M\crNA
Manchester Numerical Analysis

Stefan Güttel

The RKFIT algorithm for nonlinear rational approximation

MANCHESTER
1824

Registration open for the GAMM ANLA workshop in Cologne, September 7-8, 2017

gamm-workshop.uni-koeln.de

Invited speakers: Pierre Gosselet, Oliver Rheinbach, Wim Vanroose

Registration fee: 40 Euro

Rational least squares fitting (scalar form)

Given data pairs $(\lambda_1, f_1), \ldots, (\lambda_N, f_N)$, find $r_n(z) = \frac{p_n(z)}{q_n(z)}$ such that

$$\sum_{j=1}^{N} |f_j - r_n(\lambda_j)|^2 \to \text{“}\min_{r_n}\text{”}.$$

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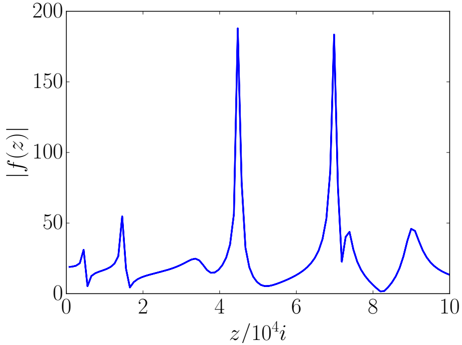
Example:

- λ_j = given sampling points (frequencies)
- $f_j = f(\lambda_j)$ = transfer function measurements
- $r_n(z)$ = low-order model



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Introduce

- $A = \operatorname{diag}(\lambda_j) \in \mathbb{C}^{N\times N}$,
- $F = \operatorname{diag}(f_j) = f(A) \in \mathbb{C}^{N\times N}$,
- $\mathbf{b} = \left[1, \ldots, 1\right]^T \in \mathbb{R}^N$.

Then

$$\sum_{j=1}^{N} |f_j - r_n(\lambda_j)|^2 = \|f(A)\mathbf{b} - r_n(A)\mathbf{b}\|_2^2.$$

Rational least squares fitting (matrix form)

More generally, given $\{A, F\} \subset \mathbb{C}^{N\times N}$ and $\mathbf{b} \in \mathbb{C}^N$, we aim to solve

$$\|F\mathbf{b} - r_n(A)\mathbf{b}\|_2^2 \to \min$$

with the minimum taken over all rational functions $r_n(z) = \frac{p_n(z)}{q_n(z)}$.

This is a nonlinear weighted rational least squares problem on $\Lambda(A)$.

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Observation

If $q_n(z) = \prod_{\substack{j=1 \\ \xi_j \neq \infty}}^{n} (z - \xi_j)$ was known, the LS problem would be linear:

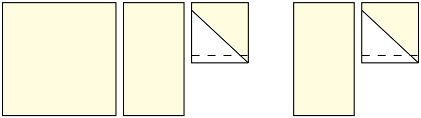
Find vector $r_n(A)\mathbf{b}$ via orthogonal projection onto rational Krylov space

$$\mathscr{Q}_{n+1}(A, \mathbf{b}, q_n) := q_n(A)^{-1} \underbrace{\operatorname{span}\{\mathbf{b}, A\mathbf{b}, \ldots, A^n\mathbf{b}\}}_{\mathscr{K}_{n+1}(A,\mathbf{b})}.$$

Rational Arnoldi decompositions

The rational Arnoldi algorithm [Ruhe 94] is used to compute a rational Arnoldi decomposition of the form

$$A \quad V_{n+1} \quad \underline{K_n} \quad = \quad V_{n+1} \quad \underline{H_n}$$



where

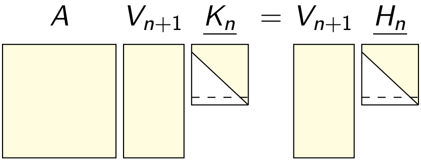
- the columns of V_{n+1} are an orthonormal basis of $\mathscr{Q}_{n+1}(A, \mathbf{b}, q_n)$,
- first column of V_{n+1} is $\mathbf{v}_1 = \mathbf{b}/\|\mathbf{b}\|_2$,
- $(\underline{H_n}, \underline{K_n})$ is unreduced upper-Hessenberg $(n+1) \times n$ pencil,
- the quotients $\{h_{j+1,j}/k_{j+1,j}\}_{j=1}^{n}$ are roots of $q_n(z) = \prod_{\substack{j=1 \\ \xi_j \neq \infty}}^{n} (z - \xi_j)$.

What can we say about uniqueness of such decompositions?

Rational implicit Q theorem [Berljafa & Güttel 2015]

Let $A \in \mathbb{C}^{N \times N}$ satisfy an orthonormal rational Arnoldi decomposition $AV_{n+1}\underline{K_n} = V_{n+1}\underline{H_n}$ with poles $\xi_j = h_{j+1,j}/k_{j+1,j}$.
Then the matrix V_{n+1} and the pencil $\left(\underline{H_n}, \underline{K_n}\right)$ are essentially uniquely determined by the first column of V_{n+1} and the poles $\xi_1, \ldots, \xi_n$.

$\Longrightarrow$ Allows us to move poles ξ_j by changing first column of V_{n+1}:



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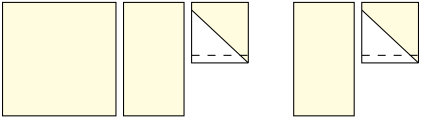
insert rotation $\overbrace{P_{n+1}P_{n+1}^*}$ $\overbrace{P_{n+1}P_{n+1}^*}$

$$A \quad V_{n+1} \quad \underline{K_n} = V_{n+1} \quad \underline{H_n}$$



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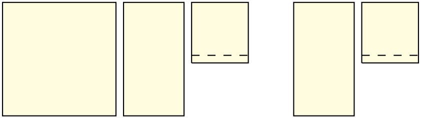
rotate basis to $\widetilde{V}_{n+1} = V_{n+1}P_{n+1}$

$$A \quad \widetilde{V}_{n+1} \quad \underline{\widetilde{K}_n} = \widetilde{V}_{n+1} \quad \underline{\widetilde{H}_n}$$



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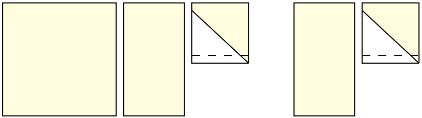
QZ transform on lower $n \times n$ part of pencil $(\underline{\widehat{H}_n}, \underline{\widehat{K}_n})$

$$A \quad \widehat{V}_{n+1} \quad \underline{\widehat{K}_n} = \widehat{V}_{n+1} \quad \underline{\widehat{H}_n}$$



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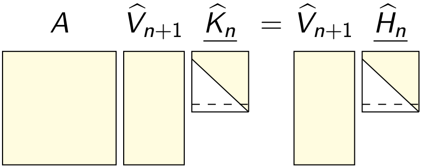

Read off new poles $\widehat{\xi}_j := \widehat{h}_{j+1,j}/\widehat{k}_{j+1,j}$ from subdiagonal elements

Rational Krylov fitting $\|F\mathbf{b} - r_n(A)\mathbf{b}\|_2 \to \min$

Take initial poles $\xi_1, \ldots, \xi_n$ and iterate:

1. Compute orthonormal basis V_{n+1} for $\mathscr{Q}_{n+1}(A, \mathbf{b}, q_n)$.
2. Solve the following linear problem:

Find $\widehat{\mathbf{v}} \in \mathscr{Q}_{n+1}(A, \mathbf{b}, q_n)$ such that $F\widehat{\mathbf{v}}$ is best approximated by an element of $\mathscr{Q}_{n+1}(A, \mathbf{b}, q_n)$, i.e.,

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

3. Move $\widehat{\mathbf{v}}$ to the first column of V_{n+1} and find new poles $\widehat{\xi}_1, \ldots, \widehat{\xi}_n$.

We call this algorithm **RKFIT** [Berljafa & Güttel 2015].

Convergence result: Exactness

Theorem (Berljafa & Güttel 2017)

Assume that $\mathscr{K}_{2n+1}(A, \mathbf{b}) = \mathrm{span}\{\mathbf{b}, A\mathbf{b}, \ldots, A^{2n}\mathbf{b}\}$ *is not A-invariant and that* $F = p_n(A)q_n^\star(A)^{-1}$ *for some* $p_n, q_n^\star \in \mathscr{P}_n$*. Then, in exact arithmetic, RKFIT will find* $q_n^\star$ *in a single iteration independent of the initial guess* q_n*.*

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- A similar result has been shown by [Lefteriu & Antoulas 2013] for the vector fitting (VFIT) algorithm by [Gustavsen & Semlyen 1999]. See also [Drmac, Gugercin, Beattie 2015].
- VFIT is based on a representation of p_n and q_n in barycentric form, with an implicit pole reallocation by changing weights.
- RKFIT differs from VFIT by its basis representation (partial fractions vs orthogonal rational functions) and the normalization of p_n/q_n.

Degree revelation

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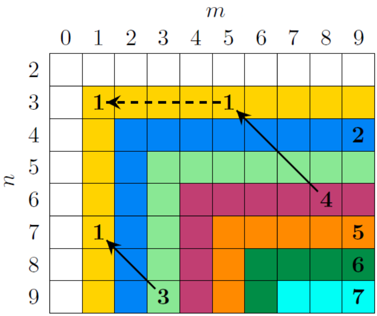
Let $M := (I - V_{n+1} V_{n+1}^*) F V_{n+1}$. *Then* $d = \dim(\operatorname{null} M) - 1$ *is the largest integer such that* F *is of type* $(n-d, n-d)$.

- We have implemented automatic degree reduction based on the numerical rank of N.
- Everything can be generalized to rational functions $r_{mn}(z) = p_m(z)/q_n(z)$ of nondiagonal type (m, n).



RKFIT is part of our MATLAB Rational Krylov Toolbox:

`www.rktoolbox.org`

RKFIT can be used to solve problems of the form

$$\|F\mathbf{b} - r_{mn}(A)\mathbf{b}\|_2 \to \min_{r_{mn}},$$

or more generally

$$\sum_{j=1}^{k} \|F^{[j]}B - r_{mn}^{[j]}(A)B\|_F^2 \to \min_{r_{mn}},$$

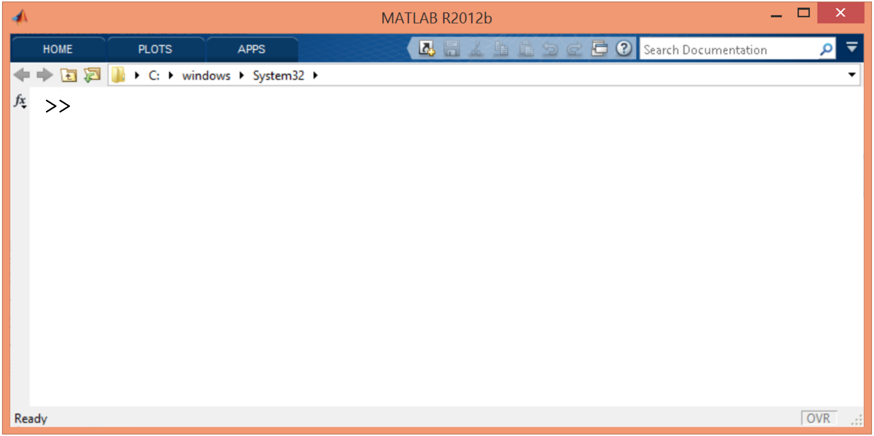
where $B = [\mathbf{b}_1, \ldots, \mathbf{b}_\ell]$ and all $r_{mn}^{[j]}(z)$ share the same denominator $q_n(z)$.

RKToolbox Demo: filter design via RKFIT

Type (99, 100) dual bandpass filter on [0, 10] via nonlinear LS fit to

$$f([2,3]) = 1, \quad f([6,8]) = 2, \quad \text{otherwise } f(x) = 0.$$

Compute partial fraction expansion in multiple precision arithmetic.



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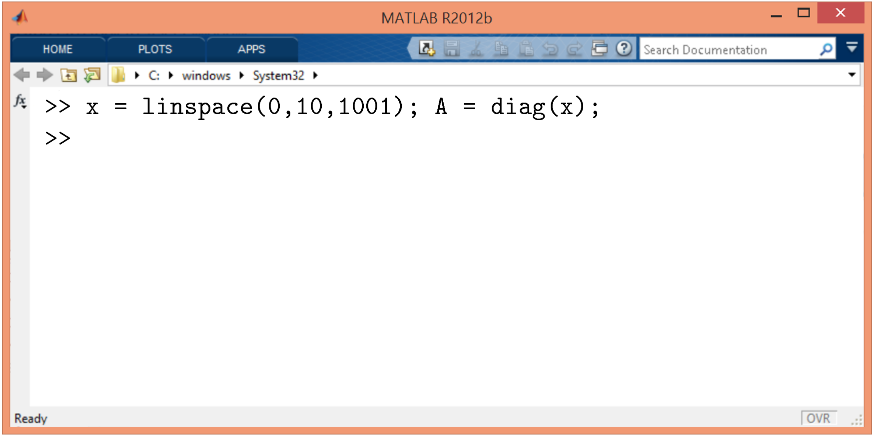

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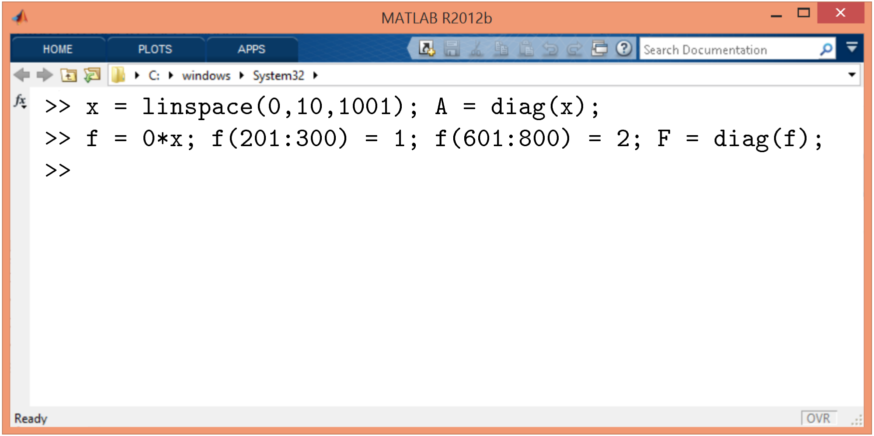

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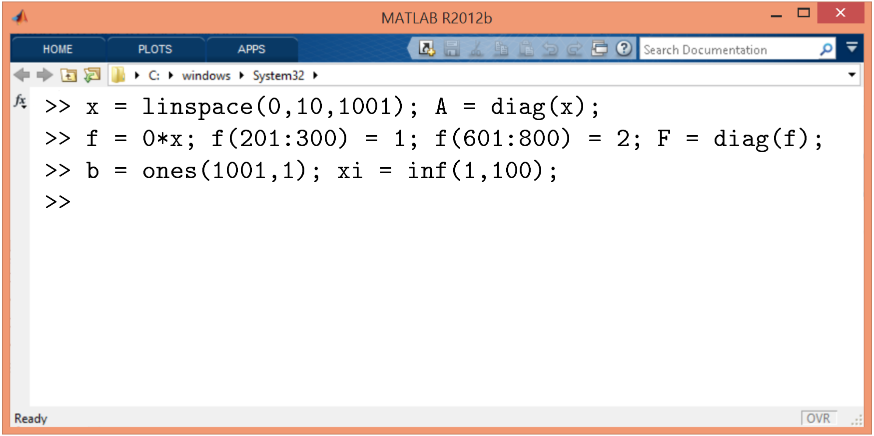

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>> f = 0*x; f(201:300) = 1; f(601:800) = 2; F = diag(f);
>> b = ones(1001,1); xi = inf(1,100);
>> param.k = -1; param.real = 1; param.reduction = 0;
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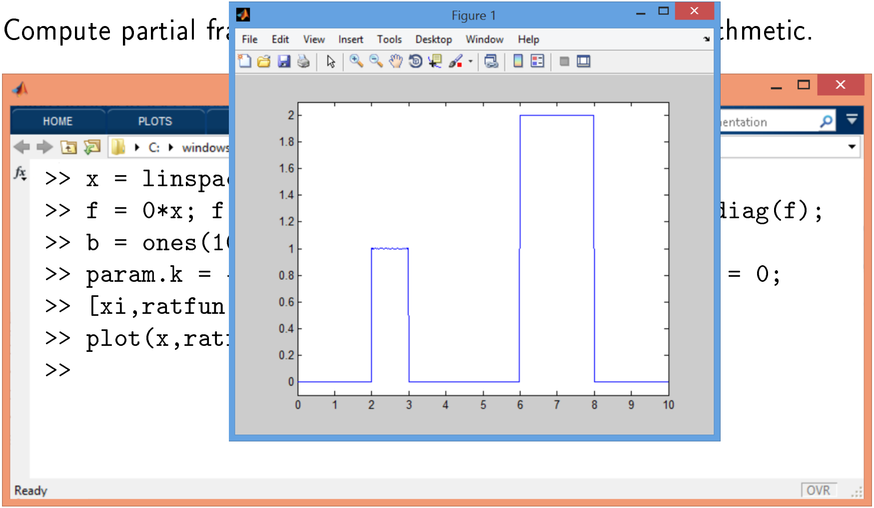

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>> [resid,xi,absterm,cnd] = residue(mp(ratfun));
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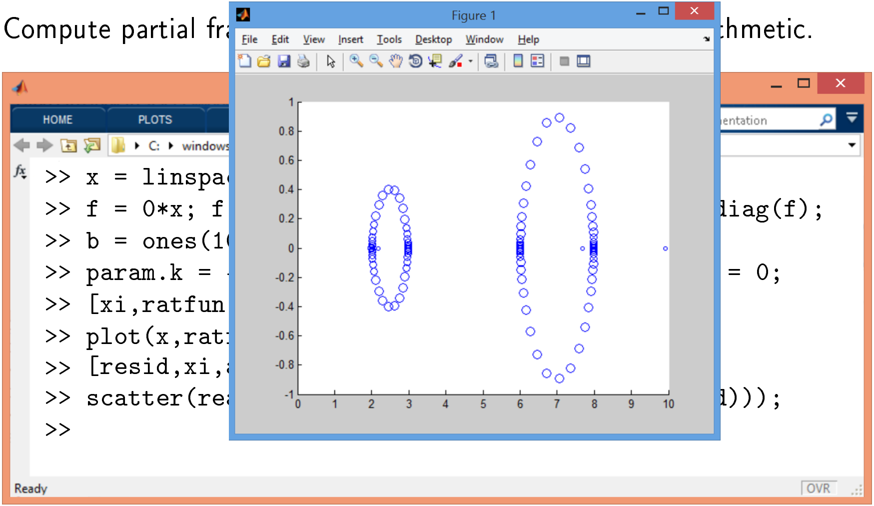

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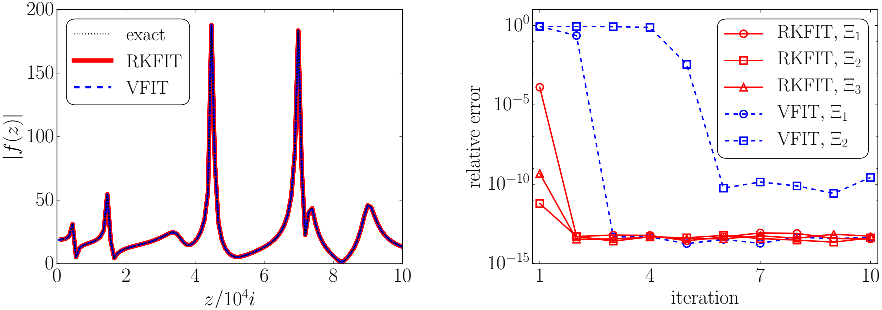
>> scatter(real(xi),imag(xi),64+4*log10(abs(resid)));
>> disp(cnd)
1.0165e+07
```

Example 1: Fitting a SISO transfer function

- $A = \text{diag}(1\text{i} \cdot \text{linspace}(-10^5, 10^5, 200))$
- $F = f(A)$, with a type $(19, 18)$ rational function $f(z) = \overline{f(\overline{z})}$
- comparing to vector fitting



- $\Xi_1 = \left[1\text{i} \cdot \text{logspace}(3, 5, 9), \quad -1\text{i} \cdot \text{logspace}(3, 5, 9)\ \right]$
- $\Xi_2 = \left[1\text{i} \cdot \text{logspace}(6, 9, 12), -1\text{i} \cdot \text{logspace}(6, 9, 12)\right]$
- $\Xi_3 = \left[\infty, \ldots, \infty\right], \quad |\Xi_3| = 18$

Example 2: Fitting multiple functions with common poles

Given $\{A, F^{[1]}, \ldots, F^{[k]}\} \subset \mathbb{C}^{N \times N}$ and a unit 2-norm vector $\mathbf{b} \in \mathbb{C}^N$.

Find rational functions $r_n^{[j]} = \dfrac{p_n^{[j]}}{q_n}$ with common denominator such that

$$\sum_{j=1}^{k} \|F^{[j]}\mathbf{b} - r_n^{[j]}(A)\mathbf{b}\|_2^2 \to \min.$$

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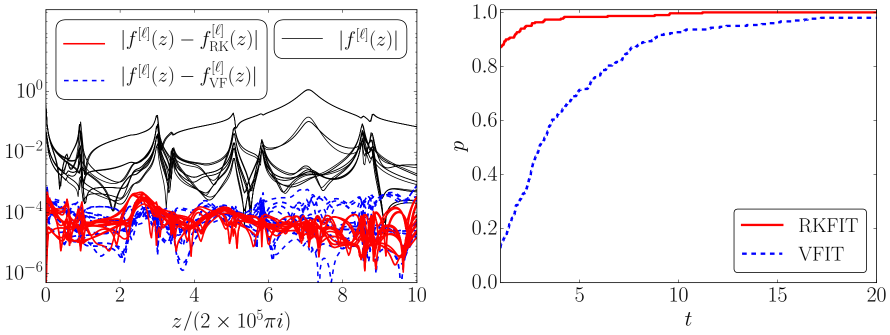
In pole reallocation step of RKFIT consider the SVD of

$$\begin{bmatrix} F^{[1]}V_{n+1} - V_{n+1}\left(V_{n+1}^* F^{[1]} V_{n+1}\right) \\ F^{[2]}V_{n+1} - V_{n+1}\left(V_{n+1}^* F^{[2]} V_{n+1}\right) \\ \vdots \\ F^{[k]}V_{n+1} - V_{n+1}\left(V_{n+1}^* F^{[k]} V_{n+1}\right) \end{bmatrix}.$$

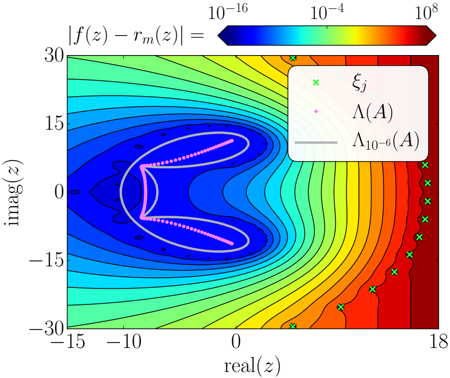
Example 2: Fitting a MIMO system

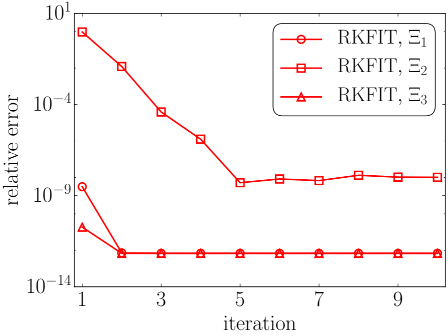
- Fitting all elements of the 3×3 transfer function of the ISS 1R problem from [Chahlaoui & Van Dooren 2002].
- $N = 300 + 300, \quad n = 50$
- $f^{[j]}(\overline{z}) = \overline{f^{[j]}(z)}, \quad j = 1, \ldots, 9$



Example 3: Exponential of a nonnormal matrix

- Given $A = -5 \cdot \text{grcar}(100, 3)$,
- $F = \exp(A)$ and $\mathbf{b} = [1, \ldots, 1]^T$,
- find $r_{16}(z)$ such that $\exp(A)\mathbf{b} \approx r_{16}(A)\mathbf{b}$.





$\Xi_1 = [0, 0, \ldots, 0]$ | $\Xi_2 = [-10, -10, \ldots, -10]$ | $\Xi_3 = [\infty, \infty, \ldots, \infty]$

Conclusions

- Matrix reformulation of rational least squares problem.
- Connection to rational Krylov spaces and pole selection problem.
- Implicit Q theorem allows for stable pole reallocation.
- RKFIT algorithm for solving nonlinear rational LS problem.
- RKFIT more general than vector fitting [Gustavsen/Semlyen 1999].
- RKFIT based on discrete orthogonal rational functions $\Rightarrow$ Robust?
- Convergence analysis? (Virtually none, neither for vector fitting.)
- Rational Krylov Toolbox: `www.rktoolbox.org`

M. Berljafa and S. Güttel, *Generalized rational Krylov decompositions with an application to rational approximation*, SIAM J. Matrix Anal. Appl., 36:894–916, 2015.

M. Berljafa and S. Güttel, *The RKFIT algorithm for nonlinear rational approximation*, SIAM J. Sci. Comput., accepted for publication in 2017.