Rational Least Squares Fitting using Krylov Spaces

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Joint work with Stefan Güttel.

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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

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

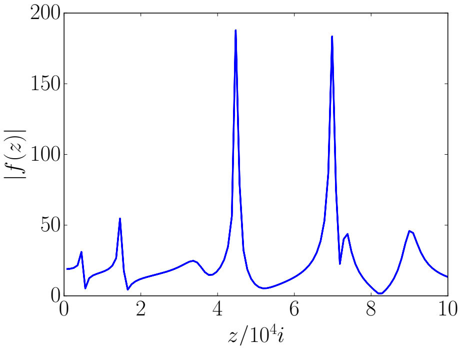
Example:

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

- given sampling frequencies

$f_j = f(\lambda_j)$

- available transfer function measurements



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Example:

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- given sampling frequencies

$f_j = f(\lambda_j)$

- available transfer function measurements

- $A = \mathrm{diag}(\lambda_j)$
- $F = \mathrm{diag}(f_j) = f(A)$
- $\mathbf{b} = \begin{bmatrix}1, \dots, 1\end{bmatrix}^T$

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

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 spaces

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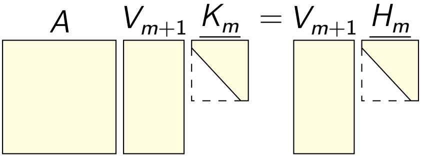
- Rational Krylov space

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



- $\mathcal{R}V_{m+1} = \mathcal{Q}_{m+1}(A, \mathbf{v}, q_m)$
- $(\underline{H_m}, \underline{K_m})$ 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

Pole reallocation is achieved by replacing the starting vector

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

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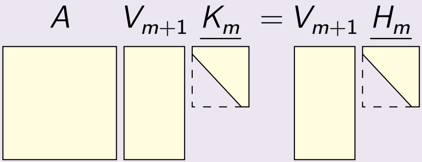

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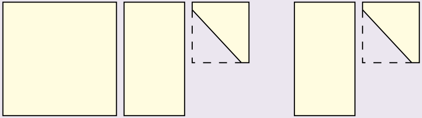
$$A \quad V_{m+1} \; \underline{K_m} = V_{m+1} \; \underline{H_m}$$



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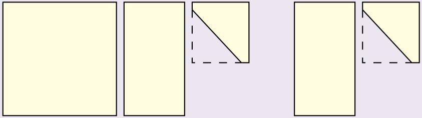

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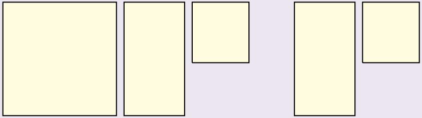

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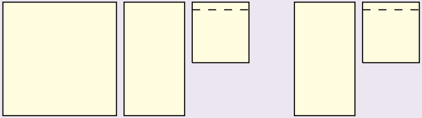

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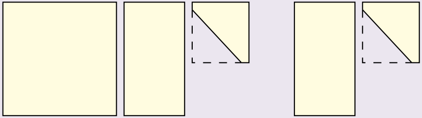

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Rational least squares fitting

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

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

Rational Krylov Fitting (RKFIT) for $\|F\mathbf{v} - r_m(A)\mathbf{v}\|_2^2 \to \min$

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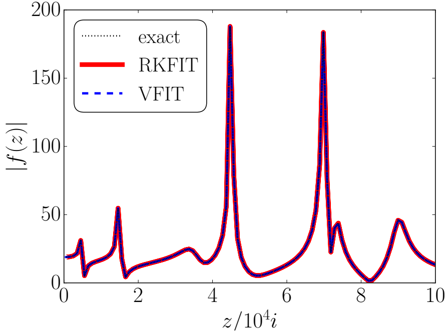
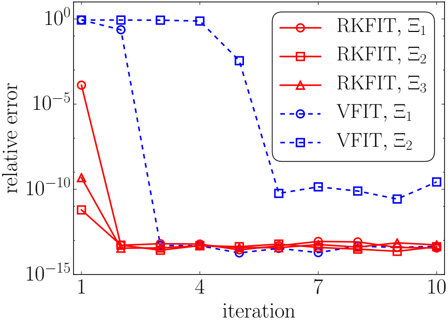
Approximate solution r_m is given implicitly as
$r_m(A)\mathbf{v} = V_{m+1}V_{m+1}^*F\mathbf{v}$, where $\mathcal{R}V_{m+1} = \mathcal{Q}_{m+1}(A, \mathbf{v}, q_m)$.

Fitting an artificial frequency response

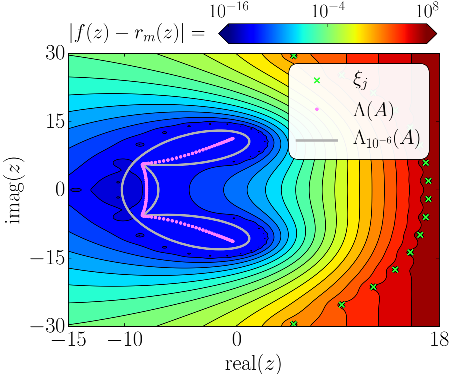
- f is a $(19, 18)$ rational function, $f(\overline{z}) = \overline{f(z)}$
- $N = 200$

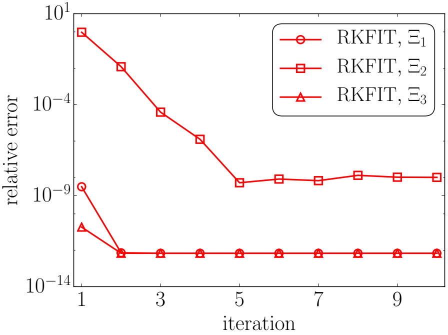




- $\Xi_1 = \left[\text{logspace}(3, 5, 9), \ \overline{\text{logspace}(3, 5, 9)}\ \right]$
- $\Xi_2 = \left[\text{logspace}(6, 9, 12), \overline{\text{logspace}(6, 9, 12)}\right]$
- $\Xi_3 = \left[\infty, \ldots, \infty\right], |\Xi_3| = 18$

- $A = -5\,\mathrm{grcar}(100, 3)$
- $F = f(A)$, 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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Summary

- Introduced RKFIT. Based on
  - discrete orthogonal rational functions, and
  - pole reallocation within $\mathcal{Q}_{m+1}(A, \mathbf{v}, q_m)$.
- Observed better numerical stability than VFIT.
- Can fit many functions with the same set of poles.
- Use only real arithmetic with “complex conjugate data”.

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References

M. Berljafa and S. Güttel, *A Rational Krylov Toolbox for MATLAB*, MIMS EPrint 2014.56. Available at `http://guettel.com/rktoolbox/`.

M. Berljafa and S. Güttel, *Generalized rational Krylov decompositions with an application to rational approximation*, MIMS EPrint 2014.59.

B. Gustavsen and A. Semlyen, *Rational approximation of frequency domain responses by vector fitting*, IEEE Trans. Power Del., 14 (1999), pp. 1052–1061.

Avoiding complex arithmetic

Let $Q \in \mathbb{C}^{N\times N}$ be unitary. Then

$$\begin{aligned}\|F\mathbf{v} - r_m(A)\mathbf{v}\|_2 &= \|\,(QFQ^*)\,(Q\mathbf{v}) - Qr_m(A)Q^*\,(Q\mathbf{v})\,\|_2 \\ &= \|\,(QFQ^*)\,(Q\mathbf{v}) - r_m(QAQ^*)\,(Q\mathbf{v})\,\|_2.\end{aligned}$$

$$F = \begin{bmatrix} f & \\ & \overline{f}\end{bmatrix}, \quad A = \begin{bmatrix} \mathrm{i}\lambda & \\ & -\mathrm{i}\lambda\end{bmatrix}, \quad \mathbf{v} = \begin{bmatrix} 1 \\ 1\end{bmatrix}, \quad Q = \frac{\sqrt{2}}{2}\begin{bmatrix} 1 & 1 \\ -\mathrm{i} & \mathrm{i}\end{bmatrix}$$

$$QFQ^* = \begin{bmatrix} \Re(f) & -\Im(f) \\ \Im(f) & \Re(f)\end{bmatrix}, \quad QAQ^* = \begin{bmatrix} & -\lambda \\ \lambda & \end{bmatrix}, \quad Q\mathbf{v} = \begin{bmatrix} \sqrt{2} \\ 0\end{bmatrix}$$

Back.

Vector functions with identical poles

Given: $\{A, F_1, \ldots, F_k\} \subset \mathbb{C}^{N \times N}$, and a unit 2-norm vector $\mathbf{v} \in \mathbb{C}^N$.

Find rational functions $r_m^{[\ell]} = \dfrac{p_m^{[\ell]}}{q_m}$ with common denominator s.t.

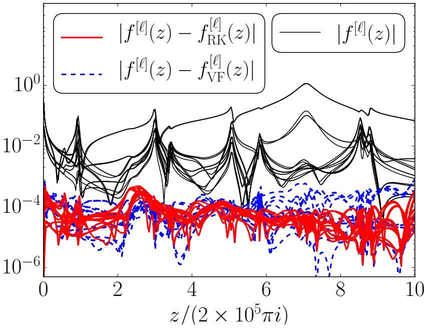
$$\sum_{\ell=1}^{k} \|F_\ell \mathbf{v} - r_m^{[\ell]}(A)\mathbf{v}\|_2^2 \to \min.$$

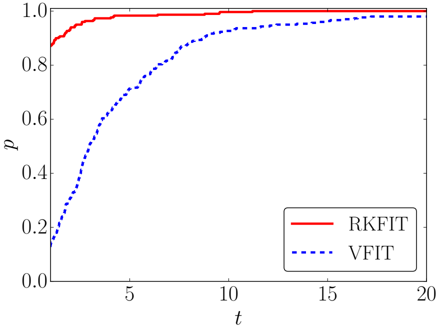
In step 2 of RKFIT consider the SVD of

$$\begin{bmatrix} F_1 V_{m+1} - V_{m+1}\left(V_{m+1}^* F_1 V_{m+1}\right) \\ F_2 V_{m+1} - V_{m+1}\left(V_{m+1}^* F_2 V_{m+1}\right) \\ \vdots \\ F_k V_{m+1} - V_{m+1}\left(V_{m+1}^* F_k V_{m+1}\right) \end{bmatrix}.$$

Vector functions with identical poles, an example

- Fitting all elements of the admittance matrix of a six-terminal system (power system distribution network).
- $N = 300 + 300, \quad m = 25 + 25$
- $f^{[\ell]}(\bar{z}) = \overline{f^{[\ell]}(z)}, \quad \ell = 1, \ldots, 21$





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