Nonlinear Evolution Equations and Linear Algebra
Cagliari (Sardinia, Italy), September 2-5, 2013

Parameter selection strategies for the Arnoldi-Tikhonov method

S. Gazzola, P. Novati, and M. R. Russo
Department of Mathematics, University of Padua, Italy

Introduction

Consider a linear system

$$Ax = b, \quad A \in \mathbb{R}^{N\times N}.$$

We assume that

- the singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_N > 0$ of A quickly decay and cluster at zero;
- the available right-hand side is affected by additive Gaussian white noise, i.e. $b = b^{ex} + e = Ax^{ex} + e$;
- the Discrete Picard Condition (DPC) holds: $|u_i^T b^{ex}| \simeq \sigma_j$.

Problems like this arise in a variety of applications, especially solving inverse problems, i.e. when one wants to reconstruct the cause of an observed effect.
Because of the bad conditioning of A and the errors in b, some sort of regularization should be employed in order to find a meaningful approximation of the exact solution x^{ex}.

Arnoldi-Tikhonov regularization method

To regularize the available system we employ the well-established Tikhonov method that, in its general form, consists in solving the problem

$$\min_{x\in\mathbb{R}^N} \left\{ \|Ax - b\|_2^2 + \lambda \|L(x - x_0)\|_2^2 \right\},$$

where $L \in \mathbb{R}^{P\times N}$ ($P \leq N$) is the regularization matrix, $\lambda > 0$ is the regularization parameter and $x_0 \in \mathbb{R}^N$ is an initial guess for the solution; in the special case $L = I_N$ and $x_0 = 0$ the problem is said to be in standard form.
The Arnoldi-Tikhonov (AT) method solves the regularized system by projecting it into a Krylov subspace

$$\mathcal{K}_m(A, r_0) = \text{span}\{r_0, Ar_0, \ldots, A^{m-1}r_0\},\ r_0 = b - Ax_0,\ m \ll N,$$

of increasing dimension. An orthonormal basis for $\mathcal{K}_m(A, r_0)$ is computed by the Arnoldi algorithm that, in matrix form, leads to the decomposition

$$AW_m = W_{m+1}\bar{H}_m,$$

where $W_m = [w_1, \ldots, w_m] \in \mathbb{R}^{N\times m}$ has orthonormal columns that span $\mathcal{K}_m(A, r_0)$ and $\bar{H}_m \in \mathbb{R}^{(m+1)\times m}$ is upper Hessenberg.
Imposing the regularized solution $x_{m,\lambda}$ to belong to the space $x_0 + \mathcal{K}_m(A, r_0)$, i.e. substituting $x = x_0 + W_m y$ into the regularized problem, we obtain

$$y_{m,\lambda} = \arg\min_{y\in\mathbb{R}^m} \left\| \begin{pmatrix} \bar{H}_m \\ \sqrt{\lambda_m} L_m \end{pmatrix} y - \begin{pmatrix} \|r_0\|_2 e_1 \\ 0 \end{pmatrix} \right\|_2^2.$$

Remark 1: in this formulation, the original regularization matrix is projected onto $x_0 + \mathcal{K}_m(A, r_0)$, i.e. $L_m = W_m^T L W_m$.
Remark 2: this method is effective only if a proper regularization parameter $\lambda = \lambda_m$ is set at each iteration and a stopping criterion is specified.

Generalized Cross Validation

The Generalized Cross Validation (GCV) is a popular $\|e\|_2$-free, statistics-based strategy that prescribes to choose the regularization parameter minimizing the prediction errors for all the data elements; the basic idea behind GCV is that a good choice of the regularization parameter should accurately predict missing data. GCV has already been adopted in the TSVD, Tikhonov, iterative, Lanczos-hybrid settings.
In the AT framework (assume $x_0 = 0$), at each iteration m, one chooses

$$\lambda_m = \arg\min_{\lambda>0} G_m(\lambda),\ G_m(\lambda) := \frac{\left\|\bar{H}_m y_{m,\lambda} - b\right\|_2^2}{\left(N - m + \sum_{i=1}^m \frac{\lambda}{\left(\gamma_i^{(m)}\right)^2 + \lambda}\right)^2}$$

where $\gamma_i^{(m)}$, $i = 1, \ldots, m$ are the generalized singular values of $(\bar{H}_m, L_m)$.
Remark 1: at the denominator of $G_m(\lambda)$, the term $(N - m)$ accounts for the iterative feature of the AT method while the sum accounts for the projected Tikhonov regularization.
Remark 2: sometimes $G_m(\lambda)$ is pretty flat near the minimum; in this case the GCV strategy may fail.
To decide when to stop the iterations one monitors the relative changes in the residuals associated to AT method and the progression of the sequence $\{\lambda_m\}_{m\geq 1}$.

Theoretical estimates

Convergence of the Arnoldi algorithm

Theorem 1. *Let us assume that A is severely ill-conditioned (i.e. $\sigma_j = O(e^{-\alpha j})$, $\alpha > 0$) and that b^{ex} satisfies the DPC. Then, if b^{ex} is the starting vector of the Arnoldi process, we have*

$$h_{m+1,m} = O\left(m^{3/2}\sigma_m\right).$$

Approximation of the SVD

Let us denote the SVD of $\bar{H}_m \in \mathbb{R}^{(m+1)\times m}$ by
$$\bar{H}_m = \bar{U}_{m+1}\Sigma^{(m)}\bar{V}_m^T.$$

Proposition 2. *Let $U_{m+1}^{(m)} := W_{m+1}\bar{U}_{m+1}$ and $V_m^{(m)} := W_m\bar{V}_m$. Then*

$$\left\|A - U_{m+1}^{(m)}\Sigma^{(m)}V_m^{(m)T}\right\|_2 = \left\|A(I - W_m W_m^T)\right\|_2.$$

After some considerations involving A^T and using some heuristics, one obtains the bound

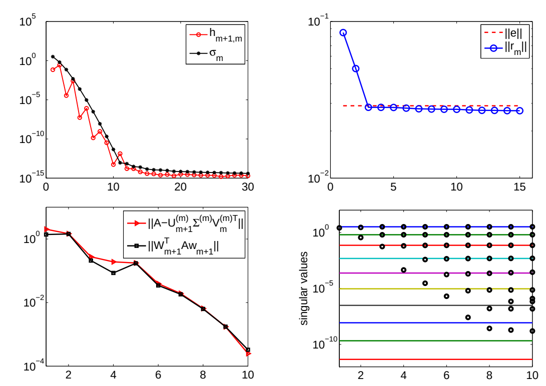
$$\left\|A - U_{m+1}^{(m)}\Sigma^{(m)}V_m^{(m)T}\right\|_2 \simeq \left\|W_{m+1}^T A w_{m+1}\right\|_2.$$

Behavior of $\|\mathbf{r}_\mathbf{m}^{\mathbf{GMRES}}\|_2$

Let us define the $N \times m$ matrices $\widetilde{V}_m^{ex} = \left[A^i b^{ex}/\|A^i b^{ex}\|_2\right]_{i=0,\ldots,m-1}$ and $\widetilde{V}_m = \left[A^i b/\|A^i b\|_2\right]_{i=0,\ldots,m-1}$. r_m^{ex} denotes the residual of the GMRES applied to $Ax = b^{ex}$; one can express
$$\|r_m^{ex}\|_2 = \|b^{ex} - \widetilde{V}_{m+1}s^{ex}\|_2, \text{ where } s^{ex} \in \mathbb{R}^m,\ e_1^T s^{ex} = 0.$$

Proposition 3. *The norm of the GMRES residual satisfies*

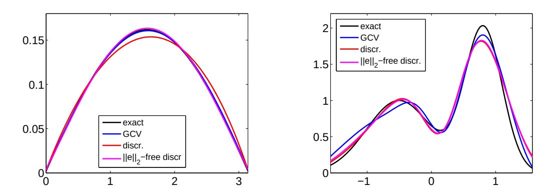
$$\|r_m^{GMRES}\|_2 \leq \eta(m)\|e\|_2, \quad \eta(m) = 1 + \frac{\|r_m^{ex}\|_2 + \left\|\left(\widetilde{V}_{m+1} - \widetilde{V}_{m+1}^{ex}\right)s^{ex}\right\|_2}{\|e\|_2}.$$



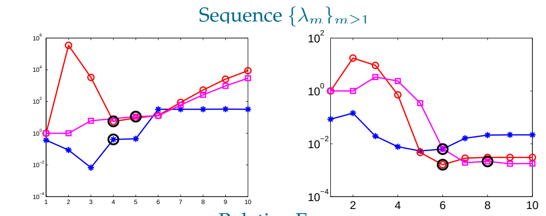
Numerical experiments

Left column: `baart`; right column: `shaw` (both from *Regularization Tools*). Matrix size: $N = 120$. Noise level $\|e\|_2/\|b^{ex}\|_2 = 10^{-2}$.

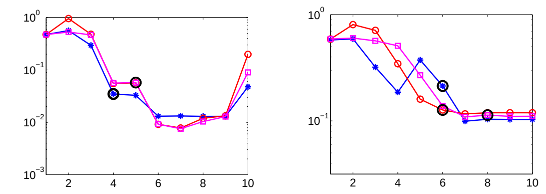
Reconstructed solutions



Sequence $\{\lambda_m\}_{m>1}$



Relative Errors



References

[1] P. Novati, M.R. Russo. *A GCV based Arnoldi-Tikhonov regularization method*. Submitted (2013), http://arxiv.org/abs/1304.0148.

[2] S. Gazzola, P. Novati, M.R. Russo. *Embedded techniques for choosing the parameter in Tikhonov regularization*. Submitted (2013), http://arxiv.org/pdf/1307.0334v1.

The discrepancy principle for the AT method

$\|e\|_2$ known

The discrepancy principle prescribes to choose the regularization parameter that solves the nonlinear equation

$$\phi_m(\lambda) := \|b - Ax_{m,\lambda}\|_2 = \eta\|e\|_2,\ \eta > 1\,(\simeq 1).$$

In the AT setting, at each step m, the following linear approximation of the discrepancy function is considered

$$\phi_m(\lambda) \simeq \phi_m(0) + \lambda\beta_m,$$

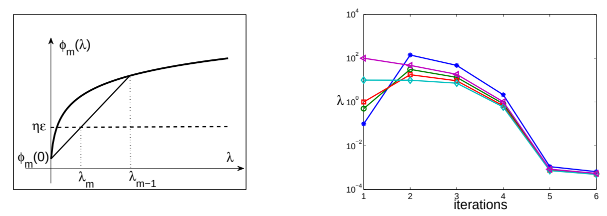
where $\phi_m(0)$ is the norm of the GMRES residual and

$$\beta_m = \frac{\phi_m(\lambda_{m-1}) - \phi_m(0)}{\lambda_{m-1}}.$$

The value λ_{m-1} is the one considered at the previous iteration (λ_0 is given by the user, and the strategy is very stable w.r.t. this initial choice).
To select the next parameter λ_m one solves the linear equation $\phi_m(0) + \lambda\beta_m = \eta\|e\|_2$ w.r.t. λ and gets

$$\lambda_m = \left|\frac{\eta\|e\|_2 - \phi_m(0)}{\phi_m(\lambda_{m-1}) - \phi_m(0)}\right|\lambda_{m-1}.$$

We stop when the norm of the discrepancy associated to the current solution $x_{m,\lambda_{m-1}}$ lies below the threshold $\eta\|e\|_2$.
Remark 1: this approach is equivalent to performing just one step of a secant zero finder at each iteration of the AT method; therefore this strategy is called secant update method.
Remark 2: the secant update method acts simultaneously as a parameter choice strategy and as a stopping criterion.



$\|e\|_2$ unknown (*embedded technique*)

Assuming that, after a few iterations, the norm of the GMRES residual stabilizes around $\|e\|_2$, one can consider the following parameter update strategy

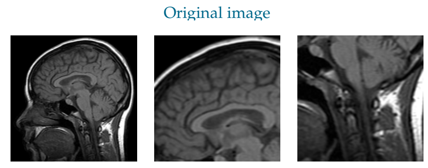
$$\lambda_m = \left|\frac{\eta\phi_{m-1}(0) - \phi_m(0)}{\phi_m(\lambda_{m-1}) - \phi_m(0)}\right|\lambda_{m-1}.$$

In this case one stops the iterations monitoring the relative changes in the GMRES residuals and in the discrepancies.

Image deblurring & denoising

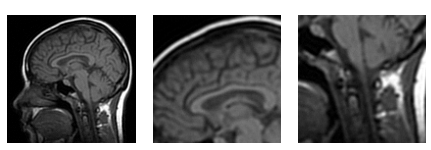
In this test problem, the blur is Gaussian symmetric and the corresponding matrix A is block Toeplitz with Toeplitz blocks. The size of the original image is 256 pixels, therefore $A \in \mathbb{R}^{65536\times 65536}$. A is generated by the function `blur`, whose parameters are `band`$= 7$, `sigma`$= 2$. The regularization matrix employed is a discretization of the first derivative operator. The noise level is 10^{-3}.

Original image



Corrupted image

Restored by AT method equipped with GCV (10^{th} iteration)



Restored by AT method equipped with $\|e\|_2$-free discrepancy principle (10^{th} iteration)