Levenberg-Marquardt methods for the solution of noisy nonlinear least squares problems: Regularization of ill-posed problems and cheap solution of large scale problems

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Ill-posed least squares problems

Let us consider the following least squares problem: given $\mathcal{X}, \mathcal{Y}$ Hilbert spaces, $F : \mathcal{X} \rightarrow \mathcal{Y}$, nonlinear, continuously differentiable and $y \in \mathcal{Y}$, solve

$$\min_{x \in \mathcal{X}} \|F(x) - y\|^2.$$

Definition

The problem is well-posed if:

1. $\forall y \in \mathcal{Y}$ it exists a solution $x \in \mathcal{X}$,
2. the solution is unique,
3. property of stability holds.

The problem is ill-posed if one or more of the previous properties do not hold.

Ill-posed problems

- Let us consider problems of the form

$$\min_{x\in\mathbb{R}^n} \|F(x) - y\|^2, \qquad x \in (\mathbb{R}^n, \|\cdot\|_2),\ y \in (\mathbb{R}^m, \|\cdot\|_2),$$

  with $F : \mathbb{R}^n \to \mathbb{R}^m$ and $m \geq n$, arising from the discretization of an ill-posed problem.

- In a realistic situation the data y are affected by noise, we have at disposal only y^δ such that:

$$\|y - y^\delta\| \leq \delta$$

  for some positive δ .

- We can handle only a noisy problem:

$$\min_{x\in\mathbb{R}^n} \|F(x) - y^\delta\|^2.$$

Need for regularization

- As stability does not hold, the solutions of the original problem do not depend continuously on the data.
  $\Longrightarrow$ The solutions of the noisy problem may not be meaningful approximations of the original problem solutions.

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  $\Longrightarrow$ The solutions of the noisy problem may not be meaningful approximations of the original problem solutions.
- For ill-posed problems there are no finite bounds on the inverse of the Jacobian of F around a solution of the original problem.
- Classical methods used for well-posed systems are not suitable in this contest.

$$\Downarrow$$

Need for regularization.

Outline

First part - zero-residual problems: $F(x) = y^\delta$

We consider a fixed noise level δ.
We propose a regularizing trust-region approach.

Second part - non-zero residual problems: $\min_{x\in\mathbb{R}^n} \|F(x) - y^\delta\|^2$

It does not exist x such that $F(x) - y = 0$.
1) First extend the trust-region approach to small residual problems.
2) Then we consider problems with a noise level δ that can vary.
We propose a Levenberg-Marquardt method for large-scale problems.

Levenberg-Marquardt method

- It is an iterative method. Let denote x_k the iterate at iteration k.
- Given $x_k \in \mathbb{R}^n$ and $\lambda_k > 0$, we denote with $J \in \mathbb{R}^{m\times n}$ the Jacobian matrix of F. The step $p_k \in \mathbb{R}^n$ is the minimizer of

$$m_k^{LM}(p) = \frac{1}{2}\|F(x_k) - y + J(x_k)p\|^2 + \frac{1}{2}\lambda_k\|p\|^2.$$

- p_k is the solution of

$$(B_k + \lambda_k I)p_k = -g_k$$

with $B_k = J(x_k)^T J(x_k)$, $g_k = J(x_k)^T(F(x_k) - y)$.

- Set $\Phi(x) = \frac{1}{2}\|F(x) - y^\delta\|^2$, and compute

$$\rho_k(p_k) = \frac{\Phi(x_k) - \Phi(x_k + p_k)}{m_k^{LM}(0) - m_k^{LM}(p_k)}.$$

- Given $\eta \in (0, 1)$:
  - If $\rho_k < \eta$ then set $\lambda_{k+1} > \lambda_k$ and $x_{k+1} = x_k$.
  - If $\rho_k \geq \eta$ then set $\lambda_{k+1} \leq \lambda_k$ and $x_{k+1} = x_k + p_k$.

Trust-region methods

- Given $x_k \in \mathbb{R}^n$, the step $p_k \in \mathbb{R}^n$ is the minimizer of

$$\min_p m_k^{TR}(p) = \frac{1}{2}\|F(x_k) - y + J(x_k)p\|^2,$$
$$\text{s.t. } \|p\| \le \Delta_k,$$

  with $\Delta_k > 0$ trust-region radius.
- Set $\Phi(x) = \frac{1}{2}\|F(x) - y^\delta\|^2$, and compute

$$\rho_k(p_k) = \frac{\Phi(x_k) - \Phi(x_k + p_k)}{m_k^{TR}(0) - m_k^{TR}(p_k)}.$$

- Given $\eta \in (0, 1)$:
  - If $\rho_k < \eta$ then set $\Delta_{k+1} < \Delta_k$ and $x_{k+1} = x_k$.
  - If $\rho_k \ge \eta$ then set $\Delta_{k+1} \ge \Delta_k$ and $x_{k+1} = x_k + p_k$.

Trust-region methods

It is possible to prove that p_k solves

$$(B_k + \lambda_k I)p_k = -g_k$$

for some $\lambda_k \geq 0$ such that

$$\lambda_k(\|p_k\| - \Delta_k) = 0,$$

where we have set $B_k = J(x_k)^T J(x_k)$ and $g_k = J(x_k)^T (F(x_k) - y)$.

$\Rightarrow$ Trust-region methods are Levenberg-Marquardt methods!

First part: zero-residual problems

Consider

$$F(x) = y^{\delta},$$

with δ fixed noise level, and let $x^{\dagger}$ be a solution of $F(x) = y$.

Iterative regularization methods generate a sequence $\{x_k^\delta\}$. If the process is stopped at iteration $k^*(\delta)$ the method is supposed to guarantee the following properties:

- $x^\delta_{k^*(\delta)}$ is an approximation of $x^\dagger$;
- $\{x^\delta_{k^*(\delta)}\}$ tends to $x^\dagger$ if δ tends to zero;
- local convergence to $x^\dagger$ in the noise-free case.

There are many methods of this class in the literature, they are analyzed only under local assumptions, the definition of globally convergent approaches is still an open task.

Standard trust-region

Standard trust-region

The step p_k solves

$$(B_k + \lambda_k I)p_k = -g_k$$

for some $\lambda_k \geq 0$ such that

$$\lambda_k(\|p_k\| - \Delta_k) = 0.$$

- B_k is ill-conditioned.
- In trust-region methods the trust region is eventually inactive: $\|p_k\| < \Delta_k \to \lambda_k = 0$.
- It is not a regularization method!

How to obtain a regularizing method?

Noisy problem

$$\min_{x \in \mathbb{R}^n} \frac{1}{2} \|F(x) - y^\delta\|^2$$

Exact problem

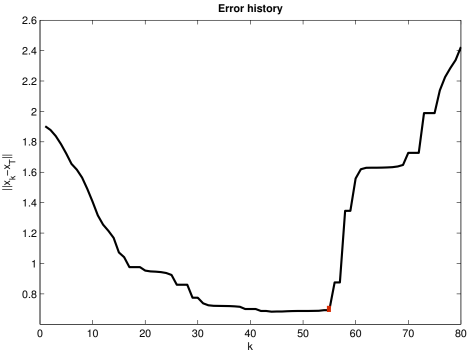
$$\min_{x \in \mathbb{R}^n} \frac{1}{2} \|F(x) - y\|^2$$

1. stopping criterion
2. small steps

1) Stopping criterion: with noisy data the process is stopped at iteration $k^*(\delta)$ such that $x^\delta_{k^*(\delta)}$ satisfies the discrepancy principle:

$$\|F(x^\delta_{k^*(\delta)}) - y^\delta\| \leq \tau\delta < \|F(x^\delta_k) - y^\delta\|$$

for $0 \leq k < k^*(\delta)$ and $\tau > 1$ suitable parameter.

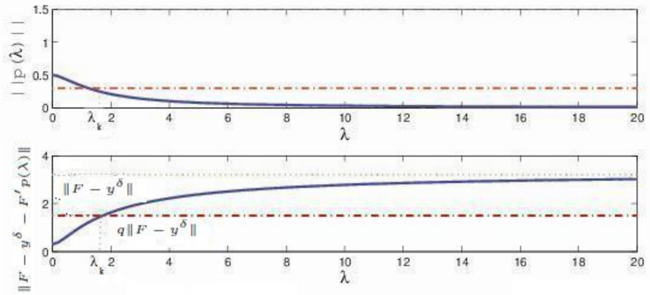


SEMI CONVERGENCE

Plot of the error $\|x^\delta_k - x^\dagger\|$ versus iteration number.

Regularizing trust-region

2) q-condition: $\|F(x_k^\delta) - y^\delta + J(x_k^\delta)p\| \geq q\|F(x_k^\delta) - y^\delta\|,\ q \in (0,1)$



$\rightarrow$ If $\Delta_k \leq \frac{1-q}{\|B_k\|}\|g_k^\delta\|$ then p_k satisfies the q-condition and the trust region is active.

Algorithm : k-th iteration of regularizing trust-region

Given x_k^δ, $\eta \in (0,1)$, $\gamma \in (0,1)$, $0 < C_{\min} < C_{\max}$.
Exact data: y, $q \in (0,1)$.
Noisy data: y^δ, $q \in (0,1)$, $\tau > 1/q$.

1. Compute $B_k = J(x_k^\delta)^T J(x_k^\delta)$ and $g_k^\delta = J(x_k^\delta)^T (F(x_k^\delta) - y^\delta)$.
2. Choose $\Delta_k \in \left[C_{\min} \|g_k^\delta\|, \min\left\{ C_{\max}, \frac{1-q}{\|B_k\|} \right\} \|g_k^\delta\| \right]$
3. Repeat
   3.1 Compute the solution p_k of trust-region problem.
   3.2 Compute
   $$\rho_k(p_k) = \frac{\Phi(x_k^\delta) - \Phi(x_k^\delta + p_k)}{m_k^{TR}(0) - m_k^{TR}(p_k)}$$
   with $\Phi(x) = \frac{1}{2}\|F(x) - y^\delta\|^2$, $m_k^{TR}(p) = \frac{1}{2}\|F(x_k^\delta) + J(x_k^\delta)p\|^2$.
   3.3 If $\rho_k(p_k) < \eta$,set $\Delta_k = \gamma \Delta_k$.

   Until $\rho_k(p_k) \geq \eta$.
4. Set $x_{k+1}^\delta = x_k^\delta + p_k$.

Local analysis

- **Assumption 1** For index $\bar{k}$ it exist positive ρ and c such that
  1. the system $F(x) = y$ is solvable in $B_\rho(x^\delta_{\bar{k}})$;
  2. for $x, \tilde{x} \in B_{2\rho}(x^\delta_{\bar{k}})$

$$\|F(x) - F(\tilde{x}) - J(x)(x - \tilde{x})\| \leq c\|x - \tilde{x}\|\|F(x) - F(\tilde{x})\|.$$

  For well-posed systems: $\|F(x) - F(\tilde{x}) - J(x)(x - \tilde{x})\| \leq c\|x - \tilde{x}\|^2$.

- **Assumption 2**: It exists positive K_J such that

$$\|J(x)\| \leq K_J$$

for all $x \in \mathcal{L} = \{x \in \mathbb{R}^n \;\; s.t. \;\; \Phi(x) \leq \Phi(x_0)\}$.

Theoretical results

Lemma

The method generates a sequence $\{x_k^\delta\}$ such that:
1) the trust-region is active, i.e. $\lambda_k > 0$,
2) error decreases monotonically: $\|x_{k+1}^\delta - x^\dagger\| < \|x_k^\delta - x^\dagger\|$,
for $k \geq \bar{k}$, with $\bar{k} < k^*(\delta)$ for noisy data.

Theorem

If $\delta = 0$ the sequence $\{x_k\}$ converges to a solution x^* of $F(x) = y$ such that $\|x^* - x^\dagger\| \leq \rho$.
If $\delta > 0$ the discrepancy principle is satisfied after a finite number of iterations $k^*(\delta)$ and the sequence $\{x_{k^*(\delta)}^\delta\}$ converges to a solution of $F(x) = y$ if δ tends to zero.

$\rightarrow$ **Regularizing method**, [S. Bellavia, B. Morini, E. R., COAP, 2016].

Test problems

- Four nonlinear ill-posed systems arising from the discretization of nonlinear first-kind Fredholm integral equation are considered, they model gravimetric and geophysics problems:

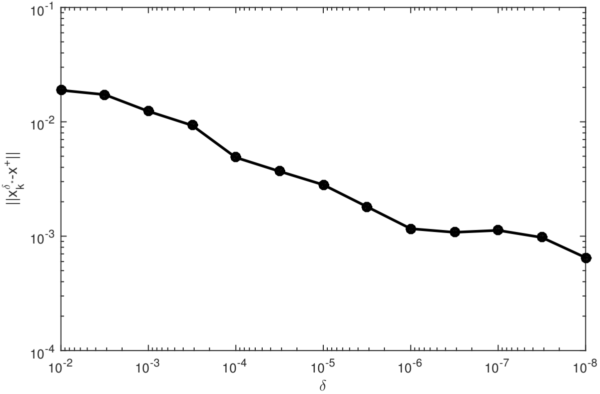
$$\int_0^1 k(t, s, x(s))ds = y(t), \qquad t \in [0, 1],$$

  P1,**P2**, [Vogel, 1990], **P3**,**P4** [Kaltenbacher,2007];

- Their kernel is of the form

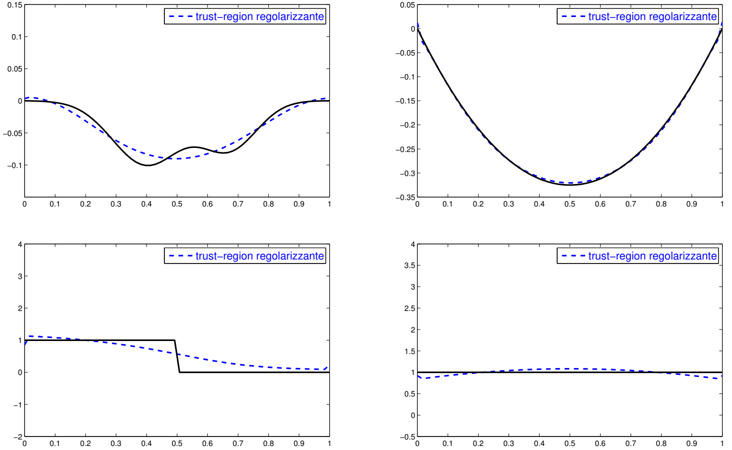
$$\begin{aligned} k(t, s, x(s)) &= log\left(\frac{(t-s)^2 + H^2}{(t-s)^2 + (H - x(s))^2}\right); \\ k(t, s, x(s)) &= \frac{1}{\sqrt{1 + (t-s)^2 + x(s)^2}}; \end{aligned}$$

Regularizing properties of the method.



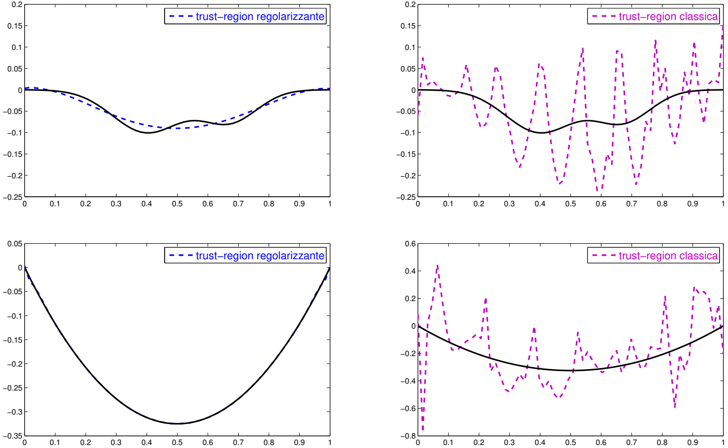
Semilogarithmic plot of the error $||x^{\delta}_{k^*(\delta)} - x^{\dagger}||$ as a function of the noise level δ.

Computed solution approximations



Blue: regularizing TR, **Solid line**: solution of the original problem.

Comparison between regularizing and standard trust-region



Left: regularizing TR, **Right**: standard TR , **Solid line**: solution of the original problem.

Second part - non-zero residual problems

We consider non-zero residual problems:
it does not exist x such that $F(x) - y = 0$.

Small residual problems

- We extend the approach for zero-residual problems to small residual problems. → We propose an **elliptical trust-region approach.**
- Let us assume that J is full rank, but ill-conditioned, with ill-conditioning due to smallest singular value close to zero, as often happens in these applications.

At a generic iteration k, given $\Delta_k > 0$, the following problem is solved:

$$\min_p m_k(p) := \frac{1}{2}\|F(x_k^\delta) - y^\delta + J(x_k^\delta)p\|^2,$$
$$\text{s.t. } \|(B_k)^{-\frac{1}{2}} p\| \leq \Delta_k.$$

Regularizing properties

To maintain the regularizing properties of the trust-region approach we assume equivalent conditions on the gradient instead on the function.

1. **discrepancy principle** :

$$\|J(x^\delta_{k^*(\delta)})^T(F(x^\delta_{k^*(\delta)}) - y^\delta)\| \leq \tau\delta < \|J(x^\delta_k)^T(F(x^\delta_k) - y^\delta)\|$$

2. **q-condition**:

$$\|J(x^\delta_k)^T(F(x^\delta_k) - y^\delta + J(x^\delta_k)p_k)\| \geq q\|J(x^\delta_k)^T(F(x^\delta_k) - y^\delta)\|$$

If $\Delta_k \leq \frac{1-q}{\|B_k\|^2}\|(B_k)^{1/2}g^\delta_k\|$ then p_k satisfies the q-condition and the trust-region is active.

- **Assumption1**: there exists $\bar{k}$ s.t. a solution exists in $B_\rho(x_{\bar{k}})$ and for $x, \tilde{x} \in B_{2\rho}(x_{\bar{k}})$

$$\|\nabla f(\tilde{x}) - \nabla f(x) - J(x)^T J(x)(\tilde{x} - x)\| \leq (c\|\tilde{x} - x\| + \sigma)\|\nabla f(x) - \nabla f(\tilde{x})\|.$$

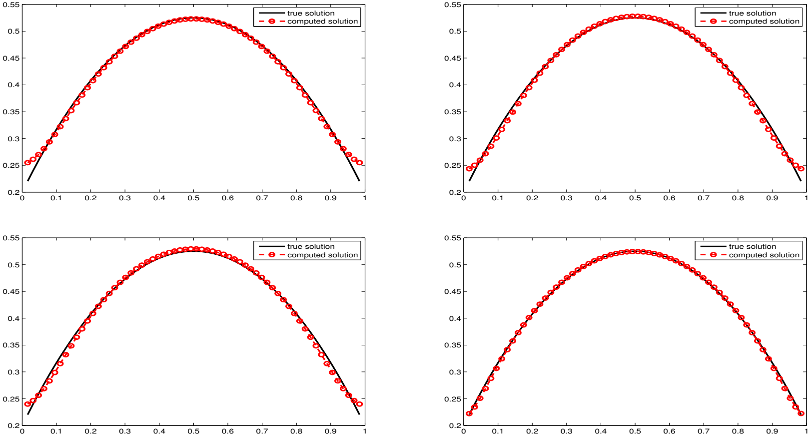
$$\nabla^2 f(x) = J(x)^T J(x) + S(x) = J(x)^T J(x) + \sum_{j=1}^{m} (F_j(x) - y_j)\nabla^2 F_j(x).$$

- **Assumption2**: $\|S(x^\dagger)\| \leq \sigma < q < 1$ (small residual problems)

$$\Downarrow$$

Regularizing method.

Pb. Freh2, $x_0^\delta = (-0.3, \dots, -0.3)^T$. Plot of the true and the computed solution for decreasing noise level, $\delta = 10^{(-(k+1)/2)}$, k=4,5,6,7.



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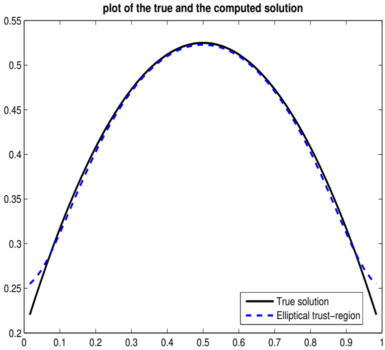

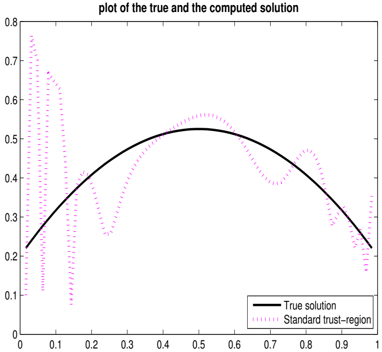

Left: elliptical TR, **Right**: standard TR , **Solid line**: solution of the original problem

Large scale non-zero residual problems

- Collaboration with S. Gratton, CERFACS, Enseeiht-INP, Toulouse.
- Data Assimilation: weather forecasting, oceanography.
- It is possible to modify the noise on the data δ_k during the optimization process. $\rightarrow$ Need for a strategy to control the noise.
- Large-scale non-zero residual ill-posed problems

We propose a Levenberg-Marquardt method, globally convergent as the noise level tends to zero.

- At each iteration we have to solve linear systems of the form:

$$(J(x_k^{\delta_k})^T J(x_k^{\delta_k}) + \lambda_k I)p_k = -g_k^{\delta_k}.$$

- We have to compute:

$$\rho_k^{\delta_k}(p_k) = \frac{\Phi^{\delta_k}(x_k^{\delta_k}) - \Phi^{\delta_k}(x_k^{\delta_k} + p_k)}{m_k(0) - m_k(p_k)}.$$

- If the noise is too high the reduction in Φ^{δ_k} can be just an effect of the presence of the noise.

Noise control

Noise control

Let

$$\delta_k \leq \frac{1}{2}\lambda_k^{\alpha}\|p\|^2,$$

for $\alpha \in (\frac{1}{2}, 1]$. If

$$\rho_k^{\delta_k}(p_k) = \frac{\Phi^{\delta_k}(x_k^{\delta_k}) - \Phi^{\delta_k}(x_k^{\delta_k} + p_k)}{m_k(0) - m_k(p_k)} > \eta$$

then also

$$\rho_k(p_k) = \frac{\Phi(x_k^{\delta_k}) - \Phi(x_k^{\delta_k} + p_k)}{m_k(0) - m_k(p_k)} > \eta.$$

$\rightarrow$ True reduction in the noise-free objective function Φ

Algorithm : k-th iteration of regularizing Levenberg-Marquardt

Given $\alpha \in \left(\frac{1}{2}, 1\right]$, δ_0, $\eta_1 \in (0,1)$, $\eta_2 > 0$, $\lambda_{\max} > \lambda_{\min} > 0$, $\gamma > 1$, x_0 and $\lambda_{\max} > \lambda_0 \geq \lambda_{\min}$.

Compute $f^{\delta_0}(x_0)$. For $k = 0, 1, 2, \ldots$

1. Compute a solution p_k of the LM subproblem.
2. If $\delta_k \leq \frac{1}{2}\lambda_k^{\alpha}\|p_k\|^2$, compute $\Phi^{\delta_k}(x_k^{\delta_k} + p_k)$, else reduce δ_k and go back to 1.
3. Compute

$$\rho_k(p_k) = \frac{\Phi^{\delta_k}(x_k^{\delta_k}) - \Phi^{\delta_k}(x_k^{\delta_k} + p_k)}{m_k(0) - m_k(p_k)}.$$

3.1 If $\rho_k^{\delta_k}(p_k) \geq \eta_1$, then set $x_{k+1}^{\delta_k} = x_k^{\delta_k} + p_k$ and

$$\lambda_{k+1} = \begin{cases} \min\{\gamma\lambda_k, \lambda_{\max}\} & \text{if } \|g_k^{\delta_k}\| < \eta_2/\lambda_k, \\ \max\{\lambda_k, \lambda_{\min}\} & \text{if } \|g_k^{\delta_k}\| \geq \eta_2/\lambda_k. \end{cases}$$

3.2 Otherwise set $x_{k+1}^{\delta_k} = x_k^{\delta_k}$, $\lambda_{k+1} = \gamma\lambda_k$.

Inexact step

Large-scale problems: approximate solution of LM subproblem

p provides the sufficient Cauchy decrease:

$$m_k(0) - m_k(p_k) \geq \frac{\theta}{2} \frac{\|g_k^{\delta_k}\|^2}{\|J(x_k)\|^2 + \lambda_k}, \qquad \theta > 0.$$

The Levenberg-Marquardt step computed as

$$(J(x_k^{\delta_k})^T J(x_k^{\delta_k}) + \lambda_k I) p_k = -g_k^{\delta_k} + r_k$$

for a residual r_k satisfying $\|r_k\| \leq \epsilon_k \|g_k^{\delta_k}\|$, with ϵ_k small enough achieves the Cauchy decrease.

Assumptions

Let $\mathcal{L} = \{x \mid f(x) \leq f(x_0)\}$, $x^\dagger$ a local minimum of function f.

- Assumption 1: It exists $K > 0$ such that $\|J(x)\| \leq K$ for all $x \in \mathcal{L}$.
- Assumption 2: f has Lipschitz continuous gradient on $\mathcal{L}$: $\|g(x) - g(y)\| \leq L\|x - y\|$ for all $x, y \in \mathcal{L}$.
- Assumption 3: Let H the Hessian matrix of function f, $H(x^\dagger) \succeq 0$, H is Lipschitz continuous: $\|H(x) - H(y)\| \leq M\|x - y\|$ for all $x, y \in \mathcal{L}$, and let $0 < l \leq L < \infty$ such that $l\, I_n \preceq H(x^\dagger) \preceq L\, I_n$ with I_n the identity matrix of size n.

Theoretical results

- **Global convergence**: Let Assumptions 1 and 2 hold. Then

$$\lim_{k\to\infty} \delta_k = 0, \qquad \lim_{k\to\infty} \|g(x_k^{\delta_k})\| = 0.$$

- **Parameters λ_k**: It exists $\bar{k} > 0$ such that $\lambda_k = \lambda_{\max}$ for all $k \geq \bar{k}$.
- **Asymptotic step behaviour** Let p_k satisfy the Cauchy decrease. Then

$$\left\| \frac{g_k^{\delta_k}}{\|p_k\|(\lambda_k + K^2)} + \frac{p_k}{\|p_k\|} \right\|^2 = O\left(\frac{1}{\lambda_k}\right)$$

  If λ_k is large enough p_k tends to a steepest descent step with step-length $\frac{1}{\lambda_{\max}}$.
- **Local Convergence perturbed steepest descent**: Let Assumptions 1,2 and 3 hold and let $p_k^{SD} = -\frac{1}{\lambda_{\max}} g_k^{\delta_k}$ with $\frac{1}{\lambda_{\max}} < \frac{1}{L}$. If the starting guess x_0 is close enough to $x^\dagger$, the method converges.

Numerical Results

Test 1 - Reconstruct electrical conductivity of the soil with respect to depth, starting from electromagnetic data, $n = 20$, $m = 40$, [Deidda, Fenu, Rodriguez, 2014.]
Test 2 - Fredholm equation of the first kind, $n = 640$, $m = 1000$, [Vogel, 1990].

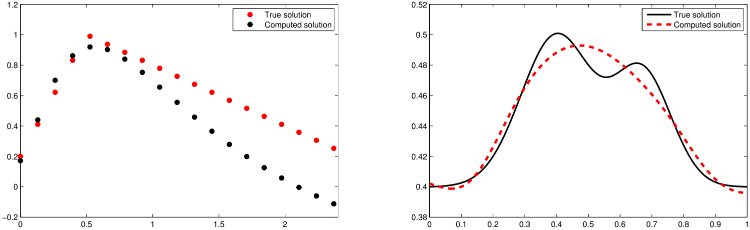

Figure: True and computed solutions for Test 1 (left) and Test 2 (right).

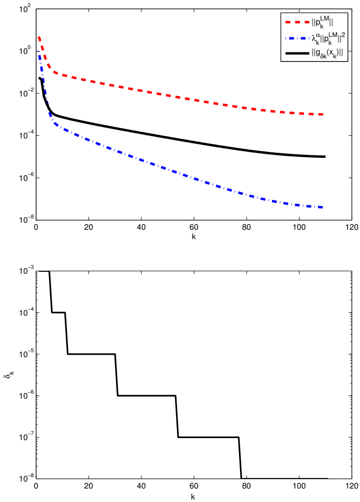

Figure: Decrease of $\|p_k\|$, $\lambda_k^{\alpha}\|p_k\|^2$, $\|g_{\delta_k}(x_k)\|$ (up) and decrease of δ_k (bottom) for Test 1.

Conferences and visiting

- Poster: 'Levenberg-Marquardt method for ill-posed large scale nonlinear least squares problems', OIP2016, Modena, 19/09/2016-21/09/2016.
- 'Support Vector Machine classification applied to the parametric design of centrifugal pumps', SIMAI 2016, Milano 13/09/2016-16/09/2016.
- Visiting at INP-ENSEEIHT, Toulouse, for a collaboration with Prof. Serge Gratton on ill-posed nonlinear least-squares problems, June-July 2016.
- 'Regularizing trust-region approaches for ill-posed nonlinear systems and nonlinear least squares', 20th Conference of the International Linear Algebra Society (ILAS), Leuven, Belgium, 11/07/2016-15/07/2016, invited speaker.
- 'Numerical methods for optimization problems: an application to energetic districts', 19th European Conference on Mathematics for Industry ECMI, Santiago de Compostela, Spain, 13/06/2016-17/06/2016, invited speaker for receiving the **degree award 'Hansjörg Wacker Memorial Prize'**.

- 'Solving ill-posed nonlinear systems with noisy data: a regularizing trust-region approach', 'PING - Inverse Problems in Geophysics' Workshop Firenze, 6/04/2016.
- 'A regularization trust-region approach for ill-posed nonlinear systems', Workshop 'Optimization and Data Assimilation', CERFACS, Toulouse (France), 13/01/2016-15/01/2016.
- November 21-22, 2015, 'On an Adaptive Regularization for Ill-posed Nonlinear Systems and its Trust-Region Implementation' Networking in Numerical Analysis 2015, a two day meeting in Bertinoro', Bertinoro (FC).
- September 12, 2015, 'On an Adaptive Regularization for Ill-posed Nonlinear Systems and its Trust-Region Implementation' , XX Congresso UMI, Siena.
- ISMP 2015, 22nd International Symposium on Mathematical Programming, Pittsburgh (USA), 12/07/2015- 17/07/2015.
- June 21-26, 2015, CIME course 'Exploiting Hidden Structure in Matrix Computations. Algorithms and Applications', Cetraro (CS).

Research Outputs

- S.Bellavia, B.Morini, E.Riccietti, *On an adaptive regularization for ill-posed nonlinear systems and its trust-region implementation* (COAP, 2016).
- E.Riccietti, J.Bellucci, M.Checcucci, M.Marconcini, A.Arnone, *Support Vector Machine classification applied to the parametric design of centrifugal pumps*, submitted.
- E.Riccietti, S.Bellavia, S.Sello, *Numerical methods for optimization problems arising in energetic districts*, ECMI proceeding, submitted.
- S.Bellavia, E.Riccietti, *Trust-region methods for ill-posed nonlinear least-squares problems*, in preparation.
- S.Bellavia, S.Gratton, E.Riccietti, *Levenberg-Marquardt method for ill-posed large scale nonlinear least squares problems*, in preparation.