

Near-optimal continuation pairs

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1 Introduction

The MATLAB code provided here reproduces the numerical example from [2, Sec. 3.4]. This example demonstrates the effectiveness of the near-optimal strategy for selecting continuation pairs $(\eta_j/\rho_j, t_j)$ used for the expansion of a rational Krylov space during the execution of the rational Arnoldi algorithm; see [2, Alg. 2.1] and [2, Sec. 2], where the notion of continuation pairs is introduced. In [2, Sec. 2-3] we propose and analyze a framework for selecting these continuation pairs in such a way as to minimize the growth of the condition number of the rational Krylov basis undergoing the Gram–Schmidt process in order to avoid numerical stability problems. The motivation for this work is to provide a robust parallel rational Arnoldi algorithm where numerical instability problems have been reported. For more details we refer to [2] and the references therein.

2 MATLAB code

In the remainder we provide and briefly comment on the MATLAB code. A detailed discussion of the example itself is provided in [2, Sec. 3.4]. We first setup the problem, similar to the one from [1, Sec. 5.3].

```
N = 1000; n = 300; m = 16;

% Surrogate problem to get the poles.
A = -5*gallery('grcar', n, 3);
b = ones(n, 1);
xi = rkfit(expm(full(A)), A, b, inf(1, m));

% Actual problem.
```

```
A = -5*gallery('grcar', N, 3);
b = ones(N, 1);
```

For the near-optimal continuation strategy we use FOM(2) and FOM(3).

```
ucf = @(AB, nu, mu, x, param) ...
    util_continuation_fom(AB, nu, mu, x, param);

param = struct('continuation', 'near-optimal', ...
    'continuation_solve', ucf, ...
    'continuation_bounds', true, ...
    'orth', 'MGS', ...
    'reorth', 1);
```

In the remainder we run the rational Arnoldi algorithm using `rat_krylov` first with FOM(2), and then with FOM(3) for the prediction of near-optimal continuation pairs.

```
for cntm = 2:3
    % Use FOM(cntm) to predict near-optimal continuation pairs.
    param.continuation_m = cntm;

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

    % This holds the norms of  $\widehat{f}_{j+1}$ .
    Delta = out.Fhat;

    % The following correspond to [2, eq. (3.20)].
    delta_u = 1 + 2*out.fhat + out.Fhat.^2;
    delta_l = 1 - 2*out.fhat;

    cond_number = @(X) arrayfun(@(j) cond(X(:, 1:j+1)), ...
        1:size(X, 2)-1);

    % Bound from [2, Thm. 3.6].
    Bound = cumprod((1+Delta)./(1-Delta));
    % Analogous bound based on [2, eq. (3.20)].
    bound = sqrt(cumprod(delta_u./delta_l));

    figure(cntm-1)
    subplot(3, 1, 1:2)
    semilogy(Bound, 'bo-'), hold on
    semilogy(bound, 'bs-')
    semilogy(cond_number(out.W), 'r-')
    semilogy(out.Fhat, 'ko--')
    semilogy(out.fhat, 'ks--')

    legend('Bound_j', 'bound_j', '\kappa(W_{j+1})', ...
        'f_j', 'P_j f_j', 'location', 'NorthWest')

    xmin = 1;
    xmax = m;
    ymin = min([1, min(out.fhat)]);
```

```

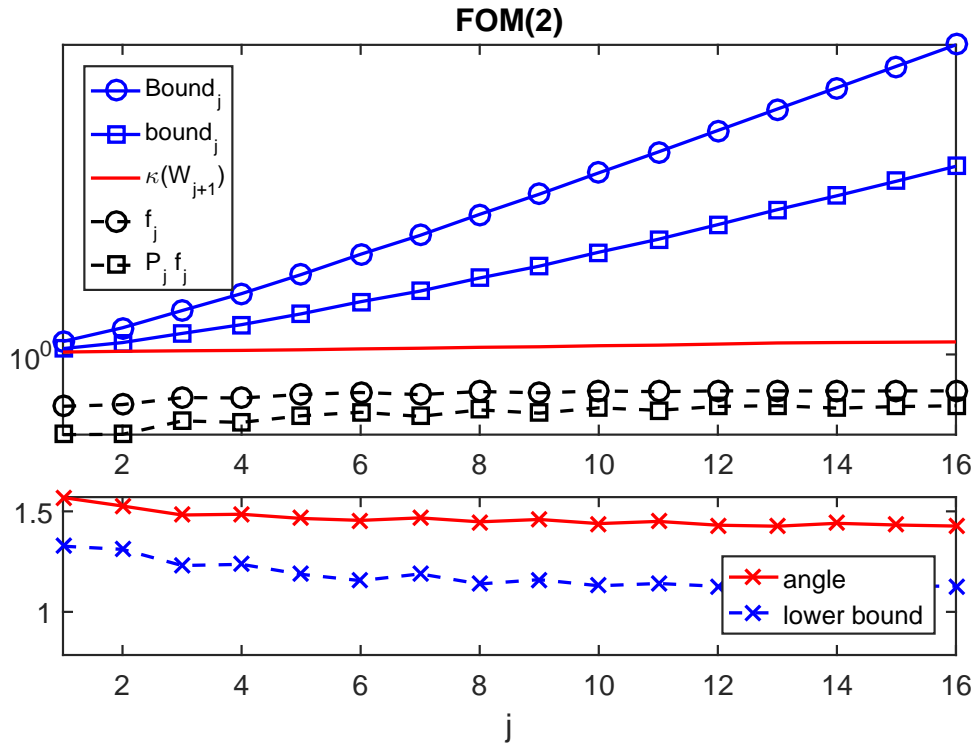
ymax = max(Bound);

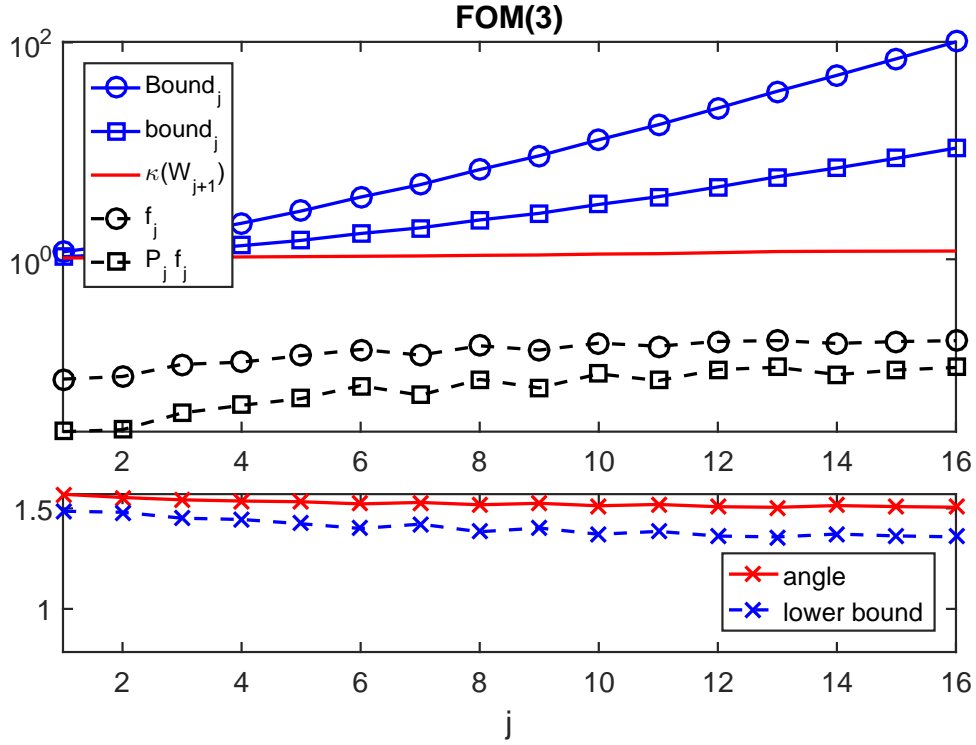
axis([xmin xmax ymin ymax])
title(['FOM(' num2str(cntm) ')'])

W = out.W;
for j = 1:m
    num = norm(W(:, j+1)-V(:, 1:j)*(V(:, 1:j)'*W(:, j+1)));
    dnm = norm(V(:, 1:j)*(V(:, 1:j)'*W(:, j+1)));
    % Angle between w_{j+1} and range(V_j).
    angl(j) = atan(num/dnm);
    % Corresponding lower bound given by [2, Cor. 3.4].
    angl_bound(j) = atan(1/out.Fhat(j)-1);
end

subplot(3, 1, 3)
plot(angl, 'rx-'), hold all
plot(angl_bound, 'bx--')
axis([xmin xmax pi/4 pi/2])
legend('angle', 'lower bound', 'location', 'SouthEast')
xlabel('j')
end

```





3 Links to other examples

Here is a list of other numerical illustrations of parallelization strategies: Overview of the parallelization options

TEM example from [1, Sec. 5.1]

Inlet example from [1, Sec. 5.2]

Waveguide example from [1, Sec. 5.3]

4 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. *Parallelization of the rational Arnoldi algorithm*, SIAM J. Sci. Comput., 39(5):S197–S221, 2017.