Preconditioning CGNE-Iterations for Inverse Problems*

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Abstract

The conjugate gradient method applied to the normal equations (CGNE) is known as one of the most efficient methods for the solution of (non-symmetric) linear equations. By stopping the iteration according to a discrepancy principle, CGNE can be turned into a regularization method. We show that CGNE can be accelerated by preconditioning in Hilbert scales, derive (optimal) convergence rates with respect to data noise for the preconditioned method, and illustrate the theoretical results by numerical tests.

1 Introduction

In this paper we investigate the solution of linear inverse problems

$$Tx = y, \tag{1}$$

where $T : \mathcal{X} \to \mathcal{Y}$ is a linear operator between Hilbert spaces $\mathcal{X}$ and $\mathcal{Y}$. Throughout the paper we assume that a solution $x^\dagger$ of (1) exists, but that only perturbed (measured) data y^δ with

$$\|y - y^\delta\| \le \delta \tag{2}$$

are available. If the inverse problem (1) is ill-posed, e.g., if the operator T is compact with infinite dimensional range, then a solution of (1) does not depend continuously on the data and *regularization methods* have to be used to get reasonable approximations for the solution $x^\dagger$.

The probably most well-known regularization method is Tikhonov regularization (cf. [4, 6]), where an approximate solution of (1) is found as the solution of the regularized normal equations

$$T^*Tx + \alpha I = T^*y, \qquad \text{for some} \quad \alpha > 0. \tag{3}$$

For large scale inverse problems, in particular, if a solution or even the assembling of the full equation (1) or the corresponding normal equation (3) is not possible or computationally expensive, iterative algorithms are an attractive alternative to Tikhonov regularization, since they usually only require applications of the operator T respectively its adjoint T^*, i.e., matrix-vector multiplications for discretized problems. Examples of are inverse problems governed by PDEs, e.g., in parameter identification, where T is only defined implicitly via the solution of the underlying differential equation. Although most parameter identification problems are nonlinear, equations of the form (1) usually appear in a numerical solution via linearization, e.g., in Newton-type methods.

Iterative algorithms are turned into regularization methods by stopping after an adequate number of steps, which may be determined a-priori, i.e., the number of iterations is fixed in advance and does not depend on the iterates x_k^δ of the algorithm. The second and for many reasons preferable strategy

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is to stop the iteration by an *a posteriori* stopping rule. The widely used discrepancy principle (cf. [4, 13]) determines the stopping index k_* according to

$$\|y^\delta - Tx^\delta_{k_*}\| \le \tau\delta < \|y^\delta - Tx^\delta_k\|, \qquad 0 \le k < k_*. \tag{4}$$

Among a variety of iterative algorithms for the solution of (1), the conjugate gradient method based on the normal equations (CGNE) has turned out to be very efficient with respect to computational complexity, i.e., it has been shown (similar as in the well-posed case) that the conjugate gradient method is the fastest method among a rather wide class of semi-iterative (Krylov subspace) methods (cf., e.g., [4, 7]), which are of the form

$$x^\delta_{k+1} = \sum_{j=0}^{k} \mu_{k,j} x^\delta_j + \omega_k T^*(y^\delta - Tx^\delta_k). \tag{5}$$

A method (5) is called linear if the weights $\mu_{k,j}$, ω_k do not depend on x^δ_k or y^δ, and thus are defined a-priori. For a rather complete analysis of conjugate gradient type methods for ill-posed problems we refer to [7].

In this paper we investigate the acceleration of conjugate gradient methods in Hilbert scales. Such a preconditioning strategy has been applied previously for the acceleration of linear (semi-)iterative methods for linear and nonlinear inverse problems [1, 2, 3]. The analysis of the CGNE-method in Hilbert scales is however significantly different and requires a separate investigation.

The outline of this article is as follows: In Section 2 we recall the basic results on (iterative) regularization in Hilbert scales and the regularizing properties of the CGNE method. We formulate the Hilbert scale version of the CGNE method (HSCGNE) and analyze its convergence properties for inverse problems in Section 3. The assumptions needed for our investigations are verified for several examples in Section 4, and the outcomes of numerical tests illustrating the theoretical results are presented.

2 On regularization in Hilbert scales and the method of conjugate gradients for ill-posed problems

In this section we the most important results on regularization in Hilbert scales and the convergence (rates) of the CGNE method for inverse problems, which will be needed later on for our analysis.

2.1 Regularization in Hilbert scales

Regularization in Hilbert scales was introduced by Natterer [14] in order overcome saturation and improve convergence rates for Tikhonov regularization. In [16], Landweber iteration, which for nonlinear problems exhibits similar saturation phenomena as Tikhonov regularization (i.e., optimal convergence only for $x^\dagger - x_0 \in \mathcal{R}((T^*T)^\mu)$, $\mu \le 1/2$), has been investigated in Hilbert scales again with the aim to obtain optimal convergence also for the case $\mu > 1/2$.

In [1, 2, 3], the application of Hilbert scales to (semi-)iterative regularization methods has been analyzed from a different point of view: if one chooses $s < 0$, the Hilbert scale operator L^{-2s} appearing in Algorithm 1 acts as a preconditioner and leads to a reduction of the number of iterations needed to satisfy a discrepancy criterion (4).

Before we sketch the most important results on Hilbert scale regularization, we shortly recall the definition of a Hilbert scale (see [11]):

Definition 1 *Let L be a densely defined, unbounded, selfadjoint, strictly positive operator in $\mathcal{X}$. Then $(\mathcal{X}_s)_{s\in\mathcal{R}}$ denotes the Hilbert scale induced by L, if $\mathcal{X}_s$ is the completion of $\bigcap_{k=0}^\infty D(L^k)$ with respect to the Hilbert space norm $\|x\|_s := \|L^s x\|_{\mathcal{X}}$; obviously $\|x\|_0 = \|x\|_{\mathcal{X}}$ (see [11] or [4, Section 8.4] for details).*

In order to be able to carry out the convergence analysis in Hilbert scales (with $s < 0$), we make some assumptions on the inverse problem (1) and thereby restrict the choice of an appropriate Hilbert scale (cf. [1, 3]):

Assumption 1

(A1) $Tx = y$ *has a solution* $x^\dagger$.

(A2) $\|Tx\| \le \overline{m}\|x\|_{-a}$ *for all* $x \in \mathcal{X}$ *and some* $a > 0, \overline{m} > 0$. *Moreover, the extension of* T *to* $\mathcal{X}_{-a}$ *(again denoted by* T*) is injective.*

Remark 1 Note that with $L = T^*T$, condition (A2) is always satisfied for $a \le 1/2$. Such a choice is however inappropriate from a numerical point of view, since already the application of L^{-2s} for some $-a/2 \le s < 0$ (cf. Algorithm 1), is at least as difficult as solving the original problem (1). The standard analysis of regularization methods in Hilbert scales requires a stronger condition than (A2), namely (cf, e.g., [14, 15])

$$\|Tx\| \sim \|x\|_{-a} \qquad \text{for all} \quad x \in \mathcal{X}, \tag{6}$$

where the number a can be interpreted as the *degree of ill-posedness.* However, if $s < 0$, an estimate from below (possibly in a weaker norm), e.g.,

$$\|Tx\| \ge \underline{m}\|x\|_{-\tilde{a}} \quad \text{for all} \quad x \in \mathcal{X} \quad \text{and some} \quad \tilde{a} \ge a,\, \underline{m} > 0, \tag{7}$$

is only needed to interpret the natural source condition (cf. [1, 3])

$$x^\dagger - x_0 = L^{-s}(B^*B)^{\frac{u-s}{2(a+s)}} w, \quad \text{for some} \quad w \in \mathcal{X},\ \|w\| \le \rho \tag{8}$$

in terms of the Hilbert scale $\{\mathcal{X}_s\}_{s\in\mathcal{R}}$.

The following proposition, which is taken from [3], draws some conclusions from Assumption 1.

Proposition 1 *Let Assumption 1 hold. Then Condition (A2) is equivalent to*

$$\mathcal{R}(T^*) \subset \mathcal{X}_a \qquad \textit{and} \qquad \|T^*w\|_a \le \overline{m}\|w\| \quad \textit{for all} \quad w \in \mathcal{Y}. \tag{9}$$

Moreover for all $\nu \in [0,1]$ *it holds that* $\mathcal{D}((B^*B)^{-\frac{\nu}{2}}) = \mathcal{R}((B^*B)^{\frac{\nu}{2}}) \subset \mathcal{X}_{\nu(a+s)}$ *and*

$$\|(B^*B)^{\frac{\nu}{2}}x\| \quad \le \quad \overline{m}^\nu \|x\|_{-\nu(a+s)} \qquad \textit{for all} \quad x \in \mathcal{X} \tag{10}$$

$$\|(B^*B)^{-\frac{\nu}{2}}x\| \quad \ge \quad \overline{m}^{-\nu} \|x\|_{\nu(a+s)} \qquad \textit{for all} \quad x \in \mathcal{D}((B^*B)^{-\frac{\nu}{2}}) \tag{11}$$

Furthermore, (7) *is equivalent to*

$$\begin{aligned} \mathcal{X}_{\tilde{a}} \subset \mathcal{R}(T^*) \quad \textit{and} \quad & \|T^*w\|_{\tilde{a}} \ge \underline{m}\|w\| \\ & \textit{for all} \quad w \in \mathcal{N}(T^*)^\perp \ \textit{with}\ T^*w \in \mathcal{X}_{\tilde{a}} \end{aligned} \tag{12}$$

and if (7) *holds, then it follows for all* $\nu \in [0,1]$ *that* $\mathcal{X}_{\nu(\tilde{a}+s)} \subset \mathcal{R}((B^*B)^{\frac{\nu}{2}}) = \mathcal{D}((B^*B)^{-\frac{\nu}{2}})$ *and*

$$\|(B^*B)^{\frac{\nu}{2}}x\| \quad \ge \quad \underline{m}^\nu \|x\|_{-\nu(\tilde{a}+s)} \qquad \textit{for all} \quad x \in \mathcal{X} \tag{13}$$

$$\|(B^*B)^{-\frac{\nu}{2}}x\| \quad \le \quad \underline{m}^{-\nu} \|x\|_{\nu(\tilde{a}+s)} \qquad \textit{for all} \quad x \in \mathcal{X}_{\nu(\tilde{a}+s)}. \tag{14}$$

The following result concerning convergence (rates) of iterative regularization methods in Hilbert scales under Assumptions (A1), (A2) can be found in [1, 3]. For the corresponding result for more general regularization methods and under the stronger condition 6, cf. [4, 14, 17].

Theorem 1 *Let (A1), (A2) hold,* $s \ge -a/2$ *and* x_k^δ *be generated by an iterative regularization method* g_k *satisfying*

$$\sup_{\lambda\in(0,1]} \lambda^\mu |r_k(\lambda)| \le c_\mu (k+1)^{-\mu}, \qquad 0 \le \mu \le \mu_0$$

for some $\mu_0 > 1/2$ *and with* $r_k(\lambda) := 1 - \lambda g_k(\lambda)$.

If $k_* = k_*(\delta, y^\delta)$ *is determined by the discrepancy principle* (4) *with sufficiently large* $\tau > 1$*, and* $x^\dagger$ *satisfies the source condition* (8) *with some* $0 < u \le 2(a+s)\mu_0 - a$*, then*

$$\|x_k^\delta - x^\dagger\| = O(\delta^{\frac{u}{a+u}}). \tag{15}$$

For the proof of this result and some discussion concerning the source condition (8) and the optimality of the rates (15), we refer to [1, 3]. As we will show below, a similar result also holds for the CGNE iteration in Hilbert scales.

2.2 Regularization by CGNE

The conjugate gradient method [8] is known as one of the most powerful iterative algorithms for solving symmetric positive definite problems. One possible way to approach also nonsymmetric problems, is to apply the CG method to the normal equations $T^*Tx = T^*y^\delta$. A reformulation of the corresponding algorithm yields the conjugate gradient method applied to the normal equations. The CGNE iteration (cf., e.g., [7, Algorithm 2.4] or Algorithm 1 with $L = I$) belongs to the class of Krylov subspace method, i.e., assuming that $x_0 = 0$, the iterates x_k are elements of the kth Krylov subspace

$$\mathcal{K}_k(T^*y^\delta, T^*T) = \mathrm{span}\{T^*y^\delta, \ldots, (T^*T)^{k-1}T^*y^\delta\}. \tag{16}$$

We assume that we want to solve (1) with perturbed data y^δ. The iterates x_k^δ and the residuals $d_k^\delta = y^\delta - Tx_k^\delta$ can be expressed via polynomials

$$x_k^\delta = g_k(T^*T; y^\delta)T^*y^\delta \quad \text{and} \quad d_k = r_k(T^*T; y^\delta)x^\dagger. \tag{17}$$

In contrast to linear semi-iterative methods, the residual and iteration polynomials r_k, g_k of CGNE depend on y^δ, which makes CGNE a nonlinear iterative (regularization) method, i.e., the regularization operators $R_k(y^\delta) := g_k(T^*T; y^\delta)T^*$ used to define the regularized solution depend themselves on the data. An important consequence is that no *a priori* stopping criterion of the form $k_* = k_*(\delta, x^\dagger)$ can make CGNE a regularization method, i.e., $R_k(y^\delta)$ is in general a discontinuous operator (cf. [4, Chapter 7]). On the other hand, CGNE can be turned into an order-optimal regularization method by stopping according to the discrepancy principle (4):

Theorem 2 *(cf. [4, Theorem 7.12.]) If $y \in \mathcal{R}(T)$, y^δ satisfies (2) and if the iteration is stopped according to the discrepancy principle (4) at $k_* = k_*(\delta, y^\delta)$, then CGNE is an order-optimal regularization method. If $T^\dagger y = (T^*T)^\mu w$ with $\|w\| \le \rho$ and μ, $\rho > 0$, then*

$$\|T^\dagger y - x_{k_*}^\delta\| \le c\rho^{\frac{1}{2\mu+1}}\delta^{\frac{2\mu}{2\mu+1}} \quad \text{and} \quad k_* = O(\delta^{-\frac{1}{2\mu+1}}).$$

An important property, which alternatively characterizes CGNE, is that the iterates x_k^δ satisfy the following optimality condition (cf. [4, Theorem 7.3]),

$$\|y^\delta - Tx_k^\delta\| = \min\{\,\|y^\delta - Tx\| : x - x_0 \in \mathcal{K}_k(T^*(y^\delta - Tx_0), T^*T)\}, \tag{18}$$

which implies that CGNE is the method with minimal stopping index k_* under all Krylov-subspace methods of the form (17), in particular all semi-iterative regularization methods. The following result provides a tighter estimate of the iteration numbers to be expected for certain classes of inverse problems:

Theorem 3 *(cf. [4, Theorem 7.14]) Let T be a compact operator and assume that the source condition $T^\dagger y \in \mathcal{R}((K^*K)^\mu)$ holds with for some μ. If the singular values σ_n of T decay like $O(n^{-\alpha})$ for some $\alpha > 0$, then*

$$k_*(\delta, y^\delta) = O\Big(\delta^{-\frac{1}{(2\mu+1)(\alpha+1)}}\Big). \tag{19}$$

If the singular values decay like $O(q^n)$ with some $q < 1$, then

$$k_*(\delta, y^\delta) = O\big(\max\{-\log(\delta), 1\}\big). \tag{20}$$

Remark 2 At first sight, the iteration number estimates of Theorem 3 are somewhat surprising. The standard convergence theory for CGNE applied to well-posed problems yields

$$k(\epsilon) = O(\kappa \ln(\epsilon)), \qquad \kappa = \mathrm{cond}(T), \tag{21}$$

where $k(\epsilon)$ denotes the number of iterations necessary to reduce the residual by a factor ϵ. Thus one would expect that the iteration numbers increase with increasing ill-posedness. However, conditions (19) and (20) imply that only a few singular values are larger than δ, and the components of the residual (and the error) corresponding to the eigenvectors of these singular values are reduced very efficiently by conjugate gradient type methods. Note that components of the data y^δ belonging to the eigenspaces of singular values $\sigma_n < \delta$ can in principle not be distinguished from noise.

3 Convergence analysis of the Hilbert scale CGNE algorithm

As mentioned in Remark 2, the performance of conjugate gradient iterations for well-posed problems is tightly coupled to the condition number of the involved operators (matrices), and the convergence of CG respectively CGNE applied to badly conditioned matrix equations arising, e.g., from finite element simulations, may be accelerated significantly by appropriate preconditioning techniques, i.e., by reducing the condition number of the system to be solved.

In view of Theorem 3 and the subsequent remark, the situation is different for inverse problems, where the iteration numbers depend on the ill-posedness of the equation in the opposite way. This is due to the fact that the spectrum of a compact operator (for many inverse problems T is compact) accumulates (only) at 0 and just the error components corresponding to (the few) large singular values of T give a significant contribution to the residual. As we will see below (cf. Remark 4), preconditioning in Hilbert scales can be interpreted as reducing the ill-posedness (condition number) of the problem. Thus, it is unclear, what effect our preconditioning strategy has on the performance of CGNE for inverse problems (1).

For the rest of this paper, we consider the following (preconditioned) Hilbert scale version of the CGNE method:

Algorithm 1 (HSCGNE)

$x_0 = x_*$; $d_0 = y - Tx_0$; $w_0 = T^* d_0$; $p_1 = s_0 = L^{-2s} w_0$

for $k = 1, 2, \ldots$, unless $s_{k-1} = 0$, compute

$$
\begin{aligned}
q_k &= Tp_k \\
\alpha_k &= \tfrac{\langle s_{k-1}, w_{k-1} \rangle}{\|q_k\|^2} \\
x_k &= x_{k-1} + \alpha_k p_k \\
d_k &= d_{k-1} - \alpha_k q_k \\
w_k &= T^* d_k \\
s_k &= L^{-2s} w_k \\
\beta_k &= \tfrac{\langle s_k, w_k \rangle}{\langle s_{k-1}, w_{k-1} \rangle} \\
p_{k+1} &= s_k + \beta_k p_k
\end{aligned}
$$

if $\|d_k\| \le \tau\delta$, stop (discrepancy principle)

Remark 3 By choosing $L = I$, Algorithm 1 reduces to to the standard CGNE method (cf. [4, Algorithm 7.1]). For typical problems, we have in mind, the main effort of the algorithm is the application of the operators T and $L^{-2s}T^*$. Usually, the operator L is chosen to be a simple differential operator, and the fractional powers L^{-2s} can be implemented efficiently, e.g. via FFT or multi-level techniques. Hence, the numerical effort of one step of Algorithm 1 is essentially the same as for standard CGNE and the number of iterations (stopping index) can be seen as a measure for the performance of the algorithm.

Remark 4 Under Assumption (A2), the inverse problem (1) can be understood as equation on $\mathcal{X}_s$, i.e., let $\tilde{T} : \mathcal{X}_s \to \mathcal{Y}$ denote the extension of T to $\mathcal{X}_s$ and solve

$$\tilde{T}x = y, \tag{22}$$

over $\mathcal{X}_s$. Note that the adjoint of $\tilde{T}$ with respect to $\mathcal{X}_s$ and $\mathcal{Y}$ is given by $\tilde{T}' = L^{-2s}T^*$, and thus Algorithm 1 can be viewed as standard CGNE iteration for (22) on the space $\mathcal{X}_s$. For $s < 0$ problem (22) is less ill-posed than the original problem (1). To see this, just consider the case $L^{-s} = (T^*T)^{-\frac{1}{4}}$. Then (22) is only half as ill-posed as (1), which can easily be seen from the singular value decomposition.

The subsequent convergence analysis of the HSCGNE method for inverse problems is based on the corresponding theory for CGNE presented in [4, Section 7] and [7, Section 3]. The considerations of the previous remark and Theorem 2 directly yield the following result:

Corollary 1 *Let Assumption 1 hold, x_k^δ be defined by Algorithm* (1), *and $k_* = k_*(\delta, y^\delta)$ be determined by the discrepancy principle* (4). *If the source condition* (8) *holds, then with $\tilde{\mu} = \frac{u-s}{2a}$,*

$$\|x_{k_*}^\delta - x^\dagger\|_s = O(\delta^{\frac{2\tilde{\mu}}{2\tilde{\mu}+1}}). \tag{23}$$

PROOF. With the above notation, we have

$$x^\dagger - x_0 = L^{-s}(B^*B)^{\frac{u-s}{2(a+s)}}w = (L^{-2s}T^*T)^{\frac{u-s}{2(a+s)}}L^{-s}w = (\tilde{T}^*\tilde{T})^{\frac{u-s}{2(a+s)}}v,$$

with $L^{-s}w =: v \in \mathcal{X}_s$. The rest follows immediately by Theorem 2. □

In the above corollary stability and optimal convergence is stated only with respect to the weak norm in $\mathcal{X}_s$ ($s \le 0$ by assumption). In the following we show that Algorithm 1 yields optimal convergence rates also with respect to the original norm in $\mathcal{X}_0 = \mathcal{X}$.

Throughout this section, let κ be defined by

$$\kappa := \begin{cases} \text{smallest index with } s_\kappa = 0, \\ +\infty \text{ if } s_k \neq 0 \text{ for all } k > 0. \end{cases} \tag{24}$$

For the proof of the main theorems, we require the following auxiliary results:

Lemma 1 *Let (A1), (A2), and* (8) *hold. Then, for $0 < k \le \kappa$,*

$$\|y^\delta - Tx_k^\delta\| \le \delta + c|r_k'(0)|^{-\frac{u+a}{2(a+s)}}\rho. \tag{25}$$

PROOF. Rewrite (22) as

$$B\xi = y^\delta, \qquad \xi = L^s x \in \mathcal{X},$$

with B as in Assumption 1. Now, $\xi^\dagger - \xi_0 = L^{-s}(x^\dagger - x_0) = (B^*B)^{\frac{u-s}{2(a+s)}}w$ by (8). The result then follows analogously to Lemma 7.10 in [4] by replacing T, x by B, ξ and μ by $\frac{u-s}{2(a+s)}$. □

Lemma 2 *Assume that (A1), (A2) and* (8) *hold. Then, for $0 < k \le \kappa$,*

$$\|x_k^\delta - x^\dagger\| \le c\,(\rho^{\frac{a}{u+a}}\delta_k^{\frac{u}{u+a}} + |r_k'(0)|^{\frac{a}{2(a+s)}}), \tag{26}$$

where $\delta_k := \max(\|Tx_k^\delta - y^\delta\|, \delta)$.

PROOF. Let $\{E_\lambda\}$, $\{F_\lambda\}$ denote the spectral families associated with the operators B^*B respectively BB^*. Then we have, cf. [4, Lemma 7.11],

$$\begin{aligned} \|x_k^\delta - x^\dagger\| &= \|L^{-s}(\xi_k^\delta - \xi^\dagger)\| \le \|(B^*B)^{\frac{s}{2(a+s)}}(\xi_k^\delta - \xi^\dagger)\| \\ &\le \|E_\epsilon(B^*B)^{\frac{s}{2(a+s)}}r_k(B^*B)(B^*B)^{\frac{u-s}{2(a+s)}}w\| \\ &\qquad + \|E_\epsilon(B^*B)^{\frac{s}{2(a+s)}}g_k(B^*B)B^*(y - y^\delta)\| + \epsilon^{-\frac{a}{2(a+s)}}\|y - B\xi_k^\delta\| \\ &\le \|\lambda^{\frac{u}{2(a+s)}}r_k(\lambda)\|_{\mathcal{C}[0,\epsilon]}\rho + \|\lambda^{\frac{a+2s}{2(a+s)}}g_k(\lambda)\|_{\mathcal{C}[0,\epsilon]}\delta + \epsilon^{-\frac{a}{2(a+s)}}(\|y^\delta - Tx_k^\delta\| + \delta). \end{aligned}$$

Like in the proof of Lemma 7.11 in [4], we have for $\epsilon < \lambda_{1,k}$ (where $\{\lambda_{i,k}\}$ denotes the increasing sequence of roots of the polynomial r_k) that r_k is convex in $[0, \epsilon]$ and hence

$$0 \leq \lambda^{\frac{a+2s}{2(a+s)}} g_k(\lambda) = \left(\frac{1-r_k(\lambda)}{\lambda}\right)^{\frac{a}{2(a+s)}} \left(1-r_k(\lambda)\right)^{\frac{a+2s}{2(a+s)}} \leq |r_k'(0)|^{\frac{a}{2(a+s)}}$$

holds for $0 \leq \lambda \leq \epsilon$. Therefore,

$$\|x_k^\delta - x^\dagger\| \leq \epsilon^{\frac{u}{2(a+s)}} \rho + |r_k'(0)|^{\frac{a}{2(a+s)}} \delta + 2\epsilon^{-\frac{a}{2(a+s)}} \delta_k =: f(\epsilon).$$

Note that $f(\epsilon)$ is monotonically decreasing in $(0, \epsilon_*)$ and increasing in (ϵ_*, ∞), with $\epsilon_*^{\frac{u+a}{2(a+s)}} = \frac{2a}{u}\frac{\delta_k}{\rho}$. The rest of the proof follows the lines of the proof of Lemma 7.11 in [4]. □

Combining the previous lemmata yields the following convergence rate result:

Theorem 4 *Let (A1), (A2) hold, and Algorithm 1 be stopped according to the discrepancy principle* (4) *with $k_* = k_*(\delta, y^\delta)$. If the source condition* (8) *holds, then*

$$\|x_{k_*}^\delta - x^\dagger\| = O(\delta^{\frac{u}{a+u}}). \tag{27}$$

Proof. Note, that by Lemma 1, we have with $k = k_*(\delta, y^\delta)$,

$$|r_{k-1}'(0)| \leq c\left(\frac{\rho}{\delta}\right)^{\frac{2(a+s)}{u+a}}.$$

Replacing T and x by B and ξ, and $\frac{2}{2\mu+1}$ by $\frac{2(a+s)}{u+a}$, the result follows with obvious modifications of the proof of Theorem 7.12 in [4]. □

Remark 5 The convergence rates in Theorem 4 also hold in the stronger norm $|\!|\!| x_{k_*}^\delta - x^\dagger |\!|\!|$ defined by

$$|\!|\!| x |\!|\!| := \|(B^*B)^{\frac{s}{2(a+s)}} L^s x\|,$$

which is the norm of the shifted Hilbert scale space (cf. [3])

$$\mathcal{X}^s := \mathcal{D}((B^*B)^{\frac{s}{2(a+s)}} L^s).$$

One can show that the corresponding rates are order optimal; cf. [1, 3] for a similar treatment of Landweber iteration and semi-iterative methods in Hilbert scales. Note that HSCGNE has no saturation, i.e., Theorem 4 holds for all $u > 0$. If the stronger condition (6) holds instead of (A2) and if $0 < u \leq a + 2s$, then the spaces $\mathcal{R}(L^{-s}(B^*B)^{\frac{u-s}{2(a+s)}})$ and $\mathcal{R}((T^*T)^{\frac{u}{2a}})$ coincide with equivalent norms, cf. [1, Remark 3.7]; in particular, (8) amounts to $x^\dagger - x_0 \in \mathcal{R}(T^*T)^\mu$ with $\mu = \frac{u}{2a}$.

Next we show that similar to Theorem 3, the number of iterations can be bounded more tightly for certain classes of operators T^* :

Theorem 5 *Let Assumptions (A1), (A2) hold, $B := TL^{-s}$ be a compact operator and* (8) *hold. If the singular values $\tilde{\sigma}_n$ of B decay like $O(n^{-\tilde{\alpha}})$ with some $\tilde{\alpha} > 0$, then*

$$k_*(\delta, y^\delta) = O\left(\delta^{-\frac{a+s}{(a+u)(\tilde{\alpha}+1)}}\right).$$

If the singular values decay like $O(\tilde{q}^n)$ with some $\tilde{q} < 1$, then

$$k_*(\delta, y^\delta) = O\Big(\max(-\log(\delta), 1)\Big).$$

Proof. The proof follows the lines of the proof of Theorem 7.14 in [4]; we only mention the main differences: For given y^δ, denote by $\{r_k\}$ the residual polynomials of CGNE applied to (22) with operator $\tilde{T} : \mathcal{X}_s \to \mathcal{Y}$. Not that we have

$$y^\delta - Tx_k^\delta = r_k(BB^*)y^\delta,$$

and that the following extremal property holds:

$$\|y^\delta - Tx_k^\delta\| = \min\{\|y^\delta - Tx\| : x - x_0 \in \mathcal{K}_k(L^{-2s}T^*(y^\delta - Tx_0), L^{-2s}T^*T)\}.$$

This in turn implies that

$$\|y^\delta - Tx_k^\delta\| \le \|p_k(BB^*)y^\delta\|,$$

for arbitrary polynomials $\{p_k\}$ with $p_k(0) = 1$. The rest follows the lines of the proof of [4, Theorem 7.14]. □

Remark 6 If the stronger condition (6) holds, and $0 < u \le a + 2s$, then one can compare the above estimate with Theorem 3 in the following way: By Proposition 1 we have $(B^*B)^{\frac{\nu}{2}} \sim L^{-\nu(a+s)}$ and $(T^*T)^{\frac{\nu}{2}} \sim L^{-\nu a}$ for $|\nu| \le 1$. Consequently, if the singular values of T decay like $O(n^{-\alpha})$, the corresponding singular values of B decay like $O(n^{-\tilde{\alpha}})$, with $\tilde{\alpha} = \alpha\frac{a+s}{a}$. Additionally, cf. Remark 5 or [1, Remark 3.7], one has $\mathcal{R}(L^{-s}(B^*B)^{\frac{u-s}{2(a+s)}}) = \mathcal{R}((T^*T)^\mu)$ for $u \le a + 2s$ and with $\mu = \frac{u}{2a}$. This implies that the stopping index for for a preconditioned method (we write $k_*(\delta, y^\delta; s)$ in order to emphasize the dependence on s) satisfies

$$k_*(\delta, y^\delta; s) \le O(\delta^{-f(s)}) \qquad \text{with} \qquad f(s) = \frac{a+s}{(a+u)(\alpha\frac{a+s}{a} + 1)},$$

which is a strictly increasing function of s. Thus stopping index of HSCGNE with $s < 0$ can be expected to be smaller than for standard CGNE. Note, that for $s = 0$ (no preconditioning; standard CGNE) we have

$$f(0) = \frac{a}{(a+u)(\alpha+1)} = \frac{1}{(2\mu+1)(\alpha+1)}$$

which coincides with the estimate of Theorem 3 for standard CGNE.

Remark 7 In [2], Hilbert scales over the image space $\mathcal{Y}$ have been used for the preconditioning of iterative regularization methods. This enables to apply the Hilbert scale framework also to problems satisfying

$$\|T^*y\| \le \|y\|_{-a}, \qquad \text{for some } a > 0 \tag{28}$$

instead of (A2). Here $\|y\|_r = \|L^r y\|_{\mathcal{Y}}$, i.e., the operator L acts on the space $\mathcal{Y}$ and generates a scale of spaces $\{\mathcal{Y}_r\}_{r\in\mathbb{R}}$. We only mention that such an approach is in principle also applicable for preconditioning of CGNE. Note however that under the relaxed assumption (28) without a lower bound, the discrepancy principle is in general not an adequate stopping rule, and therefor different stopping rules have to be considered.

4 Examples and numerical tests

The aim of this section is to verify condition $(A2)$ for some examples and to illustrate the effect of preconditioning applied to CGNE iterations for ill-posed problems. As outlined above, we are especially interested in the reconstruction of non-smooth solutions, and therefor choose solutions with jumps in our numerical tests. Throughout, the data are constructed numerically (on finer grids) and are additionally perturbed by adding randomly distributed noise.

Example 1 (An inverse source problem in an elliptic PDE)

Let Ω be a bounded domain in $\mathbb{R}^n$, $n = 2, 3$ with smooth boundary $\partial\Omega \in \mathcal{C}^{1,1}$. We consider the operator $T : L_2(\Omega) \to L_2(\Omega)$ defined by $Tf = u$, with

$$Au := -\nabla \cdot (q\nabla u) + p \cdot \nabla u + cu = f, \qquad u|_{\partial\Omega} = 0, \tag{29}$$

with sufficiently smooth parameters given q, p and c. Assume that A is uniformly elliptic; then a solution u of (29) lies in $H^2(\Omega)\cap H_0^1(\Omega)$ and satisfies $\|u\|_{H^2} \sim \|f\|_{L_2}$, i.e., A is an isomorphism between $H^2(\Omega)\cap H_0^1(\Omega)$ and $L_2(\Omega)$. For preconditioning, we use the Hilbert scale induced by $L^2u = -\Delta u$ over the space $X = L_2(\Omega)$ with $\mathcal{X}_2 = H^2(\Omega)\cap H_0^1(\Omega)$. Then we have $T \sim L^{-2}$, and thus (A2) holds with $a = 2$. Moreover, the stronger condition (6) holds.

For a numerical test, we set $\Omega = [0,1]^2$, $q = c = 1$, $p = 0$, $s = -a/2 = -1$, and try to identify the function

$$f^\dagger = \operatorname{sign}(x - 0.5)\cdot \operatorname{sign}(y - 0.5)$$

from $f_0 = 0$ as a starting value. In this setting, we have $f^\dagger - f_0 \in \mathcal{R}((T^*T)^\mu)$ for all $0 \le \mu < 1/8$, or equivalently, $f^\dagger \in \mathcal{X}_r^s$ for all $r < 1/2$.

$\frac{\delta}{\|u^\delta - u_0\|}$	it(cg)	err(cg)	it(hscg)	err(hscg)
0.016	14	0.3418	6	0.4291
0.008	18	0.2966	8	0.3887
0.004	30	0.2439	10	0.2955
0.002	44	0.2050	13	0.2579

Table 1: Iteration numbers and errors $\|x_{k_*}^\delta - x^\dagger\|$ for CGNE (cg) and HSCGNE (hscg) respectively; Example 1

In this 2D example the eigenvalues of T behave like $\sigma_n \sim \frac{1}{n}$, which by Theorems 3, 5 and Remark 6 yields the following estimates for the stopping indices: $k_*^{(cg)} = O(\delta^{-\frac{2}{5}})$ and $k_*^{(hscg)} = O(\delta^{-\frac{4}{15}})$. The iteration numbers actually observed are listed in Table 1 and yield $k_*^{(cg)} \sim \delta^{-0.56}$ and $k_*^{(hscg)} \sim \delta^{-0.36}$. We think that the deviation from the predicted results is mainly due to the small iteration numbers where calculating the rates is somewhat sensitive. We want to mention that although the errors of the reconstruction obtained with HSCGNE are a bit larger than those of CGNE, in particular the jumps in $x^\dagger$ are resolved much better by the preconditioned method. This can be explained by the fact that the HSCGNE updates are less smooth than those without preconditioning.

Example 2 (A slightly degenerate Fredholm integral equation of the first kind)

Let $T : L_2[0,1] \to L_2[0,1]$ be defined by

$$(Tx)(s) = \int_0^1 s^{1/2} k(s,t)x(t)dt,$$

with the standard Green's kernel

$$k(s,t) = \begin{cases} s(1-t)\,, & t > s\,, \\ t(1-s)\,, & s \ge t\,. \end{cases}$$

For application of our preconditioning strategy we have to verify (A2) for an appropriate choice of a Hilbert scale: First note that

$$(T^*y)(t) = (1-t)\int_0^t s^{3/2}y(s)ds + t\int_t^1 s^{1/2}(1-s)y(s)ds,$$

with $(T^*y)(0) = (T^*y)(1) = 0$. Furthermore, one can show that $(T^*y)'' = (\cdot)^{1/2}y$. Hence,

$$\mathcal{R}(T^*) = \{w \in \mathcal{H}^2[0,1]\cap \mathcal{H}_0^1[0,1] : (\cdot)^{-1/2}w'' \in \mathcal{L}_2[0,1]\}.$$

We define the Hilbert scale operator L by

$$L^s x := \sum_{n=1}^\infty (n\pi)^s \langle x, x_n \rangle x_n, \qquad x_n := \sqrt{2}\sin(n\pi\cdot),$$

which yields $L^2x = -x''$. With this choice, we have

$$\mathcal{R}(T^*) \subsetneq \mathcal{X}_2 := \mathcal{H}^2[0,1] \cap \mathcal{H}^1_0[0,1]$$

and additionally,

$$\mathcal{R}(T^*) \supset \mathcal{X}_{2.5} := \{w \in \mathcal{H}^{2.5}[0,1] \cap \mathcal{H}^1_0[0,1] : \rho^{-1/2}w'' \in \mathcal{L}_2[0,1]\},$$

with $\rho(t) = t(1-t)$. By Theorem 11.7 in [12], it follows that

$$\|w\|^2_{2.5} \simeq \|w''\|^2_{\mathcal{H}^{1/2}} + \|\rho^{-1/2}w''\|^2_{\mathcal{L}_2}$$

and thus for $T^*y \in \mathcal{X}_{2.5}$,

$$\begin{aligned}
\|T^*y\|^2_{2.5} &\sim \|(\cdot)^{1/2}y\|^2_{H^{1/2}} + \|\rho^{-1/2}(\cdot)^{1/2}y\|^2_{\mathcal{L}_2} \\
&\geq \|(\cdot)^{1/2}y\|^2_{\mathcal{L}_2} + \|\rho^{-1/2}(\cdot)^{1/2}y\|^2_{\mathcal{L}_2} \\
&= \left(\int_0^1 ty(t)^2dt + \int_0^1 (1-t)^{-1}y(t)^2dt\right) \geq c\|y\|^2_{\mathcal{L}_2}.
\end{aligned}$$

Together with $\|T^*y\|_2 = \|(\cdot)^{1/2}y\| \leq \|y\|$ and Proposition 1 it follows that there exist constants $0 < \underline{m} \leq \overline{m} < \infty$ such that

$$\underline{m}\|x\|_{-2.5} \leq \|Tx\| \leq \overline{m}\|x\|_{-2}. \tag{30}$$

For a numerical test, we consider the reconstruction of the unknown function

$$x^\dagger(s) = 2t - \operatorname{sign}(2t-1) - 1, \tag{31}$$

and choose $s = -1$ and $x_0 = 0$. Note, that $x^\dagger$ is discontinuous at $t = 1/2$, and thus we only have $x^\dagger \in H^{1/2-\epsilon}(\Omega)$ for arbitrary $\epsilon > 0$, which implies that $x^\dagger$ lies at most in $\mathcal{X}_{1/2} \supset \mathcal{X}^s_{1/2}$. Thus, one cannot expect faster convergence than $\|x^\delta_k - x^\dagger\| = O(\delta^{1/5})$. In view of Theorem 4, we expect to get the optimal convergence rates $\|x^\delta_{k_*} - x^\dagger\| = O(\delta^{1/5})$ for both, the preconditioned and the standard CGNE method. The iteration numbers and errors obtained by numerical simulation are listed in Table 2.

$\delta/\|y\|$	it(cg)	err(cg)	it(hscg)	err(hscg)
0.016	5	0.3892	4	0.3595
0.008	6	0.3328	5	0.3135
0.004	9	0.2842	6	0.2669
0.002	12	0.2498	7	0.2388

Table 2: Iteration numbers and errors $\|x^\delta_{k_*} - x^\dagger\|$ the CGNE and HSCGNE method; Example 2.

Example 3 (An Abel integral equation)

Let $T : L_2[0,1] \to L_2[0,1]$ be defined by

$$(Tx)(s) := \frac{1}{\sqrt{\pi}} \int_0^s \frac{x(t)}{\sqrt{s-t}}dt, \tag{32}$$

and consider the approximate reconstruction of x from noisy data y^δ with $\|y - y^\delta\| \leq \delta$, where $y = Tx^\dagger$ denotes the unperturbed data. One can show that

$$(T^2x)(s) = \int_0^s x(t)dt, \tag{33}$$

and thus inverting T essentially amounts to differentiation of half order; more precisely, cf. [5],

$$\mathcal{R}(T) \subset \mathcal{H}^r[0,1], \qquad \text{for all} \quad 0 \leq r < 1/2. \tag{34}$$

Now consider the Hilbert scale induced by

$$L^{2s}x = \sum_{n=0}^{\infty} \lambda_n^s \langle x, x_n \rangle x_n, \qquad x_n(t) = \sqrt{2}\sin(\lambda_n(1-t)), \quad \lambda_n = (n+1/2)\pi, \tag{35}$$

over $\mathcal{X} = L_2[0,1]$ with $\mathcal{D}(L^2) = \mathcal{X}_2 = \{x \in H^1[0,1] : x(1) = 0\}$. Then one can show that $\mathcal{R}(T^*T) \subset \mathcal{X}_r$ for all $r < 2$, and (A2) holds for any $a = 1 - \epsilon$ with $\epsilon > 0$. This allows the choice $s = -(1-\epsilon)/2$, and hence the iterations can be preconditioned with $L^{1-\epsilon}$, which for small ϵ essentially corresponds to differentiation of order 1/2, and can be realized efficiently via (35) and FFT.

As a numerical test, we again try to identify the density (31) from noisy measurements of $y = Tx^\dagger$ and an initial guess $x_0 = 0$. With the Hilbert scale defined by (35) one has $x^\dagger \in \mathcal{X}_u$ for all $u < 3/2$. We wet $s = -1$, which is the limiting case of allowed choices. By (34) it follows that the singular values of T decay like $\sigma_n \sim n^{-1/2}$, which in view of Theorems 3 and 5 yields the estimates $k_* \sim \delta^{-1/3}$ for CGNE and $k_* \sim \delta^{-1/5}$ for HSCGNE. The iteration numbers and errors realized in our numerical tests are listed in Table 3.

$\delta/\|y\|$	it(xg)	err(cg)	it(hscg)	err(hscg)
0.02	6	0.1355	4	0.1270
0.01	8	0.1085	5	0.0935
0.005	10	0.0817	6	0.0715
0.0025	14	0.0538	7	0.0523

Table 3: Iteration numbers and errors $\|x_{k_*}^\delta - x^\dagger\|$ for CGNE and HSCGNE; Example 3.

The observed rates for the stopping indices are $k_*^{(cg)} \sim \delta^{-0.39}$ and $k_*^{(hscg)} \sim \delta^{-0.26}$, and the convergence rates are $\|x_{k_*}^\delta - x^\dagger\| \sim \delta^{0.43}$ for both iterations, which is in good correspondence to the rate $O(\delta^{\frac{3}{7}})$ predicted by the theory.

Example 4 (An exponentially ill-posed problem)

Let us consider the backwards heat equation $Tu = f$ with $T : L_2[0,1] \to L_2[0,1]$ defined by $Tf = u(\cdot, t_1)$ and u denoting the solution of

$$-u_t + u_{xx} = 0, \qquad u(0,t) = u(1,t) = 0, \qquad u(x,0) = f(x). \tag{36}$$

The operator T is selfadjoint, with eigenvalues $\lambda_n = e^{-n^2\pi^2 t_1}$ and associated eigenfunctions $\psi_n = \sqrt{\frac{2}{\pi}}\sin(n\pi\cdot)$. Consequently, the inverse problem of solving $Tf = u$ is exponentially ill-posed.

We consider this problem as a model for more complicated severely ill-posed problems and investigate its solution by CGNE and HSCGNE. For preconditioning, we use

$$Lf = \sum_{n=0}^{\infty} n\pi \langle f, \psi_n \rangle \psi_n, \qquad \psi_n = \sqrt{2}\sin(n\pi\cdot)$$

over $\mathcal{X} = L_2[0,1]$ and with $X_1 = H_0^1[0,1]$. This choice implies that for all $0 \le a < 2.5$ there exists an $\overline{m}_r > 0$ such that

$$\|Tf\| \le \overline{m}_r \|f\|_{-a}.$$

Thus, (A2) holds for every $0 \le a < 2.5$. On the other hand, an estimate (7) from below cannot be satisfied for any $\tilde{a}$.

We want to mention that a source condition $L^s f^\dagger \in \mathcal{R}((B^*B)^\mu)$ or $f^\dagger \in \mathcal{R}((T^*T)^\mu)$ for some $\mu > 0$ is of course very strong, i.e., it means that $f^\dagger$ has to be analytic. Thus, for exponentially ill-posed problems usually *logarithmic source conditions* are used, and only logarithmic convergence rates can be expected (cf. [9, 10]), and it would be interesting to extend our theory also to this case. Note, however, that only components corresponding to singular values $\sigma_n \ge \delta$ will play a role in the reconstruction of $x^\dagger$, and thus for finite noise-levels $\delta \ge \delta_0 > 0$ even exponentially ill-posed problems behave numerically like a few times differentiation (cf., e.g., [3]).

As a concrete numerical test we try to identify

$$f^\dagger(x) := 2x - \mathrm{sign}(2x-1) - 1,$$

from noisy measurements of $u(\cdot,1)$, where u satisfies (36) with $t_1 = 0.01$. As initial guess, we choose $f_0 = 0$. In Table 4, we list the iteration numbers of the numerical reconstructions for CGNE and the preconditioned version HSCGNE.

$\delta/\|y\|$	it(cg)	err(cg)	it(hscg)	err(hscg)
0.016	2	0.4866	2	0.4808
0.008	5	0.4148	3	0.4144
0.004	5	0.4149	3	0.4144
0.002	5	0.4149	3	0.4145

Table 4: Iteration numbers and errors $\|x^\delta_{k_*} - x^\dagger\|$ for CGNE and HSCGNE; Example 4.

According to Theorems 3 and 5, the stopping indices for CGNE and HSCGNE are bounded by $k_*(\delta, y^\delta) \le c\,(1+|\log\delta|)$ for exponentially ill-posed problems, which explains that the observed iteration numbers are almost independent of the noise level. The convergence rates are $\|e^\delta_{k_*}\| \sim \delta^{0.065}$ for both methods. As expected, the numerically realized rates further decrease when with smaller noise levels.

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