Near best rational approximation and spectral methods

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Part I

Near best interpolation

Introduction

A very old and very classical problem...

Given a real, continuous function $f(x)$ on $[-1, 1]$, find a *good* polynomial approximation

Possible solutions

- Best (minimax) polynomial approximation according to the norm
$$\|f\| := \|f\|_\infty = \max_{-1 \le x \le 1} |f(x)|$$
- Polynomial least squares approximation
- Interpolating polynomial

Linear minimax approximation

Problem

Given linearly independent functions $\{\varphi_k\}$ find

$$\min_{a_k} \left\| f(x) - \sum_{k=0}^{n} a_k \varphi_k(x) \right\|$$

Solution

a_k such that $f - \sum a_k \varphi_k$ equi-oscillates, i.e. $n+2$ extremal points of equal magnitude and alternating sign

Example: minimax polynomial approximation

Take $\varphi_k(x) = x^k$ for $k = 0, 1, \ldots, n$

Interpolating polynomial

Take $n+1$ points $x_0, x_1, \ldots, x_n$ and construct polynomial $p_n(x)$ such that

$$f(x_i) = p_n(x_i), \quad i = 1, 2, \ldots n$$

Choice of interpolation points?
It is well-known that

$$f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0) \cdots (x - x_n)$$

where ξ depends on x and $x_0, x_1, \ldots, x_n$ and f

Try to choose $x_0, \ldots, x_n$ such that $f - p_n$ equi-oscillates ...

Equi-oscillating polynomial on $[-1, 1]$

Find points $x_0, \ldots, x_n$ such that $(x - x_0) \cdots (x - x_n)$ equi-oscillates on $[-1, 1]$

- Chebyshev polynomial

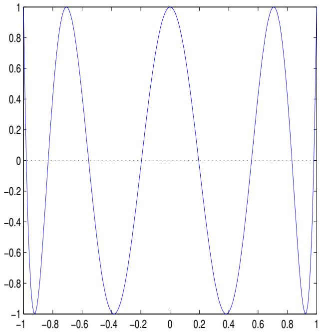
  $$T_{n+1}(x) = \cos((n+1) \arccos x)$$

- Zeros are given by

  $$x_k = \cos \frac{\pi(2k+1)}{2(n+1)}$$

  for $k = 0, \ldots, n$

- Interpolation in x_k is near best



Alternative interpretation

From

$$f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0) \cdots (x - x_n)$$

it follows that

$$\|f - p_n\| \leq \frac{\max_{-1 \leq t \leq 1} f^{(n+1)}(t)}{(n+1)!} \|(x - x_0) \cdots (x - x_n)\|$$

Minimising $\|(x - x_0) \cdots (x - x_n)\|$ over $x_0, \ldots, x_n$ leads to the Chebyshev zeros

The unique monic polynomial of degree $n + 1$ which deviates least from zero in the infinity norm, is a scaled Chebyshev polynomial

How good is near best?

Let f be a continuous function on $[-1, 1]$, p_n its polynomial interpolant in the Chebyshev zeros, and p_n^* its best approximation on $[-1, 1]$ according to the infinity norm. Then

$$\|f - p_n\| \leq \left(2 + \frac{2}{\pi} \log n\right) \|f - p_n^*\|$$

- If $n < 10^5$ we loose at most 1 digit
- If $n < 10^{66}$ we loose at most 2 digits

If f is analytic in an ellipse with foci ± 1 and semimajor/minor axis lengths $a \geq 1$ and $b \geq 0$, then

$$\|f - p_n\| = O((a + b)^{-n}), \quad n \to \infty$$

Rational generalisation

What if f has singularities close to $[-1, 1]$?

Example

Take

$$f(x) = \frac{1}{\varepsilon^2 + x^2}, \quad 0 < \varepsilon \ll 1$$

with poles at $\pm \mathrm{i}\varepsilon$

Then $\|f - p_n\| = O((1+\varepsilon)^{-n})$

Polynomial interpolation converges too slowly!

Near best fixed pole rational interpolation

Let poles $\alpha_1, \ldots, \alpha_m$ be given (real or complex conjugate) and put

$$\pi_m(x) = (x - \alpha_1) \cdots (x - \alpha_m)$$

Then

$$f(x) - \frac{p_n(x)}{\pi_m(x)} = \frac{[\pi_m(\xi)f(\xi)]^{(n+1)}}{(n+1)!} \frac{(x - x_0) \cdots (x - x_n)}{\pi_m(x)}$$

when

$$f(x_i) = \frac{p_n(x_i)}{\pi_m(x_i)}, \quad i = 0, 1, \ldots, n$$

Linear minimax approximation

Problem

Given linearly independent functions $\{\varphi_k\}$ find

$$\min_{a_k} \left\| f(x) - \sum_{k=0}^{n} a_k \varphi_k(x) \right\|$$

Solution

a_k such that $f - \sum a_k \varphi_k$ equi-oscillates, i.e. $n+2$ extremal points of equal magnitude and alternating sign

Example: minimax rational approximation

Take $\varphi_k(x) = x^k / \pi_m(x)$ for $k = 0, 1, \ldots, n$

Near best fixed pole rational interpolation

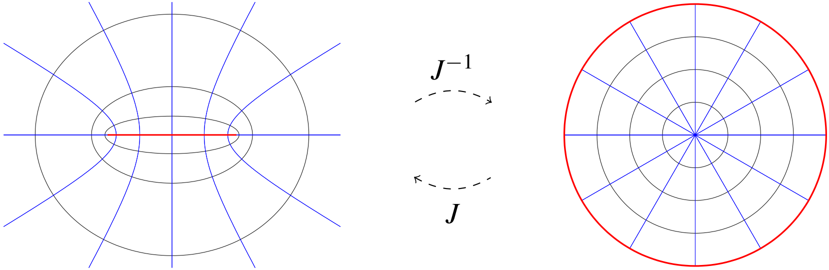
Problem statement

Given π_m, find $x_0, \ldots, x_n$ with $n + 1 \geq m$ such that $\|q_{n+1}/\pi_m\|$ is minimal, where $q_{n+1}(x) = (x - x_0) \cdots (x - x_n)$
(equivalently: such that q_{n+1}/π_m equi-oscillates)

History

- Special case studied by Markoff, 1884
- General case solved by Bernstein, 1937
- Discussed in Appendix A of Achieser's "Theory of Approximation", 1956
- Only theoretical solution, no properties, computational aspects, ...

Joukowski transformation



$$x = J(z) = \frac{1}{2}\left(z + \frac{1}{z}\right)$$

$$z = x - \sqrt{x^2 - 1}$$

Solution

- Let $\{\alpha_1, \dots, \alpha_m\}$ denote zeros of π_m
- Put $\beta_k = J^{-1}(\alpha_k)$ for $k = 1, \dots, m$
- Define B_m by

$$B_m(z) = \frac{z - \beta_1}{1 - \beta_1 z} \cdots \frac{z - \beta_m}{1 - \beta_m z}$$

Then

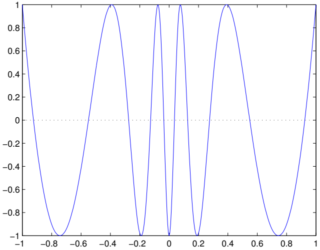
$$\mathcal{T}_n(x) = \frac{1}{2}\left(z^{n-m} B_m(z) + \frac{1}{z^{n-m} B_m(z)}\right)$$

is a rational function in x of the form $q_n(x)/\pi_m(x)$.
The interpolation points $x_0, \dots, x_n$ are the zeros of $\mathcal{T}_{n+1}(x)$.

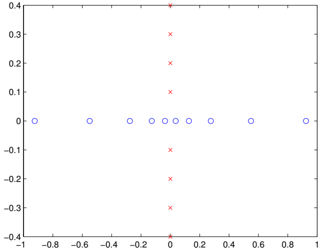
Equi-oscillating rational function on $[-1, 1]$

Example

$\pi_m(x) = \prod_{k=1}^{m/2}(x^2 + k^2\omega^2)$ where $\omega = 0.1$



$\mathcal{T}_n(x)$



Poles & zeros

Note

Poles attract zeros (see later: electrostatic interpretation)

Why bother?

Can we not just do rational interpolation in the (polynomial) Chebyshev points (zeros of Chebyshev polynomial T_n)?

- If $\alpha_1, \ldots, \alpha_m$ correspond to poles of f close to the interval, then $\|\pi_m f - p_n\|$ will be small (enlarging the ellipse of analyticity)
- However, dividing by π_m can destroy this advantage and $\|f - p_n/\pi_m\|$ may not be small
- If poles gather near the interior of the interval, Chebyshev zeros are useless
- Application: differential equations with interior layers

Example

Let

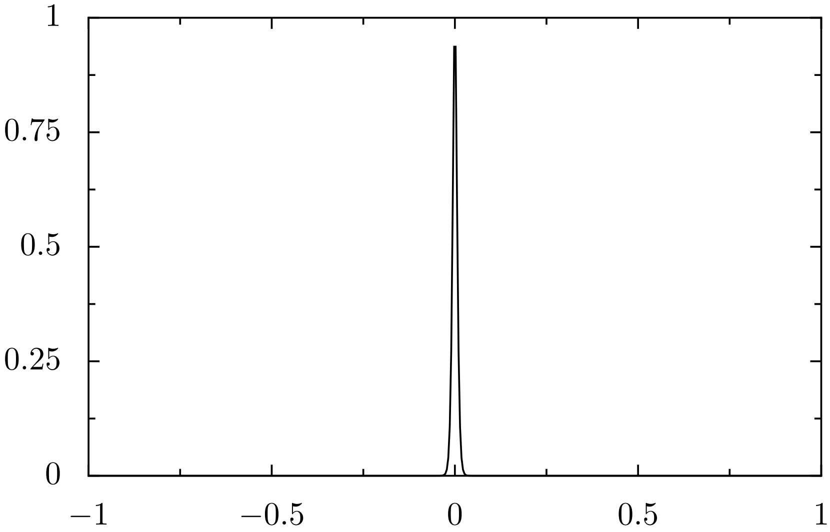
$$f(x) = \frac{\pi x/\omega}{\sinh(\pi x/\omega)}$$

This function has simple poles at $\pm \mathrm{i}k\omega$ for $k = 1, 2, \ldots$

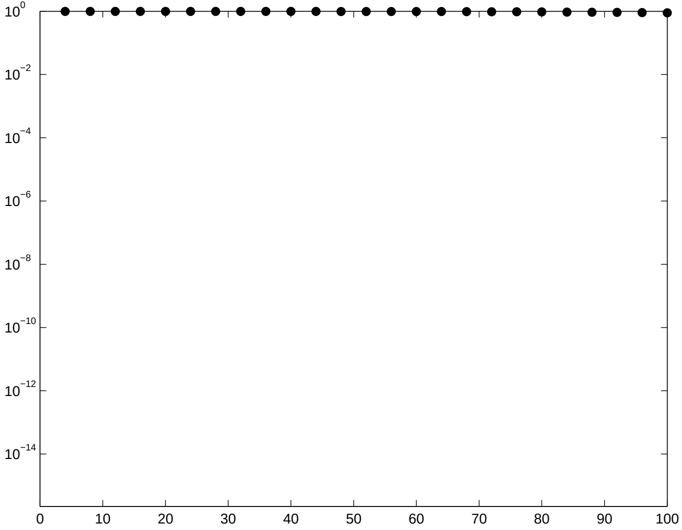
- Interpolate by p_{n-1} in zeros of T_n
- Interpolate by p_{n-1}/π_{n-2}
  - in zeros of T_n
  - in zeros of $\mathcal{T}_n$

Plot interpolation error $\|f - p_{n-1}\|$ and $\|f - p_{n-1}/\pi_{n-2}\|$ for the case $\omega = 0.01$

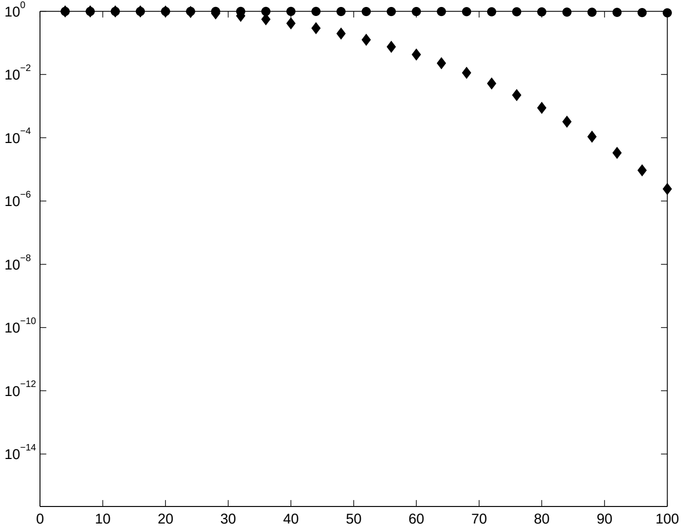
Graph of $f(x)$



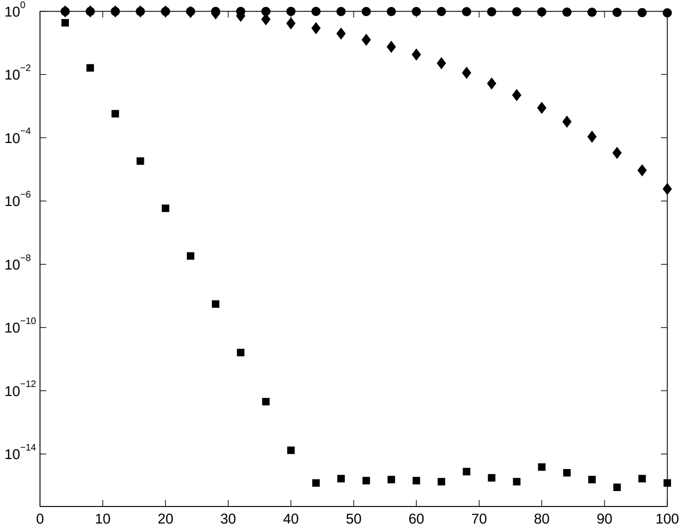
Interpolation error as function of n



Interpolation error as function of n



Interpolation error as function of n



Part II

Properties

Properties of T_n and $\mathcal{T}_n$

Definition

$$T_n(x) = \frac{1}{2}\left(z^n + \frac{1}{z^n}\right)$$
$$\mathcal{T}_n(x) = \frac{1}{2}\left(z^{n-m}B_m(z) + \frac{1}{z^{n-m}B_m(z)}\right)$$

Orthogonality property

$$\int_{-1}^{1} T_j(x)T_k(x)\frac{dx}{\sqrt{1-x^2}} = 0, \quad j \neq k$$
$$\int_{-1}^{1} \mathcal{T}_j(x)\mathcal{T}_k(x)\frac{dx}{\sqrt{1-x^2}} = 0, \quad j \neq k, \quad j,k \geq m$$

Properties of T_n and $\mathcal{T}_n$

Three term recurrence

It is well known that

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

for $n = 1, 2, \ldots$

Writing

$$\mathcal{T}_n(x) = \frac{q_n(x)}{\pi_n(x)}$$

where

$$\begin{aligned} \pi_n(x) &= (x - \alpha_1) \cdots (x - \alpha_n), \quad n \leq m \\ &= \pi_m(x), \quad n > m \end{aligned}$$

we can extend the definition for $\mathcal{T}_n$ to $n < m$ using the theory of orthogonal rational functions

They satisfy the recurrence relation

$$\mathcal{T}_n(x) = \left(A_n \frac{x}{1 - x/\alpha_n} + B_n \frac{1 - x/\alpha_{n-1}}{1 - x/\alpha_n} \right) \mathcal{T}_{n-1}(x) + C_n \frac{1 - x/\bar{\alpha}_{n-2}}{1 - x/\alpha_n} \mathcal{T}_{n-2}(x)$$

for $n = 1, 2, \ldots$ with $\mathcal{T}_0 = 1$ and $\mathcal{T}_{-1} = 0$

The recurrence coefficients A_n, B_n and C_n are known explicitly

Explicit formulas for the recurrence coefficients

$$A_n = 2\frac{(1-\beta_n\beta_{n-1})(1-|\beta_{n-1}|^2)}{(1+\beta_{n-1}^2)(1+\beta_n^2)}$$

$$B_n = -\frac{(1-|\beta_{n-1}|^2)(\beta_n+\bar{\beta}_{n-2})+(\beta_{n-1}+\bar{\beta}_{n-1})(1-\beta_n\bar{\beta}_{n-2})}{(1+\beta_n^2)(1-\beta_{n-1}\bar{\beta}_{n-2})}$$

$$C_n = -\frac{(1-\beta_n\bar{\beta}_{n-1})(1+\bar{\beta}_{n-2}^2)}{(1-\beta_{n-1}\bar{\beta}_{n-2})(1+\beta_n^2)}$$

Interpolation points as eigenvalues

From the three term recurrence it follows immediately that the zeros of $T_n(x)$ are the eigenvalues of

$$\begin{bmatrix} 0 & 1 & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ & & \ddots & \ddots & \\ & & \ddots & & \frac{1}{2} \\ & & & \frac{1}{2} & 0 \end{bmatrix}$$

Explicitly:

$$x_k = \cos \frac{\pi(2k+1)}{2n}, \quad k = 0, 1, \ldots, n-1$$

Interpolation points as eigenvalues

The zeros of $\mathcal{T}_n(x)$ are also the generalised eigenvalues of the matrix pencil $(J_n, J_nD_n - S_n + I_n)$, where

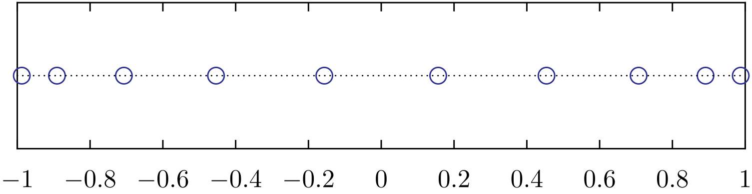
$$J_n = \begin{bmatrix} -\frac{B_1}{A_1} & \frac{1}{A_1} & & & \\ -\frac{C_2}{A_2} & -\frac{B_2}{A_2} & \frac{1}{A_2} & & \\ & \ddots & \ddots & \ddots & \\ & & & -\frac{C_n}{A_n} & -\frac{B_n}{A_n} \end{bmatrix}, D_n = \begin{bmatrix} 0 & & & \\ & \frac{1}{\alpha_1} & & \\ & & \ddots & \\ & & & \frac{1}{\alpha_{n-1}} \end{bmatrix}$$

$$S_n = 2\mathrm{i} \begin{bmatrix} 0 & & & \\ & \frac{\Im(\alpha_1)C_3}{|\alpha_1|^2 A_3} & & \\ & & \ddots & \\ & & & \frac{\Im(\alpha_{n-2})C_n}{|\alpha_{n-2}|^2 A_n} \end{bmatrix}$$

Electrostatic interpretation of the zeros

Chebyshev polynomials

- Put n positive unit charges on $(-1, 1)$ to move freely
- Fix positive charges of magnitude $1/4$ on -1 and 1
- Equilibrium position of unit charges corresponds to zeros of T_n



Chebyshev rational functions

Denote by $\tilde{\alpha}_k$ the m eigenvalues of the matrix

$$\begin{bmatrix} \alpha_1 & & \\ & \ddots & \\ & & \alpha_m \end{bmatrix} + \frac{1}{n-m}\mathbf{w}\mathbf{w}^T$$

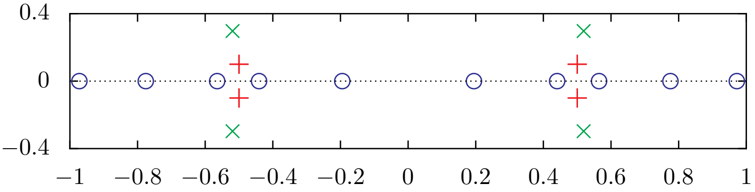
where $\mathbf{w} = [\sqrt{w_1}, \cdots, \sqrt{w_m}]^T$ and $w_k = (1 - \beta_k^2)/(2\beta_k)$

These $\tilde{\alpha}_k$ are *ghost poles*

If m fixed and $n \to \infty$, then they converge to the real poles

Chebyshev rational functions

- Put n positive unit charges on $(-1, 1)$ to move freely
- Fix positive charges of magnitude $1/4$ at -1 and 1
- Fix negative charges of magnitude $1/2$ at each α_k and $\tilde{\alpha}_k$
- Equilibrium position of unit charges corresponds to zeros of $\mathcal{T}_n$



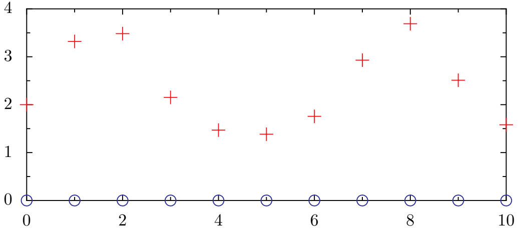
Part III

Spectral collocation methods

Approximating the derivative

Example

Uniform grid $x_0, \ldots, x_n$ with $x_{j+1} - x_j = h$ and function values $f(x_j) = f_j$



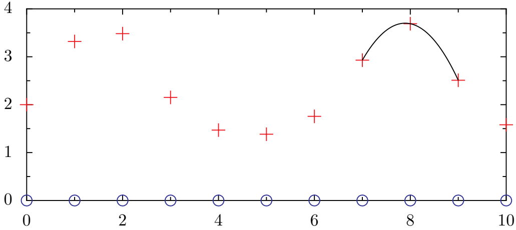
Finite difference approximation

$$f'(x_j) \approx \frac{f_{j+1} - f_{j-1}}{2h}$$

Approximating the derivative

Example

Uniform grid $x_0, \ldots, x_n$ with $x_{j+1} - x_j = h$ and function values $f(x_j) = f_j$



Finite difference approximation

$$f'(x_j) \approx \frac{f_{j+1} - f_{j-1}}{2h}$$

Differentiation matrix

Writing down this approximation for each j gives

$$\begin{bmatrix} f_0' \\ \\ \vdots \\ \\ f_n' \end{bmatrix} \approx h^{-1} \begin{bmatrix} 0 & \frac{1}{2} & & & -\frac{1}{2} \\ -\frac{1}{2} & 0 & \ddots & & \\ & & \ddots & & \\ & & \ddots & 0 & \frac{1}{2} \\ \frac{1}{2} & & & -\frac{1}{2} & 0 \end{bmatrix} \begin{bmatrix} f_0 \\ \\ \vdots \\ \\ f_n \end{bmatrix}$$

Differentiation becomes sparse matrix-vector multiplication

$$\mathbf{f}' \approx D\mathbf{f}$$

Differential equation

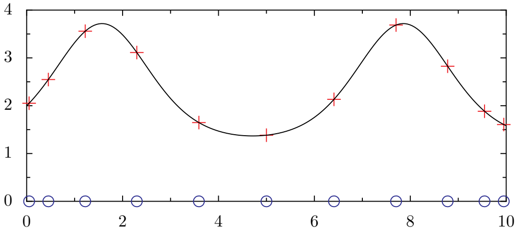
$$f'(x) + f(x) = g(x)$$

becomes linear system

$$(D + I)\mathbf{f} = \mathbf{g}$$

Spectral collocation

- Use global interpolant (polynomial or rational function) instead of local
- Dense differentiation matrices instead of sparse
- $O(e^{-cn})$ convergence instead of $O(n^{-2})$ or $O(n^{-4})$



Boundary value problems

Boundary conditions

If boundary conditions are given in 1 and -1, then we need those points as interpolation points

- either use zeros of T_n or $\mathcal{T}_n$, and include -1 and 1
- or use the extrema (which already include -1 and 1)

Polynomial case

Extrema of T_n are given by the zeros of U_{n-1} together with the points -1 and 1, where U_{n-1} is a Chebyshev polynomial of the second kind

Rational case

Extrema of $\mathcal{T}_n$ are given by the zeros of $\mathcal{U}_{n-1}$ together with the points -1 and 1, where $\mathcal{U}_{n-1}$ is a Chebyshev rational function of the second kind

Solution with boundary/interior layer

If the solution $f(x)$ changes abruptly (almost discontinuously) in a small region of $[-1, 1]$, then

- polynomial interpolation converges too slowly
- rational interpolation is appropriate

How do we choose the poles?
Obtain rough approximation of $f(x)$ using

- boundary layer analysis, or
- polynomial interpolation, or
- …

and extract poles doing some kind of Padé approximation

Interior layer problem

Solve the boundary value problem

$$\epsilon \frac{d^2 f}{dx^2} + x \frac{df}{dx} + xf = 0, \quad -1 < x < 1$$

with boundary values $f(-1) = e$ and $f(1) = 2/e$ where $0 < \epsilon \ll 1$
Asymptotic estimate for $\epsilon \to 0$ gives

$$f(x) \approx \left(\frac{1}{2} \operatorname{erf} \left(\frac{x}{\sqrt{2\epsilon}} \right) + \frac{3}{2} \right) e^{-x}$$

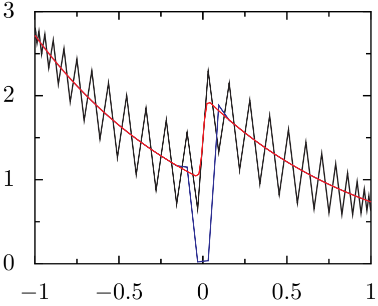
Padé approximation of erf function provides poles

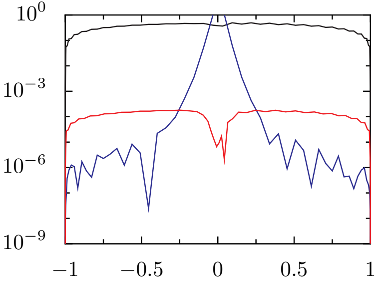
Solution for $\epsilon = 0.0002$

Spectral method with $n = 50$ and $m = 10$

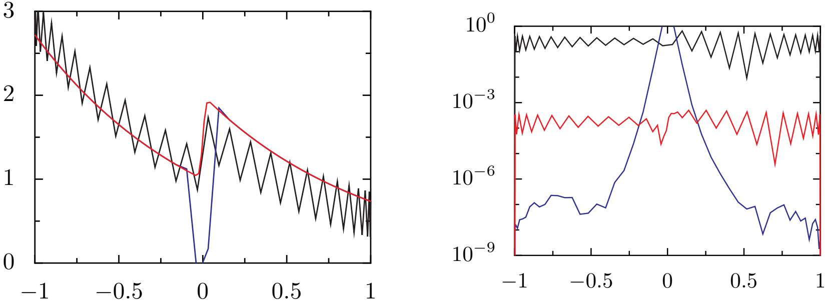
Using

- Polynomial interpolant in zeros of T_n
- Rational interpolant in zeros of T_n
- Rational interpolant in zeros of $\mathcal{T}_n$

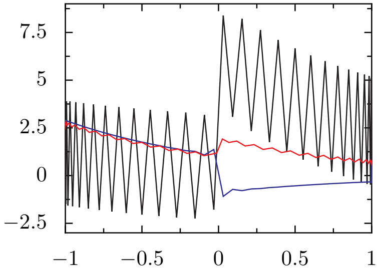


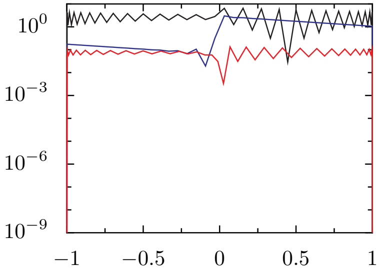


Using the extrema

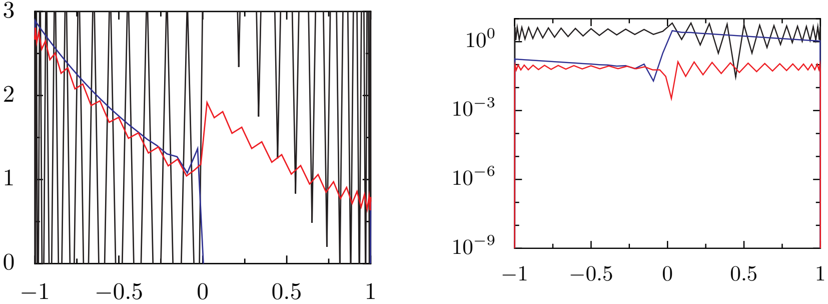


Chebyshev-Padé instead of asymptotic





Chebyshev-Padé instead of asymptotic

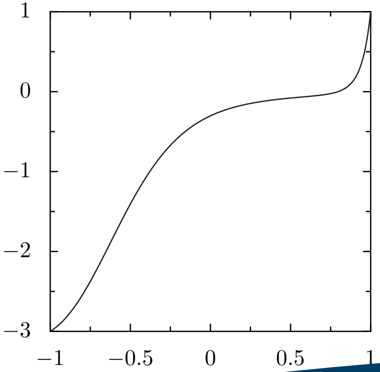


Boundary layer problem

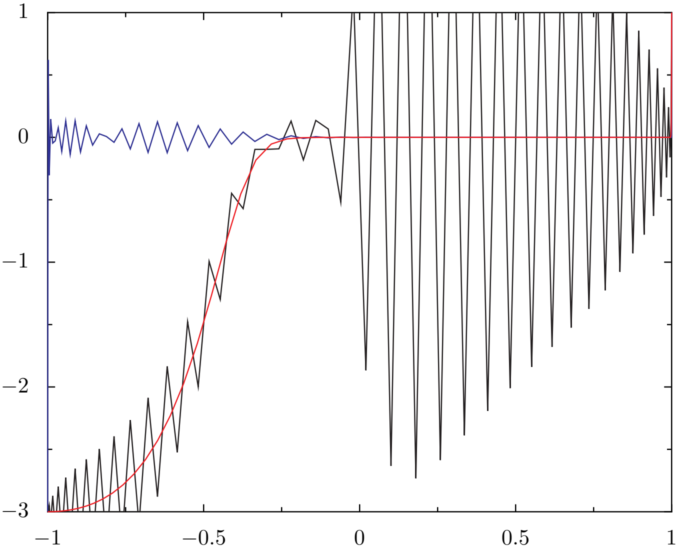
Solve the boundary value problem

$$4\epsilon\frac{d^2f}{dx^2} - 2\left(\frac{x+1}{2} - a\right)^2 \frac{df}{dx} - \frac{x+1}{2}f = 0, \quad -1 < x < 1$$

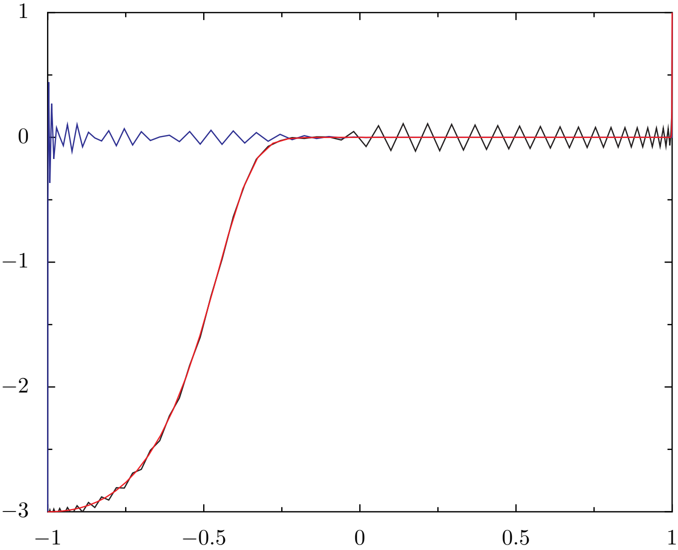
with boundary values $f(-1) = -3$ and $f(1) = 1$ where $0 < \epsilon \ll 1$
Example: $\epsilon = 0.01$, $a = 0.4$



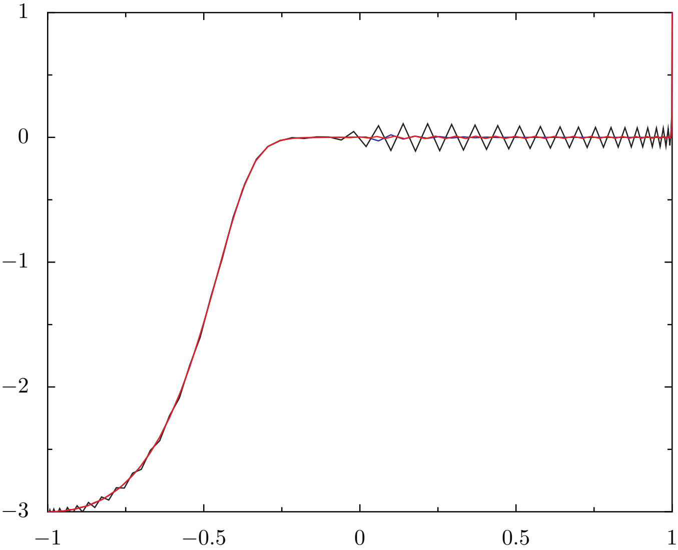
$\epsilon = 0.0001$, zeros, asymptotic, $n = 80$, $m = 20$



Same with extrema instead of poles



Same with Padé instead of asymptotic



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