CHEM1047 - Week 7 Lecture 2 - Polynomial series and interpolants, part II

☐ *Section 7.5 of Steiner, "The Chemistry Maths Book", 2nd edition.*

1. Convergence tests for Taylor series

The approximation provided by a Taylor series is only good in the vicinity of the point x_0 – the closer, the better. When that is not the case, the series can misbehave – adding further terms would make the approximation worse (Figure 1). This may be seen for $x=3$ in the logarithm series from the previous lecture – that series was only intended to be used around $x=1$.

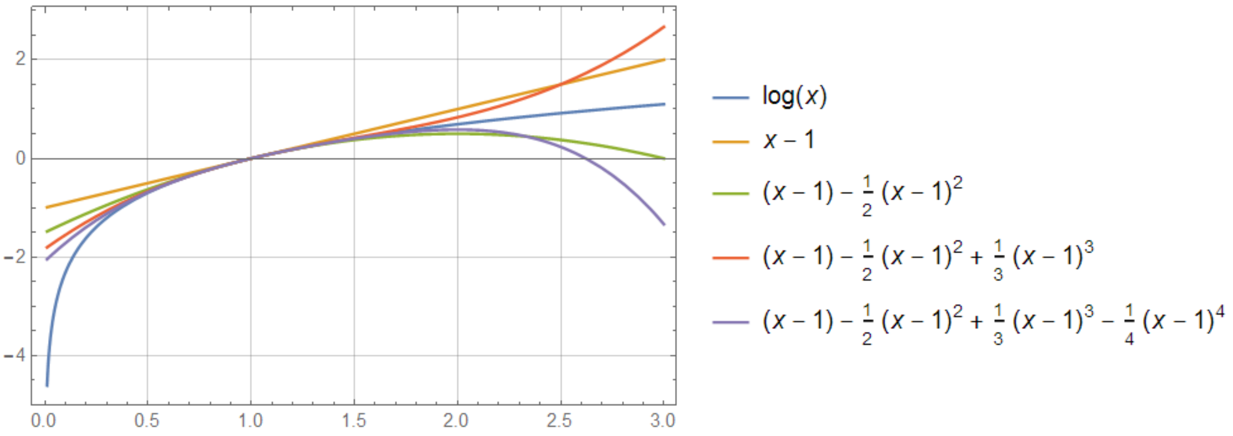

Figure 1. *Natural logarithm function and its Taylor series around x_0=1, truncated at orders 1, 2, 3, and 4.*

This situation is called *divergence.* An important question is about the interval in which a given Taylor series is guaranteed to be free of divergences. The following tests are useful:

D'Alembert's test (also called *ratio test*):

A series $\sum_{n=0}^{\infty} a_n$ converges if $\lim_{n\to\infty}\left|\frac{a_{n+1}}{a_n}\right|<1$ and diverges if $\lim_{n\to\infty}\left|\frac{a_{n+1}}{a_n}\right|>1$.

Cauchy's test (also called *root test*):

A series $\sum_{n=0}^{\infty} a_n$ converges if $\lim_{n\to\infty}\sqrt[n]{a_n}<1$ and diverges if $\lim_{n\to\infty}\sqrt[n]{a_n}>1$.

If both limits above are equal to 1, the question remains open. The interval of x values for which the series converges is called its *radius of convergence*.

Even when they do slowly converge, the series for which the tests above give no answer are undesirable in practice – they are computationally expensive and insufficiently accurate.

Example 1: demonstrate that the following Taylor series converges for any value of x

$$\sum_{n=0}^{\infty}\frac{x^n}{n!}$$

Solution: using the ratio test, we conclude that, for any finite value of x

$$\lim_{n\to\infty}\left|\frac{x^{n+1}/(n+1)!}{x^n/n!}\right| = \lim_{n\to\infty}\left|\frac{x}{n+1}\right| = 0$$

The limit is always smaller than 1, and therefore the series always converges.

Example 2: find the convergence radius for the following series

$$\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}(x-1)^n$$

Solution: using the ratio test, we get

$$\lim_{n\to\infty}\left|\frac{\dfrac{(-1)^{n+2}}{n+1}(x-1)^{n+1}}{\dfrac{(-1)^{n+1}}{n}(x-1)^n}\right| = \lim_{n\to\infty}\left|\frac{n}{n+1}(x-1)\right| = |(x-1)|<1 \quad\Rightarrow\quad 0<x<2$$

This explains the deterioration of accuracy observed in Figure 1 for $x=3$.

2. Polynomial interpolation

Consider a function defined or measured at $N+1$ specific points $\{x_k, f(x_k)\}$. We can ask the following question: does there exist a polynomial of order N

$$y(x)=\sum_{n=0}^{N}a_n x^n \tag{1}$$

that would be equal to $f(x_k)$ at each point x_k?

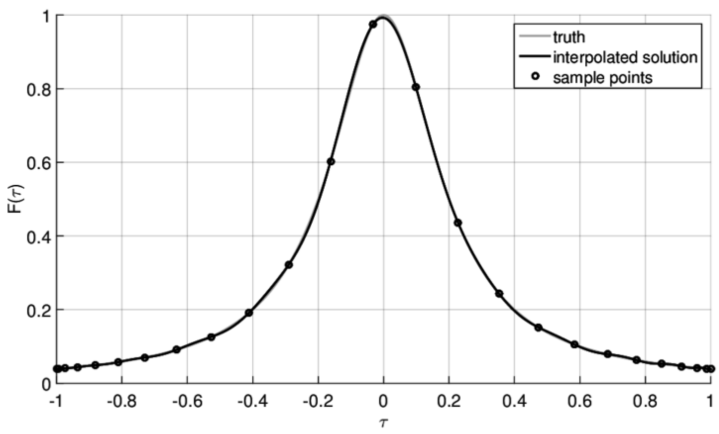

Figure 2. *A typical experimental data set (from NMR spectroscopy) and its interpolating polynomial.*

An example is shown in Figure 2. Such a polynomial would be useful because it would give us a function, and therefore allow us to use analytical methods that normally require continuity. The question formally leads to the following system of equations:

$$\left\{ f(x_k) = \sum_{n=0}^{N} a_n x_k^n \right._{k=0}^{N+1} \tag{2}$$

that must be solved for the coefficients a_n. A simple solution was obtained by Lagrange:

$$y(x) = \sum_k f(x_k) C_k(x), \qquad C_k(x) = \prod_{m \neq k} \frac{x - x_m}{x_k - x_m} \tag{3}$$

This is known as *Lagrange polynomial*. Due to stability problems illustrated in Figure 2, it is not recommended to use interpolating polynomials of order greater than four. If the grid has more points, the function should be interpolated piecewise.

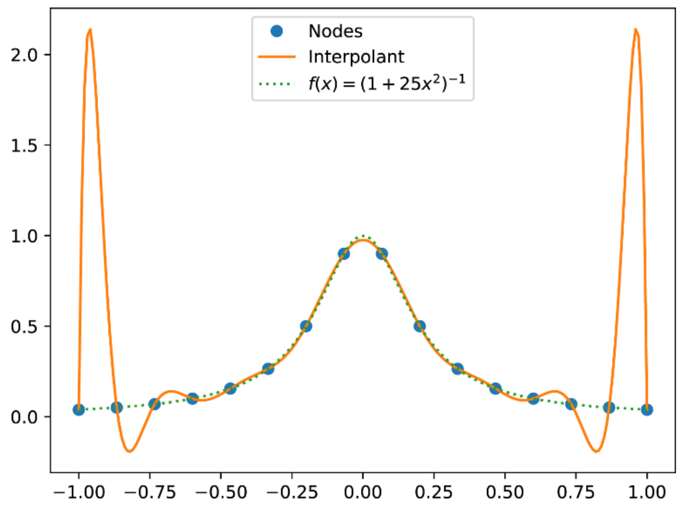

Figure 3. *An illustration of the instability in high-order Lagrange interpolants. The curve shown in Figure 2 is a piecewise interpolation by a cubic polynomial.*

Example 3: find the Lagrange interpolant for the function taking the following values: $f(-1) = 1/2$, $f(0) = 0$, $f(1) = 2$. Calculate the value of the interpolant at $x = 1/2$.

Solution: we can number the points to have $x_1 = -1,\ x_2 = 0,\ x_3 = 1$; Equation (3) then yields

$$y(x) = f(x_1)C_1(x) + f(x_2)C_2(x) + f(x_3)C_3(x) = \frac{1}{2}C_1(x) + 2C_3(x)$$

where the functions may be computed from their definition

$$C_1(x) = \frac{x - x_2}{x_1 - x_2}\frac{x - x_3}{x_1 - x_3} = \frac{x(x-1)}{2}, \qquad C_3(x) = \frac{x - x_1}{x_3 - x_1}\frac{x - x_2}{x_3 - x_2} = x(x+1)$$

with the result that

$$y(x) = \frac{5x^2 + 3x}{4}, \qquad y(1/2) = \frac{11}{16}$$