RATIONAL KRYLOV SEQUENCES AND ORTHOGONAL RATIONAL FUNCTIONS

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Problem formulation

Suppose A is an N by N real symmetric positive-definite matrix, and $q \in \mathbb{R}^N$. We seek numerical approximations to matrix functions, mainly for the computation of

$$y = f(A)q.$$

In the literature, attention has been given to functions like e.g. $x^{\frac{1}{2}}, x^{-\frac{1}{2}}, \exp(-tx^{\frac{1}{2}}), \ldots$, and their combinations. These functions find applications in various fields of applied mathematics and statistics, like e.g. in the solution of various differential problems.
It is well known (see e.g. [1]) that the standard Lanczos spectral decomposition, which seeks polynomial approximations to y belonging to the Krylov subspaces

$$K_{m+1}(A, q) = \text{span}\{q, Aq, A^2q, \ldots, A^mq\}, \quad m \ll N,$$

in general, is not effective since the convergence of polynomial approximations may be very slow. Therefore, we seek rational approximations to y belonging to rational Krylov subspaces.

Rational Krylov sequences

Suppose the sequence of numbers $\mathcal{M} = \{\mu_0 = \mu_1, \mu_2, \ldots, \mu_m\} \subset \mathbb{R}_0^+$, with $\mathcal{M} \cap \sigma(A) = \emptyset$, is given, and define the factors

$$\begin{aligned} Z_k(A) &= (I + \mu_k A)^{-1} A = A(I + \mu_k A)^{-1} \\ &= \frac{A}{I + \mu_k A}, \quad k = 1, 2, \ldots, m, \end{aligned}$$

and products

$$b_0(A) \equiv I, \quad b_k(A) = Z_k(A) b_{k-1}(A) = b_{k-1}(A) Z_k(A), \quad k = 1, 2, \ldots, m.$$

Then the rational Krylov subspace $K_{m+1}(A, q, \mathcal{M})$ with poles in $\{-\mu_1^{-1}, \ldots, -\mu_m^{-1}\}$ is given by

$$\begin{aligned} K_{m+1}(A, q, \mathcal{M}) &= \text{span}\{b_0(A)q, b_1(A)q, \ldots, b_m(A)q\} \\ &= \text{span}\{q^0, q^1, \ldots, q^m\}, \end{aligned}$$

where the sequence of vectors $q^0, \ldots, q^m$ forms an orthonormal system of vectors. Under certain conditions on the poles in $\mathcal{M}$, these orthonormal vectors do satisfy the following three-term recurrence relation:

$$Aq^{k-1} = \beta_{k-2}(I + \mu_{k-2}A)q^{k-2} + \alpha_{k-1}(I + \mu_{k-1}A)q^{k-1} + \beta_{k-1}(I + \mu_k A)q^k.$$

Let $Q_m = [q^0, \ldots, q^{m-1}]$,

$$J_m = \begin{bmatrix} \alpha_0 & \beta_0 & 0 & \cdots & 0 \\ \beta_0 & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \beta_{m-2} \\ 0 & \cdots & 0 & \beta_{m-2} & \alpha_{m-1} \end{bmatrix} \quad \text{and} \quad D_m = \begin{bmatrix} \mu_0 & 0 & \cdots & 0 \\ 0 & \mu_1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \mu_{m-1} \end{bmatrix}.$$

Then it follows that

$$Q_m^T A Q_m = J_m(I_m - D_m J_m)^{-1} + R_m,$$

where R_m is an $N \times N$ real symmetric matrix with $\text{rank}(R_m) \leq 1$, given by

$$R_m = \beta_{m-1}\mu_m g_m h_m^T, \quad g_m = Q_m^T A q^m, \quad h_m = (I_m - J_m D_m)^{-1} e_m,$$

and e_m is the mth vector of the canonical basis of $\mathbb{R}^m$.
Because the matrix $J_m(I_m - D_m J_m)^{-1} = (I_m - J_m D_m)^{-1} J_m$ is real symmetric, their exist m real eigenvalues $\lambda_1, \ldots, \lambda_m$ and an orthonormal set of eigenvectors $u_1, \ldots, u_m$ so that

$$(I_m - J_m D_m) U_m \Lambda_m = J_m U_m,$$

where $U_m = [u_1, \ldots, u_m]$ and

$$\Lambda_m = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \lambda_m \end{bmatrix}.$$

Accordingly, we define the mth approximation of y as (cfr. [2])

$$y^{(m)} = Q_m U_m f(\Lambda_m) U_m^T \|q\|_2 e^1,$$

where e^1 represents the first vector of the canonical basis of $\mathbb{R}^N$.

Computing Q_m and J_m

Define the vectors $x^{k-1}, y^{k-1} \in \mathbb{R}^N$ by

$$\begin{aligned} x^{k-1} &= Z_k(A)\left\{\beta_{k-2}(\mu_k - \mu_{k-2})q^{k-2} + q^{k-1}\right\} - \beta_{k-2}q^{k-2} \\ y^{k-1} &= [I + (\mu_{k-1} - \mu_k)Z_k(A)]q^{k-1}. \end{aligned}$$

Then it follows that

$$\begin{aligned} \alpha_{k-1} &= \frac{(q^l)^T x^{k-1}}{(q^l)^T y^{k-1}}, \quad l \in \{0, \ldots, k-1\} \\ \beta_{k-1} &= \|x^{k-1} - \alpha_{k-1}y^{k-1}\|_2 \\ q^k &= \beta_{k-1}^{-1}\left(x^{k-1} - \alpha_{k-1}y^{k-1}\right). \end{aligned}$$

Further, with the initial conditions $q^{-1} = \mathbf{0}$ and $q^0 = q/\|q\|_2$, it holds for $k = 1$ that

$$x^0 = Z_1(A)q^0 \quad \text{and} \quad y^0 = q^0.$$

Finally, if $\mu_k \neq 0$, we need to solve

- 1 system of equations whenever $\mu_k = \mu_{k-1}$ and/or $\mu_k = \mu_{k-2}$ or
- 2 systems of equations whenever $\mu_k \neq \mu_{k-1}$ and $\mu_k \neq \mu_{k-2}$

per iteration, to compute the vectors x^{k-1} and y^{k-1}. Therefore, it is advisable to

- limit the number of different values in $\mathcal{M}$,
- use a sorted list of numbers so that the values in $\mathcal{M}$ do not change too often,
- use a Cholesky factorization for the matrix $(I + \mu_k A)$ each time $\mu_k \neq \mu_{k-1}$.

Numerical example

Consider the second order differential operator

$$L = -c\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right), \quad c > 0,$$

on the unit square $(0, 1) \times (0, 1)$, with Dirichlet boundary conditions. After discretizing L on a uniform meshgrid, with meshsize $\delta = 1/(n+1)$ in both directions, using central differences, we obtain a real symmetric positive-definite block-tridiagonal $N \times N$ matrix A, with $N = n^2$. We then seek approximations to the solution of the following time-periodic problem:

$$\begin{aligned} &\frac{d}{dt}y(t) + (A + 0.6I)y(t) = \exp(-0.4t)q, \quad t \in [0, T], \\ &y(0) = y(T), \end{aligned}$$

where $q \in \mathbb{R}^N$ and $y(t) \in \mathbb{R}^N$ are discretizations of the function $q(x, y)$, respectively $y(x, y, t)$. The exact solution to this problem is given by $y(t) = f(A, t)q$, where $f(a, t)$ is defined as

$$f(a, t) = \frac{\exp(-0.4t)}{a + 0.2} - \frac{[1 - \exp(-0.4T)]\exp(-(a + 0.6)t)}{(a + 0.2)[1 - \exp(-(a + 0.6)T)]}.$$

For $t = 0$ or $t = T$ we get that

$$f(a) = f(a, 0) = f(a, T) = \frac{\exp(-0.4T)[1 - \exp(-(a + 0.2)T)]}{(a + 0.2)[1 - \exp(-(a + 0.6)T)]}.$$

Note that $f(a)$ has a singularity in $a = -3/5$, while $f(\infty) = 0$. In the case of one multiple pole $-\mu^{-1}$, however, it follows from [2] that the optimal value is $\mu = T$.
Let $n = 50$, $c = 0.1$, $T = 0.01$ and $q(x, y) = x(1 - x)y(1 - y)$. The following figures then show the relative error-norm

$$e = \|y^{(m)} - f(A)q\|_2 / \|f(A)q\|_2$$

as a function of the number of iterations m for the case of one multiple pole (Fig. 1 and 2), and for the case of two different poles (Fig. 3).

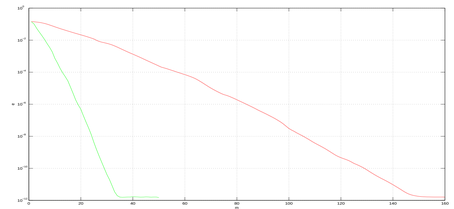

FIGURE 1: Relative error e as a function of the number of iterations m for the case of $\mu = 0$, respectively $\mu = 0.01$.

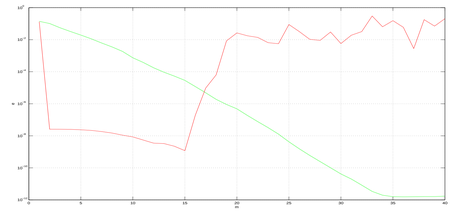

FIGURE 2: Relative error e as a function of the number of iterations m for the case of $\mu = 5/3$, respectively $\mu = 0.01$.

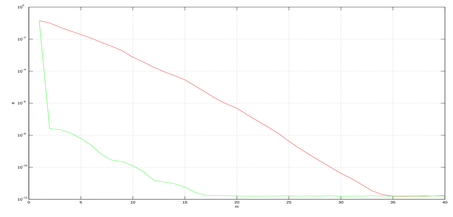

FIGURE 3: Relative error e as a function of the number of iterations m for the case of $\mu_0 = \mu_1 = 5/3$ and $\mu_2 = \ldots = \mu_{40} = 0.01$, compared with the case in which $\mu = 0.01$.

References

[1] V. Druskin and L. Knizhnerman, *"Two polynomial methods for calculating functions of symmetric matrices"*, Comput. Maths. Math. Phys., **29**(6):112-121, 1989.

[2] I. Moret and P. Novati, *"A rational Krylov method for solving time-periodic differential equations"*, Appl. Num. Math., 58:212-222, 2008.