Padé Approximations

And Continued Fractions

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Topics

- Theory
- Examples
- Applications

Motivation

- If a power series representation of a function diverges it indicates the presence of singularities
- This divergence reflect that a polynomial cannot appropriately approximate the function near the singularities
- Want to find a way to represent the function in question with a convergent expression.
- Want a summation algorithm that only requires a finite number of terms of a divergent series
- An answer is Padé Approximations

[0] Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

Theory

An asymptotic expansion can be expressed by replacing the power series $\sum c_n z^n$ by a ratio of two similar functions:

$$P_M^N(z) = \frac{\sum_{n=0}^{N} a_n z^n}{\sum_{n=0}^{M} b_n z^n}$$

This sequence of rational functions is a Padé Approximation.

[0] Fornberg, B., Calculation of weights in finite difference formulas, SIAM Rev. 40:685-691, 1998.

Generalizing Taylor Expansion

$$P_M^N(z) = \frac{\sum_{n=0}^{N} a_n z^n}{\sum_{n=0}^{M} b_n z^n}$$

Generalizes the Taylor expansion with equal degrees of freedom

$$T_{M+N}(z) = \sum_{n=0}^{M+N} c_n z^n$$

Which are equivalent for $M = 0$

[0] Fornberg, B., Calculation of weights in finite difference formulas, SIAM Rev. 40:685-691, 1998.

Choosing Coefficients

$$\text{Taking:} \quad P_M^N(z) = \frac{\sum_{n=0}^{N} a_n z^n}{\sum_{n=0}^{M} b_n z^n}$$

- Normalized by letting $b_0 = 1$ without loss of generality
- Must choose the remaining $(M + N + 1)$ coefficients
- Choose $a_0, a_1, ..., a_{N-1}, a_N, b_1, b_2, ..., b_{M-1}, b_M$ such that the first $(M + N + 1)$ terms of the Taylor expansion of $P_M^N(z)$ match the first $(M + N + 1)$ terms of the power series $\sum c_n z^n$

[0] Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

Choosing Coefficients In Practice

$$P_M^N(z) = \frac{\sum_{n=0}^{N} A_n z^n}{\sum_{n=0}^{M} B_n z^n}, \quad T_{M+N}(z) = \sum_{n=0}^{M+N} c_n z^n$$

Equate the Taylor Expansion

$$\frac{a_0 + a_1 x + a_2 x^2 + \ldots}{1 + b_1 x + b_2 x^2 + \ldots} = c_0 + c_1 x + c_2 x^2 + \ldots$$

Multiply over yields coefficient relations:

$$\begin{aligned}
a_0 &= c_0 \\
a_1 &= c_1 + c_0 b_1 \\
a_2 &= c_2 + c_1 b_1 + c_0 b_2 \\
a_3 &= c_3 + c_2 b_1 + c_1 b_2 + c_0 b_3 \\
&\ldots
\end{aligned}$$

[0] Fornberg, B., Calculation of weights in finite difference formulas, SIAM Rev. 40:685-691, 1998.

Specifying Degree

$$a_0 = c_0$$
$$a_1 = c_1 + c_0 b_1$$
$$a_2 = c_2 + c_1 b_1 + c_0 b_2$$
$$\dots$$

The above system of equations at first appears underdetermined. However, recall

$$P_M^N(z) = \frac{\sum_{n=0}^{N} A_n z^n}{\sum_{n=0}^{M} B_n z^n}, \quad T_{M+N}(z) = \sum_{n=0}^{M+N} c_n z^n$$

Take the degree of the numerator and denominator to be N and M respectively, and truncate the Taylor expansion to M+N+1 terms

[0] Fornberg, B., Calculation of weights in finite difference formulas, SIAM Rev. 40:685-691, 1998.

Example: Coefficients

Given $T_5(x)$, determine $P_3^2(x)$
$M + N = 5,\ N = 2,\ M = 3$ Then:

$$a_0 = c_0$$
$$a_1 = c_1 + c_0 b_1$$
$$a_2 = c_2 + c_1 b_1 + c_0 b_2$$

no more a's available $\Rightarrow$

$$\boxed{\begin{aligned} 0 &= c_3 + c_2 b_1 + c_1 b_2 + c_0 b_3 \\ 0 &= c_4 + c_3 b_1 + c_2 b_2 + c_1 b_3 \\ 0 &= c_5 + c_4 b_1 + c_3 b_2 + c_2 b_3 \end{aligned}}$$

no more b's avail.

past limit $O(x^{2+3+1})$

Solve for b_1, b_2, b_3 and then a_0, a_1, a_2

[0] Fornberg, B., Calculation of weights in finite difference formulas, SIAM Rev. 40:685-691, 1998.

The Padé Approximate

- A key feature of the Padé is not needing to know the full power series representation of a function to construct a Padé approximate. Just the first $(M+N+1)$ terms
- Padé Approximation often allows approximations to be found outside the radius of convergence of a power series expansion
- Padé Approximation can also accelerate convergence
- Often if $\sum c_n z^n$ is the power series representation of $f(z)$ then $P_M^N(z) \to f(z)$ as $M, N \to \infty$ EVEN if $\sum c_n z^n$ is a divergent series
- Consider the convergence of Padé sequences $P_0^j, P_1^{1+j}, P_2^{2+j}, P_3^{3+j}, \ldots$ with $N = M + j$, j fixed and $M \to \infty$
- $j = 0$ is the diagonal sequence
- Computationally convenient as they only contain algebraic terms. No integration

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[0] Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

[0] Fornberg, B., Calculation of weights in finite difference formulas, SIAM Rev. 40:685-691, 1998.

Padé Approximate Example

Consider $\frac{1}{(1+x)}$ with Taylor expansion $f(x) = 1 - x + x^2 - x^3 + \ldots$
The Padé approximate of f(x) has padé table:

		N - order of numerator				
		0	1	2	3	....
	0	1	$1 - x$	$1 - x + x^2$	$1 - x + x^2 - x^3$	
M -	1	$\frac{1}{1+x}$	$\frac{1}{1+x}$	$\frac{1}{1+x}$	....	
order of denomi-nator	2	$\frac{1}{1+x}$	$\frac{1}{1+x}$	....		
	3	$\frac{1}{1+x}$	....			
	....	....				

In a Padé table the main diagonal and the diagonal immediately bellow it commonly give the best result.

[0] Fornberg, B., Calculation of weights in finite difference formulas, SIAM Rev. 40:685-691, 1998.

Computational Convenience

- The Padé approximate is computationally convenient as it only contain algebraic terms.
- Further, the Padé approximate can be expressed in terms of determinants

Computational Convenience Cont.

The Padé approximate $P_M^N(z) = \frac{\sum_{n=0}^{N} A_n z^n}{\sum_{n=0}^{M} B_n z^n}$ can be found through simple matrix operations

- First the coefficients of the denominator $B_1, B_2, ..., B_{M-1}, B_M$ (recall $B_0 = 1$) can be found by solving the matrix equation:

$$\alpha \begin{bmatrix} B_1 \\ B_2 \\ \dots \\ B_{M-1} \\ B_M \end{bmatrix} = - \begin{bmatrix} a_{N+1} \\ a_{N+2} \\ \dots \\ a_{N+M-1} \\ a_{N+M} \end{bmatrix}$$

- Where α is an MxM matrix with entries $\alpha_{ij} = a_{N+i-j}$ $(1 \leq i, j \leq M)$

[0]Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

Computational Convenience Cont.[2]

- Second the coefficients of the numerator $A_0, A_1, ..., A_{N-1}, A_N$ can be found by solving:

$$A_N = \sum_{j=0}^{n} a_{n-j} B_j, \quad \text{where} \quad 0 \leq n \leq N$$

- where $B_j = 0$ for $j > M$

[0]Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

Computational Convenience Cont.[3]

The two preceding equations are derived by equating coefficients of $1, z, \ldots, z^{N+M}$ in:

$$\sum_{j=0}^{N+M} a_j z^j \sum_{k=0}^{M} B_k z^k - \sum_{n=0}^{N} A_n z^n = O(z^{N+M+1})$$

Which is a restatement of the definition of a Padé approximate as can be seen here:

$$\sum_{j=0}^{N+M} a_j z^j \sum_{k=0}^{M} B_k z^k - \sum_{n=0}^{N} A_n z^n = O(z^{N+M+1})$$

$$\sum_{j=0}^{N+M} a_j z^j = \frac{\sum_{n=0}^{N} A_n z^n}{\sum_{k=0}^{M} B_k z^k} + O(z^{N+M+1}) \implies P_M^N(z) = \frac{\sum_{n=0}^{N} A_n z^n}{\sum_{n=0}^{M} B_n z^n}$$

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[0] Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

Application

- Evaluating Taylor expansions outside their radius of convergence

- Determining weights in FD formulas

Evaluating Taylor Expansions

Evaluating Taylor expansions outside their radius of convergence.

Example 3: Approximate $f(2)$ when we only know the first few terms in the expansion $f(x) = 1 - \frac{1}{2}x + \frac{1}{3}x^2 - \frac{1}{4}x^3 + \frac{1}{5}x^4 - + \ldots \left(= \frac{\ln(1+x)}{x}\right.$, but only if $\left.|x| < 1\right)$.

The Padé table below is laid out like Table 3, but shows only the numerical values for $x = 2$ and, in parenthesis, the errors in these compared to $\frac{1}{2}\ln 3 \approx 0.5493$.

TABLE 4

Truncated power series expansion compared to values from main Padé diagonal

		N - order of numerator					
		0	1	2	3	4	....
M - order of denominator	0	1 (0.4507)	0 (-0.5493)	1.3333 (0.7840)	-0.6667 (-1.2160)	2.5333 (1.9840)	
	1		0.5714 (0.0221)				
	2			0.5507 (0.0014)			
	3				0.5494 (0.0001)		
	4					0.5493 (0.0000)	
	....						....

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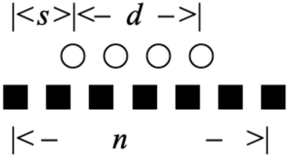
[0] Fornberg, B., Calculation of weights in finite difference formulas, SIAM Rev. 40:685-691, 1998.

Determining FD Weights

Determining weights in FD formulas

Recall that a Finite Difference Stencil is of the form:



With s (real), d (integer ≥ 0), $n(integer > 0)$,■ entries for f, ○ entries for $f^{(m)}$.

[0] Fornberg, B., Calculation of weights in finite difference formulas, SIAM Rev. 40:685-691, 1998.

Determining FD Weights

Given this structure, the optimal weights in the stencil can be calculated with this symbolic code:

$$t = PadeApproximant[x^s * (Log[x]/h)^m, x, 1, n, d];$$
$$CoefficientList[Denominator[t], Numerator[t], x]$$

First discovered in 1998, in Fornberg, B., Calculation of weights in finite difference formulas, SIAM Rev. 40:685-691, 1998.

[0] Fornberg, B., Calculation of weights in finite difference formulas, SIAM Rev. 40:685-691, 1998.

Determining FD Weights

<u>Example 5:</u> The choice `s=0, d=2, n=2, m=2` describes a stencil of the shape

○ ○ ○

■ ■ ■

for approximating the second derivative (since m = 2). The algorithm produces the output

$$\left\{\left\{\frac{h^2}{12}, \frac{5h^2}{6}, \frac{h^2}{12}\right\}, \{1, -2, 1\}\right\},$$

corresponding to the implicit 4th order accurate formula for the second derivative:

$$\tfrac{1}{12} f''(x-h) + \tfrac{5}{6} f''(x) + \tfrac{1}{12} f''(x+h) \approx \tfrac{1}{h^2}\{f(x-h) - 2f(x) + f(x+h)\}$$

[0] Fornberg, B., Calculation of weights in finite difference formulas, SIAM Rev. 40:685-691, 1998.

Continued Fractions

- There are several variations of the Padé Approximation
- Most notably, continued fractions
- Recast the power series into continued-fraction form rather than rational function-form

[0]Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

Continued Fractions Defined

A continued fraction is an infinite sequence of fractions.
The$(N+1)^{th}$ member of the sequence, call it $F_N(z)$, has the form:

$$F_N(z) = \cfrac{c_0}{1 + \cfrac{c_1 z}{1 + \cfrac{c_2 z}{1 + \ddots \cfrac{c_{N-1} z}{1 + c_N z}}}}$$

The coefficients $c_0, c_1, ..., c_{N-1}, c_N$ can be determined by taking the Taylor expansion of $F_N(z)$ and comparing them to the coefficients of the original power series.

[0] Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

Quick Continued Fraction Example

Representing $\sqrt{2}$ as a continued fraction:

$$\sqrt{2} = 1 + \frac{1}{1+\sqrt{2}}$$

$$\sqrt{2} = 1 + \frac{1}{2 + \frac{1}{1+\sqrt{2}}}$$

$$\sqrt{2} = 1 + \frac{1}{2 + \frac{1}{2+\frac{1}{1+\sqrt{2}}}}$$

$$\sqrt{2} = 1 + \frac{1}{2 + \frac{1}{2+\frac{1}{2+\frac{1}{1+\dots}}}}$$

Continued Fractions and Padé

Gaol is to represent a Padé approximate as a continued fraction. To do this, the Padé approximate must meet some conditions:

- Consider $P^M_{M+1}(z)$ and $P^M_M(z)$, and the Padé sequence $P^0_0(z), P^0_1(z), P^1_1(z), P^1_2(z), P^2_2(z), P^2_3(z), \ldots$
- The sequence is normal if every member of the sequence exists and no two members are equal
- If the sequence is normal then the $(N+1)^{th}$ term has the continued fraction representation $F_N(z)$ and the coefficients $c_0, c_1, \ldots, c_{N-1}, c_N$ are the same for each term in the sequence

$$F_N(z) = \cfrac{c_0}{1 + \cfrac{c_1 z}{1 + \cfrac{c_2 z}{1 + \ddots \cfrac{c_{N-1} z}{1 + c_N z}}}}$$

[0] Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

Continued Fractions and Padé Cont.

Given the Padé sequence is normal:

- $P^M_{M+1}(z)$ is obtained by replacing $c_N z$ with $\frac{c_N z}{1+c_{N+1}z}$ in $P^M_M(z)$ where $N = 2M$
- $P^{M+1}_{M+1}(z)$ is obtained by replacing $c_N z$ with $\frac{c_N z}{1+c_{N+1}z}$ in $P^M_{M+1}(z)$ where $N = 2M + 1$

[0] Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

Continued Fractions and Padé Advantage

Resulting Advantage:

- When Padé approximates are written as a ratio of polynomials (rational functions) every coefficient must be recalculated from one member to the next.
- When Padé approximates are written as a single continued fraction only one coefficient must be recalculated from one member to the next.
- Proof on pg. 397 of Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

[0] Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

Evaluating Padé Continued Fractions

Can evaluate $F_N(z)$ directly. Or at a little extra cost $F_0(z), F_1(z), F_2(z), F_3(z)...$ can be evaluated as well leading to $F_N(z)$

Given

$$F_N(z) = \frac{R_N(z)}{S_N(z)}$$

For $N = 1, 2, 3, ...,$ $R_N(z)$ and $S_N(z)$ satisfy the recurrence relations:

$$R_{N+1}(z) = R_N(z) + c_{N+1} z R_{N-1}(z)$$
$$S_{N+1}(z) = S_N(z) + c_{N+1} z S_{N-1}(z)$$

For $N = 1, 2, 3, ...,$ where $R_{-1}(z) = 0$, $S_{-1}(z) = 1$ and$R_0(z) = c_0$, $S_0(z) = 1$

[0]Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

Convergence

Example 1 *Padé approximants may diverge where Taylor approximants converge.* Consider the function $y(x) = (x+10)/(1-x^2) = \sum_{n=0}^{\infty} a_n x^n$, where $a_{2n} = 10$ and $a_{2n+1} = 1$. This Taylor series converges for $|x| < 1$.

The Padé approximant $P_1^N(x)$ for this series is

$$P_1^N(x) = \sum_{n=0}^{N-2} a_n x^n + \frac{a_{N-1} x^{N-1}}{1 - a_N x / a_{N-1}}.$$

Thus, if N is even, $P_1^N(x)$ has a simple pole at $x = \frac{1}{10}$. Consequently, the Padé sequence $P_1^0, P_1^1, P_1^2, P_1^3, \ldots$ does not converge to $y(x)$ throughout $|x| < 1$.

- Shows that the zeros of the denominator function can affect the convergence of a Padé approximation
- To prove that a Padé approximation converges, must show that poles of the Padé approximants not belonging to the function be approximated (extraneous poles) move out of that region as $N \to \infty$

[0] Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

Convergence Cont.

Example 5 *Convergence of Padé approximants for* e^z. The continued fraction coefficients of e^z are $c_0 = -c_1 = 1$, $c_{2n} = 1/(4n-2)$, $c_{2n+1} = -1/(4n+2)$ $(n \geq 1)$. For these values of c_n, (8.4.8*b*) becomes the following system of equations:

$$S_{2M+1} - S_{2M} = -\frac{z}{4M+2} S_{2M-1}, \tag{8.5.10a}$$

$$S_{2M} - S_{2M-1} = \frac{z}{4M-2} S_{2M-2}, \qquad M \geq 1. \tag{8.5.10b}$$

We transform this system into a single difference equation of higher order by solving (8.5.10*b*) for S_{2M-1} and substituting the result into (8.5.10*a*):

$$S_{2M+2} - S_{2M} = \frac{z^2}{16M^2 - 4} S_{2M-2}, \qquad M \geq 1. \tag{8.5.11}$$

A local asymptotic analysis of this difference equation (see Prob. 8.39) yields

$$S_{2M}(z) = C(z)\left[1 - \frac{z^2}{16M} + O(M^{-2})\right], \qquad M \to \infty, \tag{8.5.12a}$$

for some function $C(z) \neq 0$. Combining (8.5.12*a*) into (8.5.10*b*) gives

$$S_{2M-1}(z) = C(z)\left[1 - \frac{z}{4M} - \frac{z^2}{16M} + O\left(\frac{1}{M^2}\right)\right], \qquad M \to \infty. \tag{8.5.12b}$$

Substituting (8.5.12) into (8.5.1) gives

$$F_N - F_{N-1} \sim \frac{\sigma_N z^N \sqrt{N}}{2^N N!} D(z), \qquad N \to \infty, \tag{8.5.13}$$

where $D(z)$ is a function of z (but not N) and $\sigma_N = 1, 1, -1, -1, 1, 1, -1, \ldots$ when $N = 0, 1, 2, 3, 4, 5, 6, \ldots$. By contrast, if $T_N = \sum_{n=0}^{N-1} z^n/n!$ is the sum of the first N terms of the Taylor series for e^z, then

$$T_N - T_{N-1} = \frac{z^N}{N!}. \tag{8.5.14}$$

[0]Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

Convergence *Cont.*[2]

In the previous example (example 5)

- The factor 2^{-N} causes the Padé sequence to converge far more rapidly than the Taylor sequence

[0] Bender, C. M. and Orszag, S. A., Advanced MathematicalMethods for Scientists and Engineers, McGraw Hill (1978),reprinted by Springer (1999).

References

- [1] Bender, C. M. and Orszag, S. A., Advanced Mathematical Methods for Scientists and Engineers, McGraw Hill (1978), reprinted by Springer (1999).

- [2] Fornberg, B. and Weideman, J.A.C., A numerical methodology for the Painlevé equations, J. Comp. Phys. 230 (2011), 5957-5973.

- [3] Fornberg, B., Calculation of weights in finite difference formulas, SIAM Rev. 40:685-691, 1998.