Iterative regularization for nonsmooth inverse problems

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**Motivation**

**Inverse problem:** find

- unknown parameter $u^\dagger$
  
  e.g., heat source, diffusion constant, thermal conductivity, heat capacity, latent heat density, ...

**given**

- measurement $y$
- model $S : u \mapsto y$, e.g., solution of PDE

$\mapsto$ solve

$$S(u) = y$$

**Problem:** measurement $y = y^\delta$ **noisy**, range of $S$ not **closed**

$\mapsto$ ill-posed, needs **regularization**
Regularization

Solve approximate, **stable** problem:

1. Tikhonov regularization $\leadsto$ optimal control
2. Iterative regularization, e.g., Landweber iteration

\[ u_{n+1} = u_n + w_n S'(u_n)^* (y^\delta - S(u_n)) \quad n = 1, \ldots, N \]

- $S'(u)$ Fréchet derivative, $S'(u)^*$ adjoint
- Stopping index $N = N(\delta) < \infty$ regularization parameter
- Regularization: $N(\delta) \to \infty$, $u_{N(\delta)} \to u^\dagger$ for $\delta \to 0$

Here: $S$ solution operator for **non-smooth PDE**

$\leadsto$ **not** Fréchet differentiable
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3 Bouligand–Landweber iteration

4 Bouligand–Levenberg–Marquardt iteration

5 Numerical examples
Non-smooth equation

\[-\Delta y + \max\{0, y\} = u\]

solution operator \( S : u \mapsto y \ (:= S(u)) \)

- well-posed (in suitable – standard – spaces)
- Lipschitz continuous
- completely continuous (\( \mapsto \) ill-posed)
- not Fréchet differentiable unless \(|\{x : y(x) = 0\}| = 0\)
- model for membrane under water, plasma MHD equilibrium
- can be extended to arbitrary \( f(y) \) piecewise differentiable
- simplified model for sharp phase transition (Stefan problem)
Non-smooth equation

\[-\Delta y + \max\{0, y\} = u\]

solution operator \( S : u \mapsto y \ (:= S(u)) \)

- not Fréchet differentiable unless \( |\{x : y(x) = 0\}| = 0 \)
- but: directionally differentiable

Directional derivative \( S'(u; h) =: \eta \) solves

\[-\Delta \eta + 1_{\{y=0\}} \max(0, \eta) + 1_{\{y>0\}} \eta = h\]

not linear in \( h \) \( \Rightarrow \) not useful for algorithm
Non-smooth equation

Bouligand subdifferential

\[ \partial_B S(u) := \begin{cases} G \text{ linear} \\ \text{there is } \{u_n\} \text{ Gâteaux differentiable with } \\ u_n \to u \text{ and } S'(u_n; h) \to G h \text{ for all } h \end{cases} \]

\[ -\Delta \eta + 1_{\{y > 0\}} \eta = h \]

\[ G_u : h \mapsto \eta \]

- \( G_u \in \partial_B S(u) \) Bouligand derivative [Christof/Meyer/Walter/C.]
- \( u \mapsto G_u \) uniformly bounded (in right spaces)
- linear \( \rightsquigarrow \) use for Landweber in place of \( S'(u) \)
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Bouligand–Landweber iteration

\[ u_{n+1}^\delta = u_n^\delta + w_n G_{u_n^\delta}^* (y^\delta - S(u_n^\delta)), \quad n = 0, 1, 2, \ldots, N(\delta) \]

- \( S : u \mapsto y \) non-smooth
- \( y^\delta \) with \( \|y^\delta - y^\dagger\| \leq \delta, \quad y^\dagger = S(u^\dagger) \) (assume unique)
- \( u_0^\delta = u_0 \) starting point
- \( w_n \) step sizes
- stopping index \( N(\delta) \) by discrepancy principle:

\[ \|y^\delta - S(u_{N(\delta)}^\delta)\|_Y \leq \tau \delta < \|y^\delta - S(u_n^\delta)\|_Y, \quad 0 \leq n < N(\delta) \]

(modified Landweber iteration [Scherzer ’95])
Well-posedness

Assume:

1. \(\{G_u\}\) uniformly bounded
2. generalized tangential cone condition (GTCC)

\[
\|S(u') - S(u) - G_u(u' - u)\| \leq \mu \|S(u') - S(u)\| \quad \text{for all } u, u' \in B_\rho(u^\dagger)
\]

non-smooth PDE: satisfied for \(1 > \mu > C(\{|x : y^\dagger(x) = 0|\})\)

3. \(u_0 \in B_\rho(u^\dagger)\)

Then (under conditions on \(\mu, \tau, \omega_n\)):

- \(u_\delta^n \in B_\rho(u^\dagger)\) for all \(n \leq N(\delta)\)
- \(\delta > 0: N(\delta) < \infty\) and \(\|u_\delta^n - u^\dagger\| < \|u_{n-1}^\delta - u^\dagger\|\) for \(n \leq N(\delta)\)
- \(\delta = 0: N(\delta) = \infty\) and \(u_0^n \rightarrow u^\dagger\) for \(n \rightarrow \infty\)
Regularization

Goal: show that \( u_{N(\delta)}^\delta \rightarrow u^\dagger \) for \( \delta \rightarrow 0 \)

Standard proof: combine

1. monotonicity: \( \| u_n^\delta - u^\dagger \| < \| u_{n-1}^\delta - u^\dagger \| \) for \( n \leq N(\delta) \)

2. stability: \( u_n^\delta \rightarrow u_n^0 \) for all \( n = 1, \ldots \)

Problem:

- stability requires continuity of \( u \mapsto G_u \)
- \( u \mapsto G_u \) not continuous for \( S \) non-smooth
- \( \leadsto \) use asymptotic stability
Asymptotic stability

Definition

Iterative method generating \( \{u_\delta^n\}_{n \leq N(\delta)} \) asymptotically stable for \( \delta \to 0 \) if exists subsequence \( \{\delta_k\} \) with:

- For all \( 0 \leq n \leq \bar{N} := \lim_{k \to \infty} N(\delta_k) \in \mathbb{N} \cup \{\infty\} \)
  \[
  u_{\delta_k}^n \to \tilde{u}_n \quad \text{as } k \to \infty
  \]
  for some \( \tilde{u}_n \in \bar{B}_U(u^\dagger, \rho) \)

- If \( \bar{N} = \infty \),
  \[
  \tilde{u}_n \to u^\dagger \quad \text{as } n \to \infty
  \]

- \( \tilde{u}_n \) generated by perturbed noise-free iteration

- perturbation needs to vanish for \( n \to \infty \)
Asymptotic stability

Bouligand–Landweber iteration

\[ u_{n+1}^\delta = u_n^\delta + w_n G_{u_n^\delta}^* \left( y^\delta - S(u_n^\delta) \right), \quad n = 0, 1, 2, \ldots, N(\delta) \]

- asymptotically stable for non-smooth PDE
  (proof uses GTCC and compact embedding for \( R(G_u^*) \))
- \( \rightsquigarrow \) regularization (under conditions on \( \mu, \tau, w_n \)):

\[ u_{N(\delta)}^\delta \to u^\dagger \quad \text{for} \quad \delta \to 0 \]
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Levenberg–Marquardt iteration

\[ u^\delta_{n+1} = \text{argmin}_{u \in D(S)} \| S'(u^\delta_n)(u - u^\delta_n) - y^\delta - S(u^\delta_n) \|^2 + \alpha_n \| u - u^\delta_n \|^2 \]

\[ = u^\delta_n + \left( \alpha_n I + S'(u^\delta_n)^* S'(u^\delta_n) \right)^{-1} S'(u^\delta_n)^* \left( y^\delta - S(u^\delta_n) \right) \]

- \( \alpha_n = \alpha_0 r^n, \ r < 1 \) \footnote{Kaltenbacher et al. '08}
- stopping by discrepancy principle \footnote{Q. Jin '10}
- TCC + transfer operator property

\[ S'(u_2) = Q(u_1, u_2)S'(u_1) \quad \text{Q linear, near identity} \]

- \( \leadsto \) stable, convergent regularization
- \( N(\delta) = O(1 + | \log \delta |) \)
Bouligand–Levenberg–Marquardt iteration

\[ u_{n+1}^\delta = \arg\min_{u \in D(S)} \| G_{u_n^\delta} (u - u_n^\delta) - y^\delta - S(u_n^\delta) \|^2 + \alpha_n \| u - u_n^\delta \|^2 \]

\[ = u_n^\delta + \left( \alpha_n I + G_{u_n^\delta}^* G_{u_n^\delta} \right)^{-1} G_{u_n^\delta}^* \left( y^\delta - S(u_n^\delta) \right) \]

- \( \alpha_n = \alpha_0 r^n, r < 1 \)
- stopping by discrepancy principle
- GTCC + transfer operator property (holds for non-smooth PDE)

\[ G_{u_2} = Q(u_1, u_2)G_{u_1} \quad Q \text{ linear, near identity} \]

- \( \leadsto \) asymptotically stable, convergent regularization
- \( N(\delta) = O(1 + |\log \delta|) \)
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Numerical example

\[-\Delta y + \max\{0, y\} = u\]

- finite element discretization
- semismooth Newton method for solution (evaluation of $S$)
- constructed exact solution $u^\dagger$ with $|\{x : y^\dagger(x) = 0\}| > 0$
- random Gaussian noise: $\|y^\delta - y^\dagger\| = \delta$
- $\mu = 0.1, \quad \tau = 1.4, \quad \rho = 5, \quad w_n = \frac{2-2\mu}{L^2}, \quad \bar{L} = 5 \times 10^{-2}$
- compare two starting points:
  1. $u_0 \equiv 0$
  2. $\bar{u}_0$ satisfying $u^\dagger - u_0 \in \mathcal{R}(G_u^*)$ (generalized source condition)
Numerical example: results with $u_0$

(a) Bouligand–Landweber

(b) Bouligand–Levenberg–Marquardt

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Numerical example: results with $\bar{u}_0$

(a) Bouligand–Landweber

(b) Bouligand–Levenberg–Marquardt

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Alternatives

Alternative approaches:

1. Nesterov acceleration of Bouligand–Landweber

2. Bouligand–Newton method

→ Newton step ill-posed:

1. iterative regularization of Newton step

2. Tikhonov regularization of Newton step
Nesterov–Bouligand–Landweber

\[
\begin{align*}
    u_{n+1}^\delta &= \hat{u}_n^\delta + w_n G^*_\hat{u}_n^\delta \left( y^\delta - S(\hat{u}_n^\delta) \right) \\
    \hat{u}_{n+1}^\delta &= u_{n+1}^\delta + \frac{n - 1}{n + 2} (u_{n+1}^\delta - u_n^\delta)
\end{align*}
\]

- Nesterov acceleration of gradient descent
  [Neubauer ’17, Hubmer/Ramlau ’18]

- stopping by discrepancy principle

- smooth case: \( N(\delta) = \Theta(\delta^{-1}) \)

- but asymptotic stability unclear
Nesterov–Bouligand–Landweber

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Nesterov–Bouligand–Newton

\[ s_{k+1} = \hat{s}_k + G_{u_n}^* \left( y^\delta - S(u_n) - G_{u_n} \hat{s}_k \right) \]

\[ \hat{s}_{k+1} = s_{k+1} + \frac{k - 1}{k + 2} (s_{k+1} - s_k) \]

\[ \ldots \]

\[ u_{n+1}^\delta = u_n^\delta + s_k \]

- **Bouligand–Newton** iteration \( G_{u_n}^* s = y^\delta - S(u_n^\delta) \)
- regularized solution by **Nesterov-accelerated gradient** method
- outer iteration: stopped by discrepancy principle
- inner iteration: stopped by linearized discrepancy principle (inner residual < \( \mu \) outer residual)
- count total number of Nesterov steps
Nesterov–Bouligand–Newton

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CG–Bouligand–Newton

\[
\begin{align*}
    s_{k+1} &= \alpha_k \hat{s}_k \\
    \hat{s}_{k+1} &= \beta_k \hat{s}_k + y^\delta - S(u_n^\delta) - G_{u_n^\delta} s_{k+1} \\
    &\quad \ldots \\
    u_{n+1}^\delta &= u_n^\delta + s_K
\end{align*}
\]

- **Bouligand–Newton** iteration \( G_{u_n^\delta} s = y^\delta - S(u_n^\delta) \)
- regularized solution by **conjugate gradient** method
  (optimal two-point method for s.p.d. linear systems)
- outer iteration: stopped by discrepancy principle
- inner iteration: stopped by linearized discrepancy principle
  (inner residual < \( \mu \) outer residual)
- count total number of CG steps

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Tikhonov–Bouligand–Newton

\[ s_K \approx \arg\min_s \frac{1}{2} \| G_{u_n^\delta} s + S(u_n^\delta) - y^\delta \|^2 + \frac{a_n}{2} \| s + u_n^\delta \|^2 \]

\[ u_{n+1}^\delta = u_n^\delta + s_K \]

- **Bouligand–Newton** iteration \( G_{u_n^\delta} s = y^\delta - S(u_n^\delta) \)
- regularized solution by **Tikhonov regularization**
  \( \leadsto \) **Iteratively Regularized Bouligand–Gauß–Newton Method**
  [Kaltenbacher et al. ’97, ’98]

- outer iteration: stopped by discrepancy principle
- inner iteration: **CG**, stopped by linearized discrepancy principle
- choice \( a_n(\mu, \tau, \rho) \) (residual norm)
- count total number of **CG** steps

**Motivation Non-smooth equation Landweber Levenberg–Marquardt Examples**
Tikhonov–Bouligand–Newton

Motivation Non-smooth equation Landweber Levenberg–Marquardt Examples

(a) $u_0 = 0$

(b) $u_0 = \bar{u}_0$
Conclusion

Summary

- iterative regularization using Bouligand derivatives
- inverse source problems for non-smooth PDEs
- convergence under asymptotic stability

Outlook

- convergence rates under source condition
- Tikhonov–Bouligand–Newton method
- other non-smooth equations, variational inequalities
- coefficient inverse problems

Preprints, Python/Julia codes:
http://www.uni-due.de/mathematik/agclason/clason_pubs.php