Moving the poles of a rational Krylov space

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Contents

1 Rational Krylov spaces

A rational Krylov space is a linear vector space of rational functions in a matrix times a vector [5]. Let A be a square matrix of size $N \times N$, $\boldsymbol{b}$ an $N \times 1$ nonzero 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

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

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 $\mathcal{Q}_{m+1}$. The rational Krylov sequence method by Ruhe [5] computes an orthonormal basis V_{m+1} of $\mathcal{Q}_{m+1}$. The first column of V_{m+1} can be chosen as $V_{m+1}\boldsymbol{e}_1 = \boldsymbol{b}/\|\boldsymbol{b}\|_2$. 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 $(m+1) \times m$.

2 The poles of a rational Krylov space

Given a rational Arnoldi decomposition of the above form, it can be shown [1] that the poles ξ_j of the associated rational Krylov space are the generalized eigenvalues of the lower $m \times m$ subpencil of $(\underline{H_m}, \underline{K_m})$. Let us verify this at a simple example by first constructing a rational Krylov space associated with the $m = 5$ poles $-1, \infty, -\mathrm{i}, 0, \mathrm{i}$. The matrix A

is of size $N = 100$ and chosen as the `tridiag` matrix from MATLAB's `gallery`, and $\boldsymbol{b}$ is the first canonical unit vector. The `rat_krylov` command is used to compute the quantities in the rational Arnoldi decomposition:

```
N  = 100;
A  = gallery('tridiag', N);
b  = eye(N, 1);
m  = 5;
xi = [-1, inf, -1i, 0, 1i];
[V, K, H] = rat_krylov(A, b, xi);
```

Indeed, the rational Arnoldi decomposition is satisfied with a residual norm close to machine precision:

```
format shorte
disp(norm(A*V*K - V*H) / norm(H))
```

```
   3.5143e-16
```

And the chosen poles ξ_j are the eigenvalues of the lower $m \times m$ subpencil:

```
disp(eig(H(2:m+1,1:m),K(2:m+1,1:m)))
```

```
  -1.0000e+00 + 0.0000e+00i
          Inf + 0.0000e+00i
   0.0000e+00 - 1.0000e+00i
   0.0000e+00 + 0.0000e+00i
   0.0000e+00 + 1.0000e+00i
```

3 Moving the poles explicitly

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 [1] and implemented in the functions `move_poles_expl` and `move_poles_impl`.

For example, let us move the poles of the above rational Krylov space $\mathcal{Q}_{m+1}$ to the points $-1, -2, \ldots, -5$:

```
xi_new = -1:-1:-5;
[KT, HT, QT, ZT] = move_poles_expl(K, H, xi_new);
```

The output of `move_poles_expl` are unitary matrices Q and Z, and transformed upper Hessenberg matrices $\underline{\breve{K}_m} = Q\underline{K_m}Z$ and $\underline{\breve{H}_m} = Q\underline{H_m}Z$, so that the lower $m \times m$ part of the pencil $(\underline{\breve{H}_m}, \underline{\breve{K}_m})$ has as generalized eigenvalues the new poles $\breve{\xi}_j$:

```
disp(eig(HT(2:m+1,1:m),KT(2:m+1,1:m)))
```

```
  -1.0000e+00 + 0.0000e+00i
  -2.0000e+00 + 1.4085e-15i
  -3.0000e+00 - 7.2486e-16i
  -4.0000e+00 + 1.6407e-16i
  -5.0000e+00 - 2.4095e-16i
```

Defining $\breve{V}_{m+1} = V_{m+1}Q^*$, the transformed rational Arnoldi decomposition is

$$A\breve{V}_{m+1}\underline{\breve{K}_m} = \breve{V}_{m+1}\underline{\breve{H}_m}.$$

This can be verified numerically by looking at the residual norm:

```
VT = V*QT';
disp(norm(A*VT*KT - VT*HT) / norm(HT))
```

```
   6.8004e-16
```

It should be noted that the function `move_poles_expl` can be used to move the m poles to arbitrary locations, including to infinity, and even to the eigenvalues of A. In latter case, the transformed space $\breve{V}_{m+1}$ does not correspond to a rational Krylov space generated with starting vector $\breve{V}_{m+1}\boldsymbol{e}_1$ and poles $\breve{\xi}_j$, but must be interpreted as a *filtered* rational Krylov space. Indeed, the pole relocation problem is very similar to that of applying an implicit filter to the rational Krylov space [3,4]. See also [1] for more details.

4 Moving the poles implicitly

Assume we are given a nonzero vector $\breve{\boldsymbol{b}} \in \mathcal{Q}_{m+1}$ with coefficient representation $\breve{\boldsymbol{b}} = V_{m+1}\boldsymbol{c}$, where $\boldsymbol{c}$ is a vector with $m+1$ entries. The function `move_poles_impl` can be used to obtain a transformed rational Arnoldi decomposition with starting vector $\breve{\boldsymbol{b}}$.

As an example, let us take $\boldsymbol{c} = [0, \ldots, 0, 1]^T$ and hence transform the rational Arnoldi decomposition so that $\breve{V}_{m+1}\boldsymbol{e}_1 = \boldsymbol{v}_{m+1}$, the last basis vector in V_{m+1}:

```
c = zeros(m+1,1); c(m+1) = 1;
[KT, HT, QT, ZT] = move_poles_impl(K, H, c);
VT = V*QT';
```

The poles of the rational Krylov space with the modified starting vector can again be read off as the generalized eigenvalues of the lower $m \times m$ part of $(\underline{\breve{H}_m}, \underline{\breve{K}_m})$:

```
disp(eig(HT(2:m+1,1:m),KT(2:m+1,1:m)))
```

```
   3.2914e+00 - 5.5756e-02i
   1.8705e+00 - 1.2100e-01i
   7.7852e-01 - 9.2093e-02i
   1.9752e-01 - 3.0824e-02i
   4.4392e-03 - 3.5884e-04i
```

This implicit pole relocation procedure is key element of the RKFIT algorithm described in [1,2].

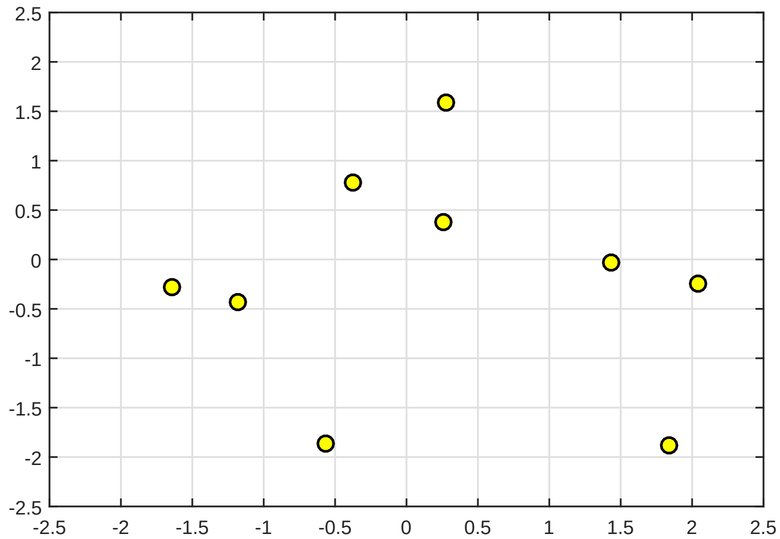
5 Some fun with moving poles

To conclude this example, let us consider a 10×10 random matrix A, a random vector $\boldsymbol{b}$, and the corresponding 6-dimensional rational Krylov space with poles at $-2, -1, 0, 1, 2$:

```
A  = (randn(10) + 1i*randn(10))*.5;
b  = randn(10,1) + 1i*randn(10,1);
m  = 5;
xi = -2:2;
[V, K, H] = rat_krylov(A, b, xi);
```

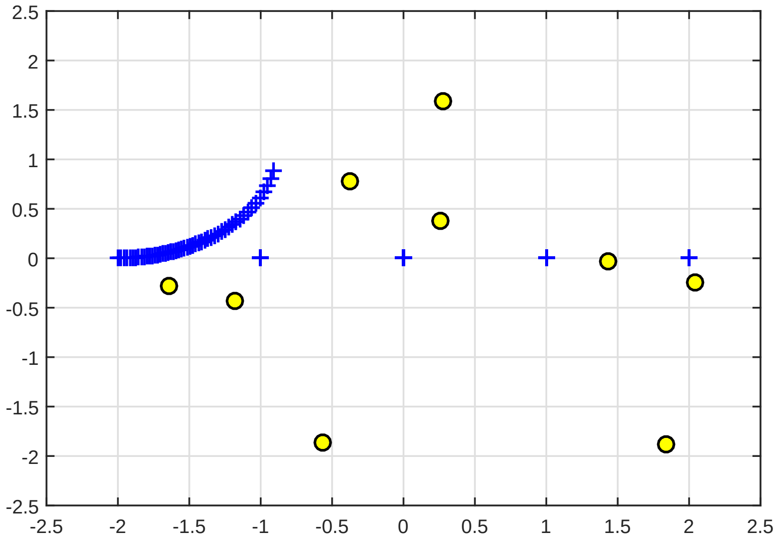
Here are the eigenvalues of A:

```
figure
plot(eig(A),'ko','MarkerFaceColor','y')
axis([-2.5,2.5,-2.5,2.5]), grid on, hold on
```



We now consider a t-dependent coefficient vector $\boldsymbol{c}(t)$ such that $V_{m+1}\boldsymbol{c}(t)$ is continuously "morphed" from $\boldsymbol{v}_1$ to $\boldsymbol{v}_2$. The poles of the rational Krylov space with the transformed starting vector $V_{m+1}\boldsymbol{c}(t)$ are then plotted as a function of t.

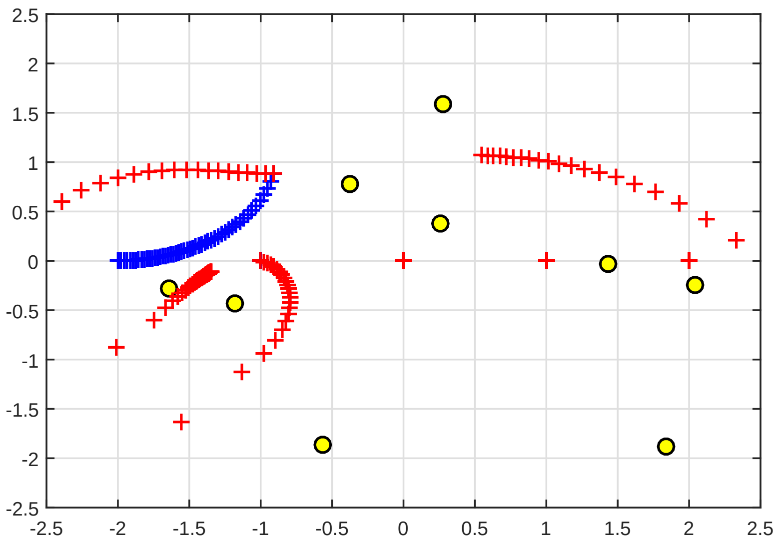
```
for t = linspace(1,2,51),
  c = zeros(m+1,1);
  c(floor(t))   = cos(pi*(t-floor(t))/2);
  c(floor(t)+1) = sin(pi*(t-floor(t))/2);
  [KT, HT, QT] = move_poles_impl(K, H, c);% transformed pencil
  xi_new = sort(eig(HT(2:m+1,1:m),KT(2:m+1,1:m))); % new poles
  plot(real(xi_new), imag(xi_new), 'b+')
end
```



As one can see, only one of the five poles starts moving away from -2, with the remaining four poles staying at their positions. This is because "morphing" the starting vector from $\boldsymbol{v}_1$ to $\boldsymbol{v}_2$ only affects a two-dimensional subspace of $\mathcal{Q}_{m+1}$ which includes the vector $\boldsymbol{b}$ and is itself a rational Krylov space, and this space is parameterized by one pole only.

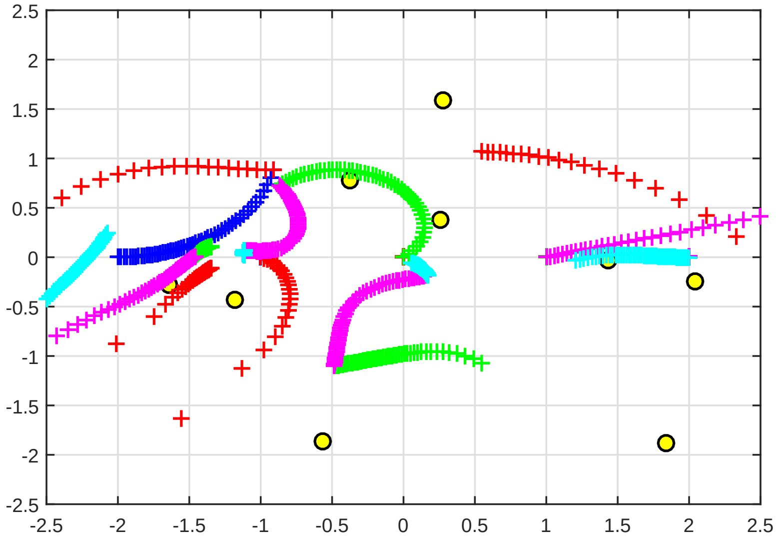
As we now continue morphing from $\boldsymbol{v}_2$ to $\boldsymbol{v}_3$, another pole starts moving:

```
for t = linspace(2,3,51),
  c = zeros(m+1,1);
  c(floor(t))   = cos(pi*(t-floor(t))/2);
  c(floor(t)+1) = sin(pi*(t-floor(t))/2);
  [KT, HT, QT, ZT] = move_poles_impl(K, H, c);
  xi_new = sort(eig(HT(2:m+1,1:m),KT(2:m+1,1:m)));
  plot(xi_new, 'r+')
end
```



Morphing from $\boldsymbol{v}_3$ to $\boldsymbol{v}_4$, then to $\boldsymbol{v}_5$, and finally to $\boldsymbol{v}_6$ will eventually affect all five poles of the rational Krylov space:

```
for t = linspace(3, 5.99, 150)
  c = zeros(m+1,1);
  c(floor(t))   = cos(pi*(t-floor(t))/2);
  c(floor(t)+1) = sin(pi*(t-floor(t))/2);
  [KT, HT, QT, ZT] = move_poles_impl(K, H, c);
  xi_new = sort(eig(HT(2:m+1, 1:m), KT(2:m+1, 1:m)));
  switch floor(t)
   case 3, plot(xi_new', 'g+')
   case 4, plot(xi_new', 'm+')
   case 5, plot(xi_new', 'c+')
  end
end
```



6 References

[1] 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.

[2] M. Berljafa and S. Güttel. *The RKFIT algorithm for nonlinear rational approximation,* SIAM J. Sci. Comput., 39(5):A2049–A2071, 2017.

[3] G. De Samblanx and A. Bultheel. *Using implicitly filtered RKS for generalised eigenvalue problems*, J. Comput. Appl. Math., 107(2):195–218, 1999.

[4] G. De Samblanx, K. Meerbergen, and A. Bultheel. *The implicit application of a rational filter in the RKS method*, BIT, 37(4):925–947, 1997.

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