Padé approximation

An asymptotic expansion (or a Taylor expansion) can often be accelerated quite dramatically (or turned from divergent to convergent) by being rearranged into a ratio of two such expansions.

A Padé approximation

$$P_M^N(x) = \frac{\sum_{n=0}^{N} a_n x^n}{\sum_{n=0}^{M} b_n x^n} \qquad (1)$$

(normalized by $b_0 = 1$) generalizes the Taylor expansion with equally many degrees of freedom

$$T_{M+N}(x) = \sum_{n=0}^{M+N} c_n x^n \qquad (2)$$

(the two being the same in case $M = 0$). The Padé coefficients are normally best found from a Taylor expansion:

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

Multiplying up the denominator gives the following equivalent set of coefficient relations

$$\begin{array}{lcl} a_0 & = & c_0 \\ a_1 & = & c_1 + c_0\, b_1 \\ a_2 & = & c_2 + c_1\, b_1 + c_0\, b_2 \\ a_3 & = & c_3 + c_2\, b_1 + c_1\, b_2 + c_0\, b_3 \\ \ldots & & \ldots \end{array} \qquad (3)$$

With the c_i given, each new line introduces two new unknowns, a_i and b_i. The system would appear to be severely underdetermined. However, if we specify the degree of the numerator to be N, of the denominator to be M, and of the truncated Taylor expansion to be M+N, there will be just as many equations as unknowns (ignoring all terms that are $O(x^{M+N+1})$). We can then solve for all the unknown coefficients, as the following example shows:

Example 1: Given $T_5(x)$, determine $P_3^2(x)$.

In this case of $M = 2$, $N = 3$, $M+N = 5$, the system (3) becomes 'cut off' as follows

$$
\begin{array}{lll|l|l|l}
 & & a_0 & = c_0 & & \\
 & & a_1 & = c_1 + c_0\, b_1 & & \\
 & & a_2 & = c_2 + c_1\, b_1 + c_0\, b_2 & & \\
\hline
\text{no more } a\text{'s} & \Rightarrow & 0 & = c_3 + c_2\, b_1 + c_1\, b_2 + c_0\, b_3 & \text{no} \\
\text{available} & & 0 & = c_4 + c_3\, b_1 + c_2\, b_2 + c_1\, b_3 & \text{more} \\
 & & 0 & = c_5 + c_4\, b_1 + c_3\, b_2 + c_2\, b_3 & b\text{'s avail.} \\
\hline
 & & \multicolumn{2}{l|}{\text{past limit } O(x^{2+3+1})} & \\
\end{array}
$$

The bottom three equations can be solved for b_1, b_2, b_3, after which the top three explicitly give a_1, a_2, a_3. This same idea carries through for any values of M and N.

◊

A key usage of Padé approximations is to extract the information from power series expansions with only a few known terms. Transformation to Padé form usually accelerates convergence, and often allows good approximations to be found even outside a power series expansion's radius of convergence (which, in case of divergent asymptotic expansions, may be zero).

Example 2: Find the increasing order Padé approximations for $f(x) = 1 - x + x^2 - x^3 + -\ldots$.

The Padé table based on the truncated Taylor sums becomes:

TABLE 3

Beginning of Padé table for $f(x) = 1 - x + x^2 - x^3 + -\ldots$

		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	$\frac{1}{1+x}$	....			
	....	....				

The main diagonal (and the diagonal below it) usually gives the best results. This example is trivial in that every entry with $M > 0$ happens to recover the exact result.

◊

Application 1: 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)	
	....						....

◊

Example 4: Comparison of Taylor- and Padé approximations for $f(z) = \int_0^\infty \frac{e^{-t}}{1+zt}\,dt$.

The *Stieltjes' function* $f(x)$ is singular for $z < 0$, but well defined for other values of z - including values in the complex plane away from the negative real axis. Figure 1 shows Im($f(z)$) for $z = x + iy$ in the domain $[-3,3]\times[-3,3]$ - the jump along $x < 0$ is obvious.

We can try to Taylor expand $f(z)$ around $z = 0$. Several approaches lead to the same expansion, e.g.

(i) Repeated integration by parts,

(ii) Noting that $f(z)$ satisfies $z^2 f'(z) + (1+z) f(z) - 1 = 0$, $f(0) = 1$, leading to recursion relations for the Taylor coefficients,

(iii) Expanding $\frac{1}{1+zt} = 1 - (zt) + (zt)^2 - (zt)^3 + - \ldots$ and then utilizing that $\int_0^\infty t^k e^{-t}\,dt = k!$.

With all of the approaches, the result becomes the same:

$$f(z) \sim \sum_{k=0}^{\infty} (-z)^k k!\ ,$$

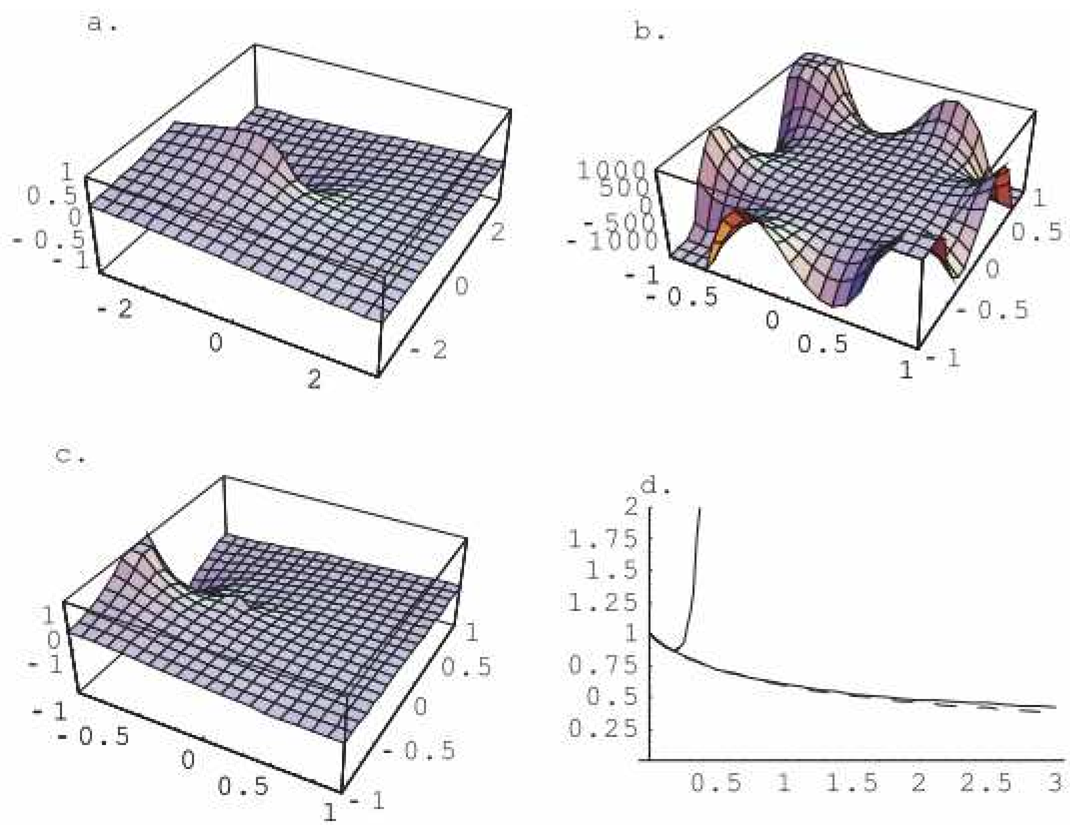
which diverges for all values of $z \neq 0$. Truncation after the sixth power gives

$$T_6(z) \sim 1 - z + 2z^2 - 6z^3 + 24z^4 - 120z^5 + 720z^6 \quad .$$

Predictably, this gives nonsense when evaluated over [-1,1]×[-1,1] (imaginary part shown in Figure 1 b). However, when $T_6(z)$ is converted to the Padé approximation

$$P_3^3(z) = \frac{1 + 11z + 26z^2 + 6z^3}{1 + 12z + 36z^2 + 24z^3} \tag{4}$$

we recover a quite respectable approximation of the original function (Figure 1 c; the rational approximation $P_3^3(z)$ has even arranged for singularities along the negative real axis in an automatic attempt to mimic the line of discontinuity there). Finally, Figure 1 d compares, on the positive real axis $x > 0$, the original function (dashed) with $T_6(z)$ and $P_3^3(z)$). Somehow, the everywhere divergent power series expansion did still contain information about the function, and rearranging this into Padé form has recovered it.



Figures 1 a-d. Stieltjes' function and its Taylor- and Padé approximations.

a. Imaginary part of $f(z) = \int_0^\infty \frac{e^{-t}}{1+zt}dt$,

b. $\mathrm{Im}(T_6(z))$,

c. $\mathrm{Im}(P_3^3(z))$,

d. Comparison for $z > 0$ between $f(z)$ (dashed curve), $P_3^3(z)$ (solid curve - just above it), and $T_6(z)$ (solid curve, rapidly growing).

◊

Application 2: Determining weights in FD formulas and Linear Multistep Methods (LMM) for solving ODEs.

Finite Differences (FD) approximate derivatives by combining nearby function values using a set of *weights*. An extremely simple FD formula for approximating $f'(x)$ can be obtained can be obtained directly from the definition of a derivative, as illustrated in Figure 2.

-

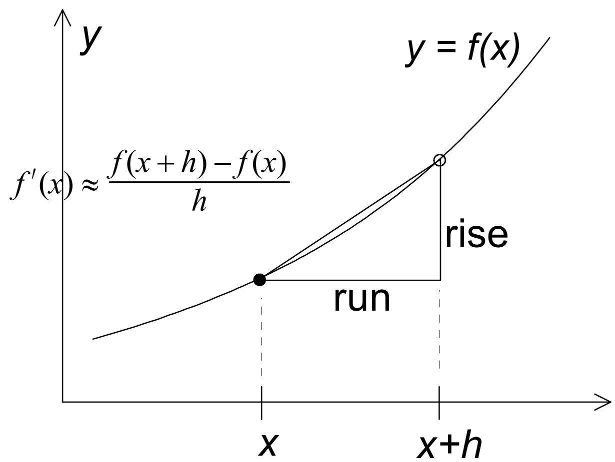


Figure 2. Illustration of the approximation $f'(x) \approx \frac{\text{rise}}{\text{run}} = \frac{f(x+h)-f(x)}{h}$, increasingly accurate as $h \to 0$.

Taylor expansion of $f(x+h)$ gives

$$\frac{f(x+h)-f(x)}{h} = f'(x) + \frac{hf''(x)}{2!} + \frac{h^2 f'''(x)}{3!} + \ldots \quad = f'(x) + O(h^1)$$

and verifies that the approximation is accurate to *first order*. The FD *weights* at the *nodes* x and $x+h$ are in this case $[-1 \;\; 1]/h$. The FD *stencil* can graphically be illustrated as

$$\begin{array}{llcll} \bigcirc & & \leftarrow & \text{entry for } f' & \text{value } \{1\} \\ \blacksquare & \blacksquare & \leftarrow & \text{entries for } f & \text{values } \{-\frac{1}{h}, \frac{1}{h}\} \\ \uparrow & \uparrow & & & \\ x & x+h & \leftarrow & \text{spatial locations} & \end{array} \tag{5}$$

In this and subsequent stencil illustrations, the open circle indicates a typically unknown derivative value, and the filled squares typically known function values. The stencil shape in (5) can be greatly generalized: We can ask what the optimal weights are in a FD formula that relates values of $f^{(m)}(x)$ at some locations with values of $f(x)$ at other locations, as illustrated in (6):

$\mid<s>\mid<-\ d\ ->\mid$	$\leftarrow$	s (real), d (integer ≥ 0); in figure taking values 3/2 and 3 resp.	
○ ○ ○ ○	$\leftarrow$	entries for $f^{(m)}$	(6)
■ ■ ■ ■ ■ ■ ■	$\leftarrow$	entries for f	
$\mid<-\quad n \quad ->\mid$	$\leftarrow$	n (integer > 0), in figure taking value 6.	

Here, the three numbers s, d, and n completely describe the stencil shape. It transpires (first discovered in 1998 [1]) that the optimal weights in this stencil can be calculated in just two lines of symbolic algebra code, with a Padé approximation as its key ingredient. In Mathematica 7 and higher, these two lines are:

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

The next two examples below illustrate typical applications of this algorithm:

<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:

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

◊

<u>Example 6:</u> The choice `s=-2, d=2, n=1, m=1` describes a stencil of the shape

○ ○ ○

      ■ ■

for approximating the first derivative. The output

$$\left\{\left\{\frac{5h}{12}, -\frac{4h}{3}, \frac{23h}{12}\right\}, \{-1, 1\}\right\}$$

is readily rearranged as

$$f(x+h) = f(x) + \frac{h}{12}(23f'(x) - 16f'(x-h) + 5f'(x-2h)) ,$$

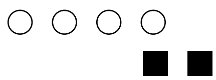
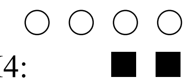
which we recognize as the third order Adams-Bashforth method for solving ODEs.

◊

We can further note that the all the main classes of LMM methods (Adams-Bashforth, Adams-Moulton, and Backward Differentiation) arise all as special cases of (6), with $m = 1$ and for different choices for s, d, and n. This algorithm provides the weights for all these cases. With $m = 1$ and accuracy of order p :

Adams-Bashforth	$(p \geq 1)$	$s = 1 - p,$	$d = p - 1,$	$n = 1.$
Adams-Moulton	$(p \geq 2)$	$s = 2 - p,$	$d = p - 1,$	$n = 1.$
Backward Differentiation	$(p \geq 1)$	$s = -p,$	$d = p,$	$n = 0.$

We have already illustrated the FD stencil shape associated with the AB3 scheme (and written down its coefficients explicitly). Thinking again of the t-axis as going to the right, the stencil shapes for the fourth order accurate AB4, AM4 and BD4 schemes become as follows:

AB4:  , AM4:  , BD4: 

Reference:

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