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Wavelet-Accelerated Tikhonov-Phillips Regularization with applications

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1 Introduction

1.1 Tikhonov-Phillips Regularization of Ill-Posed Problems

Many technical and physical problems can be mathematically modeled by operator equations (1) of the first kind,

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

where x is the searched-for information under observed data y. We mention only a few typical examples: medical imaging, see e.g. [16, 20], and inverse scattering problems, see e.g. [6].

To fix the mathematical setup we consider A (throughout the paper) as a compact non-degenerate linear operator acting between the real Hilbert spaces X and Y. In this setting the problem (1) is *ill-posed*, that is, its minimum norm solution x^+ does not depend continuously on the right hand side y. Small perturbations in y may cause dramatic changes in x^+. This instability has to be taken into account by any solution technique for (1). The more as only a perturbation y^δ of the exact but unknown data y is available in general. The perturbation of y is caused by noise which can not be avoided in real-life applications due to the specific experiment and due to the limitations of the measuring apparatus. The perturbed data y^δ are assumed to satisfy $\| y - y^\delta \|_Y \le \delta$ with an a-priori known *noise level* $\delta > 0$.

One of the theoretically best understood and most often used stabilization techniques for (1) is *Tikhonov-Phillips regularization* where the linear equation (1) is replaced by the minimization problem

$$\begin{aligned} &\textit{find } x_\alpha^\delta \in X \textit{ which minimizes} \\ &T_\alpha(x) = \| Ax - y^\delta \|_Y^2 + \alpha \|x\|_X^2 \ . \end{aligned} \tag{2}$$

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Here, $\alpha > 0$ is the *regularization parameter*. The idea of Tikhonov-Phillips regularization (2) is to control the influence of the data error in the regularized solution x_α^δ by adding a penalty term. The unique minimizer of (2) is given as the unique solution of the regularized normal equation

$$(A^*A + \alpha I)\, x_\alpha^\delta = A^* y^\delta \ . \tag{3}$$

The high art of regularization is the determination of the regularization parameter $\alpha = \alpha(\delta, y^\delta)$ such that x_α^δ converges to x^+ as $\delta \to 0$. Examples for such parameter selection strategies are presented in Section 3.

In this paper we introduce two methods to speed up the solution process of (3) which even can be combined. Both methods employ wavelet techniques. For the reader's convenience we therefore give a brief overview on the wavelet theory in the next subsection.

In Section 2 we present a fast multilevel iteration for the solution of a discrete version of the normal equation (3). The theoretical results we achieve are illustrated by numerical examples where the abstract operator equation (1) will be an integral equation. Finally, we discuss the potential of our multilevel method for solving the $3D$-reconstruction problem in computerized tomography.

Any iterative scheme for solving (3) requires the multiplication of a vector by the operator $A^*A + \alpha I$ (resp. a matrix version thereof). Typically, this operator (matrix) will be dense. Therefore, operator compression techniques will speed up any iterative solver. Such methods are considered in Section 3. First, we study compression schemes from a theoretical point of view and then we discuss two ways of computing such compressions. We report on results obtained by applying this approach to hyperthermia treatment planning.

1.2 A Compact Course to Wavelets

We give a brief overview to the univariate theory. Multivariate wavelets, for instance, can be generated from univariate ones by tensor products. We refer to e.g. [10, 17] for a comprehensive introduction to wavelets.

The starting point is the concept of a *refinable* or *scalable* function $\varphi \in L^2(\mathbb{R})$ which is compactly supported and satisfies the following *refinement* or *scaling* equation

$$\varphi(\cdot) = \sqrt{2} \sum_{k \in \mathbb{Z}} h_k \, \varphi(2 \cdot - k) \ . \tag{4}$$

The finite sequence $\{h_k\}_{k \in \mathbb{Z}}$ of real numbers is called mask or filter corresponding to φ. Taking the Fourier transform on both sides of (4) we realize that any non-trivial scaling function has a non-vanishing mean value. Without loss of generality we therefore assume

$$\int_{\mathbb{R}} \varphi(t) \, dt = 1 \ . \tag{5}$$

Further, we require that the integer translates of φ generate a Riesz system in $L^2(\mathbb{R})$, i.e. we have the norm equivalence

$$\Big\| \sum_{k\in\mathbb{Z}} a_k \; \varphi(\cdot\, - \, k) \Big\|_{L^2} \sim \|a\|_{\ell^2} \quad \text{for all} \quad a \in \ell^2(\mathbb{Z}) \ . \tag{6}$$

We use the notation $f \sim g$ to indicate the existence of two positive constants c_1 and c_2 such that $c_1 f \leq g \leq c_2 f$.

Typical examples for scaling functions with the above requirements are B-splines, several kinds of box-splines and the Daubechies scaling functions whose integer translates are even orthonormal.

Using the scaling function φ we define subspaces V_l of $L^2(\mathbb{R})$ by

$$V_l := \overline{\operatorname{span}\{\, \varphi_{l,k} \,|\, k \in \mathbb{Z}\,\}}, \quad l \in \mathbb{Z}, \tag{7}$$

where

$$f_{l,k}(\cdot) := 2^{l/2} \; f\big(2^l \, \cdot - k\big)$$

for any $f \in L^2(\mathbb{R})$. The closure in (7) is taken with respect to the L^2-norm. The spaces V_l are nested by (4), $V_l \subset V_{l+1}$, and $\{\, \varphi_{l,k} \,|\, k \in \mathbb{Z}\,\}$ is a Riesz basis of V_l by (6). By (4), (5) and (6) it follows that

$$\bigcap_{l\in\mathbb{Z}} V_l = \{0\} \quad \text{and} \quad \overline{\bigcup_{l\in\mathbb{Z}} V_l} = L^2(\mathbb{R}) \ .$$

To any scaling function φ satisfying (5) and (6) there exists a function ψ such that

$$W_l := \overline{\operatorname{span}\{\, \psi_{l,k} \,|\, k \in \mathbb{Z}\,\}}, \quad l \in \mathbb{Z},$$

coincides with the orthogonal complement of V_l in V_{l+1}: $V_{l+1} = V_l \oplus W_l$. Moreover,

$$\{\, \psi_{l,k} \,|\, l \in \mathbb{Z},\ k \in \mathbb{Z}\,\} \tag{8}$$

is an orthonormal basis of $L^2(\mathbb{R})$. The function ψ is called *orthogonal wavelet.* In general ψ does not inherit the compact support from φ. This disadvantage can be avoided by relaxing the requirements. We speak of *pre-wavelets* if the spaces W_l are mutually orthogonal and the wavelet system (8) is only a Riesz basis in $L^2(\mathbb{R})$.

There exists a family, the Daubechies family, of compactly supported orthogonal wavelets, see [10]. The smoothness of the Daubechies wavelets increases monotonically with their support. Also, there exists a family, the Chui-Wang family, of compactly supported pre-wavelets, see [4]. The Chui-Wang wavelets are spline functions. Their corresponding scaling functions are the B-splines.

Both wavelet families can be adapted to bounded intervals, see [4, 5].

The wavelet space W_l is a subspace of V_{l+1}. Therefore, the wavelet ψ can be expanded with respect to the Riesz basis $\{\, \varphi_{1,k} \,|\, k \in \mathbb{Z}\,\}$ of V_1. Consequently, there exists a unique sequence $g \in \ell^2(\mathbb{Z})$ of real numbers such that

$$\psi(\cdot) = \sqrt{2} \sum_{k\in\mathbb{Z}} g_k \; \varphi(2 \cdot - k) \tag{9}$$

holds true. The sequence g is finite if ψ has a compact support.

Any $f \in L^2(\mathbb{R})$ can be represented by

$$f = \sum_{k \in \mathbb{Z}} c_k(f)\, \varphi_{0,k} + \sum_{l \in \mathbb{N}_0} \sum_{k \in \mathbb{Z}} d_{l,k}(f)\, \psi_{l,k} \ . \tag{10}$$

If the scaling function φ is q-times continuously differentiable then we have the norm equivalence, see [19, 7],

$$\|f\|^2_{H^s} \sim \sum_{k \in \mathbb{Z}} |c_k(f)|^2 + \sum_{l \in \mathbb{N}_0} 2^{2\,s\,l} \sum_{k \in \mathbb{Z}} |d_{l,k}(f)|^2, \quad 0 \le s \le q, \tag{11}$$

where $\|f\|^2_{H^s} = \int_{\mathbb{R}} (1+|\xi|^2)^s\, |\widehat{f}(\xi)|^2\, d\xi$ is the norm of the Sobolev space $H^s(\mathbb{R}) = \{f \in L^2(\mathbb{R}) \mid \|f\|_{H^s} < \infty\}$. Here, $\widehat{f}$ denotes the Fourier transform of f.

2 A Multilevel Iteration for Tikhonov-Phillips Regularization

When it comes to a numerical realization of the Tikhonov-Phillips regularization one has to project the normal equation (3) to a finite dimensional subspace of X. The most commonly used projection technique in combination with Tikhonov-Phillips regularization is the method of least squares, see e.g. [15] and [24]. Here we get the finite dimensional regularized normal equation

$$(A_l^* A_l + \alpha I)\, x_l = A_l^* y^\delta, \tag{12}$$

with $A_l = AP_l$ where $P_l : X \to V_l$ is the orthogonal projection onto a finite dimensional subspace $V_l \subset X$.

We require two essential properties of the sequence $\{V_l\}_l$ of finite dimensional approximation spaces: it should be expanding, that is, $V_l \subset V_{l+1}$, and it should be dense in X, that is, $\overline{\cup_l V_l} = X$. With these properties at hand the solution $x_l^{\delta,\alpha}$ of (12) converges to the minimum norm solution x^+ of (1) as $l \to \infty$ and $\delta \to 0$, provided α is determined according to the parameter choice strategies introduced in [24].

In the remainder of this section we will present an efficient multilevel iteration for the resolution of (12) *under the general assumption of a fixed noise level* δ.

2.1 Multilevel Splitting

The basis of all multilevel iterations is the decomposition of the approximation space into subspaces. Therefore, we introduce the splitting $V_{l+1} = V_l \oplus W_l$ where W_l is the X-orthogonal complement of the approximation space V_l with respect to the larger space V_{l+1}. Here, $\oplus$ denotes the X-orthogonal sum. Inductively, we yield the multilevel splitting (13) of V_l,

$$V_l = V_{l_{\min}} \oplus \bigoplus_{j = l_{\min}}^{l-1} W_j, \quad l_{\min} \le l-1, \tag{13}$$

where $l_{\min}$ is called the coarsest level of the splitting. By Q_j we denote the X-orthogonal projection from X onto W_j.

The convergence behavior of the multilevel iteration will depend on the decay rate of the quantity

$$\gamma_l = ||A - A_l|| = ||A(I - P_l)|| \tag{14}$$

as $l \to \infty$. For a proof of $\gamma_l \to 0$ as $l \to \infty$ see e.g. [14].

In the next lemma we show that compact operators vanish asymptotically on the complement spaces W_l.

Lemma 1. *Let V_l and W_l be the spaces defined above and let $A : X \to Y$ be a compact linear operator. Then,*

$$||AQ_l|| \leq \gamma_l \to 0 \quad as \quad l \to \infty$$

with γ_l defined in (14).

Proof. The orthogonality of V_l and W_l yields $P_l Q_l = 0$. Therefore, $||AQ_l|| = ||A(I - P_l)Q_l|| \leq ||A(I - P_l)|| = \gamma_l$. □

For our further considerations and for the description of the iteration it will be convenient to reformulate (12) as a variational problem

$$\text{find } x_l^{\delta,\alpha} \in V_l : \quad a\big(x_l^{\delta,\alpha}, v_l\big) = \big\langle A_l^* y^\delta, v_l \big\rangle_X \quad \text{for all } v_l \in V_l \tag{15}$$

with the bilinear form $a : X \times X \to \mathbb{R}$,

$$a(u, v) := \langle Au, Av \rangle_Y + \alpha \langle u, v \rangle_X$$

which is symmetric and positive definite. The form a induces the energy norm $||\cdot||_a^2 = a(\cdot,\cdot)$ on X.

The operators $\mathcal{A}_l := A_l^* A_l + \alpha P_l : V_l \to V_l$ and $\mathcal{B}_l := Q_l A^* A Q_l + \alpha Q_l : W_l \to W_l$ are related to the bilinear form a via $a(u_l, v_l) = \langle \mathcal{A} u_l, v_l \rangle$ for all $u_l, v_l \in V_l$ and $a(w_l, z_l) = \langle \mathcal{B} w_l, z_l \rangle$ for all $w_l, z_l \in W_l$, respectively.

The strengthened Cauchy inequalities we present now are crucial for the later convergence analysis. Basically, they indicate that the spaces V_l and W_l as well as W_l and W_m are not only X-orthogonal but also asymptotically orthogonal with respect to the inner product on X induced by a.

Theorem 2. *Let V_l and W_m be defined as above and let $m \geq l$. The strengthened Cauchy inequality*

$$|a(v_l, w_m)| \leq \min\{1, \gamma_m/\sqrt{\alpha}\} \; ||v_l||_a \; ||w_m||_a \tag{16}$$

holds true for all $v_l \in V_l$ and for all $w_m \in W_m$. Further, let $j \neq l$. Then,

$$|a(w_j, w_l)| \leq \min\{1, \gamma_l/\sqrt{\alpha}\} \; \min\{1, \gamma_j/\sqrt{\alpha}\} \; ||w_j||_a \; ||w_l||_a \tag{17}$$

for all $w_j \in W_j$ and for all $w_l \in W_l$.

Proof. Since v_l and w_m are X-orthogonal we have that $a(v_l, w_m) = \langle Av_l\,, Aw_m\rangle_Y$. Further,

$$\begin{aligned} |a(v_l, w_m)| &= \left|\left\langle A_l\mathcal{A}_l^{-1/2}\mathcal{A}_l^{1/2}v_l\,,\, AQ_m\mathcal{B}_m^{-1/2}\mathcal{B}_m^{1/2}w_m\right\rangle_Y\right| \\ &\le \left\|A_l\mathcal{A}_l^{-1/2}\right\|\,\left\|\mathcal{A}_l^{1/2}v_l\right\|_X\,\left\|AQ_m\mathcal{B}_m^{-1/2}\right\|\,\left\|\mathcal{B}_m^{1/2}w_m\right\|_X \\ &\le \left\|A_l\mathcal{A}_l^{-1/2}\right\|\,\left\|\,v_l\,\right\|_a\,\left\|AQ_m\right\|\,\left\|\mathcal{B}_m^{-1/2}\right\|\,\left\|\,w_m\,\right\|_a. \end{aligned}$$

Using arguments from spectral theory it is easy to verify that $\|A_l\,\mathcal{A}_l^{-1/2}\,\| \le 1$ and $\|\mathcal{B}_m^{-1/2}\| \le \alpha^{-1/2}$. Thus, (16) is proved by $\|AQ_m\| \le \gamma_m$ (Lemma 1). The second inequality (17) can be proved in the very same way. □

2.2 The Multilevel Iteration

Motivation and Definition. The general idea of multilevel methods is to approximate the original large scale problem (in our situation: (12)) by a sequence of related auxiliary problems on smaller scales which can be solved very cheaply. If the auxiliary problems are designed in a proper way their combination should result in a fair approximation to our original problem, see e.g. [28].

Now, we introduce the concept of subspace corrections, see [28]. Suppose that we have a given approximation u_l^{old} to the solution $x_l^{\delta,\alpha}$ of (12). If the residue $r_l^{\text{old}} = \mathcal{A}_l\,u_l^{\text{old}} - A_l^* y^\delta$ is small we are done. Otherwise, we consider the equation

$$\mathcal{A}_l\,e_l \;=\; r_l^{\text{old}} \tag{18}$$

for the error $e_l := u_l^{\text{old}} - x_l^{\delta,\alpha}$. Instead of the large scale problem (18) we solve restricted equations with respect to each of the subspaces of the splitting (13):

$$\begin{aligned} \mathcal{B}_j\,\mathsf{e}_j &= Q_j\,r_l^{\text{old}}, \quad \text{for } l_{\min} \le j \le l-1, \qquad (19)\\ \mathcal{A}_{l_{\min}}\,e_{l_{\min}} &= P_{l_{\min}}\,r_l^{\text{old}}\;. \end{aligned}$$

We observe that

$$\alpha\,\|w_j\|_X^2 \;\le\; \langle\mathcal{B}_j w_j, w_j\rangle_X \;=\; a(w_j, w_j) \;\le\; \left(1 + \gamma_j^2/\alpha\right)\,\alpha\,\|w_j\|_X^2 \tag{20}$$

for all $w_j \in W_j$ which is an immediate consequence of Lemma 1. Hence, $\mathcal{B}_j$ can be approximated well by $\alpha\,I$ on W_j and

$$\widetilde{\mathsf{e}}_j \;=\; \alpha^{-1}\,Q_j\,r_l^{\text{old}}, \quad \text{for } l_{\min} \le j \le l-1,$$

may be viewed as reasonable approximations to the e_j's defined in (19). Finally we are in a position to define the *subspace correction* of u_l^{old} relative to W_j by

$$u_{W_j}^{\text{new}} \;:=\; u_l^{\text{old}} \;-\; \widetilde{\mathsf{e}}_j \;=\; u_l^{\text{old}} \;-\; \alpha^{-1}\,Q_j\left(\mathcal{A}_l\,u_l^{\text{old}} - A_l^* y^\delta\right)$$

and relative to $V_{l_{\min}}$ by

$$u_{V_{l_{\min}}}^{\text{new}} \;:=\; u_l^{\text{old}} \;-\; e_{l_{\min}} \;=\; u_l^{\text{old}} \;-\; \mathcal{A}_{l_{\min}}^{-1}\,P_{l_{\min}}\left(\mathcal{A}_l\,u_l^{\text{old}} - A_l^* y^\delta\right)\;.$$

Starting with an approximation $u_l^\mu \in V_l$ the (Jacobi-like) *additive Schwarz iteration* produces a new iterate by performing the subspace corrections simultaneously, that is,

$$u_l^{\mu+1} = u_l^\mu - \mathcal{C}_{l,l_{\min}}^{\text{add}} \left(\mathcal{A}_l u_l^\mu - A_l^* y^\delta\right), \quad \mu = 0,1,2,\dots , \tag{21}$$

with an arbitrary starting guess $u_l^0 \in V_l$ and with

$$\mathcal{C}_{l,l_{\min}}^{\text{add}} = \mathcal{A}_{l_{\min}}^{-1} P_{l_{\min}} + \alpha^{-1} \sum_{j=l_{\min}}^{l-1} Q_j .$$

Algebraic Structure of the Iteration. Here we give a detailed description of the algebraic structure of the Schwarz iteration (21). Therefore, we assume that X is a function space over the compact interval $[a,b]$, $X = L^2(a,b)$ for example. The results obtained can easily be generalized to tensor product spaces, e.g. $X = L^2\big([a,b] \times [c,d]\big)$.

Let φ be a compactly supported scaling function satisfying (4). For convenience, we neglect – just for now – necessary boundary modifications and suppose that

$$V_l = \operatorname{span}\big\{\varphi_{l,k} \mid k = 0,\dots,n_l - 1\big\} \subset X$$

for all $l \geq l^\star > 0$. Further, let W_l be spanned by the pre-wavelet ψ, that is,

$$W_l = \operatorname{span}\big\{\psi_{l,k} \mid k = 0,\dots,m_l - 1\big\} .$$

Since the sum of two functions $f_l = \sum_k c_k^l \varphi_{l,k} \in V_l$ and $q_l = \sum_k d_k^l \psi_{l,k} \in W_l$ is in V_{l+1}, it can be expressed by $f_l + q_l = \sum_k c_k^{l+1} \varphi_{l+1,k}$. Applying both refinement equations (4) and (9) we get the relation

$$c_k^{l+1} = \sum_i h_{k-2i}\, c_i^l + \sum_j g_{k-2j}\, d_j^l$$

which we write in matrix notation as

$$c^{l+1} = H_{l+1}^t c^l + G_{l+1}^t d^l . \tag{22}$$

Clearly, $H_{l+1} : \mathbb{R}^{n_{l+1}} \to \mathbb{R}^{n_l}$ and $G_{l+1} : \mathbb{R}^{n_{l+1}} \to \mathbb{R}^{m_l}$.

The solution $x_l^{\delta,\alpha}$ of the variational problem (15) resp. of the normal equation (12) can be expanded in the basis of V_l as $x_l^{\delta,\alpha} = \sum_k (\xi_l)_k \varphi_{l,k}$. The vector $\xi_l \in \mathbb{R}^{n_l}$ of the expansion coefficients is the unique solution of the linear system

$$\mathbf{A}_l\, \xi_l = \beta_l \tag{23}$$

where the entries of the positive definite matrix $\mathbf{A}_l$ and of the right-hand side β_l are given by

$$(\mathbf{A}_l)_{i,j} = \big\langle A\varphi_{l,i}, A\varphi_{l,j}\big\rangle_Y + \alpha \big\langle \varphi_{l,i}, \varphi_{l,j}\big\rangle_X,$$

$$(\beta_l)_j = \big\langle y^\delta, A\varphi_{l,j}\big\rangle_Y .$$

The following lemma enables matrix representations of the operators $Q_j\mathcal{A}_l$, $l_{\min} \le j \le l-1$, and $\mathcal{A}_{l_{\min}}^{-1} P_{l_{\min}} \mathcal{A}_l$ which are the building blocks of the Schwarz iteration (21). For a proof see [25].

Lemma 3. *Define the restrictions*

$$\mathcal{H}_{l,j} := H_{j+1}\, H_j\, \cdots\, H_{l-1}\, H_l\, : \mathbb{R}^{n_l} \to \mathbb{R}^{n_j},$$
$$\mathcal{G}_{l,j} := G_{j+1}\, H_j\, \cdots\, H_{l-1}\, H_l\, : \mathbb{R}^{n_l} \to \mathbb{R}^{m_j}$$

for $j \le l-2$ *and set* $\mathcal{H}_{l,l-1} := H_l$ *and* $\mathcal{G}_{l,l-1} := G_l$.

For $v_l = \sum_k c_k^l \varphi_{l,k} \in V_l$ *we have that*

$$Q_j \mathcal{A}_l v_l \;=\; \sum_{k=0}^{n_l-1} \left(\mathcal{G}_{l,j}^t\, \mathbf{B}_j^{-1}\, \mathcal{G}_{l,j}\, \mathbf{A}_l\, c^l \right)_k \varphi_{l,k}, \quad l_{\min} \le j \le l-1,$$

where $\mathbf{B}_j$ *is the Gramian matrix* $(\mathbf{B}_j)_{r,s} = \langle \psi_{j,r}, \psi_{j,s} \rangle_X$, *and*

$$\mathcal{A}_{l_{\min}}^{-1} P_{l_{\min}} \mathcal{A}_l v_l \;=\; \sum_{k=0}^{n_l-1} \left(\mathcal{H}_{l,l_{\min}}^t\, \mathbf{A}_{l_{\min}}^{-1}\, \mathcal{H}_{l,l_{\min}}\, \mathbf{A}_l\, c^l \right)_k \varphi_{l,k}\;.$$

Now, the abstract additive iteration (21) translated into an iteration acting on (23) reads

$$z_l^{\mu+1} \;=\; z_l^{\mu} \;-\; \mathbf{C}_{l,l_{\min}}^{\text{add}} \left(\mathbf{A}_l z_l^{\mu} \;-\; \beta_l \right), \quad \mu = 0, 1, 2, \ldots, \tag{24}$$

with an arbitrary starting guess $z_l^0 \in \mathbb{R}^{n_l}$ and where

$$\mathbf{C}_{l,l_{\min}}^{\text{add}} \;=\; \mathcal{H}_{l,l_{\min}}^t\, \mathbf{A}_{l_{\min}}^{-1}\, \mathcal{H}_{l,l_{\min}} \;+\; \alpha^{-1} \sum_{j=l_{\min}}^{l-1} \mathcal{G}_{l,j}^t\, \mathbf{B}_j^{-1}\, \mathcal{G}_{l,j}\;.$$

Remark. In applying the iteration (24) one has to solve a linear system with band matrix $\mathbf{B}_j$ on each level j during the multilevel process. However, this does not slow down the iteration. Since the entries of $\mathbf{B}_j$ do not depend on j one can precompute a Cholesky decomposition of $\mathbf{B}_j$ independently of $j \ge l^\star$.

Employing the additive structure of $\mathbf{C}_{l,l_{\min}}^{\text{add}}$ the multiplication of the residue by $\mathbf{C}_{l,l_{\min}}^{\text{add}}$ can be done in parallel. This leads to a significant speed up if the iteration is implemented on a parallel machine. Since the subspaces of the splitting (13) do not intersect the communication between processors is reduced to a minimum.

Convergence Analysis. Provided a mild decay assumption on γ_j (14) we have the convergence result stated in Theorem 4.

In general, an exact computation of γ_j is impossible. However, upper bounds are often available. In the sequel we will therefore work with such an upper bound.

Theorem 4. *Let η_l be an upper bound of γ_l ($\gamma_l \le \eta_l$) satisfying*

$$\eta_l \le \eta_{l-1} \quad \text{and} \quad \sum_{j=l_{\min}}^{l-1} \eta_j \le C_\eta \, \eta_{l_{\min}} \tag{25}$$

with a positive constant C_η which does neither depend on l nor on $l_{\min}$. Let $\{u_l^\mu\}_\mu$ be sequence generated by the Schwarz iteration (21). *If $\sigma_{l_{\min}} := \eta_{l_{\min}}/\sqrt{\alpha} \le 1$ then*

$$\left\| u_l^\mu - x_l^{\delta,\alpha} \right\|_a \le \rho^\mu \left\| u_l^0 - x_l^{\delta,\alpha} \right\|_a$$

with the convergence rate

$$\rho = 2\, C_\eta \, (C_\eta + 2) \, \sigma_{l_{\min}} \ . \tag{26}$$

Proof. We roughly sketch the proof. For more details we refer to [25].

It is well known, see e.g. [13], that $\rho_{\mathrm{a}} = \max\{|1-\Gamma_1|, |1-\Gamma_2|\}$ where Γ_1 and Γ_2 are positive constants such that

$$\Gamma_1 \, |||\, v_l \,|||^2 \le \|\, v_l \,\|_a^2 \le \Gamma_2 \, |||\, v_l \,|||^2 \tag{27}$$

holds true for all $v_l \in V_l$. Here, the norm $|||\cdot|||$ on V_l is given by $|||\, v_l \,|||^2 := \|\, P_{l_{\min}} v_l \,\|_a^2 + \alpha \sum_{j=l_{\min}}^{l-1} \|\, Q_j v_l \,\|_X^2$. Using the Cauchy inequalities (16), (17) and the estimate (20) one can show that (27) is satisfied with

$$\Gamma_1 = 1/\left(1 + 2\, C_\eta \left(1 + (C_\eta + 1)\, \sigma_{l_{\min}} \right) \sigma_{l_{\min}} \right)$$

and

$$\Gamma_2 = \left(1 + \sigma_{l_{\min}}^2 \right) \left(1 + 2\, C_\eta \, \sigma_{l_{\min}} \right) \ .$$

□

Numerical Examples. Here we present some numerical experiments to illustrate the theoretical result of Theorem 4.

The ill-posed problem under consideration is the integral equation

$$Af(\cdot) = \int_0^1 k(\cdot, t)\, x(t)\, dt = y(\cdot) \tag{28}$$

where $A : L^2(0,1) \to L^2(0,1)$ is the integral operator with the non-degenerate and square integrable kernel $k(x,y) = x - y$, if $x \ge y$ and $k(x,y) = 0$, otherwise.

As finite dimensional approximation space $V_l \subset L^2(0,1)$ we choose the space of piecewise linear functions with respect to the discretization step-size $s_l = 2^{-l}$. Then, the splitting (13) becomes just the pre-wavelet splitting of the linear spline space, see [3].

Remark. The numerical realization of (21) for the solution of (28) based on spline spaces and on the spaces of the Daubechies scaling functions can be found in some detail in [25]. Also, implementation issues as well as the computational complexity are discussed.

We provide numerical approximations to the convergence rate ρ (26). In the present situation the assumptions (25) are met with $\eta_l = C_k\, s_l^2$ and $C_\eta = 4/3$ resulting in

$$\rho \le C_A\, s_{l_{\min}}^2 / \sqrt{\alpha} \tag{29}$$

with a constant C_A independent of l, $l_{\min}$ and α.

By our first experiment we check the decay rate 2 of ρ as $l_{\min} \to \infty$. Figure 2.2 displays approximations to $\rho = \rho(l)$ and the quotient $q_l := \rho(l)/\rho(l-1)$ as functions of the approximation level l with $l_{\min} = l - 5$ and $\alpha = 10^{-4}$.

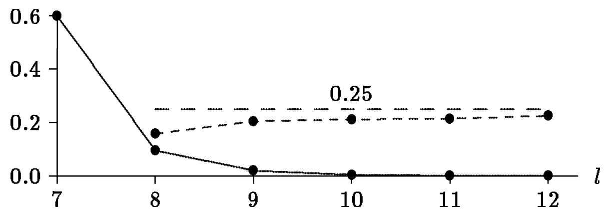

Fig. 1. Approximations to the convergence rate $\rho = \rho(l)$ (solid curve) and the quotient $q_l = \rho(l)/\rho(l-1)$ (dashed curve) for $l_{\min} = l - 5$ and $\alpha = 10^{-4}$. The theoretical bound 0.25 for q_l is drawn as a dashed straight line.

Now we show approximations to $\rho = \rho(l)$ where the coarsest level $l_{\min}$ is fixed to be 2, see Fig. 2.2. In the latter setting the iteration converges for $\alpha = 0.001$ and $\alpha = 0.005$ and Theorem 4 predicts convergence rates which are uniformly bounded in l.

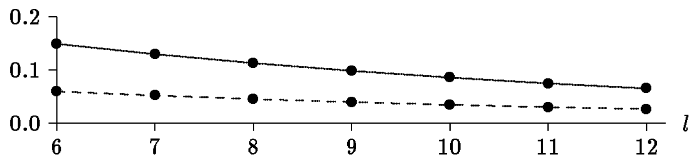

Fig. 2. Convergence rates $\rho = \rho(l)$ for $l_{\min} = 2$. Solid curve: $\alpha = 0.001$, dashed curve: $\alpha = 0.005$.

2.3 Multilevel Approach to Cone Beam Reconstruction

The ultimate goal is an implementation of the above introduced multilevel iteration for the reconstruction of a three-dimensional object from finitely many cone beam X-ray projections.

In the following we investigate what we may expect in this application from a theoretical point of view.

Speaking in mathematical terms the reconstruction problem can be formulated as the operator equation (30) of the first kind,

$$Df = g^\delta, \tag{30}$$

where the cone beam (or divergent beam) transform D is given as

$$Df(a,\omega) := \int_0^\infty f(a + t\,\omega)\; dt, \quad a \in \mathbb{R}^3,\; w \in S^2 \;.$$

Physically, one can think of a as the position of the X-ray source emitting an X-ray into the direction ω (S^2 denotes the unit sphere in $\mathbb{R}^3$). In the sequel we assume that the searched-for density function f has compact support in the unit box $\square = [0,1]^3$ and is square integrable, i.e. $f \in L^2(\square)$.

If Γ, the set of all source points a, is compact and does not intersect $\square$ then D maps $L^2(\square)$ continuously to $L^2(\Gamma \times S^2)$, see e.g. [20].

Now we apply the method of least squares together with a Tikhonov-Phillips regularization to (30). As approximation space V_l we choose tensor product B-spline spaces with respect to the step-size $s_l = 2^{-l}$. Thus we have to solve

$$(D_l^* D_l + \alpha\, I)\, f_l \;=\; D_l^* g^\delta, \tag{31}$$

where $D_l = DP_l$ and P_l is the orthogonal projection from $L^2(\square)$ onto V_l.

To set up our multilevel iteration we need the complement spaces W_l, cf. Sect. 2.1. But these spaces are just the tensor product spline wavelet spaces, see [3]. Hence, the multilevel iteration (21) for solving (31) is well-defined.

Lemma 5. *Suppose that we have complete data, that is, $\Gamma = \partial B$ where ∂B is the boundary of an open Ball B containing the box: $\square \subset B$. Then, the convergence rate ρ (26) of the multilevel iteration (21) acting on (31) fulfills*

$$\rho \le C_D \sqrt{s_{l_{\min}}/\alpha} \tag{32}$$

where $l_{\min}$ is the coarsest level in the underlying wavelet splitting of the tensor product B-Spline space V_l. The positive constant C_D does neither depend on l, $l_{\min}$ nor on α.

Consequently, the iteration converges if $l_{\min}$ is sufficiently large.

Proof. The assertion follows by Theorem 4 as soon as we are able to verify that $\gamma_l = \|D(I - P_l)\| \le C\sqrt{s_l}$.

To establish such an estimate we note a relation between the cone beam transform D and the parallel beam transform L defined by

$$Lf(x,\vartheta) := \int_{\mathbb{R}} f(x + t\,\vartheta)\; dt, \quad \vartheta \in S^2,\; x \in \vartheta^\perp \;.$$

Let the radius of B be r. Then,

$$\int_{S^2}\int_{\Gamma} |Df(a,\omega)|^2\,|\langle a,\omega\rangle|\;da\,d\omega \;=\; 2r\int_{S^2}\int_{\omega^\perp} |Lf(x,\omega)|^2\;dx\,d\omega$$

which follows by a change of coordinates in the inner integral on the left-hand side: set $a = x + \langle a,\omega\rangle\omega$ where x is the orthogonal projection of a onto $\omega^\perp$ and where $|\langle a,\omega\rangle|\,da = r\,dx$. By our assumptions on B and $\Box$ there is an $\epsilon > 0$ such that $Df(a,\omega) = 0$ for $|\langle a,\omega\rangle| \geq \epsilon$. Hence,

$$||Df||_{L^2(\Gamma\times S^2)} \;\leq\; \sqrt{2r/\epsilon}\;||Lf||_{L^2(T)}$$

where T is the tangent bundle $T = \big\{(x,\vartheta)\,|\,\vartheta\in S^2,\; x\in\vartheta^\perp\big\}$.

As in the proof of Theorem 5.1 in [20] we show that

$$||Lf||_{L^2(T)} \;\leq\; C_L\;||f||_{H^{-1/2}} \quad \text{for all}\;\; f\in\mathcal{C}_0^\infty(\Box),$$

where $||f||^2_{H^\beta} = \int_{\mathbb{R}^3}\big(1+||\xi||^2\big)^\beta\,|\widehat{f}(\xi)|^2\;d\xi$. Here, $\widehat{f}$ is the Fourier transform of f. Denoting the closure of $\mathcal{C}_0^\infty(\Box)$ with respect to $||\cdot||_{H^{-1/2}}$ by $H_0^{-1/2}(\Box)$, we finally have

$$||Df||_{L^2(\Gamma\times S^2)} \;\leq\; \sqrt{2r/\epsilon}\;C_L\;||f||_{H^{-1/2}} \quad \text{for all}\;\; f\in H_0^{-1/2}(\Box)\;\;.$$

The dual space to $H_0^{-1/2}(\Box)$ is $H^{1/2}(\Box) = \big\{v\,|\,\text{there is a } u\in L^2(\mathbb{R}^3) \text{ such that } ||u||_{H^{1/2}} < \infty \text{ and } u|_\Box = v\big\}$ with norm $||v||_{H^{1/2}(\Box)} = \inf\big\{||u||_{H^{1/2}}\,|\,u|_\Omega = v\big\}$, see e.g. [27, Chap. 17.2]. The norm in $H^{1/2}(\Box)$ can also be expressed by

$$||v||_{H^{1/2}(\Box)} \;=\; \sup\Big\{\,|(v,u)|\,/\,||u||_{H^{-1/2}}\,\Big|\,u\in H_0^{-1/2}(\Box)\Big\}$$

where $(\cdot,\cdot)$ denotes the duality pairing which can be considered as an extension of the $L^2(\Box)$ inner product onto $H^{1/2}(\Box)\times H_0^{-1/2}(\Box)$. This yields

$$\begin{aligned} ||D^*g||_{H^{1/2}(\Box)} &= \sup\Big\{\,|(D^*g,f)|\,/\,||f||_{H^{-1/2}}\,\Big|\,f\in H_0^{-1/2}(\Box)\Big\} \\ &= \sup\Big\{\,|\langle g,Df\rangle_{L^2(\Gamma\times S^2)}|\,/\,||f||_{H^{-1/2}}\,\Big|\,f\in H_0^{-1/2}(\Box)\Big\} \\ &\leq \sqrt{2r/\epsilon}\;C_L\;||g||_{L^2(\Gamma\times S^2)}\;\;. \end{aligned}$$

Relying on approximation results for tensor product B-splines, see e.g. [26], the proof ends by

$$\begin{aligned} ||(I-P_l)D^*g||_{L^2(\Box)} &\leq C_S\;\sqrt{s_l}\;||D^*g||_{H^{1/2}(\Box)} \\ &\leq C_S\;\sqrt{2r/\epsilon}\;C_L\;||g||_{L^2(\Gamma\times S^2)}\;\sqrt{s_l} \end{aligned}$$

which implies that $\gamma_l = ||(I-P_l)D^*|| \leq C_S\;\sqrt{2r/\epsilon}\;C_L\;\sqrt{s_l}$. □

Remark. Compared to the decay rate 2 of ρ in (29) (as $s_{l_{\min}} \to 0$), the decay rate 1/2 of ρ in (32) is poor. This difference comes from the different smoothing properties of the operators A (28) and D expressed in Sobolev scales.

The assumptions of Lemma 5 are somewhat unrealistic. In commercial scanners finitely many source positions are distributed on a curve Γ surrounding the object and at each source position only finitely many X-ray projections are taken. Mostly, Γ is a planar circle.

From now on we therefore consider the cone beam transform as a mapping with finite dimensional image space, i.e.

$$D : L^2(\square) \to \mathbb{R}^{p \cdot q},$$

where p is the number of source positions on Γ and q is the number of X-rays emitted at each source position.

In this setting the structure of the linear system being equivalent to (31), cf. (23), is suited in particular for applying an iterative solver. Let $\{\varphi_{l,k} \mid k \in \mathcal{I}_l\}$ be the B-spline basis of V_l. The system matrix $\mathbf{A}_l$ can be written as

$$\mathbf{A}_l = \mathbf{D}_l^t \mathbf{D}_l + \alpha \mathbf{G}_l$$

with

$$(\mathbf{D}_l)_{(i,j),k} = D\varphi_{l,k}(a_i, \omega_{i,j}) \quad \text{and} \quad (\mathbf{G}_l)_{m,k} = \langle \varphi_{l,m}, \varphi_{l,k} \rangle_{L^2(\square)} .$$

Here, a_i, $1 \le i \le p$, are the discrete source positions on Γ and $\omega_{i,j}$, $1 \le j \le q$, are the directions of the X-rays emitted at source position a_i. Since the basis functions in V_l have a local support (the width of the support is proportional to s_l), both matrices $\mathbf{D}_l$ and $\mathbf{G}_l$ are sparse, that is, almost all of their entries are zero. This is obvious for the Gramian $\mathbf{G}_l$. At the source position a_i only a few X-rays hit the support of $\varphi_{l,k}$ which explains the sparsity of $\mathbf{D}_l$.

So, we can employ sparse matrix techniques to store $\mathbf{D}_l$ as well as $\mathbf{G}_l$ and hence $\mathbf{A}_l$. Additionally, the evaluation of the residue, which has to be done at each iteration step, cf. (24), can be realized very efficiently.

Our theoretical results indicate that it might be worth to tackle the cone beam reconstruction problem by the introduced multilevel iteration. However, only an implementation on a parallel computer can finally settle the question whether this algorithm yields satisfactory results in a reasonable run-time.

3 The use of approximating operators

Again we consider Tikhonov regularization for solving (1), i.e. we consider

$$x_\alpha^\delta = (A^*A + \alpha I)^{-1} A^* y^\delta \quad , \tag{33}$$

where $\|y - y^\delta\| \le \delta$ and A is a compact operator between Hilbert spaces X, Y

$$A : X \to Y \quad .$$

Now assume that a family of approximating operators $\{A_h\}$ is given with

$$||A - A_h|| \leq h \tag{34}$$

and that A is replaced by A_h in (33). Hence we study the approximation properties of

$$x^\delta_{\alpha,h} = (A^*_h A_h + \alpha I)^{-1} A^*_h y^\delta \quad . \tag{35}$$

The introduction of the operators $\{A_h\}$ serves two purposes. First of all any numerical method for computing (33) always requires a finite dimensional approximation of the operator equation (1), cf. Section 2. Secondly we may aim at choosing a sparse or compressed approximation A_h which will yield faster algorithms – this is our main intention for introducing A_h.

The choice of α and h determine the approximation properties of $x^\delta_{\alpha,h}$. We will choose α according to a discrepancy principle of the form (or some modification thereof)

$$||A_h x^\delta_{\alpha,h} - y^\delta|| = \tau\delta, \tag{36}$$

where $\tau > 1$. This still describes an idealized situation: in practice one never aims at solving (36) precisely, one rather chooses α from a sequence of test parameters and determines $\alpha_N \in \{\alpha_n = q^n \alpha_0 | n \in \mathbb{N}\}$ by requiring

$$||A_h x^\delta_{\alpha_N,h} - y^\delta|| \leq \tau\delta \tag{37}$$

$$||A_h x^\delta_{\alpha_n,h} - y^\delta|| > \tau\delta \quad \text{for} \quad n < N \quad . \tag{38}$$

Hence the overall algorithm for computing $x^\delta_{\alpha,h}$ requires to solve $(N+1)$ operator equations

$$(A^*_h A_h + \alpha_n I)x = A^*_h y^\delta, \quad n = 0, 1, \ldots, N \quad . \tag{39}$$

Thus an efficient procedure for obtaining sparse approximations A_h in connection with a reliable strategy for selecting the approximation level h will greatly reduce the numerical cost of the algorithm. Our main objective in this chapter is to determine an approximation level $h(\delta, \alpha)$ such that $x^\delta_{\alpha,h}$ exhibits optimal convergence rates. Note that the approximation level $h(\delta, \alpha)$ may change with α during the search process for the optimal regularization parameter α_N. This will later be used to choose coarser approximations for larger values of α.

As usual we assume that the generalized solution x^+ lies in the range of $(A^*A)^\nu$, that is,

$$x^+ = (A^*A)^\nu v, \quad ||v|| \leq \varrho \quad . \tag{40}$$

Moreover we restrict ourselves to smoothness assumptions of the order

$$0 \leq \nu \leq \frac{1}{2} \quad ,$$

since higher order regularity of x^+ does not further improve the convergence rate of $||x_\alpha^{\delta,h} - x^+||$. This is consistent with the theory of a posteriori parameter selection for classical Tikhonov regularization since – even when using the exact operator A – applying a discrepancy functional of type (36) limits optimal convergence rates to the range $0 \le \nu \le 1/2$. To avoid unnecessary notation we furthermore assume that A_h is a compact operator and that

$$\overline{\text{range}\,(A)} = Y, \quad ||y^\delta|| > \delta, \quad ||A||,\, ||A_h|| \le 1 \ . \tag{41}$$

Notation. A missing index of $x^\delta_{\alpha,h}$ indicates that the related quantity is zero, for instance, $x_{\alpha,h}$ denotes the solution of (35) with exact data y.

We will frequently use the singular value decomposition for a compact operator A, which is denoted by $\{u_n, v_n, \sigma_n\}$ where $u_n \in X$, $v_n \in Y$ are the singular vectors and $\sigma_n > 0$ are the singular values.

The starting for this investigation is a basic estimate which reveals the three error contributions in estimating $||x^\delta_{\alpha,h} - x^+||$. This result is – in principle – contained in Lemma 2.5 of [22]. However we include the full proof since we will need some intermediate steps again later.

Lemma 6. *Let x^+ be the generalized solution of $Ax = y$ and let $x^\delta_{\alpha,h}$ be defined by* (35)*. Assume that $||y - y^\delta|| \le \delta$ and that x^+ obeys* (40)*. Then,*

$$||x^\delta_{\alpha,h} - x^+|| \le \frac{\delta}{2\sqrt{\alpha}} + \frac{h||x^+||}{\sqrt{\alpha}} + \alpha^\nu c_{\nu,\alpha}(v)$$

where

$$c^2_{\nu,\alpha}(v) = \sum_{n\ge 0} \left\{ \frac{\alpha^{1-\nu}\sigma_n^{2\nu}}{(\sigma_n^2 + \alpha)} \ \langle v, u_n\rangle \right\}^2 \le \{(1-\nu)^{1-\nu}\nu^\nu \varrho\}^2 \ .$$

Proof. We follow the proof of Lemma 2.5 in [22]. Equation (40) and inserting the singular value decomposition yields

$$||(A^*A + \alpha I)^{-1} x^+|| \le \tilde{c}_\nu \alpha^{\nu-1} \ ||v|| \ .$$

Moreover we need the following estimates for a compact operator T, they follow from standard estimates using the singular value decomposition of T:

$$||(T^*T + \alpha I)^{-1} T^*|| \le \frac{1}{2\sqrt{\alpha}}, \qquad ||(T^*T + \alpha I)^{-1}|| \le \alpha^{-1},$$

$$||T(T^*T + \alpha I)^{-1} T^*|| \le 1,$$

where $T = A$ or $T = A_h$. Now we have

$$||x^\delta_{\alpha,h} - x^+|| \le ||x^\delta_{\alpha,h} - x_{\alpha,h}|| + ||x_{\alpha,h} - x_\alpha|| + ||x_\alpha - x^+||$$

where those three terms can be estimated as follows

$$\begin{aligned}\|x_\alpha - x^+\| &= \| \, (A^*A+\alpha I)^{-1}A^*Ax^+ - x^+\| \\ &= \alpha\|(A^*A+\alpha I)^{-1}x^+\| \\ &\le c_{\nu\alpha}(v)\alpha^\nu\|\rho\|\,,\end{aligned}$$

$$\|x_{\alpha,h} - x_\alpha\| = \|(A_h^*A_h+\alpha I)^{-1}A_h^*y - (A^*A+\alpha I)^{-1}A^*y\| \ .$$

Now we observe that

$$\begin{aligned}&\left\{(A_h^*A_h+\alpha I)^{-1} - (A^*A+\alpha I)^{-1}\right\} \\ &= (A_h^*A_h+\alpha I)^{-1}\left[(A^*A) - (A_h^*A_h)\right](A^*A+\alpha I)^{-1} \\ &= (A_h^*A_h+\alpha I)^{-1}\left\{(A^*-A_h^*)A + A_h^*(A-A_h)\right\}(A^*A+\alpha I)^{-1} \ .\end{aligned}$$

Inserting this identity and $y - A(A^*A+\alpha I)^{-1}A^*y = \alpha(AA^*+\alpha I)^{-1}y$ we obtain

$$\begin{aligned}\|x_{\alpha,h} - x_\alpha\| &= \|(A_h^*A_h+\alpha I)^{-1}(A_h^*-A^*)\left[y - A(A^*A+\alpha I)^{-1}A^*y\right] \\ &\qquad + (A_h^*A_h+\alpha I)^{-1}A_h^*(A-A_h)(A^*A+\alpha I)^{-1}A^*y\| \\ &\le \frac{1}{\alpha}h\,\alpha\,\|(AA^*+\alpha I)^{-1}Ax^+\| \ + \frac{1}{2\sqrt{\alpha}}\,h\,\|x^+\| \\ &\le h\,\|x^+\|/\sqrt{\alpha} \ .\end{aligned}$$

Finally,

$$\|x_{\alpha,h}^\delta - x_{\alpha,h}\| = \|(A_h^*A_h+\alpha I)^{-1}A_h^*(y^\delta - y)\| \le \frac{\delta}{2\sqrt{\alpha}}$$

concludes the proof. □

Remark. Lemma 6 describes the different contributions to the error $\|x_{\alpha,h}^\delta - x^+\|$. The approximation error $\alpha^\nu c_{\alpha\nu}(v)$ as well as the influence of the data error $\frac{\delta}{2\sqrt{\alpha}}$ are the same as for Tikhonov regularization with exact operator A. In addition the operator error introduces a new term of the order $\frac{h\|x^+\|}{\sqrt{\alpha}}$. Of course $\|x^+\|$ is not precisely known, but, since A has been scaled to $\|A\| \le 1$, we have $\|x^+\| \le \varrho$.

The total error $\| \, x_{\alpha,h}^\delta - x^+ \, \|$ depends on the choice of h and α. To begin with let us choose h to be fixed for all α and let us determine α according to a modified discrepancy principle:

$$\text{choose } \alpha \ \text{ s.t.} \quad \| \, A_h \, x_{\alpha,h}^\delta - y^\delta \| = \tau\delta + \sigma h \ . \tag{42}$$

Various types of discrepancy principles, both in terms of the functional on the left hand side and the expression on the right hand side have been investigated, see [11, 12, 15, 22].

Investigating a posteriori strategies of this sort always starts by proving that choosing α according to (42) is equivalent to a discrepancy principle with exact data and exact operator, see e.g. [21].

Lemma 7. *Let $\tau > 2$, $\sigma > \frac{9}{4}||x^+||$, and assume that α is chosen according to* (42). *Then, x_α satisfies a discrepancy principle*

$$||Ax_\alpha - y|| = \tilde{\tau}\delta + \tilde{\sigma}h \ ,$$

where $|\tau - \tilde{\tau}| \le 2$, $|\sigma - \tilde{\sigma}\ | \ \le \frac{9}{4}\ ||x^+||$, in particular $\tilde{\tau} > 0$, $\tilde{\sigma} > 0$.

Proof. The term $||Ax_\alpha - y||$ can be extended as follows:

$$\begin{aligned} ||Ax_\alpha - y|| &= ||A(A^*A + \alpha I)^{-1}A^*y - y|| \\ &= ||\,(A - A_h)\underbrace{(A^*A + \alpha I)^{-1}A^*y}_{=\,x_\alpha} + A_h(x_\alpha - x_{\alpha,h}) + A_h(x_{\alpha,h} - x^\delta_{\alpha,h}) \\ &\qquad + \ \left[A_h\ x^\delta_{\alpha,h} - y^\delta\right] + \left(y^\delta - y\right)\ || \ . \end{aligned}$$

These five terms have to be estimated separately,

$$||(A - A_h)(A^*A + \alpha I)^{-1}A^*y|| \le h\ ||(A^*A + \alpha I)^{-1}A^*Ax^+|| \le h\ ||x^+|| \ .$$

Now we use the same modifications as in the proof of Lemma 6 for $||x_\alpha - x_{\alpha,h}||$.

$$\begin{aligned} ||A_h(x_\alpha - x_{\alpha,h})|| &= ||A_h\ \left[(A^*A + \alpha I)^{-1}A - (A_h^*A_h + \alpha I)^{-1}A_h^*\right]y|| \\ &\le \frac{1}{2\sqrt{\alpha}}\ h\ \alpha||(AA^* + \alpha I)^{-1}Ax^+|| \ + \ h\ ||x^+|| \\ &\le \frac{1}{4}h||x^+|| + h||x^+|| \ , \\ ||A_h(x_{\alpha,h} - x^\delta_{\alpha,h})|| &= ||A_h(A_h^*A_h + \alpha I)^{-1}A_h^*(y - y^\delta)|| \ \le \ \delta \ , \\ ||A_hx^\delta_{\alpha,h} - y^\delta|| &= \tau\delta + \sigma h, \\ ||y^\delta - y|| &\le \delta \ . \end{aligned}$$

Combining these estimates yields

$$||Ax_\alpha - y|| \le \tau\delta + \sigma h \ + \ \frac{9}{4}\ ||x^+||\ h \ + 2\delta$$

and similarly by the inverse triangle inequality we have

$$||Ax_\alpha - y|| > (\tau - 2)\,\delta + \left(\sigma - \frac{9}{4}||x^+||\right)h \ .$$

□

Now we can deal with y and A instead of y^δ and A_h. This gives rise to an estimate for the a posteriori chosen regularization parameter α.

Lemma 8. *Let α be chosen according to* (42) *then*

$$(\tilde{\tau}\delta + \tilde{\sigma}h)^2 = \alpha^{2\nu+1}\ d^2_{\alpha,\nu}(v)$$

or equivalently

$$\alpha = (\tilde{\tau}\delta + \tilde{\sigma}h)^{\frac{2}{2\nu+1}}\ d_{\alpha,\nu}^{-\frac{2}{2\nu+1}}(v)$$

Proof. The proof is based on the same type of arguments as used in [21]. Applying the results of the previous lemmata yields

$$(\tilde{\tau}\delta + \tilde{\sigma}h)^2 = ||Ax_\alpha - y||^2 = ||(A(A^*A + \alpha I)^{-1}A^* - I)Ax^+||^2$$
$$= \sum_{n\geq 0} \left(\frac{\sigma_n^2}{\sigma_n^2 + \alpha} - 1\right)^2 (\sigma_n \sigma_n^{2\nu})^2 \ |\langle v,\, u_n\rangle|^2$$
$$= \alpha^{2\nu+1} \underbrace{\sum_{h\geq 0} \frac{\sigma_n^{4\nu+2}\alpha^{1-2\nu}}{(\sigma_n^2 + \alpha)^2} \ |\langle\, v,\, u_n\rangle|^2}_{=\ d^2_{\alpha,\nu}(v)} \ .$$

□

Now we can combine the above estimate for α with Lemma 6. First one should note that inserting the singular value decomposition shows that $d_{\alpha,\nu}(v)$ is bounded for $0 \leq \nu \leq 1/2$ and by the Hölder inequality one obtains, see e.g. [21],

$$c_{\alpha,\nu}(v)\ d_{\alpha,\nu}^{\frac{-2\nu}{2\nu+1}}(v) \leq c\ .$$

Lemma 6 now be reformulated as

$$||x^\delta_{\alpha,h} - x^+|| \leq \frac{\delta \cdot d_{\alpha,\nu}^{\frac{1}{2\nu+1}}(v)}{2(\tilde{\tau}\delta + \tilde{\varepsilon}h)^{\frac{1}{2\nu+1}}} + \frac{h||x^+||\ d_{\alpha,\nu}^{\frac{1}{2\nu+1}}(v)}{(\tilde{\tau}\delta + \tilde{\varepsilon}h)^{\frac{1}{2\nu+1}}} + \alpha^\nu c_{\alpha,\nu}(v)$$
$$\leq C(\delta + h)^{\frac{2\nu}{2\nu+1}}\ .$$

Theorem 9. *If* $0 \leq \nu \leq 1/2$ *and if* α *is chosen according to the discrepancy principle* (42) *then*

$$||x^\delta_{\alpha,h} - x^+|| \ = \ O\left((\delta + h)^{\frac{2\nu}{2\nu+1}}\right)\ .$$

If the operator error h is linked to the data error by

$$h \ = \ O(\delta)\ ,$$

then an order optimal convergence rate is achieved by the modified Tikhonov–regularization.

Remark. As always we can strengthen the estimate if $0 \leq \nu < 1/2$ to

$$||x^\delta_{\alpha,h} - x^+|| \ = \ o\left((\delta + h)^{\frac{2\nu}{2\nu+1}}\right)\ .$$

Now we consider the algorithm where α is chosen by testing various parameters

$$\alpha \in \{\alpha_n \mid \alpha_n = q^n \alpha_0 \}$$

according to

$$\|A_h x^\delta_{\alpha_N,h} - y^\delta\| \le \tau\,\delta + \sigma\, h, \tag{43}$$

$$\|A_h x^\delta_{\alpha_n,h} - y^\delta\| > \tau\,\delta + \sigma\, h \quad \text{for} \quad n < N \ . \tag{44}$$

As we will see in the following, a little bit stronger assumptions on the choice of τ and σ insure the same convergence properties as in Theorem 9. As the main ingredient we need the equivalent of Lemma 7.

Lemma 10. *If α_N is chosen according to* (43) *with $\tau > 2/q$ and $\sigma > 9\|x^+\|/4q$ then there exist $\tilde{\tau} > 0$ and $\tilde{\sigma} > 0$ s.t. x_{α_N} satisfies the discrepancy principle*

$$\|Ax_{\alpha_N} - y\| = \tilde{\tau}\,\delta + \tilde{\sigma}\, h \ .$$

Proof. We compare α_N with the parameter α^*, which stems from solving the discrepancy principle (42) exactly. Since the functional $\|A_h x^\delta_{\alpha,h} - y^\delta\|$ increases monotonically with α (this can be seen by expressing this functional in terms of the singular functions of A_h) we have

$$q\ \alpha^* < \alpha_N \le \alpha^*$$

and

$$\|A_h x^\delta_{q\alpha^*,h} - y^\delta\| \le \|A_h x^\delta_{\alpha_N,h} - y^\delta\| \le \tau\delta + \sigma h \ .$$

A lower estimate is obtained by $(q < 1)$

$$\begin{aligned}
\|A_h x^\delta_{q\alpha^*,h} - y^\delta\| &= \left(\sum \left(\frac{(\sigma^h_n)^2}{(\sigma^h_n)^2 + q\alpha^*} - 1 \right)^2 (\langle y^\delta, v^h_n \rangle)^2 \right)^{1/2} \\
&\ge q \left(\sum \left(\frac{(\sigma^h_n)^2}{(\sigma^h_n)^2 + \alpha^*} - 1 \right)^2 (\langle y^\delta, v^h_n \rangle)^2 \right)^{1/2} \\
&= q \|A_h x^\delta_{\alpha^*,h} - y^\delta\| \\
&\ge q(\tau\delta + \sigma h) \ .
\end{aligned}$$

Combining both estimates therefore shows that $x^\delta_{\alpha_N,h}$ satisfies a discrepancy principle with (τ^*, σ^*) where $q\tau \le \tau^* \le \tau$ and $q\sigma \le \sigma^* \le \sigma$. In particular $\tau^* > 2$ and $\sigma^* > 9\|x^+\|/4$, hence Lemma 7 applies. □

Remark. The above lemma implies that choosing α from a decreasing sequence $\alpha = q^n\alpha_0$, $(q < 1)$, yields optimal convergence rates in connection with the discrepancy principle (43).

So far we have discussed to which extend A may be replaced by an approximating operator A_h, where A_h is kept fixed for all possible values of the regularization parameter α. However since we choose α by testing different values of the regularization parameter we would also like to link the quality of the approximation $||A - A_h||$ to α. This will allow us to use coarser approximations for large values of α. The approximation only has to be refined as α gets small.

Let us consider approximation levels of the type

$$h = O(\delta^p \alpha^q) \tag{45}$$

where $0 \le p, q \le 1$ and the regularization parameter is assumed to be bounded above by $\alpha \le \alpha_0$.

All the previous estimates remain valid in this case, in particular we obtain

$$||x^\delta_{\alpha,h} - x^+|| \ = \ O\left((\delta + h)^{\frac{2\nu}{2\nu+1}}\right) \quad . \tag{46}$$

But now h depends on α and we need an additional upper bound for the regularization parameter α. Simply using $\alpha \le \alpha_0$ would yield a suboptimal convergence rate $O(\delta^{2\nu q/(2\nu+1)})$. But, since we expect that asymptotically the regularization parameter of our modified scheme behaves similar to the standard Tikhonov regularization where $(0 \le \nu \le 1/2)$

$$\alpha = O(\delta^{2/(2\nu+1)}) \le c\delta \quad ,$$

we anticipate asymptotically at least $\alpha = O(\delta)$. In order to make this statement precise let us reconsider the relation between δ, h and α as described in Lemma 8,

$$(\tilde{\tau}\delta + \tilde{\sigma}h)^2 = \alpha^{2\nu+1} \left(d_{\alpha,\nu}(v)\right)^2 \quad .$$

Up to here we have used this relation to obtain an upper bound on $1/\sqrt{\alpha}$ by proving that $d_{\alpha,\nu}(v)$ itself is bounded for $0 \le \nu \le 1/2$. Now we need an upper bound for α itself. The proof of Lemma 8 begins with

$$(\tilde{\tau}\delta + \tilde{\sigma}h)^2 = \alpha^2 \sum_{n \ge 0} \frac{\sigma_n^{4\nu+2}}{(\sigma_n^2 + \alpha)^2} \ |\langle\, v, u_n \,\rangle\,|^2 \ .$$

Since $(\sigma_n^2 + \alpha)^2 \le (\sigma_0^2 + \alpha_0)^2 \le c_0$ is bounded we obtain a lower bound for the right hand side by

$$(\tilde{\tau}\delta + \tilde{\sigma}h)^2 \ge \alpha^2 c \sum_{n \ge 0} \sigma_n^{4\nu+2} \ |\langle v,\, u_n\rangle|^2 = \alpha^2 c ||A(A^*A)^\nu v||^2 = \alpha^2 c ||Ax^+||^2 \ .$$

Our assumptions on the computability of the discrepancy principle (41) stated $||Ax^+|| = ||Ax^+ - y^\delta + y^\delta|| \ge ||y^\delta|| - \delta > 0$. Hence we obtain

$$(\tilde{\tau}\delta + \tilde{\sigma}h)^2 \ge c\alpha^2 \quad . \tag{47}$$

Let us now insert the adaptive approximation level $h = O(\delta^p \alpha^q)$.

Lemma 11. *If $h = O(\delta^p \alpha^q)$, where we assume that*

$$0 < p, q, \quad p + q = 1 ,$$

and if $\|Ax^+\| > 0$ then

$$\alpha = O(\delta) .$$

Remark. We expect an even faster decay, namely $\alpha = O(\delta^{2/(2\nu+1)})$. However, this is not obvious for a posteriori parameter selection. Nevertheless applying the above estimate allows us to show optimal convergence rates.

Proof. We have to consider two cases. First assume that $\tilde{\tau}\delta \geq \tilde{\sigma}h$. Then we obtain directly by (47)

$$\alpha^2 \leq c\delta^2 .$$

Secondly, assume that $\tilde{\tau}\delta < \tilde{\sigma}h$. Then,

$$\alpha^2 \leq ch^2 = O(\delta^p \alpha^q)^2$$

which implies $(p + q = 1)$

$$\alpha^{2-2q} = O(\delta^{2p}) \quad \text{or} \quad \alpha = O(\delta) .$$

□

Theorem 12. *If $h = O(\delta^p \alpha^q)$, with $0 < p, q,\ p + q = 1$, and if α is chosen by the modified discrepancy principle* (42)*, then*

$$\|x^\delta_{\alpha,h} - x^+\| = O(\delta^{2\nu/(2\nu+1)}) .$$

Proof. Combining (46) and Lemma 11 gives the desired result. □

Remark. The above theorem shows that we can e.g. chose $p = q = 1/2$ and still obtain optimal convergence rates. Such a choice is preferable for large values of α which is the case in the beginning of our iterative search for the optimal regularization parameter.

Optimal convergence rates cannot be achieved in general if $p + q < 1$.

3.1 Computing approximating families $\{A_h\}$

Replacing A by A_h serves two purposes: first of all any numerical implementation of Tikhonov regularization requires a finite dimensional approximation and secondly one may aim at approximations which have a sparse structure leading to accelerated algorithms. The conventional way of satisfying the first requirement is to replace A by AP_h, where P_h is a projector onto a finite dimensional subspace, see e.g. [24]. However this leads in general to dense matrices. An exception arises when using a singular function system of A, which leads to a diagonal matrix. But those singular functions are in general not known or difficult to construct.

In the following we will discuss two possibilities. Truncated singular value decompositions fall in the class $A_h = AP_h$. But – as usual – they are not recommended for practical applications, nevertheless they achieve optimal convergence rates for a wider range of discrepancy principles. As a second possibility we will apply wavelet techniques in a lazy fashion: we assume that A has been discretized and reduced to a matrix formulation by any standard discretization which might be suitable for the application at hand. Then this matrix is compressed by computing its two–dimensional discrete wavelet transform and discarding small coefficients. This yields an approximating operator which cannot be expressed as $A_h = AP_h$.

Truncated singular value decomposition. Let us assume that the singular value decomposition of A is denoted by $\{u_n, v_n, \sigma_n\}$ and let $n(h)$ denote the index s.t. $|\sigma_n| \le h$ for all $n \ge n(h)$. Then a family of approximating operators is defined by

$$A_h x := \sum_{n \le n(h)} \sigma_n \, \langle x, u_n \rangle \, v_n \quad .$$

Obviously we have $||A - A_h|| \le h$. In this situation we can describe the regularized solution explicitly by

$$x^\delta_{\alpha,h} \; = \sum_{n \le n(h)} \frac{\sigma_n}{\sigma_n^2 + \alpha} \, \langle y^\delta, v_n \rangle \, u_n \quad . \tag{48}$$

In the previous chapter we considered a discrepancy principle with a modified right hand side, namely $\tau\delta + \sigma h$. However this modification is not necessary when using the truncated singular value decomposition.

Theorem 13. *Let $\{A_h\}$ be defined by truncated singular decompositions, choose*

$$h = c_1 \delta^p \alpha^q, \quad 1/2 \le q, \quad 1/3 < p,$$

and determine α by

$$||A_h x^\delta_{\alpha,h} - y^\delta|| = \tau\delta \quad .$$

If $\tau > 2$ and $0 \le \nu \le 1/2$ then

$$||x^\delta_{\alpha,h} - x^+|| \; = \; O(\delta^{2\nu/(2\nu+1)}) \quad .$$

Proof. The central part of the proofs in the previous section is contained in Lemma 7, which allows to deal with the exact data and the full operator A. The proof of this Lemma consists of estimating five terms. All of them can be expressed with the help of the singular value decomposition. The first term gives ($Ax^+ = y$):

$$(A - A_h)(A^*A + \alpha I)^{-1} A^* A x^+ = \sum_{n > n(h)} \sigma_n \, \frac{\sigma_n^2}{\sigma_n^2 + \alpha} \, \langle x^+, u_n \rangle \, v_n \quad .$$

Hence its norm is bounded by a multiple of

$$h^3/\alpha = c_1 \delta^{3p} \alpha^{3q-1} \ .$$

Since $p > 1/3$ and $\alpha \leq \alpha_0$ this norm can be bounded by $c_2\delta$, where $c_2 = O(\delta^{3p-1})$ can be chosen arbitrarily small as δ tends to zero.

The second term vanishes since $x_\alpha - x_{\alpha,h}$ contains only contributions to singular values smaller than h which are in the kernel of A_h. The other terms remain the same. Hence $\tau > 2$ guarantees that x_α obeys the same discrepancy principle with a $\tilde{\tau} > 0$. This, via Lemma 8, gives the relation

$$\tilde{\tau}^2 \delta^2 = \alpha^{2\nu+1} d^2_{\alpha,\nu} \ .$$

Now we have to revise the basic error estimate of Lemma 6 in the light of the truncated singular value decompositions. Here the second term, the operator error is given by

$$\|x_{\alpha,h} - x_\alpha\| \leq h^2/\alpha = c_1^2 \delta^{2/3} \ .$$

The remaining terms can be estimated in the standard fashion:

$$\|x^\delta_{\alpha,h} - x^+\| \ = \ O(\delta^{2\nu/(2\nu+1)}) \ .$$

□

Wavelet compression techniques. Another possibility for constructing approximating operators arises from applying wavelet techniques. The theory of sparsifying or compressing general operators by wavelet techniques has been extensively studied in [2, 8], for applications to compact operators and inverse problems see e.g. [9, 23]. Wavelet–vaguelette decompositions are also considered in the last paper. They can be precomputed and serve as a good compromise between singular functions and finite elements: they also lead to diagonal matrices, moreover the wavelets may be chosen compactly supported.

There exist various ways of achieving a wavelet compression of integral operators with kernel $k(s,t)$. One can e.g. apply a two-dimensional discrete wavelet transform to k to obtain a two-dimensional version of the expansion (10). Discarding all coefficients on scales l smaller than h or using a threshold t, that is, discarding those $d_{l,k}$-coefficients on all scales which are smaller than t leads to compressed operators. In both cases one obtains error estimates by either applying Lemma 1 or the norm equivalence (11). For a more detailed analysis in the framework of ill–posed problems see [9].

A lazy method for accelerating the regularization method is to discretize the operator with an arbitrary Galerkin–type approach. This is rather suitable for many applications where e.g. a triangular model (or tetrahedral model) has been build with large effort and a volume integration technique has lead to a full matrix of large dimension. After computing the wavelet transform of this matrix one can easily either apply thresholding or truncation.

We will only shortly examplify the order of acceleration which can be achieved when this approach is used for optimizing hyperthermia treatment planning, see [18]. For an introduction to the mathematical problems of hyperthermia we refer to [1].

The related matrix has been compressed by thresholding using the Daubechies wavelet with 6 coefficients. The following table shows the number of zeroes obtained for various levels of thresholding.

t_h	n_h	e_h
0.01	47.7%	0.016
0.015	56.8%	0.026
0.05	81.2%	0.0826
0.1	90.93%	0.146
0.25	97.8%	0.27

Different choices t_h of the thresholding parameter t lead to different approximating operators A_h. In the above table n_h denotes the percentage of highpass–coefficients which were set to zero. The deviation e_h is computed by

$$e_h^2 = \frac{\sum_{i,j}(a_{ij} - a_{ij}^h)^2}{\sum_{i,j} a_{ij}^2}$$

which only gives a very rough upper bound to the approximation error. Here, a_{ij} and a_{ij}^h denote the entries of A and A^h, respectively. Typical values for the threshold (discarding about 90% of the wavelet coefficients) resulted – due to the overhead cost for computing the wavelet transforms – in a speed up factor of about 7, without distorting the result visibly.

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