Regularizing trust-region approaches for ill-posed nonlinear systems and nonlinear least squares

Elisa Ricciietti
Università degli Studi di Firenze
Dipartimento di Matematica e Informatica 'Ulisse Dini'

Joint work with Stefania Bellavia, Benedetta Morini

ILAS 2106, Leuven, July 11-15 2016.

Ill-posed least squares

Let us consider the following least squares problem: given $F : \mathbb{R}^n \rightarrow \mathbb{R}^m$ with $m \geq n$, nonlinear, continuously differentiable and $y \in \mathbb{R}^m$, solve

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

$\rightarrow$ We are interested in ill-posed problems.

Ill-posed problems

The problem is ill-posed if:

1. $\forall y \in \mathbb{R}^m$ the existence and uniqueness of the solution $x \in \mathbb{R}^n$ of the problem are not guaranteed,
2. stability does not hold: the solutions do not depend continuously on the data.

Noisy case

- In a realistic situation only noisy data y^δ are given:

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

  where δ is the noise level.
- The solution does not depend continuously on the data that are noisy: the solution of the noisy problem is not a good solution of the original one.
- As the problem is ill-posed, no finite bounds on the inverse of the norm of the Jacobian matrix: classical methods used for well-posed problems are not suitable in this contest.

$$\Downarrow$$

Need for regularization

Outline

- Introduction to iterative regularization methods.
- Description of Levenberg-Marquardt method and of its regularizing variant.
- Description of a new regularizing trust-region approach, obtained by a suitable choice of the trust region radius .
- Regularization and convergence properties of the new approach.
- Numerical tests: we compare the new trust-region approach to the regularizing Levenberg-Marquardt and standard trust-region methods.
- Open issues and future developments.

Iterative regularization methods

Hypothesis: it exists $x^\dagger$ solution of $\min \frac{1}{2}\|F(x) - y\|^2$.

Definition

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:

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

Regularizing methods for zero residual problems

- Landweber (gradient-type method)[Hanke, Neubauer, Scherzer, 1995,Kaltenbacher, Neubauer, Scherzer, 2008]
- Truncated Newton - Conjugate Gradients [Hanke,1997, Rieder, 2005]
- Iterative Regularizing Gauss-Newton [Bakushinsky, 1992, Blaschke, Neubauer, Scherzer, 1997]
- Levenberg-Marquardt [Hanke,1997,2010,Vogel 1990, Kaltenbacher, Neubauer, Scherzer, 2008]
- Trust region methods [Wang, Yuan 2002,Bellavia, Morini, R. 2016]

Most of these methods are analyzed only under local assumptions.

Levenberg-Marquardt method

- Given $x_k^\delta \in \mathbb{R}^n$ 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

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

- $p_k = p(\lambda_k)$ is the solution of

$$(J(x_k^\delta)^T J(x_k^\delta) + \lambda_k I)p_k = -J(x_k^\delta)^T(F(x_k^\delta) - y^\delta).$$

- The step is then used to compute the new iterate

$$x_{k+1}^\delta = x_k^\delta + p_k.$$

Regularizing Levenberg-Marquardt (LM) method for zero residual problems

The regularizing properties are given by two choices:

- The parameter $\lambda_k > 0$ satisfies:

$$\|F(x_k^\delta) - y^\delta + J(x_k^\delta)p(\lambda_k)\| = q\|F(x_k^\delta) - y^\delta\|$$

  with $q \in (0,1)$;

- With noisy data the process is stopped at iteration $k^*(\delta)$ such that $x_{k^*(\delta)}^\delta$ satisfies the discrepancy principle:

$$\|F(x_{k^*(\delta)}^\delta) - y^\delta\| \leq \tau\delta < \|F(x_k^\delta) - y^\delta\|$$

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

[Hanke, 1997,2010]

Local analysis

Assumption

Given the starting guess x_0, it exist positive ρ and c such that

- the system $F(x) = y$ is solvable in $B_\rho(x_0)$;
- for $x, \tilde{x} \in B_{2\rho}(x_0)$

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

- Due to the ill-posedness of the problem it is not possible to assume that a finite bound on the inverse of the Jacobian matrix exists.
- The Jacobian may be singular at the solution.

Regularizing properties of the LM method

Choosing λ_k solution of

$$\|F(x_k^\delta) - y^\delta + J(x_k^\delta)p(\lambda_k)\| = q\|F(x_k^\delta) - y^\delta\|$$

and stopping the process when the discrepancy principle

$$\|F(x_{k^*(\delta)}^\delta) - y^\delta\| \leq \tau\delta < \|F(x_k^\delta) - y^\delta\|$$

is satisfied, Hanke proves that:

Lemma

- *With exact data ($\delta = 0$): local convergence to $x^\dagger$,*
- *With noisy data ($\delta > 0$): Choosing x_0 close to $x^\dagger$ the discrepancy principle is satisfied after a finite number of iterations $k^*(\delta)$ and $\{x_{k^*(\delta)}^\delta\}$ converges to a solution of $F(x) = y$ if δ tends to zero.*

Regularizing method.

Drawbacks of the LM approach

- The existence of $\lambda_k > 0$ s.t.
  $\|F(x_k^\delta) - y^\delta + J(x_k^\delta)p(\lambda_k)\| = q\|F(x_k^\delta) - y^\delta\|$
  is guaranteed only whenever x_k is close to a solution.
- If λ_k does not exists it is not clear how to choose λ: from a computational point of view the choice of λ is crucial.
- Global convergence is not enforced either in the noise-free case.

Drawbacks of the LM approach

- The existence of $\lambda_k > 0$ s.t.
  $\|F(x_k^\delta) - y^\delta + J(x_k^\delta)p(\lambda_k)\| = q\|F(x_k^\delta) - y^\delta\|$
  is guaranteed only whenever x_k is close to a solution.
- If λ_k does not exists it is not clear how to choose λ: from a computational point of view the choice of λ is crucial.
- Global convergence is not enforced either in the noise-free case.

On the other hand,Trust-Region methods are LM methods.

Can we obtain more robust regularizing methods than the Hanke's LM approach and enforce global convergence in the noise-free case?

First step in proving regularization properties of Trust-Region methods: [Wang, Yuan, 2002]

Standard TR approach: observations

- The trial step p_k is solution to:

$$\min_{\|p\|\leq\Delta_k} m_k^{TR}(p) = \|F(x_k^\delta) - y^\delta + J(x_k^\delta)p\|^2.$$

- The role of Δ_k is to provide global convergence of the procedure.
- The solution p_k of the TR subproblem is a LM step as it is the solution of the linear system

$$(J(x_k^\delta)^T J(x_k^\delta) + \lambda_k I)p = -J(x_k^\delta)^T (F(x_k^\delta) - y^\delta)$$

with $\lambda_k \geq 0$ s.t. $\lambda_k(\|p_k\| - \Delta_k) = 0$.

Standard TR approach: observations

As $\lambda_k(\|p_k\| - \Delta_k) = 0$:

- If the minimum norm solution p^* of

$$J(x_k^\delta)^T J(x_k^\delta) p = -J(x_k^\delta)^T (F(x_k^\delta) - y^\delta)$$

  satisfies $\|p^*\| \leq \Delta_k$ then $\lambda_k = 0$ and $p_k = p(0)$;
- Otherwise $\lambda_k \neq 0$, $\|p_k\| = \Delta_k$ and $p_k = p(\lambda_k)$ is a Levenberg-Marquardt step.

Standard TR approach: observations

As $\lambda_k(\|p_k\| - \Delta_k) = 0$:

- If the minimum norm solution p^* of

$$J(x_k^\delta)^T J(x_k^\delta)p = -J(x_k^\delta)^T (F(x_k^\delta) - y^\delta)$$

  satisfies $\|p^*\| \leq \Delta_k$ then $\lambda_k = 0$ and $p_k = p(0)$;
- Otherwise $\lambda_k \neq 0$, $\|p_k\| = \Delta_k$ and $p_k = p(\lambda_k)$ is a Levenberg-Marquardt step.

The standard trust-region does not ensure regularizing properties, trust-region should be active to have a regularizing method:

$$\|p_k\| = \Delta_k.$$

Goals

We modify the standard trust-region to have:

- monotone decay of the function

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

- the q-condition to hold:

$$\|F(x_k^\delta) - y^\delta + J(x_k^\delta)p(\lambda_k)\| \geq q\|F(x_k^\delta) - y^\delta\|.$$

- the same regularizing properties of Levenberg-Marquardt method.

The q-condition is a relaxed reformulation of

$$\|F(x_k^\delta) - y^\delta + J(x_k^\delta)p(\lambda_k)\| = q\|F(x_k^\delta) - y^\delta\|.$$

Trust-region radius choice

Let $B_k = J(x_k^\delta)^T J(x_k^\delta)$ and $g_k = J(x_k^\delta)^T (F(x_k^\delta) - y^\delta)$.

Lemma

Let p_k the solution of trust-region problem. If

$$\Delta_k \leq \frac{1-q}{\|B_k\|}\|g_k\|$$

then p_k satisfies the q-condition.

Trust-region radius choice

Let $B_k = J(x_k^\delta)^T J(x_k^\delta)$ and $g_k = J(x_k^\delta)^T (F(x_k^\delta) - y^\delta)$.

Lemma

Let p_k the solution of trust-region problem. If

$$\Delta_k \leq \frac{1-q}{\|B_k\|}\|g_k\|$$

then p_k satisfies the q-condition.

- Trust region radius choice:

$$\Delta_k \in \left[C_{\min}\|g_k\|, \min\left\{ C_{\max}, \frac{1-q}{\|B_k\|} \right\} \|g_k\| \right]$$

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

$$\|F(x^\delta_{k^*(\delta)}) - y^\delta\| \leq \tau\delta < \|F(x_k^\delta) - y^\delta\| \quad \text{with} \quad \tau > 1$$

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 $g_k = J(x_k^\delta)^T (F(x_k^\delta) - y^\delta)$.
2. Choose $\Delta_k \in \left[C_{\min}\|g_k\|, \min\left\{ C_{\max}, \frac{1-q}{\|B_k\|} \right\} \|g_k\| \right]$
3. Repeat

   3.1 Compute the solution p_k of trust-region problem.

   3.2 Compute

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

   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 $\pi_k(p_k) < \eta$,set $\Delta_k = \gamma \Delta_k$.

   Until $\pi_k(p_k) \geq \eta$.

4. Set $x_{k+1}^\delta = x_k^\delta + p_k$.

Solution of the TR subproblem

At each iteration we have to deal with the solution of

$$\min_{\|p\| \leq \Delta_k} m_k^{TR}(p) = \|F(x_k^\delta) - y^\delta + J(x_k^\delta)p\|^2.$$

that is equivalent to

$$(J(x_k^\delta)^T J(x_k^\delta) + \lambda_k I)p = -J(x_k^\delta)^T (F(x_k^\delta) - y^\delta)$$

for a parameter λ_k such that:

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

Small scale problems

- As the TR is active, to compute parameters λ_k we have to solve the following non linear equation:

$$\|p(\lambda)\| = \Delta_k.$$

- We used Newton method to solve this reformulation of the condition:

$$\psi(\lambda) = \frac{1}{\|p(\lambda)\|} - \frac{1}{\Delta_k} = 0.$$

  that is more suitable to the application of Newton method.
- Each Newton iteration requires Cholesky factorization of $J(x_k^\delta)^T J(x_k^\delta) + \lambda_k I$.

Large scale problems

- CGLS is applied to the linear system

$$J(x_k^\delta)p = -(F(x_k^\delta) - y^\delta)$$

- If the initial guess is zero, the sequence of computed approximations is increasing in norm.
- As a consequence, it is acceptable to stop iterating as soon as the trust-region boundary is reached, because no further iterates giving a lower value of $\|J(x_k^\delta)p + F(x_k^\delta)\|$ will be inside the trust region.
- Then, once the trust-region is left the process is stopped and the previous iteration (still inside the TR) is taken as an approximation of the subproblem solution.
- In the trust-region the q-condition is satisfied, due to the choice of trust-region radius.

Convergence analysis: noise free case

- $\lim_{k\to\infty} \|g_k\| = 0$ so the trust-region radius tends to zero.

Assumption

There exists $\bar{k}$ s.t. the system $F(x) = y$ is solvable in $B_\rho(x_{\bar{k}})$ and for $x, \tilde{x} \in B_{2\rho}(x_{\bar{k}})$
$\|F(x) - F(\tilde{x}) - J(x)(x - \tilde{x})\| \leq c\|x - \tilde{x}\|\|F(x) - F(\tilde{x})\|.$

Convergence analysis: noise free case

- $\lim_{k\to\infty} \|g_k\| = 0$ so the trust-region radius tends to zero.

Assumption

There exists $\bar{k}$ s.t. the system $F(x) = y$ is solvable in $B_\rho(x_{\bar{k}})$ and for $x, \tilde{x} \in B_{2\rho}(x_{\bar{k}})$
$\|F(x) - F(\tilde{x}) - J(x)(x - \tilde{x})\| \leq c\|x - \tilde{x}\|\|F(x) - F(\tilde{x})\|$.

Lemma

For $k \geq \bar{k}$

- *trust-region is active, i.e. $\lambda_k > 0$;*
- *Error monotonic decrease: $\|x_{k+1} - x^\dagger\| < \|x_k - x^\dagger\|$;*

Theorem

The sequence $\{x_k\}$ converges to a solution x^* of $F(x) = y$ such that $\|x^* - x^\dagger\| \leq \rho$.

Convergence analysis: noisy case

Lemma

Let $\bar{k} < k^*(\delta)$. *For* $\bar{k} \le k < k^*(\delta)$

- *the trust-region is active, i.e.* $\lambda_k > 0$;
- x_k^δ *belongs to* $B_{2\rho}(x_{\bar{k}}^\delta)$ *and to* $B_\rho(x^\dagger)$;
- $\|x_{k+1}^\delta - x^\dagger\| < \|x_k^\delta - x^\dagger\|$;

Theorem

- *The discrepancy principle is satisfied after a finite number of iterations* $k^*(\delta)$,
- *The sequence* $\{x_{k^*(\delta)}^\delta\}$ *converges to a solution of* $F(x) = y$ *if* δ *tends to zero.*

Regularizing method.

Test problems

We consider small scale 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 trust-region implementation

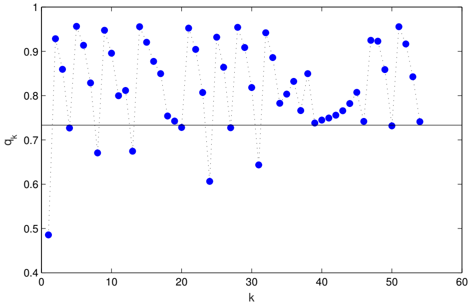
Trust-region radius update:

$$\Delta_k = \mu_k \|F(x_k^\delta) - y^\delta\|, \qquad \mu_k = \begin{cases} \frac{1}{6}\mu_{k-1} & \text{if } q_{k-1} < q \\ 2\mu_{k-1} & \text{if } q_{k-1} > \nu q \\ \mu_{k-1} & \text{otherwise} \end{cases}$$

with $q_k = \frac{\|F(x_k^\delta) - y^\delta + J(x_k^\delta)p_k\|}{\|F(x_k^\delta) - y^\delta\|}$, and $\nu = 1.1$.

- This choice preserves convergence to zero if $\delta = 0$.
- In the update the fulfilment of q-condition is considered.

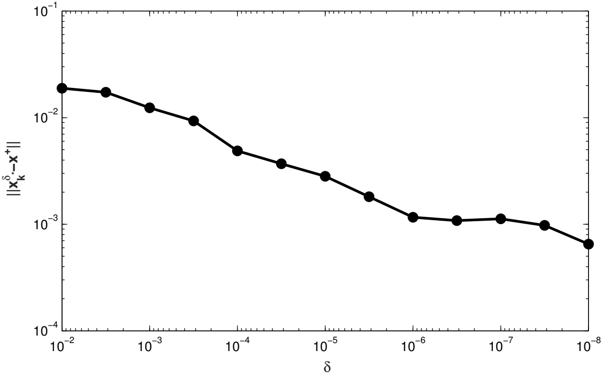
Regularizing properties



- $=$ Values of $q_k = \frac{\|F(x_k^\delta) - y^\delta + J(x_k^\delta)p_k\|}{\|F(x_k^\delta) - y^\delta\|}$, solid line: $q = 1.1/\tau$.

The q-condition is satisfied in most of the iterations even if not explicitly imposed.

Regularizing properties of the method.



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

Comparison between regularizing TR-LM, $\delta = 10^{-2}$.

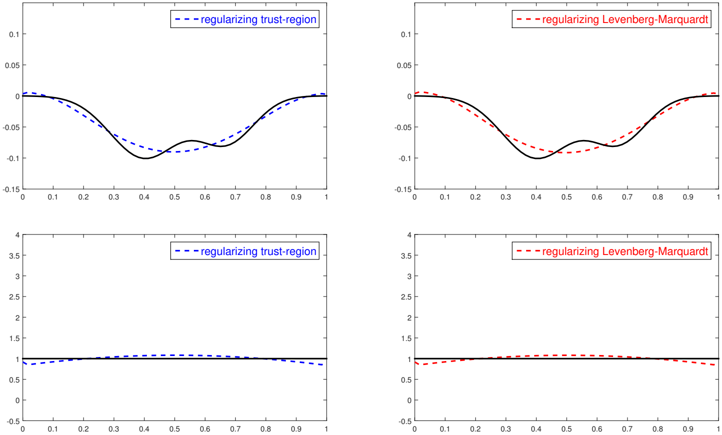
Problem	x_0	Regularizing TR it	nf	cf	Regularizing LM it	nf	cf
P1	$0\,e$	20	21	6	17	18	4
	$-0.5\,e$	29	30	6	22	23	4
	$-1\,e$	35	36	5	24	25	4
	$-2\,e$	40	41	5	25	26	4
P2	$0\,e$	30	31	5	*	*	*
	$0.5\,e$	25	26	5	*	*	*
	$1\,e$	29	30	5	22	23	5
	$2\,e$	37	39	5	25	26	5
P3	$x_0(1.25)$	15	16	4	12	13	4
	$x_0(1.5)$	17	18	4	14	15	4
	$x_0(1.75)$	19	20	4	15	16	4
	$x_0(2)$	22	23	4	16	17	4
P4	$x_0(1,1)$	17	18	5	10	11	4
	$x_0(0.5,0)$	20	21	4	*	*	*
	$x_0(1.5,1)$	22	23	4	15	16	4
	$x_0(1.5,0)$	26	27	4	*	*	*

it=iterations, **nf**=function evaluations, **cf**=mean number of Cholesky factorizations.

$*$=failure, reached maximum number of iterations or convergence to a solution of the noisy problem

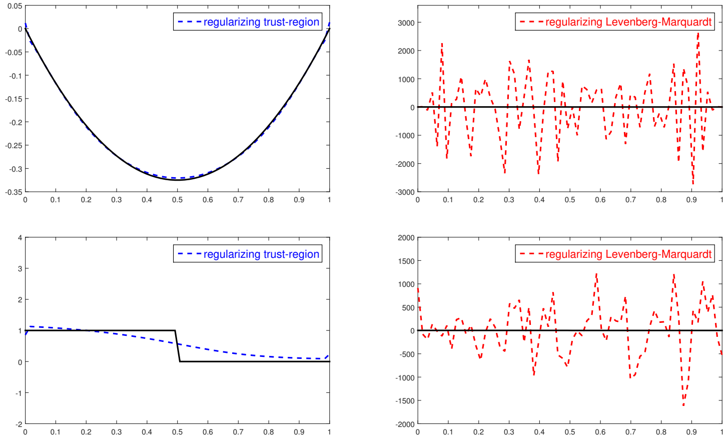
$e = (1, \dots, 1)^T$, **P3:** $(x_0(\alpha))_j = (-4\alpha + 4)s_j^2 + (4\alpha - 4)s_j + 1$, **P4:** $x_0(\beta, \chi) = \beta - \chi s_j$, s_j grid points, $j = 1, \dots, n$.

Comparison between regularizing TR and LM, $\delta = 10^{-2}$



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

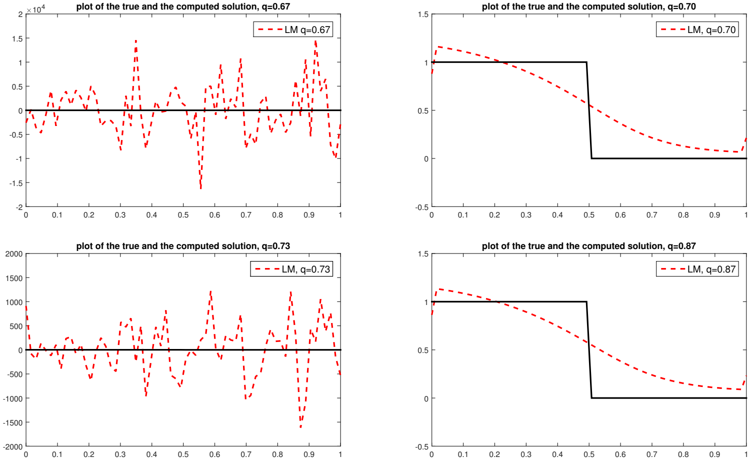
Comparison between regularizing TR e LM, $\delta = 10^{-2}$



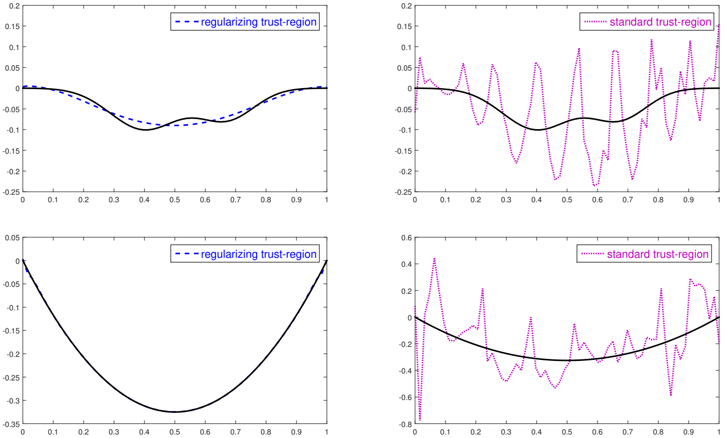
Left: regularizing TR , **Right**: regularizing LM , **Solid line**: solution of the original problem.

The q-condition

The condition imposed by Hanke is strongly dependent on the choice of the value of free parameter q. Values of $q = 0.67,\ 0.70,\ 0.73,\ 0.87,\ \delta = 10^{-2}$.



Comparison between regularizing and standard trust-region



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

Open issues and future developments

- We are currently working on designing new methods for non zero residual ill-posed problems,
  - elliptical trust-region approach to solve small scale small residual problems,
  - Levenberg-Marquardt approach for large scale problems.
- In many applications bounds on the variables must be enforced: methods able to handle bounds and ill-posedness are needed.
- Results for zero residual problems in:
  Bellavia, Morini, R., On an adaptive regularization for ill-posed nonlinear systems and its trust-region implementation, COAP, 2016

Open issues and future developments

- We are currently working on designing new methods for non zero residual ill-posed problems,
  - elliptical trust-region approach to solve small scale small residual problems,
  - Levenberg-Marquardt approach for large scale problems.
- In many applications bounds on the variables must be enforced: methods able to handle bounds and ill-posedness are needed.
- Results for zero residual problems in:
  Bellavia, Morini, R., On an adaptive regularization for ill-posed nonlinear systems and its trust-region implementation, COAP, 2016

THANK YOU FOR YOUR ATTENTION!

Open issues: Convergence to the infinite dimensional solution.

Let $\mathcal{X}, \mathcal{Y}$ be Hilbert spaces, $F_\infty : \mathcal{X} \to \mathcal{Y}$, $y_\infty \in \mathcal{Y}$. The nonlinear system is the discretization of a infinite dimensional problem: find $x_\infty \in \mathcal{X}$ such that $F_\infty(x_\infty) = y_\infty$. We are interested in the convergence of the discrete solution $\hat{x}_n(s) = \sum_{j=1}^{n} \Phi_j(s) x_j$ to a solution of the infinite dimensional problem as $n \to \infty$.

Theorem

The sequence $\{\hat{x}_n\}$ has a weakly convergent subsequence $\{\hat{x}_k\}$.

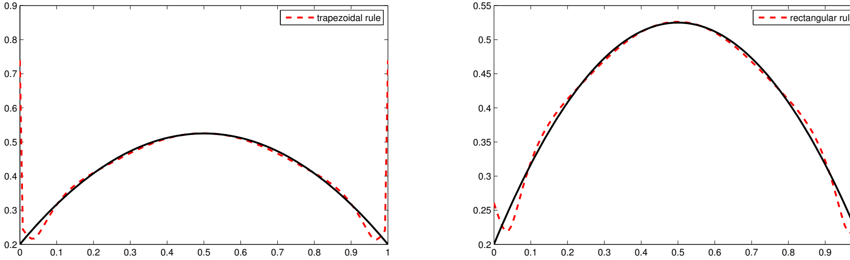
Theorem

The sequence $\{\|F_\infty(\hat{x}_k) - y_\infty\|\}$ converges to zero as k tends to infinite, i.e. the weak limit x^* of sequence $\{\hat{x}_k\}$ is a solution of the original problem, $F_\infty(x^*) = y_\infty$.

Open issues: peaks

- Problem: when solving the nonlinear system obtained computing the integral by the trapezoidal rule, the approximated solution shows peaks at the end points of the interval. Peaks are higher and higher as the starting guess moves away from the solution and the noise increases.
- When solving the nonlinear system obtained computing the integral by the rectangular rule, the approximated solution does not show peaks at the end points of the interval.

Computed solution



Computed solution, $x_0 = 1e$, $\delta = 1.e-2$. **Left**: trapezoidal rule, **Right**: rectangular rule, **Solid line**: solution of the original problem.

Comparison of the nonlinear systems

- Trapezoidal rule: the resulting nonlinear system is

$$\frac{1}{2}k(t_i, s_1, x_1)+1k(t_i, s_2, x_2)+\cdots+1k(t_i, s_{n-1}, x_{n-1})+\frac{1}{2}k(t_i, s_n, x_n) = y(t_i),$$

$$i = 1, \ldots, n.$$

- Rectangular rule: the resulting nonlinear system is

$$1k(t_i, s_1, x_1)+1k(t_i, s_2, x_2)+\cdots+1k(t_i, s_{n-1}, x_{n-1})+1k(t_i, s_n, x_n) = y(t_i),$$

$$i = 1, \ldots, n.$$

Linear system: trapezoidal rule

We solve $(J^T J + \lambda I)p(\lambda) = -J^T(F - y^\delta)$. Let $n = 5$.

$$J = \begin{pmatrix} \frac{1}{2}\partial_1 k(t_1, s_1, x_1) & 1\partial_2 k(t_1, s_2, x_2) & . & 1\partial_4 k(t_1, s_4, x_4) & \frac{1}{2}\partial_5 k(t_1, s_5, x_5) \\ . & . & . & . & . \\ . & . & . & . & \\ . & . & . & . & . \\ \frac{1}{2}\partial_1 k(t_5, s_1, x_1) & 1\partial_2 k(t_5, s_2, x_2) & . & 1\partial_4 k(t_5, s_4, x_4) & \frac{1}{2}\partial_5 k(t_5, s_5, x_5) \end{pmatrix}$$

We denote $k_{i,j} = k(t_i, s_j, x_j)$ $i, j = 1, \dots, n$.

$$J^T J =$$

$$\begin{pmatrix} \frac{1}{4}\sum_{i=1}^5 \partial_1 k_{i,1}\partial_1 k_{i,1} & \frac{1}{2}\sum_{i=1}^5 \partial_1 k_{i,1}\partial_2 k_{i,2} & . & \frac{1}{2}\sum_{i=1}^5 \partial_1 k_{i,1}\partial_4 k_{i,4} & \frac{1}{4}\sum_{i=1}^5 \partial_1 k_{i,1}\partial_5 k_{i,5} \\ \frac{1}{2}\sum_{i=1}^5 \partial_2 k_{i,2}\partial_1 k_{i,1} & 1\sum_{i=1}^5 \partial_2 k_{i,2}\partial_2 k_{i,2} & . & 1\sum_{i=1}^5 \partial_2 k_{i,2}\partial_4 k_{i,4} & \frac{1}{2}\sum_{i=1}^5 \partial_2 k_{i,2}\partial_5 k_{i,5} \\ . & . & . & . & . \\ \frac{1}{2}\sum_{i=1}^5 \partial_4 k_{i,5}\partial_1 k_{i,1} & 1\sum_{i=1}^5 \partial_4 k_{i,5}\partial_2 k_{1,2} & . & 1\sum_{i=1}^5 \partial_4 k_{i,5}\partial_4 k_{i,4} & \frac{1}{2}\sum_{i=1}^5 \partial_4 k_{i,5}\partial_5 k_{i,5} \\ \frac{1}{4}\sum_{i=1}^5 \partial_4 k_{i,5}\partial_1 k_{i,1} & \frac{1}{2}\sum_{i=1}^5 \partial_5 k_{i,5}\partial_2 k_{1,2} & . & \frac{1}{2}\sum_{i=1}^5 \partial_5 k_{i,5}\partial_4 k_{i,4} & \frac{1}{4}\sum_{i=1}^5 \partial_5 k_{i,5}\partial_5 k_{i,5} \end{pmatrix}$$

Linear system: rectangular rule

We solve $(J^T J + \lambda I)p(\lambda) = -J^T(F - y^\delta)$. Let $n = 5$.

$$J = \begin{pmatrix} 1\partial_1 k(t_1, s_1, x_1) & 1\partial_2 k(t_1, s_2, x_2) & . & 1\partial_4 k(t_1, s_4, x_4) & 1\partial_5 k(t_1, s_5, x_5) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1\partial_1 k(t_5, s_1, x_1) & 1\partial_2 k(t_5, s_2, x_2) & . & 1\partial_4 k(t_5, s_4, x_4) & 1\partial_5 k(t_5, s_5, x_5) \end{pmatrix}$$

We denote $k_{i,j} = k(t_i, s_j, x_j)$ $i, j = 1, \dots, n$.

$$J^T J =$$

$$\begin{pmatrix} 1\sum_{i=1}^5 \partial_1 k_{i,1}\partial_1 k_{i,1} & 1\sum_{i=1}^5 \partial_1 k_{i,1}\partial_2 k_{i,2} & . & 1\sum_{i=1}^5 \partial_1 k_{i,1}\partial_4 k_{i,4} & 1\sum_{i=1}^5 \partial_1 k_{i,1}\partial_5 k_{i,5} \\ 1\sum_{i=1}^5 \partial_2 k_{i,2}\partial_1 k_{i,1} & 1\sum_{i=1}^5 \partial_2 k_{i,2}\partial_2 k_{i,2} & . & 1\sum_{i=1}^5 \partial_2 k_{i,2}\partial_4 k_{i,4} & 1\sum_{i=1}^5 \partial_2 k_{i,2}\partial_5 k_{i,5} \\ . & . & . & . & . \\ 1\sum_{i=1}^5 \partial_4 k_{i,5}\partial_1 k_{i,1} & 1\sum_{i=1}^5 \partial_4 k_{i,5}\partial_2 k_{1,2} & . & 1\sum_{i=1}^5 \partial_4 k_{i,5}\partial_4 k_{i,4} & 1\sum_{i=1}^5 \partial_4 k_{i,5}\partial_5 k_{i,5} \\ 1\sum_{i=1}^5 \partial_4 k_{i,5}\partial_1 k_{i,1} & 1\sum_{i=1}^5 \partial_5 k_{i,5}\partial_2 k_{1,2} & . & 1\sum_{i=1}^5 \partial_5 k_{i,5}\partial_4 k_{i,4} & 1\sum_{i=1}^5 \partial_5 k_{i,5}\partial_5 k_{i,5} \end{pmatrix}$$

SVD decomposition: trapezoidal rule

Let consider matrix $J^T J$ SVD decomposition.

- $J^T J = U \Sigma U^T$
- $cond(J^T J) = 10^6$, $\lambda = 15.7$, $cond(J^T J + \lambda I) = 1.2\ 10^0$
- $\sigma = diag(\Sigma) = \begin{pmatrix} 3.8\ 10^0 \\ 8.5\ 10^{-2} \\ 2.3\ 10^{-3} \\ 7.1\ 10^{-5} \\ 1.6\ 10^{-6} \end{pmatrix}, \qquad p = \begin{pmatrix} -7.6\ 10^{-2} \\ -1.7\ 10^{-1} \\ -1.8\ 10^{-1} \\ -1.7\ 10^{-1} \\ -7.6\ 10^{-2} \end{pmatrix}$
- $U = \begin{pmatrix} -0.24 & -0.44 & 0.58 & 0.56 & 0.32 \\ -0.54 & -0.56 & 0.04 & -0.44 & -0.46 \\ -0.56 & 3.5\ 10^{-8} & -0.56 & -7.3\ 10^{-8} & 0.61 \\ -0.54 & 0.56 & 0.04 & 0.44 & -0.46 \\ -0.24 & 0.44 & 0.58 & -0.56 & 0.32 \end{pmatrix}$

SVD decomposition: rectangular rule

Let consider matrix J^TJ SVD decomposition.

- $J^TJ = U\Sigma U^T$
- $cond(J^TJ) = 10^6$, $\lambda = 17.4$, $cond(J^TJ + \lambda I) = 1.3\ 10^0$
- $\sigma = diag(\Sigma) = \begin{pmatrix} 5.1\ 10^0 \\ 1.8\ 10^{-1} \\ 5.8\ 10^{-3} \\ 1.3\ 10^{-4} \\ 1.8\ 10^{-6} \end{pmatrix}, \qquad p = \begin{pmatrix} -1.8\ 10^{-1} \\ -2.0\ 10^{-1} \\ -2.1\ 10^{-1} \\ -2.0\ 10^{-1} \\ -1.8\ 10^{-1} \end{pmatrix}$
- $U = \begin{pmatrix} -0.41 & -0.60 & 0.55 & -0.38 & -0.17 \\ -0.46 & -0.38 & -0.19 & 0.60 & 0.5 \\ -0.48 & -4.1\ 10^{-8} & -0.57 & -1.4\ 10^{-6} & -0.66 \\ -0.46 & 0.38 & -0.19 & -0.60 & 0.50 \\ -0.41 & 0.60 & 0.55 & 0.38 & -0.17 \end{pmatrix}$