Near best rational approximation and spectral methods

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Part I

Near best interpolation
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

$$
\|f\| := \|f\|_{\infty} = \max_{-1 \leq x \leq 1} |f(x)|
$$

- 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 $\xi$ 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

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

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

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

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

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

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

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

Polynomial interpolation converges too slowly!
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

$$f(x_i) = \frac{p_n(x_i)}{\pi_m(x_i)}, \quad i = 0, 1, \ldots, n$$
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 \( k = 0, 1, \ldots, n \)
Problem statement
Given \( \pi_m \), 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 \( q_{n+1}/\pi_m \) 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

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

\[ z = x - \sqrt{x^2 - 1} \]
Near best fixed pole rational interpolation

Solution

- Let \( \{\alpha_1, \ldots, \alpha_m\} \) denote zeros of \( \pi_m \)
- Put \( \beta_k = J^{-1}(\alpha_k) \) for \( k = 1, \ldots, m \)
- 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 \( x_0, \ldots, x_n \) are the zeros of \( \mathcal{T}_{n+1}(x) \).
Equi-oscillating rational function on $[-1, 1]$

Example

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

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 $\pi_m$ 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 \( \pm ik \omega \) for \( k = 1, 2, \ldots \)

- Interpolate by \( p_{n-1} \) in zeros of \( T_n \)
- Interpolate by \( p_{n-1} / \pi_{n-2} \)
  - in zeros of \( T_n \)
  - in zeros of \( T_n \)

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 $T_n$

Definition

$$T_n(x) = \frac{1}{2} \left( z^n + \frac{1}{z^n} \right)$$

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

Orthogonality property

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

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

$$\pi_n(x) = (x - \alpha_1) \cdots (x - \alpha_n), \quad n \leq m$$
$$= \pi_m(x), \quad n > m$$

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

\[ T_n(x) = \left( A_n \frac{x}{1 - x/\alpha_n} + B_n \frac{1 - x/\alpha_{n-1}}{1 - x/\alpha_n} \right) T_{n-1}(x) \]

\[ + C_n \frac{1 - x/\bar{\alpha}_{n-2}}{1 - x/\alpha_n} T_{n-2}(x) \]

for \( n = 1, 2, \ldots \) with \( T_0 = 1 \) and \( T_{-1} = 0 \)

The recurrence coefficients \( A_n, B_n \) and \( C_n \) are known explicitly.
Explicit formulas for the recurrence coefficients

\[ A_n = 2 \frac{(1 - \beta_n \beta_{n-1})(1 - |\beta_{n-1}|^2)}{(1 + \beta^2_n)(1 + \beta^2_{n-1})} \]

\[ B_n = -\frac{(1 - |\beta_{n-1}|^2)(\beta_n + \beta_{n-2}) + (\beta_{n-1} + \beta_{n-2})(1 - \beta_n \beta_{n-2})}{(1 + \beta^2_n)(1 - \beta_{n-1} \beta_{n-2})} \]

\[ C_n = -\frac{(1 - \beta_n \beta_{n-1})(1 + \beta^2_{n-2})}{(1 - \beta_{n-1} \beta_{n-2})(1 + \beta^2_n)} \]
Interpolation points as eigenvalues

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

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

Explicitly:

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

The zeros of $T_n(x)$ are also the **generalised eigenvalues** of the matrix pencil $(J_n, J_nD_n - S_n + I_n)$, where

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

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

$$
\begin{bmatrix}
\alpha_1 \\
\vdots \\
\alpha_m
\end{bmatrix} + \frac{1}{n-m} \mathbf{ww}^T
$$

where $\mathbf{w} = [\sqrt{w_1}, \ldots, \sqrt{w_m}]^T$ 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 \(\alpha_k\) and \(\tilde{\alpha}_k\)
- Equilibrium position of unit charges corresponds to zeros of \(T_n\)
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

\[
\begin{bmatrix}
  f'_0 \\
  \vdots \\
  f'_n
\end{bmatrix}
\approx h^{-1}
\begin{bmatrix}
  0 & \frac{1}{2} & \cdots & -\frac{1}{2} \\
  -\frac{1}{2} & 0 & \cdots & \vdots \\
  \vdots & \vdots & \ddots & \vdots \\
  \frac{1}{2} & \cdots & 0 & \frac{1}{2}
\end{bmatrix}
\begin{bmatrix}
  f_0 \\
  \vdots \\
  f_n
\end{bmatrix}
\]

Differentiation becomes sparse matrix-vector multiplication

\[
f' \approx Df
\]

Differential equation

\[
f'(x) + f(x) = g(x)
\]

becomes linear system

\[
(D + I)f = g
\]
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 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
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 \( f(1) = \frac{2}{e} \) where \( 0 < \epsilon \ll 1 \)

Asymptotic estimate for \( \epsilon \to 0 \) gives

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

Padé approximation of \( \text{erf} \) 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 $T_n$
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