CHEM1033 - Week 8 Lecture - Power series and their convergence

Chapter 7 of Steiner, "The Chemistry Maths Book", 2nd edition.

Approximations in physical sciences

A common problem in all areas of physics and chemistry is that, while the fundamental equations governing a particular process are known, the solutions to those equations are in practice incomputable because they lead to very large datasets or require very large number of mathematical operations. In such cases, a question that is commonly asked is: "what is the simplest possible mathematical procedure that would produce the required result *with acceptable accuracy*?" – the problem of computing *the exact answer* is replaced with the problem of computing *a good enough answer* within the range of the parameter values that may realistically be expected to occur within the system. Such solutions are called "approximations". They are not expected to produce accurate answers in all situations, but may be designed to produce sufficiently accurate answers within some pre-determined ranges.

Taylor series

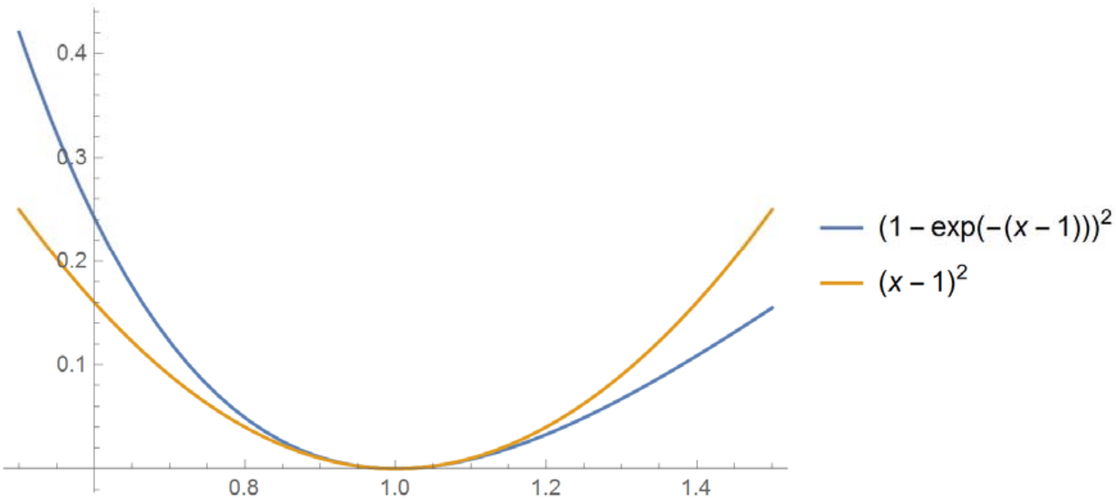
A situation frequently arises in physical sciences and engineering when the value of a particular function is only required approximately and in close vicinity of a particular point (often zero). A good example from chemistry is the *high temperature approximation*, when the Boltzmann exponential is approximated by a linear function in suituations when the energy difference ΔE is small:

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

It is also often found that some functions may be locally approximated well by a polynomial. A graphical illustration for the example of a Morse potential:

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

(an energy function that describes vibrations in simple diatomic molecules) is given below.



More generally, we can ask the question of whether a *sufficiently well-behaved*[1] function $f(x)$ can be *approximated* in the vicinity of some point x_0 by the following polynomial expression:

[1]This is a loaded term in mathematics. For our purposes here, all required derivatives of the function must exist and be continuous – this is required for the formal proofs that we do not give in this course for lack of time.

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

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

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

If we solve the equations on the right of this expression for the corresponding coefficients and put them into Equation (4), we obtain:

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

where $n!$ (pronounced *"n factorial"*) is a shorthand for $1 \cdot 2 \cdot 3 \cdot \ldots \cdot n$. By convention, $0! = 1$. In the special case when $x_0 = 0$ Equation (6) is called McLaurin series. For a given function, the Taylor expansion is unique – only one set of coefficients may exist. The general recipe for computing the Taylor series of a function 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 your chosen point x_0.
4. Assemble the Taylor series.

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

Solution: we should keep computing derivatives until we see a regularity in them that would allow us to generalize to arbitrary order. In this case, the procedure is quite simple:

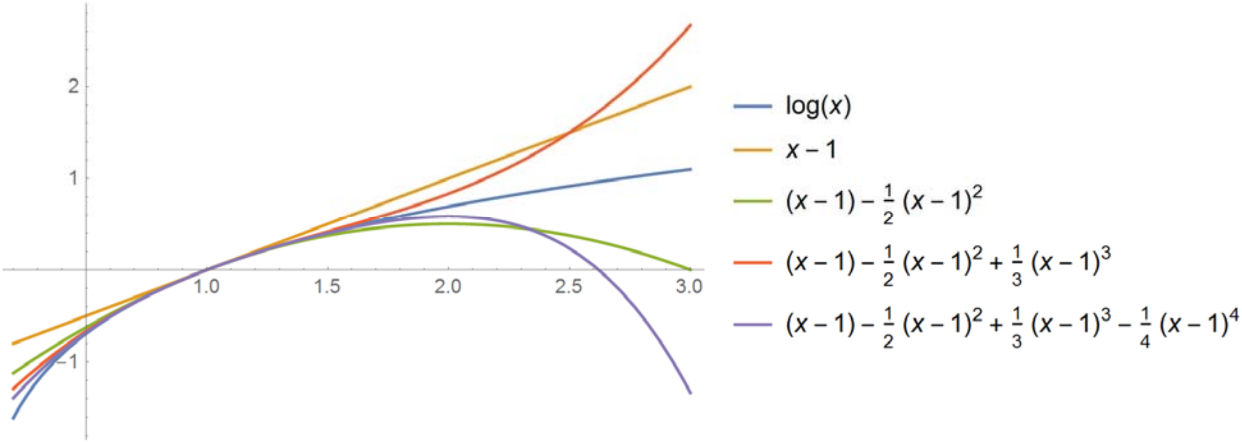
$$\begin{cases} f^{(0)}(x) = \ln x \\ f^{(1)}(x) = +x^{-1} \\ f^{(2)}(x) = -1 \cdot x^{-2} \\ f^{(3)}(x) = +1 \cdot 2 \cdot x^{-3} \\ f^{(4)}(x) = -1 \cdot 2 \cdot 3 \cdot x^{-4} \\ \ldots \end{cases} \quad \Rightarrow \quad \begin{cases} f^{(n=0)}(x) = \ln x \\ f^{(n>0)}(x) = (-1)^{n+1} (n-1)! \, x^{-n} \end{cases} \tag{7}$$

and therefore the Taylor series is:

$$\ln x = \ln x_0 + \sum_{n=1}^{\infty} \frac{(-1)^{n+1}(n-1)!}{n!} \frac{1}{x_0^n} (x - x_0)^n = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} (x-1)^n \tag{8}$$

Accuracy of a truncated Taylor expansion

It is obvious that even a computer cannot in practice calculate infinitely many terms. With a finite number of terms, a Taylor series would be an *approximation*. A good example is Equation (8):



A reasonable question is about the accuracy of this approximation. Exact calculation of the error is not possible (that would be equivalent to computing infinitely many terms), but the following estimates are 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 remainder

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

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

where $O\left[(x-x_0)^{N+1}\right]$ stands for "some number of the order of $(x-x_0)^{N+1}$" and θ is a hard to predict number between x and x_0.

Convergence tests and convergence radius

The approximation provided by a Taylor series is only good in the vicinity of the point x_0 – the closer, the better. In some cases, notably for the logarithm series in Example 1, adding further terms might actually make the approximation *worse*: around $x=3$, the linear approximation is actually the closest to the logarithm. This situation is called a *divergence* and another reasonable question is about the interval in which a given Taylor series is guaranteed to be free of divergences.

D'Alembert test (*aka* 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 test (*aka* 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 either of the limits above are equal to 1, then the question remains open. The interval of x values for which the series converges is called its *convergence radius*. Slowly convergent series are usually avoided in practical calculations because they are computationally expensive and insufficiently accurate in finite precision arithmetic that is used by modern computers.

Example 2: demonstrate that the following series for the exponential function converges everywhere

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

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

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

Example 3: find the convergence radius of the logarithm series from Example 1.

Solution: using the ratio test, we get

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

This explains the apparent deterioration of accuracy observed above for $x = 3$.

Week 9 workshop exercises

Steiner, 2nd edition: section 7.9, problems 41-43, 48, 49, 52-57.

Extra difficulty exercises for the brave

Steiner, 2nd edition: section 7.9, problems 66, 77, 79, 80.