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AN ITERATIVE STABILIZATION METHOD FOR THE EVALUATION OF UNBOUNDED OPERATORS

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Abstract. We investigate a stable iterative approximate evaluation method for closed unbounded operators such as those that occur frequently in inverse problems. Convergence theorems, as well as order of approximation results, are proved for both *a priori* and *a posteriori* schemes for choosing the stopping index of the iteration.

1. Introduction

Numerous inverse problems in the mathematical sciences may be formulated as operator equations of the first kind, $Ky = x$, where K is a compact linear operator acting on a Hilbert space (see e.g. [3]). The accepted solution of such an inverse problem is $y = K^\dagger x$, where $K^\dagger$ is the Moore-Penrose generalized inverse of K. The principal difficulty in dealing with such an inverse problem lies not in the computation of $K^\dagger$ but in the intrinsic ill-posed nature of the problem. This ill-posedness is manifested by the fact that $K^\dagger$ is, except in trivial cases (see e.g. [1], pp. 116-118), a closed but *unbounded* linear operator. The upshot is instability: vanishingly small errors in the data x can express themselves as unbounded perturbations in the generalized solution $y = K^\dagger x$. An effective solution procedure therefore consists of two ingredients: an approximation of $K^\dagger$ and a stabilization procedure to damp spurious oscillations.

This note is a theoretical investigation of the second part of this process as a problem in its own right. That is, we consider the problem of stabilized approximate evaluation of a closed unbounded linear operator, given approximate data that is not necessarily in the domain of the operator. By stabilized evaluation we mean that the value of the unbounded operator at a given vector in its domain is approximated by applying certain *bounded* linear operators to approximate data vectors that are not necessarily in the domain of the unbounded operator. The beginning of a general scheme of stable evaluation is sketched in [2], but in this note we investigate in some detail a specific iterative stabilization method that is inspired by functional interpolation. Our main interest is convergence theory. We provide convergence results and orders of convergence with respect to the error amplitude in the data

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which are arbitrarily near to the optimal order for both *a priori* and *a posteriori* choices of the iteration number.

2. An iterative method

Suppose $L : \mathcal{D}(L) \subseteq H_1 \to H_2$ is a closed linear operator defined on a dense subspace $\mathcal{D}(L)$ of a Hilbert space H_1 and taking values in a Hilbert space H_2. In many applications the challenge is to evaluate L at a vector $x \in \mathcal{D}(L)$, given an approximate data vector $x^\delta \in H_1$ satisfying $\|x - x^\delta\| \le \delta$, where δ is a known "noise amplitude" in the data. Given such an approximation $x^\delta \in H_1$ to a vector $x \in \mathcal{D}(L)$, we treat a specific method of forming stable (i.e., continuous in x^δ) approximations $y_n(x^\delta)$ to Lx with the property that $y_{n(\delta)}(x^\delta) \to Lx$ as $\delta \to 0$ if $n = n(\delta) \to \infty$ in an appropriate fashion. Our primary interest is convergence theory, including order of convergence results. In the case $x^\delta \in \mathcal{D}(L)$, it follows that Lx^δ converges to Lx whenever $\{Lx^\delta\}$ is Cauchy, since L is closed: however, as L is unbounded, in general it can happen that Lx^δ might not converge to anything. Note that since generally $x^\delta \notin \mathcal{D}(L)$ it simply will not do to take Lx^δ as an approximation to Lx.

Morozov [7] (Chapter IV) has investigated stable approximations to Lx of the form

$$y_\alpha^\delta = L(I + \alpha L^* L)^{-1} x^\delta, \tag{1}$$

where α is a positive regularization parameter. This method requires a new inversion for each new choice of the parameter α and, as is shown in [4], has a best possible order of approximation $\|Lx - y_\alpha^\delta\| = O(\delta^{2/3})$, where δ is the noise amplitude in the data. The iteration method investigated here requires only a single inversion (see the illustration in the final section) and is capable of achieving orders of approximation arbitrarily close to the optimal order $O(\delta)$, that is, the order of the noise amplitude in the data.

The method we propose makes crucial use of an idea that Lardy [6] employed in a different context, namely von Neumann's theorem, which asserts that each of the operators

$$\widetilde{L} := (I + L^* L)^{-1} \quad \text{and} \quad \widehat{L} := (I + LL^*)^{-1}$$

is bounded and self-adjoint and the operators $L\widetilde{L}$ and $L^*\widehat{L}$ are bounded contractions (see e.g. [8], p. 307). We note that $L\widetilde{L}x = \widehat{L}Lx$ for all $x \in \mathcal{D}(L)$ and hence

$$LP(\widetilde{L})x = P(\widehat{L})Lx \quad \text{for all} \quad x \in \mathcal{D}(L) \tag{2}$$

and any polynomial P.

Our approach to stabilization is motivated by the fact that L is an extension of the operator $L\widetilde{L}\widetilde{L}^{-1}$. This suggests approximations of the form $y_n^\delta = Lx_n^\delta$, where $x_n^\delta = \widetilde{L}T_n(\widetilde{L})x^\delta$ and T_n are continuous functions on $[0,1]$ that approximate $1/t$ in some sense (see [2] for some general results along these lines). Note that, since the operators $L\widetilde{L}$ and $T_n(\widetilde{L})$ are bounded, the approximations $y_n^\delta = (L\widetilde{L})T_n(\widetilde{L})x^\delta$ are *stable*, that is, continuous with respect to x^δ, for each n. We consider a simple iterative approximation scheme suggested by interpolatory function theory.

Let T_n be the polynomial of degree not greater than $n-1$ that interpolates the function $f(t) = 1/t$ at $t = \beta_1^{-1}, \beta_2^{-1}, \ldots, \beta_n^{-1}$, where $\{\beta_j\}$ are positive numbers satisfying $1 \geq \beta_n \to 0$ as $n \to \infty$ and $\sum \beta_j \to \infty$, that is,

$$T_n(t) = \frac{1}{t}\left(1 - \prod_{j=1}^{n}(1-\beta_j t)\right).$$

Note that $\{T_n\}$ is given iteratively by $T_1(t) = \beta_1$ and

$$T_{n+1}(t) = \beta_{n+1} + (1-\beta_{n+1}t)\,T_n(t), \quad n = 1, 2, \ldots. \tag{3}$$

Given an approximation $x^\delta \in H_1$ to $x \in \mathcal{D}(L)$ we therefore study the approximations y_n^δ to Lx defined by

$$y_{n+1}^\delta = \beta_{n+1} L\widetilde{L}x^\delta + \left(I - \beta_{n+1}\widehat{L}\right) y_n^\delta, \quad n = 0, 1, \ldots, \qquad y_0^\delta = 0. \tag{4}$$

Equivalently we may formulate this as $y_n^\delta = Lx_n^\delta$, where

$$x_{n+1}^\delta = \beta_{n+1}\widetilde{L}x^\delta + \left(I - \beta_{n+1}\widetilde{L}\right) x_n^\delta, \quad n = 0, 1, \ldots, \qquad x_0^\delta = 0. \tag{5}$$

Our analysis will use iteratively defined sequences $\{y_n\}$ and $\{x_n\}$ which satisfy the same relationships using the ideal data vector x rather than the available data vector x^δ

$$y_{n+1} = \beta_{n+1} L\widetilde{L}x + \left(I - \beta_{n+1}\widehat{L}\right) y_n, \quad n = 0, 1, \ldots, \qquad y_0 = 0, \tag{6}$$

$$x_{n+1} = \beta_{n+1}\widetilde{L}x + \left(I - \beta_{n+1}\widetilde{L}\right) x_n, \quad n = 0, 1, \ldots, \qquad x_0 = 0. \tag{7}$$

The convergence of the method will depend on the parameter

$$\sigma(n) = \sum_{j=1}^{n} \beta_j.$$

Theorem 2.1. *Suppose $x \in \mathcal{D}(L)$ and $\|x - x^\delta\| \leq \delta$. If $n = n(\delta) \to \infty$ while $\delta^2\sigma(n(\delta)) \to 0$, then $\|Lx - y_{n(\delta)}^\delta\| \to 0$.*

Proof. We begin by considering the approximations with "clean" data, that is, the approximations y_n and x_n defined by equations (6) and (7), respectively. We then have

$$Lx - Lx_n = L\left(\prod_{j=1}^{n}(I - \beta_j\widetilde{L})\right)x = \left(\prod_{j=1}^{n}(I - \beta_j\widehat{L})\right)Lx.$$

However, since $\beta_j \in (0,1]$ and $\sum_{j=1}^{\infty}\beta_j = \infty$ we see that

$$\lim_{n\to\infty}\prod_{j=1}^{n}(1-\beta_j t) = \begin{cases} 1, & t = 0, \\ 0, & t \in (0,1], \end{cases}$$

in a uniformly bounded fashion. Therefore, in applying the spectral theorem to the self-adjoint bounded operator $\widehat{L}$ we find that

$$Lx - y_n = \left(\prod_{j=1}^{n}(I - \beta_j\widehat{L})\right)Lx \to 0, \quad \text{as} \quad n \to \infty.$$

Note that $y_n = L\widetilde{L}T_n(\widetilde{L})x$ and since $R(\widetilde{L}) \subseteq \mathcal{D}(L^*L)$ we have

$$y_n - y_n^\delta = L\widetilde{L}T_n(\widetilde{L})(x - x^\delta) \in \mathcal{D}(L^*).$$

The stability error may be bounded as follows:

$$
\begin{aligned}
\|y_n - y_n^\delta\|^2 &= \langle L^*L\widetilde{L}T_n(\widetilde{L})(x - x^\delta), \widetilde{L}T_n(\widetilde{L})(x - x^\delta)\rangle \\
&= \langle (I - \widetilde{L})T_n(\widetilde{L})(x - x^\delta), \widetilde{L}T_n(\widetilde{L})(x - x^\delta)\rangle \qquad (8)\\
&\le \delta^2 \|(I - \widetilde{L})T_n(\widetilde{L})\| \|\widetilde{L}T_n(\widetilde{L})\|.
\end{aligned}
$$

By (3)

$$|(1-t)T_{n+1}(t)| \le \beta_{n+1} + |(1-t)T_n(t)|$$

and hence

$$\max_{t\in[0,1]} |(1-t)T_n(t)| \le \sum_{j=1}^{n} \beta_j = \sigma(n).$$

Therefore, since $|tT_n(t)| \le 1$, we obtain from (8) that

$$\|y_n - y_n^\delta\|^2 \le \delta^2 \sigma(n),$$

and so

$$\|Lx - y_n^\delta\| \le \|Lx - y_n\| + \delta\sqrt{\sigma(n)}, \tag{9}$$

giving the result.

3. A priori stopping scheme

To obtain a convergence rate we will use the inequality

$$0 \le (1 - tT_n(t))t^\nu \le t^\nu \prod_{j=1}^{n} e^{-t\beta_j} = t^\nu e^{-\sigma(n)t}$$

for $t \in [0,1]$ and $\nu > 0$. The function on the right of the inequality above achieves for $t \in [0,1]$ a maximum value of $\nu^\nu (e\sigma(n))^{-\nu}$ and hence

$$|(1 - tT_n(t))t^\nu| \le \left(\frac{\nu}{e}\right)^\nu \sigma(n)^{-\nu} \tag{10}$$

for $t \in [0,1]$.

Theorem 3.1. *If $x \in \mathcal{D}(L)$ and $Lx \in R(\widehat{L}^\nu)$ for some $\nu > 0$, then*

$$\|Lx - y_n\| = O(\sigma(n)^{-\nu}),$$

where y_n is defined by (6).

Proof. Suppose that $Lx = \widehat{L}^\nu w$. Then by the spectral theorem and inequality (10) we have

$$
\begin{aligned}
\|Lx - y_n\| &= \|Lx - L\widetilde{L}T_n(\widetilde{L})x\| = \|Lx - \widehat{L}T_n(\widehat{L})Lx\| \\
&= \|(I - \widehat{L}T_n(\widehat{L}))\widehat{L}^\nu w\| \le \left(\tfrac{\nu}{e}\right)^\nu \sigma(n)^{-\nu}\|w\| = O(\sigma(n)^{-\nu}).
\end{aligned}
$$

Combining Theorem 3.1 with inequality (9) we obtain:

Theorem 3.2. *Suppose $x \in \mathcal{D}(L)$, $\|x - x^\delta\| \le \delta$ and $Lx \in R(\widehat{L}^\nu)$ for some $\nu > 0$. If the iteration parameter $n = n(\delta)$ is chosen so that $\sigma(n(\delta)) \sim \delta^{-2/(2\nu+1)}$, then*

$$\|y_{n(\delta)}^\delta - Lx\| = O(\delta^{2\nu/(2\nu+1)}).$$

4. A posteriori stopping scheme

Under appropriate conditions this method can achieve order of convergence rates that are arbitrarily close to the optimal order $O(\delta)$ by use of an *a posteriori* choice of the iteration parameter rather than with an *a priori* choice as in Theorem 3.2. In fact, note that the vectors defined by equations (7) and (6) satisfy

$$y_n = L\left(I - \prod_{j=1}^{n}\left(I - \beta_j \widetilde{L}\right)\right) x = Lx_n, \tag{11}$$

where

$$x_n = \left(I - \prod_{j=1}^{n}\left(I - \beta_j \widetilde{L}\right)\right) x, \quad x_0 = 0, \tag{12}$$

and $\{y_n^\delta\}$ and $\{x_n^\delta\}$ satisfy the same relationships, respectively, with x replaced by x^δ. The approximations $\{x_n^\delta\}$ can be compared with the available data x^δ in order to monitor the convergence of $\{y_n^\delta\}$ to Lx. First note that $x_n^\delta \to x^\delta$ as $n \to \infty$ and

$$\|x^\delta - x_n^\delta\| = \left\|\left(I - \beta_n \widetilde{L}\right)(x^\delta - x_{n-1}^\delta)\right\| \le \|x^\delta - x_{n-1}^\delta\|.$$

We assume that for a given constant $\tau > 1$, the signal-to-noise ratio (i.e., the ratio of the signal amplitude $\|x^\delta\|$ and the noise amplitude δ) is not less than τ. That is, we assume that

$$\|x^\delta - x_0^\delta\| = \|x^\delta\| \ge \tau\delta.$$

There is then a first value $n = n(\delta) \ge 1$ of the iteration index for which

$$\|x^\delta - x_{n(\delta)}^\delta\| < \tau\delta. \tag{13}$$

Note that this iteration number is chosen in an *a posteriori* manner as the computation proceeds. The remainder of our discussion is patterned on the general line of reasoning in [5].

Lemma 4.1. *If $x_{n(\delta)}$ is given by* (12) *where $n(\delta)$ satisfies* (13), *then*

$$\|x - x_{n(\delta)}\| \le (\tau + 1)\delta.$$

Proof. From (12), using the approximate data x^δ in one case and "clean" data $x \in \mathcal{D}(L)$ in the other, we have

$$x_{n(\delta)}^\delta - x_{n(\delta)} = \left(I - \prod_{j=1}^{n(\delta)}(I - \beta_j \widetilde{L})\right)(x^\delta - x).$$

Now

$$\begin{aligned} x - x_{n(\delta)} &= x^\delta - x_{n(\delta)}^\delta + x - x^\delta + x_{n(\delta)}^\delta - x_{n(\delta)} \\ &= x^\delta - x_{n(\delta)}^\delta + \left(\textstyle\prod_{j=1}^{n(\delta)}(I - \beta_j \widetilde{L})\right)(x - x^\delta). \end{aligned}$$

Since $\|I - \beta_j \widetilde{L}\| \le 1$, we have by (13)

$$\|x - x_{n(\delta)}\| \le \tau\delta + \|x - x^\delta\| \le (\tau + 1)\delta.$$

$\square$

We now need an inequality.

Lemma 4.2. *For $\mu > 0$, $\|\widehat{L}^\mu z\| \le \|z\|^{1/(2\mu+1)}\|\widehat{L}^{\mu+1/2}z\|^{2\mu/(2\mu+1)}$.*

Proof. Let $\{E_\lambda\}$ be a resolution of the identity for H_2 generated by the bounded self-adjoint operator $\widehat{L} : H_2 \to H_2$. By Hölder's inequality

$$\begin{array}{rcl} \|\widehat{L}^\mu z\|^2 & = & \int_0^1 1 \cdot \lambda^{2\mu} d\|E_\lambda z\|^2 \\ & \le & \left(\int_0^1 1 d\|E_\lambda z\|^2\right)^{1/(2\mu+1)} \left(\int_0^1 \lambda^{2\mu+1} d\|E_\lambda z\|^2\right)^{2\mu/(2\mu+1)} \\ & = & \|z\|^{2/(2\mu+1)} \left(\|\widehat{L}^{\mu+1/2} z\|^2\right)^{2\mu/(2\mu+1)}. \end{array}$$

Lemma 4.3. *If $x \in \mathcal{D}(L)$ and $x = \widetilde{L}^\mu w$ for some $w \in \mathcal{D}(L)$, then*

$$\|Lx - Lx_{n(\delta)}\| = O(\delta^{\mu/(\mu+1)}).$$

Proof. From (11) and (2) we find

$$\begin{array}{rcl} Lx - Lx_{n(\delta)} & = & L\left(\prod_{j=1}^{n(\delta)}(I - \beta_j \widetilde{L})\right)\widetilde{L}^\mu w \\ & = & \left(\prod_{j=1}^{n(\delta)}(I - \beta_j \widehat{L})\right)\widehat{L}^\mu Lw = \widehat{L}^\mu z_{n(\delta)}, \end{array}$$

where $z_{n(\delta)} = \left(\prod_{j=1}^{n(\delta)}(I - \beta_j \widehat{L})\right) Lw$ and hence $\|z_{n(\delta)}\| \le \|Lw\|$.

Applying the previous lemma, we find

$$\begin{array}{rcl} \|Lx - Lx_{n(\delta)}\| & \le & \|Lw\|^{1/(2\mu+1)}\|\widehat{L}^{\mu+1/2} z_{n(\delta)}\|^{2\mu/(2\mu+1)} \\ & = & \|Lw\|^{1/(2\mu+1)}\|\widehat{L}^{1/2}(Lx - Lx_{n(\delta)})\|^{2\mu/(2\mu+1)}. \end{array} \tag{14}$$

However, since $\|x - x_{n(\delta)}\| \le (\tau + 1)\delta$ and $\|L\widetilde{L}\| \le 1$,

$$\begin{array}{rcl} \|\widehat{L}^{1/2}(Lx - Lx_{n(\delta)})\|^2 & = & \langle \widehat{L}(Lx - Lx_{n(\delta)}), Lx - Lx_{n(\delta)}\rangle \\ & = & \langle \widehat{L}L(x - x_{n(\delta)}), Lx - Lx_{n(\delta)}\rangle \\ & = & \langle L\widetilde{L}(x - x_{n(\delta)}), Lx - Lx_{n(\delta)}\rangle \\ & \le & (\tau + 1)\delta\|Lx - Lx_{n(\delta)}\|. \end{array}$$

Therefore (14) gives

$$\|Lx - Lx_{n(\delta)}\| = O(\delta^{\mu/(2\mu+1)})\|Lx - Lx_{n(\delta)}\|^{\mu/(2\mu+1)},$$

that is,

$$\|Lx - Lx_{n(\delta)}\| = O(\delta^{\mu/(\mu+1)}).$$

□

Theorem 4.1. *Suppose that $x \in \mathcal{D}(L)$ and $x = \widetilde{L}^\mu w$ for some $w \in \mathcal{D}(L)$ and $\mu > 1/2$. If $x \in H_1$ satisfies $\|x - x^\delta\| \le \delta$ and $n(\delta)$ is chosen by (13), then*

$$\|Lx - Lx^\delta_{n(\delta)}\| = \begin{cases} O(\delta^{(2\mu-1)/(2\mu)}) & , \quad \mu \le 1, \\ O(\delta^{\mu/(\mu+1)}) & , \quad \mu \ge 1. \end{cases}$$

Proof. First note from (12) that

$$(x_{n-1} - x^\delta_{n-1}) - (x - x^\delta) = -\left(\prod_{j=1}^{n-1}\left(I - \beta_j \widetilde{L}\right)\right)(x - x^\delta)$$

and hence by (13)

$$
\begin{aligned}
& \|x_{n(\delta)-1} - x\| \\
= \quad & \|x^\delta_{n(\delta)-1} - x^\delta + (x_{n(\delta)-1} - x^\delta_{n(\delta)-1}) - (x - x^\delta)\| \\
\geq \quad & \|x^\delta_{n(\delta)-1} - x^\delta\| - \left\| \left(\prod_{j=1}^{n(\delta)-1} \left(I - \beta_j \widetilde{L} \right) \right) (x - x^\delta) \right\| \\
\geq \quad & \tau\delta - \delta = (\tau - 1)\delta.
\end{aligned} \tag{15}
$$

If $x = \widetilde{L}^\mu w$, then by (10)

$$\|x_{n-1} - x\| = \left\| (I - \widetilde{L} T_{n-1}(\widetilde{L})) \widetilde{L}^\mu w \right\| = O(\sigma(n-1)^{-\mu}).$$

However, $\sigma(n)/\sigma(n-1) \to 1$ as $n \to \infty$ and hence $\sigma(n-1)^{-\mu} = O(\sigma(n)^{-\mu})$, therefore

$$\|x_{n(\delta)-1} - x\| = O(\sigma(n(\delta))^{-\mu}).$$

In light of (15), we obtain

$$\sigma(n(\delta)) = O(\delta^{-1/\mu}). \tag{16}$$

By the stability estimate in the proof of Theorem 2.1 we then have

$$\|Lx^\delta_{n(\delta)} - Lx_{n(\delta)}\| = \|y^\delta_{n(\delta)} - y_{n(\delta)}\| \leq \delta\sqrt{\sigma(n(\delta))} = O(\delta^{(2\mu-1)/(2\mu)}).$$

Combining this with the previous lemma gives the result. □

We note that this result says that rates of order arbitrarily close to optimal order may in principle be obtained by use of the *a posteriori* iteration number choice criterion (13).

5. An illustration

The previous sections present a theoretical investigation of an aspect of operator approximation theory, specifically the determination of asymptotic convergence orders, with respect to error amplitude, of an iterative stabilized evaluation method that arises out of functional interpolation. The analysis has been carried out in the general context of Hilbert space, but a number of issues related to applications and computational implementation remain to be addressed elsewhere. These include best values of constants and parameters, discretizations and inversion techniques. In this brief section we illustrate the method with a simple specific example to indicate the basics of the computation.

Suppose for instance that $\beta_j = 1/j$. The stabilized approximations to Lx, given a data vector x^δ not necessarily lying in the domain of L, are the vectors Lx^δ_n, where x^δ_n satisfy $x^\delta_0 = 0$ and

$$x^\delta_{n+1} = 1/(n+1)\widetilde{L}x^\delta + \left(I - 1/(n+1)\widetilde{L} \right) x^\delta_n, \quad n = 0, 1, \ldots. \tag{17}$$

This illustrates a key difference between the iterative method, in which the approximations are controlled by the iteration index n, and the method (1), in which the parameter α controls the approximations. In (17) the single inversion required to find $\widetilde{L}$ serves all steps of the process, while in (1), each change in the parameter α requires a new inversion.

It is instructive to phrase the iteration (17) in terms of the corrections Δ_n^δ that update the approximations, namely

$$x_{n+1}^\delta = x_n^\delta + \Delta_n^\delta,$$

where the corrections Δ_n^δ satisfy

$$(I + L^*L)\Delta_n^\delta = (x^\delta - x_n^\delta)/(n+1). \tag{18}$$

We see that the "data defect" $x^\delta - x_n^\delta$ does double duty: it is used in (18) to compute the corrections Δ_n^δ that update the approximations, and its norm is monitored to choose the stopping index via (13).

The computational nature of the basic problem (18) varies with the operator L. For example, in the case when L is the differentiation operator defined on the dense subspace

$$\mathcal{D}(L) = \{u \in L^2[0,1] : u \text{ absolutely continuous}, \quad u' \in L^2[0,1]\},$$

the correction Δ_n^δ is the solution u of the two-point boundary value problem

$$\begin{aligned} u - u'' &= h, \\ u'(0) = u'(1) &= 0, \end{aligned} \tag{19}$$

where $h = (x^\delta - x_n^\delta)/(n+1)$. The operator $\widetilde{L}$ is then the compact linear integral operator on $L^2[0,1]$ whose kernel is the Green's function for (19). When the data vector $x^\delta(t)$ is known for (almost) all $t \in [0,1]$, the iteration (17) may therefore be carried out explicitly until the condition (13) is satisfied. On the other hand, if only a discrete sample of x^δ is known on some grid, the iteration may be carried out in finite dimensions by applying a finite difference approximation to (19). The problem in the implicit iteration (18) then has the same matrix for all n, and hence the matrix factorizations used to solve the basic linear system need be computed only once and then used in all steps of the iteration process.

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