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Tikhonov regularization and matrix function evaluation

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Introduction and Motivations

We consider ill-conditioned linear systems

$$Ax = b$$

We mainly focus the attention on **full-rank** problems in which the singular values of A decay gradually to zero.

We want to construct an iterative solver able to overcome some of the typical drawback of the classical iterative solvers:

- **Semi-convergence**: the iterates initially approach the solution but quite rapidly diverge
- **Strong dependence on the parameter-choice strategy**: in order to prevent divergence a reliable stopping criterium has to be used
- **Poor accuracy**: typically holds for Krylov type methods based on the use of A^TA (CGLS)

Reformulation of the problem

The basic idea is to solve the system $Ax = b$ in two steps, first solving in some way the regularized system

$$(A + \lambda I)\, x_\lambda = b$$

and then recovering the solution x from the system

$$(A + \lambda I)^{-1} Ax = x_\lambda$$

that is equivalent to compute

$$x = f(A)x_\lambda$$

where

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

By the definition of f the attainable accuracy depends on the conditioning of $(A + \lambda I)^{-1} A$. Theoretically the best situation is attained defining λ such that

$$\kappa(A + \lambda I) = \kappa((A + \lambda I)^{-1} A)$$

In the SPD case taking

$$\lambda = \sqrt{\lambda_1 \lambda_N} \approx 1/\sqrt{\kappa(A)}$$

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 computation of the matrix function

The Arnoldi Algorithm

For the computation of $f(A)x_\lambda$ we use the standard Arnoldi method projecting the matrix A onto the Krylov subspaces generated by A and x_λ

$$K_m(A, x_\lambda) = span\{x_\lambda, Ax_\lambda, ..., A^{m-1}x_\lambda\}$$

For the construction of the subspaces $K_m(A, x_\lambda)$ the Arnoldi algorithm generates an orthonormal sequence $\{v_j\}_{j\geq 1}$, with $v_1 = x_\lambda / \|x_\lambda\|$, such that $K_m(A, x_\lambda) = span\{v_1, v_2, ..., v_m\}$. For every m,

$$AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^T.$$

where $V_m = [v_1, v_2, ..., v_m]$, H_m is an upper Hessenberg matrix with entries $h_{i,j} = v_i^T A v_j$ and e_j is the j-th vector of the canonical basis of $\mathbb{R}^m$.

The m-th Arnoldi approximation to $x = f(A)x_\lambda$ is defined as

$$x_m = \|x_\lambda\|\, V_m f(H_m) e_1$$

At each step of the Arnoldi algorithm we have to compute the vector $w_j = Av_j$. The method theoretically converges in a finite number of steps. For the computation of $f(H_m)$ we employ the Schur-Parlett algorithm (Golub and Van Loan 1983).

Extension to Tikhonov regularization

The method can be extended to problems in which the exact right hand side b is affected by noise. We assume to work with a perturbed right-hand side $\widetilde{b} = b + e_b$. Given λ and H we solve the regularized system

$$(A^TA + \lambda H^TH)x_\lambda = A^T\widetilde{b}.$$

and then we approximate x by computing

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

where $Q = \left(H^TH\right)^{-1}\left(A^TA\right)$. As before, for the computation of $f(Q)x_\lambda$ we use the standard Arnoldi method projecting the matrix Q onto the Krylov subspaces generated by Q and x_λ. Now, at each step we have to compute the vectors $w_j = Qv_j$, $j \geq 1$, with $v_1 = x_\lambda / \|x_\lambda\|$, that is, to solve the systems $\left(H^TH\right) w_j = \left(A^TA\right) v_j$.

Theoretical error analysis

The field of values of A is defined as

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

THEOREM 1 *Assume that $F(A) \subset \mathbb{C}^+$. Then for the error $E_m := f(A)x_\lambda - \|x_\lambda\| V_m f(H_m)e_1$ we have*

$$\|E_m\| \leq K \frac{\lambda}{a^{m+1}} \prod_{i=1}^{m} h_{i+1,i} \|x_\lambda\|,$$

where $a > 0$ is the leftmost point of $F(A)$ and $2 \leq K \leq 11.08$ (Crouzeix 2007; in the symmetric case $K = 1$).

The rate of convergence is almost independent of the choice of λ, and is closely related with the rate of the decay of $\prod_{i=1}^{m} h_{i+1,i}$.

THEOREM 2 *Let σ_j, $j \geq 1$, be the singular values of an operator A. If*

$$\sum_{j\geq 1} \sigma_j^p < \infty \text{ for a certain } p > 0$$

then

$$\prod_{i=1}^{m} h_{i+1,i} \leq \left(\frac{\eta e p}{m}\right)^{m/p} \quad where \quad \eta \leq \frac{1+p}{p} \sum_{j\geq 1} \sigma_j^p$$

- 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.
- Each Arnoldi-based method (CG, FOM, GMRES) shows the same rate of convergence

Error analysis in computer arithmetics

ASP. We assume that x_λ, solution of $(A + \lambda I)\, x_\lambda = b$, is approximated by $\overline{x}_\lambda$ with an accuracy depending on the choice of λ and the method used. In this way, the Arnoldi algorithm actually constructs the Krylov subspaces $K_m(A, \overline{x}_\lambda)$. We obtain

$$\|E_m\| \leq \|f(A)\overline{x}_\lambda - \|\overline{x}_\lambda\| V_m f(H_m)e_1\| + \|f(A)\,(x_\lambda - \overline{x}_\lambda)\|$$

- For small λ, $f(A) \approx I$ and $\|E_m\| \approx \|x_\lambda - \overline{x}_\lambda\|$. The method is not able to improve the accuracy of the solution of the initial system.
- For large λ we have that $x_\lambda \approx \overline{x}_\lambda$, but even assuming that $\|f(A)\,(x_\lambda - \overline{x}_\lambda)\| \approx 0$, we have another lower bound due the ill-conditioning of $f(A)$.

ATP. The error is given by

$$E_m := f(Q)x_\lambda - p_{m-1}(Q)\overline{x}_\lambda$$

(p_{m-1} interpolates f at the eigenvalues of Q) where $(A^TA + \lambda H^TH)x_\lambda = A^Tb$ and $(A^TA + \lambda H^TH)\overline{x}_\lambda = A^T\widetilde{b}$. As before

$$\|E_m\| \leq \|f(Q)\overline{x}_\lambda - p_{m-1}(Q)\overline{x}_\lambda\| + \|f(Q)\,(x_\lambda - \overline{x}_\lambda)\|.$$

Theoretically we may choose λ very large, thus oversmoothing, in order to reduce the effect of noise. Unfortunately, as before, $f(Q)$ may be ill-conditioned for λ large. A compromise for the selection of λ is necessary but contrary to the ASP method, it is difficult to design a theoretical strategy.

Numerical experiments

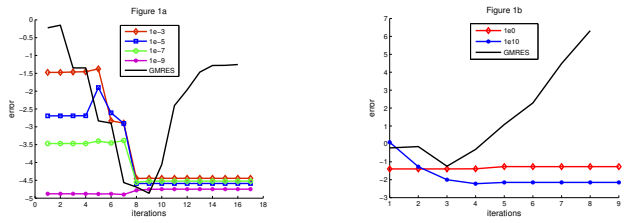

Figure 1 - Stability behaviour of the error for the ASP method (1a) and the ATP method (1b) for different values of λ for the problem BAART 240.

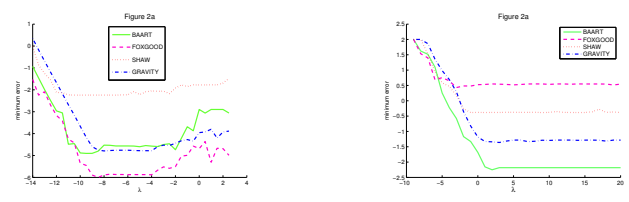

Figure 2 - Maximum attainable accuracy with respect to the choice of lambda and with right-hand side affected by Gaussian noise $\sigma = 10^{-3}$ (2b). The dimension of each problem is $N = 160$.

An example of image restoration

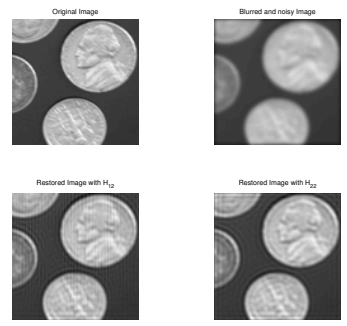

Image restoration of
a 100×100 subimage of `coins.png`
from MATLAB's Image Processing Toolbox with $\lambda = 100$.

As filters we consider

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

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

Conclusions

- Both methods are stable w.r.t. the choice of the number of iterations, i.e. they do not require a reliable stopping rule
- They are as fast and accurate as the most effective iterative solvers
- W.r.t. classical preconditioned iterative solvers, only one linear system with the preconditioner has to be solved
- They do not require an accurate parameter-choice strategy for λ

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