Research Article

Anatoly Bakushinsky and Alexandra Smirnova*

A study of frozen iteratively regularized Gauss–Newton algorithm for nonlinear ill-posed problems under generalized normal solvability condition

https://doi.org/10.1515/jiip-2019-0099
Received December 4, 2019; revised January 16, 2020; accepted January 21, 2020

Abstract: A parameter identification inverse problem in the form of nonlinear least squares is considered. In the lack of stability, the frozen iteratively regularized Gauss–Newton (FIRGN) algorithm is proposed and its convergence is justified under what we call a generalized normal solvability condition. The penalty term is constructed based on a semi-norm generated by a linear operator yielding a greater flexibility in the use of qualitative and quantitative a priori information available for each particular model. Unlike previously known theoretical results on the FIRGN method, our convergence analysis does not rely on any nonlinearity conditions and it is applicable to a large class of nonlinear operators. In our study, we leverage the nature of ill-posedness in order to establish convergence in the noise-free case. For noise contaminated data, we show that, at least theoretically, the process does not require a stopping rule and is no longer semi-convergent. Numerical simulations for a parameter estimation problem in epidemiology illustrate the efficiency of the algorithm.

Keywords: Regularization, ill-posed problems, parameter estimation in epidemiology

MSC 2010: 35R25, 47J06, 65F22, 65J20, 65L08, 65M30, 65R30

1 Introduction

Consider an applied inverse problem of minimizing the functional

$$\Omega(q) := \frac{1}{2}\|F(q) - f\|^2, \quad F\colon \mathcal{D}_F \subseteq \mathcal{H} \to \mathcal{H}_1, \tag{1.1}$$

where $\mathcal{H}$ and $\mathcal{H}_1$ are Hilbert spaces, and the nonlinear operator, F, is fitted to some (generally limited) noise contaminated data, f_δ,

$$\|f - f_\delta\| \le \delta. \tag{1.2}$$

Let $\hat{q}$ be a minimizer of $\Omega(q)$ such that

$$\|F(\hat{q}) - f\| = \inf_{q\in\mathcal{D}_F} \|F(q) - f\| = 0. \tag{1.3}$$

Suppose F is Fréchet differentiable in a neighborhood $\mathcal{O}_\eta(\hat{q})$ to be specified below. Throughout this paper we assume that F' is Lipschitz-continuous, i.e.,

$$\|F'(u) - F'(v)\| \le \mathcal{L}\|u - v\| \quad \text{for any } u, v \in \mathcal{O}_\eta(\hat{q}), \tag{1.4}$$

***Corresponding author: Alexandra Smirnova,** Department of Mathematics and Statistics, Georgia State University, Atlanta, USA, e-mail: asmirnova@gsu.edu
Anatoly Bakushinsky, Federal Research Center “Computer Science and Control” of Russian Academy of Sciences, Moscow, Russia, e-mail: bakush@isa.ru

but not regular in a sense that neither $F'(\hat{q})$ nor $F'^*(\hat{q})F'(\hat{q})$ is boundedly invertible. Hence, the problem of minimizing (1.1) is ill-posed, and any algorithm used to solve this problem numerically has to be regularized. To that end, we penalize $\Omega(q)$ (see [28]):

$$\Omega_\tau(q) := \frac{1}{2}\|F(q) - f_\delta\|^2 + \frac{\tau}{2}\|T(q-\xi)\|^2, \tag{1.5}$$

with T being a surjective linear operator between two Hilbert spaces, and $\mathcal{H}$ and $\mathcal{H}_2$ satisfying, for any $h \in \mathcal{H}$, the condition

$$(T^*Th, h) \geq m\|h\|^2, \quad m > 0. \tag{1.6}$$

A much needed flexibility in our choice of $T \in L(\mathcal{H}, \mathcal{H}_2)$, along with a suitable reference element, $\xi \in \mathcal{D}_F \subseteq \mathcal{H}$, allows to incorporate some problem-specific a priori information, which is not covered by the operator F or the data, f_δ. In certain cases, T maps spline expansion coefficients to the physical space, where the unknown solution is actually defined. In other cases, it scales the respective components of q when the solution consists of multiple unknown parameters, some of which are on different levels of magnitude [26]. By linearizing the fidelity term in (1.5) around the current iteration point, q_k, and setting $\tau = \tau_k > 0$, one gets a strongly convex quadratic functional

$$\Omega_{\tau_k}(q; q_k) := \frac{1}{2}\|F(q_k) - f_\delta + F'(q_k)(q - q_k)\|^2 + \frac{\tau_k}{2}\|T(q-\xi)\|^2, \tag{1.7}$$

whose unique global minimum yields what is known as the classical iteratively-regularized Gauss–Newton (IRGN) method, introduced by Bakushinsky for $T = I$, see [2, 3, 6, 7, 11, 15–17, 29], and later extended to $T \neq I$ in [25, 26]. Its "frozen" version to be investigated in this paper is obtained by replacing $F'(q_k)$ with $F'(q_0)$, which enables us to save time and storage on recomputing F' at each iteration step. Thus, one arrives at the following regularized numerical procedure:

$$q_{k+1} = q_k - [F'^*(q_0)F'(q_0) + \tau_k T^*T]^{-1}\{F'^*(q_0)(F(q_k) - f_\delta) + \tau_k T^*T(q_k - \xi)\}, \quad q_0 \in \mathcal{O}_\eta(\hat{q}). \tag{1.8}$$

Note that condition (1.6) guarantees that iterations (1.8) are well defined even when $F'^*(q_0)F'(q_0)$ is not positive definite, and

$$\big\|[F'^*(q_0)F'(q_0) + \tau_k T^*T]^{-1}\big\| \leq \frac{1}{\tau_k m}.$$

Under various nonlinearity conditions, algorithms similar to (1.8) have been considered by many authors in both Hilbert and Banach spaces (see, for example, [14, 19, 20]). In [19], convergence in a Banach space is justified under the assumption that for some constant $C_0 > 0$, and for each u, v in a neighborhood of q_0, there exists a linear operator $R_u^v : \mathcal{H}_1 \to \mathcal{H}_1$ such that

$$F'(v) = R_u^v F'(u), \quad \|R_u^v - I\| \leq C_0, \tag{1.9}$$

which means that in some neighborhood of q_0 the operator $F'(v)$ remains essentially the same for all v up to a certain perturbation by R_u^v. This assumption was first introduced in [13] in order to prove convergence rates of the Landweber iteration method for nonlinear ill-posed problems. It was further used to study convergence rates of other iterative solution methods (see [7, 17, 23] and references therein).

While the results based on nonlinearity conditions are important, they are not applicable to inverse problems with highly nonlinear operators, where these conditions are not satisfied or are hard to verify. In our study, we take a different route. Rather than restricting the nonlinearity of the operator, we leverage the nature of ill-posedness in order to establish convergence of iterative scheme (1.8) without using (1.9) or any other condition of this kind. As such, our analysis does not in any way limit the nonlinearity of the parameter-to-data map, F, and covers a large class of nonlinear least squares. It is based on what we call *the generalized normal solvability condition* (GNSC), that is, for $q_0 \in \mathcal{O}_\eta(\hat{q})$ and $T \in L(\mathcal{H}, \mathcal{H}_2)$, introduced in (1.7), the image, $\mathcal{R}(F'(q_0)(T^*T)^{-1/2})$, is a closed subspace in $\mathcal{H}_1$. Here for any $A \in L(\mathcal{H}, \mathcal{H}_1)$, $\mathcal{R}(A)$ is defined as

$$\mathcal{R}(A) := \{v \in \mathcal{H}_1,\ v = Au,\ u \in \mathcal{H}\}.$$

Recall that minimization problems are still ill-posed under GNSC if we have $\mathcal{N}(F'(q_0)(T^*T)^{-1/2}) \neq 0$ and/or

$\mathcal{R}(F'(q_0)(T^*T)^{-1/2}) \neq \mathcal{H}_1$, and they need to be regularized. However, the spectrum of a normally solvable operator has a remarkable property: even though 0 is still in the spectrum due to ill-posedness, there exists $\mu_0 > 0$ such that

$$\sigma((F'(q_0)(T^*T)^{-1/2})^* F'(q_0)(T^*T)^{-1/2}) \subseteq \{0\} \cup [\mu_0^2, \|F'(q_0)(T^*T)^{-1/2}\|^2]. \tag{1.10}$$

This "hole" in the spectrum is a real game changer. Due to inclusion (1.10), the regularized pseudo-inverse operator, $[F'^*(q_0)F'(q_0) + \tau_k T^*T]^{-1}F'^*(q_0)$, remains bounded (which is not true for general ill-posed problems where the upper bound is $\frac{1}{2\sqrt{m\tau_k}}$). And that is the reason the nonlinearity of the operator F no longer has to be restricted in the convergence analysis (see Section 2 for more details).

In the linear case, for $T = I$, normally solvable ill-posed operator equations have been thoroughly studied by Vainikko and Veretennikov [30]. And in [4, 18], Bakushinsky and Kokurin investigated convergence rates of iteratively regularized Gauss–Newton-type algorithms under the assumption that $\mathcal{R}(F'(\hat{q}))$ is a closed subspace in $\mathcal{H}_1$.

Our interest in regularized numerical algorithms based on normal solvability conditions is primarily motivated by inverse problems in epidemiology, where infinite dimensional time dependent disease parameters must be recovered from finite incidence data. However, unstable problems of recovering infinite solutions from finite data sets occur in many other fields, including biomedical imaging, gravitational sounding, and hydraulics. Clearly, the GNSC is fulfilled when one of the spaces, $\mathcal{H}$ or $\mathcal{H}_1$, is finite dimensional. The GNSC also holds if $F'(q_0)(T^*T)^{-1/2}$ is a Fredholm operator [4, 18]. Further examples can also be found in [12].

The main result of this paper, presented in Theorem 2.2, is estimate (2.17), which shows that algorithm (1.8) does not actually need a stopping rule, since (at least theoretically, if one does not account for other sources of noise rather than noise in the data) the error on the solution goes down as $k \to \infty$. That is, unlike most iteratively regularized methods for nonlinear ill-posed problems, the process is not semi-convergent and there is no danger to over-fit. This is a remarkable property that greatly simplifies the numerical implementation of (1.8).

The paper is organized as follows. In Section 2, theoretical analysis of the new regularization algorithm (1.8) is offered, and the stability of (1.8) with respect to noise in the input data is justified. Numerical experiments aimed at parameter estimation from real epidemiological data are presented in Section 3, followed by conclusions and future plans discussed in Section 4.

2 Convergence analysis of the regularization algorithm

In this section, we establish the regularizing properties of the iterative scheme (1.8) and show that, under some natural assumptions on $q_0, \xi \in \mathcal{D}_F \subseteq \mathcal{H}$,

$$\limsup_{k\to\infty} \|q_k - \hat{q}\| \leq \Delta\delta, \quad \Delta > 0.$$

The following lemma is instrumental for our convergence analysis.

Lemma 2.1 ([30, p. 153]). *An operator $A \in L(\mathcal{H}, \mathcal{H}_1)$ has a closed range $\mathcal{R}(A) \subseteq \mathcal{H}_1$ if and only if*

$$\mu := \inf\{\|Au\| : u \in \mathcal{H},\ u \perp \mathcal{N}(A), \|u\| = 1\} > 0,$$

where

$$\mathcal{N}(A) := \{u \in \mathcal{H},\ Au = 0\}.$$

According to Lemma 2.1,

$$\mu_0 := \inf\{\|F'(q_0)(T^*T)^{-1/2}u\| : u \in \mathcal{H},\ u \perp \mathcal{N}(F'(q_0)(T^*T)^{-1/2}),\ \|u\| = 1\} > 0. \tag{2.1}$$

Suppose $\|q_0 - \hat{q}\| \leq l\tau_0 + \Delta\delta$ for some $l, \Delta > 0$, see [5]. Let $\{\tau_k\}$ be a sequence of regularization parameters satisfying the conditions

$$\tau_k \geq \tau_{k+1} > 0, \quad \sup_{k\in N\cup\{0\}} \frac{\tau_k}{\tau_{k+1}} = d < \infty, \quad \lim_{k\to\infty} \tau_k = 0, \tag{2.2}$$

and assume, by induction, that for any $0 < j \le k$,

$$\|q_j - \hat{q}\| \le l\tau_j + \Delta\delta.$$

Taking into consideration that

$$F'^*(q_0)(F(q_k) - f_\delta) = F'^*(q_0)(F(q_k) - F(\hat{q})) + F'^*(q_0)(f - f_\delta),$$

one concludes, from (1.8) and (1.4),

$$\begin{aligned} q_{k+1} - \hat{q} = q_k - \hat{q} - [F'^*(q_0)F'(q_0) + \tau_k T^*T]^{-1}\{&F'^*(q_0)F'(\hat{q})(q_k - \hat{q}) + F'^*(q_0)\mathcal{B}(q_k, \hat{q}) \\ &+ F'^*(q_0)(f - f_\delta) + \tau_k T^*T(q_k - \hat{q}) + \tau_k T^*T(\hat{q} - \xi)\}, \end{aligned} \tag{2.3}$$

where

$$\|\mathcal{B}(q_k, \hat{q})\| \le \frac{\mathcal{L}}{2}\|q_k - \hat{q}\|^2.$$

Identity (2.3) yields

$$\begin{aligned} q_{k+1} - \hat{q} = &-[F'^*(q_0)F'(q_0) + \tau_k T^*T]^{-1}F'^*(q_0)\{(F'(\hat{q}) - F'(q_0))(q_k - \hat{q}) + \mathcal{B}(q_k, \hat{q}) + f - f_\delta\} \\ &- \tau_k[F'^*(q_0)F'(q_0) + \tau_k T^*T]^{-1}T^*T(\hat{q} - \xi). \end{aligned} \tag{2.4}$$

If one estimates $[F'^*(q_0)F'(q_0) + \tau_k T^*T]^{-1}F'^*(q_0)$ using the spectral theorem for the self-adjoint operator $(F'(q_0)(T^*T)^{-1/2})^*F'(q_0)(T^*T)^{-1/2}$ and polar decomposition for the bounded linear operator $F'(q_0)(T^*T)^{-1/2}$, then one obtains (see [3, 17, 26])

$$\begin{aligned} &[F'^*(q_0)F'(q_0) + \tau_k T^*T]^{-1}F'^*(q_0) \\ &\quad = \{(T^*T)^{1/2}[(T^*T)^{-1/2}F'^*(q_0)F'(q_0)(T^*T)^{-1/2} + \tau_k I](T^*T)^{1/2}\}^{-1}F'^*(q_0) \\ &\quad = (T^*T)^{-1/2}[(F'(q_0)(T^*T)^{-1/2})^*F'(q_0)(T^*T)^{-1/2} + \tau_k I]^{-1}(F'(q_0)(T^*T)^{-1/2})^*. \end{aligned} \tag{2.5}$$

Introduce the notation

$$G_0 := F'(q_0)(T^*T)^{-1/2}. \tag{2.6}$$

Combining (2.5), (2.6) and (1.6), one derives

$$\begin{aligned} \|[F'^*(q_0)F'(q_0) + \tau_k T^*T]^{-1}F'^*(q_0)\| &= \|(T^*T)^{-1/2}[G_0^*G_0 + \tau_k I]^{-1}G_0^*\| \\ &= \|(T^*T)^{-1/2}[G_0^*G_0 + \tau_k I]^{-1}(U(G_0^*G_0)^{1/2})^*\| \\ &\le \|(T^*T)^{-1/2}[G_0^*G_0 + \tau_k I]^{-1}(G_0^*G_0)^{1/2}\| \\ &\le \frac{1}{\sqrt{m}} \sup_{\lambda \in \sigma(G_0^*G_0)} \psi(\lambda), \quad \psi(\lambda) := \frac{\sqrt{\lambda}}{\lambda + \tau_k}. \end{aligned} \tag{2.7}$$

Here $\sigma(B)$ is the spectrum of $B \in L(\mathcal{H}, \mathcal{H})$, $G_0 = U(G_0^*G_0)^{1/2}$, and U is partial isometry:

$$\|Uq\| = \|q\| \quad \text{for any } q \in \mathcal{N}(U)^\perp.$$

From polar decomposition, $G_0 = U(G_0^*G_0)^{1/2}$, it follows that $\mathcal{R}(G_0)$ is closed if and only if $\mathcal{R}((G_0^*G_0)^{1/2})$ is closed [30]. Thus, μ_0 in (2.1) is the least nonzero element in $\sigma((G_0^*G_0)^{1/2})$ or, alternatively,

$$\mu_0^2 = \min_{\lambda \in \sigma(G_0^*G_0),\, \lambda \ne 0} \lambda, \tag{2.8}$$

and $\sigma(G_0^*G_0) \subseteq \{0\} \cup [\mu_0^2, \|G_0\|^2]$. Taking into account (2.7) and (2.8) and assuming that $\tau_0 \le \mu_0^2$, one gets

$$\|[F'^*(q_0)F'(q_0) + \tau_k T^*T]^{-1}F'^*(q_0)\| \le \frac{1}{\sqrt{m}} \sup_{\lambda \in \{0\} \cup [\mu_0^2, \|G_0\|^2]} \psi(\lambda) = \frac{\psi(\mu_0^2)}{\sqrt{m}} = \frac{\mu_0}{\sqrt{m}\,(\mu_0^2 + \tau_k)} \le \frac{1}{\sqrt{m}\,\mu_0}. \tag{2.9}$$

In order to compute the upper bound for the element $[F'^*(q_0)F'(q_0) + \tau_k T^*T]^{-1}T^*T(\hat{q} - \xi)$ in (2.4), we impose a very weak source condition (weak in a sense that p can be less than $1/2$):

$$(T^*T)^{1/2}(\hat{q}-\xi) = (G_0^*G_0)^p w, \quad p>0,\ w\in\mathcal{H}. \tag{2.10}$$

Equalities (2.5) and (2.10) imply

$$\begin{aligned}[F'^*(q_0)F'(q_0)+\tau_k T^*T]^{-1}T^*T(\hat{q}-\xi) &= (T^*T)^{-1/2}[(F'(q_0)(T^*T)^{-1/2})^*F'(q_0)(T^*T)^{-1/2}+\tau_k I]^{-1},\\ (T^*T)^{1/2}(\hat{q}-\xi) &= (T^*T)^{-1/2}[G_0^*G_0+\tau_k I]^{-1}(G_0^*G_0)^p w.\end{aligned}$$

Thus, one arrives at the following estimate:

$$\|[F'^*(q_0)F'(q_0)+\tau_k T^*T]^{-1}T^*T(\hat{q}-\xi)\| \le \frac{1}{\sqrt{m}}\sup_{\lambda\in\sigma(G_0^*G_0)}\phi(\lambda), \quad \phi(\lambda) := \frac{\lambda^p}{\lambda+\tau_k}. \tag{2.11}$$

Suppose that for $0<p<1$,

$$\frac{p\tau_0}{1-p} \le \mu_0^2 \tag{2.12}$$

(this condition covers the case $\tau_0\le\mu_0^2$ when $p=1/2$). Then identity (2.8) together with (2.11) yield

$$C(p,\mu_0) := \sup_{\lambda\in\sigma(G_0^*G_0)}\phi(\lambda) = \begin{cases}\phi(\mu_0^2) = \dfrac{1}{\mu_0^{2-2p}}, & 0<p<1,\\[2ex] \phi(\|G_0\|^2) = \|G_0\|^{2p-2}, & p\ge 1.\end{cases} \tag{2.13}$$

As a result, from (1.2), (2.2), (2.4), (2.9), and (2.13), one obtains

$$\begin{aligned}\|q_{k+1}-\hat{q}\| &\le \frac{1}{\sqrt{m}\,\mu_0}\Big(\mathcal{L}\|q_0-\hat{q}\|\,\|q_k-\hat{q}\| + \frac{\mathcal{L}}{2}\|q_k-\hat{q}\|^2+\delta\Big) + \frac{C(p,\mu_0)}{\sqrt{m}}\|w\|\tau_k\\ &\le \frac{3\mathcal{L}(l\tau_0+\Delta\delta)}{2\sqrt{m}\,\mu_0}(l\tau_k+\Delta\delta) + \frac{\delta}{\sqrt{m}\,\mu_0} + \frac{C(p,\mu_0)}{\sqrt{m}}\|w\|\tau_k\\ &\le \frac{3\mathcal{L}}{2\sqrt{m}\,\mu_0}(l^2\tau_0\tau_k+2l\tau_0\Delta\delta+\Delta^2\delta^2) + \frac{\delta}{\sqrt{m}\,\mu_0} + \frac{C(p,\mu_0)}{\sqrt{m}}\|w\|\tau_k\\ &\le \frac{d}{\sqrt{m}}\Big[\frac{3\mathcal{L}l^2\tau_0}{2\mu_0}+C(p,\mu_0)\|w\|\Big]\tau_{k+1} + \frac{3\mathcal{L}}{2\sqrt{m}\mu_0}\Delta^2\delta^2 + [3\mathcal{L}l\tau_0\Delta+1]\frac{\delta}{\sqrt{m}\mu_0}.\end{aligned}$$

In order to carry out the induction step, it is sufficient to prove that the right-hand side of the above estimate does not exceed $l\tau_{k+1}+\Delta\delta$. Clearly, this will be the case if

$$\frac{d}{\sqrt{m}}\Big[\frac{3\mathcal{L}l^2\tau_0}{2\mu_0}+C(p,\mu_0)\|w\|\Big] \le l \quad\text{and}\quad \frac{3\mathcal{L}}{2\sqrt{m}\mu_0}\Delta^2\delta^2 + [3\mathcal{L}l\tau_0\Delta+1]\frac{\delta}{\sqrt{m}\mu_0} \le \Delta\delta. \tag{2.14}$$

Take $l := \frac{\mu_0\sqrt{m}}{3d\mathcal{L}\tau_0}$ and suppose that $6d^2\mathcal{L}\tau_0 C(p,\mu_0)\|w\| \le m\mu_0$. Then one derives

$$\begin{aligned}\frac{d}{\sqrt{m}}\Big[\frac{3\mathcal{L}l^2\tau_0}{2\mu_0}+C(p,\mu_0)\|w\|\Big] &= \frac{d}{\sqrt{m}}\Big[\frac{3\mathcal{L}\tau_0}{2\mu_0}\Big(\frac{\mu_0\sqrt{m}}{3d\mathcal{L}\tau_0}\Big)^2 + C(p,\mu_0)\|w\|\Big]\\ &\le \frac{\mu_0 m + 6d^2\mathcal{L}\tau_0 C(p,\mu_0)\|w\|}{6d^2\mathcal{L}\tau_0\sqrt{m}}\\ &\le \frac{\mu_0\sqrt{m}}{3d\mathcal{L}\tau_0} = l.\end{aligned}$$

The second inequality in (2.14) is equivalent to

$$\frac{3\mathcal{L}}{2\sqrt{m}\mu_0}\Delta^2\delta + \frac{1}{\sqrt{m}\mu_0} \le \Delta\Big[1-\frac{3\mathcal{L}l\tau_0}{\sqrt{m}\mu_0}\Big],$$

or, given our choice of $l := \frac{\mu_0\sqrt{m}}{3d\mathcal{L}\tau_0}$,

$$\frac{3\mathcal{L}}{2\sqrt{m}\mu_0}\Delta^2\delta + \frac{1}{\sqrt{m}\mu_0} \le \frac{\Delta(d-1)}{d}. \tag{2.15}$$

Recall that, by definition, $d > 1$. Evidently, inequality (2.15) holds if

$$\max\left\{\frac{3\mathcal{L}}{2\sqrt{m}\mu_0}\Delta^2\delta,\ \frac{1}{\sqrt{m}\mu_0}\right\} \le \frac{\Delta(d-1)}{2d}. \tag{2.16}$$

Estimate (2.16) implies

$$\delta \le \frac{(d-1)\sqrt{m}\mu_0}{3\mathcal{L}\Delta d} \quad \text{and} \quad \frac{2d}{(d-1)\sqrt{m}\mu_0} \le \Delta.$$

In particular, if one chooses $\Delta = \frac{2d}{(d-1)\sqrt{m}\mu_0}$, then $\delta \le \frac{(d-1)^2 m\mu_0^2}{6\mathcal{L}d^2}$. From the above, one concludes the following.

Theorem 2.2. *Let $F\colon \mathcal{D}_F \subseteq \mathcal{H} \to \mathcal{H}_1$, $T \in L(\mathcal{H}, \mathcal{H}_2)$, and let $\mathcal{H}$, $\mathcal{H}_1$, and $\mathcal{H}_2$ be Hilbert spaces. Assume that conditions* (1.3), (1.4), (1.6), (2.2), (2.10), *and* (2.12) *are fulfilled with $\mu_0 > 0$ introduced in* (2.1), *and $\mathcal{R}(F'(q_0)(T^*T)^{-1/2})$ is a closed subspace in $\mathcal{H}_1$. Suppose also that $q_0 \in \mathcal{O}_\eta(\hat{q})$, where*

$$\mathcal{O}_\eta(\hat{q}) := \{q \in \mathcal{D}_F \subseteq \mathcal{H},\ \|q - \hat{q}\| \le \eta\}, \quad \eta := l\tau_0 + \Delta\delta,$$

and the constants l and Δ are selected as follows:

$$l := \frac{\mu_0\sqrt{m}}{3d\mathcal{L}\tau_0} \quad \text{and} \quad \Delta := \frac{2d}{(d-1)\sqrt{m}\mu_0}.$$

Furthermore, let the noise level, δ, do not exceed the threshold:

$$\delta \le \frac{(d-1)^2 m\mu_0^2}{6\mathcal{L}d^2}.$$

Then for $\{q_k\}$ defined in (1.8) *and for $\hat{q}$ defined in* (1.3), *the following estimate holds:*

$$\|q_k - \hat{q}\| \le l\tau_k + \Delta\delta, \quad k = 0, 1, 2, \ldots, \tag{2.17}$$

provided that $T \in L(\mathcal{H}, \mathcal{H}_2)$, τ_0, and d in (2.2) *are chosen to satisfy the inequality*

$$6d^2\mathcal{L}\tau_0 C(p, \mu_0)\|w\| \le m\mu_0,$$

with $C(p, \mu_0)$ and w introduced in (2.13) *and* (2.10), *respectively.*

Remark 2.3. Estimate (2.17) shows that algorithm (1.8) does not actually need a stopping rule, since (at least theoretically, if one does not account for the rounding errors) $\|q_k - \hat{q}\|$ goes down as $k \to \infty$. However, suppose $\Delta\delta \le l\tau_0$, and assume that algorithm (1.8) is terminated the moment $l\tau_k$ is less than $\Delta\delta$ for the first time:

$$l\tau_{\mathcal{K}(\delta)} < \Delta\delta \le l\tau_k, \quad 0 \le k < \mathcal{K}(\delta).$$

Since $\Delta\delta \le l\tau_0$, conditions (2.2) imply that $\mathcal{K}(\delta)$ is correctly defined and

$$\lim_{\delta\to 0}\mathcal{K}(\delta) = \infty.$$

Then it follows from (2.17) that

$$\|q_{\mathcal{K}(\delta)} - \hat{q}\| \le 2\Delta\delta.$$

3 Numerical simulations and discussion

To validate the efficiency of algorithm (1.8), we conduct numerical experiments on stable parameter estimation from real incidence data on cholera epidemic in Peru from 1991 to 1997, see [27]. Quantification of various transmission pathways of cholera epidemics has been an important tool in control and intervention.

In our study, we adapted a dynamic model comprised of 4 equations and 8 parameters [1, 9, 21, 22]. According to this model, humans are born and die at the same rate, μ ($1/(60\cdot 52)$ weeks^{-1}). Susceptible individuals can be infected through the environment with transmission rate $\beta_e(t)$ or through human

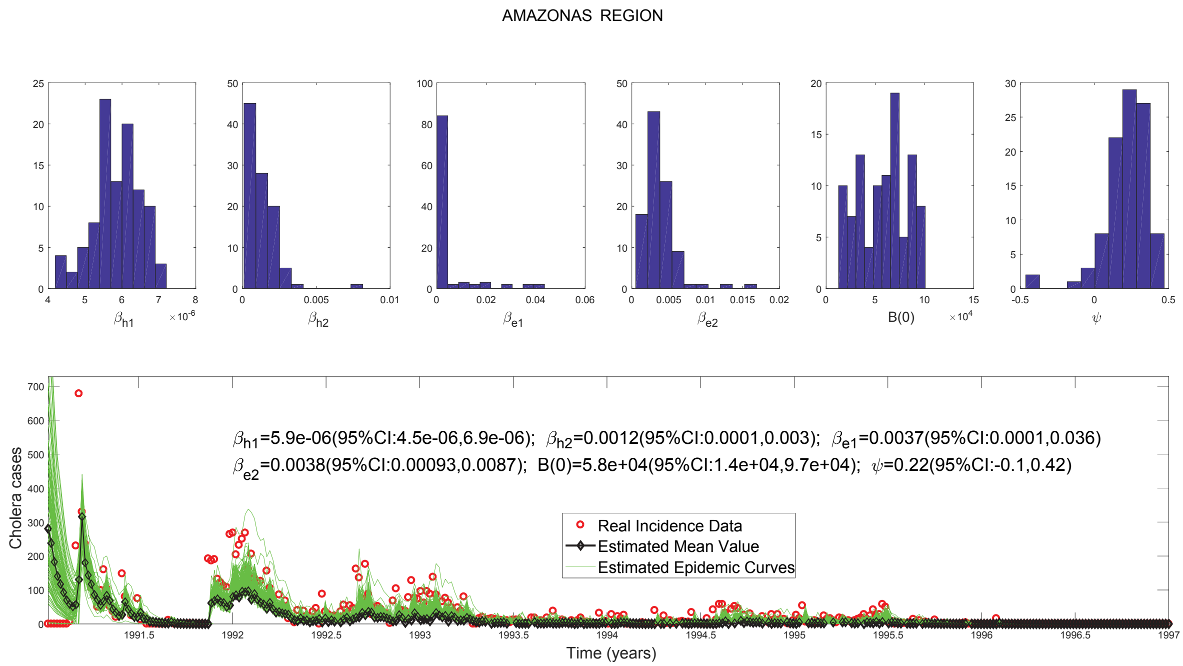

Figure 1: Reconstructed parameter values and incidence curves for cholera epidemic.

contact with transmission rate $\beta_h(t)$. Therefore, they move from susceptible to infectious classes at rates $\beta_e(t)B(t)/(B(t)+\kappa)$ (where κ is the 50% infectious dose in the environment, $10^6\,\mathrm{mL}^{-1}$, and $B(t)$ is the current concentration of vibrios in the environment) and $\beta_h(t)I(t)$, respectively [27]. Vibrios are shed by infectious individuals into the environment at the rate λ ($70\,\mathrm{mL}^{-1}\cdot\mathrm{weeks}^{-1}$), and then die at the rate ζ ($7/30\,\mathrm{weeks}^{-1}$). Infected individuals are assumed to recover and acquire protective immunity for the entire duration of the epidemic at the rate γ ($7/5\,\mathrm{weeks}^{-1}$) [27]. The overall transmission dynamics is therefore described by the following nonlinear initial value problem:

$$\frac{dS}{dt} = \mu N - \beta_h(t)S(t)I(t) - \beta_e(t)S(t)\frac{B(t)}{B(t)+\kappa} - \mu S(t), \tag{3.1}$$

$$\frac{dI}{dt} = \beta_h(t)S(t)I(t) + \beta_e(t)S(t)\frac{B(t)}{B(t)+\kappa} - \mu I(t) - \gamma I(t), \tag{3.2}$$

$$\frac{dR}{dt} = \gamma I(t) - \mu R(t), \tag{3.3}$$

$$\frac{dB}{dt} = \lambda I(t) - \zeta B(t), \tag{3.4}$$

$$S(0) = N - C_1, \quad I(0) = C_1, \quad R(0) = 0, \quad B(0) = B_1, \tag{3.5}$$

where N is the population size for a given department in Peru, C_1 is the number of cases observed in the first week in each department divided by a reporting rate, and B_1 is the initial concentration of vibrios in the environment. We assume that reported data, $f_\delta(t)$, is available for weekly incidence cases subject to an unknown reporting rate, ψ. Based on (3.1)–(3.5), the cumulative number of human cases, $C(t)$, satisfies the following differential equation:

$$\frac{dC}{dt} = \beta_h(t)S(t)I(t) + \beta_e(t)S(t)\frac{B(t)}{B(t)+\kappa}.$$

By fitting $\psi\frac{dC}{dt}$ to the reported incidence data, $f_\delta(t)$, we estimate four system parameters, two of which are time dependent: $\beta_h(t)$, $\beta_e(t)$, B_1, and ψ. The reporting rate, ψ, is a scaling factor used to adjust for possible under- or over-reporting of cases, owing to, for instance, a large proportion of asymptomatic cholera cases or false diagnostics.

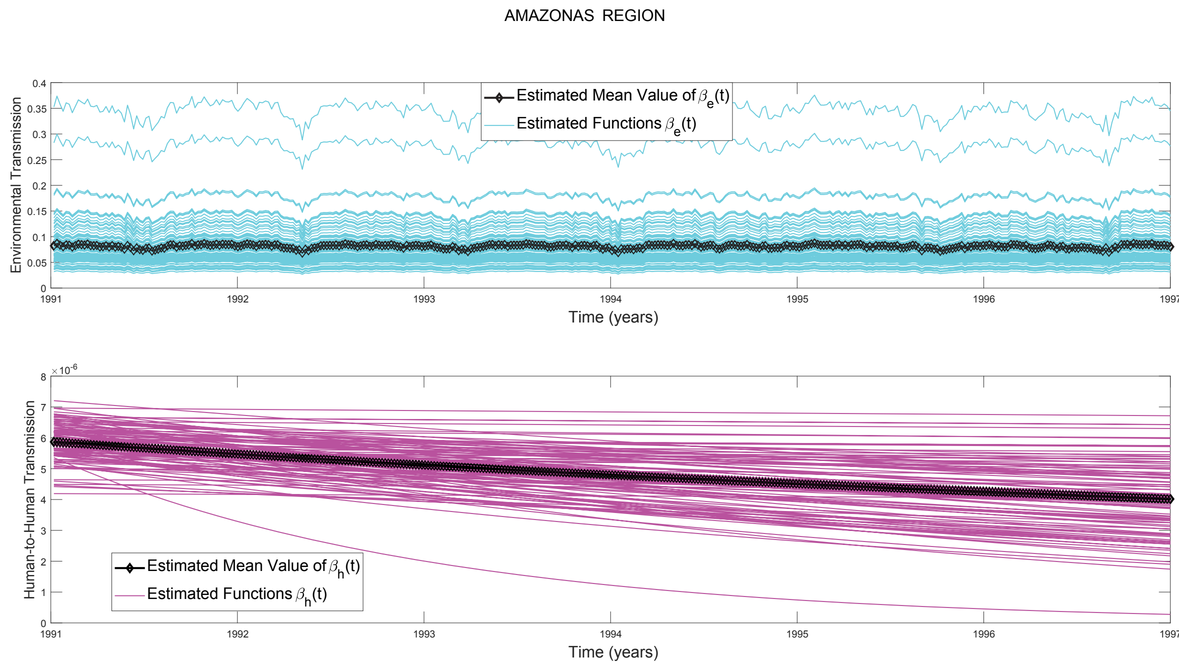

Figure 2: Reconstructed environmental and human-to-human transmission rates.

As proposed in [27], in order to estimate four unknown parameters, we replace the force of infection, $\beta_h(t)S(t)I(t) + \beta_e(t)S(t)\frac{B(t)}{B(t)+\kappa}$, with $\frac{dC}{dt}$ in the first two equations of compartmental model (3.1)–(3.5) to get linear nonhomogeneous ordinary differential equations (ODEs) for $S(t)$ and $I(t)$, respectively:

$$\frac{dS}{dt} = -\mu S(t) - \frac{dC}{dt} + \mu N, \tag{3.6}$$

$$\frac{dI}{dt} = -(\mu + \gamma)I(t) + \frac{dC}{dt}. \tag{3.7}$$

Given the initial conditions (3.5), one derives the following analytic solutions to (3.6) and (3.7):

$$S(t) = N - \exp(-\mu t)C_1 - \int_0^t \exp(-\mu(t-s))C'(s)\,ds, \tag{3.8}$$

$$I(t) = \exp(-(\mu+\gamma)t)C_1 + \int_0^t \exp(-(\mu+\gamma)(t-s))C'(s)\,ds. \tag{3.9}$$

To obtain the expression for $B(t)$ in terms of $C'(t)$, one first solves the linear ODE (3.4), then substitutes (3.9) for $I(s)$, and finally integrates by parts to eliminate the inner integral. This yields

$$\begin{aligned} B(t) = \exp(-\zeta t)B_1 &+ \frac{\lambda C_1}{\mu+\gamma-\zeta}[\exp(-\zeta t) - \exp(-(\mu+\gamma)t)] \\ &+ \frac{\lambda}{\mu+\gamma-\zeta}\int_0^t C'(s)[\exp(-\zeta(t-s)) - \exp(-(\mu+\gamma)(t-s))]\,ds. \end{aligned} \tag{3.10}$$

The next step of the algorithm is to obtain discrete analogs of (3.8)–(3.10) at the grid points $t_1, t_2, \dots, t_m$, where $t_i = i-1$, $i = 1, 2, \dots, m$, and $t_1 = 0$ is the first week of the outbreak. To fit $\psi\frac{dC}{dt}$ to the reported incidence data, $f_\delta(t)$, we replace C_1 with f_{δ_1}/ψ and $C'(s)$ with $f_\delta(s)/\psi$ under each integral in (3.8), (3.9), and (3.10). Given the discrete data, $f_\delta = [f_{\delta_1}, f_{\delta_2}, \dots, f_{\delta_m}]^\top$, reported weekly, we interpolate f_δ as follows:

$$f_\delta(0) = f_\delta(t_1) = f_{\delta_1} \quad \text{and} \quad f_\delta(t) = f_{\delta_{j+1}} \quad \text{for } t \in (t_j, t_{j+1}],\ j = 1, 2, \dots, m-1. \tag{3.11}$$

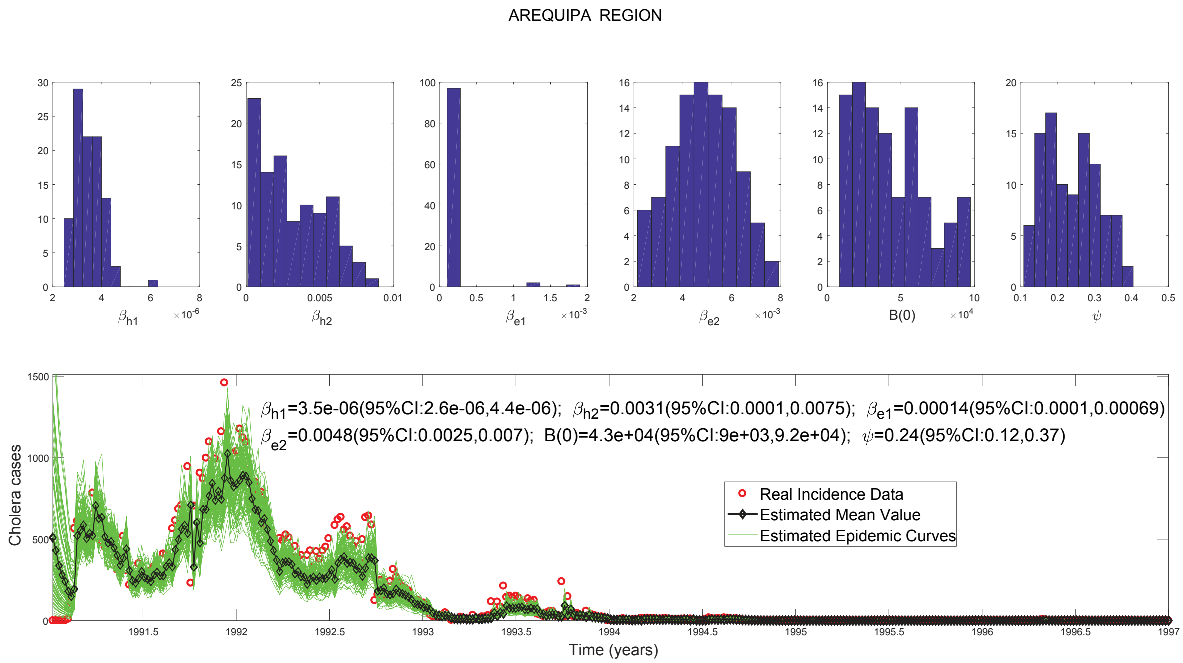

Figure 3: Reconstructed parameter values and incidence curves for cholera epidemic.

From (3.11), one concludes that

$$\begin{cases} S_1[\psi] = N - f_{\delta_1}/\psi, \\ S_i[\psi] = N - \dfrac{\exp(-\mu(i-1))f_{\delta_1}}{\psi} - \dfrac{1}{\mu\psi}\displaystyle\sum_{j=1}^{i-1} f_{\delta_{j+1}}[\exp(-\mu(i-j-1)) - \exp(-\mu(i-j))], \end{cases} \tag{3.12}$$

$i = 2, 3, \ldots, m$. Likewise, identities (3.9) and (3.10) yield

$$\begin{cases} I_1[\psi] = f_{\delta_1}/\psi, \\ I_i[\psi] = \dfrac{\exp(-(\mu+\gamma)(i-1))f_{\delta_1}}{\psi} \\ \qquad + \dfrac{1}{(\mu+\gamma)\psi}\displaystyle\sum_{j=1}^{i-1} f_{\delta_{j+1}}[\exp(-(\mu+\gamma)(i-j-1)) - \exp(-(\mu+\gamma)(i-j))], \end{cases} \tag{3.13}$$

as well as the expression for $B_i[\psi, B_1]$:

$$B_i[\psi, B_1] = \exp(-\zeta(i-1))B_1 + \frac{\lambda D_1}{(\mu+\gamma-\zeta)\psi}[\exp(-\zeta(i-1)) - \exp(-(\mu+\gamma)(i-1))] \tag{3.14}$$

$$+ \frac{\lambda}{(\mu+\gamma-\zeta)\psi}\sum_{j=1}^{i-1} f_{\delta_{j+1}}\Big[\frac{\exp(-\zeta(i-j-1)) - \exp(-\zeta(i-j))}{\zeta} \tag{3.15}$$

$$- \frac{\exp(-(\mu+\gamma)(i-j-1)) - \exp(-(\mu+\gamma)(i-j))}{\mu+\gamma}\Big], \tag{3.16}$$

$i = 2, 3, \ldots, m$. This implies that the estimation of the unknown parameters, $\beta_h(t)$, $\beta_e(t)$, B_1, ψ, can now be cast as the following nonlinear least squares problem:

$$\min_{\beta_h(t),\beta_e(t),B_1,\psi} \frac{1}{2}\Big\|\psi S[\psi](t)\Big\{\beta_h(t)I[\psi](t) + \beta_e(t)\frac{B[\psi, B_1](t)}{B[\psi, B_1](t)+\kappa}\Big\} - f_\delta\Big\|^2$$

$$= \min_{\beta_h(t),\beta_e(t),B_1,\psi} \frac{1}{2}\sum_{i=1}^{m}\Big(\psi S_i[\psi]\Big\{\beta_{h_i}I_i[\psi] + \beta_{e_i}\frac{B_i[\psi, B_1]}{B_i[\psi, B_1]+\kappa}\Big\} - f_{\delta_i}\Big)^2,$$

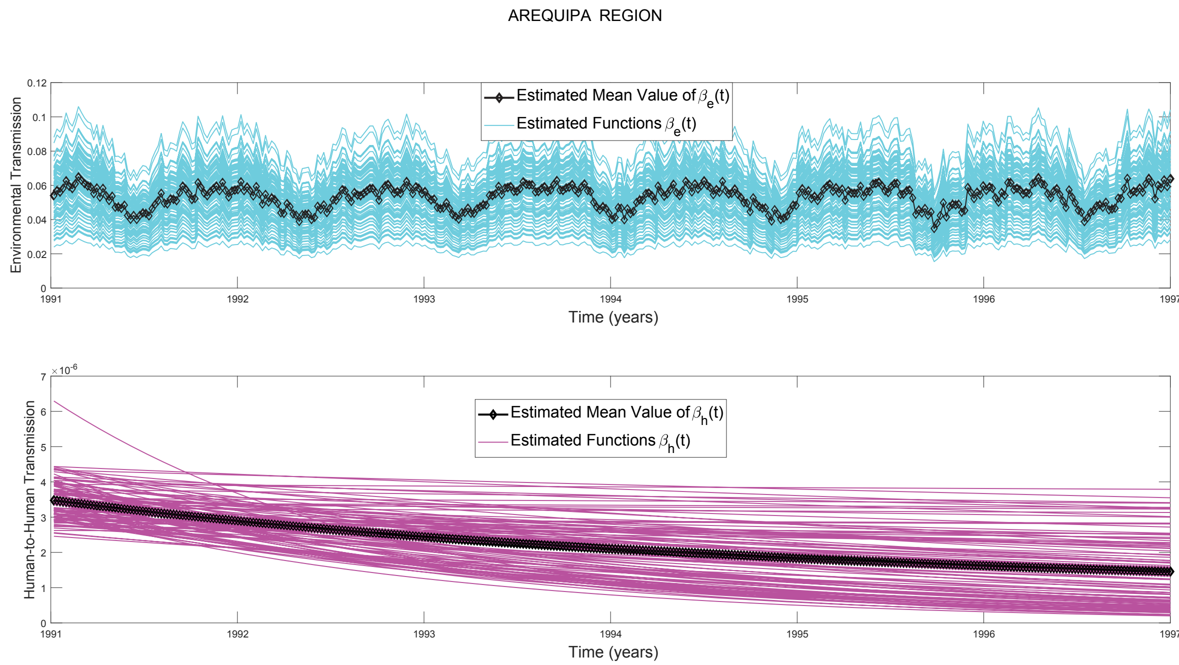

Figure 4: Reconstructed environmental and human-to-human transmission rates.

where $f_\delta = [f_{\delta_1}, f_{\delta_2}, \ldots, f_{\delta_m}]^\top$ are reported data sets for incident cases, and the expressions for $S_i[\psi]$, $I_i[\psi]$, and $B_i[\psi, B_1]$ are given by (3.12), (3.13), and (3.16), respectively. To discretize $\beta_e(t)$, as suggested in [27], we assume that the weekly temperature variation, $T(t)$, directly influences the cholera transmission rate from the environment. To reflect that, $\beta_e(t)$ is broken down into two components: $\beta_e(t) = \beta_{e1} + \beta_{e2}T(t)$, where $T(t)$ represents the mean temperature at time t for the corresponding department. Regarding $\beta_h(t)$, we assume an exponential rate of decline following the implementation of control measures, i.e., $\beta_h(t) = \beta_{h1}\exp(-\beta_{h2}t)$. This yields the following unconstrained minimization problem

$$\min_q \frac{1}{2}\|F(q) - f_\delta\|^2 := \min_q \frac{1}{2}\sum_{j=1}^{m}(F_j(q) - f_{\delta_j})^2, \quad F\colon \mathbb{R}^n \to \mathbb{R}^m,$$

with m being the number of data points and n being the size of the solution space upon discretization. In our case, n is equal to 6, since we adopt special function forms for $\beta_h(t)$ and $\beta_e(t)$, with two unknown parameters each. Hence, in the discretized solution space, we are looking to approximate $q = [\beta_{h1}, \beta_{h2}, \beta_{e1}, \beta_{e1}, B_1, \psi]^\top$. After the six unknown parameters have been recovered from the corresponding epidemic data sets using the above optimization algorithm, 100 additional incidence curves are generated via parametric bootstrap [8, 10] in order to quantify uncertainty in the estimated parameters and derive 95% confidence intervals.

All data for this test (on cholera cases and temperature fluctuations) have been provided by Dr. Gerardo Chowell from GSU School of Public Health. To avoid bias towards one particular data set, we include numerical results for two different regions: Arequipa (with population of about 1 million), and Amazonas (with population close to 370,000). To initialize the iterative process, we randomly select starting values for the unknown parameters from a uniform distribution over a certain interval. For β_{h1}, the starting values are taken from $[5 \cdot 10^{-6}, 10^{-5}]$, for β_{h2}, the values are taken from $[10^{-4}, 10^{-2}]$, for β_{e1}, the interval is $[10^{-4}, 10^{-3}]$, for β_{e2}, it is $[10^{-4}, 10^{-2}]$, for ψ, we assume the interval to be $[0.1, 0.3]$, and for B_1, the values are taken from $[10^4, 10^5]$.

Given very different levels of magnitude for the six components of the solution vector, in all our experiments T^*T is a diagonal matrix with entries selected to scale initial values of the unknowns.Without scaling (that is, with $T = I$) the process turned out to be divergent for all initial approximations considered. The general idea for choosing T^*T as a diagonal matrix to enforce scaling is as follows (see [26]). Suppose that upon discretization our solution vector consists of two subvectors, $\mathbf{x}$ and $\mathbf{y}$, that is, $q = \binom{\mathbf{x}}{\mathbf{y}}$, which are several orders of magnitude apart. Suppose also that $\tilde{x}$ is our best guess for the mean value for the components of $\mathbf{x}$, and $\tilde{y}$ is our best guess for the mean of $\mathbf{y}$ coordinates. Then one takes

$$T^*T = \begin{pmatrix} I_x & 0 \\ 0 & \omega^2 I_y \end{pmatrix},$$

where I_x and I_y are identity blocks, corresponding to $\mathbf{x}$ and $\mathbf{y}$, respectively, and $\omega = \tilde{x}/\tilde{y}$.

The numerical results presented in Figures 1–4 have been obtained after 5 iterations of algorithm (1.8). The relative discrepancies are 0.33 and 0.77 for the city of Arequipa and for Amazonas region, respectively. The problem is severely ill-posed. Even with the very aggressive disretization, the condition number of $F'^*(q_0)F'(q_0)$ for different realizations of noisy data ranges from 10^{23} to 10^{25}. To achieve the best convergence rate and, at the same time, to ensure that the process remains stable until the desired level of accuracy is reached, we choose $\tau_0 = 1$ and then drive τ_k to zero at the rate $\tau_k = \tau_0 \exp(-k)$. Without regularization, i.e., when regularization is limited to discretization only, the process turns out to be divergent. The step size for each data set is 0.1. Any step smaller than that has also worked.

It is also important to mention that parameter values recovered by FIRGN are consistent with those recovered by the Matlab built-in subfunction `lsqcurvefit`, where minimization is carried out by the Levenberg–Marquardt algorithm [24]. The elapsed time for `lsqcurvefit` varies depending on the tolerance settings, but it is considerably higher as compared to the FIRGN algorithm. On the flip side, the radius of convergence for `lsqcurvefit` is bigger than the one for FIRGN. This can probably be attributed to `lsqcurvefit` using a better-tuned line search.

4 Conclusions and discussion

A preconditioned version of a frozen iteratively regularized Gauss–Newton algorithm has been investigated. The convergence analysis is carried out under the generalized normal solvability condition, which yields convergence of the proposed scheme in the noise-free case. For noise contaminated data, estimate (2.17) implies that, at least theoretically, for this particular type of noise the process does not require a stopping rule and is no longer semi-convergent. Numerical simulations for a parameter estimation problem in epidemiology illustrate the efficiency of the algorithm. The numerical experiments have also suggested the direction of further research, that needs to include the case of nonzero residual as well as the case of noise contaminated operator.

Funding: Alexandra Smirnova is supported by NSF Grant 1818886. DMS Computational Mathematics.

References

[1] A. S. Azman, F. J. Luquero, A. Rodrigues, P. P. Palma, R. F. Grais and C. N. Banga, Urban Cholera transmission hotspots and their implications for reactive vaccination: Evidence from Bissau City, Guinea Bissau, *PLOS Neglected Tropical Diseases* **6** (2012), DOI 10.1371/journal.pntd.0001901.

[2] A. B. Bakushinskiĭ, Iterative methods for solving nonlinear operator equations without regularity. A new approach, *Dokl. Akad. Nauk* **330** (1993), no. 3, 282–284.

[3] A. B. Bakushinskiĭ and M. Y. Kokurin, *Iterative Methods for Ill-posed Operator Equations with Smooth Operators*, Springer, Dordrecht, 2004.

[4] A. B. Bakushinskiĭ and M. Y. Kokurin, An iteratively regularized Gauss–Newton method for operator equations with a normally solvable derivative in the solution (in Russian), *Izv. Vyssh. Uchebn. Zaved. Mat.* (2016), no. 8, 3–11.

[5] A. B. Bakushinsky, M. Y. Kokurin and A. Smirnova, *Iterative Methods for Ill-posed Problems. An Introduction*, Inverse Ill-posed Probl. Ser. 54, Walter de Gruyter, Berlin, 2011.

[6] B. Blaschke, A. Neubauer and O. Scherzer, On convergence rates for the iteratively regularized Gauss–Newton method, *IMA J. Numer. Anal.* **17** (1997), no. 3, 421–436.

[7] M. Burger, B. Kaltenbacher and A. Neubauer, Iterative solution methods, in: *Handbook of Mathematical Methods in Imaging. Vol. 1, 2, 3*, Springer, New York (2015), 431–470.

[8] G. Chowell, Fitting dynamic models to epidemic outbreaks with quantified uncertainty: A primer for parameter uncertainty, identifiability, and forecasts, *Infect Dis. Model.* **2** (2017), no. 3, 379–398.

[9] W. H. Curioso, J. J. Miranda and A. M. Kimball, Controlling the cholera epidemic in Peru: The community's oral rehydration units, *BMJ* **328** (2004), Article ID 777.

[10] B. Efron and R. Tibshirani, Bootstrap methods for standard errors, confidence intervals, and other measures of statistical accuracy, *Statist. Sci.* **1** (1986), no. 1, 54–77.

[11] H. W. Engl, M. Hanke and A. Neubauer, *Regularization of Inverse Problems*, Math. Appl. 375, Kluwer Academic, Dordrecht, 1996.

[12] H. W. Engl, K. Kunisch and A. Neubauer, Convergence rates for Tikhonov regularisation of nonlinear ill-posed problems, *Inverse Problems* **5** (1989), no. 4, 523–540.

[13] M. Hanke, A. Neubauer and O. Scherzer, A convergence analysis of the Landweber iteration for nonlinear ill-posed problems, *Numer. Math.* **72** (1995), no. 1, 21–37.

[14] Q. Jin, On a class of frozen regularized Gauss–Newton methods for nonlinear inverse problems, *Math. Comp.* **79** (2010), no. 272, 2191–2211.

[15] B. Kaltenbacher, Some Newton-type methods for the regularization of nonlinear ill-posed problems, *Inverse Problems* **13** (1997), no. 3, 729–753.

[16] B. Kaltenbacher and A. Neubauer, Convergence of projected iterative regularization methods for nonlinear problems with smooth solutions, *Inverse Problems* **22** (2006), no. 3, 1105–1119.

[17] B. Kaltenbacher, A. Neubauer and O. Scherzer, *Iterative Regularization Methods for Nonlinear Ill-posed Problems*, Radon Ser. Comput. Appl. Math. 6, Walter de Gruyter, Berlin, 2008.

[18] M. Y. Kokurin, Iteratively regularized methods for irregular nonlinear operator equations with a normally solvable derivative at the solution, *Comput. Math. Math. Phys.* **56** (2016), no. 9, 1523–1535.

[19] P. Mahale and S. K. Dixit, Convergence analysis of simplified iteratively regularized Gauss–Newton method in a Banach space setting, *Appl. Anal.* **97** (2018), no. 15, 2686–2719.

[20] P. Mahale and M. T. Nair, A simplified generalized Gauss–Newton method for nonlinear ill-posed problems, *Math. Comp.* **78** (2009), no. 265, 171–184.

[21] Z. Mukandavire, S. Liao, J. Wang, H. Gaff, D. L. Smith and J. G. Morris, Estimating the reproductive numbers for the 2008-2009 cholera outbreaks in Zimbabwe, *Proc. Natl. Acad. Sci. USA* **108** (2011), no. 21, 8767–8772.

[22] Z. Mukandavire, D. L. Smith and J. G. Morris, Jr., Cholera in Haiti: Reproductive numbers and vaccination coverage estimates, *Sci. Rep.* **3** (2013), Article ID 997.

[23] A. Neubauer, Some generalizations for Landweber iteration for nonlinear ill-posed problems in Hilbert scales, *J. Inverse Ill-Posed Probl.* **24** (2016), no. 4, 393–406.

[24] J. Nocedal and S. J. Wright, *Numerical Optimization*, Springer Ser. Oper. Res., Springer, New York, 1999.

[25] A. Smirnova, On convergence rates for iteratively regularized procedures with linear penalty terms, *Inverse Problems* **28** (2012), no. 8, Article ID 085005.

[26] A. Smirnova, R. A. Renaut and T. Khan, Convergence and application of a modified iteratively regularized Gauss–Newton algorithm, *Inverse Problems* **23** (2007), no. 4, 1547–1563.

[27] A. Smirnova, N. Sterrett, O. J. Mujica, C. Munayco, L. Suarez, C. Viboud and G. Chowell, Spatial dynamics and the basic reproduction number of the Cholera epidemic in Peru 1991–1997, to appear in *PLOS Neglected Tropical Diseases*.

[28] A. N. Tikhonov, A. V. Goncharsky, V. V. Stepanov and A. G. Yagola, *Numerical Methods for the Solution of Ill-posed Problems*, Math. Appl. 328, Kluwer Academic, Dordrecht, 1995.

[29] V. V. Vasin and A. L. Ageev, *Ill-posed Problems with a Priori Information*, Inverse Ill-posed Probl. Ser., VSP, Utrecht, 1995.

[30] G. M. Vaĭnikko and A. Y. Veretennikov, *Iteration Procedures in Ill-posed Problems* (in Russian), "Nauka", Moscow, 1986.