Applied Numerical Mathematics 62 (2012) 1804–1818

Contents lists available at SciVerse ScienceDirect

Applied Numerical Mathematics

www.elsevier.com/locate/apnum

Preconditioning linear systems via matrix function evaluation

P. Novati, M. Redivo-Zaglia *, M.R. Russo

Department of Mathematics, University of Padova, Italy

ARTICLE INFO

Article history:
Received 17 November 2011
Received in revised form 7 May 2012
Accepted 7 July 2012
Available online 16 July 2012

Keywords:
Ill-conditioned linear systems
Tikhonov regularization
Matrix functions
Arnoldi method

ABSTRACT

A novel preconditioned iterative method for solving discrete ill-posed problems, based on the Arnoldi algorithm for matrix functions, is presented. The method is also extended to work in connection with Tikhonov regularization. Numerical experiments arising from the solution of integral equations and image restoration are presented.

1. Introduction

In this paper we consider the solution of ill-conditioned linear systems

$$A\mathbf{x} = \mathbf{b},$$

in which we assume $A \in \mathbb{R}^{N\times N}$ to be full rank with singular values that gradually decay to 0. As reference problems we consider the linear systems arising from the discretization of Fredholm integral equation of the first kind (commonly referred to as discrete ill-posed problems [14]), where A represents the discretization of a compact operator. Most of the arguments presented here can also be applied to certain saddle point problems (see e.g. [3]) or even Vandermonde type systems arising from interpolation theory (see e.g. [10]). For important applications, involving for instance Vandermonde type systems, $\mathbf{b}$ is assumed to be error-free. On the other hand, when working with discrete ill-posed problems, one typically assumes the right-hand side $\mathbf{b}$ affected by noise. In this paper we consider both cases: $\mathbf{b}$ with and without noise.

In this framework, it is well known that many Krylov type methods such as the CG and the GMRES possess certain regularizing properties that allow to consider them as effective alternative to the popular Tikhonov regularization method, based on the minimization of the functional

$$J(\mathbf{x}, \lambda) = \|A\mathbf{x} - \mathbf{b}\|^2 + \lambda\|H\mathbf{x}\|^2 \tag{1}$$

($\|\cdot\|$ denoting the Euclidean vector norm), where $\lambda > 0$ is a given parameter and H is a regularization matrix (see e.g. [14] and [12] for a background). Indeed, since most of Krylov methods working with A or A^TA initially pick up the largest singular values of A, they can be interpreted as regularization methods in which the regularization parameter is the iteration number m. We may refer to the recent paper [2] and references therein for an analysis of the spectral approximation properties of the Arnoldi-based methods and again [14, §6] for the CG-like methods. In the framework of discrete ill-posed problems, Krylov subspace methods also present some important drawbacks. First of all we may have semi-convergence,

* Corresponding author.
E-mail addresses: novati@math.unipd.it (P. Novati), Michela.RedivoZaglia@unipd.it (M. Redivo-Zaglia), mrrusso@math.unipd.it (M.R. Russo).

0168-9274/$36.00
http://dx.doi.org/10.1016/j.apnum.2012.07.001

that is, the method initially converges but rather rapidly diverges. This phenomenon typically appears when the Krylov method is implemented with the re-orthogonalization of the Krylov vectors (as for instance in the case of the Matlab version of the GMRES, where the orthogonality of the Krylov basis is guaranteed to the machine precision by the use of the Householder transformations). In this situation, after approximating the larger singular values (oversmoothing) the method is also able to provide a good approximation to the smallest ones (undersmoothing). This allows to reach the maximum accuracy, attained for a certain m_{opt}, but at the same time a reliable stopping criterion needs to be used to avoid divergence. On the other hand, if a Krylov method is implemented without re-orthogonalization it is typically not able to produce good approximation of the smallest singular values. After say $\bar{m}$ iterations (normally with $\bar{m} < m_{\text{opt}}$, hence in a situation of oversmoothing) multiple or spurious approximations of the smallest singular values typically appear because of the loss of orthogonality, and the iteration stagnates around $\mathbf{x}_{\bar{m}}$. In this situation a valid stopping rule is no more so crucial but unfortunately the attainable accuracy is generally much poorer than the one obtained by the same method with re-orthogonalization. We refer to [14, §6.7] for an exhaustive explanation about the influence of re-orthogonalization in some classical Krylov methods.

In order to overcome these problems, in this paper we present a new method that can be referred to as a preconditioned iterative solver in which the preconditioner is either $(A+\lambda I)$ or $(A^TA+\lambda H^TH)$. In detail, in the noise-free case, the method is based on the solution of the regularized system

$$(A+\lambda I)\mathbf{x}_\lambda = \mathbf{b},$$

and then on the computation of the solution $\mathbf{x}$ as

$$\mathbf{x} = f(A)\mathbf{x}_\lambda, \tag{2}$$

where $f(z) = 1+\lambda z^{-1}$, using the standard Arnoldi method for matrix functions based on the construction of the Krylov subspaces with respect to A and $\mathbf{x}_\lambda$, that is, $K_m(A,\mathbf{x}_\lambda) = \text{span}\{\mathbf{x}_\lambda, A\mathbf{x}_\lambda, \ldots, A^{m-1}\mathbf{x}_\lambda\}$. The method can be viewed as a preconditioned iterative method, since $f(A) = A^{-1}(A+\lambda I)$. While the word *regularization* is generally used with a different meaning in the literature, Franklin in 1978 used it in [11] for the system $(A+\lambda H)\mathbf{x}_\lambda = \mathbf{b}$ when A is SPD. In [14], Hansen remembered Franklin's approach and used also the same term for this kind of system. It is worth noting that, with respect to standard preconditioned Krylov methods, in our method only one system with the preconditioner has to be solved so reducing the computational cost. Moreover it is important to point out that for problems in which the singular values of A rapidly decay to 0, as those considered in this paper, each Krylov method based on A shows a superlinear convergence (see [22, Chapter 5]). For our method, this fast convergence is preserved since we still work with A for the computation of (2) (see Section 3 for details). As we shall see, this idea, i.e., first regularize then reconstruct, will allow to solve efficiently the problem of divergence without loosing accuracy with respect to the most effective solvers.

The method can be extended to problems in which the right-hand side $\mathbf{b}$ is affected by noise by considering the matrix $(A^TA+\lambda H^TH)$ as preconditioner (cf. (1)). As before the idea is to solve the system

$$\left(A^TA+\lambda H^TH\right)\mathbf{x}_\lambda = A^T\mathbf{b},$$

and then to approximate the solution $\mathbf{x}$ by means of a matrix function evaluation

$$f(Q)\mathbf{x}_\lambda = \left(A^TA\right)^{-1}\left(A^TA+\lambda H^TH\right)\mathbf{x}_\lambda,$$

where f is as before and $Q = (H^TH)^{-1}(A^TA)$.

We need to point out that we could unify the theory taking $H = I$ for the noise-free case, and hence work always with the Krylov subspaces with respect to the matrix Q. However, since A is ill-conditioned, for evident reasons, we prefer to consider two separate situations. Thus, we shall denote by ASP (Arnoldi with Shift Preconditioner) and ATP (Arnoldi with Tikhonov Preconditioner) the approaches for noise-free and noisy problems respectively.

Besides the stability and the good accuracy, there is a third important property that holds in both cases: the reconstruction phase, that is, the matrix function computation, allows to select initially the parameter λ even much larger (heavy oversmoothing) than the one considered optimal by the standard parameter-choice analysis (L-curve, Discrepancy Principle,..., see [14] for a background), without important changes in terms of accuracy. In this sense the method is robust with respect to the choice of the parameter λ (see the filter factor analysis presented in Section 4).

We remark that the idea of using matrix function evaluations to improve the accuracy of the regularization of ill-conditioned linear systems has already been considered in [4]. However, the approach presented here is completely different since, as said before, only one regularized system needs to be solved. Indeed, in [4] the authors consider approximations belonging to the Krylov subspaces generated by $(A+\lambda I)^{-1}$ or $(A^TA+\lambda H^TH)^{-1}$ (rational Krylov approach), that require the solution of a regularized linear system at each Krylov step. Here we consider polynomial type approximations.

The paper is structured as follows. In Section 2 we provide a background about the basic features of the Arnoldi method for matrix functions and we present the methods (ASP and ATP) studied in the paper. We have chosen a parallel presentation since many aspects of the ASP and the ATP approach are very similar (as stated by the algorithms), even if, of course, the action and the choice of the parameter λ is different. Each section of the paper treats both methods, first the ASP and then the ATP, and we have chosen this kind of presentation to avoid repetitions. In Section 3 we analyze the error of the ASP

method, providing also some consideration about the error of both methods in inexact arithmetic. In Section 4 we analyze the filter factors of the methods. In Section 5 we present some numerical experiments, and a test of image restoration is shown in Section 6. Some final comments are given in Section 7.

2. The ASP and the ATP methods

As already partially explained in the introduction, the ASP method approximates the solution of the ill-conditioned system $A\mathbf{x} = \mathbf{b}$ in two steps, first solving in some way the regularized system

$$(A + \lambda I)\mathbf{x}_\lambda = \mathbf{b}, \tag{3}$$

and then recovering the solution $\mathbf{x}$ from the system

$$(A + \lambda I)^{-1} A\mathbf{x} = \mathbf{x}_\lambda, \tag{4}$$

that is equivalent to compute

$$\mathbf{x} = f(A)\mathbf{x}_\lambda \tag{5}$$

where

$$f(z) = 1 + \lambda z^{-1}. \tag{6}$$

In fact, this approach corresponds to apply a left preconditioner $A + \lambda I$ to the system $A\mathbf{x} = \mathbf{b}$. First, solving (3), we obtain the right-hand side $\mathbf{x}_\lambda$ of the preconditioned system (4), and, then, we solve it. Thus, our procedure can be considered as a two-step method, the last step being the main contribution of this paper. For the solution of the system (4) we simply used the Gaussian or the Cholesky factorization although an iterative method may be faster in many cases. In this paper, our aim was just to put forth some basic ideas. We intend to discuss the numerical aspects of our procedures (stopping rule, choice of $\lambda, \ldots$) in a forthcoming work.

Independently of the way we intend to approximate $\mathbf{x}$ from (5), this approach is a novel one because, contrarily to standard preconditioned iterative methods, the linear system (3) with the preconditioner only needs to be solved once. Of course this is possible because of the special preconditioner we are using but, in principle, the idea can be extended to any polynomial preconditioner.

For the computation of $f(A)\mathbf{x}_\lambda$ we use the standard Arnoldi method (or Lanczos in the symmetric case) projecting the matrix A onto the Krylov subspaces generated by A and $\mathbf{x}_\lambda$, that is $K_m(A, \mathbf{x}_\lambda) = \operatorname{span}\{\mathbf{x}_\lambda, A\mathbf{x}_\lambda, \ldots, A^{m-1}\mathbf{x}_\lambda\}$. For the construction of the subspaces $K_m(A, \mathbf{x}_\lambda)$, the Arnoldi algorithm generates an orthonormal sequence $\{\mathbf{v}_j\}_{j \geqslant 1}$, with $\mathbf{v}_1 = \mathbf{x}_\lambda / \|\mathbf{x}_\lambda\|$, such that $K_m(A, \mathbf{x}_\lambda) = \operatorname{span}\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_m\}$ (here and below the norm used is always the Euclidean norm). For every m, in matrix formulation, we have

$$AV_m = V_m H_m + h_{m+1,m}\mathbf{v}_{m+1}\mathbf{e}_m^T, \tag{7}$$

where $V_m = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_m]$, H_m is an upper Hessenberg matrix with entries $h_{i,j} = \mathbf{v}_i^T A\mathbf{v}_j$ and $\mathbf{e}_j$ is the j-th vector of the canonical basis of $\mathbb{R}^m$.

The m-th Arnoldi approximation to $\mathbf{x} = f(A)\mathbf{x}_\lambda$ is defined as

$$\mathbf{x}_m = \|\mathbf{x}_\lambda\| V_m f(H_m)\mathbf{e}_1 \tag{8}$$

(see [16] and the references therein for a background). For the computation $f(H_m)$, since the method is expected to produce a good approximation of the solution in a relatively small number of iterations (see Section 3), that is for $m \ll N$, one typically considers a certain rational approximation to f, or, as in our case, the Schur–Parlett algorithm, [16, Chapter 9].

We denote by ASP method the iteration (8) independently of the method chosen for solving (3). Starting from $\mathbf{v}_1 = \mathbf{x}_\lambda / \|\mathbf{x}_\lambda\|$, at each step of the Arnoldi algorithm, we only have to compute the vectors $\mathbf{w}_j = A\mathbf{v}_j$, $j \geqslant 1$. Below the algorithm used to implement the method.

ASP algorithm

Require $A \in \mathbb{R}^{N\times N}$, $\mathbf{b} \in \mathbb{R}^N$, $\lambda \in \mathbb{R}^+$
Define $f(z) = 1 + \lambda z^{-1}$
Solve $(A + \lambda I)\mathbf{x}_\lambda = \mathbf{b}$
$\mathbf{v}_1 \leftarrow \mathbf{x}_\lambda / \|\mathbf{x}_\lambda\|$
for $m = 1, 2, \ldots$ **do**
  $\mathbf{w}_m \leftarrow A\mathbf{v}_m$
  $h_{k,m} \leftarrow \mathbf{v}_k^T \mathbf{w}_m$

$\tilde{\mathbf{v}} \leftarrow \mathbf{w}_m - \sum_{k=1}^{m} h_{k,m}\mathbf{v}_k$
$h_{m+1,m} \leftarrow \|\tilde{\mathbf{v}}\|$
$\mathbf{v}_{m+1} \leftarrow \tilde{\mathbf{v}}/h_{m+1,m}$
Compute $f(H_m)$ by Schur–Parlett algorithm
$\mathbf{x}_m \leftarrow \|\mathbf{x}_\lambda\| V_m f(H_m)\mathbf{e}_1$
end for

In the above algorithm, the Arnoldi method is implemented with the modified Gram–Schmidt process. Therefore, as is well known, the theoretical orthogonality of the basis is lost quite rapidly and consequently the method is not able to pick up the singular values clustered near 0. For this reason at a certain point during the iteration (8) the method is no longer able to improve the quality of the approximation and it stagnates, typically quite close to the best attainable approximation, and almost independently of the choice λ (see Section 5).

Moreover, by the definition of f, the attainable accuracy of the method (assuming that the seed $\mathbf{x}_\lambda$ is not affected by error) depends on the conditioning of $(A+\lambda I)^{-1}A$. Denoting by $\kappa(\cdot)$ the condition number with respect to the Euclidean norm, theoretically the best situation is attained defining λ such that

$$\kappa(A+\lambda I) = \kappa\big((A+\lambda I)^{-1}A\big), \tag{9}$$

that is, the condition number of the preconditioner is equal to the condition number of the preconditioned system. It is quite easy to prove (see e.g. [4]) that in the SPD case taking $\lambda = \sqrt{\lambda_1\lambda_N}$, where λ_1 and λ_N are respectively the smallest and the largest eigenvalue of A, we obtain $\kappa(A+\lambda I) = \kappa((A+\lambda I)^{-1}A) = \sqrt{\kappa(A)}$.

The preconditioning effect of $A+\lambda I$ of course depends on the choice of λ. By (9) it is necessary to find a compromise between the preconditioning and the accuracy in the solution of the systems with $A+\lambda I$. In this sense formula (9), that theoretically represents the optimal situation also implicitly states a lower bound for the attainable accuracy. Indeed, many numerical experiments arising from the discretization of Fredholm integral equation of the first kind, in which we have examined the behavior of some classical Krylov methods such as the GMRES and the CG preconditioned with $A+\lambda I$, have revealed that we can substantially improve the rate of convergence (taking $\lambda \approx 1/\sqrt{\kappa(A)}$, see again [4] for a discussion) but we are not able to improve the accuracy over a certain limit.

The ASP method can be extended to problems in which the exact right-hand side $\mathbf{b}$ is affected by noise. Since in the presence of noise a good approximation of the exact solution may be meaningless, we extend the idea using the classical Tikhonov regularization. Moreover, many experiments have shown that the ASP method generally produces poor results for problem with noise.

We assume in particular to know only a perturbed right-hand side $\bar{\mathbf{b}} = \mathbf{b} + \mathbf{e_b}$, where $\mathbf{e_b}$ is the perturbation. Given $\lambda > 0$ and $H \in \mathbb{R}^{P\times N}$ such that H^TH is nonsingular, for approximating the solution of $A\mathbf{x} = \mathbf{b}$ we solve the regularized system

$$\big(A^TA + \lambda H^TH\big)\mathbf{x}_\lambda = A^T\bar{\mathbf{b}}, \tag{10}$$

and then we approximate $\mathbf{x}$ by computing

$$\begin{aligned}\bar{\mathbf{x}} &= \big(A^TA\big)^{-1}\big(A^TA + \lambda H^TH\big)\mathbf{x}_\lambda \\ &= f(Q)\mathbf{x}_\lambda,\end{aligned} \tag{11}$$

where f is defined by (6) and $Q = (H^TH)^{-1}(A^TA)$. As before, for the computation of $f(Q)\mathbf{x}_\lambda$ we use the standard Arnoldi method projecting the matrix Q onto the Krylov subspaces generated by Q and $\mathbf{x}_\lambda$. Now, at each step we have to compute the vectors $\mathbf{w}_j = Q\mathbf{v}_j$, $j \geqslant 1$, with $\mathbf{v}_1 = \mathbf{x}_\lambda/\|\mathbf{x}_\lambda\|$, that is, to solve the systems

$$\big(H^TH\big)\mathbf{w}_j = \big(A^TA\big)\mathbf{v}_j.$$

This means that we actually do not need Q explicitly. The algorithm is almost identical to the one given for the ASP method, apart from the two steps inserted in a box.

ATP algorithm

Require $A \in \mathbb{R}^{N\times N}$, $\bar{\mathbf{b}} \in \mathbb{R}^N$, $\lambda \in \mathbb{R}^+$
Define $f(z) = 1 + \lambda z^{-1}$
Solve $(A^TA + \lambda H^TH)\mathbf{x}_\lambda = A^T\bar{\mathbf{b}}$
$\mathbf{v}_1 \leftarrow \mathbf{x}_\lambda/\|\mathbf{x}_\lambda\|$
for $m = 1, 2, \ldots$ **do**
  Solve $(H^TH)\mathbf{w}_m = (A^TA)\mathbf{v}_m$
  $h_{k,m} \leftarrow \mathbf{v}_k^T\mathbf{w}_m$

$\tilde{\mathbf{v}} \leftarrow \mathbf{w}_m - \sum_{k=1}^{m} h_{k,m}\mathbf{v}_k$
$h_{m+1,m} \leftarrow \|\tilde{\mathbf{v}}\|$
$\mathbf{v}_{m+1} \leftarrow \tilde{\mathbf{v}}/h_{m+1,m}$
Compute $f(H_m)$ by Schur–Parlett algorithm
$\mathbf{x}_m \leftarrow \|\mathbf{x}_\lambda\| V_m f(H_m)\mathbf{e}_1$
end for

This kind of approach is somehow related with the so-called iterated Tikhonov regularization (see for instance [12] or [21]), with the important difference that now only one regularized system has to be solved.

Remark 1. The matrix Q is $H^T H$-symmetric, that is, for each $\mathbf{v}, \mathbf{w} \in \mathbb{R}^N$

$$\mathbf{v}^T \left(H^T H Q\right)^T \mathbf{w} = \mathbf{v}^T \left(H^T H Q\right)\mathbf{w} = \mathbf{v}^T A^T A\mathbf{w}.$$

Therefore, the ATP method can be symmetrized using the Lanczos process based on this new metric. However, while this approach is promising because of its reduced computational cost, some preliminary experiments have revealed that it is also quite unstable and, in general, less accurate than the ATP method. For this reason the analysis presented in the next sections does not regard this symmetric variant, and we leave it for future work.

3. Error analysis

In exact arithmetic the error of the ASP method is given by $E_m := \mathbf{x} - \mathbf{x}_m$ where $\mathbf{x}_m$ is defined by (8). If we denote by Π_{m-1} the vector space of polynomials of degree at most $m-1$, it can be seen that

$$\mathbf{x}_m = p_{m-1}(A)\mathbf{x}_\lambda, \tag{12}$$

where $\mathbf{x}_\lambda$ is the solution of (3) and $p_{m-1} \in \Pi_{m-1}$ interpolates, in the Hermite sense, the function f at the eigenvalues of H_m, the so-called Ritz values. Exploiting the interpolatory nature of the standard Arnoldi method, we notice, as pointed out also in [9], that the error can be expressed in the form

$$E_m = \|\mathbf{x}_\lambda\| g_m(A) q_m(A)\mathbf{v}_1, \quad \mathbf{v}_1 = \mathbf{x}_\lambda/\|\mathbf{x}_\lambda\|, \tag{13}$$

where

$$q_m(z) = \det(zI - H_m)$$

(see also [19]), and

$$g_m(z) := \frac{f(z) - p_{m-1}(z)}{\det(zI - H_m)}.$$

From (13), a bound for $\|E_m\|$ can be derived working with the field of values of A, defined as

$$F(A) := \left\{ \frac{\mathbf{y}^H A\mathbf{y}}{\mathbf{y}^H\mathbf{y}}, \mathbf{y} \in \mathbb{C}^N \setminus \{0\} \right\}.$$

Indeed, we can state the following result (see also the recent papers [1] and [8] for a background about the error analysis of the standard Arnoldi method for matrix functions).

Proposition 2. *Assume that $F(A) \subset \mathbb{C}^+$. Then*

$$\|E_m\| \leqslant K \frac{\lambda\|\mathbf{x}_\lambda\|}{a^{m+1}} \prod_{i=1}^{m} h_{i+1,i}, \tag{14}$$

where $a > 0$ is the leftmost point of $F(A)$ and $2 \leqslant K \leqslant 11.08$. In the symmetric case we can take $K = 1$.

Proof. From [6], we know that

$$\left\| g_m(A) \right\| \leqslant K \max_{z \in F(A)} \left| g_m(z) \right|,$$

with $2 \leqslant K \leqslant 11.08$, and hence by (13)

$$\|E_m\| \leqslant K\|\mathbf{x}_\lambda\| \max_{z \in F(A)} \left| g_m(z) \right| \left\| q_m(A)\mathbf{v}_1 \right\|.$$

Now $g_m(z)$ is a divided difference that can be bounded using the Hermite–Genocchi formula (see e.g. [7]), so that

$$\begin{aligned}|g_m(z)| &\leqslant \frac{1}{m!}\max_{\xi\in co\{z,\sigma(H_m)\}}\left|\frac{d^m}{d\xi^m}\left(1+\frac{\lambda}{\xi}\right)\right| \\ &\leqslant \max_{\xi\in co\{z,\sigma(H_m)\}}\frac{\lambda}{|\xi|^{m+1}}\end{aligned}$$

where $co\{z,\sigma(H_m)\}$ denotes the convex hull of the point set given by z and $\sigma(H_m)$. Since $\sigma(H_m)\subset F(H_m)\subseteq F(A)$, by some well known properties of the Arnoldi algorithm, and using the relation

$$\|q_m(A)\mathbf{v}_1\| = \prod_{i=1}^{m} h_{i+1,i},$$

that arises from (7) (see [20]), the result follows. □

Since a, the leftmost point of $F(A)$, can be really small for the problems we are dealing with, formula (14) can surely be considered too pessimistic with respect to what happens in practice. However, the upper bound given by (14) allows to derive some important information about the behavior of the error. First of all, it states that the rate of convergence is little influenced by the choice of λ, and this is confirmed by the analysis given in Section 4 and by the numerical experiments. Secondly, it states that, independently of its magnitude, the error decay is related with the rate of the decay of $\prod_{i=1}^{m} h_{i+1,i}$. We need the following result (cf. [22, Theorem 5.8.10]).

Theorem 3. *Let σ_j and λ_j, $j\geqslant 1$, be respectively the singular values and the eigenvalues of an operator A. Assume that $|\lambda_j|\geqslant|\lambda_{j+1}|$ and*

$$\sum_{j\geqslant 1}\sigma_j^p < \infty \quad \text{for a certain } 0<p\leqslant 1. \tag{15}$$

Let $s_m(z)=\prod_{i=1}^{m}(z-\lambda_i)$. Then

$$\|s_m(A)\| \leqslant \left(\frac{\eta e p}{m}\right)^{m/p},$$

where

$$\eta \leqslant \frac{1+p}{p}\sum_{j\geqslant 1}\sigma_j^p.$$

Of course, the hypothesis (15) is fulfilled by many problems arising from the discretization of integral equations, in many cases with p quite small. Now, using the relation [23, p. 269],

$$\prod_{i=1}^{m} h_{i+1,i} \leqslant \|s_m(A)\mathbf{v}\|$$

that holds for each monic polynomial s_m of exact degree m, we can say that Theorem 3 reveals that for discrete ill-posed problems the rate of decay of $\prod_{i=1}^{m} h_{i+1,i}$ is superlinear and depends on the p-summability of the singular values of A, i.e., on the degree of ill-posedness of the problem (cf. [17, Definition 2.42]).

In computer arithmetics, we need to assume that $\mathbf{x}_\lambda$, solution of (3) is approximated by $\bar{\mathbf{x}}_\lambda$ with an accuracy depending on the choice of λ and the method used. In this way, the Arnoldi algorithm actually constructs the Krylov subspaces $K_m(A,\bar{\mathbf{x}}_\lambda)$. Hence the error can be written as

$$\begin{aligned}\|\bar{E}_m\| &= \|f(A)\mathbf{x}_\lambda - \|\bar{\mathbf{x}}_\lambda\|V_m f(H_m)\mathbf{e}_1\| \\ &\leqslant \|f(A)\bar{\mathbf{x}}_\lambda - \|\bar{\mathbf{x}}_\lambda\|V_m f(H_m)\mathbf{e}_1\| + \|f(A)(\mathbf{x}_\lambda-\bar{\mathbf{x}}_\lambda)\|.\end{aligned} \tag{16}$$

The above formula expresses the error in two terms, one depending on the accuracy of the Arnoldi method for matrix functions and one on the accuracy in the computation of $\mathbf{x}_\lambda$. Roughly speaking we can state that for small values of λ, $f(A)\approx I$ (cf. (5)) and we have that $\|\bar{E}_m\|\approx\|\mathbf{x}_\lambda-\bar{\mathbf{x}}_\lambda\|$. This means that the method is not able to improve the accuracy provided by the solution of the initial system. For large λ we have that $\mathbf{x}_\lambda\approx\bar{\mathbf{x}}_\lambda$ because the system (3) is well conditioned, but even assuming that $\|f(A)(\mathbf{x}_\lambda-\bar{\mathbf{x}}_\lambda)\|\approx 0$ that in principle may happen even if $\|f(A)\|$ is large, we have another lower bound due to the ill-conditioning of $f(A)=A^{-1}(A+\lambda I)$ since now $A+\lambda I$ has a poor effect as preconditioner.

Regarding the optimal choice of λ we can make the following consideration. Unless the re-orthogonalization or the Householder implementation is adopted, the Arnoldi method typically stagnates around the best approximation $\mathbf{x}_{\bar{m}}$ because of the loss of orthogonality of the Krylov basis. Therefore let $c(\lambda)$ be such that

$$\left\| f(A)\bar{\mathbf{x}}_\lambda - \|\bar{\mathbf{x}}_\lambda\| V_m f(H_m)\mathbf{e}_1 \right\| \to c(\lambda) \quad \text{as } m \to N.$$

Then by (16) the optimal value of λ depends on the method used to compute $\bar{\mathbf{x}}_\lambda$ and is given by

$$\lambda_{\text{opt}} = \arg\min_{\lambda>0} \big(c(\lambda) + \left\| f(A)(\mathbf{x}_\lambda - \bar{\mathbf{x}}_\lambda) \right\| \big). \tag{17}$$

Of course the above formula is interesting only for a theoretical point of view. In practice, as mentioned in the introduction, one could try to compare the conditioning of $A + \lambda I$ and $f(A)$, by approximating the solution of

$$\kappa(A + \lambda I) = \kappa\big((A + \lambda I)^{-1} A\big), \tag{18}$$

with respect to λ. However, since the computation of $\mathbf{x}_\lambda$ comes first, it is suitable to take λ a bit larger than the solution of (18). Note that generally such solution can be approximated by $\lambda = 1/\kappa(A)$.

For the ATP method the analysis is almost identical since the error is given by

$$\bar{E}_m := f(Q)\mathbf{x}_\lambda - \|\bar{\mathbf{x}}_\lambda\| V_m f(H_m)\mathbf{e}_1,$$

where $(A^T A + \lambda H^T H)\mathbf{x}_\lambda = A^T \mathbf{b}$, $(A^T A + \lambda H^T H)\bar{\mathbf{x}}_\lambda = A^T \bar{\mathbf{b}}$, and $Q = (H^T H)^{-1}(A^T A)$. Hence, as before we have

$$\|\bar{E}_m\| \leqslant \left\| f(Q)\bar{\mathbf{x}}_\lambda - p_{m-1}(Q)\bar{\mathbf{x}}_\lambda \right\| + \left\| f(Q)(\mathbf{x}_\lambda - \bar{\mathbf{x}}_\lambda) \right\|,$$

where p_{m-1} is again defined by (12). This expression is important since it states that theoretically we may take λ very large, thus oversmoothing, in order to reduce the effect of noise and then leaving to the Arnoldi algorithm the task of recovering the solution. Unfortunately, the main problem is that, as before, $f(Q)$ may be ill-conditioned for λ large. Henceforth, even in this case we should find a compromise for the selection of a suitable value of λ, but contrary to the ASP method for noise-free problems it is difficult to design a theoretical strategy. Indeed everything depends on the problem and on the operator H. In most cases the noise on the right-hand side produces an increment of the high-frequency components of $\mathbf{b}$, that are emphasized on the solution by the nature of the problem. For this reason H is generally taken as a high-pass filter, as for instance a derivative operator, and the solution of (1) can be interpreted as a numerical approximation via penalization of the constrained minimization problem

$$\min_{\|H\mathbf{x}\|=0} \|A\mathbf{x} - \bar{\mathbf{b}}\|.$$

While in standard constrained minimization one approximates the solution taking λ very large (theoretically $\lambda \to \infty$), in our case H is hardly able to detect efficiently the effect of noise on the numerical solution so that one is forced to adopt some heuristic criterion such as the L-curve analysis. In general terms we can say that if the solution is smooth and involves only low frequencies then a high-pass filter should lead to a good approximation taking λ "large". On the other hand if the solution involves itself high frequencies as in the case of discontinuities, then it is better to undersmooth the problem so reducing the effect of the filter. We have made these considerations just to point out that a general theoretical indication on the choice of λ is not possible dealing with problems affected by error. What we can do is to derive methods able to reduce the dependence on this choice, and the ATP method seems to have some chances in this direction.

4. Filter factors

In order to understand the action of the second phase of the methods, i.e., the matrix function evaluation applied to the regularized solution (cf. (5) and (11)), below we investigate the corresponding filter factors.

Assuming for simplicity that A is diagonalizable, that is, $A = XDX^{-1}$ where $D = \text{diag}(\lambda_1, \ldots, \lambda_N)$, for the ASP method we have

$$\mathbf{x}_\lambda = \sum_{i=1}^{N} \frac{\lambda_i}{\lambda_i + \lambda} \frac{(X^{-1}\mathbf{b})_i}{\lambda_i} \mathbf{x}_i,$$

where $\mathbf{x}_i$ is the eigenvector associated with λ_i, and $(\cdot)_i$ denotes the i-th component of a vector. After the first phase, the filter factors are thus $g_i = \lambda_i(\lambda_i + \lambda)^{-1}$. Since from (12), we have $\mathbf{x}_m = p_{m-1}(A)\mathbf{x}_\lambda$, where p_{m-1} interpolates the function f at the eigenvalues of H_m, we immediately obtain

$$\mathbf{x}_m = \sum_{i=1}^{N} \frac{\lambda_i p_{m-1}(\lambda_i)}{\lambda_i + \lambda} \frac{(X^{-1}\mathbf{b})_i}{\lambda_i} \mathbf{x}_i.$$

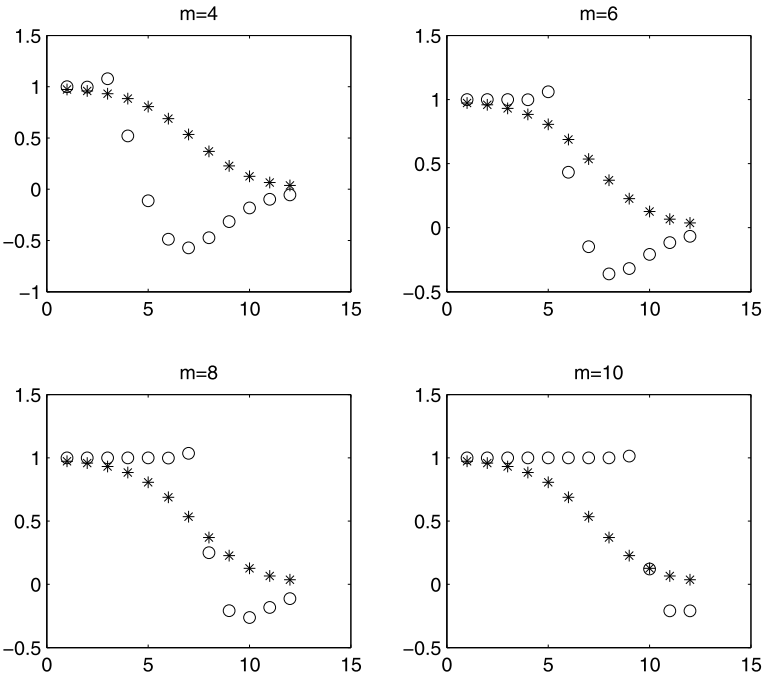

Fig. 1. Filter factors g_i (asterisk) and $f_i^{(m)}$ (circle) with $m = 4, 6, 8, 10$, for GRAVITY(12).

Therefore, at the m-th step of the ASP method the filter factors are given by

$$f_i^{(m)} = \frac{\lambda_i p_{m-1}(\lambda_i)}{\lambda_i + \lambda}, \quad i = 1, \ldots, N.$$

Let us compare, with an example, the behavior of the filter factors. Similarly to what was made in [14], we consider the problem GRAVITY taken from the Hansen's `Regularization Tools` [13,15], with dimension $N = 12$. In Fig. 1, the filter factors g_i and $f_i^{(m)}$, for $m = 4, 6, 8, 10$ are plotted. As regularization parameter we have chosen $\lambda = 1/\sqrt{\kappa(A)}$. Since the problem is SPD, for more clarity in the pictures, the eigenvalues λ_i have been sorted in decreasing order.

While the problem is rather simple the pictures clearly represent the action of the Arnoldi (Lanczos in this case) steps. Since the Arnoldi (Lanczos) algorithm initially picks up the largest eigenvalues, it automatically corrects the filters corresponding to the low-middle frequencies ($g_i \to f_i^{(m)} \approx 1$), keep damping the highest ones. The second phase thus performs a correction, but the properties of the Arnoldi algorithm guarantee that the method can still be interpreted as a regularizing approach.

For a better explanation of Fig. 1, let us assume for simplicity that the Ritz values r_j, $j = 1, \ldots, m$, are distinct (as in the example), so that we can write

$$p_{m-1}(\lambda_i) = \sum_{j=1}^{m} l_j(\lambda_i) f(r_j),$$

where l_j, $j = 1, \ldots, m$ are the Lagrange polynomials. Hence we obtain

$$f_i^{(m)} = \sum_{j=1}^{m} l_j(\lambda_i) \frac{\lambda_i}{r_j} \frac{r_j + \lambda}{\lambda_i + \lambda}, \quad i = 1, \ldots, N.$$

Since the Arnoldi algorithm ensures that $r_j \approx \lambda_j$ for $j = 1, \ldots, m$ we have $f_i^{(m)} \approx 1$ for $i \leqslant m$. For $i > m$ and when $\lambda_i \approx 0$ we have that

$$f_i^{(m)} \approx p_{m-1}(0) \frac{\lambda_i}{\lambda_i + \lambda},$$

so that the filters are close to the ones of the uncorrected scheme. Of course, numerically, the problems start to appear when the Arnoldi algorithm fails to provide good approximations of the eigenvalues of A, but it is important to observe that, at least in exact arithmetics, the choice of λ only influences the high frequencies. For this reason, at least for the ASP method, this choice is more related to the conditioning of the subproblems (cf. Section 3).

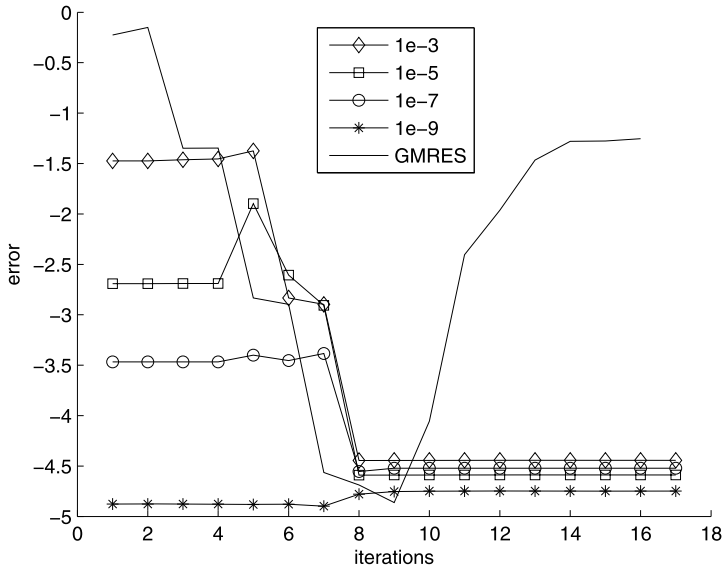

Fig. 2. Error behavior of the GMRES and the ASP method with $\lambda = 10^{-3}, 10^{-5}, 10^{-7}, 10^{-9}$, for noise-free BAART(240).

The filter factor analysis just presented remains valid also for the ATP method. Taking $H = I$ in (10) and using the SVD decomposition we easily find that the filter factors are now given by

$$f_i^{(m)} = \frac{\sigma_i^2 p_{m-1}(\sigma_i^2)}{\sigma_i^2 + \lambda}$$

and hence our considerations for the ASP method remain true also for this case. Of course for $H \neq I$ we just need to consider the GSVD. For problems with noise, the choice of λ is of great importance. Anyway we have just seen that the correction phase allows to reproduce the low frequencies independently of this choice. In this sense, in practice we can take λ even very large in order to reduce as much as possible the influence of noise.

5. Numerical experiments

This section is devoted to the numerical experiments obtained on a single processor computer Intel Core Duo T5800 with Matlab 7.9. Our goal is to prove numerically what we consider the valuable properties of the ASP and the ATP methods, that is, accuracy and speed comparable with the most effective iterative solvers, stability, and robustness of the method with respect to λ. For the experiments we consider problems taken from the `Regularization Tools Matlab` package by Hansen [13,15]. Our comparison method is the Matlab version of the GMRES, that is implemented with the Householder algorithm that guarantees the orthogonality of the Krylov basis to the machine precision. For the problems here considered the GMRES method has shown to be the most accurate, if compared to other well known methods that we can found in the literature. Since it is also quite unstable, it is generally implemented together with the discrepancy principle as stopping criterion (where it is possible of course), but not always with good results. We point out that the modified Gram–Schmidt version of the GMRES has also been considered in the experiments (even if not reported); this version is stable, but unfortunately the attainable accuracy loses one or even two order of magnitude with respect to the version implemented by Matlab. Other methods such as the CGLS and LSQR are widely inferior for the problems considered here.

In all experiments the Arnoldi algorithm for the ASP and the ATP methods, as said in Section 2, is implemented with the modified Gram–Schmidt orthogonalization, and the initial linear system is solved with the LU or the Cholesky factorization.

As first test problem we consider BAART(240) (in parentheses, as usual, we indicate the dimension N). The estimated condition number of the corresponding matrix A is around 10^{20}. We first consider the noise-free case comparing the behavior of the ASP method with GMRES, taking different values of the parameter λ. Looking at Fig. 2 we can observe that even considering a wide range of values for λ, contrary to GMRES the ASP method does not suffer from semi-convergence, that is, the error always stabilizes around the minimum. The attainable accuracy is always quite close to the one of GMRES. The number of iterations necessary to achieve the minimum accuracy is almost always the same, as expected from Proposition 2 and it depends on the spectral properties of the operator, that is, on the fast decay of $\prod_{i=1}^{m} h_{i+1,i}$ (cf. Theorem 3).

Another important observation can be made looking at the error curve corresponding to the choice of $\lambda = 10^{-9}$ (line with asterisks). Since this curve is almost flat we argue that this value of λ is probably very close to the value λ_{opt} defined by (17), that seeks for a compromise between the accuracies in the solutions of the initial linear system and in the computation of the matrix function. In other words, the method is not able to improve the accuracy provided by the solution of the

Table 1
Results for BAART(240) in the noise-free case.

	Error	Residual	λ
ASP	3.58×10^{-5} (8)	1.89×10^{-12}	10^{-3}
	2.57×10^{-5} (8)	3.86×10^{-13}	10^{-5}
	2.78×10^{-5} (8)	4.79×10^{-14}	10^{-7}
	1.26×10^{-5} (7)	1.94×10^{-12}	10^{-9}
GMRES	1.37×10^{-5} (9)	2.21×10^{-15}	

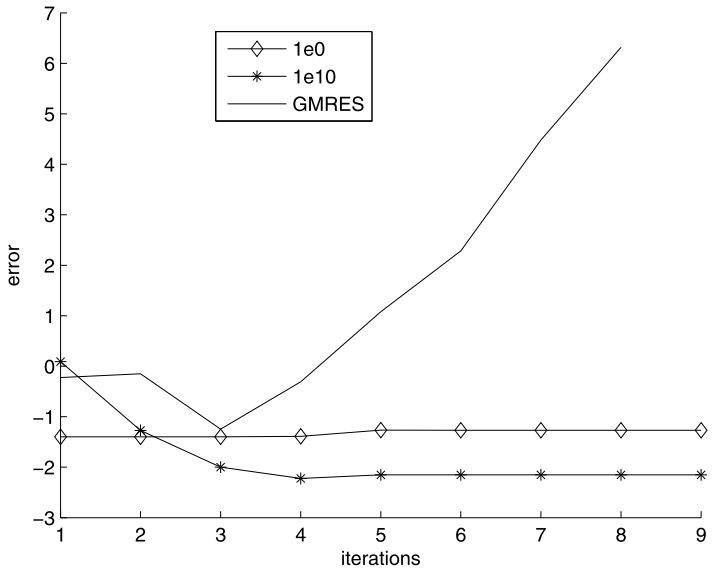

Fig. 3. Error behavior of the GMRES and the ATP method with $\lambda = 1$ and $\lambda = 10^{10}$ for BAART(240) with Gaussian noise.

initial system (see (16)). In Table 1 the minimal errors (with the iteration numbers in parentheses) and the corresponding residuals are reported.

Now we consider the same problem with right-hand side affected by noise. We try to solve $A\mathbf{x} = \mathbf{b}$ working with an inexact right-hand side $\bar{\mathbf{b}} = \mathbf{b} + \mathbf{e_b}$ where $\mathbf{e_b}$ is a noise vector of the type

$$\mathbf{e_b} = \frac{\delta \|\mathbf{b}\|}{\sqrt{N}} \mathbf{u}, \tag{19}$$

where we define $\delta = 10^{-3}$ as the relative noise level, and $\mathbf{u} = \texttt{randn(N, 1)}$, that in Matlab notation is a vector of N random components with normal distribution with mean 0 and standard deviation 1. For the ATP method, we define H as the discrete second derivative operator, that is,

$$H = \begin{pmatrix} 2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{pmatrix} \in \mathbb{R}^{N \times N},$$

and we choose $\lambda = 1$ and $\lambda = 10^{10}$. The comparison is made again with the GMRES. The error curves are plotted in Fig. 3. For $\lambda = 1$ the method does not provide a substantial improvement to the first iteration that corresponds to the Cholesky solution of the Tikhonov system. Probably this is due to the fact that $\lambda = 1$ is close to the value attainable with the L-curve analysis. Anyway it is important to notice that the method does not deteriorate that approximation during the iteration. For $\lambda = 10^{10}$ we have an effective and stable improvement with a good accuracy if compared with the one of the GMRES. In order to avoid confusion in the pictures we only consider these two values, since in the internal range the curves are similar, showing the robustness of the method with respect to the choice of the parameter λ. The results are reported in Table 2.

For a fair comparison between the ASP method and GMRES we also consider the preconditioned version of this code that we denote by PGMRES with the same preconditioner used by the ASP method, that is, $A + \lambda I$. Working again with

Table 2
Results for BAART(240) with Gaussian noise.

	Error	Residual	λ
ATP	4.00×10^{-2} (2)	2.70×10^{-4}	1
	6.01×10^{-3} (4)	2.17×10^{-4}	10^{10}
GMRES	5.66×10^{-2} (3)	2.16×10^{-4}	

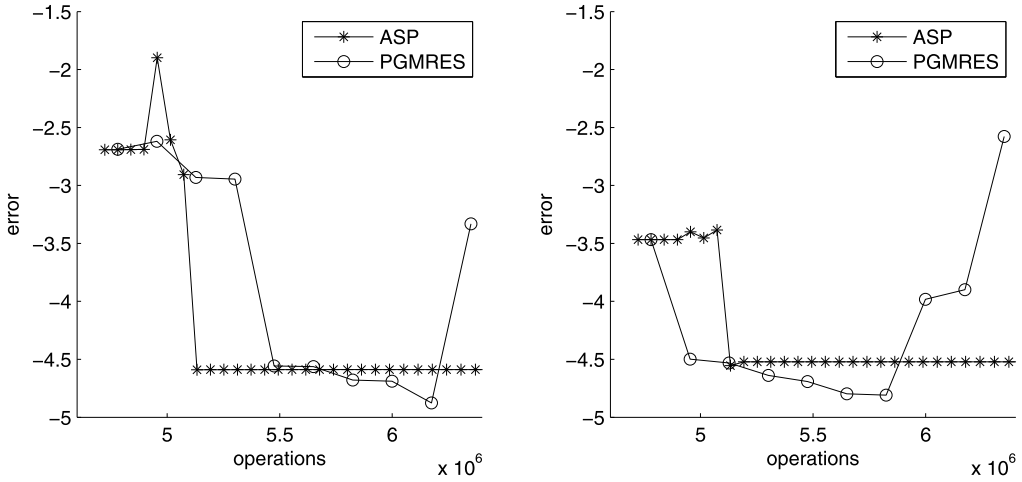

Fig. 4. Error behavior of the preconditioned GMRES and the ASP method for BAART(240) with $\lambda = 10^{-5}$ (left) and 10^{-7} (right).

Table 3
Comparison between the ASP method and the PGMRES for $\lambda = 10^{-5}, 10^{-7}$.

	Error	Residual	λ
ASP	2.57×10^{-5} (8)	3.86×10^{-13}	10^{-5}
PGMRES	1.33×10^{-5} (9)	3.92×10^{-15}	10^{-5}
ASP	2.78×10^{-5} (8)	4.79×10^{-14}	10^{-7}
PGMRES	1.55×10^{-5} (7)	3.43×10^{-13}	10^{-7}

BAART(240) with exact right-hand side, in Fig. 4 we plot the error curves with respect to the computational cost. While a flops counter is no longer available in Matlab, it is quite easy to derive these numbers knowing the algorithms. The non-vectorial operations are neglected. For both methods the systems with $A + \lambda I$ are solved by means of the LU factorization, computed only once at the beginning. Of course, each PGMRES iteration is more expensive since it requires the solution of a system with $A + \lambda I$.

The results reported in Fig. 4 reveal that the ASP is still competitive with the PGMRES in terms of accuracy and computational cost. For this example the PGMRES is a bit faster than GMRES (cf. Fig. 2) since the error curve is steeper at the beginning, but it remains unstable. Comparing also the results of these examples (Table 3) with the ones reported in Table 1, we also observe a very little improvement in terms of accuracy.

In a final example we want to show the behavior of the methods in four classical problems (BAART, FOXGOOD, SHAW and GRAVITY), with $N = 160$, changing the value of the parameter λ. Fig. 5 is representative of what happen in general for the ASP method with exact right-hand side, that is, as expected, the attainable accuracy is generally poor for small values of λ (the initial system is badly solved) and for large values of λ (the preconditioning effort is poor). In any case it is really important to observe that the maximum accuracy can be obtained without much differences for a relatively large window of values for λ, since the curves exhibit a plateau around the minimum. Indicatively, we may say that the maximum accuracy can be achieved taking λ in a range between $1/\sqrt{\kappa(A)}$ and $1/\sqrt[4]{\kappa(A)}$. The importance of this behavior is not negligible because it means that having an estimate of the conditioning of A allows to skip any pre-processing techniques to estimate the optimal value of λ.

Assume now to work with a right-hand side affected by noise, $\bar{\mathbf{b}} = \mathbf{b} + \mathbf{e_b}$, where $\mathbf{e_b}$ is a noise vector defined by (19) with noise level $\delta = 10^{-3}$. Looking at Fig. 6, we can observe that with respect to the noise-free case we do not even have the problem of oversmoothing taking λ too large, at least for the example considered. We argue that the bottleneck, for what concerns the accuracy, is represented by the effect of noise. In general, increasing the value of λ leads to a slight increase of the number of iterations. These considerations lead us to state a general strategy for an automatic parameter-choice implementation of the method:

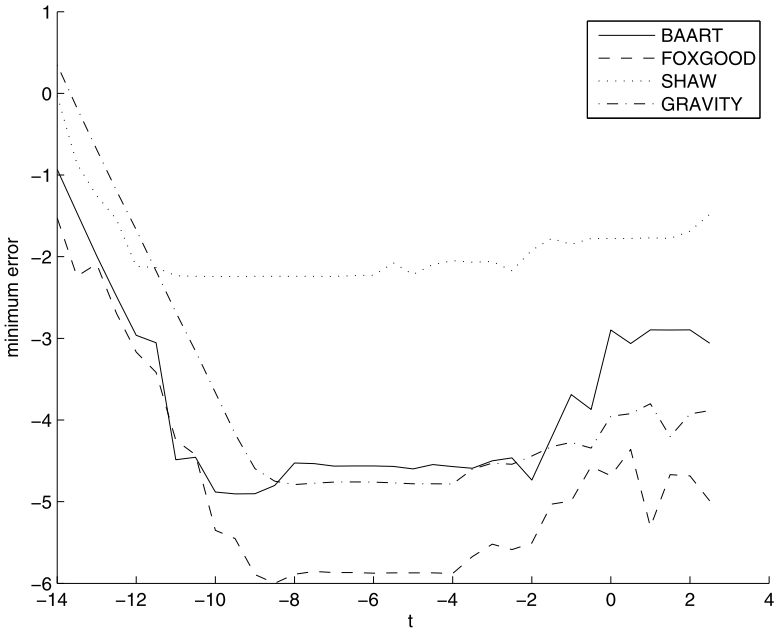

Fig. 5. Maximum attainable accuracy with respect to the choice of $\lambda = 10^t$. The dimension of each problem is $N = 160$.

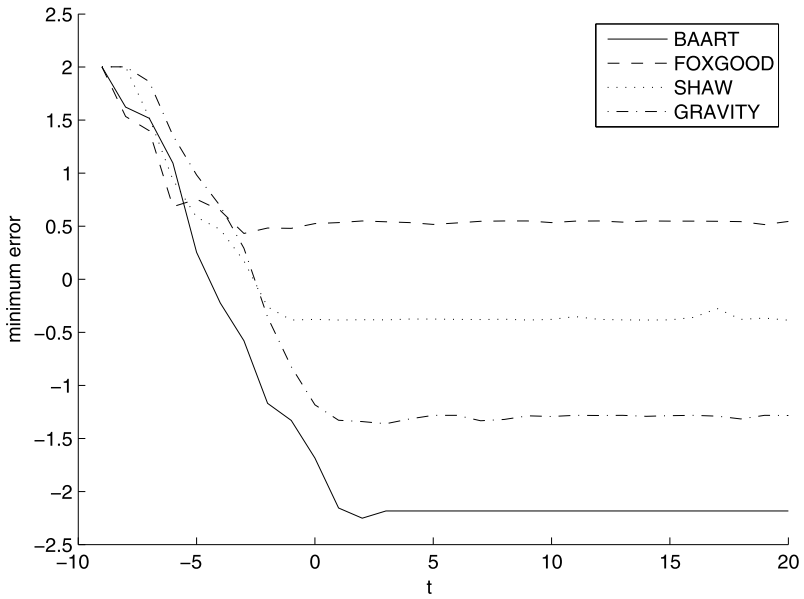

Fig. 6. Maximum attainable accuracy with respect to the choice of $\lambda = 10^t$, with right-hand side affected by noise. The dimension of each problem is $N = 160$.

1. define λ relatively "large", for instance even much larger than the point of maximum curvature of the L-curve;
2. use any parameter-choice method for m to define the stopping rule (as for instance the discrepancy principle where possible), allowing some more iterations to avoid oversmoothing (m too small, cf. Fig. 3).

Concluding we may say that for the ATP method of course there exists an optimal value of λ, say λ_{opt}, close to the corners of the L-shaped curves of Fig. 6, and a corresponding m_{opt}, that is, the minimum number of iterations to achieve the optimal accuracy. Anyway, our experiments reveal that working with $\lambda > \lambda_{\text{opt}}$ and $m > m_{\text{opt}}$, we do not have a sensible loss of accuracy nor a remarkable increase of computational cost.

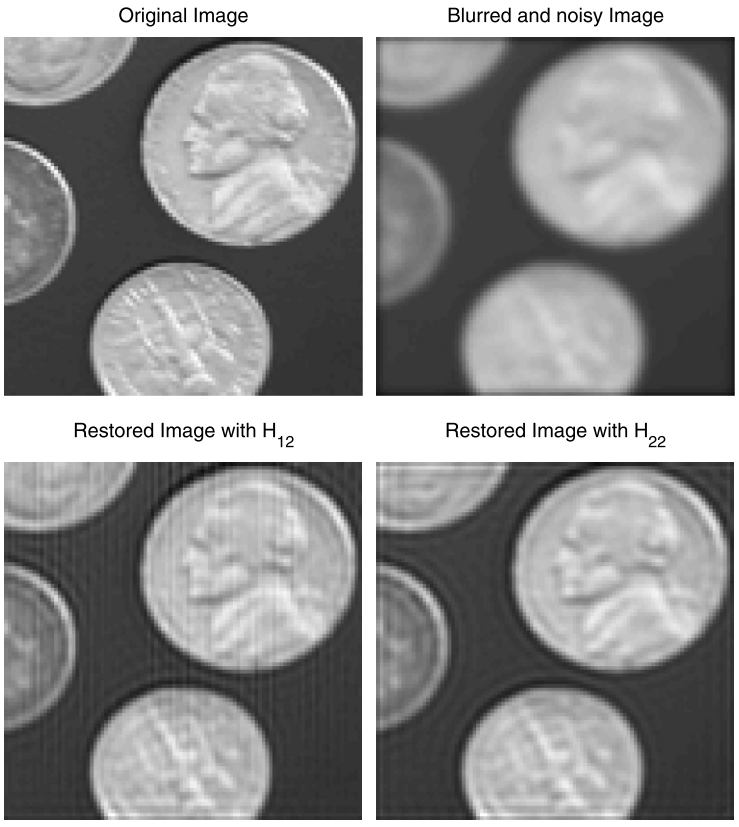

Fig. 7. Image restoration with the ATP method using $H_{1,2}$, $H_{2,2}$, and $\lambda = 100$. The results correspond to the Krylov iteration number 10 for $H_{1,2}$, and number 13 for $H_{2,2}$.

6. An example of image restoration

In this section we consider a problem of image restoration. The example is a 2D image deblurring problem which consists of recovering the original $n \times n$ image from a blurred and noisy image. The original image is denoted by X and it consists of $n \times n$ grayscale pixel values. Let $\mathbf{x} = vec(X) \in \mathbb{R}^N$, $N = n^2$, be the vector whose entries are the pixel values of the image X. Moreover, let $A \in \mathbb{R}^{N \times N}$ be the matrix representing the blurring operator, coming from the discretization of the Point Spread Function (PSF). The vector $\mathbf{b} = A\mathbf{x}$ represents the associated blurred and noise-free image. We generate a blurred and noisy image $\bar{\mathbf{b}} = \mathbf{b} + \mathbf{e_b}$, where $\mathbf{e_b}$ is a noise vector defined by (19) with $\delta = 10^{-3}$.

The matrix A is a symmetric block Toeplitz with Toeplitz blocks

$$A = \left(2\pi\sigma^2\right)^{-1} T \otimes T,$$

where T is an $n \times n$ symmetric banded Toeplitz matrix where the first row is a vector $\mathbf{v}^T$ whose elements are

$$v_j := \begin{cases} \frac{e^{-(j-1)^2}}{2\sigma^2} & \text{for } j = 1, \ldots, q, \\ 0 & \text{for } j = q+1, \ldots, n. \end{cases}$$

The parameter q is the half-bandwidth of the matrix T, and the parameter σ controls the width of the underlying Gaussian point spread function

$$h(x, y) = \frac{1}{2\pi\sigma^2} \exp\left(-\frac{x^2 + y^2}{2\sigma^2}\right),$$

which models the degradation of the image. Thus, a larger σ implies a wider Gaussian and thus a more ill-posed problem. For our experiments X is a 100×100 subimage of the image `coins.png` from Matlab's Image Processing Toolbox, shown as the first image in Fig. 7. We define $q = 6$ and $\sigma = 1.5$, so that the condition number of A is around 10^{10}. We report the results of our image restoration using two different regularization operators. In particular we consider the matrix

$$H_{1,2} = \begin{pmatrix} I \otimes H_1 \\ H_1 \otimes I \end{pmatrix}, \quad \text{where } H_1 = \begin{pmatrix} 1 & -1 & & \\ & \ddots & \ddots & \\ & & 1 & -1 \\ & & & 1 \end{pmatrix} \in \mathbb{R}^{n \times n},$$

taken from [18] (slightly modified such that $H_{1,2}^T H_{1,2}$ is nonsingular), and the matrix $H_{2,2}$ defined as the discretization of the two-dimensional Laplace operator with zero-Dirichlet boundary conditions, that is,

$$H_{2,2} = \begin{pmatrix} 4 & -1 & & -1 & \\ -1 & 4 & -1 & & -1 \\ & \ddots & \ddots & \ddots & \\ -1 & & -1 & 4 & -1 \\ & -1 & & -1 & 4 \end{pmatrix} \in \mathbb{R}^{N \times N}.$$

Fig. 7 shows that the ATP method can be fruitfully used also for this kind of problems. Due to the well marked edges, the original image involves high frequencies so that the restoration by means of the standard derivative operators is intrinsically difficult, because they are high-pass filters.

Table 4 shows that also for this kind of problems the attainable accuracy is weakly influenced by the choice of λ.

Table 4
Attainable accuracy (Euclidean norm of the error) for the image restoration with $H_{1,2}$ and $H_{2,2}$ using different values of λ. The corresponding number of iterations is indicated in parentheses.

λ	1	10^2	10^4	10^6
$H_{1,2}$	0.060 (10)	0.060 (10)	0.062 (10)	0.059 (11)
$H_{2,2}$	0.061 (12)	0.064 (13)	0.069 (13)	0.075 (13)

7. Conclusions

In this paper we have presented a new approach for the solution of discrete ill-posed problems. The basic idea is to solve the problem in two steps: first regularize and then reconstruct. We have described two methods based on this idea, the ASP method that is actually a particular preconditioned iterative solver, and the ATP method that is a method that tries to improve the approximation arising from the Tikhonov regularization. In both cases the reconstruction is performed evaluating a matrix function by means of the standard Arnoldi method. This idea can also be interpreted as a modification of the iterated Tikhonov regularization (see for instance [12] and [21]).

Being iterative, both methods should be interpreted as methods depending on two parameters, that is, λ and the number of iterations m. Actually our implementation of the Arnoldi method (modified Gram–Schmidt) is very stable so that for a fixed λ, the undersmoothing effect, theoretically determined by taking m large, in general does not deteriorate the approximation. Therefore the only important parameter is λ. Anyway, the most important property of both methods is that they do not need an accurate estimate of this parameter to work properly (cf. Section 4, Figs. 5 and 6, and Table 4). Of course this property is particularly attractive for problems in which a parameter-choice analysis is too expensive or even unfeasible as for instance for large scale problems such as the image restoration.

As possible future developments, we observe that the ASP method could be quite easily extended to work in connection with polynomial preconditioners (see e.g. [5] for a background). This can be done replacing $(A + \lambda I)^{-1}$ with a suitable $p_m(A) \approx A^{-1}$ and changing accordingly the matrix function to evaluate. Also the symmetric version of the ATP method (see Remark 1) seems quite interesting and requires further investigation.

Finally, we want to point out that the present paper was just intended to present the basic ideas and properties of the methods; in this sense, a reliable implementation with stopping criterion, choice of λ, etc., has still to be done.

Acknowledgements

The authors are grateful to the reviewers for the valuable comments and suggestions. This work was partially supported by University of Padova, Project 2010 No. CPDA104492 and by MIUR, PRIN 2008 No. 20083KLJEZ.

References

[1] B. Beckermann, L. Reichel, Error estimation and evaluation of matrix functions via the Faber transform, SIAM J. Numer. Anal. 47 (2009) 3849–3883.
[2] M. Bellalij, Y. Saad, H. Sadok, Further analysis of the Arnoldi process for eigenvalue problems, SIAM J. Numer. Anal. 48 (2010) 393–407.
[3] M. Benzi, G.H. Golub, J. Liesen, Numerical solution of saddle point problems, Acta Numer. 14 (2005) 1–137.

[4] C. Brezinski, P. Novati, M. Redivo-Zaglia, A rational Arnoldi approach for ill-conditioned linear systems, J. Comput. Appl. Math. 236 (2012) 2063–2077.
[5] C. Broyden, M.T. Vespucci, Krylov Solvers for Linear Algebraic Systems, Studies in Computational Mathematics, vol. 11, Elsevier B.V., Amsterdam, 2004.
[6] M. Crouzeix, Numerical range and numerical calculus in Hilbert space, J. Funct. Anal. 244 (2007) 668–690.
[7] C. de Boor, Divided differences, Surveys in Approximation Theory 1 (2005) 46–69.
[8] F. Diele, I. Moret, S. Ragni, Error estimates for polynomial Krylov approximations to matrix functions, SIAM J. Matrix Anal. Appl. 30 (2008) 1546–1565.
[9] M. Eiermann, O.G. Ernst, A restarted Krylov subspace method for the evaluation of matrix functions, SIAM J. Numer. Anal. 44 (2006) 2481–2504.
[10] G. Fasshauer, Meshfree Approximation Methods with MATLAB, World Scientific Publishers, Singapore, 2007.
[11] J.N. Franklin, Minimum principles for ill-posed problems, SIAM J. Math. Anal. 9 (1978) 638–650.
[12] M. Hanke, P.C. Hansen, Regularization methods for large-scale problems, Surv. Math. Ind. 3 (1993) 253–315.
[13] P.C. Hansen, Regularization Tools: A Matlab package for analysis and solution of discrete ill-posed problems, Numer. Algorithms 6 (1994) 1–35.
[14] P.C. Hansen, Rank-Deficient and Discrete Ill-Posed Problems: Numerical Aspects of Linear Inversion, SIAM, Philadelphia, 1998.
[15] P.C. Hansen, Regularization Tools version 4.0 for Matlab 7.3, Numer. Algorithms 46 (2007) 189–194.
[16] N.J. Higham, Functions of Matrices: Theory and Computation, SIAM, Philadelphia, 2008.
[17] B. Hofman, Regularization of nonlinear problems and the degree of ill-posedness, in: G. Anger, R. Gorenflo, H. Jochmann, H. Moritz, W. Webers (Eds.), Inverse Problems: Principle and Applications in Geophysics, Technology and Medicine, Akademie Verlag, Berlin, 1993.
[18] M.E. Kilmer, P.C. Hansen, M.I. Español, A projection-based approach to general-form Tikhonov regularization, SIAM J. Sci. Comput. 29 (2007) 315–330.
[19] I. Moret, P. Novati, An interpolatory approximation of the matrix exponential based on Faber polynomials, J. Comput. Appl. Math. 131 (2001) 361–380.
[20] I. Moret, P. Novati, RD-rational approximations of the matrix exponential, BIT 44 (2004) 595–615.
[21] A. Neumaier, Solving ill-conditioned and singular linear systems: a tutorial on regularization, SIAM Rev. 40 (1998) 636–666.
[22] O. Nevanlinna, Convergence of Iterations for Linear Equations, Birkhäuser, Basel, 1993.
[23] L.N. Trefethen, D. Bau, Numerical Linear Algebra, SIAM, Philadelphia, 1997.