

# Trust-region methods for rectangular systems of nonlinear equations

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# The problem

## Bound-constrained nonlinear system (BCNS)

$$\Theta(x) = 0, \quad x \in \Omega$$

- $\Theta : \mathbb{R}^n \rightarrow \mathbb{R}^m$  continuously differentiable;
  - $\Omega = \{x \in \mathbb{R}^n \text{ t.c. } l \leq x \leq u\}$ ;
  - $l \in (\mathbb{R} \cup -\infty)^n$ ,  $u \in (\mathbb{R} \cup +\infty)^n$ ;
  - any relationship between  $m$  and  $n$  is allowed.
- **Nonlinear systems** arise in several applications: differential problems, equilibrium problems, data-fitting problems.
- **Bound constraints** on the variables prevent computing solutions without physical meaning.



## System of Nonlinear Equalities and Inequalities (NEI)

$$\begin{aligned} C_E(v) &= 0, \\ C_I(v) &\leq 0, \\ l &\leq v \leq u, \end{aligned}$$

- $C_E : \mathbb{R}^p \rightarrow \mathbb{R}^{m_E}$ ,  $C_I : \mathbb{R}^p \rightarrow \mathbb{R}^{m_I}$ , continuously differentiable.
- Two alternative reformulations:
  - 1 Add a slack variable  $s \in \mathbb{R}^{m_I}$ : let  $x = (v^T, s^T)^T$

$$\Theta(x) = \begin{pmatrix} C_E(v) \\ s - C_I(v) \end{pmatrix} = 0, \quad l \leq v \leq u, \quad s \leq 0.$$

- 2 Use the function  $[t]_+ = \max\{t, 0\}^2/2$ : let  $x = v$

$$\Theta(x) = \begin{pmatrix} C_E(x) \\ \frac{\max\{C_I(x), 0\}^2}{2} \end{pmatrix} = 0, \quad l \leq x \leq u.$$



# Trust-region methods

## Trust-region methods for BCNS

- Square systems: Bellavia, Macconi and Morini, 2003-2006, Kanzow and Klug, COAP 2007,
- Underdetermined systems: Francisco, Krejić and Martínez, JCAM 2005,
- Overdetermined systems: Kanzow and Petra, OMS 2007.

## Trust-region methods for NEI

- Fletcher and Leyffer, Kluwer 2003,
- Dennis, El-Alem and Williamson, SIOPT 1999,
- Gould and Toint, ACM Trans. Math. Software 2007.

# BCNS as a bound-constrained least-squares problem

- We address the solution of BCNS considering the following **bound-constrained least-squares problem**

$$\min_{x \in \Omega} \theta(x) = \frac{1}{2} \|\Theta(x)\|_2^2.$$

- If  $x^*$  is a solution to the BCNS problem  $\Rightarrow x^*$  is a global minimizer of  $\theta$ .
- If  $x^*$  is a zero-residual solution of  $\min_{x \in \Omega} \theta(x) \Rightarrow x^*$  is a solution to the BCNS problem.
- Recent algorithms for **bound-constrained optimization** are reliable and comparable in efficiency with unconstrained algorithms.



# The scaling matrix [Coleman and Li, SIOPT 1996]

The first-order optimality conditions for a minimizer of

$$\min_{x \in \Omega} \theta(x) = \frac{1}{2} \|\Theta(x)\|_2^2$$

are equivalent to the system of nonlinear equations

$$D(x)\nabla\theta(x) = D(x)\Theta'(x)^T\Theta(x) = 0,$$

where  $D(x) = \text{diag}(|v_1(x)|, \dots, |v_n(x)|)$ , and

$$v_i(x) = \begin{cases} x_i - u_i & \text{if } (\nabla\theta(x))_i < 0, u_i < \infty \\ x_i - l_i & \text{if } (\nabla\theta(x))_i \geq 0, l_i > -\infty \\ 1 & \text{if } (\nabla\theta(x))_i < 0, u_i = \infty \\ & \text{or if } (\nabla\theta(x))_i \geq 0, l_i = -\infty \end{cases}$$

for  $i = 1, \dots, n$ .

# Outline of the methods

- Two trust-region methods for  $\min_{x \in \Omega} \theta(x) = \frac{1}{2} \|\Theta(x)\|_2^2$  are presented.

The globalization strategy employs the Coleman and Li scaling matrix.

The sequence  $\{x_k\}$  generated is feasible, i.e.  $x_k \in \Omega$ ,  $k \geq 0$ .

- The methods differ in the choice of the quadratic model used throughout the iterations.
- Formally the two methods can be stated by the following TREI framework.



# TREI framework (Trust-Region method for systems of nonlinear Equalities and Inequalities)

- Given  $x_k \in \Omega$ , let  $m_k$  be a quadratic model for  $\theta = \frac{\|\Theta\|_2^2}{2}$  at  $x_k$

$$m_k(p) = \frac{1}{2} \|\Theta'_k p + \Theta_k\|_2^2 + \frac{1}{2} \mu_k \|p\|_2^2, \quad \mu_k \geq 0$$

If  $\mu_k = 0$  for all  $k \geq 0 \Rightarrow$  Gauss-Newton method (TREI-GN).

If  $\mu_k > 0$  for all  $k \geq 0 \Rightarrow$  Levenberg-Marquardt method (TREI-LM).

- The trust-region problem (TRP) has the form:

$$\min_p \{ m_k(p) : \|p\|_2 \leq \Delta_k \}$$

- The generalized Cauchy step  $p_k^C$  along the scaled steepest descent direction  $d_k = -D_k \nabla \theta_k$  of  $\theta$  is defined as

$$p_k^C = \operatorname{argmin}_{p \in \operatorname{span}\{d_k\}} m_k(p) \quad \text{s.t.} \quad \|p\|_2 \leq \Delta_k, \quad x_k + p \in \Omega.$$



# $k$ th iteration

- **Step 0 - Input** : given  $x_k \in \Omega$ ,  $\Delta_k > 0$ ,  $\mu_k \geq 0$ .
- **Step 1 - Test for optimality** : check if  $D_k \nabla \theta_k = 0$ .
- **Step 2 - Solve the TRP** : compute a solution  $p_{tr}$  to

$$\min_p \{m_k(p) : \|p\|_2 \leq \Delta_k\}.$$

- **Step 3 - Enforce feasibility** : let  $\bar{p}_{tr}$  be s.t.

$$\bar{p}_{tr} = P_\Omega(x_k + p_{tr}) - x_k,$$

where  $P_\Omega(x)$  is the projection of  $x$  onto  $\Omega$ .



## kth iteration

- **Step 4 - Test for global convergence:**

If

$$\rho_c(\bar{p}_{tr}) = \frac{m_k(0) - m_k(\bar{p}_{tr})}{m_k(0) - m_k(p_k^C)} \geq \beta_1, \quad \beta_1 \in (0, 1),$$

Set  $p_k = \bar{p}_{tr}$ ;

Else find  $p_k = t p_k^C + (1 - t)\bar{p}_{tr}$ ,  $t \in (0, 1]$ , s.t.  $\rho_c(p_k) = \beta_1$ .

- **Step 5 - Test to accept the trial step:**

If

$$\rho_\theta(p_k) = \frac{\theta(x_k) - \theta(x_k + p_k)}{m_k(0) - m_k(p_k)} \geq \beta_2, \quad \beta_2 \in (0, 1),$$

then  $p_k$  is accepted;

Otherwise,  $p_k$  is rejected and the trust-region size  $\Delta_k$  is reduced.

# The solution of the TRP

$$\min_p \{m_k(p) : \|p\|_2 \leq \Delta_k\}$$

In the general case the unconstrained minimizer of  $m_k$  is non-unique.

- Due to the trust-region constraints, it would be convenient to use the minimum norm step.

Compute an *approximate* solution of TRP by

- the **dogleg algorithm** using the minimum norm step
- the **truncated CG method**  
(appropriate for large and sparse problems).
- The **Moré and Sorensen algorithm** has a pitfall: in the hard case, e.g. if  $m < n$ , this strategy steps to the boundary of the trust-region even when an unconstrained minimizer of  $m_k$  is safely inside.



# The minimum norm minimizer $p_k^N$ of $m_k$

The quadratic model  $m_k$  for  $\theta = \frac{\|\Theta\|_2^2}{2}$  at  $x_k$  is

$$m_k(p) = \frac{1}{2} \|\Theta'_k p + \Theta_k\|_2^2 + \frac{1}{2} \mu_k \|p\|_2^2, \quad \mu_k \geq 0.$$

- TREI-GN method ( $\mu_k = 0$ ):  $p_k^N$  has the form

$$p_k^N = -\Theta'_k{}^+ \Theta_k.$$

- TREI-LM method ( $\mu_k > 0$ ):  $p_k^N$  solves the positive definite system of equations

$$(\Theta'_k{}^T \Theta'_k + \mu_k I_n) p_k^N = -\Theta'_k{}^T \Theta_k,$$

or equivalently

$$\begin{pmatrix} I_m & -\Theta'_k \\ -\Theta'_k{}^T & -\mu_k I_n \end{pmatrix} \begin{pmatrix} z \\ p_k^N \end{pmatrix} = \begin{pmatrix} \Theta_k \\ 0 \end{pmatrix}, \quad \text{where } z \in \mathbb{R}^m.$$



# Convergence analysis

## Assumptions

Let  $L$  be an open, bounded and convex set containing  $\{x_k\}$ .

- $\Theta'(x)$  bounded in norm and Lipschitz continuous for  $x \in L$ .

(for NEI we assume  $C_E(x)$ ,  $C_I(x)$ ,  $C'_E(x)$ ,  $C'_I(x)$  bounded in norm for  $x \in L$ ,  $C'_E(x)$  and  $C'_I(x)$  Lipschitz continuous for  $x \in L$ .)

## Global convergence results

Let  $\{x_k\}$  be the sequence generated by either the TREI-GN method or the TREI-LM method.

- Every limit point of the sequence  $\{x_k\}$  is a first-order stationary point for the problem  $\min_{x \in \Omega} \theta(x) = \frac{1}{2} \|\Theta(x)\|_2^2$ .
- If  $x^*$  is a limit point of  $\{x_k\}$  and  $\Theta(x^*) = 0$ , then all the limit points of  $\{x_k\}$  solve the BCNS problem.



## Quadratic local convergence

Let  $x^*$  be a limit point of the sequence  $\{x_k\}$  s.t.  $\Theta(x^*) = 0$ .

- The sequence generated by the TREI-GN method converges quadratically to  $x^*$  if

$$\Theta'(x^*) \quad \text{is full rank}$$

- The sequence generated by the TREI-LM method converges quadratically to  $x^*$  if

$$\mu_k = O(\|\Theta_k\|_2^2),$$

and

$\|\Theta\|_2$  provides a **local error bound** near  $x^*$ .



## Error bound condition

[Kanzow, Yamashita, Fukushima, JCAM 2004] There exist  $\alpha, \rho > 0$   
s.t.

$$d(x, S) \leq \alpha \|\Theta(x)\|_2 \quad \forall x \text{ s.t. } \|x - x^*\|_2 \leq \rho$$

where

$$S = \{y \in \Omega : \Theta(y) = 0\}, \quad d(x, S) = \inf\{\|x - y\|_2, y \in S\}$$

- The error bound condition depends on  $x^*$ .
- If  $m \geq n$  and  $\Theta'(x^*)$  is full rank  $\Rightarrow$  the error bound condition is guaranteed on some neighbourhood of  $x^*$ .

The converse is not true: the local error bound is a weaker condition than the full rank condition of  $\Theta'(x^*)^T \Theta'(x^*)$  ( $m \geq n$  and  $\Theta'(x^*)$  is full rank).



# Test problems

- The TREI-GN and TREI-LM were tested on 32 problems from the *Hock-Schittkowski* test collection and from *Handbook of test problems in local and global optimization* by Floudas et al., Kluwer 1999.
- The dimensions are such that  $2 \leq m \leq 500$ ,  $2 \leq n \leq 1000$ .
- If the problems are NEI problems, the reformulation used is

$$\Theta(x) = \left( \frac{C_E(x)}{\max\{0, C_I(x)\}^2} \right) \quad l \leq x \leq u.$$





# Implementation issues

- The TREI-GN and TREI-LM methods were run under Matlab 7.0 with  $\epsilon_m \simeq 2 \cdot 10^{-16}$ .
- In the TREI-LM method we set

$$\mu_0 = 10^{-8} \|\Theta_0\|_2^2, \quad \mu_k = \min\{\mu_{k-1}, \|\Theta_k\|_2^2\}, \quad k > 0$$

[Kanzow, Yamashita, Fukushima, JCAM 2004]

- The strategy for updating the trust-region radius is the standard one.
- Successful termination:  $\|\Theta_k\|_2 \leq 10^{-6}$ .
- Failures:

$$\Delta_k \leq \sqrt{\epsilon_m};$$

300 nonlinear iterations were performed;

$$\|D_k \nabla \theta_k\|_2 \leq 100 \epsilon_m \text{ or } \|\Theta_{k+1} - \Theta_k\|_2 \leq 100 \epsilon_m \|\Theta_k\|_2.$$



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# Implementation issues: the solution of TRP

## The Dogleg algorithm

- 1 Compute the minimum norm minimizer  $p_k^N$  of  $m_k$ :
  - if  $\mu_k = 0$  by the complete orthogonal factorization of  $\Theta'_k$ ;
  - if  $\mu_k > 0$  by the QR decomposition to the least-squares pb

$$\min_p m_k(p) = \min_p \frac{1}{2} \left\| \begin{pmatrix} \Theta'_k \\ \sqrt{\mu_k} I_n \end{pmatrix} p + \begin{pmatrix} \Theta_k \\ 0 \end{pmatrix} \right\|^2.$$

If  $p_k^N$  lies inside the trust-region, stop.

- 2 Compute the **Cauchy step**

$$p_{k,c} = \operatorname{argmin}_{p \in \operatorname{span}\{-\nabla\theta_k\}} m_k(p) \quad \text{s.t.} \quad \|p\|_2 \leq \Delta_k.$$

- 3 Dogleg between  $p_{k,c}$  and  $p_k^N$ .



# Results

- All problems were run starting from three different initial guesses  $x_0$ :

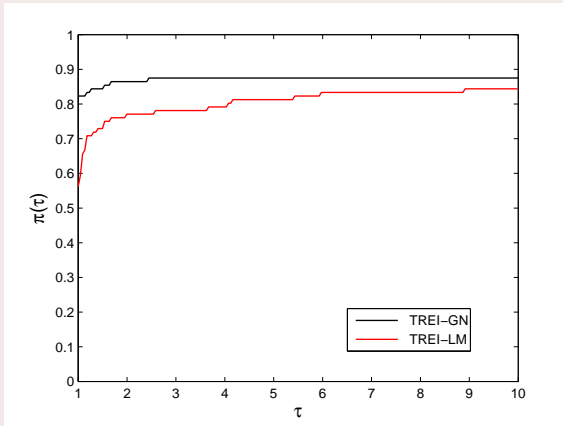
$$(x_0)_i = \begin{cases} l_i + c(u_i - l_i)/2 & \text{if } l_i > -\infty \text{ and } u_i < \infty, \\ l_i + c 10^c & \text{if } l_i > -\infty \text{ and } u_i = \infty, \\ u_i - c 10^c & \text{if } l_i = -\infty \text{ and } u_i < \infty, \\ 10(c - 1) & \text{if } l_i = -\infty \text{ and } u_i = \infty, \end{cases}$$

for  $c = 0, 1, 2$ . Then 96 runs were performed.

- The method TREI-GN and TREI-LM converged to a first-order stationary point for  $\min_{x \in \Omega} \theta(x) = \frac{1}{2} \|\Theta(x)\|_2^2$  for about 91% of the runs.

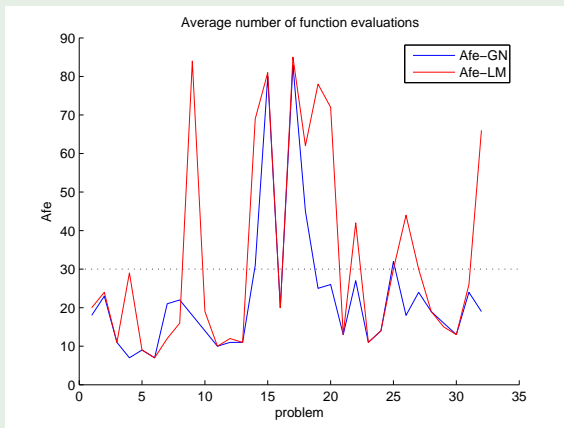


## Performance profile



We summarize the overall computational effort of the methods plotting the function  $\Theta$ -evaluation performance profile, see [Dolan, Moré, Math. Program. 2002]





Most problems were solved with a low number of  $\Theta$ -function evaluations and this number is, on average, favorable for the TREI-GN method.



# Conclusions

- We have presented two trust-region methods for solving BCNS problems based on recent developments in nonlinear optimization with simple bounds.
- At each iteration:
  - The TREI-GN method requires the minimum norm solution of a linear least-squares problem.  
For large-scale problems the use of iterative methods can reduce the cost of this task.
  - The TREI-LM method requires the solution of a positive definite system and the choice of the parameter  $\mu_k$ . This choice is critical for its numerical performances.



# Future work

- Enhancement of the global strategy: use of the filter technique in our framework;
- TRP solution: use of the truncated CG algorithm instead of the dogleg method  $\Rightarrow$  efficient solution of large problems;
- Development of software;
- Development of an efficient procedure in computing non-zero residual stationary point.





Thanks for your attention