(Multivariate) rootfinding via eigenvalues

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Joint work with Vanni Noferini (Aalto) and Alex Townsend (Cornell)
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Back to the roots seminar, KU Leuven

Bivariate rootfinding (zerofinding)

$f(x, y), g(x, y)$: bivariate functions $[-1, 1]^2 \to \mathbb{R}$

Problem: find pairs $(x_*, y_*) \in [-1, 1]^2$ s.t.

$$\begin{pmatrix} f(x_*, y_*) \\ g(x_*, y_*) \end{pmatrix} = 0$$

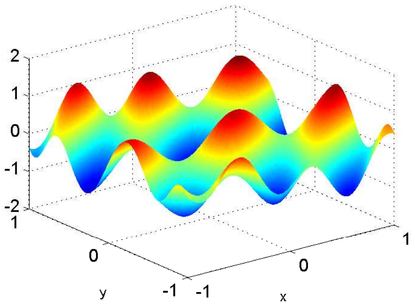
This talk (Part I): Chebfun2's `roots` [N.-Noferini-Townsend (15)]

- Speedup $O(n^6) \to\approx O(n^4)$, where n is polynomial degree
  - feasible degree: previously $n \approx 30$, now $n \approx 1000$
- Numerically stable solutions employing
  - Chebyshev interpolation via FFT
  - conditioning analysis $\Rightarrow$ local refinement for accuracy
  - stable eigensolver for polynomial eigenproblems

Bivariate rootfinding: applications

- Solving $f_x(x_*, y_*) = f_y(x_*, y_*) = 0$ gives critical points of f
  - Computing $\|f\|_\infty = \max_{x,y\in[-1,1]^2} |f(x,y)|$
  - Finding maximum/minimum values of f
- KKT conditions in optimization problems
  - e.g. ellipsoid distance, non-convex problems

$f(x, y)$



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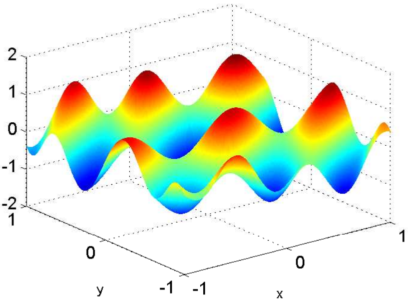
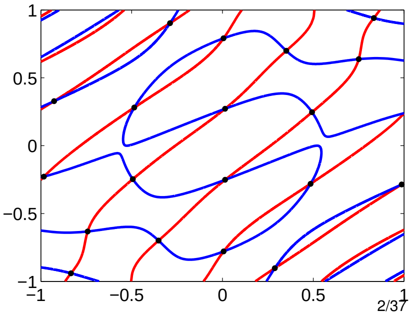


Curves $f_x(x,y) = 0, f_y(x,y) = 0$



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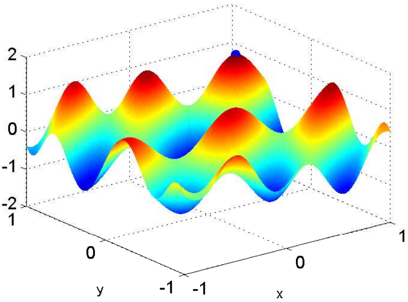

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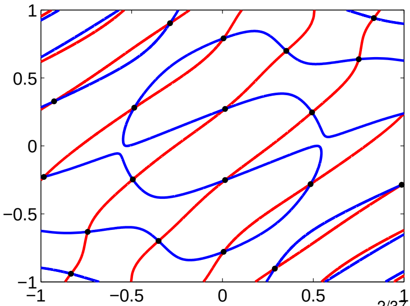


Rootfinding $f(x_*) = 0$ on $[-1, 1]$: principles

1. Approximate $f(x)$ with a polynomial $p(x)$: –[J. Boyd (02)]

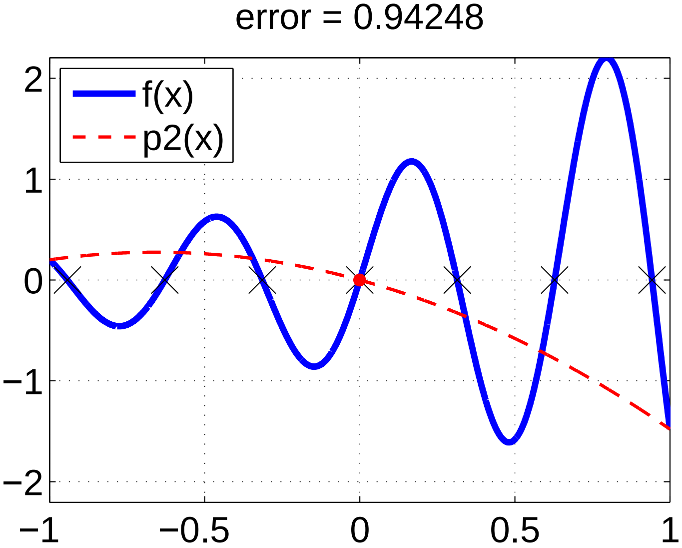
$$\|f(x) - p(x)\|_\infty = O(\epsilon)\|f(x)\|_\infty \quad \text{on} \quad [-1, 1]$$

2. Find roots of the polynomial $p(x)$ via generalized eigenvalues
– e.g. companion linearization for $p(x) = \sum_{i=0}^{n} a_i x^i$: $Yv = \lambda Xv$, where

$$(X, Y) = \left(\begin{bmatrix} a_n & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}, \begin{bmatrix} -a_{n-1} & -a_{n-2} & \dots & -a_0 \\ 1 & & & \\ & \ddots & & \\ & & 1 & \end{bmatrix} \right)$$

- The computed solutions $\widehat{x_*}$ are backward stable: $f(\widehat{x_*}) = O(\epsilon) \Leftrightarrow \tilde{f}(\widehat{x_*}) = 0$ for $\|f - \tilde{f}\|_\infty = O(\epsilon)$
- Applications: local extrema, comuting $|f(x)|$, sign$(f(x))$, $\|f\|_1 = \int_{-1}^{1} |f(x)| dx$, ...

Rootfinding $f(x) = 0$ on $[-1, 1]$: example



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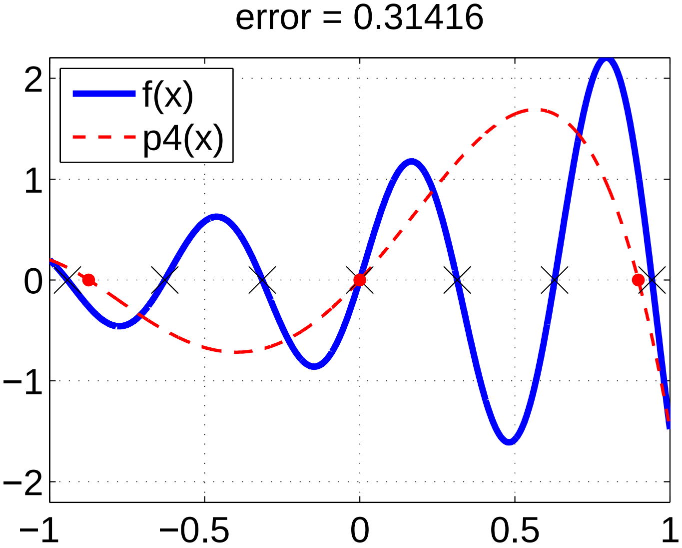

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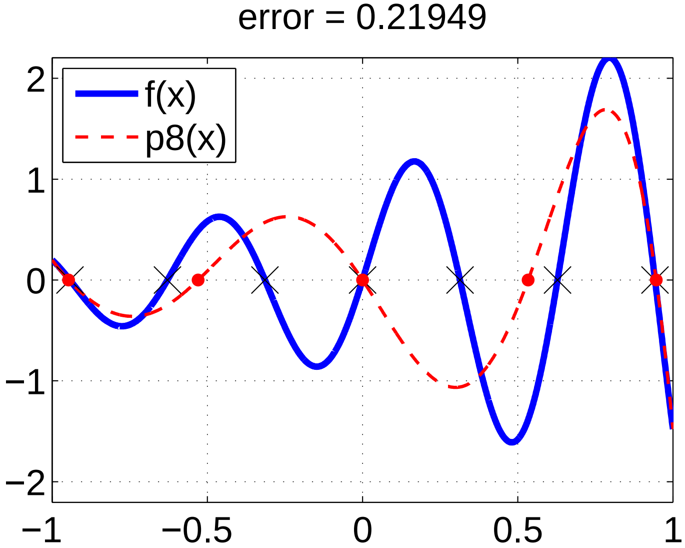

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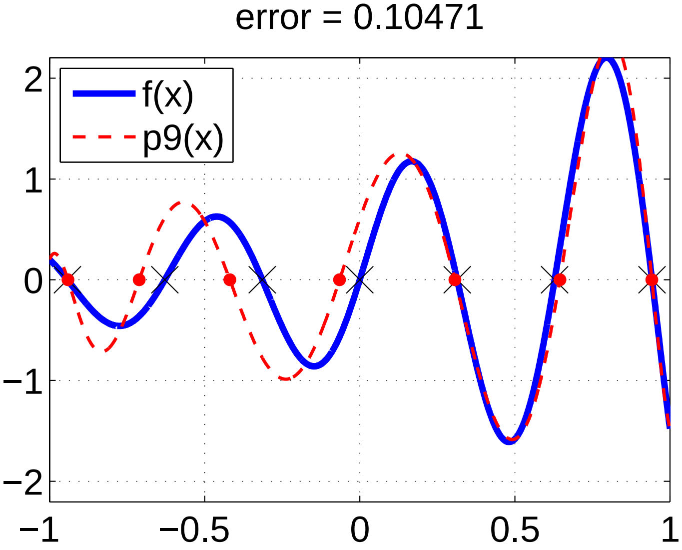

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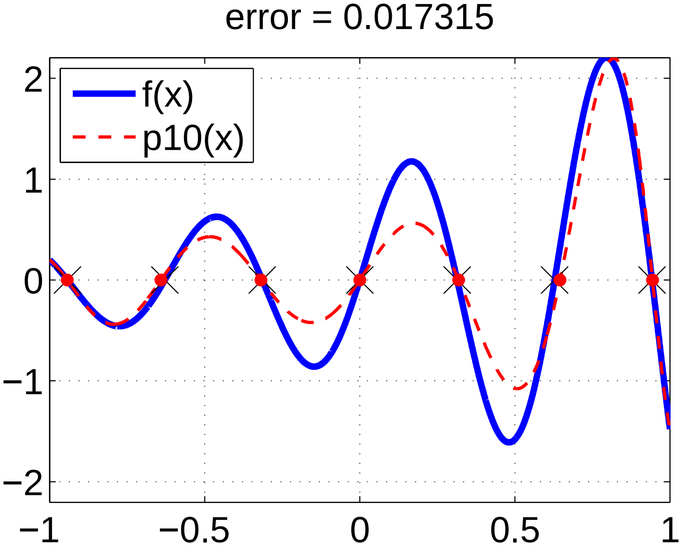

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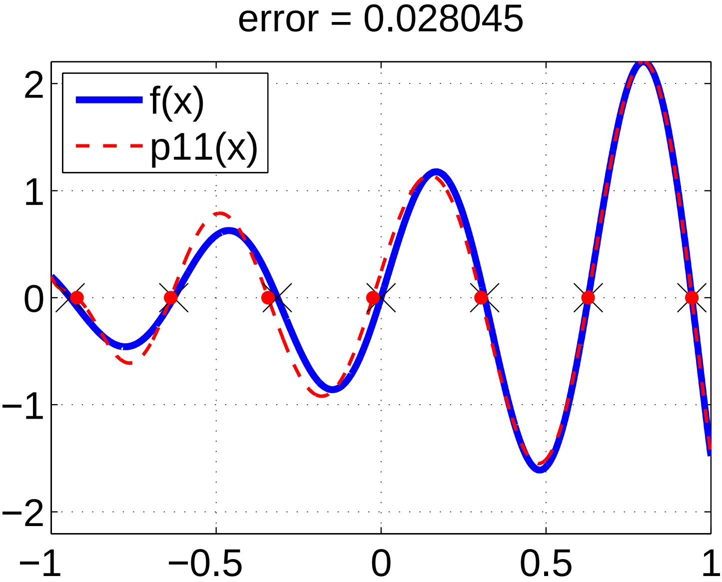

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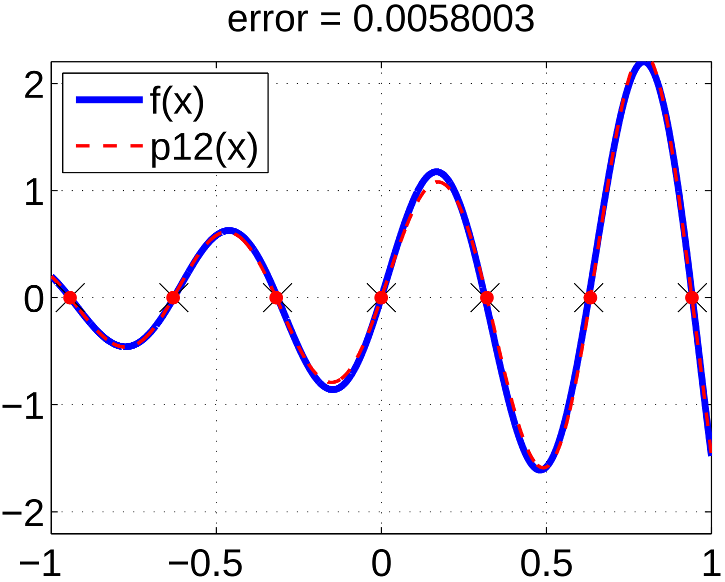

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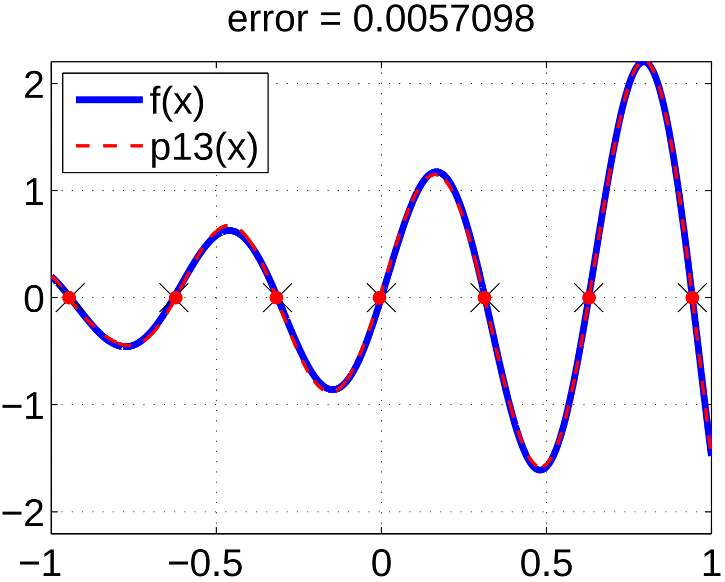

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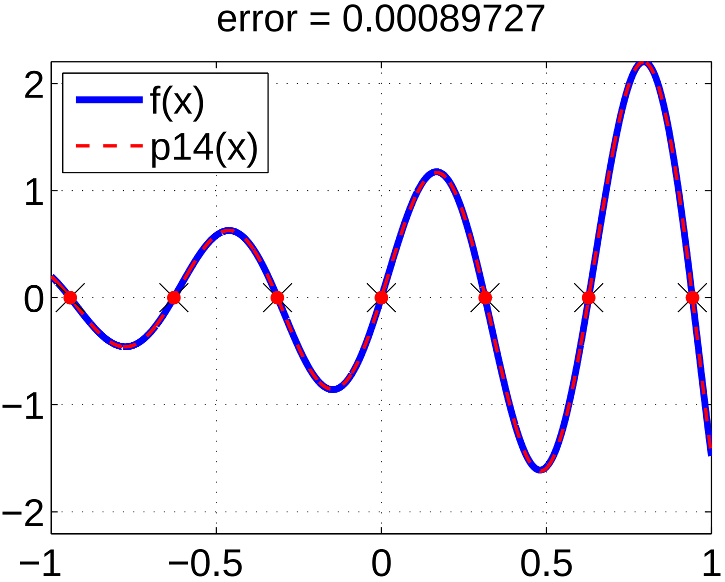

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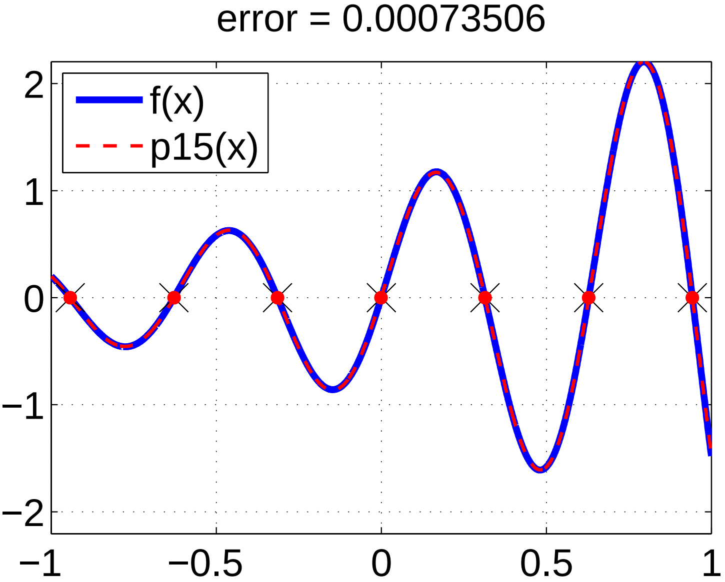

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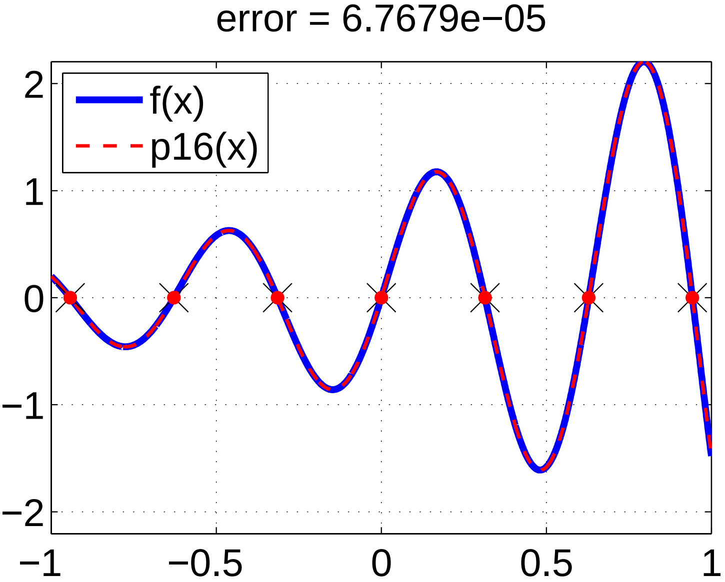

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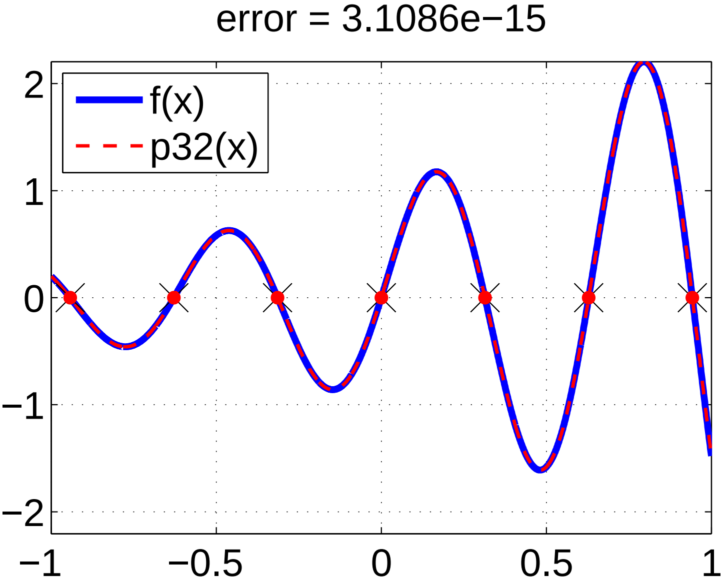

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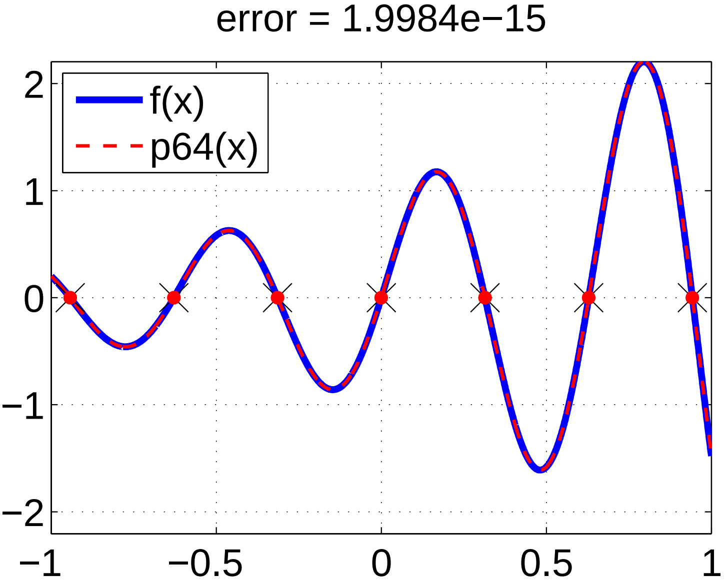

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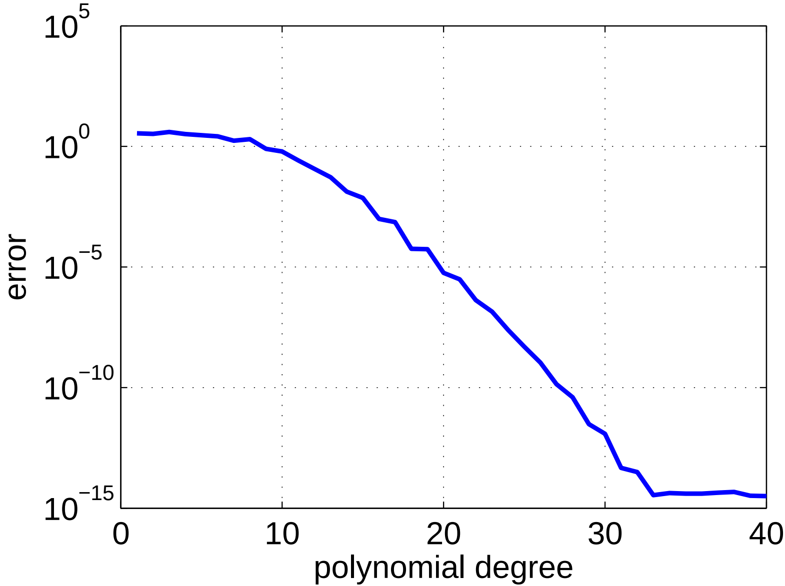
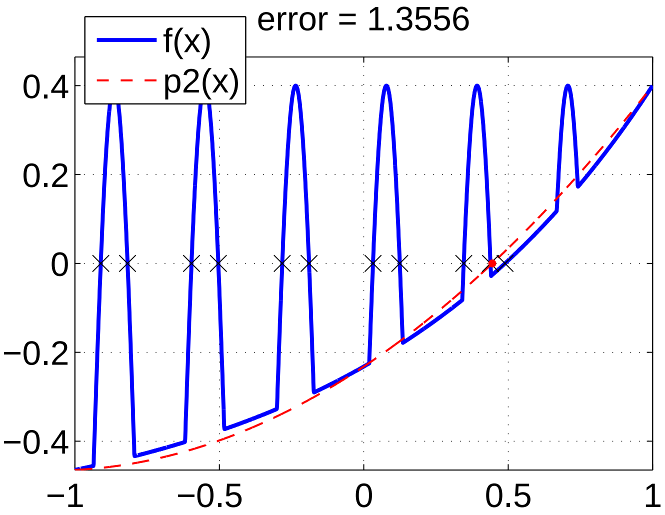


Rootfinding $f(x) = 0$ on $[-1, 1]$: zigzag example



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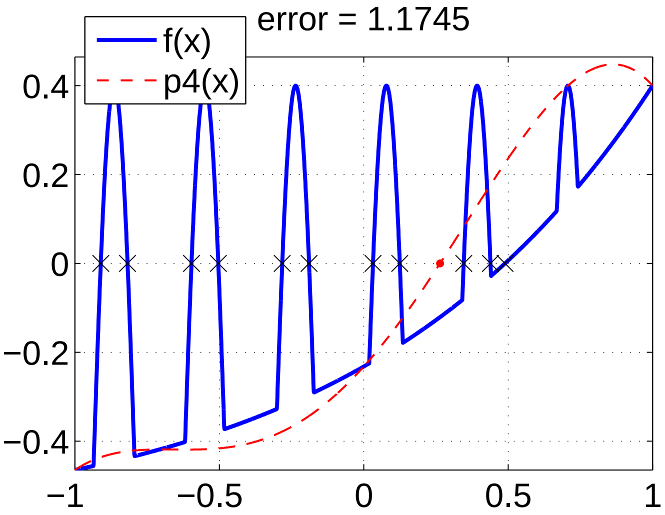

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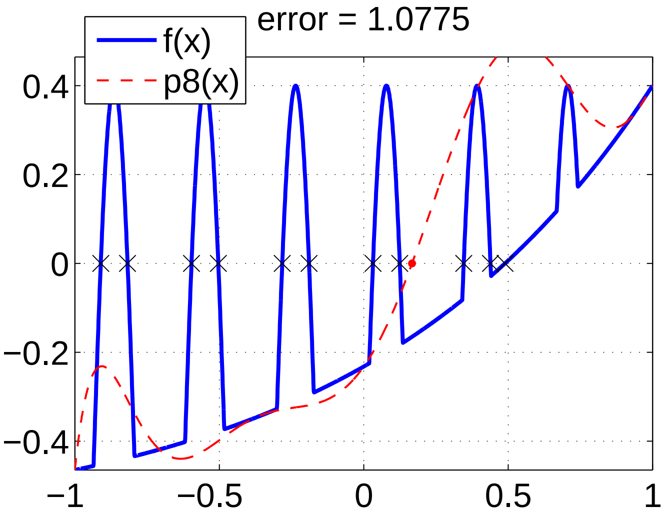

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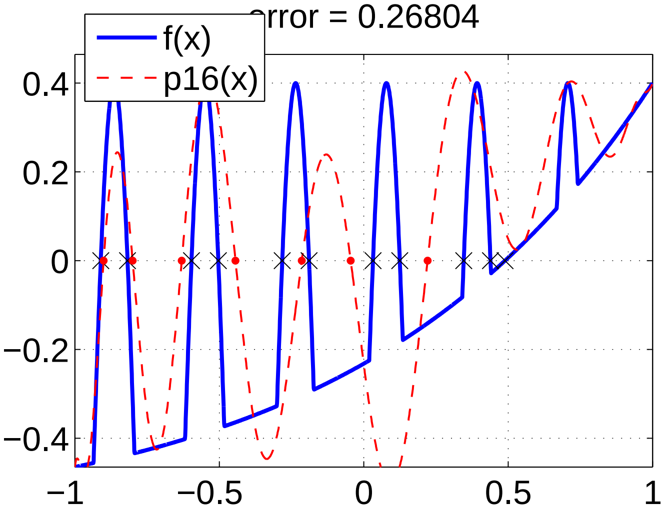

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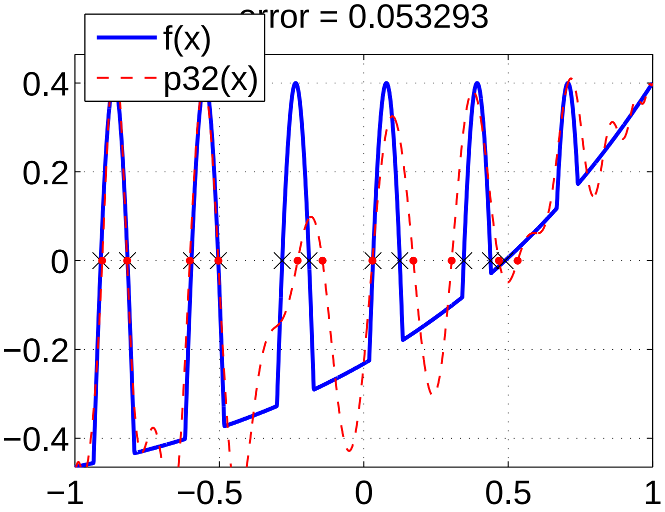

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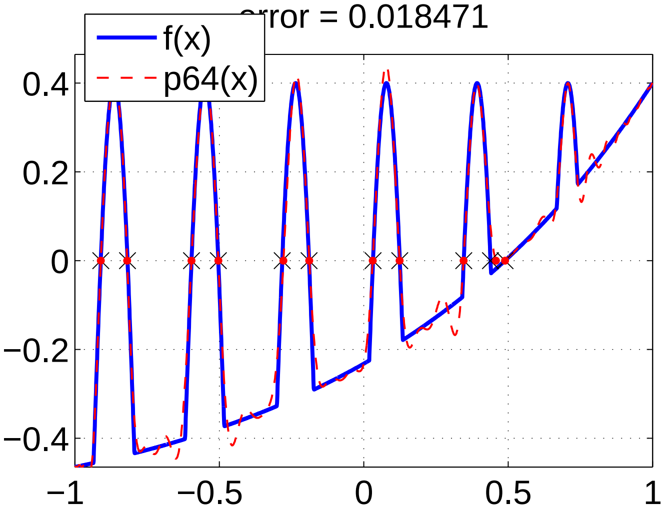

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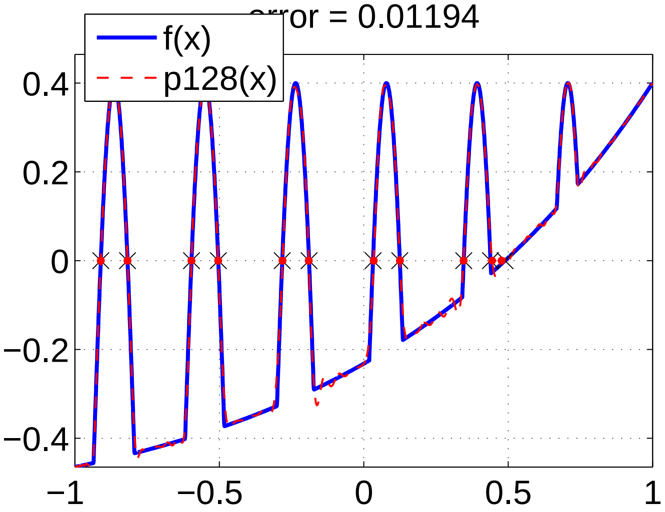

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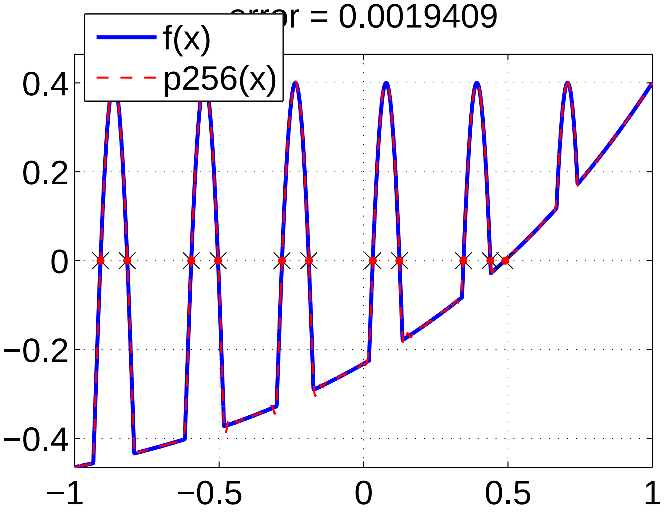

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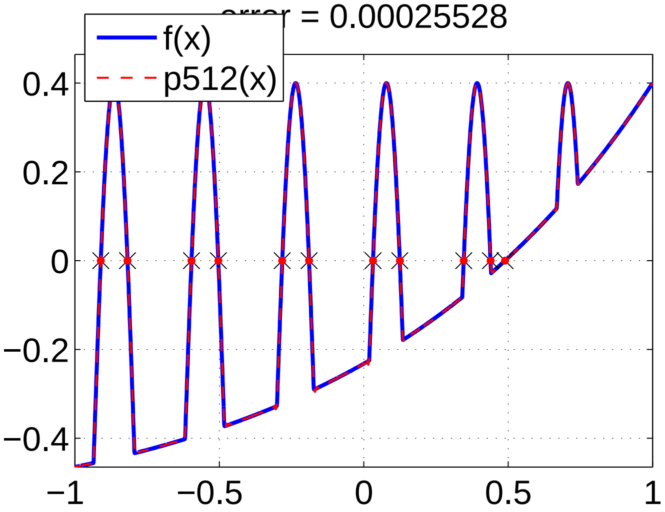

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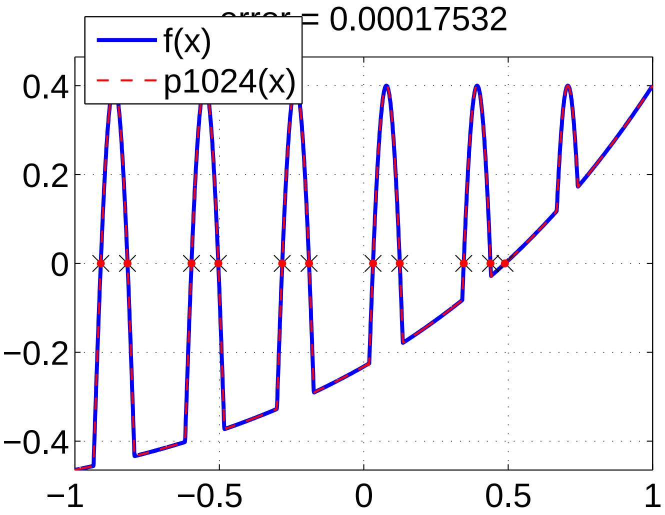

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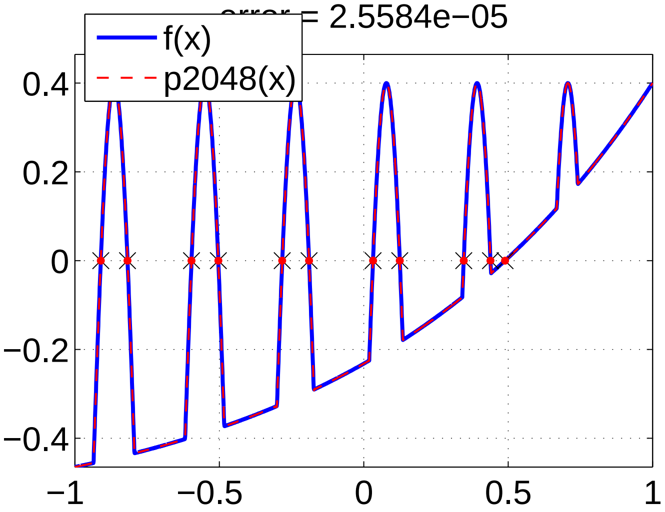

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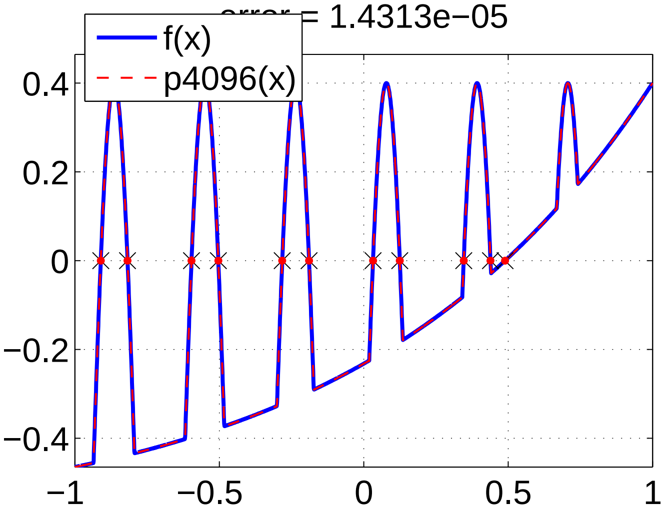

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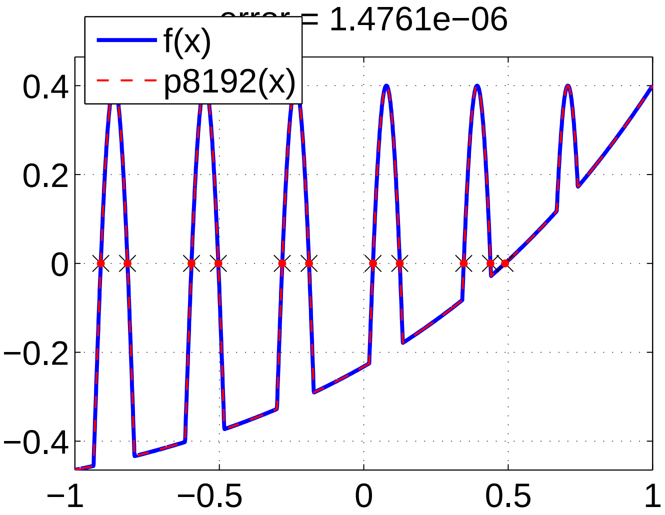

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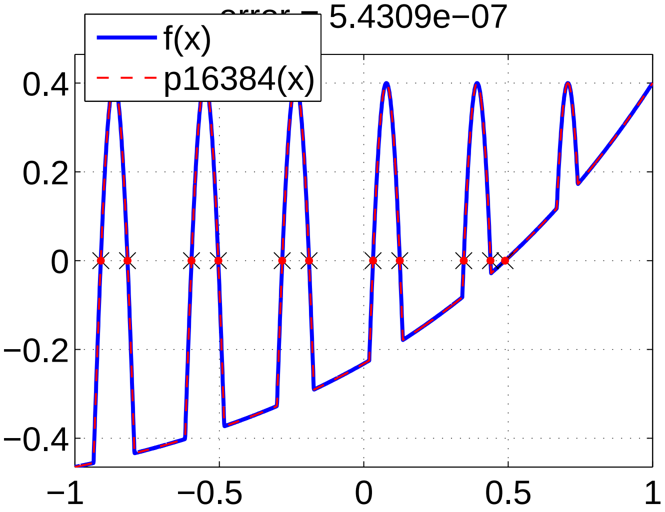

- High-degree polynomial approximation is accurate and stable

Recap: Rootfinding $f(x) = 0$ on $[-1, 1]$: principles

1. Approximate $f(x)$ with a polynomial $p(x)$:

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2. Find roots of $p(x)$ via generalized eigenvalues
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$$(X, Y) = \left(\begin{bmatrix} a_n & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}, \begin{bmatrix} -a_{n-1} & -a_{n-2} & \dots & -a_0 \\ 1 & & & \\ & \ddots & & \\ & & 1 & \end{bmatrix} \right)$$

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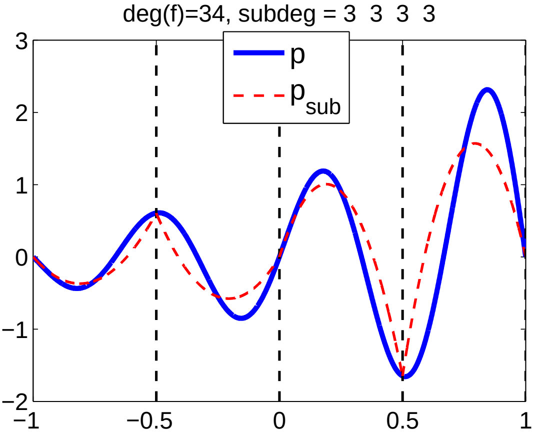
   – for p expressed in the Chebyshev basis $p(x) = \sum_{i=0}^{n} a_i T_i(x)$:

–[Good (61)]

$$(X, Y) = \left(\begin{bmatrix} a_n & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}, \frac{1}{2} \begin{bmatrix} -a_{n-1} & 1 - a_{n-2} & -a_{n-3} & \cdots & -a_0 \\ 1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 0 & 1 \\ & & & 2 & 0 \end{bmatrix} \right)$$

Solving $p_n(x) = 0$: subdivision for efficiency

- Finding $p_n(x) = 0$ via companion eigenvalues requires $O(n^3)$: dominant cost (recall interpolation is $O(n \log n)$)
- Remedy-Domain subdivision: Approximate $p_n(x)$ on smaller intervals with lower degree polynomials



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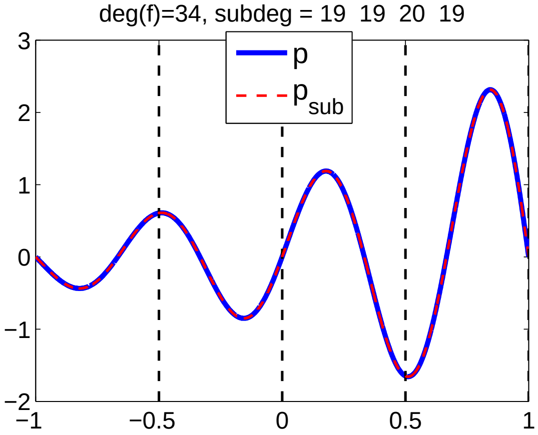


Bivariate rootfinding $f(x_*, y_*) = g(x_*, y_*) = 0$ on $[-1, 1]^2$

1. Approximate $f(x, y), g(x, y)$ with a bivariate polynomials $p(x, y), q(x, y)$ via e.g. 2D Chebyshev interpolation:

$$\|f(x, y) - p(x, y)\|_\infty = O(\epsilon)\|f(x, y)\|_\infty,$$
$$\|g(x, y) - q(x, y)\|_\infty = O(\epsilon)\|g(x, y)\|_\infty.$$

or often better: Chebfun2 [Townsend-Trefethen 13]

2. Find values of y_* via a polynomial eigenvalue problem using Bézout resultants

–[E. Bézout (1779)]

3. Find common roots of $p(x, y_*)$ and $q(x, y_*)$ via univariate rootfinding

Goal: Bivariate rootfinding of high degree

Problem: find (x_*, y_*) s.t.

$$\begin{pmatrix} p(x_*, y_*) \\ q(x_*, y_*) \end{pmatrix} = 0$$

where p, q are of degree n or less:

$$p(x,y) = \sum_{i=0}^{n} \sum_{j=0}^{n} P_{i,j} T_i(x) T_j(y), \ \ q(x,y) = \sum_{i=0}^{n} \sum_{j=0}^{n} Q_{i,j} T_i(x) T_j(y)$$

Conventionally: complexity $O(n^6)$ or worse + erroneous solutions

- reduce to $O(n^4)$ in practice
- maximum degree estimate

	max(n)	solution
Mathematica, Maple	20	$\mathbb{C}$
Our	100 ~ 2000	$\mathbb{R}$

Bézoutian of two univariate polynomials $p(x), q(x)$

$\mathcal{B}(p,q)$ is a bivariate polynomial

$$\mathcal{B}_{p,q}(s,t) = \frac{p(s)q(t) - p(t)q(s)}{s - t}$$

Express the coefficients using a symmetric matrix $B = (b_{ij})$:

$$\mathcal{B}_{p,q}(s,t) = \sum_{i,j=0}^{N-1} b_{ij} T_i(s) T_j(t).$$

- $\det B$ is the resultant of p, q:

$$\det B = \Pi_{i,j}(roots_{p_i} - roots_{q_j})$$

Theorem 1

p, q share a root $p(x_*) = q(x_*)$
$\Leftrightarrow$ B is singular with null space $[T_0(x_*), T_1(x_*), \ldots, T_{N-1}(x_*)]^T$
$\Leftrightarrow$ $\mathcal{B}_{p,q}(x_*, t) = \mathcal{B}_{p,q}(s, x_*) = 0$

Using $\mathcal{B}_{p,q}(s,t)$ for solving $p(x_*,y_*) = q(x_*,y_*) = 0$

1. Regard y as fixed in $p(x,y), q(x,y)$. $\mathcal{B}_{p,q}(s,t)$ is a bivariate polynomial

$$\mathcal{B}_{p,q}(s,t) = \frac{p_y(s)q_y(t) - p_y(t)q_y(s)}{s-t} = \sum_{i,j=0}^{N-1} b_{ij} T_i(s) T_j(t).$$

2. $B(y) = (b_{ij})$ is a matrix polynomial in y. Since $\det B(y) = 0$ iff $p_y(x), q_y(x)$ share a root, we can find y_* by solving

$$\det B(y) = 0,$$

resulting in a polynomial eigenvalue problem.

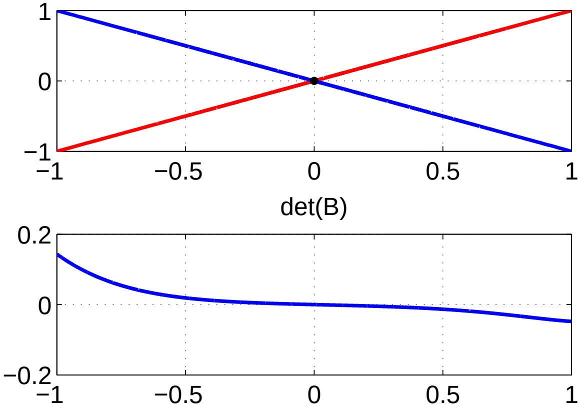
When $\deg(p_x, p_y, q_x, q_y)$ are all n, $B(y)$ is $n \times n$, degree $2n$

- Linearization is size $O(n^2) \Rightarrow \mathcal{O}(n^6)$ cost, infeasible for $n \gtrsim 50$
- Susceptible to numerical errors

$\mathcal{B}(p,q)$ for solving $p(x_*, y_*) = q(x_*, y_*) = 0$: examples

$$\mathcal{B}(p,q) = \frac{p_y(s)q_y(t) - p_y(t)q_y(s)}{s-t} = \sum_{i,j=0}^{N-1} b_{ij} T_i(s) T_j(t).$$

Let $B(y) = (b_{ij})$. We find y_* by solving $\det B(y) = 0$



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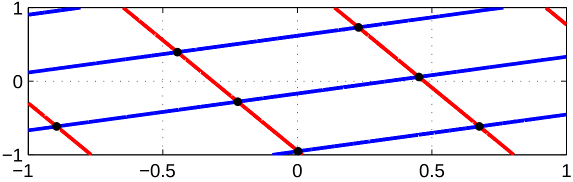
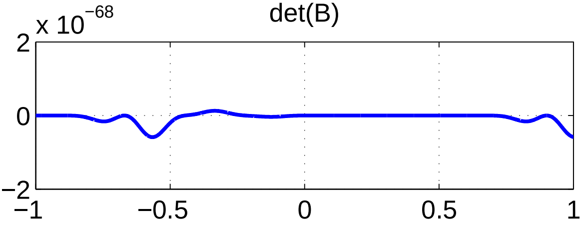
Let $B(y) = (b_{ij})$. We find y_* by solving $\det B(y) = 0$





Companion-like matrix in Chebyshev basis

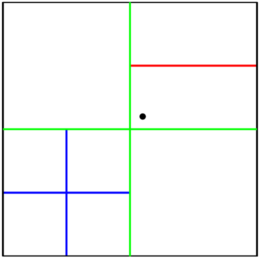
The colleague matrix pencil for a matrix polynomial $P(\lambda) = \sum_{i=0}^{M} A_i T_i(\lambda)$, $A_i \in \mathbb{R}^{N\times N}$ is

$$\lambda X + Y = \lambda \begin{bmatrix} A_M & & & \\ & I_N & & \\ & & \ddots & \\ & & & I_N \end{bmatrix} - \frac{1}{2} \begin{bmatrix} -A_{M-1} & I_N - A_{M-2} & -A_{M-3} & \cdots & -A_0 \\ I_N & 0 & I_N & & \\ & \ddots & \ddots & \ddots & \\ & & I_N & 0 & I_N \\ & & & 2I_N & 0 \end{bmatrix}.$$

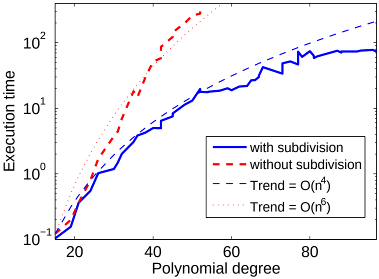
- Eigenvalues λ_* s.t. $\det P(\lambda_*) = 0$ satisfy $\det(\lambda_* X + Y) = 0$: generalized eigenvalue problem
- Other (infinitely many) linearizations available

Domain subdivision for efficiency (+stability)

- subdivide in x or/and y until the polynomial interpolants have degree 16 or less
- complexity typically $O(n^6) \to O(n^4)$



Subdivision for
$f = \sin((x - 1/10)y)\cos(1/(x + (y - 9/10) + 5)) = 0,$
$g = (y - 1/10)\cos((x + (y + 9/10)^2/4)) = 0.$



$\sin(\omega(x + y)) = \cos(\omega(x - y)) = 0$, where $\omega = 1, \ldots, 50$ (up to 20 without subdivision).

Conditioning of original problem

Suppose

- $p(x_*, y_*) = q(x_*, y_*) = 0$, $\|p\|_\infty = \|q\|_\infty = 1$
- for perturbed $\hat{p} = p + \delta p$, $\hat{q} = q + \delta q$, $\hat{p}(\hat{x}, \hat{y}) = \hat{q}(\hat{x}, \hat{y}) = 0$ for $(\hat{x}, \hat{y}) = (x_* + \delta x, y_* + \delta y)$

Then to first order in $\delta p, \delta q$,

$$0 = \begin{bmatrix} \hat{p}(\hat{x}, \hat{y}) \\ \hat{q}(\hat{x}, \hat{y}) \end{bmatrix} = \begin{bmatrix} \partial_x p(x_*, y_*) & \partial_y p(x_*, y_*) \\ \partial_x q(x_*, y_*) & \partial_y q(x_*, y_*) \end{bmatrix} \begin{bmatrix} \delta x \\ \delta y \end{bmatrix} + \begin{bmatrix} \delta p(\hat{x}, \hat{y}) \\ \delta q(\hat{x}, \hat{y}) \end{bmatrix}.$$

– A stable solution has error of size $O(\kappa_* u)$, where κ_* is the absolute condition number

$$\kappa_* = \lim_{\epsilon \to 0^+} \sup \left\{ \frac{1}{\epsilon} \min \left\| \begin{bmatrix} \delta x \\ \delta y \end{bmatrix} \right\|_2 : \hat{p}(\hat{x}, \hat{y}) = \hat{q}(\hat{x}, \hat{y}) = 0, \|\hat{p} - p\|_\infty \le \epsilon, \|\hat{q} - q\|_\infty \le \epsilon \right\},$$

It follows that $\kappa_* = \left\| \begin{bmatrix} \partial_x p(x_*, y_*) & \partial_y p(x_*, y_*) \\ \partial_x q(x_*, y_*) & \partial_y q(x_*, y_*) \end{bmatrix}^{-1} \right\|_2 := \|J^{-1}\|_2$, where J is the Jacobian matrix

Conditioning of our formulation: Bézout eigenproblem

The error in the computed eigenvalues of $B(y)$ is bounded by (conditioning)·(backward error), where the conditioning is

$$\kappa(y_*, B) = \lim_{\epsilon \to 0^+} \sup \left\{ \frac{1}{\epsilon} \min |\hat{y} - y_*| : \det \hat{B}(\hat{y}) = 0, \|B - \hat{B}\| \leq \epsilon \right\},$$

Theorem 2

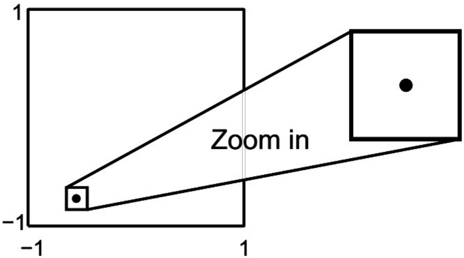
$$\frac{\kappa_*}{\left\| \begin{bmatrix} \partial_y q & -\partial_y p \\ -\partial_x q & \partial_x p \end{bmatrix} \right\|_2} \leq \kappa(y_*, B) \leq \frac{\kappa_* n}{\left\| \begin{bmatrix} \partial_y q & -\partial_y p \\ -\partial_x q & \partial_x p \end{bmatrix} \right\|_2}$$

- $\kappa_* \gg k_*$ (unstable) if $\mathrm{adj}(J) = \begin{bmatrix} \partial_y q & -\partial_y p \\ -\partial_x q & \partial_x p \end{bmatrix}$ is small

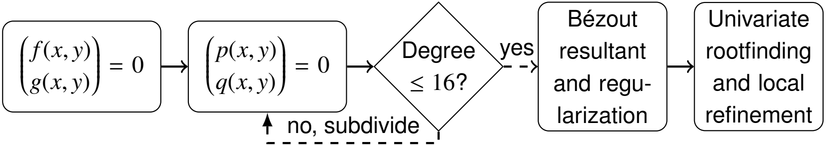
Local refinement for accuracy

$$\frac{\kappa_*}{\left\|\begin{bmatrix} \partial_y q & -\partial_y p \\ -\partial_x q & \partial_x p \end{bmatrix}\right\|_2} \leq \kappa(y_*, B) \leq \frac{\kappa_* n}{\left\|\begin{bmatrix} \partial_y q & -\partial_y p \\ -\partial_x q & \partial_x p \end{bmatrix}\right\|_2}$$

- (Bézout conditioning) $\gg$ (original conditioning) if derivatives are small: $|\partial p| \ll \|p\|_\infty$ and/or $|\partial q| \ll \|q\|_\infty$
- Remedy- Local refinement: very small region in which $\|p\|_\infty = O(|\partial p|), \|q\|_\infty = O(|\partial q|)$ (after scaling to $[-1, 1]^2$)



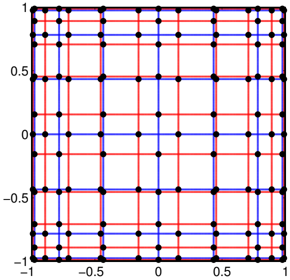
Flowchart



- dominant cost: Bézout polynomial eigenproblem
- choose first variable (hidden in Bézoutian) x or y from the size of the generalized eigenproblem (colleague linearization)
- multiple eigenvalues (e.g. solutions at (x_1, y_0), (x_2, y_0)) do not cause instability
  - Defective eigenvalues are indeed ill-conditioned
  - Non-defective eigenvalues are as well-conditioned as simple eigenvalues

Experiments

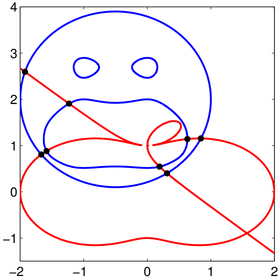
Coordinate alignment



$$(m_p, n_p, m_q, n_q) = (20, 20, 24, 30)$$

$$\begin{pmatrix} T_7(x)T_7(y)\cos(xy) \\ T_{10}(x)T_{10}(y)\cos(x^2y) \end{pmatrix} = 0$$

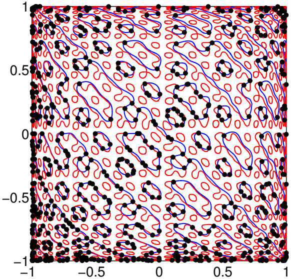
Face and apple



$$(m_p, n_p, m_q, n_q) = (10, 18, 8, 8)$$

Experiments-2

Hadamard

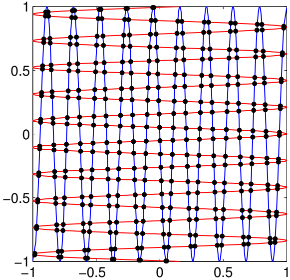


$$(m_p, n_p, m_q, n_q) = (31, 31, 63, 63)$$

$$f(x_i, x_j) = H_{32}(i, j),$$

$$g(x_i, x_j) = H_{64}(i, j)$$

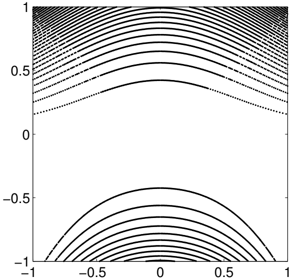
Travelling waves



$$(m_p, n_p, m_q, n_q) = (7, 63, 62, 6)$$

Experiments-3

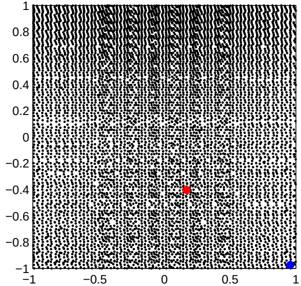
Airy



$$(m_p, n_p, m_q, n_q) = (171, 120, 569, 568)$$

$$\begin{pmatrix} \mathrm{Ai}(-13(x^2y + y^2)))) \\ J_0(500x)y + xJ_1(500y) \end{pmatrix} = 0$$

SIAM 100-Digit Challenge problem



$$(m_p, n_p, m_q, n_q) = (1781, 1204, 1781, 1204)$$

$$f(x, y) = \left(\frac{x^2}{4} + e^{\sin(100x)} + \sin(140\sin(x))\right) + \left(\frac{y^2}{4} + \sin(120e^y) + \sin(\sin(160y))\right)$$

Part I (bivariate rootfinding) Summary and future work

Summary:

- Algorithm for common zeros of two bivariate functions via Bézout resultant
- Improvements to solve polynomial interpolants of high degree up to 2000:
  - Domain subdivision for speed
  - Local refinement for resolving conditioning + removing spurious solutions

Future work:

- Trivariate (multivariate) zerofinding (many unsuccessful attempts)
- Non-analytic functions (singularities, poles,...)
- Finding appropriate initial domain in applications

Part II-a: The AAA algorithm for rational approximation

[N.-Sète-Trefethen (18)] Given $f(Z)$, $Z = \{Z_i\}_{i=1}^{M}$, find rational function r s.t.

$$\boxed{f(Z) \approx r(Z)}$$

- rationals outperform polynomials when f nonsmooth

Key ideas in AAA:

- Barycentric representation of rational functions

$$f(z) \approx r(z) = \frac{N(z)}{D(z)} = \sum_{j=0}^{n} \frac{\beta_j f_j}{z - t_j} \bigg/ \sum_{j=0}^{n} \frac{\beta_j}{z - t_j}$$

- Adaptive selection of support points, hence basis functions
- Least-squares fitting

Part II-a: The AAA algorithm for rational approximation

[N.-Sète-Trefethen (18)] Given $(f(Z), Z = \{Z_i\}_{i=1}^{M}) \leftarrow f$, find rational function r s.t.

$$\boxed{(f(Z) \approx r(Z)) \leftarrow f \approx r}$$

- rationals outperform polynomials when f nonsmooth

Key ideas in AAA:

- Barycentric representation of rational functions
  $f(z) \approx r(z) = \frac{N(z)}{D(z)} = \sum_{j=0}^{n} \frac{\beta_j f_j}{z - t_j} \Big/ \sum_{j=0}^{n} \frac{\beta_j}{z - t_j}$
- Adaptive selection of support points, hence basis functions
- Least-squares fitting

The (standard) AAA algorithm

Given sample points $\{Z_i\}_{i=1}^{M}$,

$$f(z) \approx r(z) = \frac{N(z)}{D(z)} = \sum_{j=0}^{n} \frac{\beta_j f_j}{z - t_j} \Bigg/ \sum_{j=0}^{n} \frac{\beta_j}{z - t_j}$$

---

1. $n \leftarrow n + 1$, add support point $t_n \in Z$,
2. Solve via SVD $\min_{\|\beta\|_2=1} \left\| \begin{bmatrix} \frac{f(Z_1^{(n)})-f_0}{Z_1^{(n)}-t_0} & \cdots & \frac{f(Z_1^{(n)})-f_n}{Z_1^{(n)}-t_n} \\ \vdots & \ddots & \vdots \\ \frac{f(Z_M^{(n)})-f_0}{Z_M^{(n)}-t_0} & \cdots & \frac{f(Z_M^{(n)})-f_n}{Z_M^{(n)}-t_n} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \vdots \\ \beta_n \end{bmatrix} \right\|$

Key idea: choice of support points $\{t_j\}$

Desiderata:

- Approximation error $\|f - r\|$ decreases
- “Basis matrix” $C_{ij} = \frac{1}{Z_i^n - t_j}$ well conditioned

Choice of support points $\{t_j\}$

$$f(z) \approx r(z) = \frac{N(z)}{D(z)} = \sum_{j=0}^{n} \frac{\beta_j f_j}{z - t_j} \Bigg/ \sum_{j=0}^{n} \frac{\beta_j}{z - t_j}, \qquad z \in Z^{(n)}$$

- Error after n steps: $e_n(z) := f(z) - r(z)$
- Greedy choice: take $t_{n+1} :=$ argmax$_{z \in Z}|e(z)|$
  - then $e_{n+1}(t_{n+1}) = 0$: interpolation property
- Basis $\{\frac{1}{z-t_j}\}$ chosen adaptively, depending on f

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Desiderata:

- Approximation error $\|f - r\|$ decreases
  - $\surd$ largest error position$\mapsto 0$
- "Basis matrix" $C_{ij} = \frac{1}{Z_i^n - t_j}$ well conditioned
  - $\surd$ 'localization'

Sample points in AAA

In standard AAA, the sample points Z are given in advance.

- Often, equispaced or randomly drawn points in domain
- Often $|Z| \gg n$, e.g. $|Z| = 10^4$ where degree $n \leq 100$
  (overkill? Issue when f is expensive to sample)
- When f has singularities (e.g. $f(x) = |x|$), need to cluster sample points exponentially near them (but their location is often **unknown**)

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Question: Can we automate the choice of sample points?

- Idea: Use support points to guide where more samples are needed
- Roughly: Sample three additional points between support points

Please see [Driscoll-N.-Trefethen (SISC, to appear)] for details (or chat later)

Part II-b: roots of rational functions via eigenvalues

$$r(x) = p(x) + \frac{p_1(x)}{q_1(x)} + \frac{p_2(x)}{q_2(x)} + \cdots \frac{p_n(x)}{q_n(x)}$$

- barycentric form $r(z) = \frac{N(z)}{D(z)} = \sum_{j=0}^{n} \frac{\beta_j f_j}{z-t_j} \Big/ \sum_{j=0}^{n} \frac{\beta_j}{z-t_j}$, partial fraction, continued fraction

Goal: compute the roots x_0 of r s.t. $r(x_0) = 0$

- Bisection, Newton etc...
  - unclear how to verify all roots are computed
- "polynomialization": compute roots of polynomial $r(x) \prod_{i=1}^{n} q_i(x)$ via linearization
  - taking product can cause numerical issues

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- "polynomialization": compute roots of polynomial $r(x)\prod_{i=1}^{n} q_i(x)$ via linearization
  - taking product can cause numerical issues
- This work: linearization without polynomializing
  - avoids numerical issues + easier to construct (Frobenius-style)

Companion linearization: monomial basis x^i

$$p(x) = x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0$$

The companion linearization is

$$C = \begin{bmatrix} -a_{n-1} & -a_{n-2} & \dots & -a_0 \\ 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}$$

- $\text{eig}(C) = \text{roots}(p)$

Colleague linearization: Chebyshev basis $T_i(x)$

$$p(x) = T_n(x) + a_{n-1}T_{n-1}(x) + \cdots + a_1T_1(x) + a_0T_0(x)$$

$T_i(x)$: Chebyshev polynomial

$$C = \frac{1}{2}\begin{bmatrix} -a_{n-1} & 1-a_{n-2} & -a_{n-3} & \cdots & -a_0 \\ 1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 0 & 1 \\ & & & 2 & 0 \end{bmatrix}$$

- eig(C) = roots(p)

Comrade linearization: orthogonal polynomial basis $\phi_i(x)$

$$p(x) = \phi_n(x) + a_{n-1}\phi_{n-1}(x) + \cdots + a_1\phi_1(x) + a_0\phi_0(x)$$

$\phi_i(x)$: orthogonal polynomial with recurrence

$$x\phi_i(x) = \alpha_i\phi_{i+1}(x) + \beta_i\phi_i(x) + \gamma_i\phi_{i-1}(x)$$

$$C = \begin{bmatrix} \beta_{n-1} - a_{n-1} & \gamma_{n-1} - a_{n-2} & -a_{n-3} & \cdots & -a_0 \\ \alpha_{n-2} & \beta_{n-2} & \gamma_{n-2} & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha_1 & \beta_1 & \gamma_1 \\ & & & \alpha_0 & \beta_0 \end{bmatrix}$$

- eig(C) = roots(p)
- Other extensions known: confederate (degree graded), congenial (degree bounded)..., trigonometric polynomials $c + \sum_{i=1}^{k}(a_k \sin kx + b_k \cos kx)$ [Boyd 2013]

Companion-like linearizations: how?

$$p(x) = x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0$$

For $p(\lambda) = 0$,

$$\begin{bmatrix} -a_{n-1} & -a_{n-2} & \dots & -a_0 \\ 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix} \begin{bmatrix} \lambda^{n-1} \\ \lambda^{n-2} \\ \vdots \\ 1 \end{bmatrix} = \lambda \begin{bmatrix} \lambda^{n-1} \\ \lambda^{n-2} \\ \vdots \\ 1 \end{bmatrix}$$

- Bottom $n-1$ rows: $\lambda^i = \lambda^{i-1} \cdot \lambda$
- First row: $p(x) = 0$

Companion-like linearizations: how?

$$p(x) = T_n(x) + a_{n-1}T_{n-1}(x) + \cdots + a_1T_1(x) + a_0T_0(x)$$

For $p(\lambda) = 0$,

$$\frac{1}{2}\begin{bmatrix} -a_{n-1} & 1 - a_{n-2} & -a_{n-3} & \cdots & -a_0 \\ 1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 0 & 1 \\ & & & 2 & 0 \end{bmatrix} \begin{bmatrix} T_{n-1}(\lambda) \\ T_{n-2}(\lambda) \\ \vdots \\ T_0(\lambda) \end{bmatrix} = \lambda \begin{bmatrix} T_{n-1}(\lambda) \\ T_{n-2}(\lambda) \\ \vdots \\ T_0(\lambda) \end{bmatrix}$$

- Bottom $n-1$ rows: $\frac{1}{2}(T_i(\lambda) + T_{i-2}(\lambda)) = T_{i-1}(\lambda) \cdot \lambda$
- First row: $p(\lambda) = 0$

Companion-like linearizations: how?

$$p(x) = \phi_n(x) + a_{n-1}\phi_{n-1}(x) + \cdots + a_1\phi_1(x) + a_0\phi_0(x)$$

$\phi_i(x)$: orthogonal polynomial with recurrence

$$x\phi_i(x) = \alpha_i\phi_{i+1}(x) + \beta_i\phi_i(x) + \gamma_i\phi_{i-1}(x)$$

For $p(\lambda) = 0$,

$$\begin{bmatrix} \beta_{n-1} - a_{n-1} & \gamma_{n-1} - a_{n-2} & -a_{n-3} & \cdots & -a_0 \\ \alpha_{n-2} & \beta_{n-2} & \gamma_{n-2} & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha_1 & \beta_1 & \gamma_1 \\ & & & \alpha_0 & \beta_0 \end{bmatrix} \begin{bmatrix} \phi_{n-1}(\lambda) \\ \phi_{n-2}(\lambda) \\ \vdots \\ \phi_0(\lambda) \end{bmatrix} = \lambda \begin{bmatrix} \phi_{n-1}(\lambda) \\ \phi_{n-2}(\lambda) \\ \vdots \\ \phi_0(\lambda) \end{bmatrix}$$

- Bottom $n-1$ rows: $\lambda\phi_i(\lambda) = \alpha_i\phi_{i+1}(\lambda) + \beta_i\phi_i(\lambda) + \gamma_i\phi_{i-1}(\lambda)$
- First row: $p(\lambda) = 0$

Linearization for rational function in partial fraction form

$$r(x) = p(x) + \sum_{i=1}^{n} \frac{r_i}{(x - \gamma_i)}$$

$p(x) = x^d + a_{d-1}x^{d-1} + \cdots + a_1 x + a_0$: polynomial

Note: includes root/polefinding for barycentric $r(z) = \sum_{j=0}^{n} \frac{\beta_j f_j}{z-t_j} \Big/ \sum_{j=0}^{n} \frac{\beta_j}{z-t_j}$,

$$(Cy =) \begin{bmatrix} -a_{d-1} & -a_{d-2} & \ldots & -a_0 & -r_1 & -r_2 & \ldots & r_n \\ 1 & & & & & & & \\ & 1 & & & & & & \\ & & \ddots & & & & & \\ & & & 1 & \gamma_1 & & & \\ & & & 1 & & \gamma_2 & & \\ & & & \vdots & & & \ddots & \\ & & & 1 & & & & \gamma_n \end{bmatrix} y = \lambda y, \qquad y = \begin{bmatrix} \lambda^{d-1} \\ \vdots \\ 1 \\ \frac{1}{\lambda-\gamma_1} \\ \frac{1}{\lambda-\gamma_2} \\ \vdots \\ \frac{1}{\lambda-\gamma_n} \end{bmatrix}$$

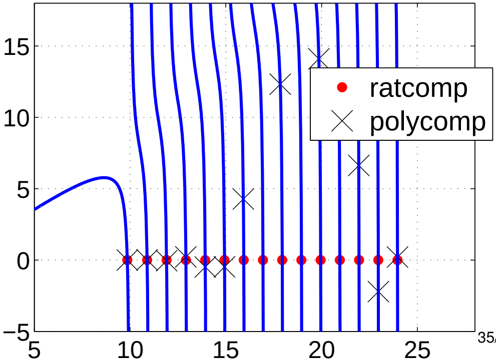
- eig(C) = roots(r) [Saad, El-Guide, Miedlar (19)]
- bottom rows: $1 + \frac{\gamma_i}{\lambda-\gamma_i} = \frac{1}{\lambda-\gamma_i} \cdot \lambda$

Example: 'Perfidious rational function'

$$r(x) = x + \sum_{i=1}^{15} \frac{1}{x-9-i}$$

- Polynomialize: $p(x) = r(x)\prod_{i=1}^{15}(x-9-i)$ has coefficients $\mathcal{O}(10^{18})$
- Rational companion: $\|C\|_2 \approx 20$
- `eig`: computes eigenvalues of $C + \epsilon\|C\|$

	$\max_i \lvert r(\hat{x}_i)\rvert$
C for $r(x)$	4e-11
C for $p(x)$	6.8e+3



Linearization for continued fractions

$$r(x) = p(x) + \cfrac{b_1}{x + a_1 + \cfrac{b_2}{x+a_2+\frac{b_3}{x+a_3+\cdots}}}$$

$p(x) = x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0$: polynomial (below shown as $*$)

$$C_0 + \lambda C_1 = \begin{bmatrix} * & b_1 & & & \\ 1 & -a_1 & -b_2 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -a_{k-1} & -b_{k-1} \\ & & & 1 & -a_k \end{bmatrix} + \lambda \begin{bmatrix} a_0 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix},$$

with eigenvector $(C_0 + \lambda C_1)x = 0, \quad x = \begin{bmatrix} \text{(poly)} \\ \vdots \\ \frac{\frac{1}{\lambda+a_k}}{\lambda+a_{k-1}+\frac{b_k}{\lambda+a_k}} \\ \frac{1}{\lambda+a_{k-1}+\frac{b_k}{\lambda+a_k}} \end{bmatrix}.$

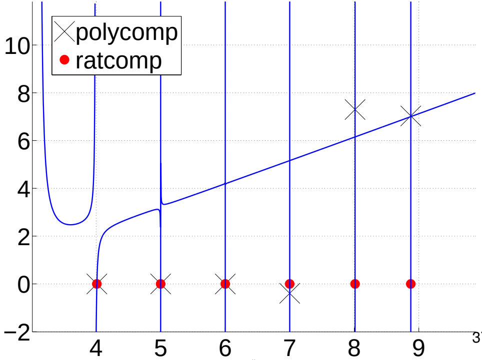
- eig(C) = roots(r) [Salazer 23]
- bottom rows: $g(x) := \frac{\frac{1}{x+a_2}}{x+a_1+\frac{b_1}{x+a_2}}$, $xg(x) = \frac{x}{x+a_{k-1}+\frac{b_k}{x+a_k}} = 1 + \frac{-a_{k-1}-\frac{b_k}{x+a_k}}{x+a_{k-1}+\frac{b_k}{x+a_k}}$

'Perfidious rational function', continued fraction

$$r(x) = x - 2 + \cfrac{1}{x - 1 + \cfrac{-1}{x+2+\cfrac{1}{x+3-\cdots+1/(x+11)}}}$$

- Polynomialize: $p(x) = r(x)\prod_{i=1}^{15}(x-9-i)$ has coefficients $\mathcal{O}(10^8)$
- Rational companion: $\|C\|_2 \approx 10$
- `eig`: computes eigenvalues of $C + \epsilon\|C\|$

	$\max_i \lvert r(\hat{x}_i)\rvert$
C for $r(x)$	4e-4
C for $p(x)$	7.2e0



Linearization for rational functions, more general form

$$r(x) = p(x) + \sum_{i=1}^{n} \left(\sum_{j=1}^{m_i} \frac{r_{ij}}{(x - \gamma_i)^j} \right), \tag{1}$$

$$C = \begin{bmatrix}
-a_d & -a_{d-1} & \dots & -a_0 & -r_{11} & \dots & -r_{1m_1} & -r_{21} & \dots & -r_{nm_n} \\
1 & & & & & & & & & \\
 & 1 & & & & & & & & \\
 & & \ddots & & & & & & & \\
 & & & 1 & \gamma_1 & & & & & \\
 & & & & \ddots & \ddots & & & & \\
 & & & & & 1 & \gamma_1 & & & \\
 & & & 1 & & & & \gamma_2 & & \\
 & & & & & & & 1 & \ddots & \\
 & & & 1 & & & & & & \gamma_n
\end{bmatrix}$$

- $\mathrm{eig}(C) = \mathrm{roots}(p)$

Conclusion and discussion

Summary

- Linearize rational function without polynomializing
  - typically reduced matrix norm, improved stability

Other things possible

- DL-type linearization
- Matrix rational functions (as opposed to scalars [Su,Bai 2011])

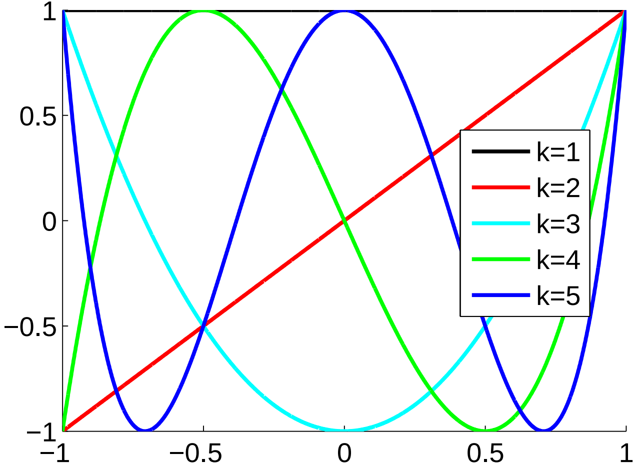
To be examined

- Conditioning
- Exploit structure (low-rank etc) in matrix case
- Trigonometric + polynomial (or rational)

Coming: more systematic framework using Schur complements (with Vanni Noferini and Maria Quintana Ponce),

Chebyshev polynomials $T_k(x)$

$$T_k(\cos\theta) = \cos k\theta$$



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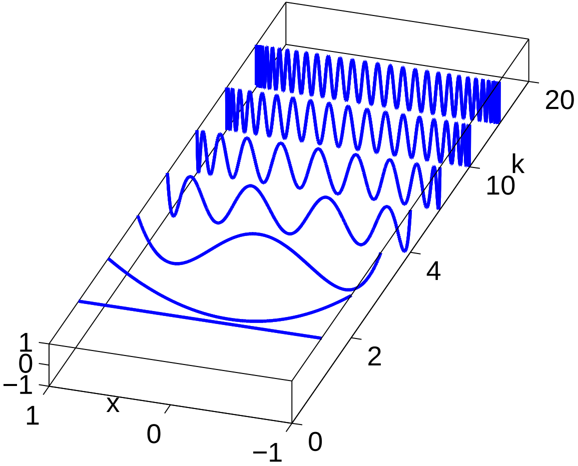

Polynomial bases and Chebyshev coefficients

$p(x)$ expressed in

- monomial basis: $p(x) = \sum_{i=0}^{n} c_i x^i$
- Chebyshev basis: $p(x) = \sum_{i=0}^{n} c_i T_i(x)$
  - For smooth $f \approx p$, $|c_n| \to 0$ as $n \to \infty$, often like $|c_n| = e^{-cn}$

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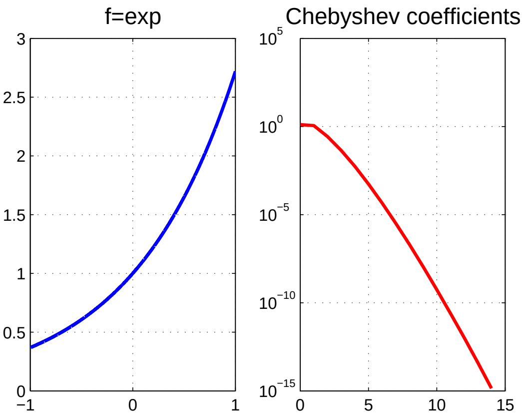

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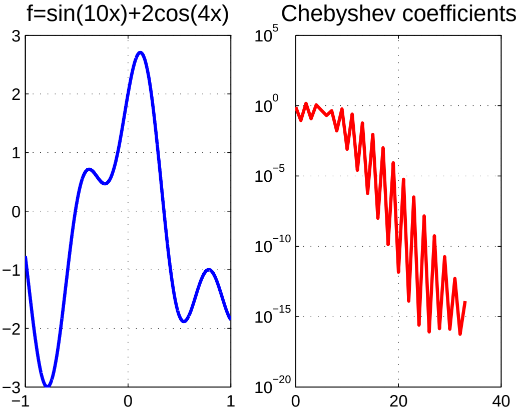
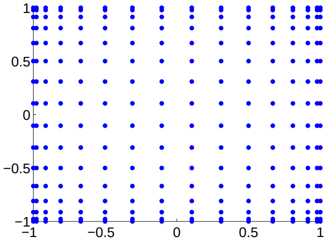


2D polynomial approximation by interpolation

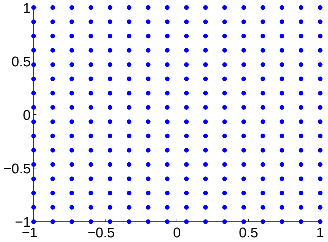
Interpolation: find $p(x,y)$ s.t.

$$f(x_i,y_j)=p(x_i,y_j),\quad i=0,1,\dots,n,\quad j=0,1,\dots,m.$$

Chebyshev points (good)



Equispaced points (bad)

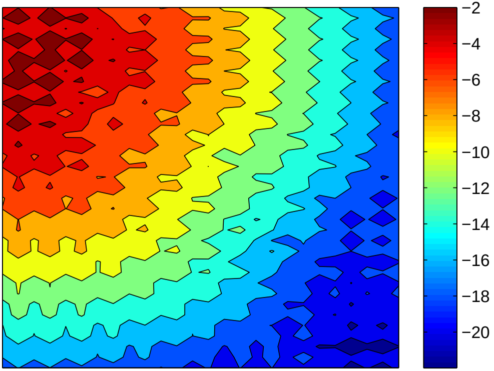


- For sufficiently smooth $f(x,y)$, with Chebyshev interpolation

$$\|f-p_{n,m}\|\le Ce^{-c\min(n,m)}$$

Bivariate polynomial approximation: $f(x,y) \approx p(x,y)$

$$p(x,y) = \sum_{i=0}^{m_p} \sum_{j=0}^{n_p} P_{ij} T_i(y) T_j(x)$$

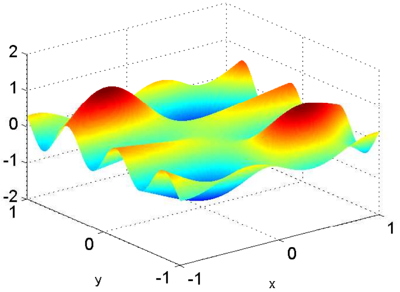


$\log_{10} |P_{ij}|$ contour plot

Bivariate Chebyshev interpolation: convergence

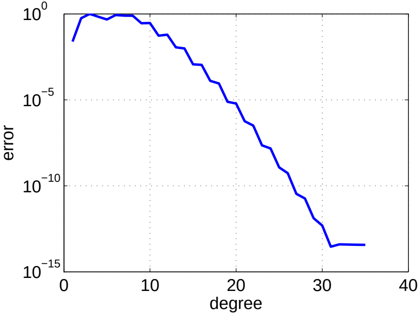
$$f(x,y) = \sin(5xy)\cos(5y)\exp((x+y)/10)$$

function



convergence:

$\|f(x,y) - p(x,y)\|_\infty$



Regularization for improved numerical stability

– $B(y)$ is nearly singular: $B(y)$ is ill-conditioned for every y

- decaying Chebyshev coefficients $\Rightarrow$ small bottom-right corner

Remedy-Regularization: partition $B(y)$ as

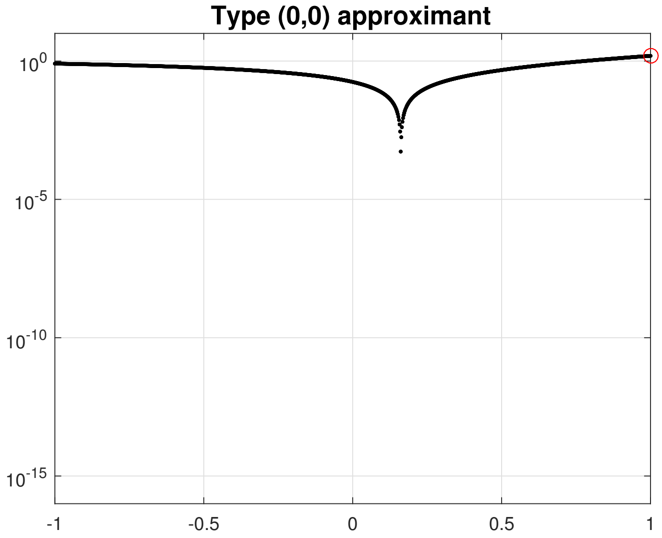
$$B(y) = \begin{bmatrix} B_1(y) & E(y)^T \\ E(y) & B_0(y) \end{bmatrix},$$

$B_1(y)$ is the largest numerically nonsingular part, i.e., for any $y_0 \in [-1, 1]$

- $||B_0(y_0)||_2 = \mathcal{O}(u)$
- $||E(y_0)||_2 = \mathcal{O}(u^{1/2})$

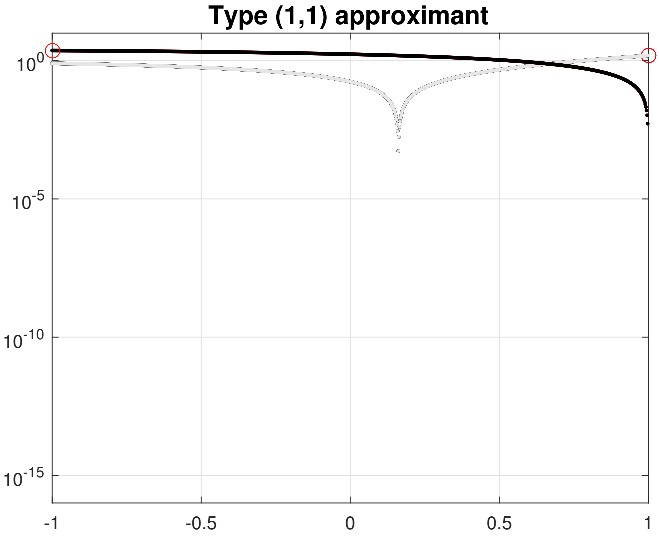
We prove eig$(B_1(y))$ are within $O(\epsilon)$ of the desired eig$(B(y))$
$\Rightarrow$ work with $B_1(y)$, “more regular” (accurate) + efficient

Example $f(x) = \mathrm{e}^x$ on $[-1, 1]$



Red circle: support points

Example $f(x) = e^x$ on $[-1, 1]$



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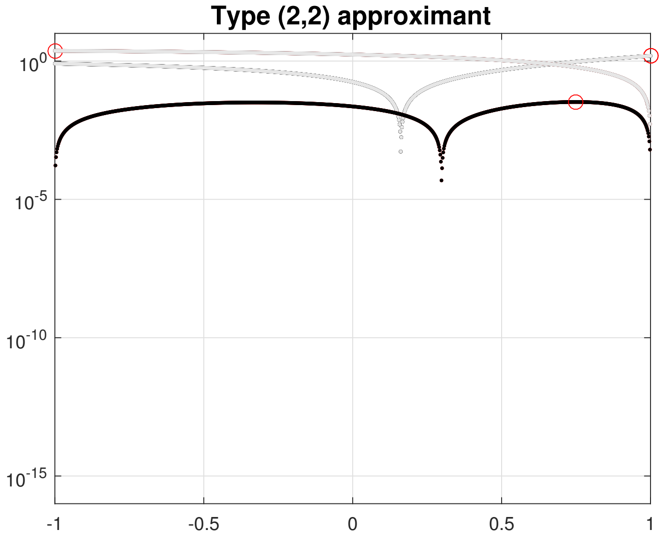

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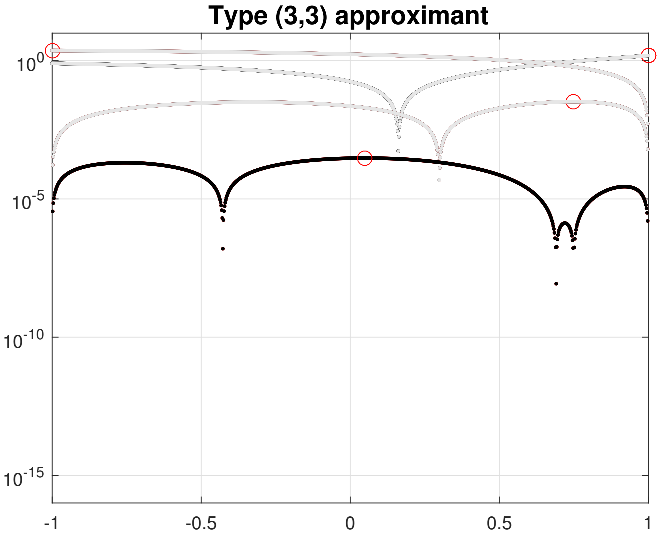

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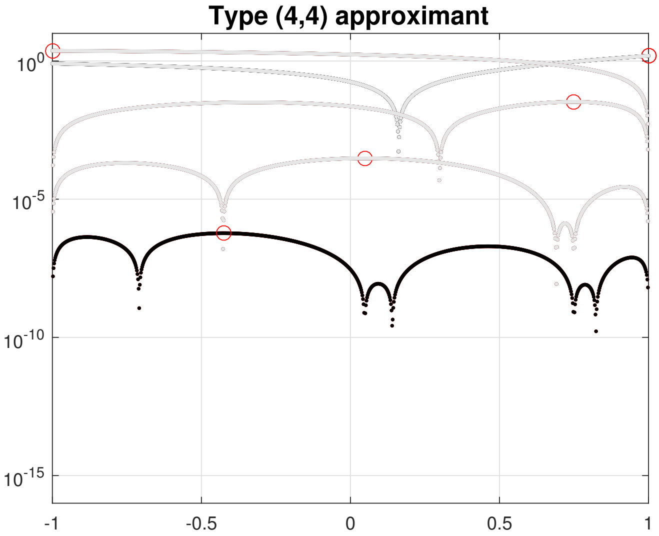

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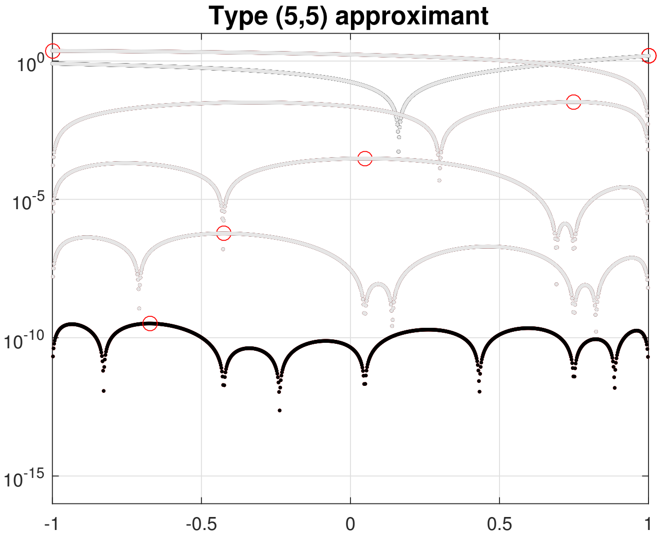

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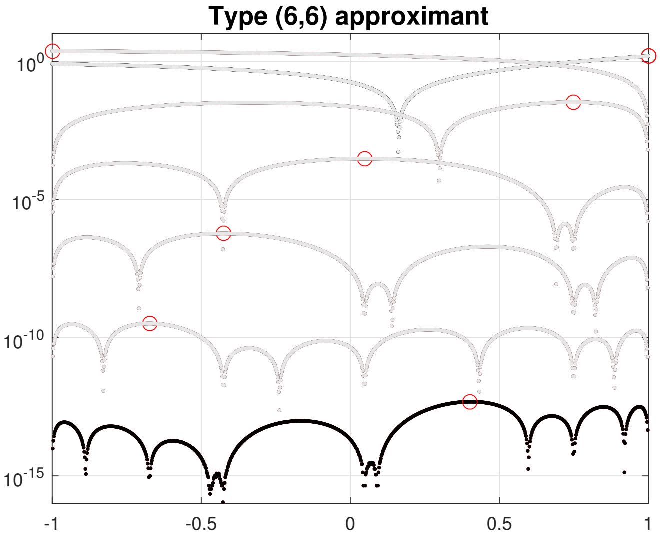

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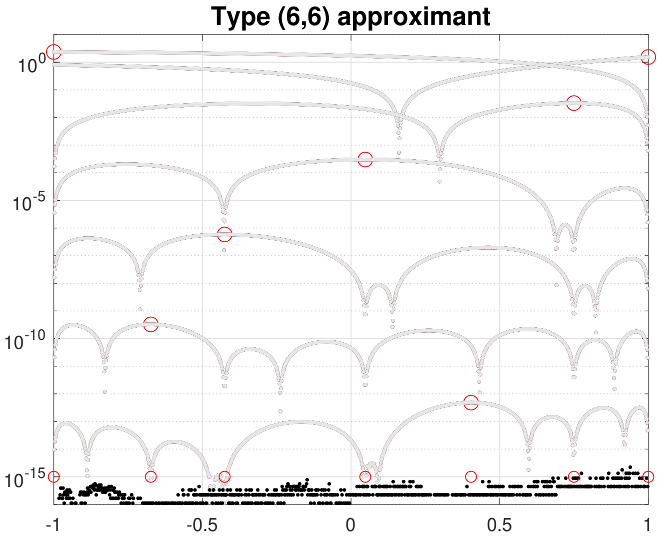

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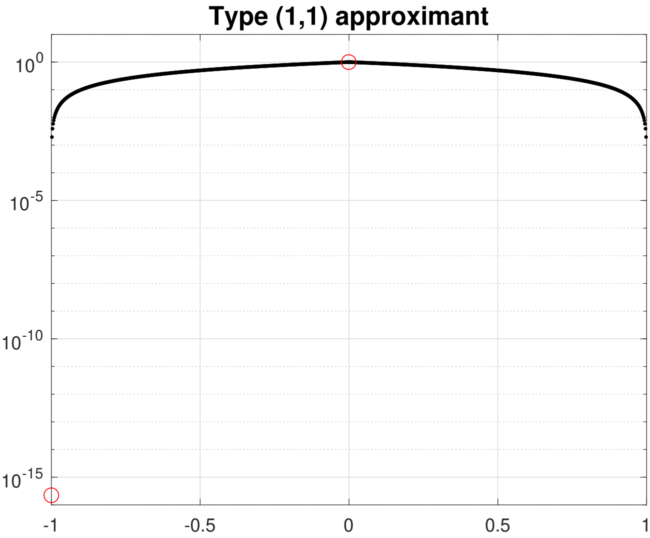

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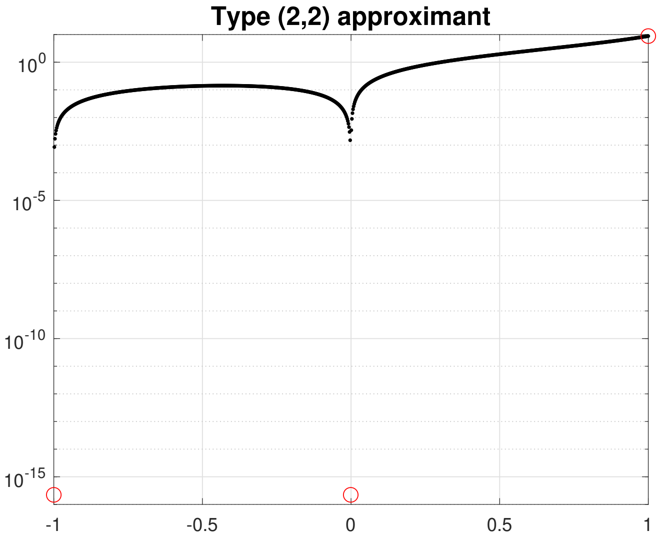

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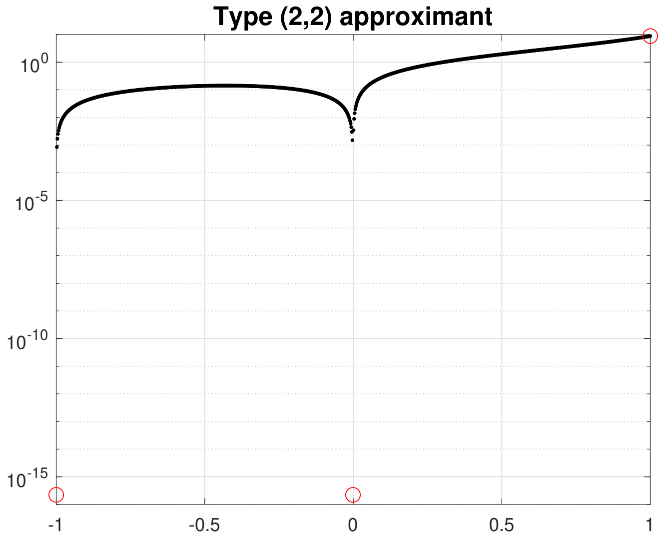

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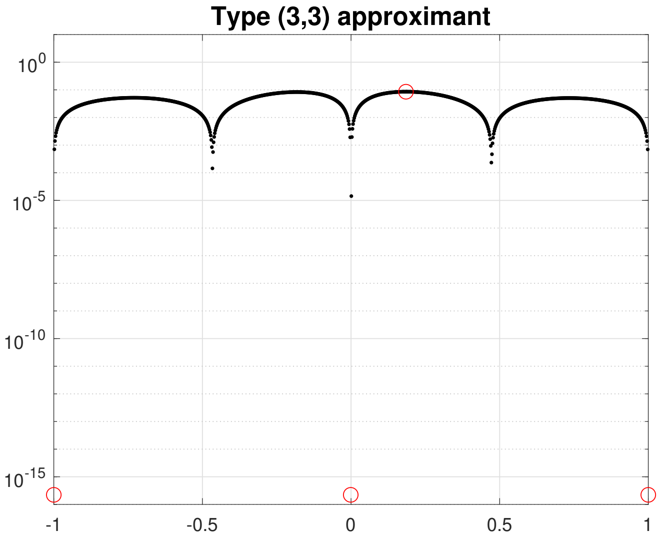

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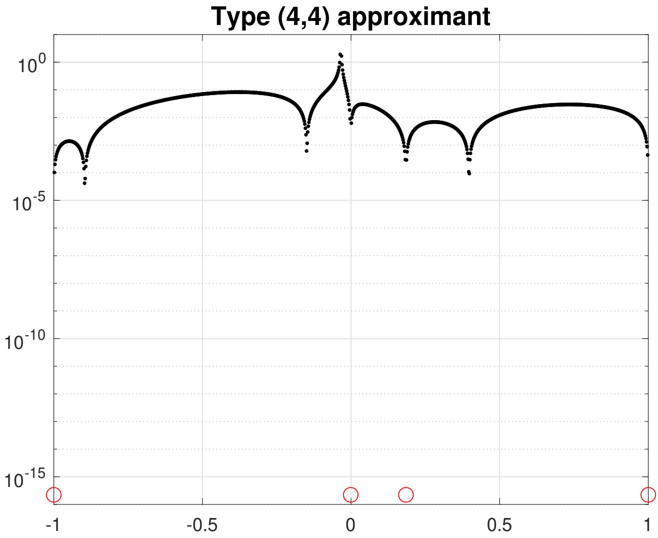

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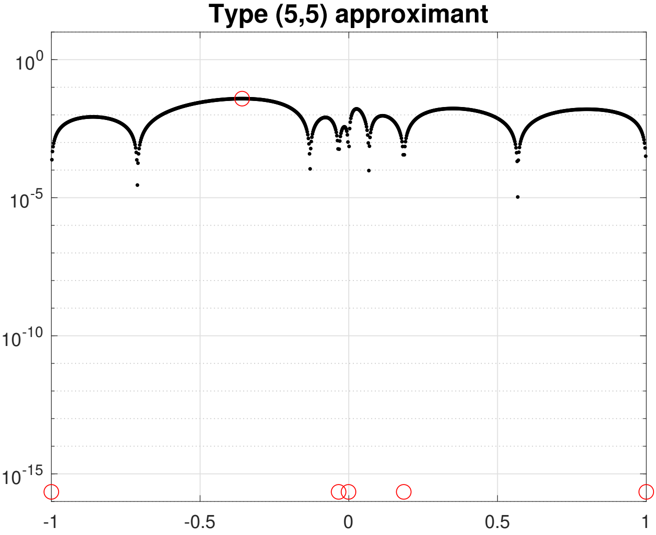

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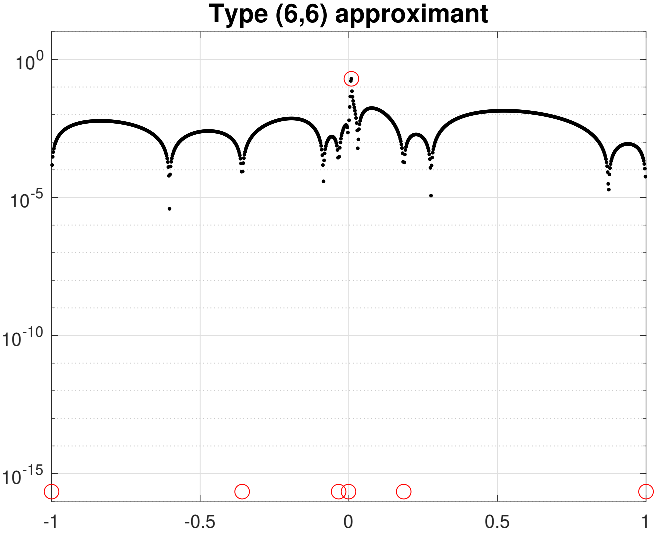

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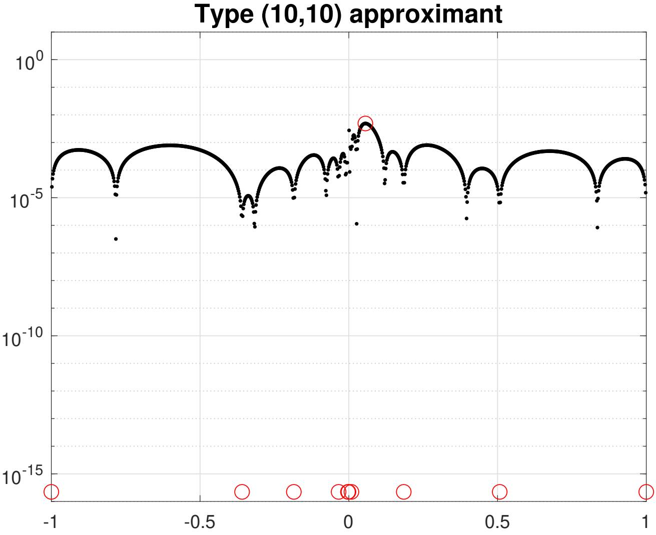

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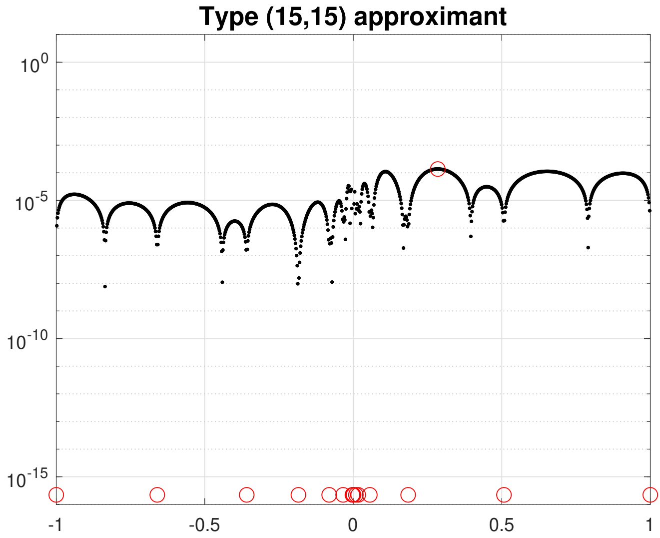

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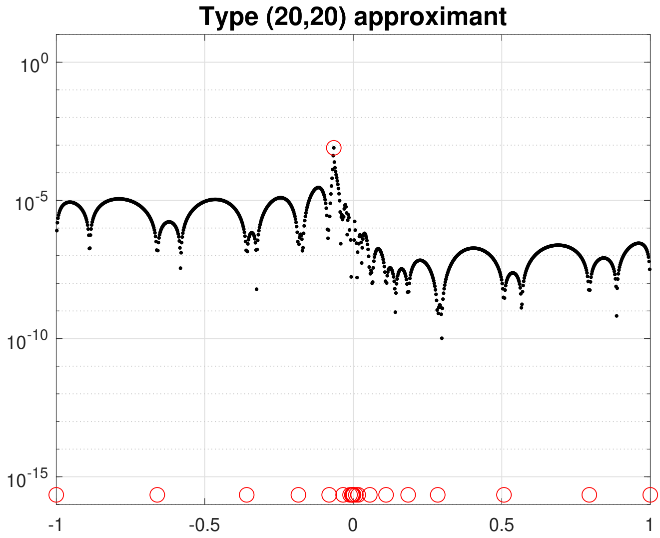

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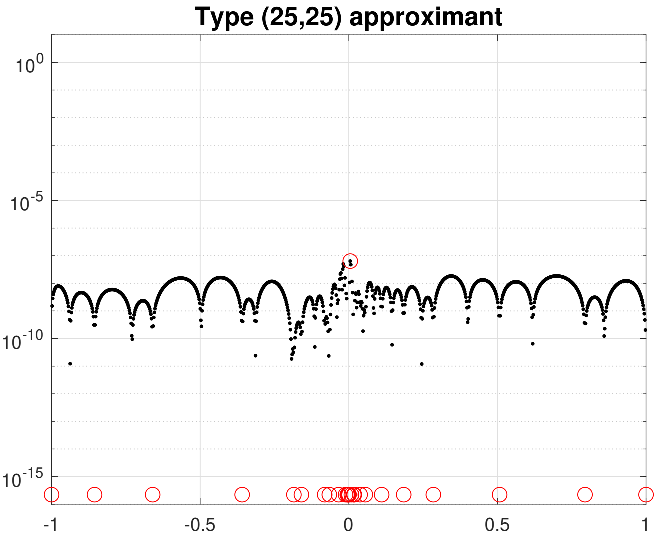

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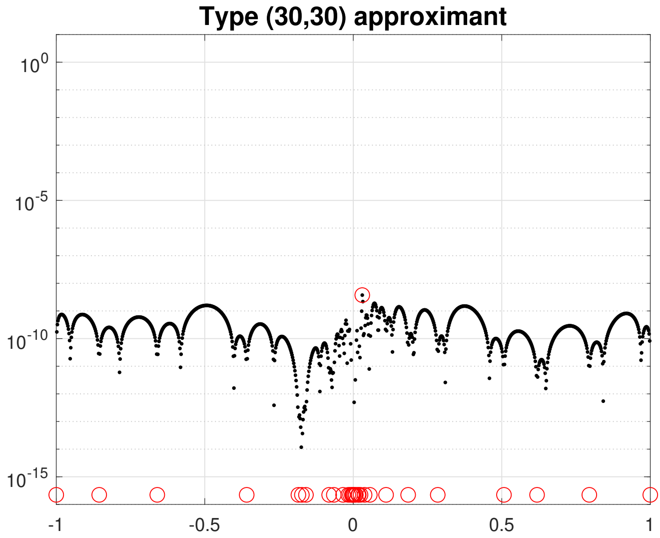

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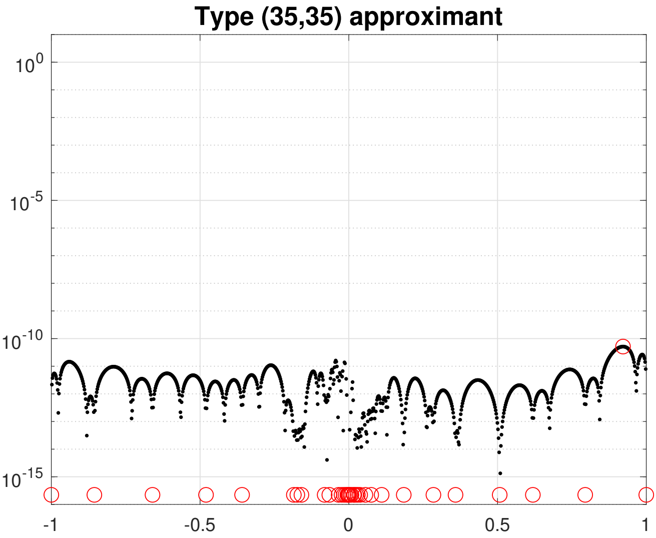

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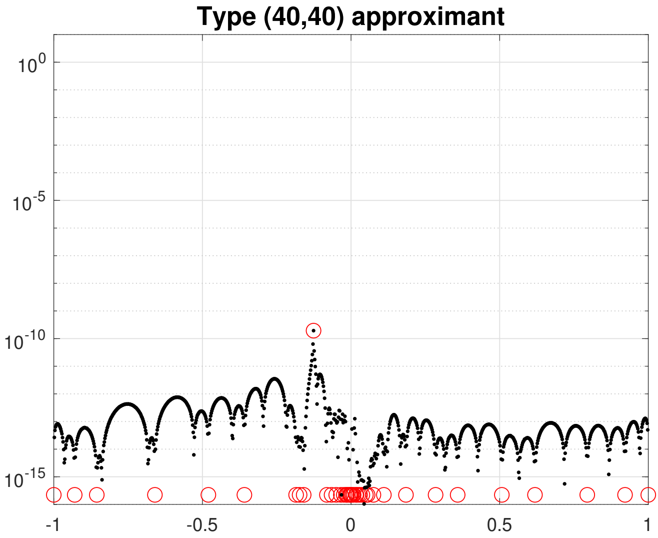
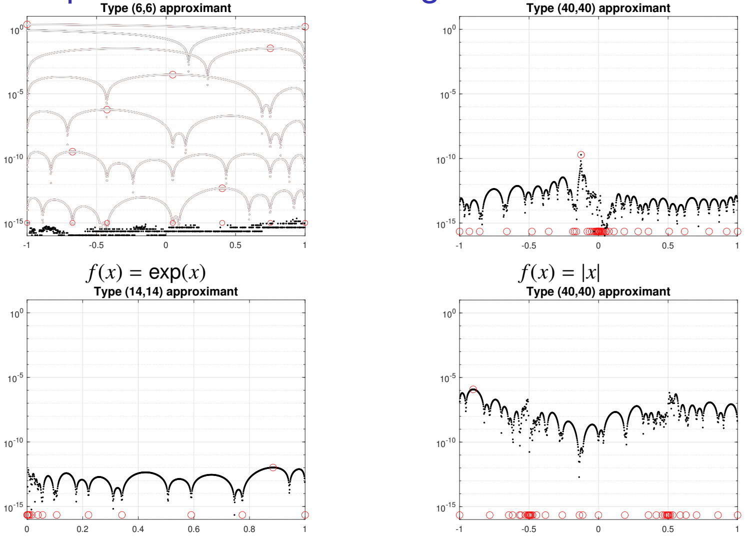


Red circle: support points

Support points cluster near singularities

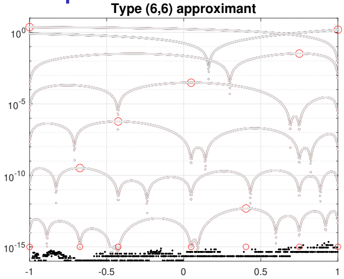


$f(x) = \exp(x)$ $\quad$ $f(x) = |x|$

$f(x) = \sqrt{x}$ $\quad$ $f(x) = |x - 0.5| + |x + 0.5|$

- For functions with singularities, support points cluster near them

Support points cluster near singularities



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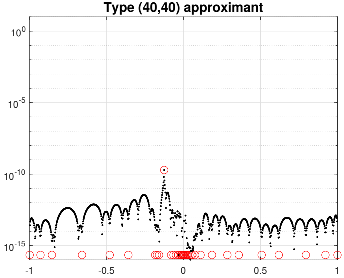

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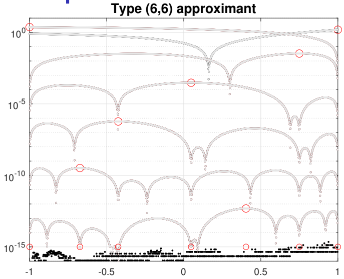
- Informally: because hard to get error small there

Support points cluster near singularities



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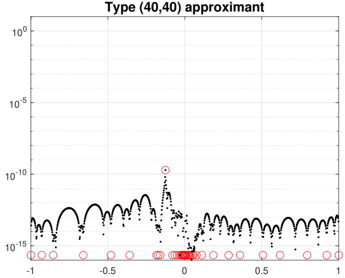
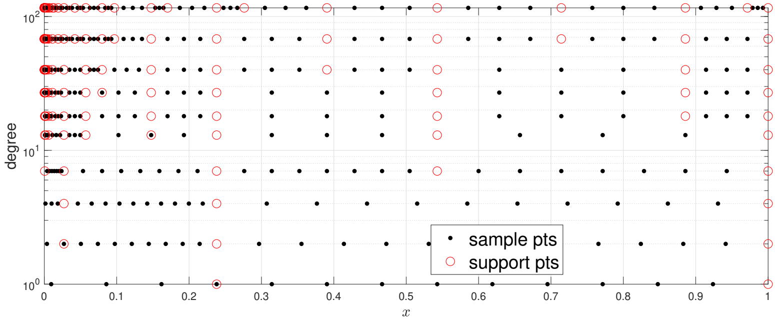


$f(x) = |x|$

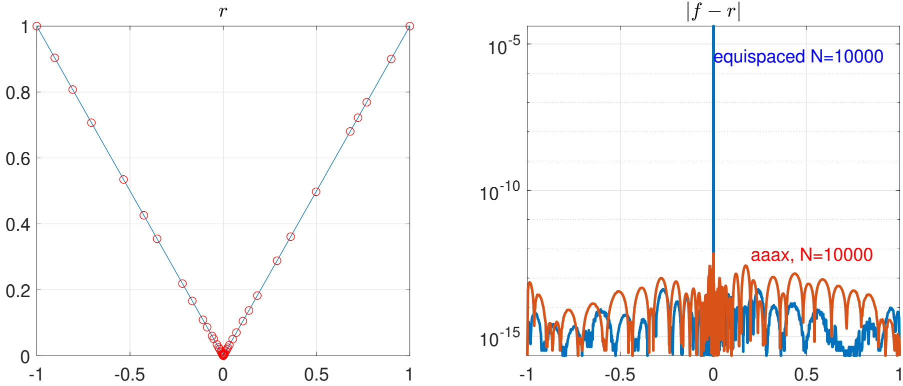
- Support points cluster near singularities
- Informally: because hard to get error small there
- Hence support points useful for clustering sample points on the fly
- We'll add three sample points between support points (i.e., six new points per step)

Continuum AAA: support+sample points

Sample points with aaax on $x > 0$, for $f(x) = |x|$:

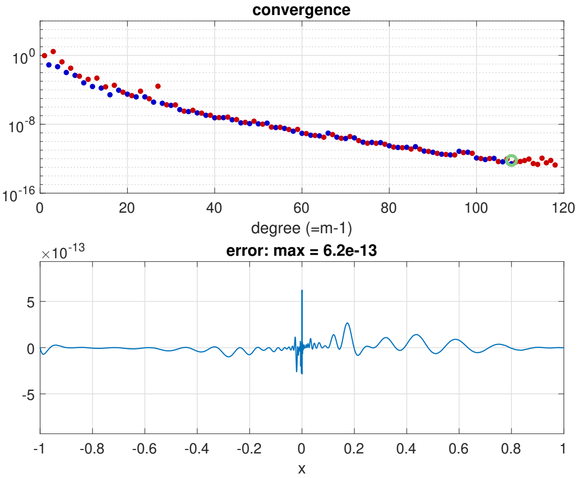


AAA vs. continuum AAA for $|x|$



- AAA with equispaced sample points yield poor error near singularity
- Continuum AAA yields good accuracy with fewer samples
- Monitor poles on $[-1, 1]$ ('bad poles'), ensure output is pole-free

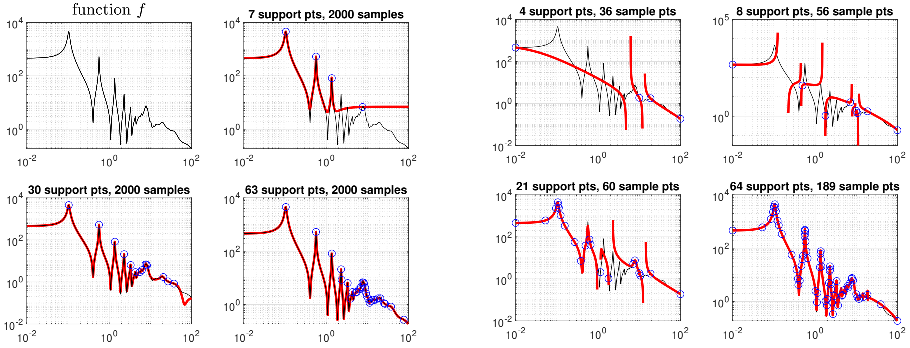
Example: `f = @(x) abs(x); r = aaax(f)`



- red: bad poles (in $[-1, 1]$) present
- green: output, pole-free on $[-1, 1]$

NICONET Beam example

$f(z) = c^T(zI - A)^{-1}b$, $A \in \mathbb{C}^{n\times n}$, $n = 348$; f expensive to evaluate



aaai succeeds with many fewer samples

Linearization and orthogonal polynomials

- Polynomial linearization entries are coefficients in the three-term recurrence, e.g. for Chebyshev

$$2xT_n(x) = T_{n+1}(x) + T_{n-1}(x)$$

- Partial fraction linearization: two-term recurrence $x\frac{1}{x-\gamma_i} = 1 + \frac{\gamma_i}{x-\gamma_i}$
- Continued fraction is historically connected to orthogonal polynomials (evaluation scheme via recursion), and the three-term recurrence gives linearization coefficients
- For non-orthogonal polynomial bases, C is dense (e.g. Hessenberg)

General rational function

$$r(x) = p(x) + \frac{p_1(x)}{q_1(x)} + \frac{p_2(x)}{q_2(x)} + \cdots \frac{p_n(x)}{q_n(x)}$$

$$C = \begin{bmatrix} * & b_1 & & & & & \\ 1 & -a_1 & -b_2 & & & & \\ & & \ddots & \ddots & b_n & & \\ & & & 1 & -a_n & & \\ 1 & & & & & \gamma_1 & \\ 1 & & & & & & \gamma_n \end{bmatrix}$$

with eigenvector $Cx = \lambda x$, $\quad x = \begin{bmatrix} \text{(poly)} \\ \vdots \\ \frac{\frac{1}{\lambda+a_k}}{\lambda+a_{k-1}+\frac{b_k}{\lambda+a_k}} \\ \frac{1}{\lambda+a_{k-1}+\frac{b_k}{\lambda+a_k}} \\ \frac{1}{\lambda-\gamma_1} \\ \vdots \\ \frac{1}{\lambda-\gamma_n} \end{bmatrix}.$

- eig(C) = roots(r)

It is a strong linearization for polynomialization

$C(\lambda)$ is a linearization for polynomial $p(\lambda) \Leftrightarrow C = E(\lambda)\begin{bmatrix} p & \\ & I \end{bmatrix}F(\lambda)$ for unimodular E, F, *strong* linearization if $\mathrm{rev}(C) = \hat{E}(\lambda)\begin{bmatrix} \mathrm{rev}(p) & \\ & I \end{bmatrix}\hat{F}(\lambda)$

- The pencil belongs to $\mathbb{L}_1$ [Mackey, Mackey, Mehrmann, Mehl SIMAX 05], although in a nonstandard polynomial basis
- $\mathbb{L}_1$ pencil is a strong linearization iff regular [YN,VN,AT preprint]
- Since our pencils are regular, they are a strong linearization

C is a linearization for $r(x)\prod_{i=1}^{n} q_i(x)$ (i.e. mathematically equivalent to polynomializing, but numerically different)

Stability in matrix $\Rightarrow$ stability in polynomial?

The computed $\hat{x}_i$ are exact eigvals of a pertubed matrix pencil:

$$\{\hat{x}_i\} = \text{eig}(\lambda(X + \Delta X) + (Y + \Delta Y))$$

But stability in polynomial means $\hat{x}_i$ are exact roots of $p + \Delta p$:

$$p(x) + \Delta p(x) = \alpha \prod_{i=1}^{n} (x - \hat{x}_i), \quad ||\Delta p|| \le \epsilon ||p||$$

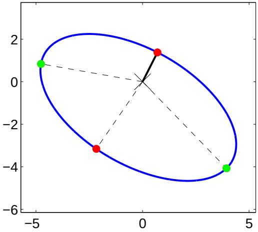
- For companion, Van Dooren and prove stability if QZ is used
- For comrade (Chebyshev + Jacobi polynomial bases), [YN and VN, Math. Comp.] proves stability, again if QZ is used (QR can be unstable)
- For rational linearization, stability is open problem

Applications: point-ellipsoid distance

Problem: find x on ellipsoid $(x-b)^T A^{-1}(x-b) = K^2$ closest to origin

- KKT conditions are

$$(x-b)^T A^{-1}(x-b) = K^2,$$
$$Ax = \lambda(x-b).$$



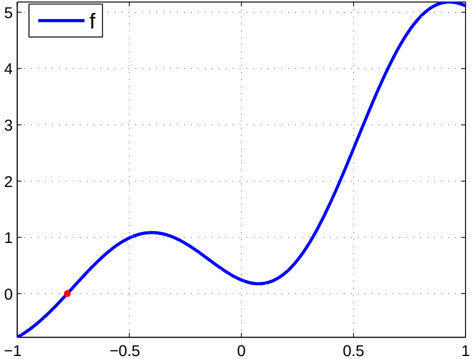
Writing $A = QDQ^T$ and $y := Q^T b$, this leads to solving for λ

$$K^2 = \sum_{i=1}^{n} \frac{d_i y_i^2}{(\lambda - d_i)^2}.$$

$$\Rightarrow \text{eigenvalues of } \begin{bmatrix} K^2 & 0 & -y_1 & 0 & -y_2 \\ 1 & d_1 & & & \\ & 1 & d_1 & & \\ 1 & & & d_2 & \\ & & & 1 & d_2 \end{bmatrix}, \text{ then } x = -(A - \lambda I)^{-1} b$$

Take-home message

- Approximate with polynomials of high degree
  - Often considered inaccurate (Newton(quadratic) > Halley (cubic)) and unstable (Vandermonde matrix...)
  - If properly implemented: accurate (global approximation instead of local) and stable (Chebyshev basis + FFT)
- Replace algorithms based on linear approximation by local sampling with high-degree polynomial approximation by global sampling(?)



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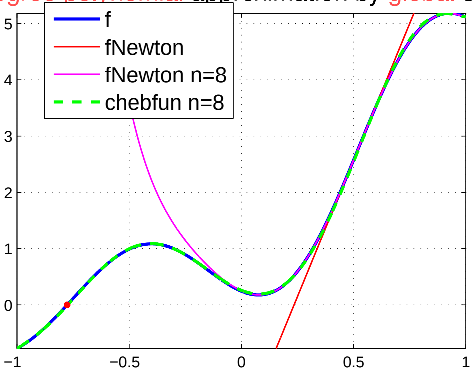
- Approximate with polynomials of high degree
  - Often considered inaccurate (Newton(quadratic) > Halley (cubic)) and unstable (Vandermonde matrix...)
  - If properly implemented: accurate (global approximation instead of local) and stable (Chebyshev basis + FFT)
- Replace algorithms based on linear approximation by local sampling with high-degree polynomial approximation by global sampling(?)



Explaining $\|f - p_n\| \leq O(\log n)\|f - p_{n,best}\|$: Lebesgue constants

- The Lebesgue constant Λ of $\{x_i\}_{i=0}^n$ is

$$\Lambda = \sup_f \frac{\|\mathcal{L}_n f\|_\infty}{\|f\|_\infty} \tag{2}$$

  Interpretation: Given data values on an $(n+1)$-point grid from sampling $\|f\|_\infty = 1$, Λ is the largest possible value of the interpolant p.

- Λ is an accurate measure of the interpolation points $\{x_i\}_{i=0}^n$:

$$\|f - p_n\|_\infty \leq (\Lambda + 1)\|f - p_{n,best}\|_\infty.$$

- Characterization using Lagrange polynomials $\ell_j(x)$ defined by $\ell(x) = \prod_{i=0}^n (x - x_i)$, $\ell_i(x) = \frac{\ell(x)}{\ell'(x_i)(x-x_i)}$:

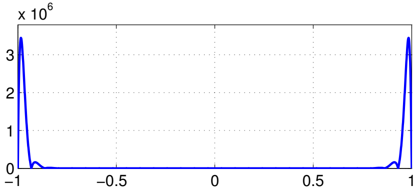
$$\Lambda = \sup_{x\in[-1,1]} \sum_{j=0}^n |\ell_j(x)|.$$

Explaining $\|f - p_n\| \le O(\log n)\|f - p_{n,best}\|$: Lebesgue function

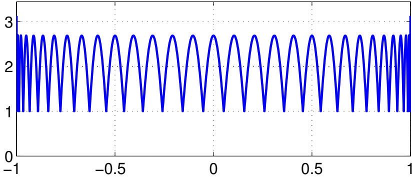
$$\Lambda = \sup_{x\in[-1,1]} \sum_{j=0}^{n} |\ell_j(x)|.$$

$\sum_{j=0}^{n} |\ell_j(x)|$ is called the Lebesgue function of $\{x_i\}_{i=0}^{n}$

$\{x_i\}_{i=0}^{n}$: Equispaced points



$\{x_i\}_{i=0}^{n}$: Chebyshev points



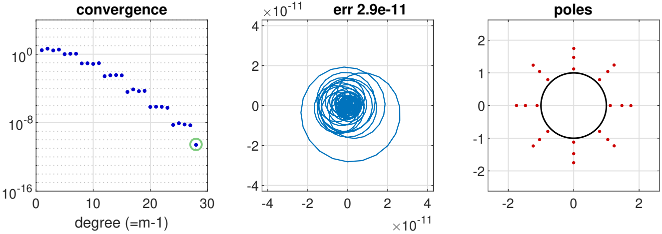
Matrix size

Resultant	Size of A_i	Degree	Size of $Cv = \lambda Ev$
Bézout (y first)	$\max(n_p, n_q)$	$m_p + m_q$	$\max(n_p, n_q)(m_p + m_q)$
Bézout (x first)	$\max(m_p, m_q)$	$n_p + n_q$	$\max(m_p, m_q)(n_p + n_q)$
Sylvester (y first)	$n_p + n_q$	$\max(m_p, m_q)$	$\max(m_p, m_q)(n_p + n_q)$
Sylvester (x first)	$m_p + m_q$	$\max(n_p, n_q)$	$\max(n_p, n_q)(m_p + m_q)$

Table: Sizes and degrees of matrix polynomials constructed from the Bézout and Sylvester resultant matrices. The product of the size of the A_i and degree is the size of the resulting generalized eigenvalue problem $Cv = \lambda Ev$, which depends on whether the x- or y-variable is solved for first. We use the Bézout resultant matrix and solve for the y-values first if $\max(n_p, n_q)(m_p + m_q) \leq \max(m_p, m_q)(n_p + n_q)$; the x-values first, otherwise.

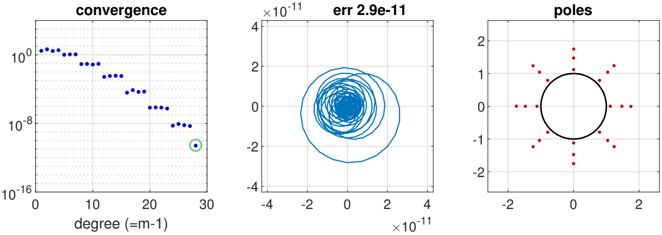
aaaz: on unit circle

Same idea, sample points on unit circle

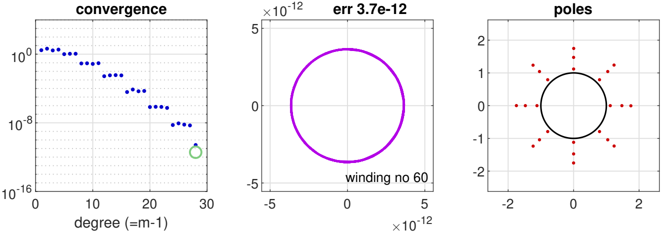


aaaz: on unit circle

Same idea, sample points on unit circle



- Poles allowed in $|z| < 1$ (mero=1) or disallowed (mero=0, here)
- with Lawson steps (find minimax approx, [N.-Trefethen 2020])



aaai: on imaginary axis

Use map

$$z = M\frac{1+w}{1-w}, \qquad w = \frac{z-M}{z+M}$$

- $z \in i\mathbb{R} \Leftrightarrow |w| = 1$
- Then apply aaaz to $f(w(z))$
- $M \in \mathbb{R}$ arbitrary, we set to 1.207