

Moving the poles of a rational Krylov space

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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 $N \times N$, \mathbf{b} an $N \times 1$ nonzero starting vector, and let $\xi_1, \xi_2, \dots, \xi_m$ 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, \mathbf{b}, ξ_j is defined as

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

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 $V_{m+1} \mathbf{e}_1 = \mathbf{b} / \|\mathbf{b}\|_2$. 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 $-1, \infty, -i, 0, i$. The matrix A is of size $N = 100$ and chosen as the `tridiag` matrix from MATLAB's `gallery`, and \mathbf{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 short e
norm(A*V*K - V*H) / norm(H)

ans =
    4.1663e-15
```

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

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

ans =
-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 \mathbf{b} and the poles ξ_j of a rational Krylov space \mathcal{Q}_{m+1} . A change of the poles ξ_j to $\check{\xi}_j$ can be interpreted as a change of the starting vector from \mathbf{b} to $\check{\mathbf{b}}$, 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 $-1, -2, \dots, -5$:

```
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 $\check{K}_m = Q \underline{K}_m Z$ and $\check{H}_m = Q \underline{H}_m Z$, so that the lower $m \times m$ part of the pencil $(\check{H}_m, \check{K}_m)$ has as generalized eigenvalues the new poles $\check{\xi}_j$:

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

ans =
-1.0000e+00 + 0.0000e+00i
-2.0000e+00 + 8.7675e-16i
-3.0000e+00 + 1.5579e-15i
-4.0000e+00 + 4.3491e-15i
-5.0000e+00 - 8.4187e-15i
```

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

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

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

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

ans =
6.8685e-15
```

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 \check{V}_{m+1} does not correspond to a rational Krylov space generated with starting vector $\check{V}_{m+1}e_1$ and poles $\check{\xi}_j$, 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 $\check{b} \in \mathcal{Q}_{m+1}$ with coefficient representation $\check{b} = V_{m+1}c$, where 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 $\tilde{\mathbf{b}}$.

As an example, let us take $\mathbf{c} = [0, \dots, 0, 1]^T$ and hence transform the rational Arnoldi decomposition so that $V_{m+1}\mathbf{e}_1 = \mathbf{v}_{m+1}$, 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 $(\underline{H}_m, \underline{K}_m)$:

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

ans =
    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].

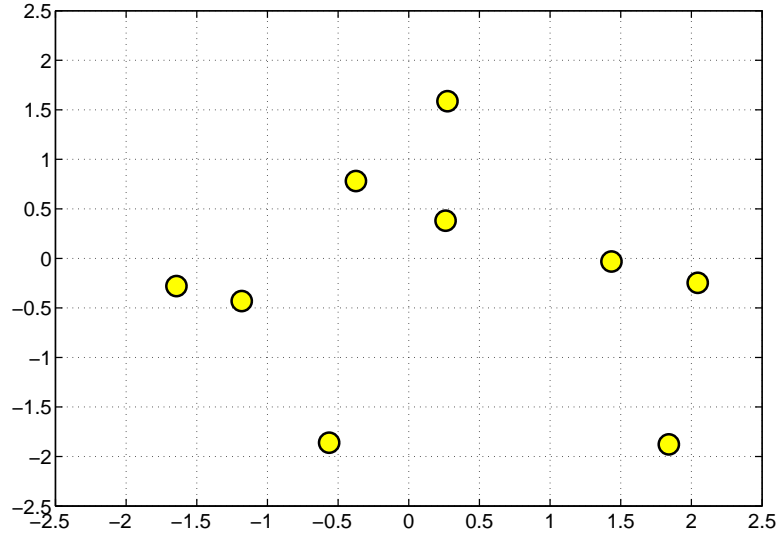
5 Some fun with moving poles

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

```
A = (randn(10) + 1i*randn(10))*0.5;
b = randn(10,1) + 1i*randn(10,1);
m = 5;
xi = -2:2; % initial poles
[V, K, H] = rat_krylov(A, b, xi);
```

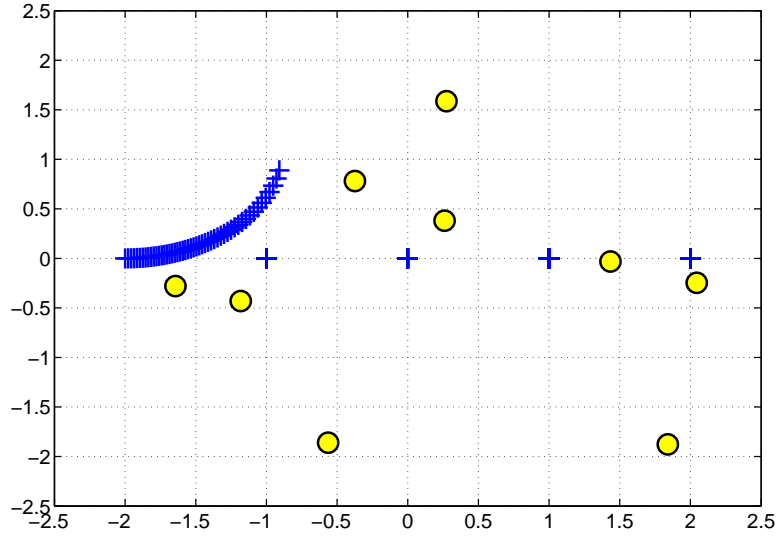
Here are the eigenvalues of A :

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

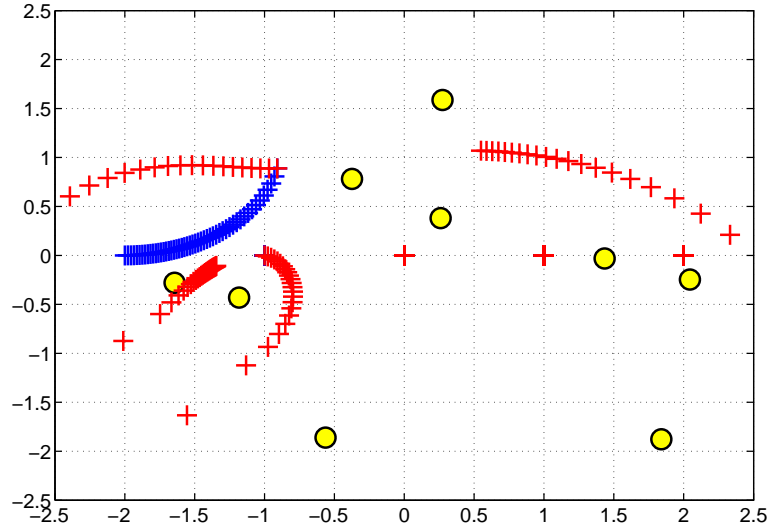
```
for t = linspace(1,2,51),
    c = zeros(m+1,1);
    c(floor(t)) = cos(pi*(t-floor(t))/2);
    c(floor(t)+1) = sin(pi*(t-floor(t))/2);
    [KT, HT, QT, ZT] = move_poles_impl(K, H, c);
% transformed pencil
    xi_new = sort(eig(HT(2:m+1,1:m),KT(2:m+1,1:m))); % new poles
    plot(real(xi_new),imag(xi_new),'b+')
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 \mathbf{v}_1 to \mathbf{v}_2 only affects a two-dimensional subspace of \mathcal{Q}_{m+1} which includes the vector \mathbf{b} and is itself a rational Krylov space, and this space is parameterized by one pole only.

As we now continue morphing from \mathbf{v}_2 to \mathbf{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
```

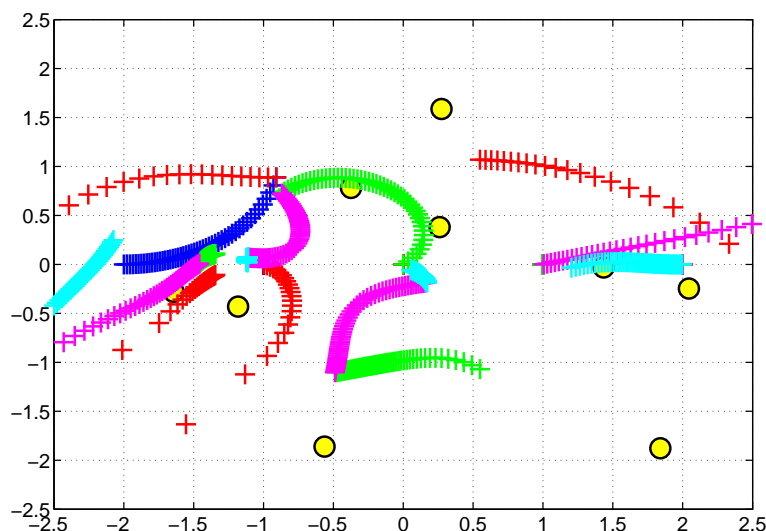


Morphing from v_3 to v_4 , then to v_5 , and finally to v_6 will eventually affect all five poles of the rational Krylov space:

```

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
end

```



6 References

- [1] M. Berljafa and S. Güttel. *Generalized rational Krylov decompositions with an application to rational approximation*, SIAM J. Matrix Anal. Appl., 2015. To appear. Available also as MIMS EPrint 2014.59 (<http://eprints.ma.man.ac.uk/2278/>).
- [2] 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.
- [3] G. De Samblanx and A. Bultheel. *Using implicitly filtered RKS for generalised eigenvalue problems*, J. Comput. Appl. Math., 107:195–218, 1999.
- [4] G. De Samblanx, K. Meerbergen, and A. Bultheel, *The implicit application of a rational filter in the RKS method*, BIT, 37:925–947, 1997.
- [5] A. Ruhe. *Rational Krylov: A practical algorithm for large sparse nonsymmetric matrix pencils*, SIAM J. Sci. Comput., 19(5):1535–1551, 1998.