3 Krylov methods for matrix functions

In the lectures we have seen several methods to compute

$$f(A)$$

for specialized f as well as general situations. All of these methods involve, in some way, direct properties of the matrix A, making most of them difficult to adapt for large and sparse problem. We will now see a method which is suitable for large and sparse problems. In many applications, it is sufficient to compute the matrix function multiplied with a vector:

$$f(A)b \tag{3.1}$$

The method we will present now is a method to compute (3.1) and which is based on Arnoldi's method.

3.1 Cauchy integral formulation

Analytic matrix functions can be characterized explicitly with the contour integrals, as follows:

$$f(A) = \frac{1}{2i\pi}\oint_\Gamma f(z)(zI - A)^{-1}\,dz,$$

where Γ is a contour enclosing all eigenvalues of A. See GVL 9.2.7 for a proof. Clearly, our quantity of interest is now

$$f(A)b = \frac{-1}{2i\pi}\oint_\Gamma f(z)((A - zI)^{-1}b)\,dz.$$

In order to approximate this expression, we will now approximate the factor involving a shifted linear system of equations

$$x = (A - zI)^{-1}b,$$

be means of Krylov subspace approximations.

3.2 Krylov approximation of shifted linear systems

A Krylov subspace is defined by an expression involving a span,

$$\mathcal{K}_m(A, b) = \text{span}(b, Ab, \ldots, A^{m-1}b).$$

Due to the fact that the span is unchanged by adding or subtracting multiplies of the vectors, one can easily verify that

$$\mathcal{K}_m(A-\sigma I,b)=\mathcal{K}_m(A,b).$$

This implies that the Krylov subspace is independent of shift. Moreover, a similar property holds for the Arnoldi factorization.

Lemma 3.2.1 *Suppose $Q_m\in\mathbb{C}^{n\times m}$, $\underline{H}_m\in\mathbb{C}^{(m+1)\times m}$ is an Arnoldi factorization associated with $\mathcal{K}_m(A,b)$,*

$$AQ_m=Q_mH_{m+1,m}+e_m^Tq_{m+1}h_{m+1,m},$$

Then, for any $\sigma\in\mathbb{C}$, $Q_m\in\mathbb{C}^{n\times m}$ and $\underline{H}_m-\sigma I$ is an Arnoldi factorization associated with $\mathcal{K}_m(A-\sigma I,b)$,

$$(A-\sigma I)Q_m=AQ_m=Q_m(H_{m+1,m}-\sigma I)+e_m^Tq_{m+1}h_{m+1,m},$$

Hence, the Arnoldi factorization associated with $\mathcal{K}_m(A-\sigma I,b)$ can be easily reconstructed from the Arnoldi factorization associated with $\mathcal{K}_m(A,b)$, by shifting hessenberg matrix H_m and using the same basis matrix Q_m.

Krylov approximation

The lectures on GMRES gave a natural procedure to extract an approximation of a linear system by means of minimizing the residual in the Krylov subspace. For the purpose of approximating $f(A)b$, via approximation of $(A-zI)^{-1}b$ we will work with a different way to extract an approximation from the Krylov subspace. We define a Krylov approximation of the linear system $Ax=b$ by

$$\tilde{x}=Q_mH_m^{-1}Q_m^Tb=Q_mH_m^{-1}e_1\|b\|. \tag{3.2}$$

This approximation can be derived by assuming that $\tilde{x}\in\mathcal{K}_m(A,b)$ and imposing that the residual is orthogonal to the mth Krylov subspace, $Q_m^T(A\tilde{x}-b)=0$.

Due to Lemma 3.2.1, the Krylov approximation of the shifted linear system $(A-\sigma I)x=b$ is

$$\tilde{x}=Q_m(H_m-\sigma I)^{-1}e_1\|b\|. \tag{3.3}$$

Note that this approximation can be computed for many σ by only computing one Arnoldi factorization.

GMRES vs (3.2): The approximation (3.2) corresponds to an element of $\mathcal{K}_m(A,b)$ such that the residual satisfies $Q_m^T(A\tilde{x}-b)=0$, whereas the GMRES approximation corresponds to an element of $\mathcal{K}_m(A,b)$ which minimizes $\min_{x\in\mathcal{K}_m(A,b)}\|Ax-b\|_2=\|A\tilde{x}-b\|_2$.

3.3 A Krylov approximation of the matrix function

By using the approximation (3.3) in the Cauchy integral formulation, we have

$$f(A)b \approx \frac{-1}{2i\pi}\oint_\Gamma f(z)Q_m(H_m - zI)^{-1}e_1\|b\|\,dz =$$
$$Q_m\frac{1}{2i\pi}\oint_\Gamma f(z)(zI - H_m)^{-1}\,dz(e_1\|b\|) = Q_m f(H_m)e_1\|b\|.$$

This serves as a justification of (what we call) the Krylov approximation of $f(A)b$, which is defined as

$$f_m := Q_m f(H_m)e_1\|b\|. \tag{3.4}$$

Note that the Krylov approximation (3.4) involves a matrix function. However, the Hessenberg matrix H_m is in general much smaller than the original problem and computing $f(H_m)$ is realitively inexpensive in comparison to carrying out the Arnoldi method.

3.4 Convergence theory

Similar to the Arnoldi method for eigenvalue problems and GMRES, the convergence can be characterized with a min-max expression. To illustrate the convergence, we present only a result for normal matrices. Unlike the other bounds in this course, the maximum is not taken over a discrete set, but a continuous convex compact set Ω containing the eigenvalues of A.

The proof of Theorem 3.4.1 is beyond the scope of the contents of the course. A proof can be found in [*Error estimation and evaluation of matrix functions via the Faber transform*, Beckermann, Reichel, SIAM J. Numer. Anal., 47:3849-3883, 2009]

Theorem 3.4.1 *Suppose $A \in \mathbb{C}^{n\times n}$ is a normal matrix and suppose $\Omega \subset \mathbb{C}$ is a convex compact set such that $\lambda(A) \subset \Omega$. Let f_m be the Krylov approximation of $f(A)b$ defined by (3.4). Then,*

$$\|f(A)b - f_m\| \le 2\|b\| \min_{p\in P_{m-1}} \max_{z\in\Omega} |f(z) - p(z)|.$$

Error interpretations

The bound gives several qualitative interpretations of the error. Sufficient conditions for fast convergence can be easily identified: The method will work well if

- $f(z)$ can be well approximated with low-order polynomials
- $\lambda(A)$ are clustered together such that Ω can be chosen small

Similar to other min-max bounds in this course, qualitative understanding can be found by bounding using particular choices of the polynomials. Let q_m be the truncated Taylor expansion

$$q_m(z) := \sum_{i=0}^{m} \frac{f^{(m)}(0)}{i!} z^m.$$

Hence, $r_m(z) = f(z) - q_m$ is the remainder term in the Taylor expansion of f. Suppose now that Ω is a subset of a disk of radius ρ centered at the origin $\Omega \subset D(\rho, 0)$. Then

$$\max_{z\in\Omega} r_m(z) \sim \frac{\rho^{m-1}}{(m-1)!}$$

and $\|f(A)b - f_m\| \le e_m \sim \frac{\rho^{m-1}}{(m-1)!} \to 0$ as $m \to \infty$. This shows that the method is convergent. The speed of convergence is usually much faster than what is predicted by this Taylor series bound.

3.5 *Example*

For many problems, the convergence is superlinear in practice. See the video demonstration

`http://www.math.kth.se/~eliasj/krylov_matfun_approx.mp4`