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


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 $\Delta E$ is small, or the temperature is high:

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

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

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

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.

![Morse potential and its polynomial approximation](image)

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:

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

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

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

$$f(x) = \sum_{n=0}^{\infty} a_n (x-x_0)^n \quad \Rightarrow \quad f(x_0) = a_0 \quad \Rightarrow \quad a_0 = \frac{f(x_0)}{0!}$$

$$f'(x) = \sum_{n=1}^{\infty} na_n (x-x_0)^{n-1} \quad \Rightarrow \quad f'(x_0) = 1 \cdot a_1 \quad \Rightarrow \quad a_1 = \frac{f'(x_0)}{1!}$$

$$f''(x) = \sum_{n=2}^{\infty} n(n-1)a_n (x-x_0)^{n-2} \quad \Rightarrow \quad f''(x_0) = 1 \cdot 2 \cdot a_2 \quad \Rightarrow \quad a_2 = \frac{f''(x_0)}{2!}$$

$$f'''(x) = \sum_{n=3}^{\infty} n(n-1)(n-2)a_n (x-x_0)^{n-3} \quad \Rightarrow \quad f'''(x_0) = 1 \cdot 2 \cdot 3 \cdot a_3 \quad \Rightarrow \quad a_3 = \frac{f'''(x_0)}{3!}$$

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

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

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:

$$\begin{align*}
  f^{(0)}(x) &= e^x & f^{(0)}(0) &= 1 \\
  f^{(1)}(x) &= e^x & f^{(1)}(0) &= 1 \\
  f^{(2)}(x) &= e^x & f^{(2)}(0) &= 1 \\
  \vdots & & \vdots \\
  f^{(n)}(x) &= e^x & f^{(n)}(0) &= 1
\end{align*}$$

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

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

$$
\begin{align*}
  f^{(0)}(x) &= \ln x \\
  f^{(1)}(x) &= +x^{-1} \\
  f^{(2)}(x) &= -1 \cdot x^{-2} \\
  f^{(3)}(x) &= +1 \cdot 2 \cdot x^{-3} \\
  f^{(4)}(x) &= -1 \cdot 2 \cdot 3 \cdot x^{-4} \\
  &\vdots \\
  f^{(n)}(x) &= (-1)^{n+1} (n-1)! x^{-n+1}
\end{align*}
$$

so

$$
\begin{align*}
  f^{(0)}(1) &= 0 \\
  f^{(1)}(1) &= +0! \\
  f^{(2)}(1) &= -1! \\
  f^{(3)}(1) &= +2! \\
  f^{(4)}(1) &= -3! \\
  &\vdots \\
  f^{(n)}(1) &= (-1)^{n+1} (n-1)!
\end{align*}
$$

and therefore the Taylor series is:

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

and therefore the Taylor series is:

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

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 x₀=1, truncated at orders 1, 2, 3, and 4.](image)

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 \(\theta\) is a hard to predict number between \(x\) and \(x_0\).