

# 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

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

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

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

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

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

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

$$\begin{aligned} a_0 &= c_0 \\ a_1 &= c_1 + c_0 b_1 \\ a_2 &= c_2 + c_1 b_1 + c_0 b_2 \\ a_3 &= c_3 + c_2 b_1 + c_1 b_2 + c_0 b_3 \\ &\dots \quad \dots \end{aligned} \quad (3)$$

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

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

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  $N$ .

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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  $f(x) = 1 - x + x^2 - x^3 + \dots$ .

The Padé table based on the truncated Taylor sums becomes:

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

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

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## 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

$$f(x) = 1 - \frac{1}{2}x + \frac{1}{3}x^2 - \frac{1}{4}x^3 + \frac{1}{5}x^4 - + \dots \quad \left( = \frac{\ln(1+x)}{x}, \text{ but only if } |x| < 1 \right).$$

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 denomi- nator	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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**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  $\text{Im}(f(z))$  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  $\frac{1}{1+zt} = 1 - (zt) + (zt)^2 - (zt)^3 + \dots$  and then utilizing that  $\int_0^\infty t^k e^{-t} dt = k!$ .

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

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

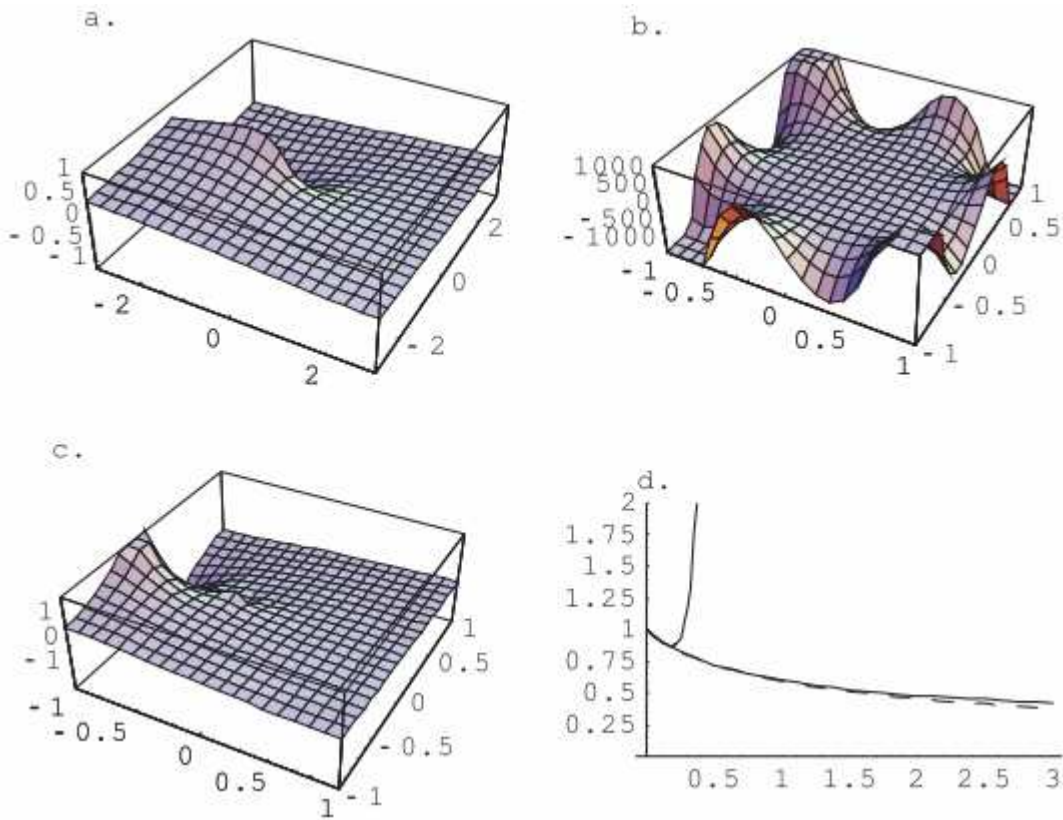
which diverges for all values of  $z \neq 0$ . Truncation after the sixth power gives

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

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

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

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.  $\text{Im}(T_6(z))$ ,
- c.  $\text{Im}(P_3^3(z))$ ,
- 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).

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**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 directly from the definition of a derivative, as illustrated in Figure 2.

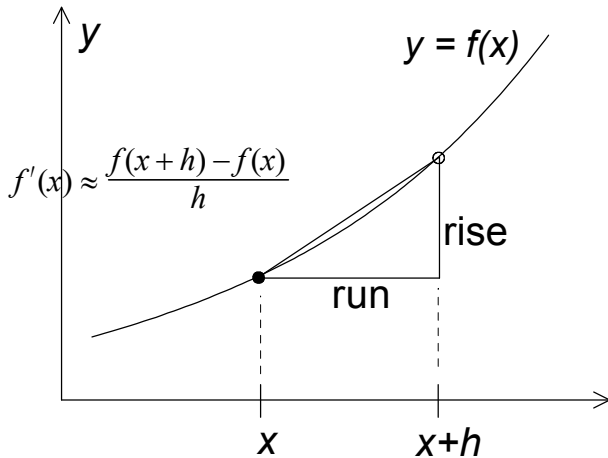


Figure 2. Illustration of the approximation  $f'(x) \approx \frac{\text{rise}}{\text{run}} = \frac{f(x+h)-f(x)}{h}$ , increasingly accurate as  $h \rightarrow 0$ .

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

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

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

$$\begin{array}{lll} \circ & \leftarrow & \text{entry for } f' \quad \text{value } \{1\} \\ \blacksquare \ \blacksquare & \leftarrow & \text{entries for } f \quad \text{values } \{-\frac{1}{h}, \frac{1}{h}\} \\ \uparrow \ \uparrow & & \\ x \ x+h & \leftarrow & \text{spatial locations} \end{array} \quad (5)$$

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):

$$\begin{array}{l}
|<s>|<- d ->| \quad \leftarrow \quad s \text{ (real), } d \text{ (integer } \geq 0\text{); in figure taking values } 3/2 \text{ and } 3 \text{ resp.} \\
\quad \circ \quad \circ \quad \circ \quad \circ \quad \leftarrow \quad \text{entries for } f^{(m)} \\
\blacksquare \blacksquare \blacksquare \blacksquare \blacksquare \blacksquare \blacksquare \quad \leftarrow \quad \text{entries for } f \\
|<- n ->| \quad \leftarrow \quad n \text{ (integer } > 0\text{), in figure taking value } 6.
\end{array} \tag{6}$$

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:

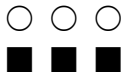
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t = PadéApproximant[x^s*(Log[x]/h)^m, {x, 1, {n, d}}];
CoefficientList[{Denominator[t], Numerator[t]}, x]

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

**Example 5:** 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

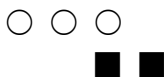
$$\left\{ \left\{ \frac{h^2}{12}, \frac{5h^2}{6}, \frac{h^2}{12} \right\}, \{1, -2, 1\} \right\},$$

corresponding to the implicit 4<sup>th</sup> order accurate formula for the second derivative:

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

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**Example 6:** 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

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

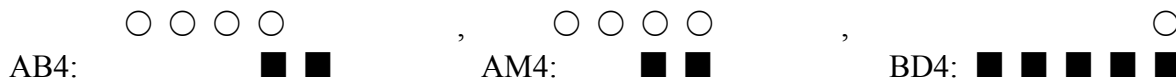
which we recognize as the third order Adams-Bashforth method for solving ODEs.

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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  $p$  :

$$\begin{array}{lll}
 \text{Adams-Bashforth} & (p \geq 1) & s = 1 - p, \quad d = p - 1, \quad n = 1. \\
 \text{Adams-Moulton} & (p \geq 2) & s = 2 - p, \quad d = p - 1, \quad n = 1. \\
 \text{Backward Differentiation} & (p \geq 1) & s = -p, \quad d = p, \quad n = 0.
 \end{array}$$

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:



## Reference:

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