Rational Least Squares Fitting using Krylov Spaces

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Joint work with Stefan Güttel.

Student Krylov Day
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Manchester Numerical Analysis

Rational least squares fitting

Given the data $(\lambda_j, f_j)_{j=1}^N$ find a rational function $r_m = \dfrac{p_m}{q_m}$ such that

$$\sum_{j=1}^{N} |f_j - r_m(\lambda_j)|^2 \to \min.$$

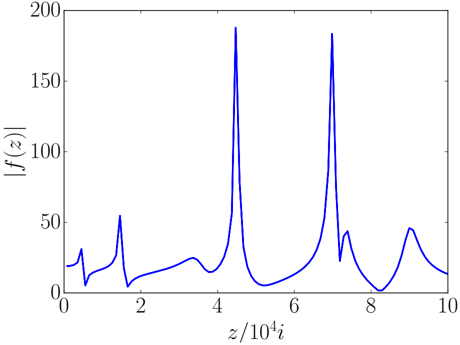
Example:

$[\lambda_1, \ldots, \lambda_N]$

- given sampling frequencies

$f_j = f(\lambda_j)$

- available transfer function measurements



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- available transfer function measurements

- $A = \mathrm{diag}(\lambda_j)$
- $F = \mathrm{diag}(f_j) = f(A)$
- $\mathbf{b} = [1, \ldots, 1]^T$

$$\sum_{j=1}^{N} |f_j - r_m(\lambda_j)|^2 = \|f(A)\mathbf{b} - \underbrace{r_m(A)\mathbf{b}}_{\in \mathcal{Q}_{m+1}(A,\mathbf{b})}\|_2^2$$

Outline

1. Rational Krylov spaces
   - Rational Arnoldi decomposition
   - Pole reallocation
2. Rational least squares approximation
   - RKFIT
   - Numerical experiments
   - A Rational Krylov Toolbox for MATLAB
3. Summary

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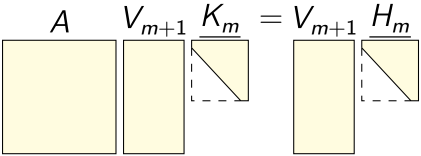
- Rational Krylov space

$$\mathcal{Q}_{m+1}(A, \mathbf{v}, q_m) := q_m(A)^{-1} \mathcal{K}_{m+1}(A, \mathbf{v}).$$



- $\mathcal{R}(V_{m+1}) = \mathcal{Q}_{m+1}(A, \mathbf{v}, q_m)$
- $(\underline{H_m}, \underline{K_m})$ unreduced upper-Hessenberg $(m+1) \times m$ pencil and such that $\{h_{j+1,j}/k_{j+1,j}\}_{j=1}^{m}$ are the roots of q_m, i.e., the poles

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For any nonzero $\breve{q}_m \in \mathcal{P}_m$ with roots disjoint from $\Lambda(A)$ there holds

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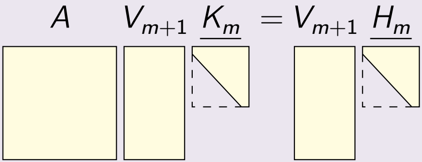

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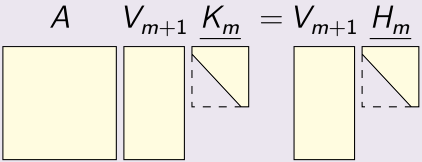

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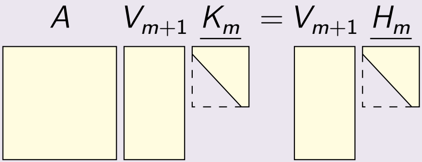
- $A\big(V_{m+1}P\big)\big(P^{-1}\underline{K_m}\big) = \big(V_{m+1}P\big)\big(P^{-1}\underline{H_m}\big)$



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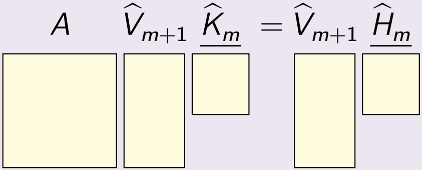

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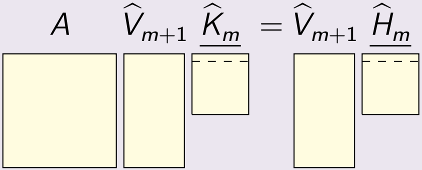

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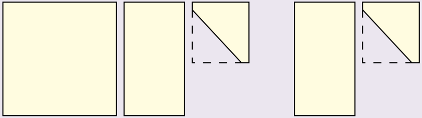
$$A \quad \breve{V}_{m+1} \; \underline{\breve{K}_m} = \breve{V}_{m+1} \; \underline{\breve{H}_m}$$



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Rational least squares fitting

Given

- $\{A, F\} \subset \mathbb{C}^{N \times N}$, and a
- unit 2-norm vector $\mathbf{v} \in \mathbb{C}^N$,

we consider the following rational least squares problem.

Find a rational function $r_m = \dfrac{p_m}{q_m}$ of type (m, m) such that

$$\|F\mathbf{v} - r_m(A)\mathbf{v}\|_2^2 \to \min.$$

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2. Solve the following linear problem.

Find $\check{\mathbf{v}} \in \mathcal{Q}_{m+1}$ s. t. $F\check{\mathbf{v}}$ is best approximated by an element of $\mathcal{Q}_{m+1}$.

$$\check{\mathbf{v}} = \underset{\substack{\mathbf{y}=V_{m+1}\mathbf{c} \\ \|\mathbf{y}\|_2=1}}{\operatorname{argmin}} \|(I - V_{m+1}V_{m+1}^*)F\mathbf{y}\|_2$$

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Compute the SVD of $FV_{m+1} - V_{m+1}\left(V_{m+1}^* FV_{m+1}\right)$.

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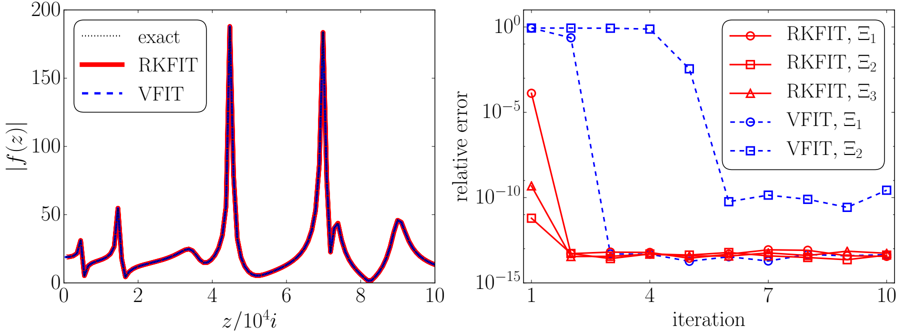
Approximate solution r_m is given implicitly as
$r_m(A)\mathbf{v} = V_{m+1}V_{m+1}^*F\mathbf{v}$, where $\mathcal{R}V_{m+1} = \mathcal{Q}_{m+1}(A, \mathbf{v}, q_m)$.

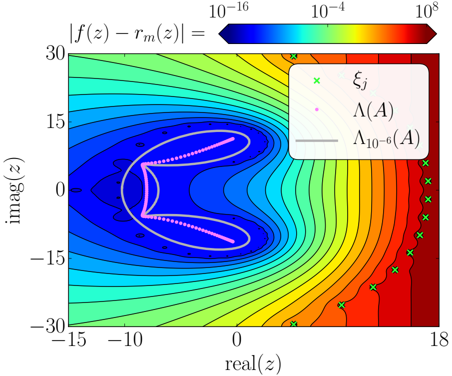
Fitting an artificial frequency response

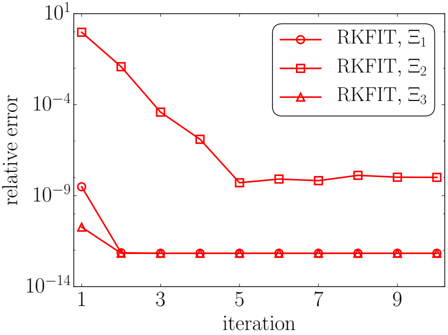
- f is a $(19, 18)$ rational function, $f(\overline{z}) = \overline{f(z)}$
- $N = 200$



- $\Xi_1 = \left[\text{logspace}(3, 5, 9), \ \overline{\text{logspace}(3, 5, 9)}\ \right]$
- $\Xi_2 = \left[\text{logspace}(6, 9, 12), \overline{\text{logspace}(6, 9, 12)}\right]$
- $\Xi_3 = \left[\infty, \ldots, \infty\right], |\Xi_3| = 18$

- $A = -5\,\mathrm{grcar}(100, 3)$
- $F = f(A)$, with $f = \exp$, and $\mathbf{v} = \begin{bmatrix} 1 & \dots & 1 \end{bmatrix}^T$





- $\Xi_1 = \mathrm{repmat}(0, \quad 1, 16)$
- $\Xi_2 = \mathrm{repmat}(-10, 1, 16)$
- $\Xi_3 = \mathrm{repmat}(\infty, \quad 1, 16)$

A Rational Krylov Toolbox for MATLAB

```
N = 100;
A = -5*gallery('grcar',N,3);
v = ones(N,1);
F = expm(A); exact = F*v;
```

```
poles = inf*ones(1, 16);
for iter = 1:3
 [poles,ratfun,misfit] = rkfit(F,A,v,poles,'real');
 rel_misfit = misfit/norm(exact);
 disp(sprintf('iter %d: %e',[iter rel_misfit]))
end
```

```
iter 1: 1.814195e-11
iter 2: 6.863362e-13
iter 3: 6.843369e-13
```

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References

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