Numerical Analysis and Computing

Lecture Notes #13
— Approximation Theory —
Rational Function Approximation

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Outline

1. Approximation Theory
   - Pros and Cons of Polynomial Approximation
   - New Bag-of-Tricks: Rational Approximation
   - Padé Approximation: Example #1
2. Padé Approximation
   - Example #2
   - Finding the Optimal Padé Approximation

Advantages of Polynomial Approximation:

[1] We can approximate any continuous function on a closed interval to within arbitrary tolerance. *(Weierstrass approximation theorem)*

[2] Easily evaluated at arbitrary values. *(e.g. Horner's method)*

[3] Derivatives and integrals are easily determined.

Disadvantage of Polynomial Approximation:

[1] Polynomials tend to be oscillatory, which causes errors. This is sometimes, but not always, fixable: — *E.g.* if we are free to select the node points we can minimize the interpolation error *(Chebyshev polynomials)*, or optimize for integration *(Gaussian Quadrature).*

Moving Beyond Polynomials: Rational Approximation

We are going to use rational functions, $r(x)$, of the form

$$r(x) = \frac{p(x)}{q(x)} = \frac{\displaystyle\sum_{i=0}^{n} p_i x^i}{1 + \displaystyle\sum_{j=1}^{m} q_i x^i}$$

and say that the degree of such a function is $N = n + m$.

Since this is a richer class of functions than polynomials — rational functions with $q(x) \equiv 1$ are polynomials, we expect that **rational approximation of degree N gives results that are at least as good as polynomial approximation of degree N.**

Caveat Emptor!

We take a fairly simplistic view of Rational / Padé approximation in what follows.

More details, theory, warnings, and best practices are found in:

Reference

LLYOD N. TREFETHEN, *Approximation Theory and Approximation Practice*. Chaper 27: Padé Approximation; and Chapter 26: Rational Interpolation and Linearized Least-Squares.

Extension of **Taylor expansion** to rational functions; selecting the p_i's and q_i's so that $r^{(k)}(x_0) = f^{(k)}(x_0)\ \forall k = 0, 1, \ldots, N$.

$$f(x) - r(x) = f(x) - \frac{p(x)}{q(x)} = \frac{f(x)q(x) - p(x)}{q(x)}.$$

Now, use the Taylor expansion $f(x) \sim \sum_{i=0}^{\infty} a_i (x - x_0)^i$, for simplicity $x_0 = 0$:

$$f(x) - r(x) = \frac{\mathbf{\sum_{i=0}^{\infty} a_i x^i \sum_{i=0}^{m} q_i x^i - \sum_{i=0}^{n} p_i x^i}}{q(x)}.$$

Next, we choose $p_0, p_1, \ldots, p_n$ and $q_1, q_2, \ldots, q_m$ so that the numerator has no terms of degree $\leq N$.

Padé Approximation: The Mechanics.

For simplicity/implementation we (sometimes) define the "indexing-out-of-bounds" coefficients:

$$\begin{cases} p_{n+1} = p_{n+2} = \cdots = p_N = 0 \\ q_{m+1} = q_{m+2} = \cdots = q_N = 0, \end{cases}$$

so we can express the **coefficients of** x^k in

$$\sum_{i=0}^{\infty} a_i x^i \sum_{i=0}^{m} q_i x^i - \sum_{i=0}^{n} p_i x^i = 0,$$

as

$$\sum_{i=0}^{k} a_i q_{k-i} = p_k, \quad k = 0, 1, \ldots, N.$$

Find the Padé approximation of $f(x)$ of degree 5, where $f(x) \sim a_0 + a_1 x + \ldots a_5 x^5$ is the Taylor expansion of $f(x)$ about the point $x_0 = 0$.

The corresponding equations are:

x^0	a_0	$-$	p_0	$=$	0
x^1	$a_0 q_1 + a_1$	$-$	p_1	$=$	0
x^2	$a_0 q_2 + a_1 q_1 + a_2$	$-$	p_2	$=$	0
x^3	$a_0 q_3 + a_1 q_2 + a_2 q_1 + a_3$	$-$	p_3	$=$	0
x^4	$a_0 q_4 + a_1 q_3 + a_2 q_2 + a_3 q_1 + a_4$	$-$	p_4	$=$	0
x^5	$a_0 q_5 + a_1 q_4 + a_2 q_3 + a_3 q_2 + a_4 q_1 + a_5$	$-$	p_5	$=$	0

Note: $p_0 = a_0$**!!!** (This reduces the number of unknowns and equations by one (1).)

We get a linear system for $p_1, p_2, \ldots, p_N$ and $q_1, q_2, \ldots, q_N$:

$$\begin{bmatrix} a_0 & & & & \\ a_1 & a_0 & & & \\ a_2 & a_1 & a_0 & & \\ a_3 & a_2 & a_1 & a_0 & \\ a_4 & a_3 & a_2 & a_1 & a_0 \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \\ q_5 \end{bmatrix} - \begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \\ p_5 \end{bmatrix} = - \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{bmatrix}.$$

If we want $n = 3$, $m = 2$: (empty entries = zeros)

$$\left[\begin{array}{cc|ccc} a_0 & & -1 & & \\ a_1 & a_0 & & -1 & \\ a_2 & a_1 & & & -1 \\ \hline a_3 & a_2 & & & \\ a_4 & a_3 & & & \end{array}\right] \begin{bmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \\ p_3 \end{bmatrix} = - \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{bmatrix}.$$

The Taylor series expansion for e^{-x} about $x_0 = 0$ is $\sum_{k=0}^{\infty} \frac{(-1)^k}{k!} x^k$, hence $\{a_0, a_1, a_2, a_3, a_4, a_5\} = \{1, -1, \frac{1}{2}, \frac{-1}{6}, \frac{1}{24}, \frac{-1}{120}\}$.

$$\left[\begin{array}{cc|ccc} 1 & & -1 & & \\ -1 & 1 & & -1 & \\ 1/2 & -1 & & & -1 \\ \hline -1/6 & 1/2 & & & \\ 1/24 & -1/6 & & & \end{array}\right] \begin{bmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \\ p_3 \end{bmatrix} = - \begin{bmatrix} -1 \\ 1/2 \\ -1/6 \\ 1/24 \\ -1/120 \end{bmatrix},$$

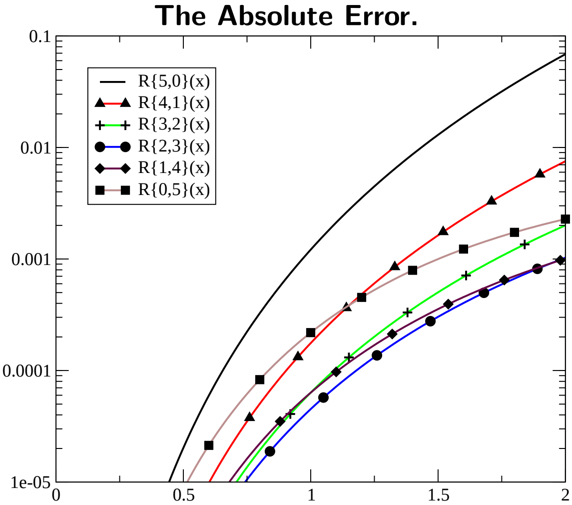
which gives $\{q_1, q_2, p_1, p_2, p_3\} = \{2/5,\ 1/20,\ -3/5,\ 3/20,\ -1/60\}$, *i.e.*

$$r_{3,2}(x) = \frac{1 - \frac{3}{5}x + \frac{3}{20}x^2 - \frac{1}{60}x^3}{1 + \frac{2}{5}x + \frac{1}{20}x^2}.$$

All the possible Padé approximations of degree 5 are:

$$
\begin{aligned}
r_{5,0}(x) &= 1 - x + \tfrac{1}{2}x^2 - \tfrac{1}{6}x^3 + \tfrac{1}{24}x^4 - \tfrac{1}{120}x^5 \\
r_{4,1}(x) &= \frac{1-\frac{4}{5}x+\frac{3}{10}x^2-\frac{1}{15}x^3+\frac{1}{120}x^4}{1+\frac{1}{5}x} \\
r_{3,2}(x) &= \frac{1-\frac{3}{5}x+\frac{3}{20}x^2-\frac{1}{60}x^3}{1+\frac{2}{5}x+\frac{1}{20}x^2} \\
r_{2,3}(x) &= \frac{1-\frac{2}{5}x+\frac{1}{20}x^2}{1+\frac{3}{5}x+\frac{3}{20}x^2+\frac{1}{60}x^3} \\
r_{1,4}(x) &= \frac{1-\frac{1}{5}x}{1+\frac{4}{5}x+\frac{3}{10}x^2+\frac{1}{15}x^3+\frac{1}{120}x^4} \\
r_{0,5}(x) &= \frac{1}{1+x+\frac{1}{2}x^2+\frac{1}{6}x^3+\frac{1}{24}x^4+\frac{1}{120}x^5}
\end{aligned}
$$

Note: $r_{5,0}(x)$ is the Taylor polynomial of degree 5.


The Absolute Error.
R{5,0}(x)
R{4,1}(x)
R{3,2}(x)
R{2,3}(x)
R{1,4}(x)
R{0,5}(x)
0.1
0.01
0.001
0.0001
1e-05
0
0.5
1
1.5
2

Maybe we should worry about division by zero? After all, the polynomials in the denominators have roots.

- $r_{5,0}(x)$: $q(x) = 1$ has no roots.
- $r_{4,1}(x)$: $q(x) = 1 + \frac{1}{5}x$ has the root -5.
- $r_{3,2}(x)$: $q(x) = 1 + \frac{2}{5}x + \frac{1}{20}x^2$ has the roots $-4 \pm 2i$.
- $r_{2,3}(x)$: $q(x) = 1 + \frac{3}{5}x + \frac{3}{20}x^2 + \frac{1}{60}x^3$ has the roots -3.6378, $-2.6811 \pm 3.0504i$.
- $r_{1,4}(x)$: $q(x) = 1 + \frac{4}{5}x + \frac{3}{10}x^2 + \frac{1}{15}x^3 + \frac{1}{120}x^4$ has the roots $-1.2357 \pm 3.4377i$, $-2.7643 + 1.1623i$.
- $r_{0,5}(x)$: $q(x) = 1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 + \frac{1}{24}x^4 + \frac{1}{120}x^5$ has the roots -2.1806, $0.2398 \pm 3.1283i$, $-1.6495 \pm 1.6939i$

For now we sweep such "minor" details under the rug; but keep in mind that troublesome things may happen, and there are potential limits to the usefulness of a particular rational expression.

The algorithm in the book looks frightening! If we think in term of the matrix problem defined earlier, it is easier to figure out what is going on:

```
% The Taylor Coefficients, a0, a1, a2, a3, a4, a5
a = [1 -1 1/2 -1/6 1/24 -1/120]';
N = length(a);   A = zeros(N-1,N-1);
% m is the degree of q(x), and n the degree of p(x)
m = 3;   n = N-1-m;
% Set up the columns which multiply q1 through qm
for i=1:m
   A(i:(N-1),i) = a(1:(N-i));
end
% Set up the columns that multiply p1 through pn
A(1:n,m+(1:n)) = -eye(n)
% Set up the right-hand-side
b = - a(2:N);
% Solve
c = A\b;
Q = [1 ; c(1:m)];  % Select q0 through qm
P = [a0 ; c((m+1):(m+n))];  % Select p0 through pn
```

Optimal Padé Approximation?

	One Point	**Optimal Points**
Polynomials	Taylor	Chebyshev
Rational Functions	Padé	???

From the example e^{-x} we can see that Padé approximations suffer from the **same problem** as Taylor polynomials – they are very accurate near **one point,** but away from that point the approximation degrades.

"Chebyshev-placement" of interpolating points for polynomials gave us an optimal (uniform) error bound over the interval.

Can we do something similar for rational approximations???

We use the **same** idea — instead of expanding in terms of the basis functions x^k, we will use the **Chebyshev polynomials**, $T_k(x)$, as our basis, *i.e.*

$$r_{n,m}(x) = \frac{\sum_{k=0}^{n} p_k T_k(x)}{\sum_{k=0}^{m} q_k T_k(x)},$$

where $N = n + m$, and $q_0 = 1$.

We also need to expand $f(x)$ in a series of Chebyshev polynomials:

$$f(x) = \sum_{k=0}^{\infty} a_k T_k(x),$$

so that

$$f(x) - r_{n,m}(x) = \frac{\sum_{k=0}^{\infty} a_k T_k(x) \sum_{k=0}^{m} q_k T_k(x) - \sum_{k=0}^{n} p_k T_k(x)}{\sum_{k=0}^{m} q_k T_k(x)}.$$

The Resulting Equations

Again, the coefficients $p_0, p_1, \ldots, p_n$ and $q_1, q_2, \ldots, q_m$ are chosen so that the numerator has zero coefficients for $T_k(x)$, $k = 0, 1, \ldots, N$, *i.e.*

$$\sum_{k=0}^{\infty} a_k T_k(x) \sum_{k=0}^{m} q_k T_k(x) - \sum_{k=0}^{n} p_k T_k(x) = \sum_{\mathbf{k=N+1}}^{\infty} \gamma_k T_k(x).$$

We will need the following relationship:

$$T_i(x) T_j(x) = \frac{1}{2} \left[T_{i+j}(x) + T_{|i-j|}(x) \right].$$

Also, we must compute (maybe numerically)

$$a_0 = \frac{1}{\pi} \int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}\, dx \quad \text{and} \quad a_k = \frac{2}{\pi} \int_{-1}^{1} \frac{f(x) T_k(x)}{\sqrt{1-x^2}}\, dx, \quad k \geq 1.$$

The 8th order Chebyshev-expansion (All Praise Maple) for e^{-x} is

$$\begin{aligned} P_8^{CT}(x) &= 1.266065878\, T_0(x) - 1.130318208\, T_1(x) + 0.2714953396\, T_2(x) \\ &\quad -0.04433684985\, T_3(x) + 0.005474240442\, T_4(x) \\ &\quad -0.0005429263119\, T_5(x) + 0.00004497732296\, T_6(x) \\ &\quad -0.000003198436462\, T_7(x) + 0.0000001992124807\, T_8(x), \end{aligned}$$

and using the same strategy — building a matrix and right-hand-side utilizing the coefficients in this expansion, we can solve for the Chebyshev-Padé polynomials of degree $(n + 2m) \leq 8$:

Next slide shows the matrix set-up for the $r_{3,2}^{CP}(x)$ approximation.

Note: Due to the "folding", $T_i(x)T_j(x) = \frac{1}{2}\left[T_{i+j}(x) + T_{|i-j|}(x)\right]$, we need $n + 2m$ Chebyshev-expansion coefficients. (Burden-Faires(8th) do not mention this, but it is "obvious" from algorithm 8.2; Example 2 (p. 519) is broken, – it needs $\tilde{P}_7(x)$.)

$$T_0(x): \tfrac{1}{2}\Big[\quad a_1 q_1 \quad + \quad a_2 q_2 \quad - \quad 2p_0 \quad = \quad 2a_0 \quad \Big]$$

$$T_1(x): \tfrac{1}{2}\Big[\quad (2a_0 + a_2) q_1 \quad + \quad (a_1 + a_3) q_2 \quad - \quad 2p_1 \quad = \quad 2a_1 \quad \Big]$$

$$T_2(x): \tfrac{1}{2}\Big[\quad (a_1 + a_3) q_1 \quad + \quad (2a_0 + a_4) q_2 \quad - \quad 2p_2 \quad = \quad 2a_2 \quad \Big]$$

$$T_3(x): \tfrac{1}{2}\Big[\quad (a_2 + a_4) q_1 \quad + \quad (a_1 + a_5) q_2 \quad - \quad 2p_3 \quad = \quad 2a_3 \quad \Big]$$

$$T_4(x): \tfrac{1}{2}\Big[\quad (a_3 + a_5) q_1 \quad + \quad (a_2 + a_6) q_2 \quad - \quad 0 \quad = \quad 2a_4 \quad \Big]$$

$$T_5(x): \tfrac{1}{2}\Big[\quad (a_4 + a_6) q_1 \quad + \quad (a_3 + a_7) q_2 \quad - \quad 0 \quad = \quad 2a_5 \quad \Big]$$

Example: Revisiting e^{-x} with Chebyshev-Padé Approximation

$\mathbf{R}^{\mathrm{CP}}_{\mathbf{4,1}}(\mathbf{x}) =$

$$\frac{1.155054\ T_0(x) - 0.8549674\ T_1(x) + 0.1561297\ T_2(x) - 0.01713502\ T_3(x) + 0.001066492\ T_4(x)}{T_0(x) + 0.1964246628\ T_1(x)}$$

$\mathbf{R}^{\mathrm{CP}}_{\mathbf{3,2}}(\mathbf{x}) =$

$$\frac{1.050531166\ T_0(x) - 0.6016362122\ T_1(x) + 0.07417897149\ T_2(x) - 0.004109558353\ T_3(x)}{T_0(x) + 0.3870509565\ T_1(x) + 0.02365167312\ T_2(x)}$$

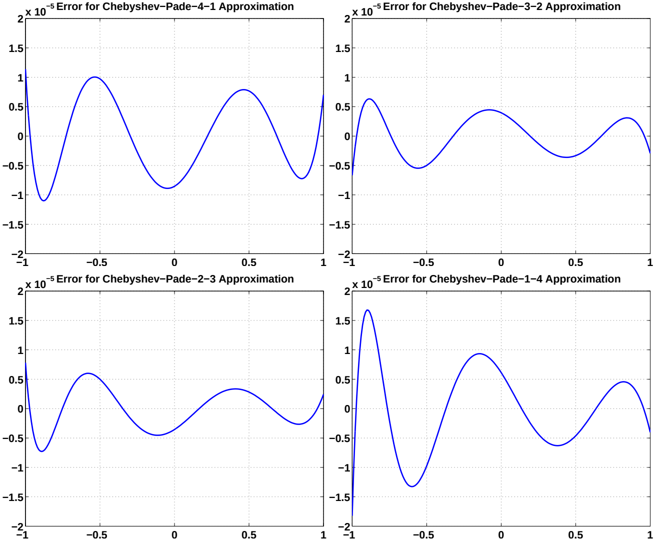
$\mathbf{R}^{\mathrm{CP}}_{\mathbf{2,3}}(\mathbf{x}) =$

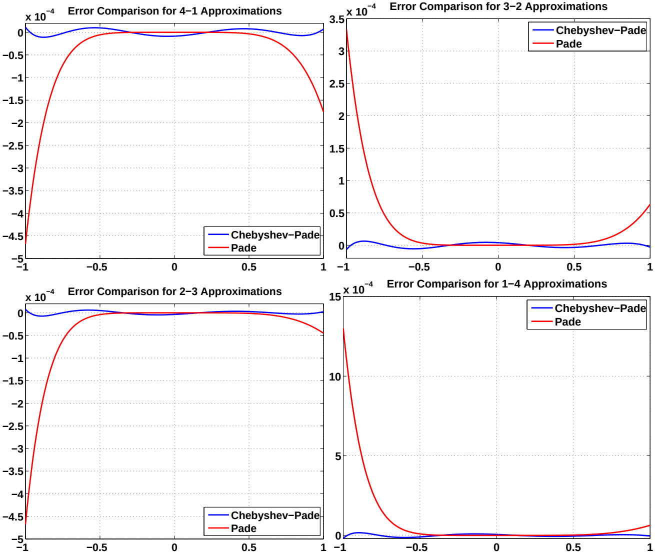
$$\frac{0.9541897238\ T_0(x) - 0.3737556255\ T_1(x) + 0.02331049609\ T_2(x)}{T_0(x) + 0.5682932066\ T_1(x) + 0.06911746318\ T_2(x) + 0.003726440404\ T_3(x)}$$

$\mathbf{R}^{\mathrm{CP}}_{\mathbf{1,4}}(\mathbf{x}) =$

$$\frac{0.8671327116\ T_0(x) - 0.1731320271\ T_1(x)}{T_0(x) + 0.73743710\ T_1(x) + 0.13373746\ T_2(x) + 0.014470654\ T_3(x) + 0.00086486509\ T_4(x)}$$

Example: Revisiting e^{-x} with Chebyshev-Padé Approximation




x 10^-4
Error Comparison for 4−1 Approximations
Chebyshev−Pade
Pade
0
−0.5
−1
−1.5
−2
−2.5
−3
−3.5
−4
−4.5
−5
−1
−0.5
0
0.5
1
x 10^-4
Error Comparison for 3−2 Approximations
Chebyshev−Pade
Pade
3.5
3
2.5
2
1.5
1
0.5
0
−1
−0.5
0
0.5
1
x 10^-4
Error Comparison for 2−3 Approximations
Chebyshev−Pade
Pade
0
−0.5
−1
−1.5
−2
−2.5
−3
−3.5
−4
−4.5
−5
−1
−0.5
0
0.5
1
x 10^-4
Error Comparison for 1−4 Approximations
Chebyshev−Pade
Pade
15
10
5
0
−1
−0.5
0
0.5
1

The Bad News — It's Not Optimal!

The Chebyshev basis does not give an optimal (in the min-max sense) rational approximation. However, the result can be used as a starting point for **the second Remez algorithm**. It is an iterative scheme which converges to the best approximation.

A discussion of how and why (and why not) you may want to use the second Remez' algorithm can be found in **Numerical Recipes in C: The Art of Scientific Computing** (Section 5.13). [You can read it for free on the web$^{(*)}$ — just Google for it!]

$^{(*)}$ The old 2nd Edition is Free, the new 3rd edition is for sale...