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# NONLINEAR OPTIMIZATION PROBLEM

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## 1. Introduction

In this contribution, we are concerned with a general nonlinear optimization problem [7]: find a local minimum $x_\star \in \mathbb{R}^n$ of function $f : \mathbb{R}^n \to \mathbb{R},\ f \in \mathcal{C}^2$ :

$$x_\star = \arg\min_{x \in \mathbb{R}^n} f(x). \tag{1}$$

The main optimization method for solving this problem has an iterative character. After choosing initial point $x_0$ we construct a sequence of points $\{x_k\}_{k \in \mathbb{N}_0}$, so that

$$x_{k+1} = x_k + \alpha_k d_k, \tag{2}$$

where $d_k$ is a direction vector and $\alpha_k$ is a steplength. A global convergence is an important assumption for the application of optimization methods. It means satisfying the condition

$$\liminf_{k \to \infty} g_k = 0, \tag{3}$$

where $g_k \equiv g(x_k) = \nabla f(x_k)$.

## 2. Trust region methods

Trust region methods [1], [8] belong to the most effective optimization methods because of their very good convergence properties. They are globally and superlinearly convergent [3], [4] and moreover they use a simple choice of the steplength. Before the definition of trust region methods we'll introduce the following notation:

$$\psi_k(d) = \frac{1}{2}\, d^T B_k d + g_k^T d$$

for a quadratic function that locally approximates the difference $f(x_k + d) - f(x_k)$,

$$w_k(x) = \frac{B_k d + g_k}{\|g_k\|}$$

for a vector used in the determination of the accuracy of a direction vector, and

$$\varrho_k(x) = \frac{f(x_k + d) - f(x_k)}{\psi_k(d)}$$

for a quotient of an actual and predicted reduction in function $f$. Matrix $B_k$ is either the Hessian matrix $G_k \equiv G(x_k) = \nabla^2_{xx} f(x_k)$ or its suitable approximation, and the norm is Euclidean.

**Definition 1** *Optimization method (2) is a trust region method if direction vectors* $d_k \in \mathbb{R}^n,\ k \in \mathbb{N}_0$, *are chosen so that*

$$\begin{aligned} \|d_k\| &\leq \Delta_k, && (4)\\ \|d_k\| &< \Delta_k \quad \Rightarrow \quad \|w_k(d_k)\| = \omega_k \leq \overline{\omega}, && (5)\\ \psi_k(d_k) &\leq -\underline{\sigma}\,\|g_k\| \min\left\{\|d_k\|,\ \frac{\|g_k\|}{\|B_k\|}\right\}, && (6) \end{aligned}$$

*where* $\overline{\omega} < 1,\ 0 < \underline{\sigma} < 1$. *Steplengths* $\alpha_k \geq 0,\ k \in \mathbb{N}_0$, *are chosen so that*

$$\begin{aligned} \varrho_k(d_k) \leq 0 \quad &\Rightarrow \quad \alpha_k = 0, && (7)\\ \varrho_k(d_k) > 0 \quad &\Rightarrow \quad \alpha_k = 1. && (8) \end{aligned}$$

*Sequence* $\Delta_k > 0,\ k \in \mathbb{N}_0$, *is constructed so that*

$$\begin{aligned} \varrho_k(d_k) < \underline{\varrho} \quad &\Rightarrow \quad \underline{\beta}\,\|d_k\| \leq \Delta_{k+1} \leq \overline{\beta}\,\|d_k\|, && (9)\\ \varrho_k(d_k) \geq \underline{\varrho} \quad &\Rightarrow \quad \Delta_k \leq \Delta_{k+1} \leq \overline{\gamma}\,\Delta_k, && (10) \end{aligned}$$

*where* $0 < \underline{\varrho} < 1,\ 0 < \underline{\beta} \leq \overline{\beta} < 1 < \overline{\gamma}$. *Matrices* $B_k,\ k \in \mathbb{N}_0$, *are constructed so that they satisfy the condition*

$$\|B_k\| \leq M \quad \forall k \in \mathbb{N}_0, \qquad (11)$$

*where constant* $M < \infty$ *is independent of* $k \in \mathbb{N}_0$.

The algorithm can be written in the following way.

**Algorithm 1** *Trust region method.*

*Choose* $x_0 \in \mathbb{R}^n,\ 0 \neq B_0 \in \mathbb{R}^{n\times n}_S,\ \Delta_0 > 0,\ \varepsilon > 0$, *compute* $f(x_0)$, *set* $k = 0$.

1. *Compute gradient* $g(x_k)$. *If* $\|g(x_k)\| < \varepsilon$, *then STOP.*

2. *Determine vector* $d_k$ *satisfying conditions (4)-(6).*

3. *Set* $x_k^+ = x_k + d_k$ *and compute values* $f(x_k^+)$ *and* $\varrho_k(d_k) = \dfrac{f(x_k^+) - f(x_k)}{\psi_k(d_k)}$.

4. *If* $\varrho_k(d_k) < \underline{\varrho}$, *update* $\Delta_{k+1}$ *according to (9).*
   *If* $\varrho_k(d_k) \geq \underline{\varrho}$, *update* $\Delta_{k+1}$ *according to (10).*

5. *If* $\varrho_k(d_k) \leq 0$, *go to step 2.*
   *If* $\varrho_k(d_k) > 0$, *update matrix* $B_{k+1} \neq 0$ *so that it satisfies condition (11), set* $x_{k+1} = x_k^+,\ f(x_{k+1}) = f(x_k^+),\ k := k + 1$ *and return to step 1.*

Trust region methods lead to a subproblem of finding minimum $d_k$ of quadratic function $\psi_k(d)$ subject to constraint $\|d\| \leq \Delta_k$. As this subproblem is solved iteratively for fixed $k$, this index can be omited. If $d_\star$ is a resulting direction vector in step $k$, the subproblem is as follows:

$$d_\star = \arg\min \psi(d) \equiv \frac{1}{2} d^T B d + g^T d, \quad \|d\| \leq \Delta. \tag{12}$$

Trust region methods are a class of methods that must satisfy conditions of Definition 1. The first class seeks an optimal step on the whole space $\mathbb{R}^n$. As computing such a vector is a difficult task, there exists the second class of methods that seeks only an approximation of the optimal step on some subspaces (e.g. Krylov subspaces) of $\mathbb{R}^n$. Conditions (4)-(6) are the only ones that computed optimal or approximated solution $d_\star$ must satisfy.

## 3. Direction determination

### *1. Use of a Cholesky decomposition and Newton's method*

We exploit optimality conditions [2] that characterize the optimal step $d_\star$ :

$$\|d_\star\| \leq \Delta, \;\; B + \xi_\star I \succeq 0, \;\; \xi_\star \geq 0, \;\; (B + \xi_\star I) d_\star = -g, \;\; (\|d_\star\| - \Delta)\, \xi_\star = 0 \tag{13}$$

and after denoting by $\lambda_1$ the smallest eigenvalue of $B$ we solve the equation

$$\phi(\xi) \equiv \frac{1}{\Delta} - \frac{1}{\|d\|} = 0, \quad \xi > \max\{0, -\lambda_1\}$$

for $\xi_\star$ by Newton's method and factorization $B + \xi I = R^T R$.

### *2. Use of a linear combination of eigenvectors*

Let $B = QDQ^T$ be the eigendecomposition of $B$, $Q = (q_1, \ldots, q_n)$. Then

$$d_\star = \sum_{i=1}^{n} c_i q_i,$$

where $c = (c_1, \ldots, c_n)^T$ is a certain vector such that $d_\star$ satisfies optimality conditions (13).

### *3. The dogleg method*

$$d_\star \in \mathrm{sp}\{g, B^{-1} g\}$$

A simple piecewise linear curve is generated, where Cauchy and Newton points $d_C = -\dfrac{g^T g}{g^T B g}\, g$ and $d_N = -B^{-1} g$ are considered.

### *4. Combination of the dogleg method and a Cholesky decomposition*

$$d_\star = \tau_1 g + \tau_2 B^{-1} g$$

Vector $\tau_\star = (\tau_1, \tau_2)^T$ is the optimal step on subspace $\mathbb{R}^2$. As this is a simple problem, a Cholesky decomposition and Newton's method approaches are used.

***5. Use of the conjugate gradient method***

$$d_\star \in \mathcal{K}_{i+1} = \mathrm{sp}\{g, Bg, B^2g, \ldots, B^ig\}$$

Vector $d_\star$ is a linear combination of $B$-orthogonal basis of Krylov subspace $\mathcal{K}_{i+1}$. A piecewise linear curve, whose final points are conjugate gradient iterations, is generated. Sequence $\{\|d_j\|\}_{j=0,1,\ldots,i}$ is monotonically increasing while sequence $\{\psi(d_j)\}_{j=0,1,\ldots,i}$ is monotonically decreasing.

***6. The preconditioned conjugate gradient method***

For large scale sparse systems there is suitable to use preconditioning of CGM with a symmetric and positive definite matrix $C$. We perform an incomplete decomposition $B \approx R^TR$, where $R$ has the same nonzero elements structure as matrix $B$, and set $C = R^TR$.

***7. Combination of the conjugate gradient and dogleg methods***

As the dogleg method uses just one step of conjugate gradient method, we can generalize this process with using more steps of CGM.

***8. Use of the Lanczos method***

Vector $d_\star \in \mathcal{K}_{i+1}$ is a linear combination of orthonormal basis, $d_\star = Q_ih_i$, where $Q_i^TBQ_i = T_i$ is a matrix form of the Lanczos method. Such an approach leads to subproblem

$$h_i = \arg\min \tilde{\psi}(h) \equiv \frac{1}{2}\, h^TT_ih + \tilde{g}^Th, \quad \|h\| \leq \Delta, \tag{14}$$

where $\tilde{g} = (\|g\|, 0, \ldots, 0)^T$, that is solved by a Cholesky decomposition and Newton's method. It is a simple problem because matrix $T_i$ is tridiagonal. Thus a sequence of approximations of the optimal step is generated. Unfortunately we cannot use preconditioning because we would loose the orthogonality of the original basis vectors and change a constraint of quadratic subproblem (12).

***9. Two new modifications of the Lanczos method***

*(a) Combined "Lanczos – conjugate gradient" method*

We choose fixed $m$ (usually small) and compute $m$ steps of the Lanczos method to obtain tridiagonal matrix $T_{m-1}$ of order $m$. Now we solve tridiagonal quadratic subproblem (14) for $h_{m-1} \in \mathbb{R}^m$ with a Cholesky decomposition of matrix $T_{m-1} + \xi I_m$ to obtain parameter $\xi_\star > 0$. Such a value is sufficient in computing an approximate solution of original subproblem (12). Finally, equation $(B + \xi_\star I)d + g = 0$ is solved by the (preconditioned) conjugate gradient method. We'll get a better approximation of the trust region step than in case $\xi_\star = 0$.

*(b) Combined "conjugate gradient – Lanczos" method*
We choose a fixed $m$ (usually small) and compute $m$ steps of the conjugate gradient method to generate Lanczos vectors. Tridiagonal matrix $T_{m-1}$ of order $m$ is obtained and now we proceed as follows. If $\|d_m\| < \Delta$, we continue with the conjugate gradient method till end because matrix $T_{m-1}$ is no longer updated. If $\|d_m\| \geq \Delta$, we solve tridiagonal quadratic subproblem (14) for $h_{m-1} \in \mathbb{R}^m$ with a Cholesky decomposition of matrix $T_{m-1}+\xi I_m$ and set $d_\star = Q_{m-1}h_{m-1}$. However, with this method we cannot use preconditioning for the same reasons as above.

***10. Parametric eigenvalue problem***

We exploit optimality conditions (13) that characterize optimal step $d_\star$, define parametr $\tau \in \mathbb{R}$, construct matrix

$$A_\tau = \begin{pmatrix} \tau & g^T \\ g & B \end{pmatrix} \in \mathbb{R}^{(n+1)\times(n+1)}$$

and observe that

$$\frac{\tau}{2} + \psi(d) = \frac{1}{2}\,(1, d^T)\, A_\tau\, (1, d^T)^T.$$

Therefore, we can rewrite subproblem (12) as

$$\min_{y\in\mathbb{R}^{n+1}} \frac{1}{2}\, y^T A_\tau y, \quad y^T y \leq 1 + \Delta^2, \quad e_1^T y = 1, \quad \text{where} \quad e_1 = (1, 0, \ldots, 0)^T.$$

This formulation suggests that we can find the desired solution in terms of an eigenpair of $A_\tau$. The main goal is to drive parameter $\tau$ to an optimal value $\tau_\star$, so that the eigenvector associated with the smallest eigenvalue of $A_{\tau_\star}$ has the form $y = (1, d_\star)^T$, where $d_\star$ is the optimal step for subproblem (12).

## 4. Numerical experiments

Algorithms were implemented in UFO [5] and tested on two collections of large scale structured testing problems with 22 optimization problems without constraints [6] for 1000 and 5000 unknowns. The results are presented in Tables 1-2, where:

- N – number of the method used
- Method – initials of the method used
- P – type of preconditioning: $0, 1, 2$ (see below)
- NIT – total number of leading iterations ($x_k$ in algorithm 1)
- NFV – total number of evaluations of function $f$
- NFG – total number of evaluations of gradient $g = \nabla f$
- NCG – total number of CGM iterations (inner iterations for $d_k$)
- T – total time

| N | Method | P | NIT | NFV | NFG | NCG | T |
|---|---|---|---|---|---|---|---|
| 1. | CHDM | 0 | 4 108 | 4 242 | 4 129 | 0 | 8.84 |
| 3. | DLM-1 | 0 | 5 731 | 5 898 | 5 751 | 0 | 10.05 |
| 3. | DLM-2 | 0 | 6 370 | 6 504 | 6 391 | 0 | 10.84 |
| 4. | DLCHM | 0 | 5 719 | 5 913 | 5 740 | 0 | 10.24 |
| 5. | CGM | 0 | 4 965 | 5 317 | 4 987 | 62 837 | 12.25 |
| 6. | PCGM | 1 | 7 639 | 7 851 | 7 659 | 8 445 | 17.03 |
| 6. | PCGM | 2 | 7 569 | 7 778 | 7 589 | 8 386 | 16.56 |
| 7. | CGDLM(5) | 0 | 3 957 | 4 104 | 3 978 | 23 463 | 8.06 |
| 8. | LM(100) | 0 | 5 076 | 5 426 | 5 097 | 71 035 | 12.97 |
| 9.(a) | LCGM(5) | 0 | 4 718 | 5 116 | 4 737 | 64 384 | 13.59 |
| 9.(a) | LCGM(5) | 1 | 6 065 | 6 183 | 6 087 | 9 188 | 12.66 |
| 9.(a) | LCGM(5) | 2 | 5 905 | 6 053 | 5 925 | 7 872 | 12.33 |
| 9.(b) | CGLM(10) | 0 | 4 986 | 5 312 | 5 007 | 75 463 | 12.45 |

**Tab. 1:** *Sum of squares minimization,* $n = 1000$.

| N | Method | P | NIT | NFV | NFG | NCG | T |
|---|---|---|---|---|---|---|---|
| 1. | CHDM | 0 | 8 391 | 8 566 | 35 824 | 0 | 2:02.44 |
| 3. | DLM-1 | 0 | 9 657 | 10 133 | 42 425 | 0 | 1:55.77 |
| 3. | DLM-2 | 0 | 9 717 | 10 195 | 42 452 | 0 | 1:52.20 |
| 4. | DLCHM | 0 | 9 625 | 10 150 | 42 260 | 0 | 1:56.05 |
| 5. | CGM | 0 | 16 894 | 19 163 | 83 933 | 358 111 | 6:04.42 |
| 6. | PCGM | 1 | 10 600 | 11 271 | 50 385 | 3 767 | 2:25.42 |
| 6. | PCGM | 2 | 10 599 | 11 269 | 50 382 | 83 | 2:26.88 |
| 7. | CGDLM(5) | 0 | 8 938 | 9 276 | 39 032 | 47 236 | 2:02.84 |
| 8. | LM(100) | 0 | 14 679 | 16 383 | 71 483 | 366 695 | 6:41.45 |
| 9.(a) | LCGM(5) | 0 | 14 906 | 16 751 | 72 727 | 355 106 | 6:26.30 |
| 9.(a) | LCGM(5) | 1 | 8 347 | 8 454 | 35 939 | 4 329 | 1:48.87 |
| 9.(a) | LCGM(5) | 2 | 8 346 | 8 454 | 35 933 | 624 | 1:49.67 |
| 9.(b) | CGLM(10) | 0 | 15 655 | 17 723 | 76 696 | 394 060 | 6:30.89 |

**Tab. 2:** *Unconstrained minimization,* $n = 5000$.

If we consider preconditioning with matrix $C$, then P = 1 or P = 2. The latter case means that before starting the iteration process we test whether solution $w_\star$ of system $Cw = -g$ satisfies condition $\|Bw_\star + g\| \leq \varepsilon\|g\|$. If this is so, we'll set $d_\star = w_\star$ and the conjugate gradient method will be omitted.

Methods number 2 and 10, which are based on the knowledge of eigenvalues, are not tested. The former method uses large dense matrix $Q$, so it is not suitable for large scale structured problems, and the latter one consumes very much CPU time for eigenpairs computation.

If NCG = 0, then the method uses matrix decompositions instead of the conjugate gradient method.

See `http://www.cs.cas.cz/~luksan/test.html` for more details.

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