A Rational Krylov Toolbox for MATLAB

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1 Overview

Thank you for your interest in the Rational Krylov Toolbox (RKToolbox). The RKToolbox is a collection of scientific computing tools based on rational Krylov techniques. The development started in 2013 and the current version 2.5 provides

- an implementation of Ruhe's rational Krylov sequence method [6, 7], allowing to control various options, including user-defined inner products, exploitation of complex-conjugate shifts, orthogonalization, rerunning [4], and parallelism [5],
- algorithms for the implicit and explicit relocation of the poles of a rational Krylov space [3],
- a collection of utility functions, e.g., for solving nonlinear eigenvalue problems,
- an implementation of RKFIT [3, 4], a robust algorithm for rational L2 approximation, including automated degree reduction, and
- the RKFUN class [4] allowing for numerical computations with rational functions, including support for MATLAB Variable Precision Arithmetic and the Advanpix Multiple Precision toolbox [1].

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This guide explains the main functionalities of the toolbox. To run the embedded MATLAB codes the RKToolbox needs to be in MATLAB's search path. For details about the installation we refer to the **Download** section on http://rktoolbox.org/.

2 Rational Krylov spaces

A rational Krylov space is a linear vector space of rational functions in a matrix times a vector. Let A be a square matrix of size $N \times N$, $\boldsymbol{b}$ an $N \times 1$ starting vector, and let $\xi_1, \xi_2, \ldots, \xi_m$ be a sequence of complex or infinite *poles* all distinct from the eigenvalues of A. Then the rational Krylov space of order $m+1$ associated with $A, \boldsymbol{b}, \xi_j$ is defined as

$$\mathcal{Q}_{m+1}(A, \boldsymbol{b}, q_m) = q_m(A)^{-1}\text{span}\{\boldsymbol{b}, A\boldsymbol{b}, \ldots, A^m\boldsymbol{b}\},$$

where $q_m(z) = \prod_{j=1,\xi_j\neq\infty}^{m}(z-\xi_j)$ is the common denominator of the rational functions associated with the rational Krylov space. The rational Krylov method by Ruhe [6, 7] computes an orthonormal basis V_{m+1} of $\mathcal{Q}_{m+1}(A, \boldsymbol{b}, q_m)$. The basis matrix V_{m+1} satisfies a rational Arnoldi decomposition of the form

$$AV_{m+1}\underline{K_m} = V_{m+1}\underline{H_m},$$

where $(\underline{H_m}, \underline{K_m})$ is an (unreduced) upper Hessenberg pencil of size $(m+1) \times m$.

Rational Arnoldi decompositions are useful for several purposes. For example, the eigenvalues of the upper $m \times m$ part of the pencil $(\underline{H_m}, \underline{K_m})$ can be excellent approximations to some of A's eigenvalues [6, 7]. Other applications include matrix function approximation and rational quadrature, model order reduction, matrix equations, nonlinear eigenproblems, and rational least squares fitting (see below).

3 Computing rational Krylov bases

Relevant functions: `rat_krylov, util_cplxpair`

Let us compute V_{m+1}, $\underline{K_m}$, and $\underline{H_m}$ using the `rat_krylov` function, and verify that the outputs satisfy the rational Arnoldi decomposition by computing the relative residual norm $\|AV_{m+1}\underline{K_m} - V_{m+1}\underline{H_m}\|_2/\|\underline{H_m}\|_2$. For A we take the `tridiag` matrix of size 100 from MATLAB's `gallery`, and $\boldsymbol{b} = [1, 0, \ldots, 0]^T$. The $m = 5$ poles ξ_j are, in order, $-1, \infty, -\mathrm{i}, 0, \mathrm{i}$.

```
N  = 100;                                % matrix size
A  = gallery('tridiag', N);
b  = eye(N, 1);                          % starting vector
xi = [-1, inf, -1i, 0, 1i];              % m = 5 poles
[V, K, H] = rat_krylov(A, b, xi);
resnorm = norm(A*V*K - V*H)/norm(H)      % residual check
```

```
resnorm =
   4.1662e-15
```

As some of the poles ξ_j in this example are complex, the matrices V_{m+1}, $\underline{K_m}$, and $\underline{H_m}$ are complex, too:

```
disp([isreal(V), isreal(K), isreal(H)])
```

```
     0     0     0
```

However, the poles ξ_j can be reordered so that complex-conjugate pairs appear next to each other using the function `util_cplxpair`. After reordering the poles, we can call the function `rat_krylov` with the `'real'` option, thereby computing a real-valued rational Arnoldi decomposition [6].

```
% Group together poles appearing in complex-conjugate pairs.
xi = util_cplxpair(xi);
[V, K, H] = rat_krylov(A, b, xi, 'real');
resnorm = norm(A*V*K - V*H)/norm(H)
disp([isreal(V), isreal(K), isreal(H)])
```

```
resnorm =
   6.4056e-15
     1     1     1
```

Our implementation `rat_krylov` supports many features not shown in the basic description above.

- It is possible the use matrix pencils (A, B) instead of a single matrix A. This leads to decompositions of the form $AV_{m+1}\underline{K_m} = BV_{m+1}\underline{H_m}$.
- Both the matrix A and the pencil (A, B) can be passed either explicitly, or implicitly by providing function handles to perform matrix-vector products and to solve shifted linear systems.
- Non-standard inner products for constructing the orthonormal bases are supported.
- One can choose between CGS and MGS with or without reorthogonalization.
- Iterative refinement for the linear system solves is supported.

For more details type `help rat_krylov`.

4 Moving poles of a rational Krylov space

Relevant functions: `move_poles_expl, move_poles_impl`

There is a direct link between the starting vector $\boldsymbol{b}$ and the poles ξ_j of a rational Krylov space $\mathcal{Q}_{m+1}$. A change of the poles ξ_j to $\breve{\xi}_j$ can be interpreted as a change of the starting vector from $\boldsymbol{b}$ to $\breve{\boldsymbol{b}}$, and vice versa. Algorithms for moving the poles of a rational Krylov space are described in [3] and implemented in the functions `move_poles_expl` and `move_poles_impl`.

Example: Let us move the $m = 5$ poles $-1, \infty, -\mathrm{i}, 0$, and i into $\breve{\xi}_j = -j$, $j = 1, 2, \ldots, 5$.

```
N  = 100;
A  = gallery('tridiag', N);
b  = eye(N, 1);
xi = [-1, inf, -1i, 0, 1i];
[V, K, H] = rat_krylov(A, b, xi);
xi_new = -1:-1:-5;
[KT, HT, QT, ZT] = move_poles_expl(K, H, xi_new);
```

The poles of a rational Krylov space are the eigenvalues of the lower $m \times m$ part of the pencil $(\breve{H}_m, \breve{K}_m)$ in a rational Arnoldi decomposition $A\breve{V}_{m+1}\breve{K}_m = \breve{V}_{m+1}\breve{H}_m$ associated with that space [3]. By transforming a rational Arnoldi decomposition we are therefore effectively moving the poles:

```
VT = V*QT';
resnorm = norm(A*VT*KT - VT*HT)/norm(HT)
moved_poles = util_pencil_poles(HT, KT).'
```

```
resnorm =
   6.8668e-15
moved_poles =
  -1.0000e+00 + 1.0476e-16i
  -5.0000e-01 - 2.1919e-16i
  -3.3333e-01 - 1.7310e-16i
  -2.5000e-01 - 2.7182e-16i
  -2.0000e-01 + 3.3675e-16i
```

5 Rational Krylov fitting (RKFIT)

Relevant function: `rkfit`

RKFIT [3, 4] is an iterative Krylov-based algorithm for nonlinear rational approximation. Given two families of $N \times N$ matrices $\{F^{[j]}\}_{j=1}^{\ell}$ and $\{D^{[j]}\}_{j=1}^{\ell}$, an $N \times n$ block of vectors B, and an $N \times N$ matrix A, the algorithm seeks a family of rational functions $\{r^{[j]}\}_{j=1}^{\ell}$ of type $(m+k, m)$, all sharing a common denominator q_m, such that the *relative misfit*

$$\text{misfit} = \sqrt{\frac{\sum_{j=1}^{\ell} \|D^{[j]}[F^{[j]}B - r^{[j]}(A)B]\|_F^2}{\sum_{j=1}^{\ell} \|D^{[j]}F^{[j]}B\|_F^2}} \to \min$$

is minimal. The matrices $\{D^{[j]}\}_{j=1}^{\ell}$ are optional, and if not provided $D^{[j]} = I_N$ is assumed. The algorithm takes an initial guess for q_m and iteratively tries to improve it by relocating the poles of a rational Krylov space.

We now show on a simple example how to use the `rkfit` function. Consider again the tridiagonal matrix A and the vector $\boldsymbol{b}$ from above and let $F = A^{1/2}$.

```
N   = 100;
A   = gallery('tridiag', N);
b   = eye(N, 1);
F   = sqrtm(full(A));
exact = F*b;
```

Now let us find a rational function $r_m(z)$ of type (m, m) with $m = 10$ such that $\|F\boldsymbol{b} - r_m(A)\boldsymbol{b}\|_2/\|F\boldsymbol{b}\|_2$ is small. The function `rkfit` requires an input vector of m initial poles and then tries to return an improved set of poles. If we had no clue about where to place the initial poles we can easily set them all to infinity. In the following we run RKFIT for at most 15 iterations and aim at relative misfit $\|F\boldsymbol{b} - r_m(A)\boldsymbol{b}\|_2/\|F\boldsymbol{b}\|_2$ below 10^{-10}. We display the error after each iteration.

```
[xi, ratfun, misfit] = rkfit(F, A, b, ...
                             repmat(inf, 1, 10), ...
                             15, 1e-10, 'real');

disp(misfit)
```

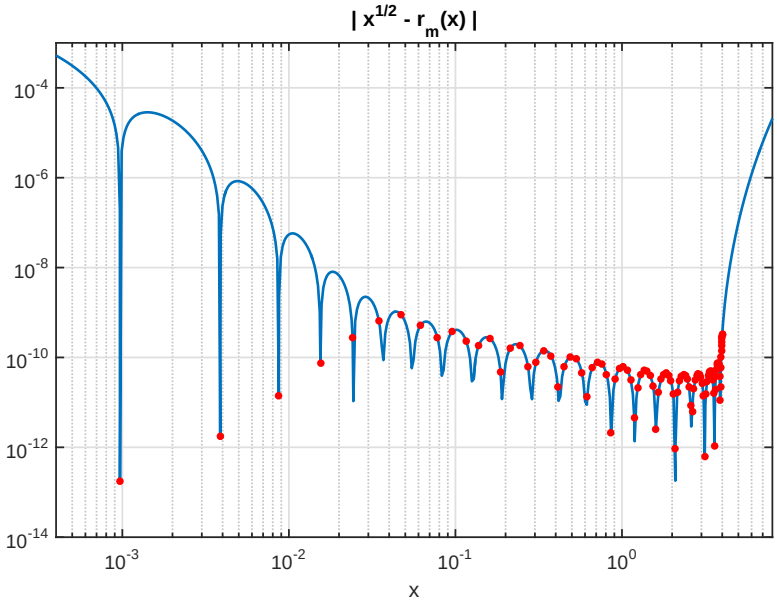
```
   7.8082e-07    1.4769e-10    4.6371e-11
```

The rational function $r_m(A)\boldsymbol{b}$ of type $(10, 10)$ approximates $A^{1/2}\boldsymbol{b}$ to about 10 decimal places. A useful output of `rkfit` is the RKFUN object `ratfun` representing the rational function r_m. It can be used, for example, to evaluate $r_m(z)$:

- `ratfun(A,v)` evaluates $r_m(A)\boldsymbol{v}$ as a matrix function times a vector,
- `ratfun(A,V)` evaluates $r_m(A)V$ as a matrix function times a matrix, e.g., setting $V = I$ as the identity matrix will return the full matrix function $r_m(A)$, or
- `ratfun(z)` evaluates $r_m(z)$ as a scalar function in the complex plane.

Here is a plot of the error $|x^{1/2} - r_m(x)|$ over the spectral interval of A (approximately $[0, 4]$), together with the values at the eigenvalues of A:

```
figure
ee = eig(full(A)).';
xx = sort([logspace(-4.3, 1, 500) , ee]);
loglog(xx,abs(sqrt(xx) - ratfun(xx))); hold on
loglog(ee,abs(sqrt(ee) - ratfun(ee)), 'r.', 'markers', 15)
axis([4e-4, 8, 1e-14, 1e-3]); xlabel('x'); grid on
title('| x^{1/2} - r_m(x) |','interpreter','tex')
```



As expected the rational function $r_m(z)$ is a good approximation of the square root over $[0, 4]$. It is, however, not a uniform approximation because we are approximately minimizing the 2-norm error on the eigenvalues of A, and moreover we are implicitly using a weight function given by the components of $\boldsymbol{b}$ in A's eigenvector basis.

Additional features of RKFIT are listed below.

- An automated degree reduction procedure [4, Section 4] is implemented; it takes place if a relative misfit below tolerance is achieved, unless deactivated.
- Nondiagonal rational approximants are supported; can be specified via an additional `param` structure.
- Utility functions are provided for transforming scalar data appearing in complex-conjugate pairs into real-valued data, as explained in [4, Section 3.5].

For more details type `help rkfit`. Some of the capabilities of `RKFUN` are shown in the following section.

6 The RKFUN class

The `rkfun` class is the fundamental data type to represent and work with rational functions. It has already been described above how to evaluate an `rkfun` object for scalar and matrix arguments by calling `ratfun(z)` or `ratfun(A,v)`, respectively. There are more than 20 other methods implemented for `rkfun`, and a list of all these can be obtained by typing `methods rkfun`. Here we provide a complete list with brief descriptions.

```
basis          - Orthonormal rational basis functions of an rkfun.
coeffs         - Expansion coefficients of an rkfun.
contfrac       - Convert an rkfun into continued fraction form.
diff           - Differentiate an rkfun.
disp           - Display information about an rkfun.
double         - Convert an rkfun into double precision (undo vpa or mp).
ezplot         - Easy-to-use function plotter.
feval          - Evaluate an rkfun at scalar or matrix arguments.
hess           - Convert an rkfun pencil to (strict) upper-Hessenberg form.
inv            - Invert an rkfun corresponding to a Moebius transform.
isreal         - Returns true if an rkfun is real-valued.
minus          - Scalar subtraction.
mp             - Convert an rkfun into Advanpix Multiple Precision format.
mrdivide       - Scalar division.
mtimes         - Scalar multiplication.
plus           - Scalar addition.
poles          - Return the poles of an rkfun.
poly           - Convert an rkfun into a quotient of two polynomials.
power          - Integer exponentiation of an rkfun.
rdivide        - Division of two rkfuns.
residue        - Convert an rkfun into partial fraction form.
rkfun          - The rkfun constructor.
roots          - Compute the roots of an rkfun.
size           - Returns the size of an rkfun.
subsref        - Evaluate an rkfun (calls feval).
times          - Multiplication of two rkfuns.
type           - Return the type (m+k,m) of an rkfun.
uminus         - Unary minus.
uplus          - Unary plus.
vpa            - Convert rkfun into MATLAB's variable precision format.
```

The names of these methods should be self-explanatory. For example, `roots(ratfun)` will return the roots of a `ratfun`, and `residue` will compute the partial fraction form. Most methods support the use of MATLAB's Variable Precision Arithmetic (VPA) or the Advanpix Multiple Precision toolbox (MP). So, for example, `contfrac(mp(ratfun))` will compute a continued fraction expansion of `ratfun` using multiple precision arithmetic. For more details on each of the methods, type `help rkfun.<method name>`. The RKFUN gallery provides some predefined rational functions that may be useful. A list of the options can be accessed as follows:

```
help rkfun.gallery
```

```
  GALLERY    Collection of rational functions.

  obj = rkfun.gallery(funname, param1, param2, ...) takes
  funname, a case-insensitive string that is the name of
  a rational function family, and the family's input
  parameters.

  See the listing below for available function families.

  constant   Constant function of value param1.
  cheby      Chebyshev polynomial (first kind) of degree param1.
  cayley     Cayley transformation (1-z)/(1+z).
  moebius    Moebius transformation (az+b)/(cz+d) with
             param1 = [a,b,c,d].
  sqrt       Zolotarev sqrt approximation of degree param1 on
             the positive interval [1,param2].
  invsqrt    Zolotarev invsqrt approximation of degree param1 on
             the positive interval [1,param2].
  sqrt0h     balanced Remez approximation to sqrt(x+(h*x/2)^2)
             of degree param3 on [param1,param2],
             where param1 <= 0 <= param2 and h = param4.
  sqrt2h     balanced Zolotarev approximation to sqrt(x+(h*x/2)^2)
             of degree param5 on [param1,param2]U[param3,param4],
             where param1 < param2 < 0 < param3 < param4 and h = param6.
  invsqrt2h  balanced Zolotarev approximation to 1/sqrt(x+(h*x/2)^2)
             of degree param5 on [param1,param2]U[param3,param4],
             where param1 < param2 < 0 < param3 < param4 and h = param6.
  sign       Zolotarev sign approximation of degree 2*param1 on
             the union of [1,param2] and [-param2,-1].
  step       Unit step function approximation for [-1,1] of
             degree 2*param1 with steepness param2.
```

Another way to create an RKFUN is to make use of MATLAB's symbolic engine. For example, `r = rkfun('(x+1)*(x-2)/(x-3)^2')` will create a rational function as expected. Alternatively, one can specify a rational function by its roots and poles (and an optional scaling factor) using the `rkfun.nodes2rkfun` function. For example, `r = rkfun.nodes2rkfun([-1,2],[3,3])` will create the same rational function as above.

7 References

[1] Advanpix LLC., *Multiprecision Computing Toolbox for MATLAB,* version 3.9.4.10481, Tokyo, Japan, 2016. http://www.advanpix.com/.

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[3] M. Berljafa and S. Güttel. *Generalized rational Krylov decompositions with an application to rational approximation,* SIAM J. Matrix Anal. Appl., 36(2):894–916, 2015.

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[6] A. Ruhe. *Rational Krylov: A practical algorithm for large sparse nonsymmetric matrix pencils,* SIAM J. Sci. Comput., 19(5):1535–1551, 1998.

[7] A. Ruhe. *The rational Krylov algorithm for nonsymmetric eigenvalue problems. III: Complex shifts for real matrices,* BIT, 34:165–176, 1994.