=\frac{2\left(y_{k}^{T} g_{k+1}-s_{k}^{T} g_{k+1}\right)}{y_{k}^{T} s_{k}}-\frac{\omega_{k}-y_{k}^{T} g_{k+1}}{y_{k}^{T} y_{k}}, \\ b_{k}=\frac{\left(y_{k}^{T} s_{k}\right)\left(\omega_{k}-y_{k}^{T} g_{k+1}\right)}{\left(y_{k}^{T} y_{k}\right)^{2}}-\frac{y_{k}^{T} g_{k+1}-s_{k}^{T} g_{k+1}}{y_{k}^{T} y_{k}} . \end{gathered}$ <br> Observe the difference between these two formulae for $a_{k}$ and $b_{k}$ computation. It is the explicit presence of the term $s_{k}^{T} g_{k+1}$ into the formulae for $a_{k}$ and $b_{k}$ computation in TTS. <br> The algorithm is presented in: <br> N. Andrei, Another three-term conjugate gradient algorithm for unconstrained optimization. Technical Report, September 11, 2013 (Please see the file ttsnc.doc) |


Fig. 1. THRCG2 versus CG-DESCENT

| 31. | TTDES | TTDES implements a three-term conjugate gradient algorithm obtained by minimizing the one-parameter quadratic model of the objective function in which the symmetrical approximation of the Hessian matrix satisfies the general quasi-Newton equation: $B_{k+1} s_{k}=\omega^{-1} y_{k}$, with $\omega \neq 0$. <br> The search direction is computed as: $d_{k+1}=-Q_{k+1} g_{k+1}=-g_{k+1}+\frac{y_{k}^{T} g_{k+1}-\omega s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}} s_{k}-\frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}} y_{k},$ <br> where $\omega=\frac{2}{\left\\|s_{k}\right\\|^{2}} \sqrt{\left\\|s_{k}\right\\|^{2}\left\\|y_{k}\right\\|^{2}-\left(y_{k}^{T} s_{k}\right)^{2}}$ <br> This choice of the parameter $\omega$ makes the condition number of $Q_{k+1}=I-\frac{s_{k}\left(y_{k}-\omega s_{k}\right)^{T}}{y_{k}^{T} s_{k}}+\frac{y_{k} s_{k}^{T}}{y_{k}^{T} s_{k}}$ <br> approach its minimum. <br> The algorithm is described in: <br> - N. Andrei, A new three-term conjugate gradient algorithm for unconstrained optimization. Numerical Algorithms, vol.68, (2015), pp.305-321. <br> - N. Andrei, Nonlinear Conjugate Gradient Methods for Unconstrained Optimization, vol. 158 Springer Optimization and Its Applications, Springer, 2020, (Chapter 9, pp.334-345) <br> (Please see the file: paper-ttdes.doc) |
| :---: | :---: | :---: |
|  |  | TTCG implements an accelerated conjugate gradient algerithm with |
| 32. | TTCG | TTCG implements an accelerated conjugate gradient algorithm with three terms, that at each iteration both the descent and the conjugacy conditions are guaranteed. <br> The search direction is computes as: $\begin{aligned} & d_{k+1}=-g_{k+1}-\delta_{k} s_{k}-\eta_{k} y_{k}, \\ & \delta_{k}=\left(1+2 \frac{\left\\|y_{k}\right\\|^{2}}{y_{k}^{T} s_{k}}\right) \frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}+\frac{y_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}, \end{aligned}$ |


|  |  | $\eta_{k}=\frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}$ <br> The algorithm is described in: <br> - N. Andrei, On three-term conjugate gradient algorithms for unconstrained optimization. Applied Mathematics and Computation, vol.219, 2013, pp.6316-6327. <br> (Please see the file AMC_17812.pdf) <br> - N. Andrei, Nonlinear Conjugate Gradient Methods for Unconstrained Optimization, vol. 158 Springer Optimization and Its Applications, Springer, 2020, (Chapter 9, pp.316-323) |
| :---: | :---: | :---: |
| 33. | NADCG | This program implements an adaptive conjugate gradient algorithm. The search direction is computed as the sum of the negative gradient and a vector determined by minimizing the quadratic approximation of the objective function at the current point. Using a special approximation of the inverse Hessian of the objective function, which depends by a positive parameter, a search direction is obtained which satisfies both the sufficient descent and the conjugacy conditions. <br> The search direction is computed as: $d_{k+1}=-g_{k+1}+\max \left\{\frac{y_{k}^{T} g_{k+1}-\omega_{k} s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}\right\} s_{k}-\frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}} y_{k},$ <br> where $\omega_{k}= \begin{cases}2 \sqrt{\tau-1} \frac{\left\\|y_{k}\right\\|}{\left\\|s_{k}\right\\|}, & a_{k} \geq \tau \\ 2 \sqrt{a_{k}-1} \frac{\left\\|y_{k}\right\\|}{\left\\|s_{k}\right\\|} & a_{k}<\tau\end{cases}$ <br> Here $a_{k}=\frac{\left\\|y_{k}\right\\|^{2}\left\\|s_{k}\right\\|^{2}}{\left(y_{k}^{T} s_{k}\right)^{2}} .$ <br> The parameter $\tau>1$ is the adaptive parameter. The algorithm is not very much sensitive the the values of $\tau$. <br> The algorith is described in the paper: <br> N. Andrei, A new adaptive conjugate gradient algorithm for large- |


|  |  | scale unconstrained optimization. Paper published into the book: "Optimization and Applications in Control and Data Science", edited by Boris Goldengorin. Springer Optimization and Its Applications, Vol.115. 2016, pp.1-16. <br> This paper is written in honour of Prof. Boris T. Polyak celebrating his 80th anniversary. <br> (Please see the file: nadcg.doc) <br> June 18, 2015 |
| :---: | :---: | :---: |
| 34. | ADCG | An adaptive conjugate gradient algorithm for large-scale unconstrained optimization. <br> The search direction is computed as $d_{k+1}=-Q_{k+1} g_{k+1}=-g_{k+1}+\frac{\left(y_{k}-t_{k} s_{k}\right)^{T} g_{k+1}}{y_{k}^{T} s_{k}} s_{k}-\frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}} y_{k},$ <br> where, $t_{k} \equiv \omega_{k}\left\\|y_{k}\right\\|^{2} / y_{k}^{T} s_{k}$ is computed as: $t_{k}=\left\{\begin{array}{cc} 2 \sqrt{\tau-1} \frac{\left\\|y_{k}\right\\|}{\left\\|s_{k}\right\\|}, & \text { if } \frac{\left\\|y_{k}\right\\|^{2}\left\\|s_{k}\right\\|^{2}}{\left(y_{k}^{T} s_{k}\right)^{2}} \geq \tau, \\ 0, & \text { otherwise }, \end{array}\right.$ <br> where $\tau>1$ is a positive constant. <br> The algorithm is described into the paper: <br> N. Andrei, An adaptive conjugate gradient algorithm for large-scale unconstrained optimization, Journal of Computational and Applied Mathematics, 292 (2016), pp.83-91. <br> May 20, 2015 |
| 35. | EIGN-SING | In this directory I placed the paper and the Fortran files: <br> N. Andrei, Eigenvalues versus singular values study in conjugate gradient algorithms for large-scale unconstrained optimization. Technical Report, July 14, 2015. (See the file: paper10.doc) The Fortran packages SVCG.FOR and NADCG.FOR implements the singular value approach and eigenvalues approach in conjugate gradient algorithms, respectively. Directory MINPACK contains 5 applications from MINPACK-II collection. <br> 1) The NADCG algorithm implements the eigenvalues clustering in conjugate gradient algorithms. The search direction is computed as: $d_{k+1}=-g_{k+1}+\max \left(\frac{y_{k}^{T} g_{k+1}-\omega_{k} s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}}, 0\right) s_{k}-\frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}} y_{k} .$ <br> where $\omega_{k}= \begin{cases}2 \sqrt{\tau-1} \frac{\left\\|y_{k}\right\\|}{\left\\|s_{k}\right\\|}, & a_{k} \geq \tau, \\ 2 \sqrt{a_{k}-1} \frac{\left\\|y_{k}\right\\|}{\left\\|s_{k}\right\\|} & a_{k}<\tau .\end{cases}$ <br> Here $a_{k}=\frac{\left\\|y_{k}\right\\|^{2} \mid s_{k} \\|^{2}}{\left(y_{k}^{T} s_{k}\right)^{2}} .$ <br> The parameter $\tau>1$ is the adaptive parameter. The algorithm is not |


|  |  | very much sensitive the the values of $\tau$. <br> 2) The SVCG algorithm implements the singular values approach (minimizing the comdition number) in conjugate gradient algorithms. The search direction is computed as: $d_{k+1}=-g_{k+1}+\frac{y_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}} s_{k}-\frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}} y_{k} .$ <br> Observe that this is a modification of the Hestenes and Stiefel conjugate gradient algorithm. <br> Some comparisons of these algorithms versus CG-DESCENT by Hager and Zhang, using 800 unconstrained optimization test problems, are as follows: <br> Please, see the paper: N. Andrei, Eigenvalues versus singular values study in conjugate gradient algorithms for large-scale unconstrained optimization. Optimization Methods and Software, vol. 32, no. 3, 2017, pp. 534-551. <br> July 14, 2015 |
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| 36. | ACGSSV | An adaptive class of nonlinear conjugate gradient algorithms is suggested. The search direction in these algorithms is given by symmetrization of the scaled Perry conjugate gradient direction [A. Perry, A modified conjugate gradient algorithm. Operations Research, 26 (1978) 1073-1078], which depends by a positive parameter. The value of this parameter is determined by minimizing the distance between the symmetrical scaled Perry conjugate gradient search direction matrix and the self-scaling memoryless BFGS update by Oren in the Frobenius norm. Two variants of the parameter in the search direction are presented as those given by: Oren and Luenberger [S.S. Oren, D. G. Luenberger, Self-scaling variable metric (SSVM) algorithms. I. Criteria and sufficient conditions for scaling a class of algorithms. Management Sci., 20 (1973/74) 845-862] and Oren and Spedicato [S.S. Oren, E. Spedicato, Optimal conditioning of selfscaling variable metric algorithms. Math. Program., 10 (1976) 70-90]. The corresponding algorithm, ACGSSV, is equipped with a vey well known acceleration scheme of conjugate gradient algorithms. <br> The algorithm is described in the paper: <br> N. Andrei, Accelerated adaptive Perry conjugate gradient algorithms based on the self-scaling memoryless BFGS update. Journal of Computational and Applied Mathematics, vol. 325, 2017, pp.149-164. (Please see the file JCAM-2017 (40).pdf) |
| 37. | DLE | A new value for the parameter in Dai and Liao conjugate gradient algorithm is presented. This is based on the clustering the eigenvalues of the matrix which determine the search direction of this algorithm. |



|  |  | equal to $10^{-8}$. <br> Fig. 1. Evolution of the error $\left\\|b-A x_{k}\right\\|$ <br> See Chapter 2 of the book: N. Andrei, "Nonlinear Conjugate Gradient Methods for Unconstrained Optimization", Spriger, 2019. <br> Example 2.1. <br> January 2, 2019 |
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| 39. | CG4 | Program for solving linear algebraic systems $A x=b$ obtained from the finite difference numerical method to discretize the two-dimensional Poisson equation. <br> The matrix $A$ has $n_{2}$ blocks $B$ on the main diagonal, where each block $B \in \mathbb{R}^{n_{1} \times n_{1}}$. Hence, $A \in \mathbb{R}^{n \times n}$, where $n=n_{1} n_{2}$. Considering $n=10,000$, the evolution of error $\left\\|b-A x_{k}\right\\|$ computed by the linear conjugate gradient algorithm for five different values of $n_{1}$ and $n_{2}$ is presented in Figure 1. <br> From Figure 1, for $n_{1}=5000$ and $n_{2}=2$, that is when there are only two blocks on the main diagonal of $A$, the linear conjugate gradient algorithm needs only 31 iterations. Therefore, the convergence is faster. On the other hand, when $n_{2}=100$, i.e. there are 100 blocks on the main diagonal of matrix $A$, then the algorithm needs 304 iterations. In other words, the smaller the number of blocks on the main diagonal of matrix $A$, the faster the convergence. |


|  |  | Fig. 1. Evolution of the error $\left\\|b-A x_{k}\right\\|$ of the linear conjugate gradient algorithm for different numbers ( $n_{2}$ ) of blocks on the main diagonal of matrix $A$. <br> Please, see the Books: <br> 1. N. Andrei, Nonlinear Conjugate Gradient Methods for Unconstrained Optimization. Springer, vol. 158 Springer Optimization and Its Applications, Springer, 2020. <br> 2. N. Andrei, Optimizare fără Restricţii - Metode de Direcţii Conjugate, MATRIXROM, Bucureşti, 2000, pp. 78-79 şi 109112. <br> (first version) March 15, 1999 (modified version) January 3, 2019 |
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| 40. | ACGSYS <br> (See: CGSYS) | ACGSYS is the accelerated version of CGSYS. This is a subroutine dedicated to compute the minimizer of a differentiable function with a large number of variables. <br> The search direction of this algorithm is a linear combination of $-g_{k+1}$ and $s_{k}$, where the coefficients in this linear combination are computed in such a way that both the descent and the conjugacy conditions to be guaranteed at every iteration $k \geq 1$. <br> Fig. 1. Performance profiles of CGSYS versus HS-DY, DL ( $t=1$ ), CGDESCENT and DESCONa <br> The accelerated version of CGSYS is described in the paper: $\mathbf{N}$. Andrei, An accelerated conjugate gradient algorithm with guaranteed descent and conjugacy conditions for unconstrained optimization. (cgsyspap.doc). March 6, 2009. |





|  |  | Applications, Springer, 2020, (Chapter 11) <br> January 18, 2020 |
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| 44. | CG3LS | Fortran program for unconstrained optimization using 6 procedures for computation of the conjugate parameter $\beta_{k}$ :Hager-Zhang, Dai-Kou, Hestenes-Stiefel, Polak-Ribière-Polyak, Dai-Yuan and minimizing the measure function $\varphi$ of Byrd and Nocedal, under the 3 line search procedures: standard Wolfe, approximate Wolfe of Hager and Zhang and improved Wolfe of Dai and Kou. <br> The program is that of Hager and Zhang (CG-DESCENT), where the formula for beta computation is modified as that given by Dai and Kou, or HS, PRP, DY, FI. <br> Please see the Book: <br> N. Andrei, Nonlinear Conjugate Gradient Methods for Unconstrained Optimization. Springer, vol. 158 Springer Optimization and Its Applications, Springer, 2020. (Chapter 8) |
|  |  | January 17, 2019 |
| 45. | CG3LSpre | Fortran program for unconstrained optimization using 6 procedures for computation of the conjugate parameter $\beta_{k}:$ PRECONDITIONED Hager-Zhang, Dai-Kou, Hestenes-Stiefel, Polak-Ribière-Polyak, DaiYuan and minimizing the measure function $\varphi$ of Byrd and Nocedal, under the 3 line search procedures: standard Wolfe, approximate Wolfe of Hager and Zhang and improved Wolfe of Dai and Kou. <br> Only the conjugate gradient parameter $\beta_{k}$ of Hager and Zhang algorithm is preconditioned with a diagonal approximation of the Hessian. <br> The program is that of Hager and Zhang (CG-DESCENT), where the formula for beta computation is modified as that given by Dai and Kou, or HS, PRP, DY, FI. <br> Please see the Book: <br> N. Andrei, Nonlinear Conjugate Gradient Methods for Unconstrained Optimization. Springer, vol. 158 Springer Optimization and Its Applications, Springer, 2020. (Chapter 1 for diagonal approximation to the Hessian and Chapter 8) |
|  |  | January 17, 2019 |
| 46. | CGALLpre | 30 conjugate gradient unconstrained optimization algorithms with standard Wolfe line search. <br> The following conjugate gradient algorithms are implemented: betatype = (1) HS, (2) FR, (3) PRP, (4) PRP+, (5) CD, (6) LS, (7) DY, (8) DL(t=1), (9) DL+, (10) SDC, (11) hDY, (12) hDY0, (13) GN, (14) HuS, (15) TAS, (16) LS-CD, (17) Birgin-Martinez, (18) BirginMartinez+, (19) scaledPRP, (20) scaledFR, (21) new cg from PRP, (22) newDY, (23) variant of newDY, (24) another variant of newDY, (25) |





|  |  | (CUBICa is the accelerated version of CUBIC.) <br> See the Book: <br> - N. Andrei, Nonlinear Conjugate Gradient Methods for Unconstrained Optimization, vol. 158 Springer Optimization and Its Applications, Springer, 2020, (Chapter 11, Section 11.4) |
| :---: | :---: | :---: |
| 49. | CGSECM | Conjugate gradient algorithm based on the equality of the Newton direction with the conjugate gradient direction and modified secant condition. The search direction is computed as: $\begin{gathered} d_{k+1}=-g_{k+1}+\beta_{k} s_{k}, \\ \beta_{k}=\max \left\{\begin{array}{c} \left.\frac{y_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}+\delta \eta}, 0\right\}-\left(1-\frac{\delta \eta}{s_{k}^{T} s_{k}}\right) \frac{s_{k}^{T} g_{k+1}}{y_{k}^{T} s_{k}+\delta \eta}, \\ \eta=6\left(f_{k}-f_{k+1}\right)+3\left(g_{k}+g_{k+1}\right)^{T} s_{k}, \\ \delta=\left\{\begin{array}{l} 0, \\ 1 \end{array}\right. \end{array} .\left\{\begin{array}{l} \text { a parameter. } \end{array}\right.\right. \end{gathered}$ |
| 50. | DESCON14 | Performances of DESCON package for solving 14 applications of unconstrained optimization. The applications are as follows: <br> 1. Weber Function (1) (Andrei, U71) <br> 2. Enzyme reaction (Andrei, U79) (A) <br> 3. Solution of a chemical reactor (A) <br> 4. Robot kinematics problem (A) <br> 5. Solar Spectroscopy (A) <br> 6. Estimation of parameters (A) <br> 7. Propan combustion in air (A) <br> 8. Gear train with minimum inertia (A) <br> 9. Human Heart Dipole. Andrei U84, pp. 65 <br> 10. Neurophysiology (A) <br> 11. Combustion application (A) <br> 12. Thermistor (A) <br> 13. Optimal design of a Gear Train (A) <br> 14. Circuit design (A) <br> Directory DESCON14: <br> - DESCON14.FOR (Fortran package with all subroutines.) <br> - FUNC14.TXT (Name of the applications) <br> - R2020T14.DOC (Technical Report.) <br> The performances of DESCON14 are presented in: <br> N. Andrei, Numerical experiments with DESCON for solving 14 applications of unconstrained optimization. AOSR - Academy of Romanian Scientists, Bucharest, Romania, Technical Report No.14/2020, June 3, 2020. (Romanian Academy Library) (10 pages) |
| 51. | CUBIC14 | June 3, 2020 <br> Performances of CUBIC package for solving 14 applications of unconstrained optimization. The applications are as follows: |




## BFGS - MODIFIED

|  |  | SBFGS |
| :--- | :--- | :--- |
| 1. | A new adaptive scaled BFGS method for unconstrained optimization <br> is presented. The third term in the standard BFGS update formula is <br> scaled in order to reduce the large eigenvalues of the approximation <br> to the Hessian of the minimizing function. Under the inexact Wolfe <br> line search conditions, the global convergence of the adaptive scaled <br> BFGS method is proved in very general conditions without assuming <br> the convexity of the minimizing function. <br> The algorithm is described in the paper: <br> N. Andrei, An adaptive scaled BFGS method for unconstrained |  |
| optimization. Numerical Algorithms, DOI: 10.1007/s1 1075-017- |  |  |
| op21-1 |  |  |
| (Please see the file: mbfgs-R2.doc) |  |  |$|$| TPSBFGS | A double parameter scaled BFGS method for unconstrained <br> optimization is presented. In this method, the first two terms of the <br> known BFGS update formula are scaled with a positive parameter <br> while the third one is scaled with another positive parameter. These <br> parameters are selected in such a way as to improve the eigenvalues <br> structure of the BFGS update. The parameter scaling the first two <br> terms of the BFGS update is determined by clustering the eigenvalues <br> of the scaled BFGS matrix. On the other hand, the parameter scaling <br> the third term is determined as a preconditioner to the Hessian of the <br> minimizing function combined with the minimization of the <br> conjugacy condition from conjugate gradient methods. |
| :--- | :--- |
| 2. | The algorithm is described in the paper: |
| DPSS | T. Andrei, A double parameter scaled BFGS method for <br> unconstrained optimization, Journal of Computational and Applied <br> Mathematics, vol.332 (2018), pp.26-44 |
| (Please see the file: JCAM-2018(43).pdf) |  |


|  |  | (a) <br> (b) <br> Fig. 1. Performance profiles of DP versus DPOL and versus DPOS. CPU time metric. $n=1000$. <br> The algorithm is described in the paper: <br> N. Andrei, A double parameter self-scaled memoryless BFGS method for unconstrained optimization. Computational and Applied Mathematics, vol. , 2020. <br> (Please see the file: COAMR1.doc) |
| :---: | :---: | :---: |
| 4. | DSBFGS (ROMANPOLYAK) | A scaled BFGS method with two parameters for unconstrained optimization is presented. In this method the first two terms of the known BFGS update formula are scaled with a positive parameter and the third one is scaled with another positive parameter. The parameter scaling the first two terms of the BFGS update is determined by clustering the eigenvalues of the scaled BFGS matrix. On the other hand, the parameter scaling the third term is determined as a preconditioner to the Hessian of the minimizing function combined with the minimization of the conjugacy condition from conjugate gradient methods. This parameter is determined to reduce the large eigenvalues, thus obtaining a better distribution of them. <br> The algorithm is described in the paper: <br> N. Andrei, A scaled BFGS method with two parameters for unconstrained optimization. <br> (Please see the file: Paper-Roman.doc) <br> May 5, 2017 |
| 5. | DNRTR | A diagonal quasi-Newton updating algorithm. The elements of the diagonal matrix approximating the Hessian are determined by minimizing both the size of the change from the previous estimate and the trace of the update, subject to the weak secant equation. <br> Figure 1 presents the performances of DNRTR versus steepest descent (SP) and versus Cauchy with Oren-Luenberger scaling in its complementary form (COL). |


|  |  |  <br> Fig. 1 Performance profiles of DNRTR versus SP and versus COL. CPU time metric. $n=100$. <br> Please see the paper: <br> N. Andrei, A diagonal quasi-Newton updating method for unconstrained optimization. Numerical Algorithms, vol.81(2), (2019), pp.575-590. |
| :---: | :---: | :---: |
|  |  | February 26, 2018 |
| 6. | YONS | A new diagonal quasi-Newton updating algorithm for unconstrained optimization is presented. The elements of the diagonal matrix approximating the Hessian, are determined as scaled forward finite differences directional derivatives of the components of the gradient. Under mild classical assumptions, the convergence of the algorithm is proved to be linear. <br> In this method the approximation Hessian $B_{k+1}$ is a diagonal matrix computed as: $B_{k+1}=Y_{k} S_{k}^{-1}$ <br> where $Y_{k}=\operatorname{diag}\left(y_{k}^{1}, \ldots, y_{k}^{n}\right)$ and $S_{k}=\operatorname{diag}\left(s_{k}^{1}, \ldots, s_{k}^{n}\right), y_{k}^{i}, i=1, \ldots n$, being the components of the vector $y_{k}$ and $s_{k}^{i}, i=1, \ldots n$, being the components of vector $s_{k}$. Therefore, the diagonal elements of the matrix $B_{k+1}$, are computed as: $b_{k+1}^{i}=y_{k}^{i} / s_{k}^{i}, i=1, \ldots, n$. In other words, $b_{k+1}^{i}=\frac{y_{k}^{i}}{s_{k}^{i}}=\frac{g_{k+1}^{i}-g_{k}^{i}}{x_{k+1}^{i}-x_{k}^{i}}=\frac{g^{i}\left(x_{k}+\alpha_{k} d_{k}\right)-g^{i}\left(x_{k}\right)}{\alpha_{k} d_{k}^{i}}, \quad i=1, \ldots n,$ <br> where $g_{k}^{i}$, is the $i$-th component of the gradient in $x_{k}$ and $d_{k}^{i}$ is the $i$ - th component of the search direction. <br> Therefore, in this approach, the element $b_{k+1}^{i}$ may be considered as an approximation of the second order derivative of function $f$, corresponding to the $i$-th diagonal element of the Hessian, computed in $x_{k+1}$ by a scaled forward finite differences directional derivative scheme. Observe that $1 / d_{k}^{i}$ is a scaling factor. <br> 1) This directory contains the following Fortran files: <br> 2) BFGS.FOR - Scaled BFGS method with Wolfe line search |



## $\rangle\rangle\rangle\rangle\rangle\rangle\rangle\rangle\rangle\rangle$

## L-BFGS

| 1. | LBFGS14 | Limited BFGS method for solving 14 applications of unconstrained <br> optimization. The applications solved by LBFGS14 are: <br> 1. Weber Function (1) (Andrei, U71) <br> 2. Enzyme reaction (Andrei, U79) (A) |
| :--- | :--- | :--- |



| Other Programs |  |  |
| :--- | :--- | :--- |
| 1. | GRADSYS | Gradient Flow Algorithm for Unconstrained Optimization. <br> The algorithm is: $\quad x_{k+1}=x_{k}+\delta x_{k}$, <br> where $\delta x_{k}$ is computed as the solution of the following linear <br> algebraic systems of equations: <br> $\left\lfloor I+h_{k} \theta \nabla^{2} f\left(x_{k}\right)\right] \delta x_{k}=-h_{k} \nabla f\left(x_{k}\right)$. <br> $\theta \in[0,1]$. If $\theta=1$ and $h_{k} \rightarrow 1$, then the algorithm is quadratically <br> convergent. |


|  |  | The algorithm is described in: <br> N. Andrei, Gradient flow algorithm for unconstrained optimization. <br> Technical Report, March 23, 2004. <br> (Please see the file diff.pdf) <br> March 23, 2004 |
| :---: | :---: | :---: |
| 2. | NEWGRAD | Relaxed Gradient Descent and a New Gradient Descent Methods for Unconstrained Optimization. <br> Mainly, the algorithm is the steepest gradient where the step-length is modified by a multiplicative parameter: $x_{k+1}=x_{k}-\theta_{k} \alpha_{k} \nabla f\left(x_{k}\right),$ <br> where $\theta_{k} \in[0,1]$ and $\alpha_{k}$ is the step-length computed by backtracking. <br> The algorithm and its theory is described in: <br> N. Andrei, Theory versus empiricism in analysis of optimization algorithms. Technical Press, Bucharest, 2004. ISBN: 973-31-2233-5. <br> N. Andrei, Criticism of the unconstrained optimization algorithms reasoning. Romanian Academy Publishing House, Bucharest, 2009. ISBN: 978-973-27-1669-4. <br> Please see the papers: <br> N. Andrei, Numerical Experiments with Gradient Descent with Backtracking for Unconstrained Optimization. March 2, 2005. (File: CGAD.DOC, 10 pages) <br> N. Andrei, Numerical Experiments with Relaxed Gradient Descent with Backtracking for Unconstrained Optimization. March 5, 2005. (File: RELAXED.DOC, 12 pages) |


|  | Constrained optimization |  |
| :---: | :---: | :---: |
| 1. | KKT | Karush-Kuhn-Tucker methods for solving inequality constraints optimization problems of the following form: $\min f(x)$ <br> subject to: $g(x) \leq 0,$ <br> where $f: R^{n} \rightarrow R$, and $g: R^{n} \rightarrow R^{m}$. It is supposed that all functions of the problem are continuousli differentiable. <br> Directorul KKT conține un număr de 8 probleme de optimizare cu restricții inegalităţi: NEWTON1.FOR, NEWTON2.FOR,... <br> NEWTON8.FOR, SIMEQ.FOR, LS.FOR. |


|  |  | Problemele sunt descrise şi rezolvate în lucrarea: N. Andrei, Metode bazate pe condițiile Karush-Kuhn-Tucker, Manuscript, 1995, cu CD. (În biblioteca mea.) |
| :---: | :---: | :---: |
|  |  | March 3, 1995 |
| 2. | PREDCOR | Interior-Point Predictor-Corrector algorithm for linear constrained optimization. <br> Directorul conține 15 exemple de probleme de optimizare cu restricţii linare utilizând metoda de punct interior, într-o implementare naivă. Sistemele de ecuaţii algebrice linare asociate metodei sun rezolvate cu subruruinele: DLINEQ.FOR (LU decomposition) şi DRESLV.FOR (Substitutions). <br> Exemplul LCPC10.FOR rezolvă aplicaţia: Chemical Equilibrium Problem. <br> December 24, 1996 |
| 3. | SPG | SIMPLE BOUNDED OPTIMIZATION by Birgin, Martinez and Rydan $\min \{f(x), l \leq x \leq u\}$ <br> where $f(x)$ is a continuously differentiable and its gradient is available. $l$ and $u$ are simple margins on the variables. It is assumed that $l \leq u$. <br> - First version: February 02, 2001 by E.G.Birgin, J.M.Martinez and M.Raydan. <br> - Final revision: April 30, 2001 by E.G.Birgin, J.M.Martinez and M.Raydan. <br> - Modified final version: May 12, 2008 by Neculai Andrei to include the safeguarded cubic interpolation. <br> The algorithm and its performances are presented in: <br> N. Andrei, Criticism of the Constrained Optimization Algorithms Reasoning, Editura Academiei Române, Bucureşti, 2015. <br> ISBN: 978-973-27-2527-6 (pp. 169-177) <br> The following applications are considered: <br> APPL1.FOR - Elastic-Plastic Torsion problem <br> APPL2.FOR - Pressure Distribution in a Journal Bearing <br> APPL3.FOR - Optimal Design with Composite Materials <br> APPL4.FOR - Ginzburg-Landau (1-dimensional) problem <br> APPL5.FOR - Steady State Combustion <br> The program MSPG.FOR implements the SPG subroutine for solving a train of 730 problems with simple bounds. The line search subroutine is modified by Neculai Andrei to include the safeguarded cubic interpolation. <br> The following examples are presented: <br> 1) SPGEX1.FOR is for minimizing the Freudenstein \& Roth function with $\mathrm{n}=1000, \ldots, 10000$. <br> 2) SPGEX2.FOR is for minimizing the Extended Penalty function with $\mathrm{n}=1000, \ldots, 10000$. <br> 3) SPGEX3.FOR is for minimizing the Broyden Tridiagonal function with $\mathrm{n}=1000, \ldots, 10000$. |


|  |  | May 12, 2008 |
| :---: | :---: | :---: |
| 4. | SPENBAR | Package for large-scale nonlinear, equality and inequality constrained optimization. |
|  |  | The optimization problem solved by SPENBAR is as follows: $\min F(x),$ |
|  |  | $c_{i}(x) \geq 0, \quad i=1, \ldots, m,$ |
|  |  | $e_{k}(x)=0, \quad k=1, \ldots, m e$, |
|  |  | $l_{j} \leq x_{j} \leq u_{j}, \quad j=1, \ldots, n,$ where all the functions |
|  |  | where all the functions are continuously differential. <br> The program implements a modified penalty-barrier method. The unconstrained optimization problems is solved by means of truncated Newton method implemented in subroutine LMQN written by Stephen Nash. |
|  |  | This directory contains 4 sub-directories (DOC, examples, PROB, REZMOD) and 4 Fortran files (HS108.FOR, IP.FOR, IP1.FOR and SPENBAR.FOR). |
|  |  | The algorithm is described in a number of papers and Technical Reports as: <br> N. Andrei, (1996) Computational Experience with a Modified PenaltyBarrier Method for Large-Scale Nonlinear Constrained Optimization. (FORTRAN subroutines) ICI Working Paper No. AMOL-96-1, February 6, 1996. |
|  |  | N. Andrei, (1996) Computational Experience with SPENBAR a Sparse Variant of a Modified Penalty-Barrier Method for Large-Scale Nonlinear, Equality and Inequality Constrained Optimization. ICI Technical Paper No. AMOL-96-4, March 11, 1996, pp.1-69. |
|  |  | N. Andrei, (2006) Numerical Examples with SPENBAR for Large-Scale Nonlinear, Equality and Inequality Constrained Optimization with Zero Columns in Jacobian Matrices. ICI Technical Paper No. AMOL-96-5, March 29, 1996. |
|  |  | N. Andrei, (2001) Numerical Examples with SPENBAR - Modified penalty barrier method for large-scale nonlinear programming problems. Part I. ICI Technical Report, ICI-TR-01/2001, Bucharest, February 2001. Technical Report placed in Library of Romanian Academy. |
|  |  | N. Andrei, (2001) Computational experience with SPENBAR. A sparse modified penalty-barrier method for large-scale nonlinear, equality and inequality, constrained optimization. Technical Report No.4/2001, February 19, 2001. (Manuscript. În biblioteca mea.) |
|  |  | N. Andrei, (2015) Criticism of the Constrained Optimization Algorithms Reasoning, Editura Academiei Române, Bucureşti, 2015. ISBN: 978-973-27-2527-6 (pp. 517-537) |


|  |  | N. Andrei, (2017) Continuous Nonlinear Optimization for Engineering Applications in GAMS Technology. Springer Optimization and Its Applications, Volume 121, Springer Science+Business Media New York 2017, ISBN: 978-3-319-58356-3, e-book ISBN: 978-3-319-58356-3, ISSN: 1931-6828, DOI: 10.1007/978-3-319-58356-3, Springer New York Heidelberg Dordrecht London, $508+$ XXIV pages. <br> OPIS.TXT contains the list of problems from SPENBAR collection. <br> February 19, 2001 |
| :---: | :---: | :---: |
| 5. | TOLMINV | Package of subroutines that calculate the the least value of a differentiable function of several variables subject to linear constraints on the values of the variables written by M.J.D. Powell. <br> TOLMIN, written by Powell, works with two-dimensional arrays and solves the problems of the following types: $\begin{aligned} & \min F(x), \\ & \text { subject to: } \\ & \qquad \begin{array}{l} a_{j}^{T} x=b_{j}, \quad j=1, \ldots, M E Q \\ a_{j}^{T} x \leq b_{j}, \quad j=M E Q+1, \ldots, m, \\ l_{i} \leq x_{i} \leq u_{i}, \quad i=1, \ldots, n . \end{array} \end{aligned}$ <br> All the subroutines of the program are modified by N. Andrei to work with vectors, without considering the spsrsity the the matrix corresponding to linear constraints. This is TOLMINV package. <br> This Directory contains three sub-directories: TOLMIN14, TOLMINMA, TOLMINVE. <br> Subdirectory TOLMIN14 includes three programs for solving constrained optimization problems as follows: <br> MAIN01.FOR is the main program for solving the nonlinear optimization problem presented in Example 14.1 in the book: <br> N. Andrei, Critica Ratiunii Algoritmilot de Optimizare cu Restrictii, Editura Academiei, 2015, pp. 629. <br> THE COMPUTED SOLUTION POINT IS <br> $0.8750081257267 \mathrm{E}-07$ $0.4629495896370 \mathrm{E}-04$ <br> $0.9999514660798 \mathrm{E}+00$ <br> $0.5001292705362 \mathrm{E}+00$ <br> $0.9999908024081 \mathrm{E}+00$ $0.4999956364708 \mathrm{E}+01$ <br> $0.3000004697421 \mathrm{E}+01$ <br> $0.1000000000000 \mathrm{E}+01$ <br> FINAL CONSTRAINT RESIDUALS $=$ <br> $0.0000 \mathrm{E}+00 \quad 0.0000 \mathrm{E}+00 \quad 1.7764 \mathrm{E}-15 \quad 0.0000 \mathrm{E}+00$ <br> Function value in optimal point $=0.2999999978913 \mathrm{E}+01$ |

MAIN02.FOR is the main program for solving the nonlinear optimization problem presented in Example 5.3 in the book:
N. Andrei, Critica Ratiunii Algoritmilot de Optimizare cu Restrictii, Editura Academiei, 2015, pp. 266.

THE COMPUTED SOLUTION POINT IS
$1 \quad 0.4002737835268 \mathrm{E}+00$
$0.1305663058260 \mathrm{E}+00$ $0.0000000000000 \mathrm{E}+00$ $0.0000000000000 \mathrm{E}+00$ $0.9033793559852 \mathrm{E}+00$ $0.4168581403599 \mathrm{E}+00$ $0.0000000000000 \mathrm{E}+00$ $0.1509334100456 \mathrm{E}+01$ $0.1522805326970 \mathrm{E}+01$ $0.5379458016316 \mathrm{E}+00$ $0.1013056630583 \mathrm{E}+01$ $0.5527662953395 \mathrm{E}+00$ $0.0000000000000 \mathrm{E}+00$ $0.0000000000000 \mathrm{E}+00$ $0.6010093996177 \mathrm{E}+00$
$X(I) \quad X(I)-X L(I)$
XU(I) -X(I)
$4.0027378 \mathrm{E}-01 \quad 1.5997262 \mathrm{E}+00$
$1.3056631 \mathrm{E}-01 \quad 1.8694337 \mathrm{E}+00$ $0.0000000 \mathrm{E}+00 \quad 2.0000000 \mathrm{E}+00$ $0.0000000 \mathrm{E}+00 \quad 2.0000000 \mathrm{E}+00$ $9.0337936 \mathrm{E}-01 \quad 1.0966206 \mathrm{E}+00$ $4.1685814 \mathrm{E}-01 \quad 1.5831419 \mathrm{E}+00$ $0.0000000 \mathrm{E}+00 \quad 2.0000000 \mathrm{E}+00$ $1.5093341 \mathrm{E}+00 \quad 4.9066590 \mathrm{E}-01$ $1.5228053 \mathrm{E}+00 \quad 4.7719467 \mathrm{E}-01$ $5.3794580 \mathrm{E}-01 \quad 1.4620542 \mathrm{E}+00$ $1.0130566 \mathrm{E}+00 \quad 9.8694337 \mathrm{E}-01$ $5.5276630 \mathrm{E}-01 \quad 1.4472337 \mathrm{E}+00$ $0.0000000 \mathrm{E}+00 \quad 2.0000000 \mathrm{E}+00$ $0.0000000 \mathrm{E}+00 \quad 2.0000000 \mathrm{E}+00$ $6.0100940 \mathrm{E}-01 \quad 1.3989906 \mathrm{E}+00$

FINAL CONSTRAINT RESIDUALS $=$

Function value in optimal point $=0.2192129651805 \mathrm{E}+02$
Execution Time: 0: 0: 0: 0
MAIN03.FOR is the main program for solving the nonlinear optimization problem presented in Example 14.3 in the book:
N. Andrei, Critica Ratiunii Algoritmilot de Optimizare cu Restrictii, Editura Academiei, 2015, pp. 266.

THE COMPUTED SOLUTION POINT IS
$0.2812500000000 \mathrm{E}+01$
$0.0000000000000 \mathrm{E}+00$
$0.7187500000000 \mathrm{E}+01$
$0.3750000000000 \mathrm{E}+01$
$0.0000000000000 \mathrm{E}+00$
$0.0000000000000 \mathrm{E}+00$
$0.0000000000000 \mathrm{E}+00$
$0.3125000000000 \mathrm{E}+01$
$0.0000000000000 \mathrm{E}+00$
$0.0000000000000 \mathrm{E}+00$
$0.0000000000000 \mathrm{E}+00$
$0.5718750000000 \mathrm{E}+02$
$0.2562500000000 \mathrm{E}+02$

| $X(I)$ | $X(I)-X L(I)$ | $X U(I)-X(I)$ |
| :--- | :--- | :--- |
| $2.8125000 \mathrm{E}+00$ | $2.8125000 \mathrm{E}+00$ | $9.7187500 \mathrm{E}+01$ |
| $0.0000000 \mathrm{E}+00$ | $0.0000000 \mathrm{E}+00$ | $1.0000000 \mathrm{E}+02$ |
| $7.1875000 \mathrm{E}+00$ | $7.1875000 \mathrm{E}+00$ | $9.2812500 \mathrm{E}+01$ |
| $3.7500000 \mathrm{E}+00$ | $3.7500000 \mathrm{E}+00$ | $9.6250000 \mathrm{E}+01$ |
| $0.0000000 \mathrm{E}+00$ | $0.0000000 \mathrm{E}+00$ | $1.0000000 \mathrm{E}+02$ |
| $0.0000000 \mathrm{E}+00$ | $0.0000000 \mathrm{E}+00$ | $1.0000000 \mathrm{E}+02$ |
| $0.0000000 \mathrm{E}+00$ | $0.0000000 \mathrm{E}+00$ | $1.0000000 \mathrm{E}+02$ |
| $3.1250000 \mathrm{E}+00$ | $3.1250000 \mathrm{E}+00$ | $9.6875000 \mathrm{E}+01$ |
| $0.0000000 \mathrm{E}+00$ | $0.0000000 \mathrm{E}+00$ | $1.0000000 \mathrm{E}+02$ |
| $0.0000000 \mathrm{E}+00$ | $0.0000000 \mathrm{E}+00$ | $1.0000000 \mathrm{E}+02$ |


|  |  |  |
| :---: | :---: | :---: |
| 6. | PSO-CO | Particle Swarm Optimization (PSO). <br> In this directory I included a number of Fortran packages for constrained optimization using the particle swarm optimization method. <br> For solving the problem $\min \left\{f(x), c_{i}(x) \leq 0, i=1, \ldots, m\right\}$ the algorithm for PSO considers the following strategy. <br> Using the PSO algorithm for unconstrained optimization minimize the penalty function: $F(x)=f(x)+h(t) H(x),$ <br> where: $\begin{aligned} & H(x)=\sum_{i=1}^{m} \theta\left(q_{i}(x)\right)\left(q_{i}(x)\right)^{\gamma\left(q_{i}(x)\right)}, \\ & q_{i}(x)=\max \left\{0, c_{i}(x)\right\}, \quad i=1, \ldots, m, \\ & \theta\left(q_{i}(x)\right)=\left\{\begin{array}{ccc} 10, & \text { dacă } & q_{i}(x)<0.001, \\ 20, & \text { dacă } & 0.001 \leq q_{i}(x)<0.1, \\ 100, & \text { dacă } & 0.1 \leq q_{i}(x)<1, \\ 300, & \text { dacă } & q_{i}(x) \geq 1, \end{array}\right. \\ & \gamma\left(q_{i}(x)\right)=\left\{\begin{array}{lll} 1, & \text { dac̆a } & q_{i}(x)<1, \\ 2, & \text { dacă } & q_{i}(x) \geq 1, \end{array}\right. \\ & h(t)=t \sqrt{t}, \end{aligned}$ <br> Here, $t$ is the number of iteration. <br> The applications solved by this method are as follows: <br> ALKI-PSO - Optimization of an alkylation process, Variant 1, <br> CAM-PSO - Shape optimization of a cam, <br> DES-PSO - Distribution of electrons on a sphere, HANG-PSO - Hanging chain, <br> MSP3-PSO - 3-stage membrane separation, <br> MSP5-PSO - A 5-stage membrane separation process, <br> PPSE-PSO - Static Power Scheduling, <br> PREC-PSO - Optimal Reactor Design, <br> TRAFO-PSO - Transformer design. <br> BRAKE-PSO - Design of a disc brake, <br> EX1-PSO - Example 1, <br> EX2-PSO - Example 2, <br> LATHE.PSO - Multi-spindle automatic lathe <br> SPRING.PSO - Minimizing the weight of a tension/compression spring <br> WESSEL.PSO - Pressure vessel |


|  |  | Please, see the book: „Critica Ratiunii Algoritmilor de Optimizare cu <br> Restrictii", Bucuresti, Editura Academiei Române, 2015, Capitolul 19. <br> See also: the paper Anale-PSO.doc and the technical report PSO.doc <br> (October 9, 2014). <br> Please, see the directory PSO-CO in CONSTRAINED-OPTIM. <br> May 21, 2014 |
| :--- | :--- | :--- |
| 7. | CAON | A collection of nonlinear optimization applications in GAMS <br> language. Se prezintă 25 de modele de optimizare neliniară, exprimate <br> in limbajul GAMS. |
| See: N. Andrei, CAON: O colectie de aplicatii de optimizare neliniară <br> in limbajul GAMS. Technical Report No.1/2011, January 31, 2011. <br> (105 pages with CD). <br> Please, see the directory CAON in CONSTRAINED_OPTIM. Please, <br> see the Technical Report: r1a11.doc. The mathematical models in <br> GAMS are placed in directory CD-GAMS. <br> January 31, 2011 |  |  |

