The parallel rational Arnoldi algorithm

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1 Introduction

Since version 2.4 of the RKToolbox, the `rat_krylov` function can simulate the parallel construction of a rational Krylov basis. This is done by imposing various nonzero patterns in a so-called continuation matrix T. Simply speaking, the j-th column of this matrix contains the coefficients of the linear combination of j rational Krylov basis vectors which have been used to compute the next $(j+1)$-th basis vector. Therefore T is an upper triangular matrix.

2 Parallelization strategies

By imposing certain nonzero patters on the continuation matrix T, we can simulate a parallel rational Arnoldi algorithm where several linear system solves are performed synchronously. Note that the typically most expensive part in the rational Arnoldi algorithm is the solution of large linear systems of equations, hence parallelizing this component can yield significant savings in computation time. There are various continuation strategies (i.e., ways to form the matrix T), each with a different numerical behaviour, and we refer to [1] for an overview. By default, the strategy `ruhe` is used, which determines the next admissible continuation vector (column of T) by computing a QR factorization of a small matrix [2]. Other available parallelization strategies are `last`, `almost-last`, and `near-optimal`. The strategy `almost-last` is the one used by Skoogh [3]. The `near-optimal` strategy is the one developed and advocated in [1]. It uses a (cheap) predictor method to anticipate the direction of the next Krylov basis vector(s) in order to determine a good continuation matrix T. By "good" we mean that the rational Krylov basis that is orthogonalized is well-conditioned, so that numerical instabilities in the Gram–Schmidt process are limited.

3 Basic usage

We now demonstrate at a simple example how to use the parallel option in `rat_krylov`. Links to the practically relevant examples are given below. First, let us define a matrix A, a starting vector $\boldsymbol{b}$, and a sequence of pole parameters, where $p = 4$ consecutive poles are pairwise distinct. Having distinct poles is a necessary requirement for parallelization.

```
load west0479
A  = west0479;
b  = ones(479,1);
xi = repmat([-50, -25, 25, 50], 1, 4);
```

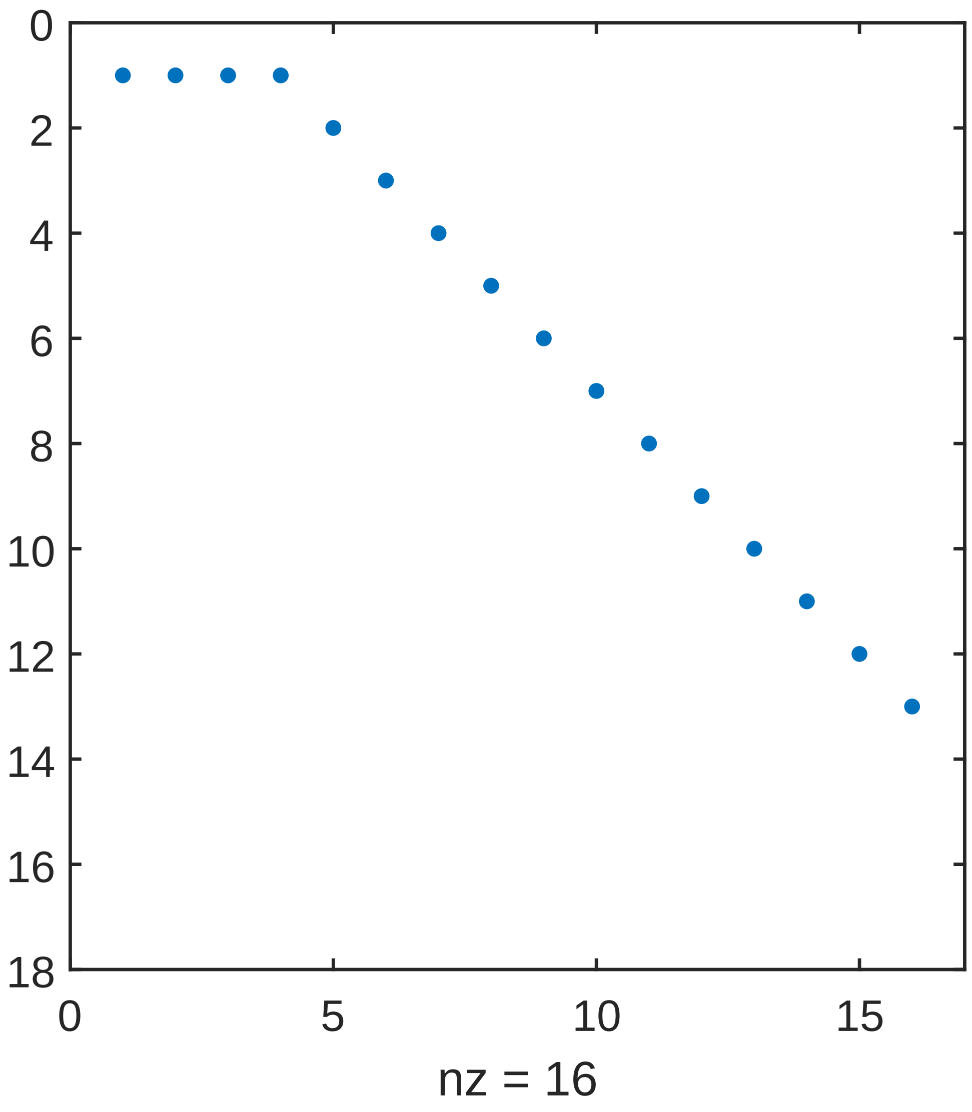
Now we can run `rat_krylov` to compute a rational Arnoldi decomposition $AV_{m+1}\underline{K_m} = V_{m+1}\underline{H_m}$, with the basis vectors in V_{m+1} being generated in parallel. This is done by specifying the continuation strategy and the `p = 4` parameter:

```
param = struct('continuation', 'almost-last', ...
               'p',            4,             ...
               'orth',         'CGS',         ...
               'reorth',       1,             ...
               'waitbar',      1 );

[V, K, H, out] = rat_krylov(A, b, xi, param);
```

The other `struct` fields specify that classical Gram-Schmidt orthogonalization has been used with reorthogonalization, the columns of the matrix pencil $(\underline{H_m}, \underline{K_m})$ have been rescaled in an attempt to improve the numerical conditioning, and a waitbar has been displayed during the computation. The output parameter `out` has several fields of interest, in particular, it returns the continuation matrix being used during the computation. Here is a spy plot of T:

```
spy(out.T)
```



We can clearly see how Skoogh's `almost-last` strategy works: in every parallel cycle, $p = 4$ rational Krylov basis vectors are computed, each from the last vector obtained on the respective parallel process in the previous parallel cycle. The output parameter `out.R` corresponds to the R factor in the implicitly computed QR factorization of the rational Krylov basis. As is explained in much more detail in [1], its condition number is an indicator for the stability of the computation. We observe that with the `almost-last` strategy this condition number is rather high:

```
R = out.R;
D = fminsearch(@(x) cond(R*diag(x)), ones(size(R, 2), 1), ...
               struct('Display','off'));
disp(cond(R*diag(D)))
```

```
   3.2177e+06
```

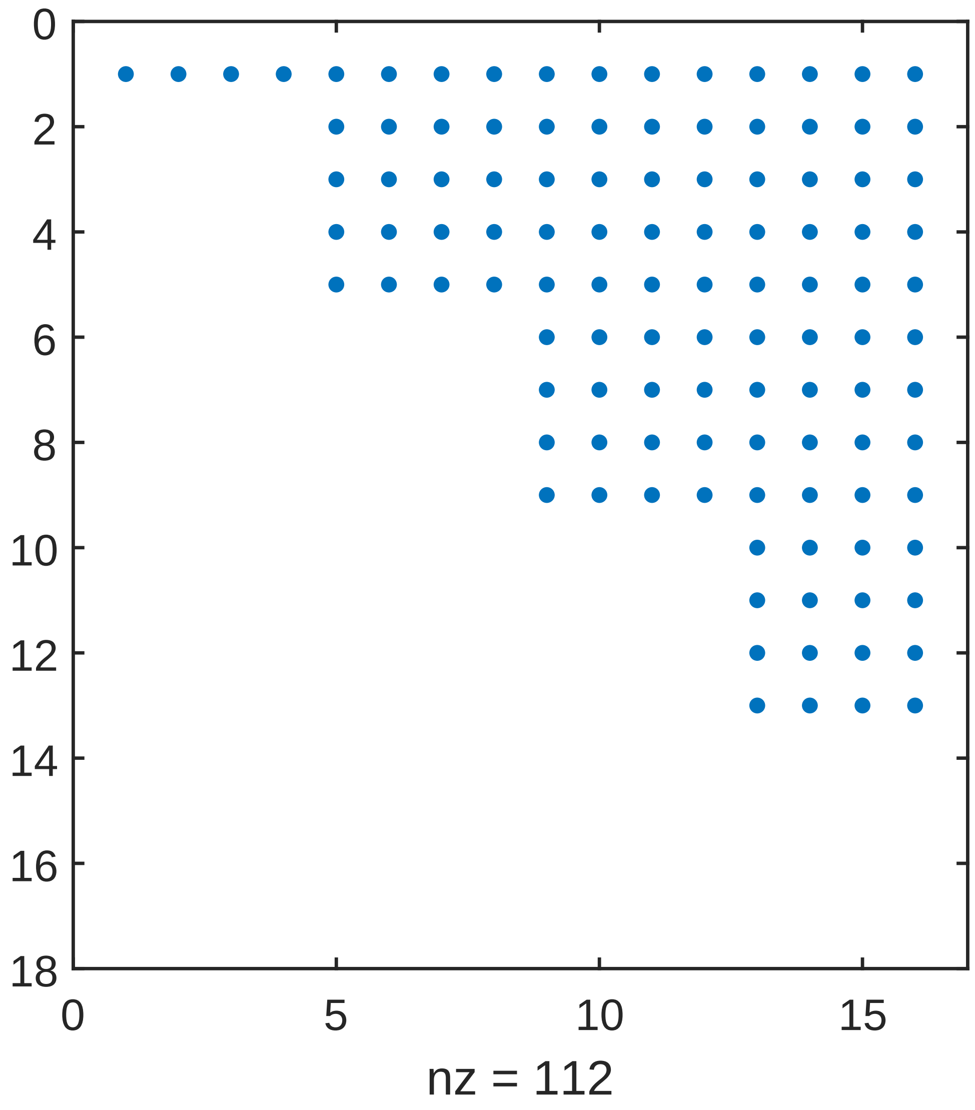
4 Near-optimal continuation strategy

To overcome, or at least reduce, the numerical problems observed with canonical parallelization strategies (such as `almost-last` and `last`), `rat_krylov` implements the `near-optimal` strategy suggested in [1]. With this strategy, a (cheap) predictor method is used to anticipate the direction of rational Krylov basis vectors before their actual computation, to infer good continuation pairs.

```
param.continuation = 'near-optimal';
[V, K, H, out] = rat_krylov(A, b, xi, param);
```

The continuation matrix T has a more dense pattern compared to the `almost-last` strategy, but still allows for $p = 4$ basis vectors to be computed in parallel:

```
spy(out.T)
```



The condition number of the basis being orthogonalized is significantly smaller:

```
R = out.R;
D = fminsearch(@(x) cond(R*diag(x)), ones(size(R, 2), 1), ...
               struct('Display','off'));
disp(cond(R*diag(D)))
```

```
   5.5275e+00
```

In fact, this basis is so close to being orthogonal, that running classical Gram-Schmidt without orthogonalization would be fine. The `near-optimal` method implemented in this simple manner is, however, computationally expensive: in fact every linear system in the rational Arnoldi algorithm has been solved twice using backslash. In a high-performance implementation one would reuse existing LU factors, or switch to an inexact predictor method like, e.g., FOM or GMRES. The predictor method is specified by a function handle in the `continuation_solve` field and the number of iterations is specified in `continuation_m`. Demonstrations of this are given in the numerical examples linked below.

5 Links to numerical examples

The numerical examples in [1] can be reproduced with the following scripts: Numerical illustration from [1, Sec. 3.4]

TEM example from [1, Sec. 5.1]

Inlet example from [1, Sec. 5.2]

Waveguide example from [1, Sec. 5.3]

6 References

[1] M. Berljafa and S. Güttel. *Parallelization of the rational Arnoldi algorithm,* SIAM J. Sci. Comput., 39(5):S197–S221, 2017.

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

[3] D. Skoogh. *A parallel rational Krylov algorithm for eigenvalue computations,* in G. Goos et al., editors, Applied Parallel Computing, volume 1541 of Lecture Notes in Computer Science, pages 521–526. Springer-Verlag, Berlin, 1998.