On an Adaptive Regularization for Ill-posed Nonlinear Systems and its Trust-Region Implementation

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Ill-posed problems

Let us consider the following inverse problem: given $F : \mathbb{R}^n \rightarrow \mathbb{R}^m$ with $m \geq n$, nonlinear, continuously differentiable and $y \in \mathbb{R}^m$, find $x \in \mathbb{R}^n$ such that

$$F(x) = y.$$

Definition

The problem is well-posed if:

1. $\forall y \in \mathbb{R}^m \; \exists x \in \mathbb{R}^n$ such that $F(x) = y$ (existence),
2. F is an injective function (uniqueness),
3. F^{-1} is a continuous function (stability).

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 $F(x) = y$ for $x \in (\mathbb{R}^n, \|\cdot\|_2)$ and $y \in (\mathbb{R}^m, \|\cdot\|_2)$, arising from the discretization of a system modeling an ill-posed problem, such that:
  - it exists a solution $x^\dagger$, but is not unique,
  - stability does not hold.
- 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:

$$F(x) = y^\delta.$$

Need for regularization

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  $\Longrightarrow$ The solutions of the noisy problem may not be meaningful approximations of the original problem solutions.

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- 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

- 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 $F(x) = y$.

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:

- $x_{k^*(\delta)}^\delta$ 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.

Existing methods

- 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]

These methods are analyzed only under local assumptions, the definition of globally convergent approaches is still an open task.

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 is the solution of

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

with $B_k = J(x_k^\delta)^T J(x_k^\delta)$, $g_k = J(x_k^\delta)^T(F(x_k^\delta) - y^\delta)$;

- The step is then used to compute the new iterate

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

Regularizing Levenberg-Marquardt method

- The parameter $\lambda_k > 0$ is chosen as the solution of:

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

  with $q \in (0,1)$;
- With noisy data the process is stopped at iteration $k^*(\delta)$ such that $x^\delta_{k^*(\delta)}$ satisfies the discrepancy principle:

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

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

[Hanke, 1997,2010]

Local analysis

Hypothesis for the local analysis:
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 $x, \tilde{x} \in B_{2\rho}(x_0)$

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

[Hanke, 1997,2010]

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.

Regularizing properties of the Levenberg-Marquardt method

Choosing λ_k as the solution of

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

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:

- With exact data ($\delta = 0$): local convergence to $x^\dagger$,
- With noisy data ($\delta > 0$): if $\tau > \frac{1}{q}$, 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.

This is a regularizing method

Trust-region methods

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

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

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

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

- Given $\eta \in (0, 1)$:
  - If $\pi_k < \eta$ then set $\Delta_{k+1} < \Delta_k$ and $x_{k+1} = x_k$.
  - If $\pi_k \geq \eta$ then set $\Delta_{k+1} \geq \Delta_k$ 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 $B_k = J(x_k^\delta)^T J(x_k^\delta)$ and $g_k = J(x_k^\delta)^T(F(x_k^\delta) - y^\delta)$.

Trust-region methods

From $\lambda_k(\|p_k\| - \Delta_k) = 0$ it follows that:

- If the minimum norm solution p^* of $B_k p = -g_k$ 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.

$$\Downarrow$$

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

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

Regularizing trust-region

- Levenberg-Marquardt and trust-region methods are strictly connected, due to the form of the step.
- As Hanke did, can we introduce a trust-region method with regularizing properties and still globally convergent?

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:

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

The q-condition is a relaxed reformulation of

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

Regularizing trust-region

We now describe the new trust-region approach that thanks to a suitable trust-region radius update ensures:

- the q-condition to hold,
- the same regularizing properties of Levenberg-Marquardt method.

Trust-region radius choice

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.

Consequence: Δ_k's choice

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

with $C_{\min}, C_{\max}$ suitable constant, $B_k = J(x_k^\delta)^T J(x_k^\delta)$ e $g_k = J(x_k^\delta)^T(F(x_k^\delta) - y^\delta)$.

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

Local analysis

Hypothesis 1: the same as for Levenberg-Marquardt method.
We assume that 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 $x, \tilde{x} \in B_{2\rho}(x^\delta_{\bar{k}})$

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

Hypothesis 2: It exists positive K_J such that

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

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

Results for $\delta = 0$

Lemma

The method generates a sequence $\{x_k\}$ *such that for* $k \geq \bar{k}$

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

Theorem

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

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

Results for $\delta > 0$

Lemma

Let $\bar{k} < k^*(\delta)$. The method generates a sequence $\{x_k^\delta\}$ such that for $\bar{k} \leq k < k^*(\delta)$

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

Theorem

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.

This is a regularizing method.

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

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

Test problems: discretization

- We chose $n = m$, interval $[0, 1]$ was discretized using n=64 equidistant grid points $t_i = (i - 1)h,\ h = 1/(n - 1),\ i = 1, \dots, n$;
- $x(s)$ was approximated by piecewise linear functions $\Phi_j(s)$ on the grid $s_j = t_j,\ j = 1, \dots, n$; $x(s) \sim \hat{x}_n(s) = \sum_{j=1}^{n} \Phi_j(s) x_j$

Test problems: discretization

- The integrals $\int_0^1 k(t_i, s, \hat{x}(s))ds$, $i = 1, \dots, n$ were approximated by the composite trapezoidal rule on the points s_j $j = 1, \dots, n$.
- The resulting nonlinear system is

$$\sum_{i=1}^{n} w_j k(t_i, s_j, \hat{x}(s_j)) = y(t_i) \qquad j = 1, \dots, n.$$

with $w_1 = w_n = \frac{1}{2}$, $w_i = 1$ for all $i \neq 1, n$.

Choice of parameters λ_k

- Parameters λ_k were computed to have an active trust-region:

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

- 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 $B_k + \lambda_k I$.

Regularizing trust-region implementation

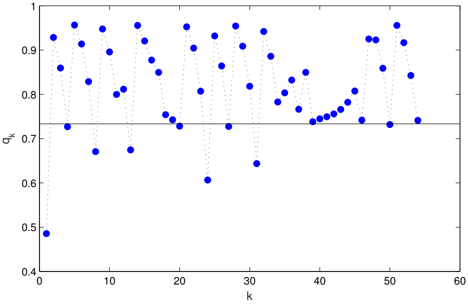
Trust-region radius update:

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

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

- Δ_k is less expensive to compute if compared to $\frac{1-q}{\|B_k\|}\|g_k\|$ but preserves convergence to zero if $\delta = 0$.
- In the update the fulfillment of q-condition is considered.

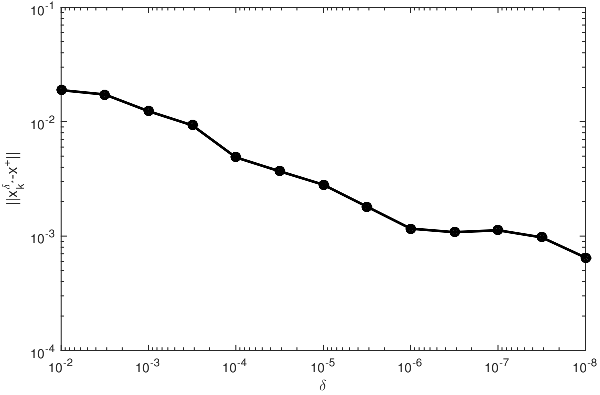
Regularizing properties



- $=$ 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 esplicitly 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	*	*	*

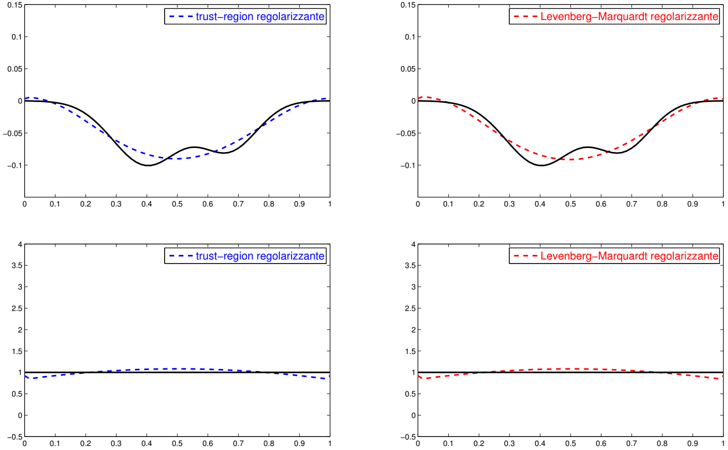
it=iterations, **nf**=function evaluations,

cf=mean number of Cholesky factorizations.

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

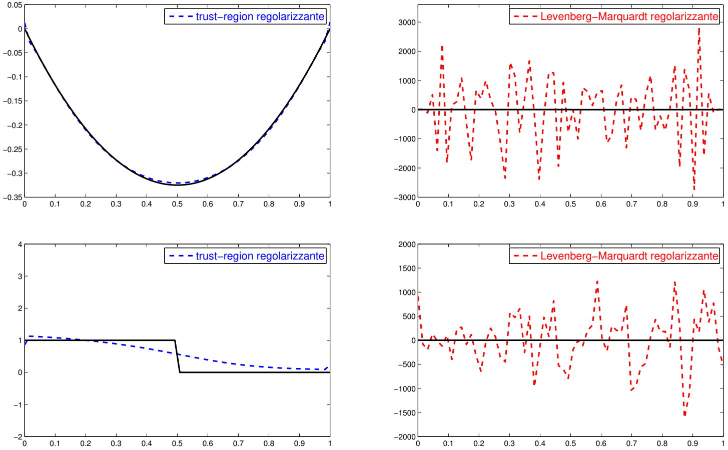
$e = (1,\dots,1)^T$, **P3:** $(x_0(\alpha))_j = (-4\alpha+4)s_j^2 + (4\alpha-4)s_j + 1$, **P4:** $x_0(\beta,\chi) = \beta - \chi s_j$, s_j grid points, $j = 1,\dots,n$.

Comparison between regularizing TR and LM



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

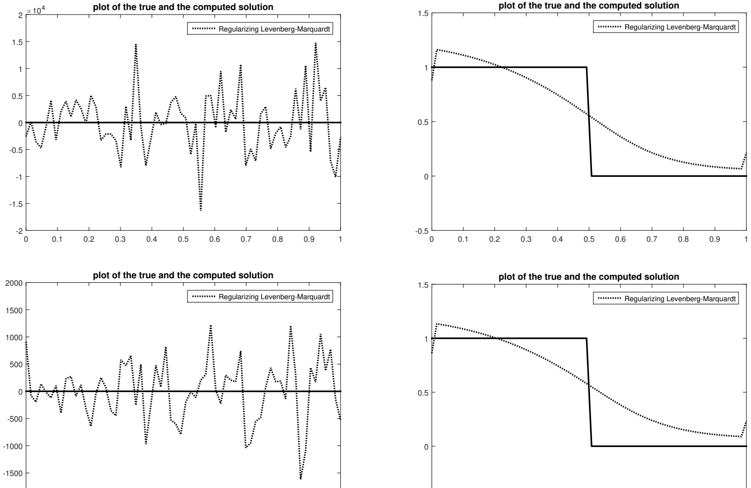
Comparison between regularizing TR e LM



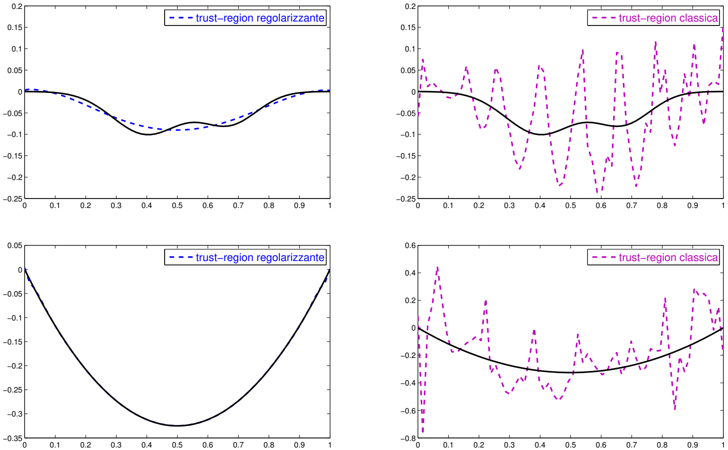
Left: regularizing TR , **Right**: regularizing LM , **Solid line**: solution of the original problem.

The q-condition

The condition imposed by Hanke is strongly dependent on the choice of the value of free parameter q. Values of $q = 0.67, 0.70, 0.73, 0.87$.



Comparison between regularizing and standard trust-region



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

Future developments

- We are now working on designing a new trust-region approach to solve nonlinear ill-posed least squares problems.

THANK YOU FOR YOUR ATTENTION!