# 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

# Polynomial Approximation: Pros and Cons.

## Advantages of Polynomial Approximation:

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## 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

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

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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 $N$.**

# Padé Approximation

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

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

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

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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 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

$$\sum_{i=0}^{\infty} a_i x^i \sum_{i=0}^{m} q_i x^i - \sum_{i=0}^{n} p_i x^i = 0, \quad k = 0, 1, \ldots, N$$

as

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

## Padé Approximation: Abstract Example



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

The corresponding equations are:

$$\begin{array}{c|lcccc}
x^0 & a_0 & - & p_0 & = & 0 \\
\hline
x^1 & a_0 q_1 + a_1 & - & p_1 & = & 0 \\
x^2 & a_0 q_2 + a_1 q_1 + a_2 & - & p_2 & = & 0 \\
x^3 & a_0 q_3 + a_1 q_2 + a_2 q_1 + a_3 & - & p_3 & = & 0 \\
x^4 & a_0 q_4 + a_1 q_3 + a_2 q_2 + a_3 q_1 + a_4 & - & p_4 & = & 0 \\
x^5 & a_0 q_5 + a_1 q_4 + a_2 q_3 + a_3 q_2 + a_4 q_1 + a_5 & - & p_5 & = & 0
\end{array}$$

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

## Padé Approximation: Abstract Example



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 $n = 3$, $m = 2$:

$$\begin{bmatrix} a_0 & & & & \\ a_1 & a_0 & & & \\ a_2 & a_1 & \mathbf{a_0} & & \\ a_3 & a_2 & \mathbf{a_1} & \mathbf{a_0} & \\ a_4 & a_3 & \mathbf{a_2} & \mathbf{a_1} & \mathbf{a_0} \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} - \begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ 0 \\ 0 \end{bmatrix} = - \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{bmatrix}.$$

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If we want $n = 3$, $m = 2$:

$$\begin{bmatrix} a_0 & & \mathbf{-1} & & \\ a_1 & a_0 & & & \\ a_2 & a_1 & \mathbf{0} & & \\ a_3 & a_2 & \mathbf{0} & a_0 & \\ a_4 & a_3 & \mathbf{0} & a_1 & a_0 \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ \mathbf{p_1} \\ 0 \\ 0 \end{bmatrix} - \begin{bmatrix} \mathbf{0} \\ p_2 \\ p_3 \\ 0 \\ 0 \end{bmatrix} = - \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{bmatrix}.$$

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If we want $n = 3$, $m = 2$:

$$\begin{bmatrix} a_0 & & -1 & & \\ a_1 & a_0 & & \mathbf{-1} & \\ a_2 & a_1 & 0 & & \\ a_3 & a_2 & 0 & \mathbf{0} & \\ a_4 & a_3 & 0 & \mathbf{0} & a_0 \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ p_1 \\ \mathbf{p_2} \\ 0 \end{bmatrix} - \begin{bmatrix} 0 \\ \mathbf{0} \\ p_3 \\ 0 \\ 0 \end{bmatrix} = - \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{bmatrix}.$$

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## Padé Approximation: Concrete Example, $e^{-x}$



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

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$$\begin{bmatrix} 1 & 0 & -1 & & \\ -1 & 1 & 0 & -1 & \\ 1/2 & -1 & 0 & 0 & -1 \\ -1/6 & 1/2 & 0 & 0 & 0 \\ 1/24 & -1/6 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \\ p_3 \end{bmatrix} = - \begin{bmatrix} -1 \\ 1/2 \\ -1/6 \\ 1/24 \\ -1/120 \end{bmatrix},$$

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

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

## Padé Approximation: Concrete Example, $e^{-x}$



All the possible Padé approximations of degree 5 are:

$$r_{5,0}(x) = 1 - x + \frac{1}{2}x^2 - \frac{1}{6}x^3 + \frac{1}{24}x^4 - \frac{1}{120}x^5$$

$$r_{4,1}(x) = \frac{1-\frac{4}{5}x+\frac{3}{10}x^2-\frac{1}{15}x^3+\frac{1}{120}x^4}{1+\frac{1}{5}x}$$

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

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

$$r_{1,4}(x) = \frac{1-\frac{1}{5}x}{1+\frac{4}{5}x+\frac{3}{10}x^2+\frac{1}{15}x^3+\frac{1}{120}x^4}$$

$$r_{0,5}(x) = \frac{1}{1+x+\frac{1}{2}x^2+\frac{1}{6}x^3+\frac{1}{24}x^4+\frac{1}{120}x^5}$$

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

## Chebyshev Basis for the Padé Approximation!

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 $q_0 = 1$.

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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)

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

## Example: Revisiting $e^{-x}$ with Chebyshev-Padé Approximation 1/5

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

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

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 do not mention this, but it is "obvious" from algorithm 8.2; Example 2 (p. 519) is broken, – it needs $\tilde{P}_7(x)$.)

## Example: Revisiting $e^{-x}$ with Chebyshev-Padé Approximation 2/5

$$
\begin{array}{ll}
T_0(x): \frac{1}{2}\Big[ & a_1 q_1 + a_2 q_2 - 2p_0 = 2a_0 \Big] \\
T_1(x): \frac{1}{2}\Big[ & (2a_0 + a_2)q_1 + (a_1 + a_3)q_2 - 2p_1 = 2a_1 \Big] \\
T_2(x): \frac{1}{2}\Big[ & (a_1 + a_3)q_1 + (2a_0 + a_4)q_2 - 2p_2 = 2a_2 \Big] \\
T_3(x): \frac{1}{2}\Big[ & (a_2 + a_4)q_1 + (a_1 + a_5)q_2 - 2p_3 = 2a_3 \Big] \\
T_4(x): \frac{1}{2}\Big[ & (a_3 + a_5)q_1 + (a_2 + a_6)q_2 - 0 = 2a_4 \Big] \\
T_5(x): \frac{1}{2}\Big[ & (a_4 + a_6)q_1 + (a_3 + a_7)q_2 - 0 = 2a_5 \Big]
\end{array}
$$

# Example: Revisiting $e^{-x}$ with Chebyshev-Padé Approximation 3/5

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

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

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

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

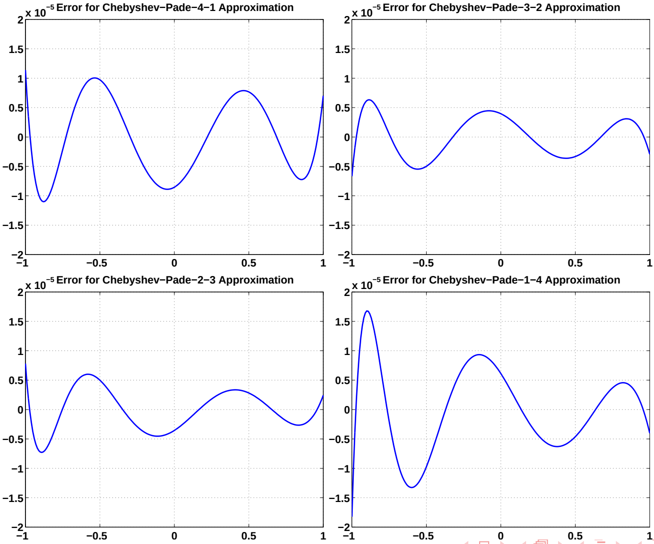
$\mathbf{R^{CP}_{2,3}(x)} =$

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

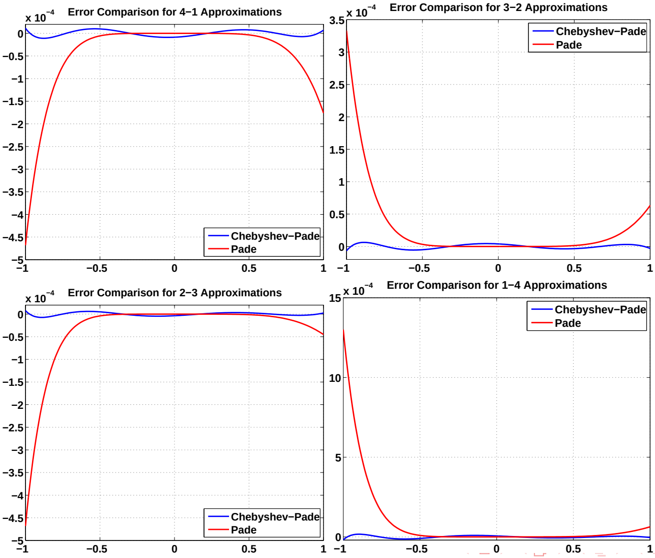
$\mathbf{R^{CP}_{1,4}(x)} =$

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

# Example: Revisiting $e^{-x}$ with Chebyshev-Padé Approximation 4/5



# Example: Revisiting $e^{-x}$ with Chebyshev-Padé Approximation 5/5



## 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...