Math 541: Numerical Analysis and Computation

Approximation Theory Rational Function Approximation

Lecture Notes #13

Joe Mahaffy Department of Mathematics San Diego State University San Diego, CA 92182-7720 mahaffy@math.sdsu.edu http://www-rohan.sdsu.edu/~jmahaffy

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Moving Beyond Polynomials: Rational Approximation.

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

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

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.

Polynomial Approximation: Pros and Cons.

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).

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Padé Approximation

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

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

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

$$f(x) - r(x) = \frac{\sum_{i=0}^{\infty} \mathbf{a}_i \mathbf{x}^i \sum_{i=0}^{m} \mathbf{q}_i \mathbf{x}^i - \sum_{i=0}^{n} \mathbf{p}_i \mathbf{x}^i}{q(x)}.$$

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 $\leq N$.

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

$$p_{n+1} = p_{n+2} = \dots = p_N = 0$$

 $q_{m+1} = q_{m+2} = \dots = q_N = 0$

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

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

as

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

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Padé Approximation: Abstract Example

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

a_0]	q_1		p_1		a_1	
a_1	a_0				q_2		p_2		a_2	
a_2	a_1	a_0			q_3	-	p_3	= -	a_3	
a_3	a_2	a_1	a_0		q_4		p_4		a_4	
a_4	a_3	a_2	a_1	a_0	q_5		p_5		a_5	

If we want n = 3, m = 2:

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

Padé Approximation: Abstract Example

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
	$a_0q_1 + a_1$	_	p_1	=	0
x^2	$a_0q_2 + a_1q_1 + a_2$	_	p_2	=	0
	$a_0q_3 + a_1q_2 + a_2q_1 + a_3$	_	p_3	=	0
x^4	$a_0q_4 + a_1q_3 + a_2q_2 + a_3q_1 + a_4$		p_4		
x^5	$a_0q_5 + a_1q_4 + a_2q_3 + a_3q_2 + a_4q_1 + a_5$	_	p_5	=	0

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

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

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

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

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

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

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All the possible Padé approximations of degree 5 are:

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

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

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

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

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

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

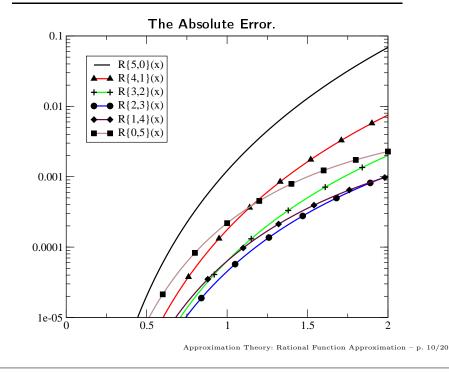
Note: $r_{5,0}(x)$ is the Taylor polynomial of degree 5.

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Padé Approximation: Matlab Code.

The algorithm in the book looks very 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, a_0, a_1, a_2, a_3, a_4, a_5
a = [1 -1 1/2 -1/6 1/24 -1/120]';
  = length(a); A = zeros(N-1, N-1);
  m is the degree of q(x), and n the degree of p(x)
  = 3; n = N-1-m;
% Set up the columns which multiply q_1 through q_m
for i=1:m
  A(i:(N-1),i) = a(1:(N-i));
end
% Set up the columns that multiply p_1 through p_n
A(1:n,m+(1:n)) = -eye(n)
% Set up the right-hand-side
b = -a(2:N);
% Solve
c = A \setminus b;
Q = [1 ; c(1:m)]; % Select q_0 through q_m
P = [a_0 ; c((m+1):(m+n))]; % Select p_0 through p_n
```



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

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

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

The 8th order Chebyshev-expansion (ALL PRAISE MAPLE) for e^{-x} is

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

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

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 $\tilde{P}_7(x)$.)

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.*

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

We will need the following relationship:

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

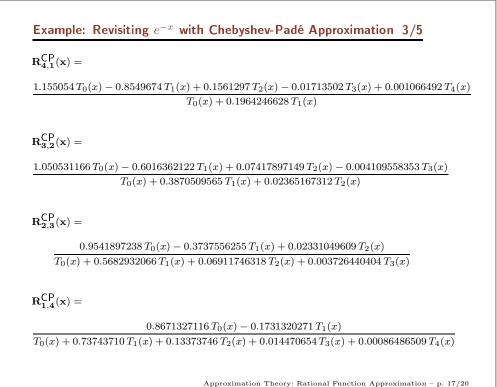
Also, we must compute (usually numerically)

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

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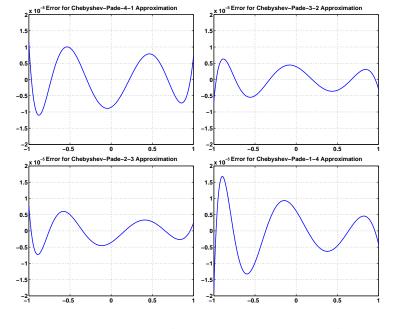
Example: Revisiting e^{-x} with Chebyshev-Padé Approximation 2/5

$$T_{0}(x): \frac{1}{2} \begin{bmatrix} a_{1}q_{1} & + a_{2}q_{2} & - 2p_{0} & = 2a_{0} \\ T_{1}(x): \frac{1}{2} \begin{bmatrix} (2a_{0}+a_{2})q_{1} & + (a_{1}+a_{3})q_{2} & - 2p_{1} & = 2a_{1} \\ T_{2}(x): \frac{1}{2} \begin{bmatrix} (a_{1}+a_{3})q_{1} & + (2a_{0}+a_{4})q_{2} & - 2p_{2} & = 2a_{2} \\ T_{3}(x): \frac{1}{2} \begin{bmatrix} (a_{2}+a_{4})q_{1} & + (a_{1}+a_{5})q_{2} & - 2p_{3} & = 2a_{3} \\ T_{4}(x): \frac{1}{2} \begin{bmatrix} (a_{3}+a_{5})q_{1} & + (a_{2}+a_{6})q_{2} & - 0 & = 2a_{4} \\ T_{5}(x): \frac{1}{2} \begin{bmatrix} (a_{4}+a_{6})q_{1} & + (a_{3}+a_{7})q_{2} & - 0 & = 2a_{5} \end{bmatrix}$$



Example: Revisiting e^{-x} with Chebyshev-Padé Approximation 5/5 Error Comparison for 3–2 Approximations x 10⁻⁴ Error Comparison for 4–1 Approximations Chebyshev-Pad -0.5 2.5 -1.5 -2 -2.5 1.5 -3 -3.5 0.5 -Chebyshev-Pac -4.5 - Pade -0.5 -0.5 0.5 -1 0 Error Comparison for 1-4 Approximations x 10⁻⁴ Error Comparison for 2–3 Approximation <u>x 10⁻⁴</u> Chebyshev-Pac -0.5 -1 -1.5 -2 -2.5 -3 -3.5 -4 5 Chebyshev-Pa - Pade -5 0.5 -0.5 0.5 Approximation Theory: Rational Function Approximation - p. 19/20

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



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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!]