Solving nonlinear eigenvalue problems

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July 2015

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1 Introduction

We consider the problem of finding eigenvalues $\lambda \in \Sigma$ and nonzero eigenvectors $\boldsymbol{x}$ of a nonlinear eigenvalue problem (NLEP)

$$A(\lambda)\boldsymbol{x} = \boldsymbol{0}.$$

Here Σ is a compact target set in the complex plane and $A(\lambda)$ is a family of $n \times n$ matrices depending analytically on λ. A popular approach for solving such problems is to approximate $A(\lambda)$ by a polynomial or rational eigenvalue problem of the form

$$Q_N(\lambda) = b_0(\lambda)D_0 + b_1(\lambda)D_1 + \cdots + b_N(\lambda)D_N,$$

where the D_j are $n \times n$ matrices, and the b_j are polynomials or rational functions in λ. Provided that the b_j can be generated by a linear recursion, the problem $Q_N(\lambda)\boldsymbol{x} = \boldsymbol{0}$ can be "linearised" into a linear pencil (A_N, B_N) of size $Nn \times Nn$, which in practice can be rather large depending on N and n.

2 The NLEIGS linearisation

The NLEIGS linearisation [3] is based on rational interpolation, with the b_j chosen as rational basis functions of the form

$$b_0(\lambda) = 1, \quad b_{j+1}(\lambda) = \frac{(\lambda - \sigma_j)}{\beta_{j+1}(1 - \lambda/\xi_{j+1})} b_j(\lambda).$$

Here, the σ_j are interpolation nodes on the boundary of Σ, and the ξ_j are poles which can be chosen freely, for example all at infinity (which leads to a polynomial interpolant) or on a singularity set Ξ of $A(\lambda)$. The advantage of employing an interpolation-based approximation $Q_N(\lambda)$ is that the matrices D_j can be obtained solely by sampling $A(\sigma_j)$, provided that the nodes σ_j are distinct. For more details we refer to [3, Section 2.1].

The numbers β_j are scaling factors which, as suggested in [3], are chosen so that $\max_{\lambda\in\Sigma} |b_j(\lambda)| \approx 1$. This scaling has the advantage that the norms $\|D_j\|_F$ give an indication of the approximation accuracy of $Q_N(\lambda)$ for $A(\lambda)$; see [3, Section 4] for more details.

3 Leja-Bagby sampling

To obtain a computationally efficient method it is desirable that $Q_N(\lambda) \approx A(\lambda)$ is a good approximation for all $\lambda \in \Sigma$ with a small degree parameter N. This suggests to use an (asymptotically) optimal rational interpolation procedure and we propose to choose the (σ_j, ξ_j) as Leja-Bagby points on (Σ, Ξ) [1, 9].

More precisely, choosing $\sigma_0 \in \Sigma$ arbitrarily, we define the nodes σ_j and poles ξ_j so that the following conditions are satisfied:

$$\max_{\lambda\in\Sigma} |s_j(\lambda)| = |s_j(\sigma_{j+1})|, \quad \min_{\lambda\in\Xi} |s_j(\lambda)| = |s_j(\xi_{j+1})|,$$

with the nodal functions s_j defined as $s_j(\lambda) = \dfrac{(\lambda-\sigma_0)\cdots(\lambda-\sigma_j)}{(\lambda-\xi_1)\cdots(\lambda-\xi_j)}$.

4 The Gun problem

We now demonstrate the above with an example taken from the problem collection [2]. We use the so-called *gun* problem, which is a model of a radio-frequency gun cavity [5]. The corresponding NLEP is

$$A(\lambda)\boldsymbol{x} = [K - \lambda M + i\sqrt{\lambda}W_1 + i\sqrt{\lambda - 108.8774^2}W_2]\boldsymbol{x} = \boldsymbol{0},$$

where K, M, W_1, W_2 are sparse 9956×9956 matrices. Let us define a function handle to the NLEP.

```
if exist('nlevp') ~= 2
  disp('Function nlevp.m not found. Can be downloaded from:')
  disp(['http://www.maths.manchester.ac.uk/our-research/research
     -groups' ...
        '/numerical-analysis-and-scientific-computing/numerical-
           analysis/' ...
        'software/nlevp/'])
  return
end

[coeffs, fun] = nlevp('gun');
n = size(coeffs{1}, 1);
A = @(lam) 1*coeffs{1} - lam*coeffs{2} + ...
    1i*sqrt(lam)*coeffs{3} + ...
    1i*sqrt(lam-108.8774^2)*coeffs{4};
```

The target set Σ for this problem is an upper-half disk with center 62500 and radius 50000. Note that the definition of $A(\lambda)$ involves two branch cuts $(-\infty, 0]$ and $(-\infty, 108.8774^2]$ caused by the square roots, and the union of these two is a good choice for the singularity set Ξ.

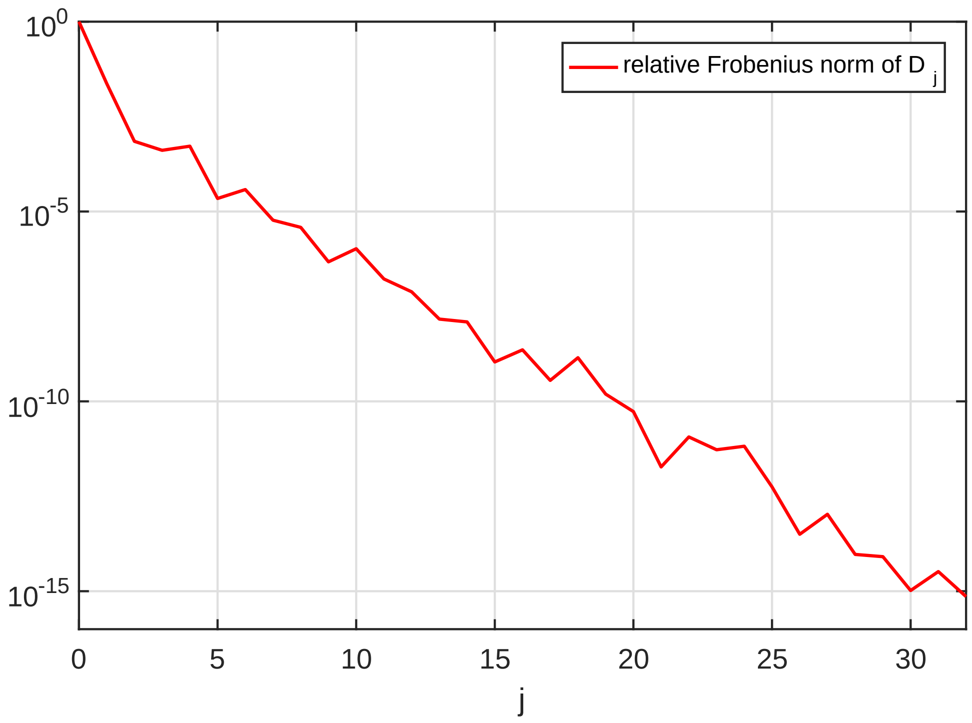
We can now use the utility function `util_nleigs` to sample the NLEP on the target set Σ using poles from the singularity set Ξ. The function requires as inputs a function handle to $A(\lambda)$, the vertices of Σ and Ξ represented by polygons, a tolerance for the sampling procedure, and the maximal number of terms.

```
Nmax  = 50;
Sigma = 62500 + 50000*exp(1i*pi*[1, linspace(0, 1)]);
Xi    = [-inf, 108.8774^2];
tol   = 1e-15;
QN    = util_nleigs(A, Sigma, Xi, tol, Nmax);
disp(QN)
```

```
        RKFUNM object of size 9956-by-9956 and type (32, 31).
        Complex sparse coefficient matrices of size 9956-by
           -9956.
        Complex-valued Hessenberg pencil (H, K) of size 33-by
           -32.
```

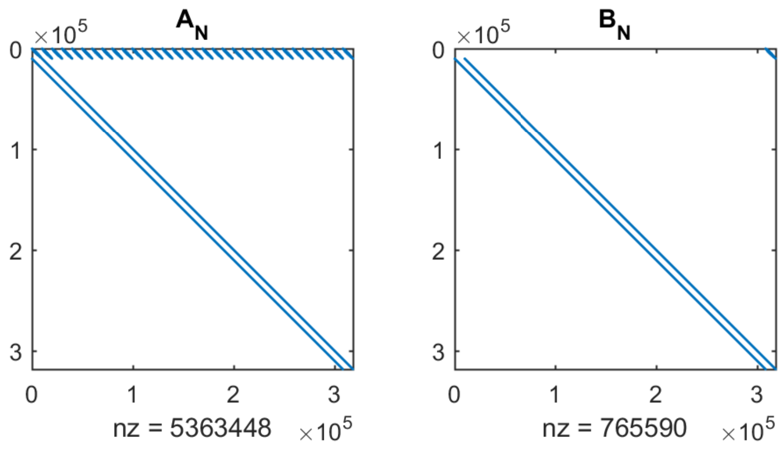
As we can see, the output of `util_nleigs` is an RKFUNM object `QN` representing $Q_N(\lambda)$, a rational matrix-valued function which interpolates $A(\lambda)$ at the nodes σ_j (i.e., $Q_N(\sigma_j) = A(\sigma_j)$ for all $j = 0, 1, \ldots, N$). We can evaluate Q_N at any point z in the complex plane by typing `QN(z)`. The `linearize` function can be used to convert Q_N into an equivalent linear matrix pencil structure $L_N(z) = A_N - zB_N$ with the same eigenvalues as Q_N. Via L_N we can also access the norms $\|D_j\|_F$ of the matrices D_j in the expansion of Q_N. Apparently, a degree of $N = 32$ was sufficient to represent $A(\lambda)$ to accuracy $\text{tol} = 10^{-15}$:

```
LN    = linearize(QN);
figure(1), semilogy(0:LN.N, LN.nrmD/LN.nrmD(1), 'r-'), grid on
legend('relative Frobenius norm of D_j'); xlabel('j')
axis([0, LN.N, 1e-16, 1])
```



Luckily this $N = 32$ is quite small due to the Leja-Bagby sampling strategy employed by `util_nleigs`. However, the full linearisation matrices (A_N, B_N) are of size $Nn \times Nn$ and hence quite large. Here is a spy plot of (A_N, B_N).

```
[AN,BN] = LN.get_matrices();
figure(2)
subplot(1,2,1), spy(AN), title('A_N')
subplot(1,2,2), spy(BN), title('B_N')
```

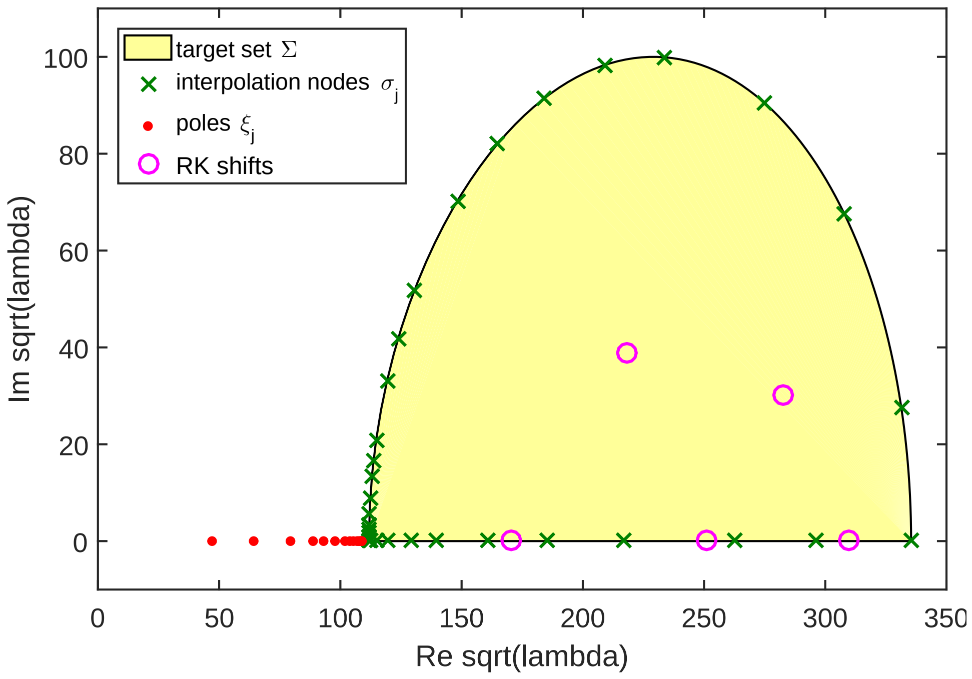


The `LN` structure provides two function handles `multiply` and `solve`, which can be used by the `rat_krylov` function to compute a rational Krylov basis for (A_N, B_N) without forming these matrices explicitly [7, 8]. For the rational Arnoldi algorithm we choose, rather arbitrarily, 5 cyclically repeated shifts in the interior of Σ.

```
shifts = [9.6e+4, 7.9e+4+1.7e+4i, 6.3e+4, 4.6e+4+1.7e+4i, 2.9e
    +4];
```

Let us first plot the target set, the sampling points σ_j, the poles ξ_j, and the shifts of the rational Krylov space:

```
figure(3)
fill(real(sqrt(Sigma)), imag(sqrt(Sigma)), [1 1 .6])
hold on
plot(sqrt(LN.sigma), 'gx', 'Color', [0 .5 0])
plot(sqrt(LN.xi(LN.xi>0))+1i*eps, 'r.', 'MarkerSize', 14)
plot(sqrt(shifts), 'mo')
xlabel('Re sqrt(lambda)'), ylabel('Im sqrt(lambda)')
legend('target set \Sigma', 'interpolation nodes \sigma_j', ...
       'poles \xi_j', 'RK shifts', 'Location', 'NorthWest')
axis([0,350,-10,110])
```



The computation of the rational Arnoldi decomposition $A_N V_{m+1} \underline{K_m} = B_N V_{m+1} \underline{H_m}$ is conveniently performed by providing the pencil structure `LN` as the first input argument to the `rat_krylov` function. Here, $m = 70$ and the starting vector is chosen at random.

Note: *The shifts in this example are cyclically repeated and the* `solve` *function provided in the* `LN` *structure attempts to reuse LU factors of $n \times n$ matrices whenever possible. The five LU factors required for this example are stored automatically as* `persistent` *variables within the* `solve` *function.*

```
v = randn(LN.N*n, 1);
shifts = repmat(shifts, 1, 14);
[V, K, H] = rat_krylov(LN, v, shifts, struct('waitbar', 1));
```

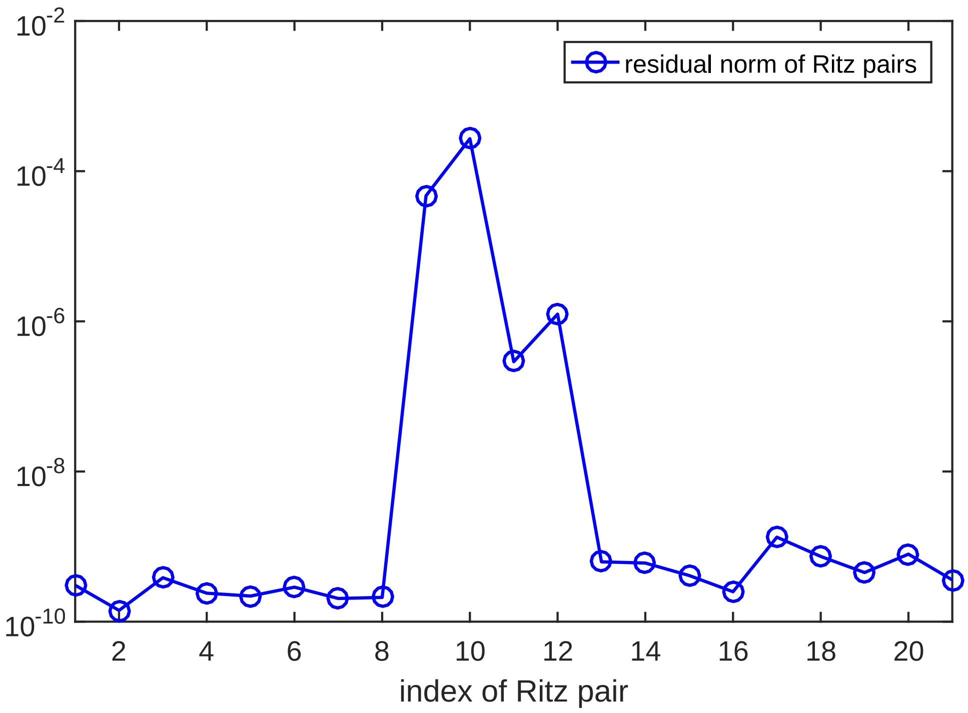
From the rational Arnoldi decomposition we can easily compute the Ritz pairs for the linearisation (A_N, B_N). In the following we extract the Ritz values in the interior of Σ and find, consistently with [3], that there are 21 Ritz values. The leading n elements of the corresponding Ritz vectors (normalised to unit norm) are then approximations to the eigenvectors $\boldsymbol{x}$ of $A(\lambda)$.

```
[X, D] = eig(H(1:end-1, :), K(1:end-1, :));
ritzval = diag(D);
ind = inpolygon(real(ritzval), imag(ritzval), ...
                real(Sigma), imag(Sigma));
ritzval = ritzval(ind);
ritzvec = V(1:n, 1:end)*(H*X(:, ind));
ritzvec = ritzvec/diag(sqrt(sum(abs(ritzvec).^2)));
disp(length(ritzval))
```

```
    21
```

Let us compute the nonlinear residual norm $\|A(\lambda)\boldsymbol{x}\|_2$ for all 21 Ritz pairs $(\lambda, \boldsymbol{x})$:

```
res = arrayfun(@(j) norm(A(ritzval(j))*ritzvec(:, j), 'fro'),
   ...
               1:length(ritzval));

figure(4)
semilogy(res, 'b-o'), xlim([1, length(res)])
legend('residual norm of Ritz pairs')
xlabel('index of Ritz pair'), hold on
```

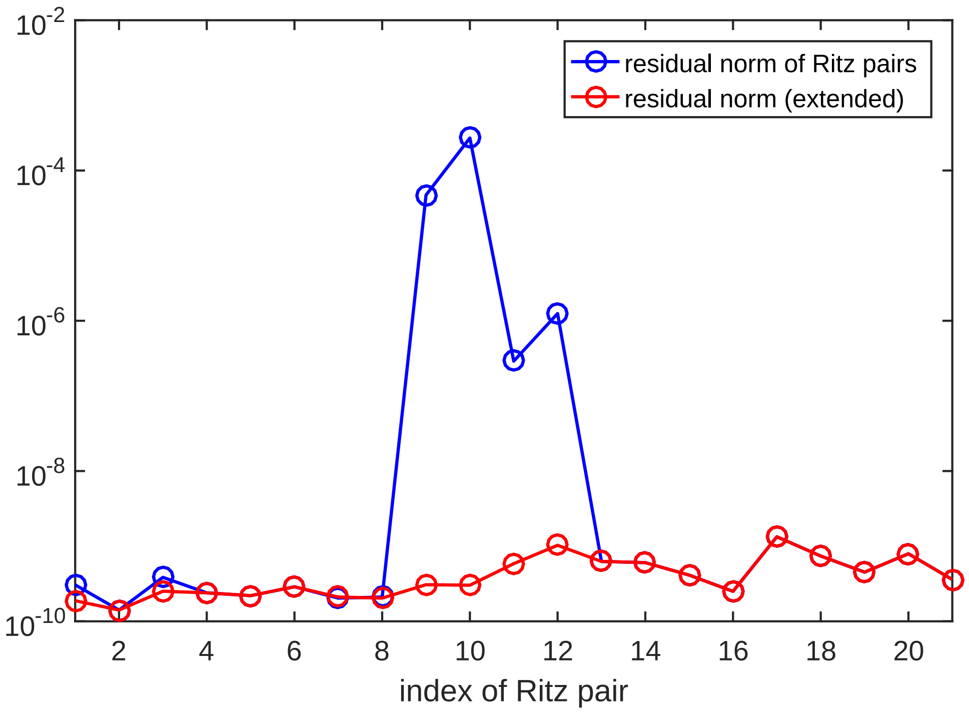


We find that all but 4 Ritz pairs are good approximations to the eigenpairs of the nonlinear problem. Let us run five more rational Arnoldi iterations by using as shift the mean of the four nonconverged Ritz values. This can be done by simply extending the existing rational Arnoldi decomposition.

```
% Use mean of Ritz values.
shifts = repmat(mean(ritzval(res>1e-8)), 1, 5);
% Extend the decomposition.
[V, K, H] = rat_krylov(LN, V, K, H, shifts, struct('waitbar',1))
   ;
```

Now let us compute the improved Ritz pairs and the corresponding nonlinear residuals exactly as above:

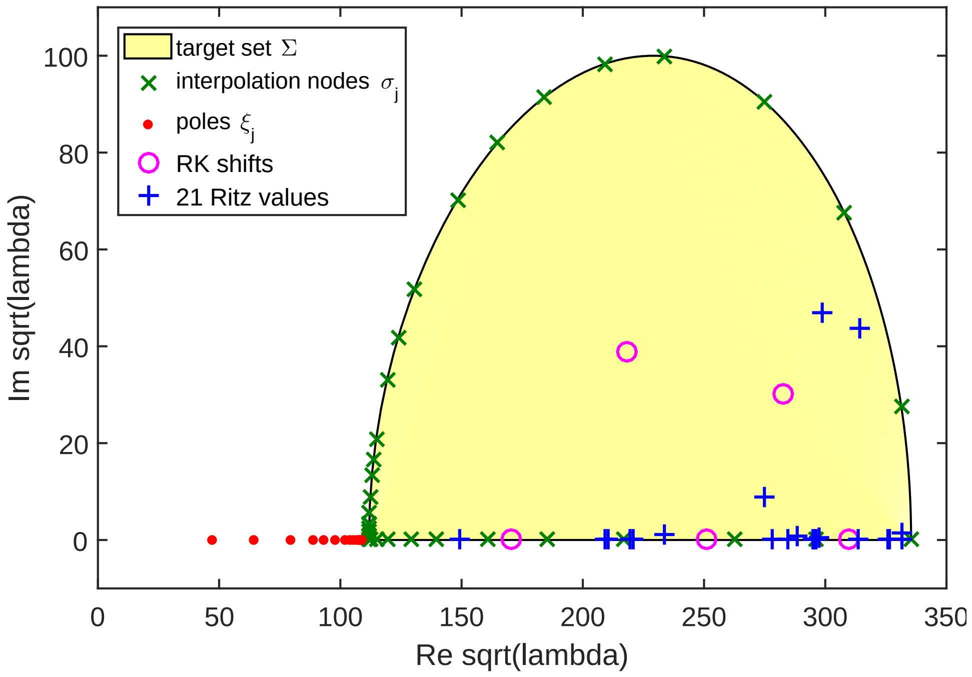
```
[X, D] = eig(H(1:end-1, :), K(1:end-1, :));
ritzval = diag(D);
ind = inpolygon(real(ritzval), imag(ritzval), ...
                real(Sigma),   imag(Sigma));
ritzval = ritzval(ind);
ritzvec = V(1:n, 1:end)*(H*X(:, ind));
ritzvec = ritzvec/diag(sqrt(sum(abs(ritzvec).^2)));

res = arrayfun(@(j) norm(A(ritzval(j))*ritzvec(:, j), 'fro'),
   ...
               1:length(ritzval));

figure(4)
semilogy(res, 'r-o')
legend('residual norm of Ritz pairs','residual norm (extended)')
```



All wanted Ritz pair are now of sufficiently high accuracy and we are done. Finally, here is a plot of the Ritz values, which coincides with [3, Figure 4(a)]:

```
figure(3)
plot(sqrt(ritzval), 'b+')
```

```
legend('target set \Sigma', 'interpolation nodes \sigma_j', ...
       'poles \xi_j', 'RK shifts', '21 Ritz values', ...
       'Location', 'NorthWest')
```



5 Variants and extensions

The linearisation computed by `util_linearise_nlep` is referred to as the "static variant of NLEIGS" in [3]. The NLEIGS algorithm, which is also available online, supports the dynamic expansion of the linearisation (A_N, B_N) as the rational Arnoldi iteration progresses. This dynamic expansion is inspired by the "infinite Arnoldi algorithm" presented in [4]. The CORK algorithm in [8] is a memory-efficient variant of NLEIGS which exploits the special structure of the Krylov basis vectors V_{m+1} associated with (A_N, B_N).

6 References

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