A Rational Krylov Toolbox for MATLAB

Mario Berljafa* Stefan Güttel*

July 14, 2015

Contents

1 Overview **1**

2 Rational Krylov spaces **1**

3 Computing rational Krylov bases **2**

4 Moving poles of a rational Krylov space **3**

5 Rational Krylov fitting (RKFIT) **4**

6 The RKFUN class **6**

7 References **7**

1 Overview

This guide explains the main functionalities of the Rational Krylov Toolbox [1]. To run the MATLAB codes it is required to download the toolbox and have it added to your MATLAB path. For details about the download we refer to http://guettel.com/rktoolbox/.

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,

*School of Mathematics, The University of Manchester, Alan Turing Building, Oxford Road, M13 9PL Manchester, United Kingdom, `m.berljafa@maths.man.ac.uk`, `stefan.guettel@manchester.ac.uk`

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

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

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 sequence method by Ruhe [5] 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 [5]. 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 200 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 =
   4.1663e-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:

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

ans =
     0     0     0
```

However, the poles ξ_j can be reordered to appear in complex conjugate pairs 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 [4].

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

resnorm =
   6.4057e-15
ans =
     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. Further, one can choose between CGS and MGS with or without reorthogonalization.
- Support for iterative refinement of linear system solutions.

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 [2] 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 $(\underline{\breve{H}_m}, \underline{\breve{K}_m})$ in a rational Arnoldi decomposition $A\breve{V}_{m+1}\underline{\breve{K}_m} = \breve{V}_{m+1}\underline{\breve{H}_m}$ associated with that space [2]. 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 =
   6.8685e-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 [2, 3] is an iterative Krylov-based algorithm for nonlinear rational approximation. Given two families of $N \times N$ matrices $\{F^{[j]}\}_{j=1}^{\ell}$ and $\{D^{[j]}\}_{j=1}^{\ell}$, a $N \times n$ block of vectors B, and a $N \times N$ 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*

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

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 at most 15 iterations of RKFIT and aim at relative misfit $\|F\boldsymbol{v} - r_m(A)\boldsymbol{v}\|_2/\|F\boldsymbol{v}\|_2$ below 10^{-10}. We display the error after each iteration.

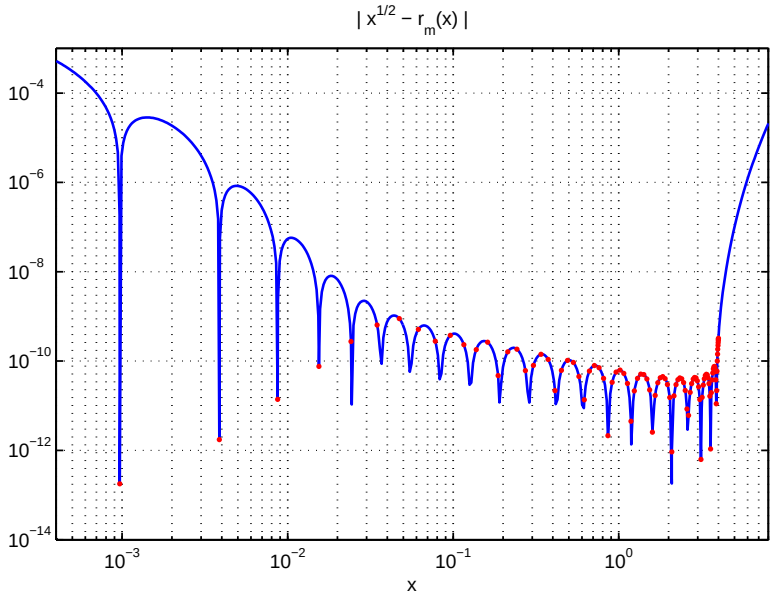
```
[xi, ratfun, misfit] = rkfit(F, A, b, ...
                             repmat(inf, 1, 10), ...
                             15, 1e-10, 'real');

misfit

misfit =
   7.8110e-07    1.4769e-10    4.6371e-11
```

The rational function $r_m(A)\boldsymbol{b}$ of type $(10, 10)$ approximates $A^{1/2}\boldsymbol{v}$ 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, 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.')
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 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 [3, 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 `help rkfun`:

```
basis          - Orthonormal rational basis functions of a rkfun.
coeffs         - Expansion coefficients of an rkfun.
contfrac       - Convert rkfun into continued fraction form.
diff           - Differentiate an rkfun.
disp           - Display information about an rkfun.
double         - Convert rkfun into double precision (undo vpa or mp).
ezplot         - Easy-to-use function plotter.
feval          - Evaluate rkfun at scalar or matrix arguments.
isreal         - Returns true if a rkfun is real.
minus          - Scalar subtraction.
mp             - Convert rkfun into Advanpix Multiple Precision format.
mrdivide       - Scalar division.
mtimes         - Scalar multiplication.
plus           - Scalar addition.
poles          - Return the poles of an rkfun.
poly           - Convert rkfun into a quotient of two polynomials.
residue        - Convert a rkfun into partial fraction form.
roots          - Compute the roots of an rkfun.
size           - Returns the size of an rkfun.
subsref        - Evaluate an rkfun (calls feval).
type           - Return the type (m+k,m) of an rkfun.
uminus         - Unary minus.
uplus          - Unary plus.
vpa            - Convert rkfun into 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 [name of method]`.

7 References

[1] M. Berljafa and S. Güttel. *A Rational Krylov Toolbox for MATLAB*, MIMS

EPrint 2014.56 (http://eprints.ma.man.ac.uk/2199/), Manchester Institute for Mathematical Sciences, The University of Manchester, UK, 2014.

[2] 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.

[3] M. Berljafa and S. Güttel. *The RKFIT algorithm for nonlinear rational approximation*, MIMS EPrint 2015.38 (http://eprints.ma.man.ac.uk/2309/), Manchester Institute for Mathematical Sciences, The University of Manchester, UK, 2015.

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

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