CHEM1047 - Week 7 Lecture 1 - Polynomial series and interpolants, part I

☐ *Section 7.6 of Steiner, "The Chemistry Maths Book", 2nd edition.*

☐ *Chapter 1 of Cockett and Doggett, "Maths for Chemists", Vol 2.*

1. Taylor series

A situation often arises when the value of a function is only required approximately around a particular point. A good example from chemistry is the high temperature limit: *Boltzmann law* may be approximated by a linear function (*i.e.* a polynomial of order 1) when either the energy difference ΔE is small, or the temperature is high:

$$\exp\left(-\frac{\Delta E}{kT}\right)\approx 1-\frac{\Delta E}{kT} \quad \text{if} \quad \Delta E \ll kT \tag{1}$$

Another illustration is *Morse potential*, which may be approximated by a quadratic function:

$$E(x)=D\left[1-e^{-a(x-x_0)}\right]^2 \approx a^2 D (x-x_0)^2 \quad \text{if} \quad |x-x_0| \ll x_0 \tag{2}$$

when the bond length x does not deviate significantly from its equilibrium value x_0 (Figure 1). In this equation, D is the energy of the chemical bond, and a is a measure of how steeply the energy rises when the bond is stretched or squeezed.

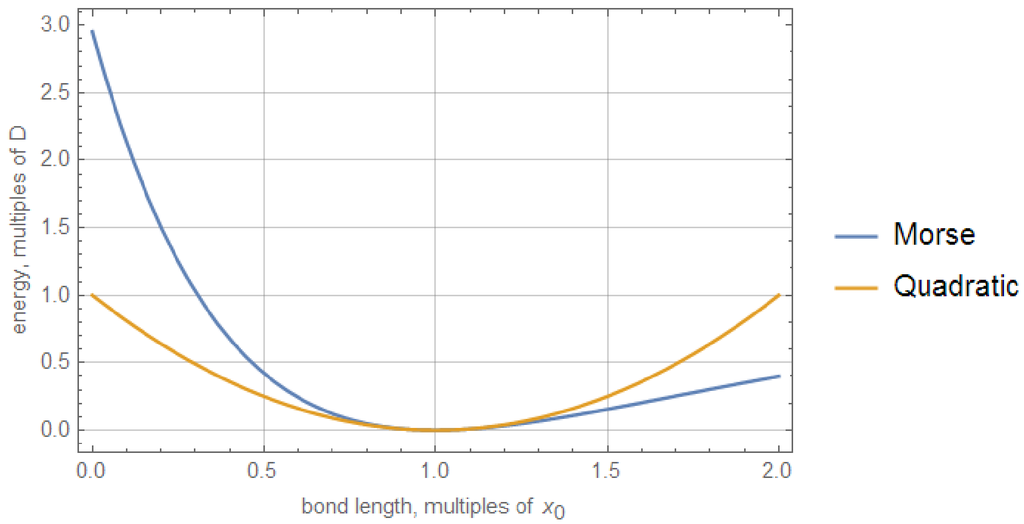

Figure 1. *Morse potential (blue line) and its polynomial approximation to second order (orange line), computed around x_0=1 and plotted using Mathematica.*

More generally, we can ask if a well-behaved function $f(x)$ can be approximated in the vicinity of some point x_0 by the following polynomial expression:

$$f(x)\approx a_0 + a_1(x-x_0)+a_2(x-x_0)^2+a_3(x-x_0)^3+\ldots \tag{3}$$

or even represented exactly if we take an infinite number of terms:

$$f(x)=\sum_{n=0}^{\infty} a_n (x-x_0)^n \tag{4}$$

Such a representation is called *Taylor series*, after *Brook Taylor* who proposed it in 1715. The coefficients a_n may be obtained by sequential differentiation of both sides of Equation (4):

$$\begin{aligned}
f(x) &= \sum_{n=0}^{\infty} a_n (x-x_0)^n && \Rightarrow \quad f(x_0) = a_0 && \Rightarrow \quad a_0 = \frac{f(x_0)}{0!} \\
f'(x) &= \sum_{n=1}^{\infty} n a_n (x-x_0)^{n-1} && \Rightarrow \quad f'(x_0) = 1\cdot a_1 && \Rightarrow \quad a_1 = \frac{f'(x_0)}{1!} \\
f''(x) &= \sum_{n=2}^{\infty} n(n-1) a_n (x-x_0)^{n-2} && \Rightarrow \quad f''(x_0) = 1\cdot 2\cdot a_2 && \Rightarrow \quad a_2 = \frac{f''(x_0)}{2!} \\
f'''(x) &= \sum_{n=3}^{\infty} n(n-1)(n-2) a_n (x-x_0)^{n-3} && \Rightarrow \quad f'''(x_0) = 1\cdot 2\cdot 3\cdot a_3 && \Rightarrow \quad a_3 = \frac{f'''(x_0)}{3!}
\end{aligned} \tag{5}$$

where $n!$ (pronounced "*n factorial*") is a shorthand for $1\cdot 2\cdot 3\cdot \ldots \cdot n$. By convention, $0! = 1$. If we now put the coefficients into Equation (4), we obtain:

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!}(x-x_0)^n \tag{6}$$

This is the definition of Taylor series. In the special case when $x_0 = 0$, Equation (6) is called *McLaurin series*. For a given function, the Taylor series is unique – only one set of coefficients exists.

The general recipe for finding the Taylor series of a function around a reference point x_0 is:

1. Compute a few derivatives, three or four are usually sufficient.
2. Try finding a pattern and therefore an expression for the *n*-th derivative.
3. Compute the numerical values of the derivatives at x_0.
4. Assemble the Taylor series.

Step 2 is optional when the complete infinite series is not required.

Example 1: find the Taylor series for the exponential function around $x_0 = 0$.

Solution: keep computing derivatives until you see a pattern in them that would allow you to generalise to arbitrary order. In this case, the pattern is simple:

$$\begin{cases} f^{(0)}(x) = e^x \\ f^{(1)}(x) = e^x \\ f^{(2)}(x) = e^x \\ \ldots \\ f^{(n)}(x) = e^x \end{cases} \Rightarrow \begin{cases} f^{(0)}(0) = 1 \\ f^{(1)}(0) = 1 \\ f^{(2)}(0) = 1 \\ \ldots \\ f^{(n)}(0) = 1 \end{cases} \tag{7}$$

and therefore the Taylor series for the exponential function around $x_0 = 0$ is:

$$e^x = \sum_{n=0}^{\infty} \frac{1}{n!} x^n \tag{8}$$

Example 2: find the Taylor series for the natural logarithm function around $x_0 = 1$.

Solution: in this case, the pattern of derivatives is more complicated and takes a while to settle:

$$\begin{cases} f^{(0)}(x) = \ln x \\ f^{(1)}(x) = +x^{-1} \\ f^{(2)}(x) = -1\cdot x^{-2} \\ f^{(3)}(x) = +1\cdot 2\cdot x^{-3} \\ f^{(4)}(x) = -1\cdot 2\cdot 3\cdot x^{-4} \\ \ldots \\ f^{(n)}(x) = (-1)^{n+1}(n-1)!\,x^{-n} \end{cases} \Rightarrow \begin{cases} f^{(0)}(1) = 0 \\ f^{(1)}(1) = +0! \\ f^{(2)}(1) = -1! \\ f^{(3)}(1) = +2! \\ f^{(4)}(1) = -3! \\ \ldots \\ f^{(n)}(1) = (-1)^{n+1}(n-1)! \end{cases} \tag{9}$$

and therefore the Taylor series is:

$$\ln x = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}(n-1)!}{n!}(x-1)^n = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n}(x-1)^n \tag{10}$$

Note that the sum runs from 1 rather than zero because the zeroth term is missing.

2. Accuracy of a truncated Taylor series

Even a computer cannot in practice calculate infinitely many terms. With a finite number of terms, a Taylor series would be an approximation. The example if Equation (10) is explored in Figure 2.

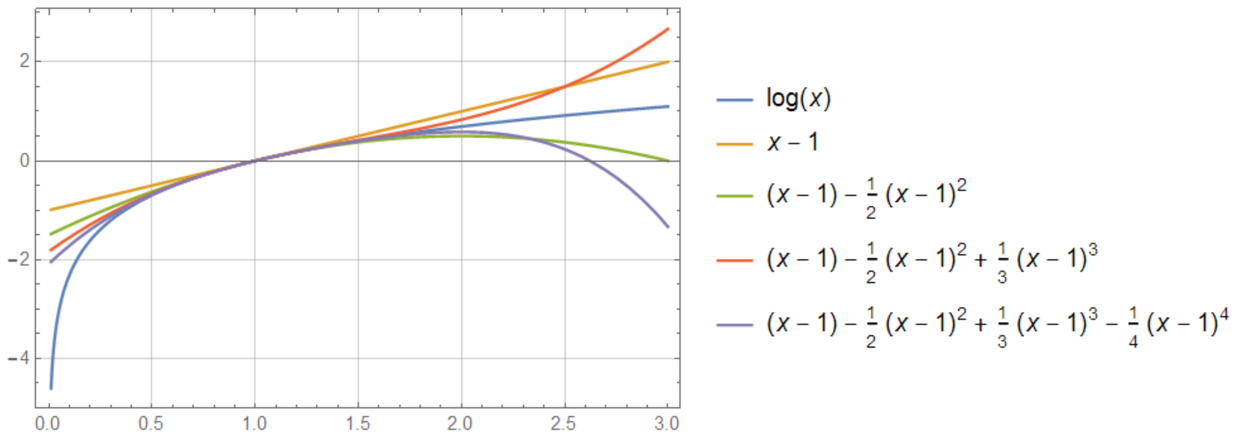

Figure 2. *Natural logarithm function and its Taylor series around x_0=1, truncated at orders 1, 2, 3, and 4.*

In the vicinity of the reference point $x_0 = 1$, the approximation is good, but its quality deteriorates as the distance from the reference point increases. This is to be expected from polynomials – for large values of the argument the leading power dominates, and the polynomial starts rising or falling steeply.

Systematic criteria exist for the approximation accuracy provided by a truncated Taylor series. An exact calculation of the error is not possible (that would be equivalent to computing infinitely many terms), but the following estimate is in practice useful:

$$f(x)=\sum_{n=0}^{N}\frac{f^{(n)}(x_0)}{n!}(x-x_0)^n+O\left[(x-x_0)^{N+1}\right]$$ - *Peano's remainder*

where $O\left[(x-x_0)^{N+1}\right]$ stands for "some number of the order of $(x-x_0)^{N+1}$". This expression may be proven by direct inspection – the next largest power in the series is $N+1$, and for small values of $x-x_0$ (the intended usage case for Taylor series) that power will dominate the error. More sophisticated error estimates exist whose derivations are outside the scope of this course, *e.g.*:

$$f(x)=\sum_{n=0}^{N}\frac{f^{(n)}(x_0)}{n!}(x-x_0)^n+\frac{f^{(N+1)}(\theta)}{(N+1)!}(x-x_0)^{N+1}$$ - *Lagrange's remainder*

where θ is a hard to predict number between x and x_0.