Polynomial and rational approximation of a function in the neighbourhood of a point

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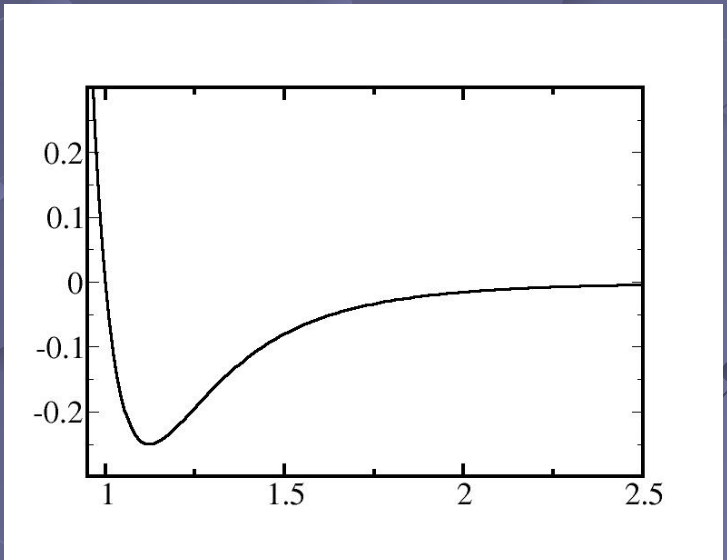
Taylor approximation

- Here, we are interested in approximating a function in a neighbourhood of a point
- The idea is to use the derivatives of the function in a point to approximate the function in a neighbourhood of that point
- It may be useful in cases where the domain we are interested in is limited

Taylor approximation

- Here, we are interested in approximating a function in a neighbourhood of a point
- Take for example a Lennard-Jones interatomic potential
- $U(r) = 4\varepsilon\,[(\sigma/r)^{12} - (\sigma/r)^{6}]$
- At low temperature, only a neighbourhood of the minimum is relevant



Taylor approximation

- The idea is to use the derivatives of the function in a point to approximate the function in a neighbourhood of that point

- The Taylor series is defined as $\Sigma^{\infty}_{n=0}$ $1/n!\, f^n(x_0)\,(x-x_0)^n$, where f^n is the n^{th} derivative of the function f

- If $x_0 = 0$, the series is called also McLaurin series

Properties of Taylor polynomials

- Taylor polynomials have useful properties
- $T_n[af+bg] = aT_n[f] + bT_n[g]$
- $T'_n[f] = T_{n-1}[f']$
-

Taylor approximation: Peano form of the remainder

- $f(x) \approx \Sigma^{n}_{j=0}\, 1/j!\, f^{j}(x_0)\, (x-x_0)^{j}$
  where f^{j} is the j^{th} derivative of the function f
- $f(x) = \Sigma^{n}_{j=0}\, 1/j!\, f^{j}(x_0)\, (x-x_0)^{j} + R_n(x)$
- Peano form of the remainder:
- $R_n(x) = O((x-x_0)^{n+1})$
- $\lim_{x->x0} R_n(x)/(x-x_0)^{n} = 0$
- Proof: based on de L'Hôpital theorem

Taylor approximation: Lagrange form of the remainder

- $f(x) = \Sigma^n_{j=0}\ 1/j!\ f^j(x_0)\ (x-x_0)^j + R_n(x)$
- Lagrange form of the remainder:
- $R_n(x) = 1/n!\ f^n(\xi)\ (x-x_0)^n$
- with ξ in (x_0, x)
- Proof

Taylor approximation: convergence

- $f(x) = \Sigma^n_{j=0}\ 1/j!\ f^j(x_0)\ (x-x_0)^j + R_n(x)$
- $R_n(x) = O((x-x_0)^{n+1})$ (Peano)
- $R_n(x) = 1/n!\ f^n(\xi)\ (x-x_0)^n$ (Lagrange)
- Lagrange form makes it possible to have upper bound for error in any point x
- Error may be large

Taylor approximation: convergence

- $f(x) = \Sigma^{\infty}_{n=0} 1/n!\, f^n(x_0)\, (x-x_0)^n$
- This series converges to the function in a neighbourhood of the expansion point
- Error formulae do not help in this
- In some cases this neighbourhood could be the whole real axis
- Example: for the exponential
- $e(x) = \Sigma^{\infty}_{n=0} 1/n!\, f^n(x_0)\, (x-x_0)^n$ for every real x

Taylor approximation: convergence

- $f(x) = \Sigma^{\infty}_{n=0} 1/n!\ f^n(x_0)\ (x-x_0)^n$

- $\arctan(x) = x - x^3/3 + x^5/5 - x^7/7 \ldots$
  $= \Sigma^{\infty}_{n=0} (-1)^n\ x^{(2n+1)}/(2n+1)$

- arctan(x) is defined in [-π/2, π/2], but the series converges to arctan(x) only for $|x| \leq 1$!

Taylor approximation: WARNING

- In other cases, it might convergence in a limited neighoburhood of the expansion point
- There are also pathological cases where the series converges to a function which is NOT the original function
- $$f(x) = \begin{cases} \exp(-1/x^2) & \text{for } x \neq 0 \\ 0 & \text{for } x = 0 \end{cases}$$

All derivatives are zero in zero, so the Taylor series is = 0 everywhere...

Taylor approximation

- $e(x) = \Sigma^{\infty}_{n=0}\ 1/n!\ f^n(x_0)\ (x-x_0)^n$ for every real x
- Of course we need to truncate the series: we approximate our function with a (Taylor) polynomial of degree N

- First-order (i.e. linear) approximation:

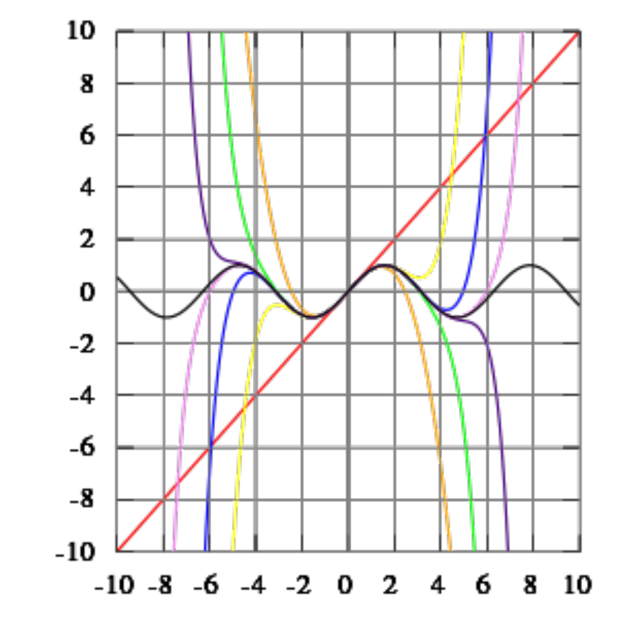
  $f(x) \approx f(x_0) + f'(x_0) * (x-x_0)$

- Quadratic approximation:

  $f(x) \approx f(x_0) + f'(x_0) * (x-x_0) + ½\ f''(x_0) * (x-x_0)^2$

Taylor polynomials

- Even when the series is convergent over the whole real axis, truncation makes the approximation good only in a neighbourhood of the expansion point
- Example: f(x) = sin(x)
- $\sin(x) = x - x^3/3! + x^5/5! - x^7/7! + \ldots$

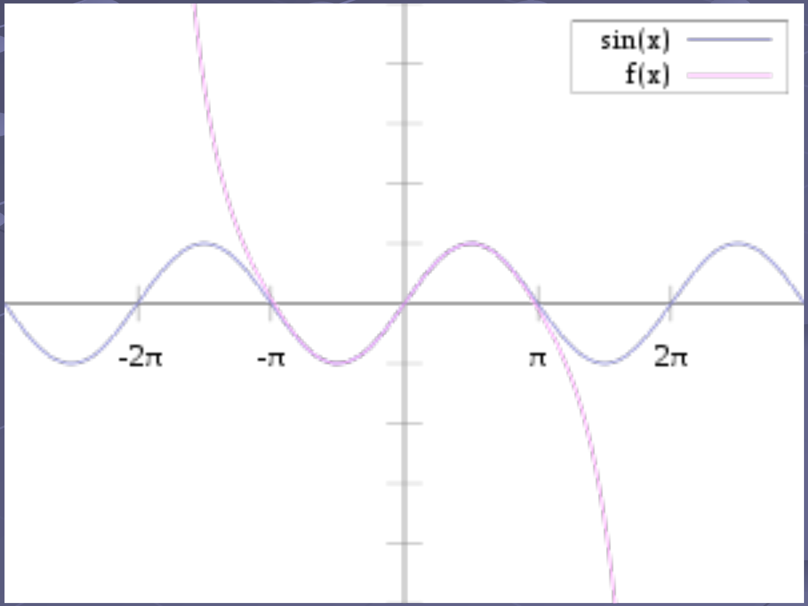


As the degree of the Taylor polynomial rises, it approaches the correct function. This image shows sin(x) and its Taylor approximations, polynomials of degree 1, 3, 5, 7, 9, 11 and 13.

http://en.wikipedia.org/wiki/Taylor_series

Taylor polynomials

- $f(x) = \sin(x)$
- $\sin(x) = x - x^3/3! + x^5/5! - x^7/7!$



sin(x) is closely approximated by its Taylor polynomial of degree 7 (pink) for a full period centered at the origin.

http://en.wikipedia.org/wiki/Taylor_series

Advantages of Taylor polynomials

- Taylor expansion approximates a function with a polynomial
- Simple form: easy to compute, to derive, to integrate...
- Systematic improvements by increasing degree, in most cases

Drawbacks of Taylor polynomials

- Taylor expansion approximates a function with a polynomial
- It may suffer from limited, slow convergence
- At high degrees, it oscillates strongly
- Bad for functions with singularities
- It diverges for x -> ±∞

Pade` approximation

- Let's generalize this to rational functions P/Q (Pade` approximation), where P and Q are polynomials
- Taylor polynomials are special cases where Q = 1
- It may even work in cases where the Taylor series does not converge
- We are still expanding around a point

Pade` approximation

- Taylor expansion approximates a function with a polynomial
- Pade` approximant provides an approximation of a given function using rational functions:

$$f(x) \approx \frac{\sum_{j=0}^{m} a_j x^j}{\sum_{j=0}^{n} b_j x^j} = \frac{p(x)}{q(x)}$$

- Usually, $b_0 = 1$

Pade` approximation

$$f(x) \approx \frac{\sum_{j=0}^{m} a_j x^j}{\sum_{j=0}^{n} b_j x^j} = \frac{p(x)}{q(x)}$$

- This is the Pade` approximant T(x) of order [m/n] if it reproduces the derivatives of f(x) to the highest possible order in 0, i.e.
- $f(0) = T(0)$
- $f'(0) = T'(0)$
- ...
- $f^{(m+n)}(0) = T^{(m+n)}(0)$
- Usually, $b_0 = 1$

Pade` approximation

$$f(x) \approx \frac{\sum_{j=0}^{m} a_j x^j}{\sum_{j=0}^{n} b_j x^j} = \frac{p(x)}{q(x)}$$

- f(0) = T(0)
- ...
- $f^{(m+n)}(0) = T^{(m+n)}(0)$
- In other words, $f(x) - T(x) = O(x^{(m+n+1)})$
- These are m+n+1 equations for m+n+2 unknowns (m +n+1 unknowns if one puts $b_0 = 1$)
- These conditions translate into conditions for the coefficients of the two polynomials

Pade` approximation

$$f(x) \approx \frac{\sum_{j=0}^{m} a_j x^j}{\sum_{j=0}^{n} b_j x^j} = \frac{p(x)}{q(x)}$$

- These conditions translate into conditions for the coefficients of the two polynomials:
- $f(x) - T(x) = f(x) – p(x)/q(x) = O(x^{(m+n+1)})$
- $f(x)q(x)-p(x) = O(x^{(m+n+1)})$

$$\sum_{j=0}^{n} b_j c_{m-j+k} = 0, k = 1, \ldots, n$$

$$\sum_{j=0}^{k} b_j c_{k-j} = a_k, k = 0, \ldots, m$$

- where $c_i = f^i(0)$
- Linear system of equations in a and b

Pade` approximation: obtaining the coefficients

$$\sum_{j=0}^{n} b_j c_{m-j+k} = 0, k = 1, \ldots, n$$

$$\sum_{j=0}^{k} b_j c_{k-j} = a_k, k = 0, \ldots, m$$

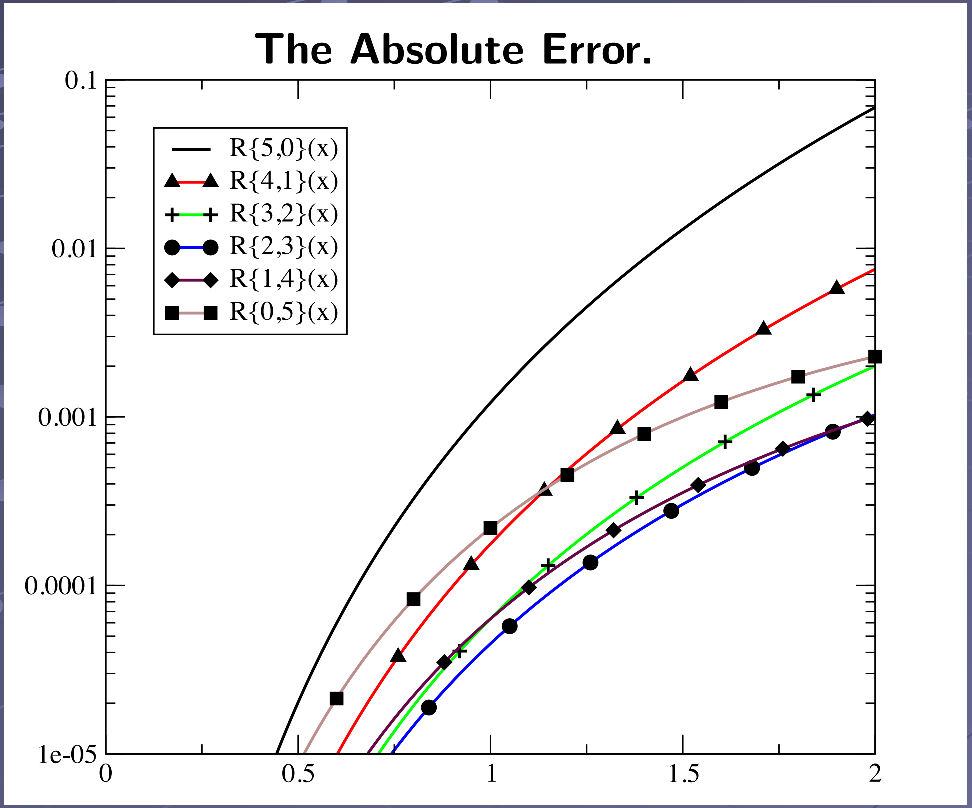
- where $c_i = f^i(0)$
- Linear system of equations in a and b
- n+m+1 equations for n+m+1 coefficients
- Method 1 to obtain coefficients: solve this linear problem

Pade` approximation: obtaining the coefficients

- Method 1 to obtain coefficients: solve the linear problem

- There are several other methods: e.g. recursive algorithm : p_n and q_n from p_{n-1} and q_{n-1}...

Pade` approximation: errors



Joe Mahaffy, San Diego State University, lecture notes

- Absolute error for e^{-x} expanded around 0
- Error lower when $n \approx m$

Pade` approximation: errors

- Explicit estimates of the error are quite complicated

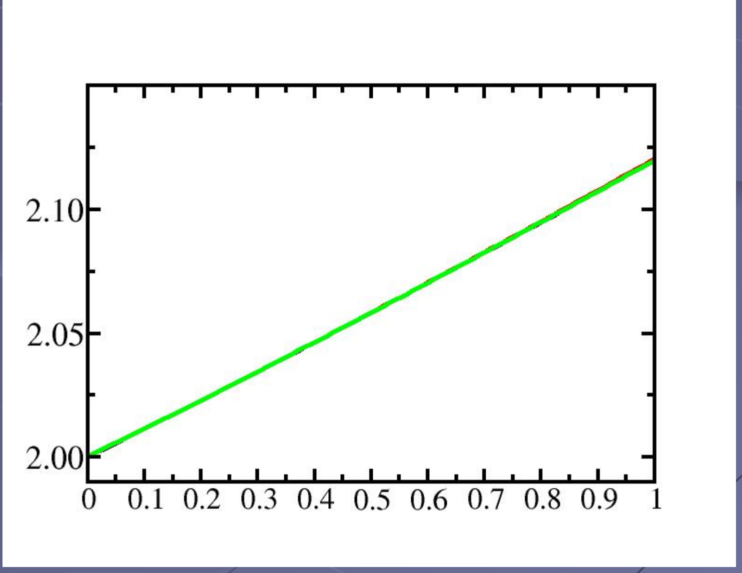
Power of Pade` approximation: one example

- Let $f(x) = (7+(1+x)^{4/3})^{1/3}$
- Taylor polynomial of order 4:

  $f(x) \approx 2 + 1/9\, x + 1/81\, x^2 - 49/8748\, x^3 + 175/78732\, x^4$
- Pade` approximant for the case m = n = 2 has

  $a_0 = 2$; $a_1 = 0.92714$; $a_2 = 0.067834$

  $b_1 = 0.40801$; $b_2 = 0.0050766$

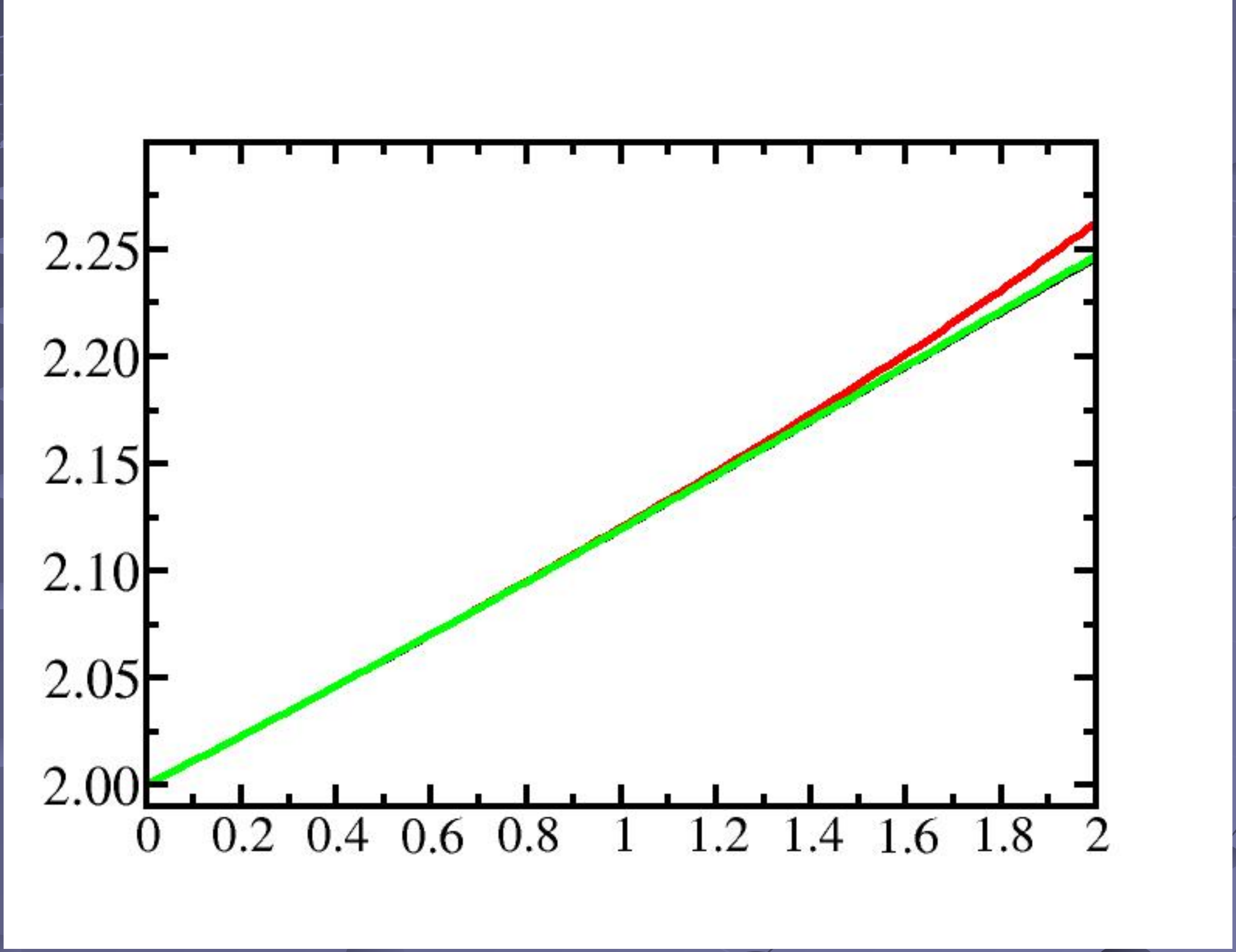


Black: f
Red: Taylor
Green: Pade`

- Good also for extrapolation

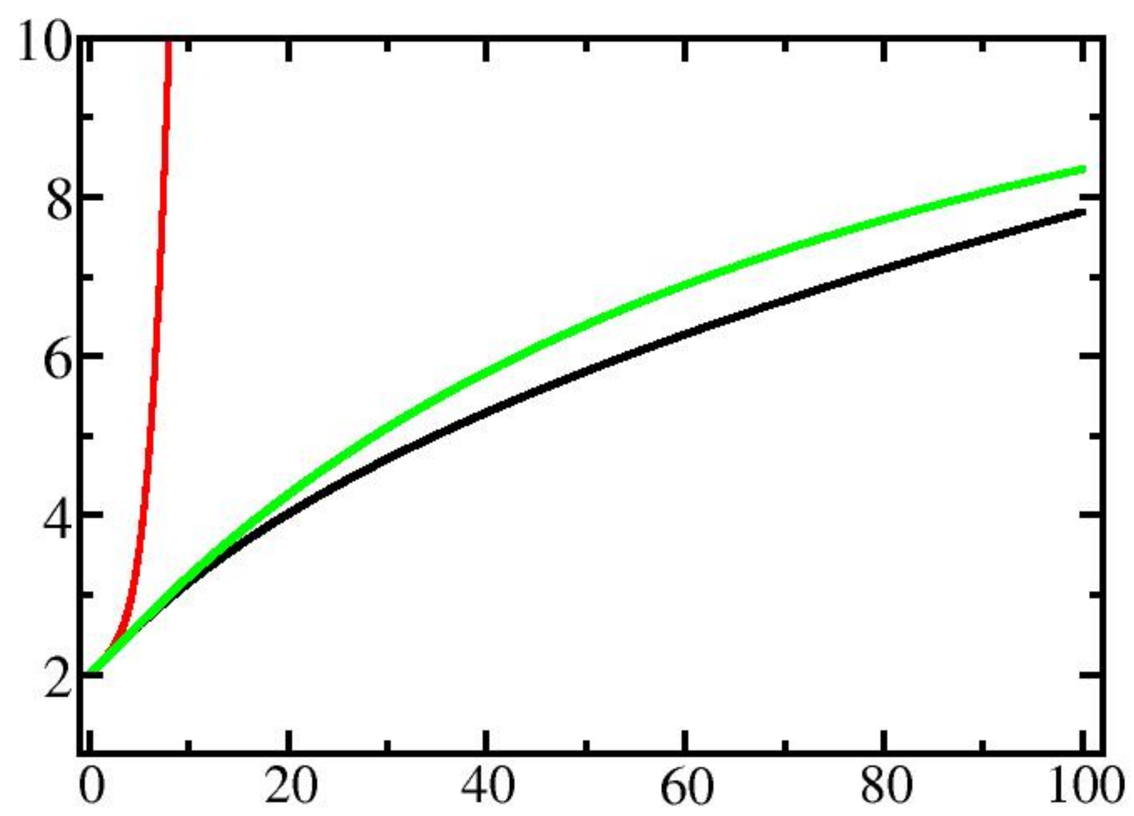
Power of Pade` approximation: one example

- Good also for extrapolation



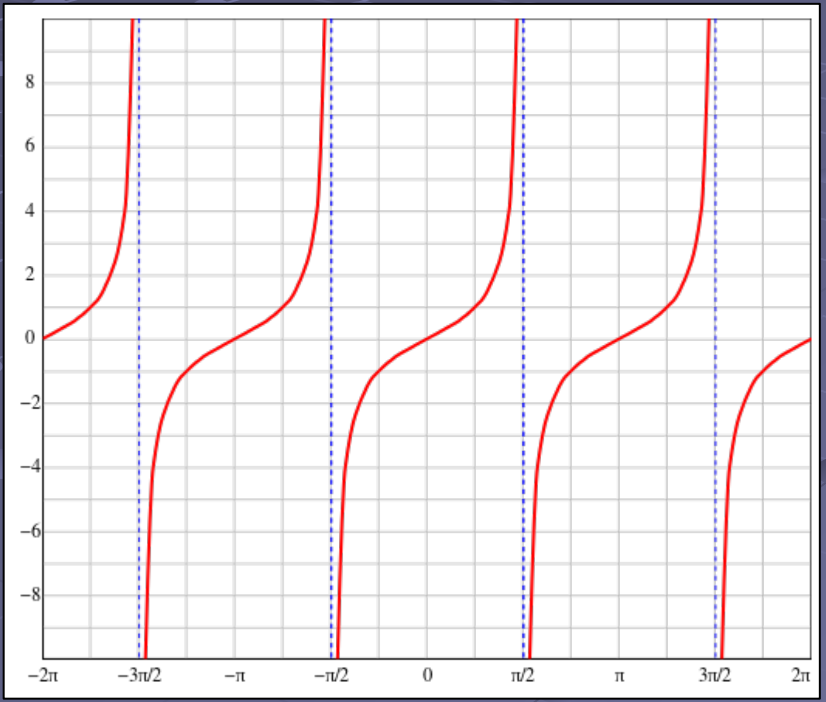
Power of Pade` approximation: one example

- Good also for extrapolation



Power of Pade` approximation: tangent

- In some cases reasons for better success of Pade` vs. Taylor is straightforward:



https://it.wikipedia.org/wiki/Tangente_(matematica)

- One can exploit the zeros of the denominator of the rational polynomial

Pade` tables

- Results are summarized in Pade` tables

Table 1: Padé table for $f(x) = e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \ldots$

1	$\frac{1}{1-x}$	$\frac{1}{1-x+\frac{1}{2}x^2}$	$\cdots$
$1+x$	$\frac{1+\frac{1}{2}x}{1-\frac{1}{2}x}$	$\frac{1+\frac{1}{3}x}{1-x+\frac{1}{6}x^2}$	$\cdots$
$1+x+\frac{1}{2}x^2$	$\frac{1+\frac{2}{3}x+\frac{1}{6}x^2}{1-\frac{1}{3}x}$	$\frac{1+\frac{1}{2}x+\frac{1}{12}x^2}{1-\frac{1}{2}x+\frac{1}{2}x^2}$	$\cdots$
$1+x+\frac{1}{2}x^2+\frac{1}{6}x^3$	$\frac{1+\frac{3}{4}x+\frac{1}{4}x^2+\frac{1}{24}x^3}{1-\frac{1}{4}x}$	$\vdots$	
$1+x+\frac{1}{2}x^2+\frac{1}{6}x^3+\frac{1}{24}x^4$	$\vdots$		
$\vdots$			

J. Kallrath: http://www.astro.ufl.edu/~kallrath/files/pade.pdf