Iteratively regularized Newton methods with general data misfit functionals and applications to Poisson data

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Outline

1. Introduction
2. An iteratively regularized Newton method
3. Important special case: Poisson data
4. Application to a phase retrieval problem
5. Conclusion

Outline

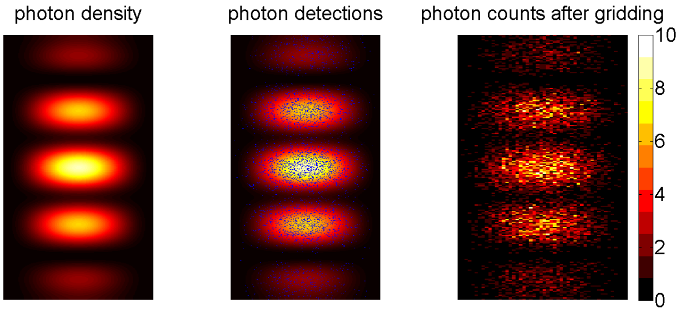
Photonic imaging

- Photonic imaging consists in counting photons which have interacted with some unknown object of interest.
- We want to reconstruct information on the unknown object $\varphi^{\dagger}$ contained in these photon counts.
- Formulation as an operator equation

$$F(\varphi) = g$$

  where g describes the photon density on the manifold where measurements are taken.
- For fundamental physical reasons, photon count data g^{obs} are Poisson distributed with mean $g^{\dagger}$ (true photon density).

Examples



- Positron Emission Tomography (PET)
- astronomical imaging
- scanning fluorescence microscopy, e.g. standard confocal, 4Pi or STED microscopy
- coherent x-ray imaging

Ill-Posedness

The forementioned problems are ill-posed in the sense that φ does not depend continuously on $F(\varphi)$. Hence, the problem cannot be solved directly or by a usual Newton method but regularization is needed.

For nonlinear F one of the most popular methods is the iteratively regularized Gauss-Newton method (IRGNM)

$$\varphi_{j+1} = \underset{\varphi \in \mathfrak{B}}{\operatorname{argmin}} \left(\left\| F'(\varphi_j; \varphi - \varphi_j) + F(\varphi_j) - g^{\mathrm{obs}} \right\|_{\mathbf{L}^2}^2 + \alpha_j \left\| \varphi - \varphi_0 \right\|_{\mathbf{L}^2}^2 \right)$$

with some initial guess $\varphi_0 \in \mathfrak{B}$.

The regularization parameters α_j control the stability and fulfill

$$\alpha_0 \leq 1, \qquad \alpha_j \searrow 0, \qquad 1 \leq \frac{\alpha_j}{\alpha_{j+1}} \leq C_{\mathrm{dec}} \qquad \text{for all} \qquad j \in \mathbb{N}.$$

Noise adjusted regularization

The IRGNM corresponds to a Gaussian noise structure. Hence,

- the information about the noise structure is ignored and
- especially for low intensity we get bad reconstructions.

Our idea is to use another data misfit functional $\mathcal{S}$ which incorporates the special structure of the noise and take

$$\varphi_{n+1} = \operatorname*{argmin}_{\varphi \in \mathfrak{B}} \mathcal{S}\left(F(\varphi_j) + F'(\varphi_j; \varphi - \varphi_j); g^{\mathrm{obs}}\right) + \alpha_j \mathcal{R}(\varphi)$$

where $\mathcal{S}\left(\cdot; g^{\mathrm{obs}}\right)$ is some convex data misfit functional and $\mathcal{R}$ some convex penalty term. For Poisson data the first choice would be the negative log-likelihood

$$\mathcal{S}\left(g; g^{\mathrm{obs}}\right) = \int_{\Omega} g - g^{\mathrm{obs}} \ln(g) \, \mathrm{d}x.$$

Alternatives

An alternative approach is nonlinear Tikhonov regularization

$$\varphi_\alpha = \operatorname*{argmin}_{\varphi \in \mathfrak{B}} \mathcal{S}\left(F(\varphi)\,; g^{\mathrm{obs}}\right) + \alpha \mathcal{R}(\varphi)$$

which has been considered by several authors:

J. M. Bardsley.
A theoretical framework for the regularization of Poisson likelihood estimation problems.
Inverse Problems and Imaging, 4:11–17, 2010.

M. Benning and M. Burger.
Error estimates for general fidelities.
Electronic Transactions on Numerical Analysis, 38:44–68, 2011.

J. Flemming.
Theory and examples of variational regularisation with non-metric fitting functionals.
Journal of Inverse and Ill-Posed Problems, 18(6):677–699, 2010.

O. Scherzer, M. Grasmair, H. Grossauer, M. Haltmeier, and F. Lenzen.
Variational Methods in Imaging.
Applied Mathematical Sciences. Springer, 2008.

Outline

Source condition I

The usual Hilbert space source condition

$$\varphi^\dagger - \varphi_0 = \Lambda\left(F'\left[\varphi^\dagger\right]^* F'\left[\varphi^\dagger\right]\right)\omega$$

implies by spectral theory and Jensen's inequality

$$\left|\left\langle \varphi_*^\dagger, \varphi - \varphi^\dagger \right\rangle\right| \leq \|\omega\| \left\|\varphi - \varphi^\dagger\right\| \Lambda\left(\frac{\left\|F'\left[\varphi^\dagger\right]\left(\varphi - \varphi^\dagger\right)\right\|^2}{\left\|\varphi - \varphi^\dagger\right\|^2}\right).$$

This is the prototype of a variational source condition.

B. Kaltenbacher and B. Hofmann.
Convergence Rates for the Iteratively Regularized Gauss-Newton Method in Banach Spaces.
Inverse Problems, 26(3):035007, 2010.

Source condition II

We will assume the following generalization:

Multiplicative variational source condition

There exists $\varphi_*^\dagger \in \partial\mathcal{R}\left(\varphi^\dagger\right) \subset \mathcal{X}'$, $\beta \geq 0$ and a concave index function $\Lambda : (0,\infty) \to (0,\infty)$ (i.e. continuous, monotonically increasing and $\Lambda(0) = 0$) such that

$$\left\langle \varphi_*^\dagger, \varphi^\dagger - \varphi \right\rangle \leq \beta \Delta\left(\varphi, \varphi^\dagger\right)^{\frac{1}{2}} \Lambda\left(\frac{\mathcal{S}\left(F\left(\varphi\right); g^\dagger\right)}{\Delta\left(\varphi, \varphi^\dagger\right)}\right) \qquad \text{for all } \varphi \in \mathfrak{B}.$$

Moreover, we assume that $t \mapsto \frac{\Lambda(t)}{\sqrt{t}}$ is monotonically decreasing.

$\Delta\left(\varphi, \varphi^\dagger\right) := \mathcal{R}\left(\varphi\right) - \mathcal{R}\left(\varphi^\dagger\right) - \left\langle \varphi_*^\dagger, \varphi - \varphi^\dagger \right\rangle$ is the Bregman distance.

Noise I

In case of $\mathcal{S}$ being the r-th power of a norm one usually assumes $\left\|g^{\mathrm{obs}} - g^{\dagger}\right\| \leq \delta$ which by the triangle inequality leads to

$$2^{1-r}\left\|g - g^{\dagger}\right\|^{r} - \delta^{r} \leq \left\|g - g^{\mathrm{obs}}\right\|^{r} \leq 2^{r-1}\left\|g - g^{\dagger}\right\|^{r} + 2^{r-1}\delta^{r}$$

for all $g \in \mathcal{Y}$.

In case of Poisson noise and the negative log-likelihood as data misfit, we obtain the following difficulties:

- The data misfit functional does not fulfill a triangle inequality.
- $\mathcal{S}\left(g; g^{\mathrm{obs}}\right)$ might be ∞ even if $\mathcal{S}\left(g; g^{\dagger}\right)$ is finite and vice versa.

Noise II

In case of $\mathcal{S}$ being the r-th power of a norm one usually assumes $\left\|g^{\mathrm{obs}} - g^{\dagger}\right\| \leq \delta$ which by the triangle inequality leads to

$$2^{1-r} \left\|g - g^{\dagger}\right\|^{r} - \delta^{r} \leq \left\|g - g^{\mathrm{obs}}\right\|^{r} \leq 2^{r-1} \left\|g - g^{\dagger}\right\|^{r} + 2^{r-1}\delta^{r}$$

for all $g \in \mathcal{Y}$.

Generalization:

Noise level

There exists some $C_{\mathrm{err}} \geq 1$ and a functional **err** : $\mathcal{Y} \to [0, \infty]$ such that

$$\frac{1}{C_{\mathrm{err}}}\mathcal{S}\left(g; g^{\dagger}\right) - \mathbf{err}\left(g\right) \leq \mathcal{S}\left(g; g^{\mathrm{obs}}\right) \leq C_{\mathrm{err}}\mathcal{S}\left(g; g^{\dagger}\right) + C_{\mathrm{err}}\mathbf{err}\left(g\right)$$

for all $g \in \mathcal{Y}$.

Nonlinearity estimate

Generalized tangential cone condition

There exist constants η (later assumed to be sufficiently small) and $C_{\mathrm{tc}} \geq 1$ such that

$$\frac{1}{C_{\mathrm{tc}}}\mathcal{S}\left(F(\psi); g^{\dagger}\right) - \eta\mathcal{S}\left(F(\varphi); g^{\dagger}\right)$$
$$\leq \mathcal{S}\left(F(\varphi) + F'(\varphi; \psi - \varphi); g^{\dagger}\right)$$
$$\leq C_{\mathrm{tc}}\mathcal{S}\left(F(\psi); g^{\dagger}\right) + \eta\mathcal{S}\left(F(\varphi); g^{\dagger}\right) \qquad \text{for all } \varphi, \psi \in \mathfrak{B}.$$

For $\mathcal{S}(g; \hat{g}) = \|g - \hat{g}\|^r$ this follows from the standard *tangential cone condition*

$$\left\|F(\varphi) - F(\psi) - F'(\varphi; \psi - \varphi)\right\| \leq \bar{\eta}\,\|F(\varphi) - F(\psi)\|.$$

Rate function and stopping rule

Our convergence rates result uses the following rate function:

$$\Theta(t) := t\Lambda^2(t).$$

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$$\begin{aligned}\mathbf{err}_j \; &:= \; \mathbf{err}\left(F(\varphi_j) + F'(\varphi_j; \varphi_{j+1} - \varphi_j)\right) \\ &\quad + C_{\mathrm{err}}\, \mathbf{err}\left(F(\varphi_j) + F'\left(\varphi_j; \varphi^\dagger - \varphi_j\right)\right)\end{aligned}$$

and use the following stopping index:

Stopping rule

We define

$$j_*(\mathbf{err}_j) := \min\left\{ j \in \mathbb{N} \;\middle|\; \Theta(\alpha_j) \le \tau\, \mathbf{err}_j \right\}$$

with some tuning parameter $\tau \ge 1$.

Rates of convergence

Convergence theorem

Let the Assumptions from above hold and let η, $\Delta\left(\varphi_0, \varphi^\dagger\right)$ and $\mathcal{S}\left(F\left(\varphi_0\right); g^\dagger\right)$ sufficiently small. Then the iterates $\left(\varphi_j\right)$ for exact data $g^{\mathrm{obs}} = g^\dagger$ fulfill

$$\Delta\left(\varphi_j, \varphi^\dagger\right) = \mathcal{O}\left(\Lambda^2\left(\alpha_j\right)\right),$$
$$\mathcal{S}\left(F\left(\varphi_j\right); g^\dagger\right) = \mathcal{O}\left(\Theta\left(\alpha_j\right)\right)$$

as $j \to \infty$, and in case of noisy data for sufficiently large $\tau \geq 1$ we get

$$\Delta\left(\varphi_{j_*}, \varphi^\dagger\right) = \mathcal{O}\left(\Lambda^2\left(\Theta^{-1}\left(\mathbf{err}_{j_*}\right)\right)\right) = \mathcal{O}\left(\frac{\mathbf{err}_{j_*}}{\Theta^{-1}\left(\mathbf{err}_{j_*}\right)}\right),$$
$$\mathcal{S}\left(F\left(\varphi_{j_*}\right); g^\dagger\right) = \mathcal{O}\left(\mathbf{err}_{j_*}\right).$$

Extensions

- Same convergence rates in terms of

$$\mathbf{err}_j := \frac{1}{C_{\mathrm{err}}} \mathbf{err}\left(F\left(\varphi_{j+1}\right)\right) + 2\eta C_{\mathrm{tc}} \mathbf{err}\left(F\left(\varphi_j\right)\right) + C_{\mathrm{tc}} C_{\mathrm{err}} \mathbf{err}\left(g^{\dagger}\right).$$

if the nonlinearity condition also holds for noisy data g^{obs}.

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  if the nonlinearity condition also holds for noisy data g^{obs}.

- Error decomposition and Lepskiĭ-type parameter choice rule in the case of an additive variational inequality

$$\left\langle \varphi_*^{\dagger}, \varphi^{\dagger} - \varphi \right\rangle \leq \beta_1 \Delta\left(\varphi, \varphi^{\dagger}\right) + \beta_2 \Lambda\left(\mathcal{S}\left(F\left(\varphi\right); g^{\dagger}\right)\right).$$

B. Hofmann, B. Kaltenbacher, C. Pöschl, and O. Scherzer.
A convergence rates result for Tikhonov regularization in Banach spaces with non-smooth operators.
Inverse Problems, 23(3):987–1010, 2007.

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- Convergence rates under Hölder-type variational inequalities with index $\nu \in \left[\frac{1}{2}, 1\right)$ in combination with a Lipschitz assumption.

Outline

Poisson data

Let $\mathcal{Y} = L^1(\Omega, \nu) \cap L^\infty(\Omega, \nu)$ for some measure space (Ω, ν), and

$$F(\varphi) \geq 0 \quad \nu - \text{a.e.} \qquad \text{for all } \varphi \in \mathfrak{B}.$$

Moreover we assume that our noisy data g^{obs} fulfills $g^{\mathrm{obs}} \geq 0$, $g^{\mathrm{obs}} = 0$ where $g^\dagger = 0$ and

$$\int\limits_{\{g^\dagger > 0\}} \frac{|g^{\mathrm{obs}} - g^\dagger|^2}{g^\dagger} \, \mathrm{d}\nu \leq \frac{1}{t}$$

for some $t > 0$.

- This is motivated by the fact that for a Poisson process the variance decays like $\frac{1}{\sqrt{t}}$ where t is proportional to the expected number of photons.
- t can be interpreted as an illumination time and we want to study the limit $t \to \infty$.

Bounding **err**

The Kullback-Leibler divergence has a singularity at 0, so we define an offset version with $e > 0$ by

$$\mathcal{S}_e\left(g; g^{\mathrm{obs}}\right) = \int_\Omega g - \left(g^{\mathrm{obs}} + e\right) \ln\left(\frac{g+e}{e}\right) \mathrm{d}x$$

for $g \geq -\frac{e}{2}$. The deterministic noise model implies

$$\left|\mathcal{S}_e(g; g^{\mathrm{obs}}) - \mathcal{S}_e(g; g^{\dagger})\right| \leq \sqrt{\frac{C}{t}}$$

for some constant $C > 0$ if $-\frac{e}{2} \leq g \leq B$. Hence the inequalities for $\mathbf{err}\left(F(\varphi) + F(\varphi; \psi - \varphi)\right),\ \varphi, \psi \in \mathfrak{B}$ are fulfilled with

$$C_{\mathrm{err}} = 1 \text{ and } \mathbf{err} \equiv \sqrt{\tfrac{C}{t}}.$$

Convergence theorem

Convergence rates

Let the Assumptions from above hold and assume that the nonlinearity condition is true for exact data. Moreover let

$$\sup_{\varphi,\psi\in\mathfrak{B}} \left\|F(\varphi) + F'(\varphi;\psi-\varphi)\right\|_{L^\infty} < \infty.$$

Then the a-priori stopping rule $j_* := \min\left\{j \in \mathbb{N} \;\middle|\; \Theta(\alpha_j) \leq \frac{\tau}{\sqrt{t}}\right\}$ with a sufficiently large parameter $\tau > 0$ leads to the convergence rates

$$\Delta\left(\varphi_{j_*}, \varphi^\dagger\right) = \mathcal{O}\left(\Lambda^2\left(\Theta^{-1}\left(t^{-1/2}\right)\right)\right),$$

$$\mathbb{KL}_e\left(F\left(\varphi_{j_*}\right); g^\dagger\right) = \mathcal{O}\left(t^{-1/2}\right).$$

Extensions

- If the nonlinearity condition also holds for noisy data g^{obs}, then the offset e can be set to 0 under a suitable variance condition on F.
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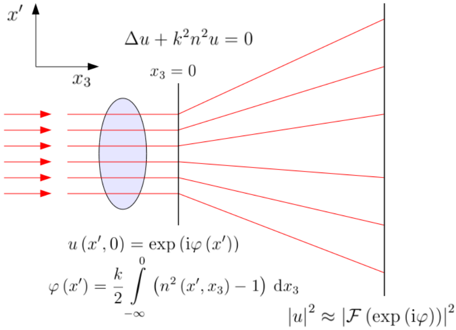
- If the nonlinearity condition also holds for noisy data g^{obs}, then the offset e can be set to 0 under a suitable variance condition on F.
  $\Rightarrow$ similar rates.
- Similar rates for a Lepskiĭ-type parameter choice rule in case of an additive variational inequality.
- Ongoing work on convergence rates in case of full stochastic data, i.e. the data are given by a Poisson process.

Outline

The setting

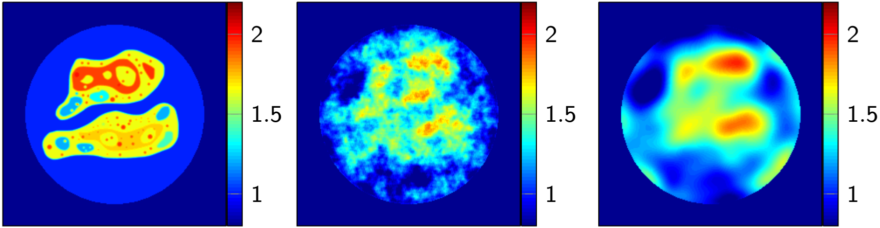


$$F : H^s(B_\rho) \longrightarrow L^\infty([-\kappa, \kappa]^2),$$

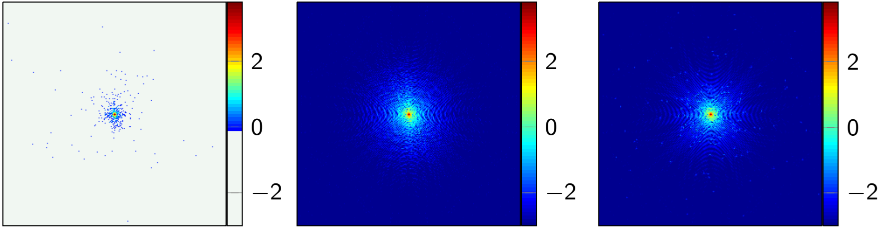
$$F(\varphi)(\xi) = \left| \int_{B_\rho} e^{-i\xi \cdot x'} e^{i\varphi(x')} \, dx' \right|^2$$

M. V. Klibanov.
On the recovery of a 2-D function from the modulus of its Fourier transform.
J. Math. Anal. Appl., 323(2):818–843, 2006.

Median results for $t = 10^4$ expected counts



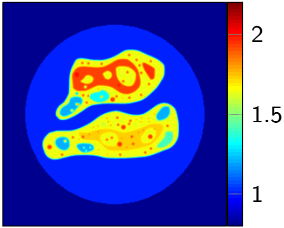
(a) exact solution (b) our algorithm (c) IRGNM



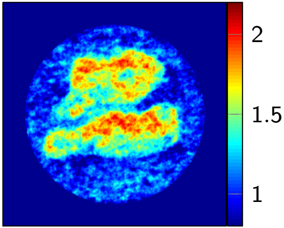
(d) observed data ($\log_{10}$) (e) exact data ($\log_{10}$) (f) our algorithm ($\log_{10}$)

K. Giewekemeyer et al, *Phys. Rev. A*, 83:023804, 2011.

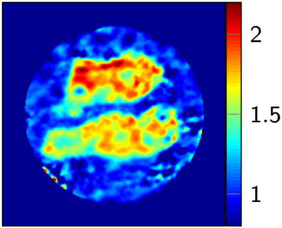
Median results for $t = 10^5$ expected counts



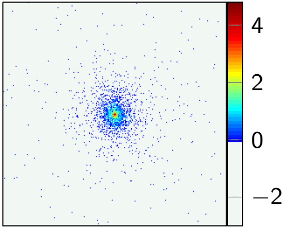
(a) exact solution



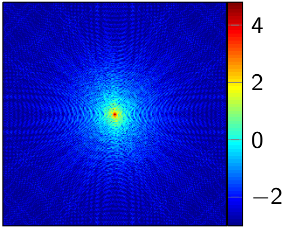
(b) our algorithm



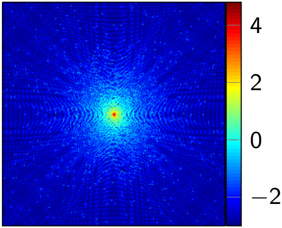
(c) IRGNM



(d) observed data ($\log_{10}$)

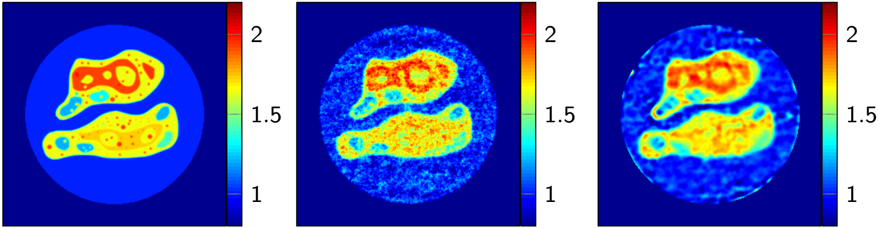


(e) exact data ($\log_{10}$)

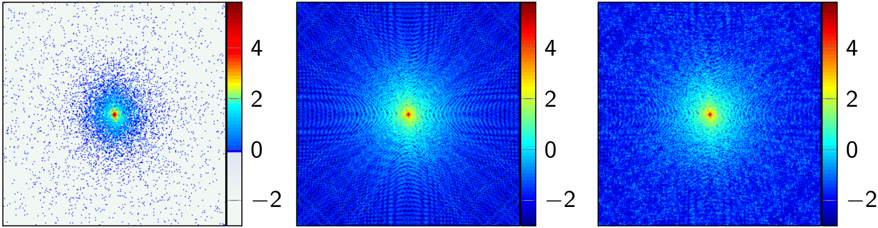


(f) our algorithm ($\log_{10}$)

Median results for $t = 10^6$ expected counts



(a) exact solution (b) our algorithm (c) IRGNM



(d) observed data ($\log_{10}$) (e) exact data ($\log_{10}$) (f) our algorithm ($\log_{10}$)

Outline

Shown results / Outlook

- Convergence analysis for iteratively regularized Newton methods with **arbitrary** data misfit functional and **arbitrary** penalty term.
- Our results include the known results for the IRGNM.
- Applications to Poisson data via choosing $\mathcal{S}$ to be the negative log-likelihood.
- Good numerical results in case of Poisson data.

T. Hohage and F. Werner.
Iteratively regularized Newton methods for general data misfit functionals and applications to Poisson data.
http://arxiv.org/abs/1105.2690v1, 2011.