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Data based regularization for discrete deconvolution problems

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Abstract We focus on the solution of discrete deconvolution problems to recover the original information from blurred signals in the presence of Gaussian white noise more accurately. For a certain class of blur operators and signals we develop a diagonal preconditioner to improve the reconstruction quality, both for direct and iterative regularization methods. In this respect, we incorporate the variation of the signal data during the construction of the preconditioner. Embedding this method in an outer iteration may yield further improvement of the solution. To estimate the optimal number of iterations in connection with (P)CGLS, we provide a comparison between different L-curve approaches, especially based on B-splines, and the Discrepancy Principle. Reconstructions of numerous discrete ill-posed model problems, arising both from realistic applications and examples generated on our own, demonstrate the effect of the presented approach.

Keywords Preconditioning · Sparse matrices · Iterative regularization · Tikhonov regularization · TSVD · CGLS · Ill-posed inverse problems

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1 Introduction

We consider the discrete ill-posed linear model problem

$$x \xrightarrow{blur} Hx \xrightarrow{noise} Hx + \eta = b \tag{1.1}$$

where $x \in \mathbb{R}^n$ is the original signal or image, $H \in \mathbb{R}^{n\times n}$ is the blur operator, $\eta \in \mathbb{R}^n$ is a vector representing the unknown perturbations such as noise or measurement

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errors, and $b \in \mathbb{R}^n$ is the observed signal and image, respectively. Our aim is to recover x as good as possible. Because H may be extremely ill-conditioned or even singular, and, because of the presence of the noise, the direct solution of (1.1) will result in a useless reconstruction dominated by noise. Consequently, to avoid this and solve (1.1) mainly on the signal subspace, corresponding to large singular values, a regularization technique has to be applied.

Direct regularization methods compute the solution via direct computation. Based on a decomposition of H, like, for instance, the QR factorization or the singular value decomposition (SVD) [6], these methods can be seen as a spectral filter acting on the singular spectrum, diminishing the deterioration of the solution by noise. Within this class we focus on the classical Tikhonov-Phillips regularization [26,27] and the truncated SVD (TSVD) [11,14]. The Tikhonov regularization can often be improved by including minimization in a seminorm. Usually, the seminorm is related to a smoothing operator like, for instance, the Laplacian.

Another class of regularization methods is based on iterative solvers, e.g., Krylov subspace methods. The usual observation, which coincides, for instance, with the Conjugate Gradient (CG) [1,5] convergence analysis is that in the first iterations the error is reduced relative to large eigenvalues. In later steps, the eigenspectrum related to noise and small eigenvalues dominates the evolution of the approximate solution. Therefore, the restoration has to stop after a few iterations before the method starts to reduce the error relative to the noise subspace. We decide to use CGLS [2] in this class as, here, it becomes possible to estimate the optimal number of iterations via discrete L-curves [12,18].

Applying a preconditioner to an iterative regularization method can have three positive effects: reduce the necessary number of iterations to reach the best reconstruction, result in a flat convergence curve such that it is easier to locate the iteration number with the best solution, or – which is considered in this paper – result in a better reconstruction of the original signal. In general, we have to expect that not all three conditions can be reached simultaneously. In [21] we show that incorporating the variation of the signal data during the construction of preconditioners and the application within iterative methods can result in better or faster reconstructions. Further and more detailed experiments revealed that it is sufficient to use a diagonal preconditioner in common regularization methods to especially improve on the reconstruction of signals which mainly consist of nearly zero components and are weakly blurred by the operator H, i.e., the signal structure is mainly preserved. Embedding this approach in an iterative reconstruction process makes it possible to further enhance on a current solution.

The outline of the paper is the following: In Section 2 we will have a closer look on the regularization methods we use for the reconstruction. Subsequently, in Section 3, we introduce a data based diagonal preconditioner to improve the reconstruction of regularization methods by incorporating the values of the signal. As the quality of (iterative) regularization methods depends on the estimation of the optimal regularization parameter (number of iterations) we briefly examine two methods for (P)CGLS on this in Section 4. Section 5 contains numerical results using the proposed approaches for several test scenarios. A conclusion with a short outlook closes the discussion in Section 6. Concerning our test scenarios, we mainly focus on discrete ill-posed problems from the package *Regularization Tools* [13], but we consider artificial problems constructed on our own using blur operators from MATLAB [23] as well.

2 Regularization methods for discrete ill-posed problems

2.1 TSVD and Tikhonov-Phillips Regularization

An intuitive approach to improve the reconstruction and circumvent the contribution of noise to the solution would be to compute the solution merely on the signal subspace. Unfortunately, an explicit splitting into the signal and noise subspace is not possible. Nevertheless, as large singular values correspond to the signal subspace, we can shrink the SVD expansion such that the solution will mostly consist of quantities corresponding to the signal part, i.e., $x_k = \sum_{i=1}^{k} (u_i^T b)\sigma_i^{-1} v_i$ which is equivalent to solving $\min_x \|x\|_2$ with subject to $\min_x \|H_k x - b\|_2$, where the rank deficient and better conditioned coefficient matrix H_k is the closest rank-k approximation to H. This direct regularization method is known as *truncated singular value decomposition* (TSVD) [11,14].

Another and one of the classical regularization methods is the *Tikhonov regularization* [27] which solves

$$\min_x \left\{ \|Hx - b\|_2^2 + \alpha^2 \|x\|_2^2 \right\} \Leftrightarrow (H^T H + \alpha^2 I)x = H^T b \tag{2.1}$$

instead of (1.1), for a fixed regularization parameter $\alpha \geq 0$. The weight α has to be chosen such that both minimization criterions yield the minimal value together: the computed solution x is as close as possible to the original problem and sufficiently regular.

For the nontrivial task of finding the optimal regularization parameter, for example, α^2 for Tikhonov, the truncation index k for the TSVD, or the number of iterations for iterative regularization methods, there exist several well-known parameter estimation methods like, for instance, the *Discrepancy Principle* [14], the *L-curve* criterion [12,18], or the *Generalized Cross Validation* (GCV) [14]. Among these, the (discrete) L-curve criterion is the most robust one [14]. Therefore, we use it for our results.

2.2 Regularization including a seminorm

Following [9,14,15], instead of using the 2-norm as a means to control the error in the regularized solution, another possibility is to use discrete smoothing norms of the form $\|Lx\|_2$ to obtain regularity. With L being a discrete approximation to a derivative operator, the *standard form* problem (2.1) can be reformulated as Tikhonov-Phillips regularization in *general form* via

$$\min_x \left\{ \|Hx - b\|_2^2 + \alpha^2 \|Lx\|_2^2 \right\} \Leftrightarrow (H^T H + \alpha^2 L^T L)x = H^T b. \tag{2.2}$$

Usually, the matrix L is an approximation to the first or second derivative operator. Consequently, rough oscillations caused by noisy components can be suppressed during the reconstruction and the regularized approximations will satisfy inherent smoothness properties. Therefore, for problems where the exact signal x is smooth, the solution of the general formulation (2.2), using a differential operator, will be smoother and thus a more accurate reconstruction.

2.3 Regularization by preconditioned iterative methods

In connection with iterative methods there is usually demand for preconditioning to accelerate the convergence by modifying the spectrum of the system. Concerning discrete ill-posed problems the application of a preconditioner can easily lead to a deterioration of the reconstruction by approximating the inverse also in the noise subspace, or by removing high-frequency components in the original signal. Therefore, an optimal preconditioner should treat the large singular values and act only on the signal part of the singular spectrum but have no effect on the smaller singular values not amplifying the noise. Following [10], such a preconditioner M should have the following properties:

- $M \approx |H|^{-1}$ on the signal subspace with $|H| = (H^T H)^{\frac{1}{2}}$, and
- $M \approx I$ or $M \approx 0$ on the noise subspace.

For circulant matrices, the eigendecomposition is known and, therefore, these conditions can be satisfied by manipulating the spectral values. Most of the preconditioners make use of properties of structured matrices but for general blur operators, this is usually not possible. In [21] we use the probing facility of MSPAI [20] in order to derive a different approximation quality on the signal and noise subspace, respectively, which in some cases leads to faster or better reconstructions.

In this paper, we use minimum-residual methods, as special projection methods, which implicitly have the desired regularization property. We focus on (P)CGLS as it is a stable way to implement the CG method on the normal equations for Least Squares problems in the general case and because the L-curve criterion can be applied [14]. In Section 4, we address to the algorithms used to estimate the regularization parameter for our results. We reconstruct the observed signal by using two-sided preconditioning within (P)CGLS according to [2]. Note that following [16], both MINRES and GMRES are not suited for the reconstruction of ill-posed image deblurring problems because they do not suppress the noise contribution sufficiently. Compared to these two methods in general, MR-II [8] and RRGMRES [3] are superior when used to reconstruct ill-posed problems.

3 Improving the regularized solution

3.1 Motivation for incorporating the signal data

In [21] we observed improved reconstructions using preconditioners which act differently around discontinuities of the signal. This can be achieved by weighting those preconditioner components which affect such local effects. Smoothing, e.g. with $M = \text{tridiag}(\frac{1}{2}, 1, \frac{1}{2})$ makes sense to remove noisy components only as long as the data is continuous. At discontinuities smoothing would cause additional errors. Therefore, we used a modified tridiagonal smoothing preconditioner with j-th row of the form $(0,\dots,0,r_{j-1},1,r_j,0,\dots,0)$ to obtain $r_j \approx \frac{1}{2}$ near continuous components, but $r_j \approx 0$ near discontinuities. Hence, it may help to incorporate the behavior of the original signal x or some approximation from previous steps, e.g., the blurred data vector b, defining the preconditioner M_b with j-th row

$$(M_b)_{j,:} := (0,\dots,0,r_{j-1},1,r_j,0,\dots,0) \ \text{ for } \ r := \left(\frac{1}{2}\cdot\frac{1}{1+\left(\rho\,|b_j - b_{j+1}|\right)^k}\right)_{j=1,\dots,n-1}.$$

The parameters ρ and k have to be chosen in such a way that discontinuities are revealed as good as possible.

Further experiments showed that it is sufficient to use a weight-free diagonal preconditioner. Nevertheless, applying smooth preconditioners, to eminently continuous data does not destroy the reconstruction process but may lead to slight quality improvement for certain problems. For signals which consist of nearly zero components and are only weakly blurred, i.e., if the signal structure is preserved, the incorporation of the signal data in form of a diagonal matrix leads to better reconstruction results. However, we want to point out that the idea of estimating the signal structure from the data may not work for inverse problems where these two domains are fundamentally different.

A motivation for the effectiveness of taking the signal values into account is the following. Assume $D_{x+\theta} := diag\big((x+\theta)_1,\dots,(x+\theta)_n\big)$ is the diagonal preconditioner built from an approximation $x+\theta$ of x, where x is the original (exact) signal and θ is some deviation from x. Note that $x+\theta$ can, but must not be the observed right-hand side b. The computed solution $\tilde{x}$, i.e., the reconstruction, can be written as $\tilde{x} = x + D_{x+\theta}\delta$, with the deviation $D_{x+\theta}\delta$. To simplify the notation we use $D := D_{x+\theta}$ and thus $\tilde{x} = x + D\delta$.

Theorem 3.1 *Assuming $(x+\theta)_{j=1,\dots,n} \neq 0$, the component-wise relative error of the reconstruction $\tilde{x}$ of the unregularized equation $H^T H\tilde{x} = H^T b$ is*

$$\left|\frac{(\tilde{x}-x)_j}{(x+\theta)_j}\right| = \left|(U\Sigma^{-1}V^T\eta)_j\right|,$$

where $U\Sigma V^T$ is the spectral decomposition of DH^T.

Proof.

$$\begin{aligned} H^T H\tilde{x} = H^T b \quad &\Leftrightarrow \quad (DH^T HD)D^{-1}\tilde{x} = DH^T b &&\Leftrightarrow\\ (DH^T HD)D^{-1}(x+D\delta) \quad &= \quad DH^T(Hx+\eta) &&\Leftrightarrow\\ (DH^T HD)D^{-1}(x+\theta-\theta+D\delta) \quad &= \quad DH^T(HDD^{-1}(x+\theta-\theta)+\eta). \end{aligned}$$

Using the identity $D^{-1}(x+\theta) =: \mathbf{1}$ and the SVD of $DH^T = U\Sigma V^T$ we obtain

$$\begin{aligned} (DH^T HD)(\mathbf{1}+\delta-D^{-1}\theta) = DH^T(HD\mathbf{1}+\eta-H\theta) \quad &\Leftrightarrow DH^T HD\delta = DH^T\eta \ \Leftrightarrow\\ (U\Sigma V^T)(U\Sigma V^T)^T\delta = (U\Sigma V^T)\eta \quad &\Leftrightarrow \delta = U\Sigma^{-1}V^T\eta. \end{aligned} \tag{3.1}$$

Therefore, using the deviation (3.1), the computed solution is $\tilde{x} = x + D(U\Sigma^{-1}V^T\eta)$. With the component-wise consideration

$$(\tilde{x}-x)_j = D_j(U\Sigma^{-1}V^T\eta)_j = (x+\theta)_j(U\Sigma^{-1}V^T\eta)_j$$

we receive the relative error with respect to the approximation $x+\theta$ as

$$\left|\frac{(\tilde{x}-x)_j}{(x+\theta)_j}\right| = \left|(U\Sigma^{-1}V^T\eta)_j\right|. \qquad \square$$

Hence, for a solution $\tilde{x} \neq 0$, the relative error is in the order of the underlying data noise η, if the elements of Σ^{-1} are not arbitrary large, i.e., $\Sigma^{-1} \in \mathscr{O}(1)$.

As the elements of Σ^{-1} usually can be arbitrary large, we get rid of the noise contribution by truncating the small singular values in the original spectral decomposition Σ_0 and denote

$$\Sigma := \left(\begin{array}{c|c} \Sigma_k & \\ \hline & 0 \end{array}\right) \qquad \text{with} \qquad \Sigma_k := diag(\sigma_1,\ldots,\sigma_k).$$

Theorem 3.2 *Assuming $(x+\theta)_{j=1,\ldots,n} \neq 0$, after truncating the small singular values, corresponding to noise, the component-wise relative error for the reconstruction $\tilde{x}$ of $(DH^THD)D^{-1}\tilde{x} = DH^Tb$ remains in the order of the underlying data noise η, i.e.,*

$$\left|\frac{(\tilde{x}-x)_j}{(x+\theta)_j}\right| = \left|(U_k\Sigma_k^{-1}V_k^T\eta)_j\right| \in \frac{1}{\sigma_k}\mathscr{O}(\eta).$$

Proof. Using (3.1) in $(DH^THD)(\mathbf{1}+\delta-D^{-1}\theta)$ we obtain

$$(U\Sigma V^T)(U\Sigma V^T)^T(\mathbf{1}+\delta-D^{-1}\theta) = U\Sigma\Sigma_0U^T(\mathbf{1}-D^{-1}\theta)+U\Sigma^2U^TU\Sigma^{-1}V^T\eta \quad \Leftrightarrow$$

$$\delta = \sum_{j=1}^{k}\left(\underbrace{\frac{\sigma_{0_j}-\sigma_j}{\sigma_j}}_{\approx 0} u_ju_j^Tu_ju_j^T\right)(\mathbf{1}-D^{-1}\theta)+\sum_{j=1}^{k}\left(\frac{1}{\sigma_j^2}u_ju_j^Tu_jv_j^T\sigma_j\right)\eta \quad \Leftrightarrow$$

$$\delta = \sum_{j=1}^{k}\left(\frac{1}{\sigma_j}u_jv_j^T\right)\eta = U_k\Sigma_k^{-1}V_k^T\eta.$$

For a solution $\tilde{x} \neq 0$ and a given truncation index k, the component-wise relative error with respect to the approximation $x+\theta$ is

$$\left|\frac{(\tilde{x}-x)_j}{(x+\theta)_j}\right| = \underbrace{\left|(U_k\Sigma_k^{-1}V_k^T\eta)_j\right|}_{=:\tilde{\eta}_j} \in \frac{1}{\sigma_k}\mathscr{O}(\eta). \qquad \square$$

It remains in the order of the underlying data noise η. Note that this is true for the 2-norm as well, as

$$\left|\frac{(\tilde{x}-x)_j}{(x+\theta)_j}\right| \leq \tilde{\eta}_j \;\Rightarrow\; \sum_{j=1}^{n}(\tilde{x}-x)_j^2 \leq \sum_{j=1}^{n}\tilde{\eta}_j^2(x+\theta)_j^2 \;\Rightarrow\; \frac{\|\tilde{x}-x\|_2}{\|x+\theta\|_2} \leq \|\tilde{\eta}\|_2 \leq \frac{1}{\sigma_k}\|\eta\|_2.$$

3.2 Data based regularization methods

Due to the given signal x or b we construct the data based preconditioner $D \in \mathbb{R}^{n\times n}$ as a diagonal matrix with entries

$$(D_x)_{ii} := |x_i| + \varepsilon \qquad \text{and} \qquad (D_b)_{ii} := |b_i| + \varepsilon,$$

respectively. The parameter ε is mandatory and should be chosen $\varepsilon \ll 1$ or $\varepsilon \in \mathscr{O}(\eta)$ if $b_i = 0$, to guarantee the non-singularity of D_b. For $b_i \neq 0$ we can choose $\varepsilon = 0$. The same holds for D_x.

Following our numerical tests, we received best results using D or D^2 depending on the regularization method. Other powers of D lead to less accurate approximations. For the TSVD the decomposition $HD = U\Sigma V^T$ leads to the modified ill-posed problem

$$(DH^T HD)D^{-1}x = DH^T b \Leftrightarrow x = DV\Sigma^{-1}U^T b$$

while for Tikhonov regularization we use the direct application of D to define an appropriate norm. We modify (2.1) to

$$\begin{aligned} &(DH^T HD)D^{-1}x = DH^T b \quad \Leftrightarrow \quad (DH^T HD + \alpha^2 I)D^{-1}x = DH^T b \quad \Leftrightarrow \\ &(H^T H + \alpha^2 D^{-2})x = H^T b \quad \Leftrightarrow \quad \min_x \left\{ \|Hx - b\|_2 + \alpha^2 \|x\|_{D^{-1}} \right\} \end{aligned} \tag{3.2}$$

Although we observed improvement for (3.2), slightly better results can be obtained by incorporating the signal values only once in the standard form of Tikhonov. Therefore, we reconstruct the signal using $D^{\frac{1}{2}}$ in

$$\min_x \left\{ \|Hx - b\|_2 + \alpha^2 \|x\|_{D^{-\frac{1}{2}}} \right\} \Leftrightarrow (H^T H + \alpha^2 D^{-1})x = H^T b.$$

Using (P)CGLS as iterative regularization method we reconstruct the observed signal by using split preconditioning with $D^{\frac{1}{2}}$. Concerning the class of iterative regularization methods, we also show the preconditioning effect for PMINRES [25] and PMR-II [8] in Section 5.2.4.

3.3 Improvement by outer iterations

It is possible to further improve on a first computed solution and start an iterative process of building diagonal preconditioners based on the current reconstruction. Following our *Regularization with Outer Iterations* (ROI) algorithm, we either use b or a first reconstruction from an unpreconditioned regularization method as initial solution $\tilde{x}^{(0)}$. For a given number of steps we construct $D_{\tilde{x}^{(s)}}$ from a previously computed reconstruction $\tilde{x}^{(s-1)}$ and compute a new solution $\tilde{x}^{(s)}$. As this approach can be applied both to direct and iterative regularization method we refer to any method presented in Section 2 by using the identifier *Regularization_method*. Note that for every call of the *Regularization_method*, there must precede a method for the estimation of the optimal regularization parameter.

ROI Improving the reconstruction by using the preconditioner $D_{\tilde{x}^{(s)}}$ in a regularization method embedded in outer iterations.

Require: $H \in \mathbb{R}^{n\times n}$, $b \in \mathbb{R}^n$, $\varepsilon \in \mathbb{R}$, steps ≥ 0, $\xi \in \mathbb{R}$
  $\tilde{x}^{(0)} \leftarrow b$ or $\tilde{x}^{(0)} \leftarrow Regularization\_method(H,b,I)$
  for $s = 1$ to steps **do**
    $(D_{\tilde{x}^{(s)}})_{ii} = |\tilde{x}_i^{(s-1)}| + \varepsilon$
    $\tilde{x}^{(s)} \leftarrow Regularization\_method(H,b,D_{\tilde{x}^{(s)}})$
    if $\|r^{(s)}\|_2 < \nu_{dp} n^{\frac{1}{2}} \xi$ **then**
      break
    end if
  end for

In general, the solution improves in the first steps. As in later steps the error saturates and the reconstruction does not change evidently, it is reasonable to perform only a few number of iterations. In most cases, it is sufficient to choose steps $\in [1,5]$. Unfortunately, the class of discrete ill-posed problems for which this approach yields improved reconstructions can not be classified exactly. The prerequisite "weakly distorting blur operators for signals containing nearly zero components" is making the method sensible or even spoiling the solution for problems which do not clearly satisfy the requested property. It turned out, that providing a heuristic stopping criterion for the outer iterations can be a resort for this problem. Following the Discrepancy Principle [14], we can stop the outer iterative process before reaching the maximum number of given steps if the residual norm $\|r^{(s)}\|_2$ drops below the expected value of the perturbation norm $\|e\|_2 = n^{\frac{1}{2}}\xi$ using the "safety factor" $\nu_{dp} = 1.5$ for $\nu_{dp}\|e\|_2 = \nu_{dp} n^{\frac{1}{2}}\xi$. Note that for this the error norm or the deviation (order of white noise) ξ has to be known in advance. Regardless, if the reconstruction should be as accurate as possible this can be a method of choice for a certain class of problems, e.g., Gaussian blurred pulse sequences or astronomical images.

4 Estimating the optimal number of iterations in (P)CGLS

Numerical regularization examples where the solution is computed iteratively by a Krylov subspace method using an appropriate stopping criterion are less frequently taken into consideration. Therefore, we introduce a discrete L-curve approach based on B-splines and smoothing and provide a comparison to the ADAPTIVEPRUNING technique [17,18] and the Discrepancy Principle [8] in Section 5.2.1. Especially the latter has not been widely considered in numerical examples in literature so far.

Our approach is slightly based upon the Algorithm FINDCORNER from [19] as we use some sort of spline method combined with a smoothing step. As a first step, we iterate to a sufficient large number of iterations within (P)CGLS, for example, $n = 200$, and compute the points $P_k = (\|r^{(k)}\|_2, \|\tilde{x}^{(k)}\|_2)$. Following [19], for many problems it is advantageous to use an intuitive logarithmic scaling of the P_k to emphasize the flat branches and the corner of the L-curve. However, when using (P)CGLS, we observed that this is no prerequisite to get well shaped L-curves. Here, our experiments showed that the usage of a linear scaling yields robust behavior of the algorithms.

Using P_k we build up a cubic spline interpolant in B-form. The B-form of our (univariate) piecewise polynomial function f is specified by its knot sequence $\|r^{(k)}\|_2$ and by its B-spline coefficient sequence. We use B-splines to receive local support along the domain to overcome the drawback that local variations in the P_k have influence on the whole function degrading the shape of the curve. We refer to the approach as B-SPLINE approach.

Due to numerical errors, local jumps in the curve lead to undesired or useless B-splines, falsifying the true corner of the curve, as, here, the curvature locally deviates from the intrinsic one. Therefore, we provide a smoothing of the original data P_k. As we observed different data ranges along the branches of the L-curve for some model problems, we perform smoothing of different magnitude along the abscissa and the ordinate via

$$\tau_x := c \cdot 10^{-2} \left| \|r^{(1)}\|_2 - \|r^{(n)}\|_2 \right| \quad \text{and} \quad \tau_y := c \cdot 10^{-2} \left| \|\tilde{x}^{(1)}\|_2 - \|\tilde{x}^{(n)}\|_2 \right|.$$

The constant c is a heuristic value and can be determined by observing the shape of the L-curve. Most of our experiments revealed $c = 10^{-2}$, i.e., almost always we use 0.01% of smoothing to receive smoother L-curves. If the residual-norm distance between two neighboring points P_i and P_j is smaller than their solution-norm distance we use the smoothing criterion

$$\left| \|r^{(i)}\|_2 - \|r^{(j)}\|_2 \right| < \tau_x, \quad \text{otherwise} \quad \left| \|\tilde{x}^{(i)}\|_2 - \|\tilde{x}^{(j)}\|_2 \right| < \tau_y.$$

If the criterion is satisfied, we include the point between P_i and P_j into the new smoothed point set S, instead of P_i and P_j. Note that the smoothing approach could be performed several times if the shape is still not smooth enough. For some model problems an additional post-smoothing step is helpful. Therefore, we remove close-by points from S which either in their residual-norm or solution-norm distance are closer to each other than 10^{-8}. Based on this new set of smoothed points S, we build the new B-spline interpolant with its corresponding piecewise polynomial function f_s.

As the optimal number of iterations for (P)CGLS is located at the point with maximum curvature, we compute the curvature at every sample S_k via

$$\kappa(S_k) = f_s''(\|r^{(k)}\|_2) \left(1 + f_s'(\|r^{(k)}\|_2)^2\right)^{-\frac{3}{2}}.$$

Hence, the corner is located at the point with absolute maximum curvature $S_{opt} = \max_k(|\kappa(S_k)|)$. Due to the smoothing approach, it is necessary to perform a back mapping of S_{opt} to locate P_{opt} on the original discrete L-curve. For this purpose, we identify the points P_i and P_j which are closest to S_{opt} via their residual-norm distance. The true corner P_{opt} is then the point with bigger absolute curvature when evaluated on f_s.

Following [9], if the perturbation norm $\|e\|_2$ (or ξ) is known within reasonable accuracy in advance, we are interested in using the DISCREPANCYPRINCIPLE as a stopping heuristic in (P)CGLS and its qualitative comparison to estimators based on L-curves, like, for example, the ADAPTIVEPRUNING algorithm or our B-SPLINE approach (see Section 5.2.1). As in (P)CGLS the series $\{r^{(k)}\}$ is monotonically decreasing, we terminate the reconstruction at iteration k if $\|r^{(k-1)}\|_2 - \|r^{(k)}\|_2 < \xi$ is satisfied. This criterion is much cheaper than, for instance, the L-curve criterion as it can be computed during each iteration. Moreover, there is no need for another invocation with the estimated k or to store every solution along the estimation process, as, here, after (P)CGLS returns, the solution is immediately available.

5 Numerical results

Besides some few model problems created on our own and from [23], we mainly focus on problems from Regularization Tools [13] by Hansen. We affect our right-hand sides with Gaussian white noise of different order, and we perform all computations on normalized values. Note that $\xi \in \mathbb{R}$ refers to the order of the white noise. If not mentioned otherwise, we use $\varepsilon = 10^{-8}$ for $D_{\tilde{x}}$ and $\tilde{x}^{(0)} = b$ as initial solution for the ROI algorithm.

5.1 Preconditioned direct regularization

For the Tikhonov regularization we use two different ways to estimate the optimal regularization parameter α. We constitute the method as OPTIMAL by using the MATLAB function `fminbnd` to search for the local minimizer α for our Tikhonov function handle. We refine the search by setting the termination tolerance to 10^{-9} = `TolX`. Providing an optimal solution has a more hypothetical character. Computing the minimal error $\min_\alpha \|x - \tilde{x}_\alpha\|_2$ illustrates the maximum obtainable improvement for a perfect estimator. Moreover, one could think of a quasi-optimal estimator by visually choosing the subjective best or sharpest image from a set of reconstructions.

Additionally, we compute an estimation via `l_corner`. Similarly to [13], we fix the size of our parameter space to $p = 200$ (number of evaluations for α_k) and perform a scaling of the various α_k in the form

$$\alpha_k = \alpha_{k+1} \left(\frac{\sigma_{max}}{\alpha_p} \right)^{\frac{1}{p-1}}, \qquad k = p-1, \ldots, 1. \tag{5.1}$$

Here $\alpha_p = \max(\sigma_{min}, 16\sigma_{max}\varepsilon_{mach})$ at which ε_{mach} denotes the machine precision and is defined as $\varepsilon_{mach} = 2.2204 \cdot 10^{-16}$ in our case. For every α_k we compute the (preconditioned) Tikhonov solution $\tilde{x}_{\alpha_k}$ and generate the points $(\|H\tilde{x}_{\alpha_k} - b\|_2, \|\tilde{x}_{\alpha_k}\|_2) = \{P_k\}$ of the L-curve. The location of the corner is performed afterwards using `l_corner`.

In case of reconstructing the signal via TSVD we estimate the regularization parameter with the ADAPTIVEPRUNING algorithm implemented in [22]. For the preconditioned TSVD solution we use the SVD of HD, compute the solution $\tilde{x}_k$ with the estimated optimal truncation parameter k via `tsvd` [13], and apply the preconditioner to the solution by $\tilde{x}_k = D_{\tilde{x}^{(s)}}\tilde{x}_k$. Similar to Tikhonov, we provide an OPTIMAL solution by computing the minimal error $\min_k \|x - \tilde{x}_k\|_2$ with respect to the true solution.

5.1.1 Example 1: 1D Gaussian blur of a constant pulse sequence

In our first example we consider the signal x_1 of size $n = 800$ which is a pulse rate with constant positive discontinuities after every 100 samples:

$$(x_1)_{100\cdot i} = 5, \quad i = 1, \ldots, 8. \tag{5.2}$$

We blur this signal with a 1D Gaussian operator `blur1D` with $band = 6$, $\sigma = 4$, and add noise of order $\xi = 0.05\%$. Here, `blur1D` is the 1D analogy of the 2D `blur` operator taken from [13] (cf. Section 5.1.2). The 2D right-hand side is reduced to appropriate size. We reconstruct the signal both in its basic way without preconditioner (denoted as I) and with the diagonal preconditioner $D_{\tilde{x}(s)}$ using ROI where s denotes the number of performed outer iterations. Note that the results for $D_{\tilde{x}(1)}$ reflect a single application of the data based preconditioner. We fix the maximum number of outer iterations to 5, i.e., steps = 5.

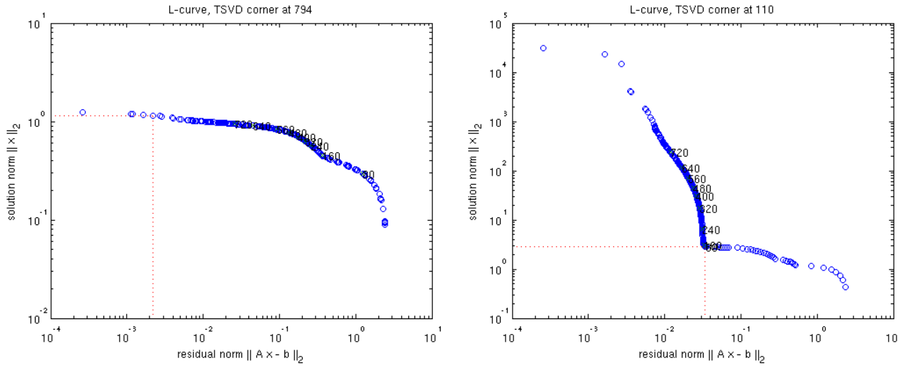
Following Table 5.1, we obtain better reconstruction of x_1 using $D_{\tilde{x}(s)}$. Performing more outer iterations leads to further improvement. In contrast to TSVD the Discrepancy Principle in ROI stops the iteration for Tikhonov (`l_corner`) after the first step. While this criterion prevents further improvement for this example, it may prevent degradation of the solution for other problems. The ADAPTIVEPRUNING algorithm yields nearly optimal estimations of the truncation index making the TSVD regularization produce saturated values similar to the OPTIMAL case. Here, and for some other model problems, we observe that after applying $D_{\tilde{x}}$, the solution norms $\|\tilde{x}\|_2$ become much bigger which results in sharper L-curves (cf. Figure 5.1). Therefore, estimators are able to locate the corner more accurately.

Table 5.1 Reconstruction errors for the signal x_1 blurred with `blur1D(800,6,4)` and affected by noise of order $\xi = 0.05\%$ using Tikhonov regularization and TSVD in algorithm ROI.

`blur1D(800,6,4)`, $n = 800$, $band = 6$, $\sigma = 4$, $\xi = 0.05\%$, $\varepsilon = 10^{-8}$, steps = 5, $(x_1)_{100\cdot i} = 5, \quad i = 1, \ldots, 8$				
Preconditioner	$\|x_1 - \tilde{x}_1\|_2 / \|x_1\|_2$ (Regularization parameter)			
	Tikhonov		TSVD	
	OPTIMAL	`l_corner`	OPTIMAL	ADAP.PRUN.
I	0.2328 (0.0418)	0.8111 (1.1503)	0.2212 (766)	0.5830 (794)
$D_{\tilde{x}(1)}$	0.0384 (0.0238)	0.2357 (0.0005)	0.0300 (82)	0.0319 (110)
$D_{\tilde{x}(2)}$	0.0224 (0.0333)	– stopped	0.0015 (8)	0.0018 (11)
$D_{\tilde{x}(3)}$	0.0176 (0.0360)	–	0.0013 (8)	0.0013 (8)
$D_{\tilde{x}(4)}$	0.0153 (0.0397)	–	0.0013 (8)	0.0013 (8)
$D_{\tilde{x}(5)}$	0.0141 (0.0419)	–	0.0013 (8)	0.0013 (8)

5.1.2 Example 2: Test problem `blur`

As a second example we consider the test problem `blur` taken from [13] which is deblurring images degraded by atmospheric turbulence blur. The matrix H is an $n^2 \times n^2$ symmetric, doubly block Toeplitz matrix that models blurring of an $n \times n$



(a) Without preconditioner. (b) With diagonal preconditioner $D_{\tilde{x}^{(1)}}$.

Fig. 5.1 Discrete L-curves for the problem `blur1D(800,6,4)` solved with TSVD without preconditioner and with $D_{\tilde{x}^{(1)}}$ using the ADAPTIVEPRUNING algorithm to estimate the truncation index.

image by an isotropic Gaussian point-spread function. The parameter σ controls the width of H and thus the amount of smoothing and ill-posedness. H is symmetric block banded and possibly positive definite depending on n and σ. We choose $H \in \mathbb{R}^{32^2 \times 32^2}$, $band = 3$, and $\sigma = 2$, i.e., we invoke `blur(32,3,2)`. We refer to the stacked right-hand side as x_2 and affect it with $\xi = 0.01\%$. Using ROI, we bound the outer iterations to steps $= 5$.

Similar to Example 1, the usage of $D_{\tilde{x}^{(s)}}$ yields better reconstructions both for Tikhonov and TSVD as illustrated in Table 5.2. The Discrepancy Principle in ROI takes effect after the first improvement for Tikhonov but it does not stop the reconstruction after the third step for TSVD producing worse results along further iterations. This reflects the inaccurate behavior of the stopping criterion which we observed for some model problems. Due to poor estimations of α using `l_corner`, we get nearly similar results for I and $D_{\tilde{x}^{(1)}}$. When using our B-SPLINE approach, for example, we obtain more distinct errors which shows the sensitivity of the estimation process.

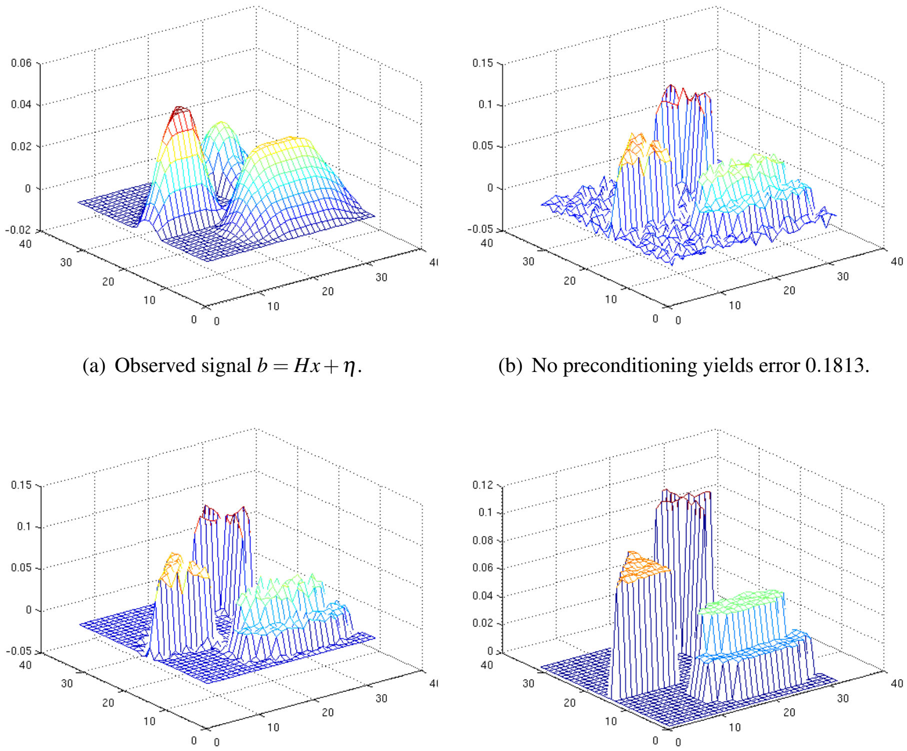
Figure 5.2 gives the mesh plots of the OPTIMAL Tikhonov solutions. Comparing 5.2 (b) and 5.2 (c) shows that using data based regularization provides a solution with better reconstruction, especially near zero values. For theoretical interest, Figure 5.2 (d) gives the solution using $D_{\tilde{x}^{(1)}}$ built from the initial solution $\tilde{x}^{(0)} = x$. Taking the exact signal values into account in most cases leads to improved reconstructions, even for more general blur operators and signals.

5.1.3 Example 3: Test problem `wing`

In our last example for direct regularization methods we consider the test problem `wing` by G. M. Wing taken from [13] where the signal is a positive flank. We invoke `wing`$(800, \frac{1}{3}, \frac{2}{3})$, affect the blurred right-hand side with white noise of order 0.1%, and perform a maximum of 5 outer iterations in ROI.

Table 5.2 Reconstruction errors for the `blur(32,3,2)` problem from [13] affected by noise of order $\xi = 0.01\%$ for Tikhonov regularization and TSVD. The reconstruction is performed with ROI.

`blur(32,3,2)`, $n = 32^2$, $band = 3$, $\sigma = 2$, $\xi = 0.01\%$, $\varepsilon = 10^{-8}$, steps $= 5$					
Precond.	$\\|x_2 - \tilde{x}_2\\|_2 / \\|x_2\\|_2$ (Regularization parameter)				
	Tikhonov			TSVD	
	OPTIMAL	`l_corner`	B-SPLINE	OPTIMAL	ADAP.PRUN.
I	0.1813 (0.0042)	0.6967 ($3 \cdot 10^{-4}$)	0.3757 (0.0670)	0.1898 (766)	0.8619 (972)
$D_{\tilde{x}^{(1)}}$	0.1148 ($5 \cdot 10^{-4}$)	0.6479 ($3 \cdot 10^{-6}$)	0.1345 (0.0012)	0.1384 (417)	0.1583 (506)
$D_{\tilde{x}^{(2)}}$	– stopped	– stopped	– stopped	0.0997 (310)	0.1243 (363)
$D_{\tilde{x}^{(3)}}$	–	–	–	0.0971 (287)	0.1247 (304)
$D_{\tilde{x}^{(4)}}$	–	–	–	0.0997 (273)	0.1309 (274)
$D_{\tilde{x}^{(5)}}$	–	–	–	0.0998 (273)	0.1789 (232)



(a) Observed signal $b = Hx + \eta$.

(b) No preconditioning yields error 0.1813.

(c) Using $D_{\tilde{x}^{(1)}}$, $\tilde{x}^{(0)} = b$ yields error 0.1148.

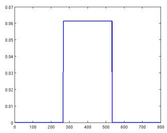
(d) Using $D_{\tilde{x}^{(1)}}$, $\tilde{x}^{(0)} = x$ yields error 0.0150.

Fig. 5.2 Impact of using $\tilde{x}^{(0)} = b$ and $\tilde{x}^{(0)} = x$ as initial solutions in algorithm ROI during OPTIMAL Tikhonov reconstruction of the problem `blur(32,3,2)`, $\xi = 0.01\%$.

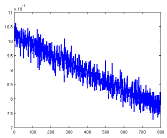
Following Table 5.3, a single application of $D_{\tilde{x}(1)}$ in the first step yields slightly worse solutions. For TSVD the stopping criterion tolerates further outer iterations and thus it becomes possible to improve the reconstruction. Although, here, for $D_{\tilde{x}(1)}$ the estimated and OPTIMAL reconstruction is worse than for the case using I, the solution becomes better for $D_{\tilde{x}(3)}$. However, the Discrepancy Principle does not prevent from spoiling the solution after 3 iterations. Note that this is an example where the signal is strongly distorted by H and the signal structure is not preserved.

Table 5.3 Reconstruction errors using Tikhonov regularization and TSVD for the `wing(800,`$\frac{1}{3}$`,`$\frac{2}{3}$`)` problem from [13] affected by noise of order $\xi = 0.1\%$. The reconstruction is performed with algorithm ROI.

`wing(800,`$\frac{1}{3}$`,`$\frac{2}{3}$`)`, $n = 800$, $\xi = 0.1\%$, $\varepsilon = 10^{-8}$, steps = 3



x_3



$Hx_3 + \eta$

Preconditioner	$\Vert x_3 - \tilde{x}_3\Vert_2 / \Vert x_3\Vert_2$ (Regularization parameter)			
	Tikhonov		TSVD	
	OPTIMAL	`l_corner`	OPTIMAL	ADAP.PRUN.
I	0.6041 (0.0038)	0.6042 (0.0035)	0.6039 (2)	0.6039 (2)
$D_{\tilde{x}(1)}$	0.6092 (0.0001)	0.6094 (0.0002)	0.6137 (3)	0.6240 (2)
$D_{\tilde{x}(2)}$	– stopped	– stopped	0.4122 (2)	0.4561 (2)
$D_{\tilde{x}(3)}$	–	–	0.3934 (2)	0.3813 (2)
$D_{\tilde{x}(4)}$	–	–	0.7248 (2)	0.6550 (2)
$D_{\tilde{x}(5)}$	–	–	1.4154 (2)	1.3208 (2)

5.2 Data based preconditioned iterative regularization

5.2.1 Estimating the number of iterations in (P)CGLS

We compare the performance between our B-SPLINE approach, the ADAPTIVEPRUNING algorithm, and the DISCREPANCYPRINCIPLE. We use a similar test scenario and the notation as presented in [17, 18] but use CGLS without preconditioner to compute the solution of our test problems. As illustrated in Table 5.4, our test problems are mainly chosen from [13], except No. 14 and No. 15 which are two ill-conditioned coefficient matrices from [23]. For the `lotkin` operator we use the smooth signal $x_i = \sin\left(\frac{i\pi}{n}\right)$ with a discontinuity in the middle $x_{\frac{n}{2}} = 4$ and for the `prolate` operator the constant pulse sequence $(x)_{100\cdot i} = 200$. To evaluate the quality of the reconstructions, we constitute $\tilde{x}_{k_{opt}}$ as the OPTIMAL solution where $k_{opt} := \min_k \Vert x - \tilde{x}_k\Vert_2$. We fix our problem size to $n = 1024$ and for each test problem p we compute regularized solutions for 10 different noise levels $\xi \in \{7 \cdot 10^{-d}, 4 \cdot 10^{-d}, 1 \cdot 10^{-d}, 7 \cdot 10^{-6}\}$ with

Table 5.4 Test problems used for the comparison of the estimation approaches. All problems from Regularization Tools use the default solution. For `lotkin` we use the signal $x_i = \sin\left(\frac{i\pi}{n}\right), x_{\frac{n}{2}} = 4$ and for `prolate` the constant pulse sequence $(x)_{100\cdot i} = 200$.

No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Name	`blur`	`deriv2-1`	`foxgood`	`gravity-1`	`spikes`	`shaw`	`wing`	`phillips`	`heat`	`tomo`	`ilaplace-1`	`gravity-3`	`baart`	`lotkin`	`prolate`
Type	Regularization Tools [13]													[23]	

$d \in \{3,4,5\}$. Similar to [18], we measure the quality of the solutions using the metric

$$Q_{p,\xi} = \frac{\|x - \tilde{x}_k\|_2}{\|x - \tilde{x}_{k_{opt}}\|_2}.$$

The minimum value $Q_{p,\xi} = 1$ is optimal, and values $Q_{p,\xi} > 10^2$ are considered off the scale and are set to 10^2.

Following Figure 5.3, the B-SPLINE approach produces solutions which are sometimes off the scale which we observed, similar to [18], for the `l_corner` approach as well. This results from the fact that a parametric spline is a function sensitive to its knot distribution making maximum curvature based methods fit only the local behavior of the L-curve and thus sometimes produce poor estimations. For the problems No. 8, 9, and 10 this approach seems to work better while for No. 3, 7, and 13 it produces worse solutions compared to the ADAPTIVEPRUNING algorithm.

The most stable behavior over all problems results from the DISCREPANCYPRINCIPLE. However, we observed that both the B-SPLINE and the ADAPTIVEPRUNING algorithm may produce better estimation. The bottom plot of Figure 5.3 illustrates a zoomed in view, where all values $Q_{p,\xi} > 10^{\frac{1}{10}}$ are set to $10^{\frac{1}{10}}$. Besides the problems No. 9, 10, 14, the results are more accurate using the ADAPTIVEPRUNING algorithm. Nevertheless, if the perturbation norm or η are known in advance and especially for model problems where the optimum is reached after a few iterations ($\lesssim 30$), the DISCREPANCYPRINCIPLE provides a cheap and robust estimation of k, yielding tolerable solutions while circumventing the drawbacks of the L-curve criterion.

Similar to [17, 18] for large scale problems, we observed in some cases that the real optimum is not located at the corner of the L-curve, but more outside along its branches which may bring up the deviation from the optimum for the L-curve based algorithms. Similar to direct regularization techniques, the estimation of the number of iterations for CGLS is sensible and depends on the smoothness and the characteristic shape of the L-curve which is not always guaranteed to be satisfied. Further difficulties may appear for model problems with slowly decaying singular values, as, here, the corner of the curve becomes less distinct. Moreover, in many practical problems the L-curve may totally lose its characteristic shape.

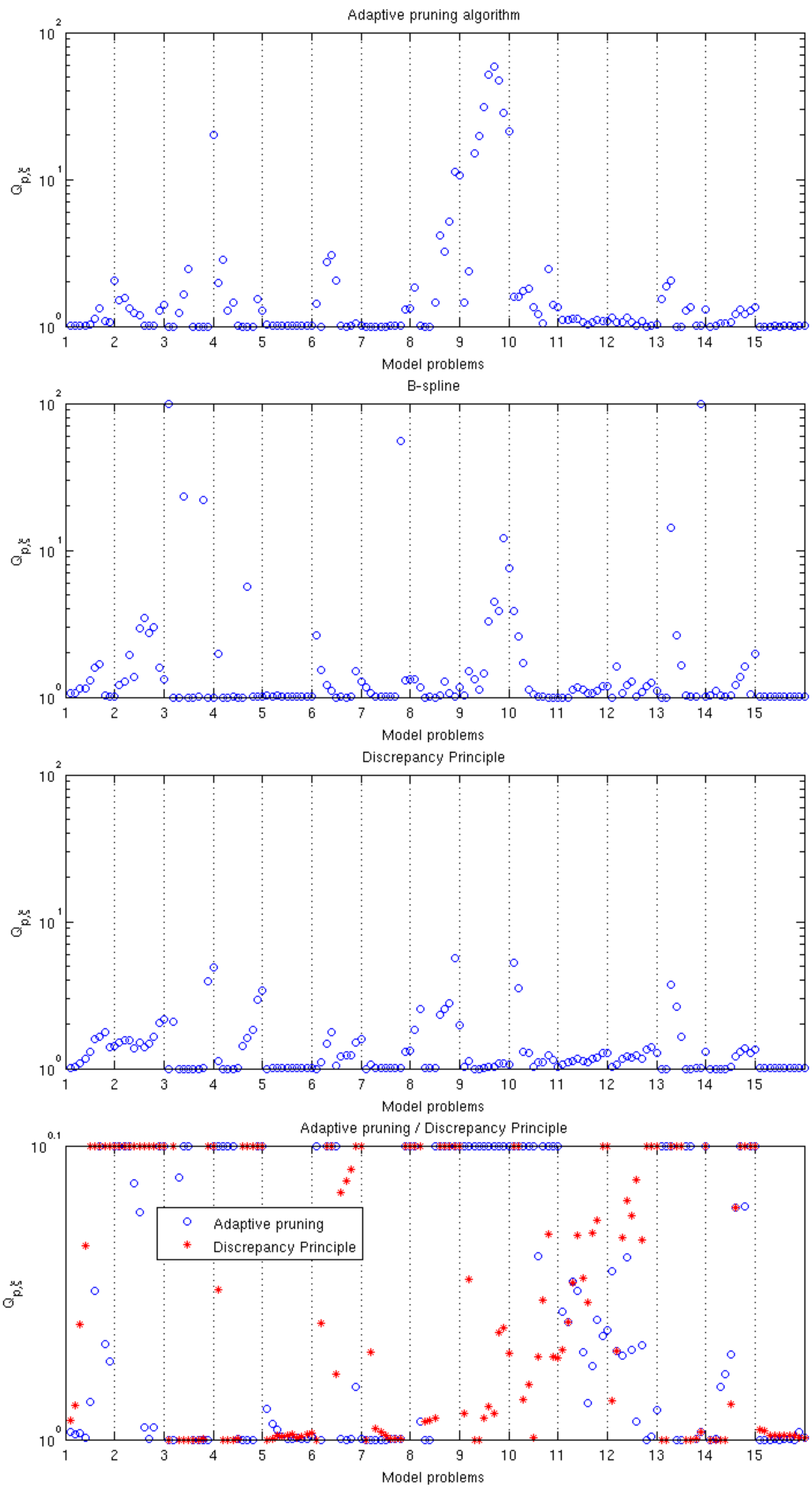


Fig. 5.3 Measure of the quality metric $Q_{p,\xi}$ for the estimation approaches used to reconstruct all model problems from Table 5.4 for ten realizations of ξ and fixed problem size $n = 1024$. A measure of one is optimal, and all values above 10^2 are set to 10^2.

5.2.2 Example 4: Test problem `prolate`

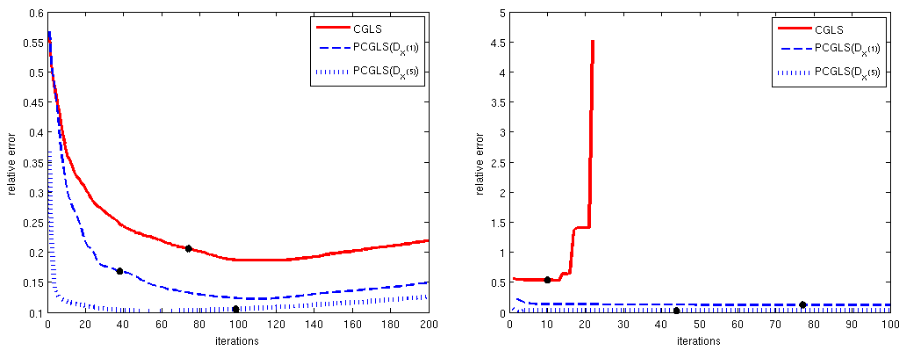
We blur our pulse sequence x_1 (5.2) with the `prolate` operator from [23] which has symmetric Toeplitz form and is severely ill-conditioned. Our model problem has order $n = 10^3$ and is positive definite as we choose $w = 0.34$, i.e., we invoke `gallery('prolate', 1000,0.34)`.

Referring to Table 5.5, we are able to further improve on a computed solution similar to the examples using direct regularization methods. As we want to show the gained accuracy in later iterations, we switch off the Discrepancy Principle within ROI to avoid the break in the outer iterations which occurs after the first step. Using B-SPLINES leads to inferior estimations of k compared to the DISCREPANCYPRINCIPLE but yields better solutions in contrast to the ADAPTIVEPRUNING algorithm. This is because the shape of the L-curve is getting degraded and the optimum no longer corresponds to the point with maximum curvature. Here, the DISCREPANCYPRINCIPLE is a robust and more accurate estimator.

Table 5.5 Reconstruction errors for x_1 (5.2) blurred with the operator `gallery('prolate',1000, 0.34)` from [23] and affected with $\xi = 0.1\%$ using (P)CGLS within algorithm ROI without stopping criterion.

`gallery('prolate',1000, 0.34)`, $n = 1000$, $\xi = 0.1\%$, $\varepsilon = 10^{-8}$, steps = 5, $(x_1)_{100 \cdot i} = 5, \quad i = 1,\ldots,10$				
Preconditioner	(P)CGLS, $\|x_1 - \tilde{x}_1\|_2 / \|x_1\|_2$ (Regularization parameter)			
	OPTIMAL	ADAPT.PRUN.	B-SPLINE	DISCR.PRINC.
I	0.5330 (13)	0.5380 (10)	0.5380 (10)	0.5404 (6)
$D_{\tilde{x}^{(1)}}$	0.1213 (78)	0.1339 (166)	0.1213 (77)	0.1355 (8)
$D_{\tilde{x}^{(2)}}$	0.0341 (5)	0.0491 (36)	0.0430 (16)	0.0392 (4)
$D_{\tilde{x}^{(3)}}$	0.0115 (2)	0.0346 (91)	0.0307 (32)	0.0146 (3)
$D_{\tilde{x}^{(4)}}$	0.0057 (2)	0.0470 (101)	0.0265 (17)	0.0069 (3)
$D_{\tilde{x}^{(5)}}$	0.0041 (2)	0.0315 (40)	0.0256 (44)	0.0048 (3)

We are interested in the convergence behavior when using $D_{\tilde{x}}$ as a preconditioner within (P)CGLS. This is illustrated for $D_{\tilde{x}^{(1)}}$ and $D_{\tilde{x}^{(5)}}$ for the problems `blur(32,3,2)` from Section 5.1.2 and `gallery('prolate',1000,0.34)` with x_1 in Figure 5.4. Applying the data based preconditioner to these problems results in flat convergence curves, especially for the `prolate` operator where CGLS starts to operate on the unwanted noise subspace after a few iterations and thus heavily spoils the reconstruction. This flattened effect is enforced along the outer iterations yielding the desirable L-shaped convergence behavior for $D_{\tilde{x}^{(5)}}$ as Figure 5.4 (a) shows. As there is no intersection between the convergence plots, the reconstruction is always more accurate in each iteration. Due to the fact that the point of maximum curvature on the L-curve does not exactly correspond to the optimal one, the estimation of k_{opt} does not always correspond to the exact optimum.



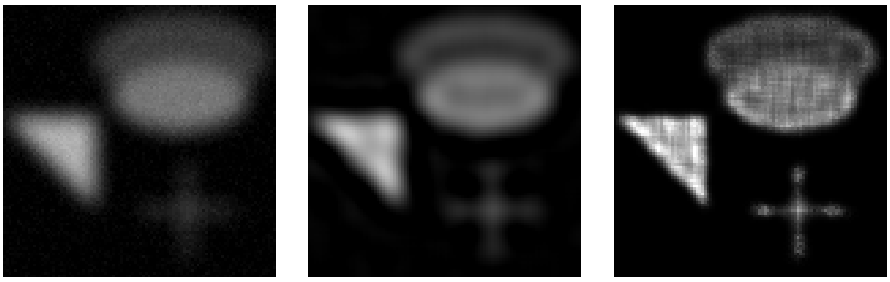
(a) Behavior for Example 2. (b) Behavior for Example 4.

Fig. 5.4 Convergence behavior of CGLS and PCGLS with $D_{\tilde{x}^{(1)}}$ and $D_{\tilde{x}^{(5)}}$ for model problems `blur(32,3,2)` (a) and `gallery('prolate',1000,0.34)` (b). The relative error $\|x-\tilde{x}\|_2/\|x\|_2$ depends on the iteration k. The black dots are the B-SPLINE estimations for the optimal number of iterations.

5.2.3 Example 5: Image test problems `blur`, `tomo` and `text_image`

We are interested in using (P)CGLS as regularization method in the ROI algorithm for two-dimensional discrete ill-posed problems and in the visual effects occurring in the solutions. We consider the problems `blur` (see Section 5.1.2), `tomo` from [13], and the image `Fig0920(a)(text_image)` from [7]. `tomo` is a tomography problem where the domain $[0;n] \times [0;n]$ is divided into n^2 cells of unit size, and a total of round(n^2) rays in random directions penetrate the domain. As a third subexample we use the quadratic cut-out $[1;150] \times [1;150]$ of the `text_image` image from [7] and blur it with the 2D Gaussian operator using $band = 4$ and $\sigma = 3$. We affect the signals resulting from `blur(100,8,4)`, `tomo(60,1)`, and `text_image` with $\xi = 0.08\%$, $\xi = 0.02\%$, and $\xi = 0.1\%$, respectively. For `blur` and `text_image` we switch off the Discrepancy Principle in ROI to illustrate the effect of 5 outer iterations. For `tomo` we limit their maximum number by 8.

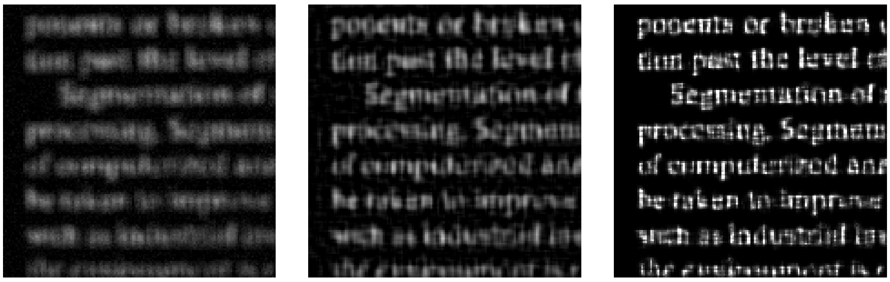
Figure 5.5 shows the solutions for the first and the third problem. For the `tomo` problem we obtained an error of 0.2027 for CGLS (B-SPLINE) on I and an error of 0.1153 for PCGLS (DISCREPANCYPRINCIPLE) for $D_{\tilde{x}^{(8)}}$. Using data based preconditioning yields higher reconstruction quality for the given model settings. Visually, there is less noise perturbation in the background as can be seen, for example, in Figure 5.5 (c). The shape of the objects is reconstructed more accurately. Compare, for instance, the white cross in Figure 5.5 (c) or the writing in Figure 5.5 (f). We additionally reconstructed the text image problem with PCGLS (DISCREPANCYPRINCIPLE) and obtained similar results with $D_{\tilde{x}^{(5)}}$ which yields an error of 0.567. Note that we were able to find model settings for these problems where data based preconditioning lead to worse results. Especially for settings affected with large noise an application of $D_{\tilde{x}}$ produces poorer reconstructions compared to I. For some of these settings the usage of outer iterations can be a remedy to circumvent this problem as, here, the reconstruction is worse for $D_{\tilde{x}^{(1)}}$ but improves along further iterations.



(a) Observed image $b = Hx + \eta$. `blur(100,8,4)`, $\xi = 0.08\%$.

(b) CGLS (B-SPLINE) on I yields error 0.3967.

(c) PCGLS (B-SPLINE) for $D_{\tilde{x}^{(5)}}$ yields error 0.3478.



(d) Observed image $b = Hx + \eta$, $\xi = 0.1\%$.

(e) CGLS (ADAPT.PRUNING) for I yields error 0.7193.

(f) PCGLS (ADAPT.PRUNING) for $D_{\tilde{x}^{(5)}}$ yields error 0.595.

Fig. 5.5 Reconstruction of model problem `blur(100,8,4)` with $\xi = 0.08\%$ in subfigures (a)–(c) and a cut-out of the image `Fig0920(a)(text_image)` from [7] blurred with the 2D Gaussian operator using *band* $= 4$, $\sigma = 3$, and $\xi = 0.1\%$ in subfigures (d)–(f). Reconstruction is perfomed with (P)CGLS in algorithm ROI with switched off Discrepancy Principle.

5.2.4 Data based preconditioning in other iterative regularization methods

We are interested in the behavior using data based preconditioning in other Krylov subspace methods as proposed in Section 3.1. We focus on the problem `blur(32,4,8)` from [13] and on the blur operator `gallery('gcdmat',1024)` from [23], which is the greatest common divisor matrix, using the point symmetric right-hand side x_4 with a positive and negative sawtooth around $\frac{n}{2}$:

$$(x_4)_{i=1:\frac{n}{2}-100,\ \frac{n}{2}+100:n} = 2,\ (x_4)_{i=\frac{n}{2}-100:\frac{n}{2}-1} = i - \frac{n}{2} + 101,\ (x_4)_{i=\frac{n}{2}:\frac{n}{2}+100} = i - \frac{n}{2} - 100.$$

We perform the reconstruction using a maximum of 5 outer iterations in ROI and use the optimal number of iterations k_{opt} within all methods.

Following Table 5.6, we receive similar results among the selected Krylov methods and obtain improved solutions using $D_{\tilde{x}}$. For the `blur` problem the Discrepancy Principle in ROI stops the reconstruction process after the first iteration. The additional theoretical results for $D_{\tilde{x}^{(1)}}$ with initial solution $\tilde{x}^{(0)} = x$ show the maximum obtainable improvement after one outer iteration if $\xi = 0\%$. For this case we always observe a strong improvement for the model problems which implies that the less b is affected by noise, the bigger the improvement will be when data based regularization is used.

Table 5.6 Reconstruction errors for various Krylov subspace methods using the optimal number of iterations for the `blur(32,4,8)` [13] and the `gallery('gcdmat',1024)` [23] problem, respectively. The reconstruction is performed with algorithm ROI using a maximum of 5 outer iterations.

`blur(32,4,8)`, $\xi = 0.015\%$, $\varepsilon = 10^{-8}$, steps = 5			
Preconditioner	$\|x - \tilde{x}\|_2 / \|x\|_2$ (Regularization parameter)		
	(P)CGLS	(P)MINRES	(P)MR-II
I	0.2648 (67)	0.2617 (82)	0.2660 (147)
$D_{\tilde{x}^{(1)}}, \tilde{x}^{(0)} = b$	0.1718 (69)	0.1684 (536)	0.1745 (243)
$D_{\tilde{x}^{(1)}}, \tilde{x}^{(0)} = x$	0.0206 (18)	0.0205 (148)	0.0199 (36)

`gallery('gcdmat',1024)`, $\xi = 0.5\%$, $\varepsilon = 10^{-8}$, steps = 5, x_4			
Preconditioner	$\|x_4 - \tilde{x}_4\|_2 / \|x_4\|_2$ (Regularization parameter)		
	(P)CGLS	(P)MINRES	(P)MR-II
I	0.4116 (25)	0.4072 (30)	0.4231 (44)
$D_{\tilde{x}^{(1)}}, \tilde{x}^{(0)} = b$	0.3033 (25)	0.3001 (95)	0.3021 (56)
$D_{\tilde{x}^{(3)}}, \tilde{x}^{(0)} = b$	0.2350 (21)	0.2340 (67)	0.2329 (42)
$D_{\tilde{x}^{(5)}}, \tilde{x}^{(0)} = b$	0.2260 (20)	0.2278 (65)	0.2216 (31)
$D_{\tilde{x}^{(1)}}, \tilde{x}^{(0)} = x$	0.1182 (11)	0.1169 (33)	0.1138 (24)

5.3 Data based regularization and regularization using smoothing norms

We are interested in a comparison between data based regularization and general form regularization using a smoothing norm. We reconstruct three signals using the T(G)SVD and a maximum of 5 outer iterations in algorithm ROI in different settings. The pulse sequence x_5 with discontinuities at

$$(x_5)_{100} = 3, \quad (x_5)_{200} = 5, \quad (x_5)_{300} = -1, \quad (x_5)_{400} = 2, \text{ and } \quad (x_5)_{500} = -8$$

is blurred with `blur1D(550,3,2)` and affected with $\xi = 0.5\%$. The smooth signals from model problems `i_laplace(550,1)` and `i_laplace(550,2)` [13] are blurred with noise $\xi = 0.4\%$ and $\xi = 0.3\%$, respectively. We obtain the first derivative approximation L_1 for the smoothing norm $\|L_1 x\|_2$ by invoking `get_l(n,1)` from [13] and reconstruct the signals by using `tgsvd`. We provide both the OPTIMAL solution and an estimation of the truncation index via the ADAPTIVEPRUNING algorithm.

Following Table 5.7, reconstructing smooth signals using smoothing norms yields improved results while for discontinuous signals data based regularization is a good choice when H is weakly distorting. Note, that for the `i_laplace(550,1)` problem data based regularization improves the reconstruction for $D_{\tilde{x}^{(1)}}$ and that the Discrepancy Principle does not circumvent spoiling the reconstruction along the outer iterations in the `i_laplace` problems.

Table 5.7 Reconstruction errors using T(G)SVD regularization for x_1 (5.2) blurred with `blur1D(550,3,2)` and the model problem `blur(20,2,4)` affected with $\xi = 0.2\%$ and $\xi = 0.3\%$, respectively.

Preconditioner	$\|x-\bar{x}\|_2 / \|x\|_2$ (Regularization parameter)	
	T(G)SVD (OPTIMAL)	T(G)SVD (ADAPTIVEPRUNING)
`blur1D(550,3,2)`, $n = 550$, $band = 3$, $\sigma = 2$, $\xi = 0.5\%$, x_5		
I	0.5875 (445)	2.5943 (548)
L_1	0.5951 (408)	0.9967 (2)
$D_{\bar{x}^{(1)}}$	0.0813 (29)	0.2311 (16)
$D_{\bar{x}^{(5)}}$	0.0094 (6)	0.0129 (5)
`i_laplace(550,1)`, $n = 550$, $\xi = 0.4\%$		
I	0.2211 (8)	0.2493 (6)
L_1	0.1042 (5)	0.1748 (4)
$D_{\bar{x}^{(1)}}$	0.1848 (7)	0.2194 (5)
$D_{\bar{x}^{(5)}}$	1.0865 (4)	1.3555 (2)
`i_laplace(550,2)`, $n = 550$, $\xi = 0.3\%$		
I	0.7926 (8)	0.8156 (5)
L_1	0.0304 (5)	0.2294 (2)
$D_{\bar{x}^{(1)}}$	1.3016 (1)	2.9878 (7)
$D_{\bar{x}^{(5)}}$	1.4655 (1)	4.0920 (3)

6 Conclusion

We considered the impact of taking the data of the observed right-hand side into account to improve on the reconstruction when using regularization methods to solve discrete deconvolution problems. As classical regularization methods we used Tikhonov-Phillips regularization and the TSVD while in the class of iterative methods we focused on (P)CGLS to compute a regular solution.

In case of model problems where H preserves the shape of the original signal, i.e., performs a weak blurring, and the right-hand side contains nearly zero components, the usage of data based regularization will improve the reconstruction, especially when the perturbation in the right-hand side is of small order and discontinuities are available. Here, incorporating the signal values in a diagonal matrix D is favorable concerning its cheap construction and inversion. Further improvement can be achieved by iteratively applying D to the solution iterates. As a heuristic stopping rule we used the Discrepancy Principle which, for some examples, showed pessimistic behavior, i.e., the outer iteration stopped although it would have been possible to further improve on the solution (see Section 5.2.2 and Section 5.2.3).

Besides using OPTIMAL solutions we investigated the results of our data based regularization approach applying estimated regularization parameters in a variety of test examples. For the direct regularization methods, we used the spline approach from [13] and the robust ADAPTIVEPRUNING algorithm [18] to estimate the corner of discrete L-curves. For (P)CGLS we proposed an approach based on FINDCORNER [19] which incorporates smoothing and the local support of B-splines. A comparison between our discrete B-SPLINE based L-curves, the ADAPTIVEPRUNING technique and the DISCREPANCYPRINCIPLE, as suggested in [9], gives further insight in the behaviour and quality of the estimation process for this Krylov method. Under the assumption of knowing the perturbation error a priori, the DISCREPANCYPRINCIPLE appears to be robust for problems where the optimum is reached after a few number of iterations ($\lesssim 30$) and is fairly cheap compared to L-curve based algorithms. Nevertheless, the presented L-curve approaches have their right to exist as they may yield more accurate estimations of the regularization parameter. Last but not least, the success of data based regularization depends on the quality of the used estimator.

It would be interesting to combine data based regularization with the stabilizing approaches of hybrid methods suggested in [4, 24]. Furthermore, a more convenient stopping rule for the outer iterations should be investigated making data based regularization applicable to general problems without downgrading existing solutions.

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