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 \( e^A \), \( e^Bx \), \( x^A \), \( \sin(A)x \), \( \cos(A)x \), 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
\[ K_m(A,q) = \text{span}\{q, Aq, A^2q, \ldots, A^{m-1}q\}, \quad m \in \mathbb{N}, \]

is, in general, not effective since the convergence of the 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 \( M = (\mu_0, \mu_1, \ldots, \mu_m) \subset \mathbb{R}_+^m \), with \( M(\cap \sigma(A)) = 0 \), is given, and define the factors
\[ Z_k(A) = (I + \mu_k A)^{-1} = \frac{A^k}{\mu_k^{N-1}}, \quad k = 1, 2, \ldots, m, \]

and products
\[ h_k(A) = I, \quad h_k(A) = Z_k(A)h_{k-1}(A) = h_{k-2}(A)Z_k(A), \quad k = 1, 2, \ldots, m. \]

Then the rational Krylov subspace \( K_{\infty}(A,q,M) \) with poles in \( -\mu_1^{-1}, \ldots, -\mu_m^{-1} \) is given by
\[ K_{\infty}(A,q,M) = \text{span}\{h_1(A)q, h_2(A)q, \ldots, h_m(A)q\} \subseteq \text{span}\{q, Aq, A^2q, \ldots, A^{m-1}q\}, \]

where the sequence of vectors \( q^0, q^1, \ldots, q^{m-1} \) forms an orthonormal system of vectors. Under certain conditions on the poles in \( M \), these orthonormal vectors do satisfy the following three-term recurrence relation:
\[ A q^k = \beta_{k-2}(I + \mu_k q^k)q^{k-2} + \alpha_{k-1}(I + \mu_k q^k)q^{k-1} + \beta_{k-1}(I + \mu_k q^k)q^k. \]

Let \( Q_{m-1}(\alpha) = [q^0, q^1, \ldots, q^{m-1}] \) and
\[ J_m = \begin{bmatrix} \alpha_0 & 0 & 0 \cdots & 0 \\ \beta_1 & \alpha_0 & 0 \cdots & 0 \\ 0 & \beta_2 & \alpha_0 \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & \beta_{m-2} \end{bmatrix} \quad \text{and} \quad D_m = \begin{bmatrix} \mu_0 & 0 & 0 \cdots & 0 \\ 0 & \mu_1 & 0 \cdots & 0 \\ 0 & 0 & \mu_2 \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & \mu_{m-1} \end{bmatrix}. \]

Then it follows that
\[
Q_{m-1}(\alpha) J_m = \rho_0 T_m(A) Q_{m-1}(\alpha) D_m,
\]

where \( T_k(A) = \text{span}\{h_k(A), h_{k+1}(A), \ldots, h_m(A)\} \subseteq K_m(A,q) \).

### Numerical example

Consider the second-order differential operator
\[ L = -\frac{d^2}{dx^2} + \frac{g}{h}, \quad x > 0, \]

on the unit square \( (0,1) \times (0,1) \), with Dirichlet boundary conditions. After discretizing \( L \) on a uniform meshgrid, with meshsize \( h = 1/(n+1) \) in each direction, 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:
\[ \frac{d}{dt} \begin{bmatrix} u(0) \\ y(0) \end{bmatrix} = \begin{bmatrix} f(u) \\ g(y) \end{bmatrix}, \quad t \in [0,T], \]

where \( u \in \mathbb{R}^N \) and \( g(t) \in \mathbb{R}^N \) are discretizations of the function \( g(x,y) \), respectively \( g(x,y,t) \). The exact solution to this problem is given by \( u(t) = f(A,t) \), where \( f(a,t) \) is defined as
\[ f(a,t) = \begin{bmatrix} \exp(-aT) \\ 1 - \exp(-aT) \exp(-a(0.6)t) \end{bmatrix} \quad a > 0. \]

For \( t = 0 \) or \( t = T \) we get that
\[ f(u,0) = f(u,T) = \begin{bmatrix} \exp(-0.4T) \\ 1 - \exp(-0.4T) \exp(-a(0.6)T) \end{bmatrix} \quad a > 0. \]

Note that \( f(a,0) \) has a singularity in \( a = -3/5 \), while \( f(a,T) \) is \( 0 \). In the case of one multiple pole \( -p^{-1} \), however, it follows from [2] that the optimal value is \( p = T \).

Let \( n = 50, e = 0.1, T = 0.01 \) and \( g(x,y,t) = x(1-x)y(1-y) \). The following figures show then the relative error-norm
\[ e = \|y^{m-1} - f(A)y^{m-1}/f(A)y^m\| \]
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).

### References
