7 Functions and approximations

Topics: infinite series, Taylor expansions, finite difference, plotting

7.1 Motivation and approach

Chemistry and physics are messy. They are full of complicated problems and equations that are sometimes (literally) impossible to solve. In these situations, approximation methods can be incredibly useful. They can be used to obtain an estimate of your answer, which can often be quite accurate, or to build intuition for how a function might behave in certain limits, like at high temperatures or short times.

The following section introduces some of the most common methods, such as Taylor expansions and finite differences for approximating functions, and provides some tips and tricks for using graphing and plots to illustrate how these approximation methods work.

7.2 Infinite series

Conceptual video: Partial sums intro by Khan Academy (6:08)
Conceptual video: Infinite series as a limit of partial sums by Khan Academy (4:48)
Conceptual video: Convergent and divergent sequences by Khan Academy (4:59)

An **infinite series** is a sum formally consisting of an infinite number of terms. If there is a sequence of infinite terms $a_1, a_2, a_3, \ldots$, then the $\boldsymbol{n^{th}}$ **partial sum** is given by

$$s_n = \sum_{i=1}^{n} a_i \,. \tag{7.1}$$

If the partial sums converge to a finite value (*i.e.* $\lim_{n\to\infty} s_n = S$), then the infinite series $\sum_{i=1}^{\infty} a_i$ is said to be **convergent** and equal to S. A necessary (but not sufficient) criteria for convergence is that $\lim_{i\to\infty} a_i = 0$.

Other series are **divergent** if their sequences of partial sums approach $\pm\infty$ or are **oscillatory** if they oscillate between two values. In general, there are many different tests for convergence.

7.3 Taylor series and Taylor expansions

Conceptual and technical video: Taylor series by 3Blue1Brown (22:19)

A **Taylor expansion** is a power series representation of a function $f(x)$ that has a continuous n^{th} derivative on an interval $a \leq x \leq b$. The Taylor series of $f(x)$ around a point a is

$$f(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}f''(a) + \frac{(x-a)^3}{3!}f'''(a) + \dots \tag{7.2}$$

$$= \sum_{n=0}^{\infty} \frac{(x-a)^n}{n!} f^{(n)}(a)\,, \tag{7.3}$$

which gives the value of the function at x in terms of the value of the function and its derivatives at a reference point a.

In practice, Taylor expansions are often truncated at a finite number of terms, and the remainder after the n^{th} term is given by

$$R_n(x) = f(x) - \sum_{m=0}^{n} \frac{(x-a)^m}{m!} f^{(m)}(a)\,. \tag{7.4}$$

Truncated expansions are often identified by the order of the last term in the approximation. For example, an approximation of $e^x \approx 1 + x$ is often referred to as an "expansion to the first order" (since the last term is the one corresponding to $n = 1$) or a "linear approximation" (since the last term is linear in x).

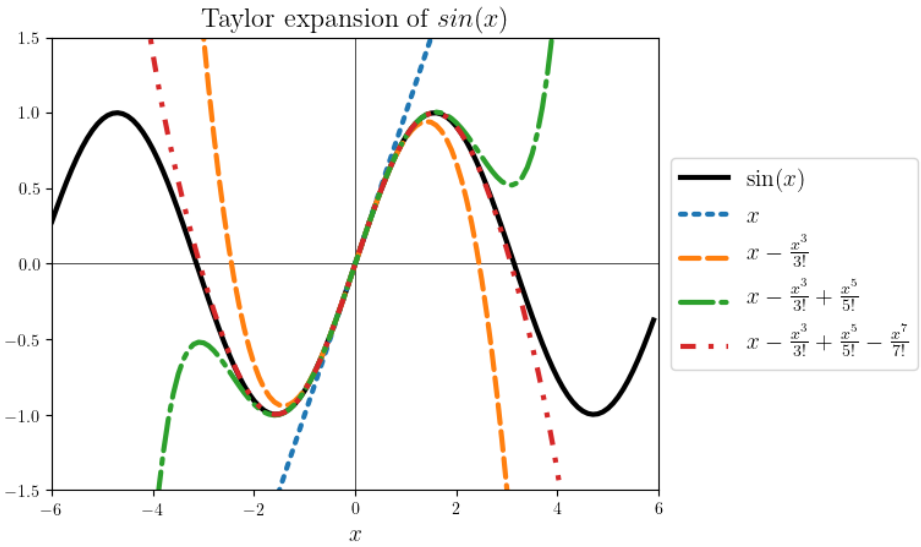
If we are approximating a function at a value x that is close to our reference point a, then $(x-a)$ is small, and powers of that difference (*i.e.* $(x-a)^n$) will shrink quickly as n increases. Therefore, we will likely be able to get a good approximation of $f(x)$ using a relatively small number of terms in our Taylor expansion. The further away from our reference point a we want to approximate $f(x)$, the more terms we will need in our expansion. This fact motivates how we might choose our reference point a.

The power series representation of a function is unique. Some examples of common Taylor series expansions are:

- $e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots = \sum_{n=0}^{\infty} \frac{x^n}{n!}$
- $\ln(1+x) = x - \frac{x^2}{2!} + \frac{x^3}{3!} - \dots = \sum_{n=1}^{\infty} (-1)^{n-1} \frac{x^n}{n!}$
- $(1+x)^m = 1 + mx + \frac{m(m-1)}{2!}x^2 + \frac{m(m-1)(m-2)}{3!}x^3 + \dots = \sum_{n=0}^{\infty} \binom{m}{n} x^n$
  - This is known as the **binomial expansion**.
- $\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \dots = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n+1}}{(2n+1)!}$

Example 7.1: Determine the series expansion for $f(x) = \cos x$ by performing a Taylor expansion around the point $a = 0$.

Below is a graphical representation of the Taylor expansion of the sine function around $x = 0$. We see that, even the lowest order term, x, approximates the sine function quite well around $x = 0$. Higher order expansions provide more accurate estimates further away from our reference point.



Power series can be differentiated or integrated term by term. Also, two power series can be added, subtracted, multiplied, or divided (so long as the denominator is not zero at $x = 0$).

7.4 Finite difference methods

Recall that the **derivative** of a function is defined as

$$\frac{df(x)}{dx} = \lim_{\varepsilon \to 0} \frac{f(x+\varepsilon) - f(x)}{\varepsilon} . \tag{7.5}$$

If ε is small, then we can approximate the derivative using the **forward finite difference**:

$$\frac{df(x)}{dx} \approx \frac{f(x+\varepsilon) - f(x)}{\varepsilon} . \tag{7.6}$$

We could also use the **backward finite difference**:

$$\frac{df(x)}{dx} \approx \frac{f(x) - f(x-\varepsilon)}{\varepsilon} \tag{7.7}$$

or the **central finite difference**:

$$\frac{df(x)}{dx} \approx \frac{f(x+\varepsilon) - f(x-\varepsilon)}{2\varepsilon} , \tag{7.8}$$

and we could use a similar approach to approximate the second derivative using, for example, the **second central difference**:

$$\frac{d^2 f(x)}{dx^2} \approx \frac{f(x+\varepsilon) - 2f(x) + f(x-\varepsilon)}{\varepsilon^2} . \tag{7.9}$$

7.4.1 Finite difference method for differential equations

Technical video: Finite differences introduction by Commutant (6:48)

If given a differential equation $f'(x)$ and an initial condition for the function $f(x_0)$, one can use the finite differences to approximate the function $f(x)$ by iteratively solving for points.

To do this, one can rearrange the forward finite difference equation to obtain

$$f'(x) = \frac{f(x+\varepsilon) - f(x)}{\varepsilon} \tag{7.10}$$

$$\varepsilon f'(x) = f(x+\varepsilon) - f(x) \tag{7.11}$$

$$f(x+\varepsilon) = f(x) + \varepsilon f'(x)\,. \tag{7.12}$$

This is called the **Euler formula**. Given a small enough step size ε and knowledge of the function and derivative evaluated a certain point, one can use this formula to approximate the function at a nearby point.

Other numerical schemes that use higher-order finite differences can be used for more accurate approximations .

Example 7.2: Given the differential equation $f'(x) = 2x$ and the initial condition $f(0) = 1$, use the Euler formula to approximate the function near $x = 0$. Use steps of $\varepsilon = 0.1$ and 0.5. Plot both of those approximations as well as the analytical solution on the same graph.

7.4.2 Stationary points

For a function $f = f(x_1, x_2, \ldots, x_n)$ defined in n dimensions, a **stationary point** $\boldsymbol{x}$ of f is one for which $\frac{\partial f}{\partial x_i}$ evaluated at $\boldsymbol{x}$ is equal to 0 for all $i = 1, \ldots, n$.

The stationary point is a **minimum** if $\frac{\partial^2 f(\boldsymbol{x})}{\partial x_i^2} > 0$ for all i, a **maximum** if $\frac{\partial^2 f(\boldsymbol{x})}{\partial x_i^2} < 0$ for all i, or otherwise a **saddle point** (*i.e.* it is a minimum in some directions and a maximum in others).

The **Hessian** is a square matrix of second-order partial derivatives of a function f, where the i, j matrix element is defined as

$$H_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}\,. \tag{7.13}$$

If the Hessian evaluated at a point $\boldsymbol{x}$ has all positive eigenvalues, then $\boldsymbol{x}$ is a minimum of f. If it has all negative eigenvalues, then $\boldsymbol{x}$ is a maximum, and if it has both positive and negative eigenvalues, then $\boldsymbol{x}$ is a saddle point.

Stationary points can be useful reference points when performing Taylor expansions.

7.5 Plotting functions

Conceptual and technical video: Solving linear systems by graphing by Khan Academy (8:30)

Sometimes, you are presented with a system of equations that are challenging to solve. Using a graphing tool, like the desmos graphing calculator, can allow you to quickly plot the equations and visually identify solutions as the intersection points.

7.5.1 Identifying functions by graphing

Often, you will encounter a function or data set to which you are trying to fit or assign a functional form. Plotting the function or data points is a good starting point, and changing the scale of the x and/or y axis to a log-scale (instead of a linear-scale) might be helpful.

First, let us review some useful properties of logarithms, regardless of the base, where a and b are constants:

- $\log(ab) = \log(a) + \log(b)$
- $\log(a/b) = \log(a) - \log(b)$
- $\log\left(a^b\right) = b\log(a)$
- $\log(1) = 0$

Additionally, for the natural log, $\ln(e) = 1$.

An **exponential function** has the general form:

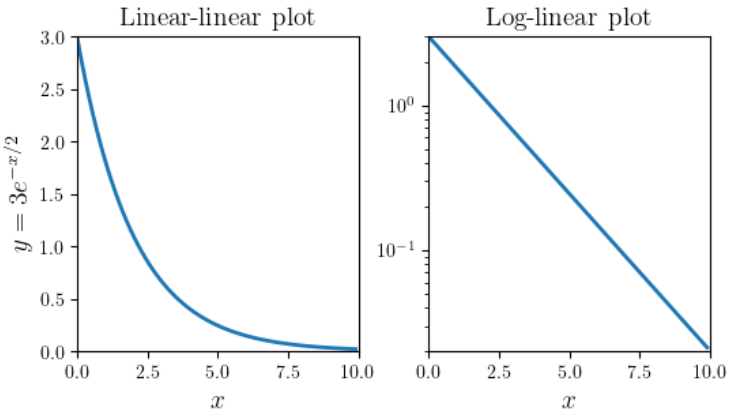
$$y = ae^{bx}\,. \tag{7.14}$$

Taking the natural log (ln) of both sides and simplifying gives:

$$\ln(y) = \ln\left(ae^{bx}\right) = \ln(a) + \ln\left(e^{bx}\right) = \ln(a) + bx\ln(e) \tag{7.15}$$

$$= \ln(a) + bx\,. \tag{7.16}$$

Therefore, if you plot an exponential function with the y-axis on a natural log scale, it will appear to have a linear relationship with the slope corresponding to the exponential factor b. Note that if you plot the function on a $\log_{10}$ scale, it will appear to have a linear relationship, but the slope will not correspond directly to b. Below is an illustration of the function $y = 3e^{-1/2}$ plotted on a linear-linear scale (left) and a log-linear scale (right).



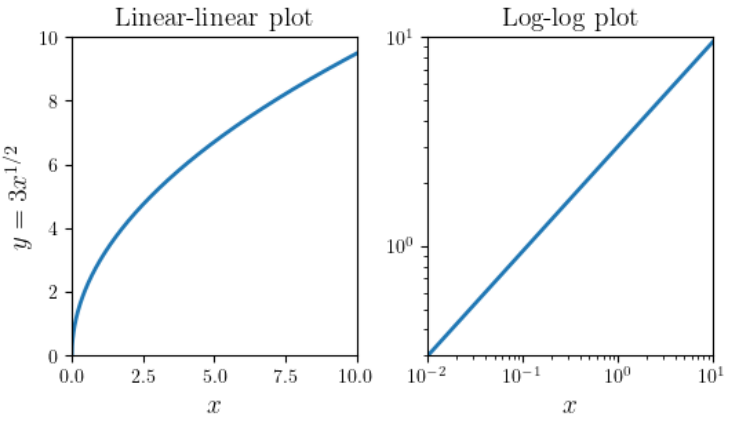
A **power law** has the general form:

$$y = ax^b \,. \tag{7.17}$$

Taking the log of both sides and simplifying gives:

$$\log(y) = \log\big(ax^b\big) = \log(a) + \log\big(x^b\big) \tag{7.18}$$
$$= \log(a) + b\log(x) \,. \tag{7.19}$$

In this case, plotting the power law with both the x and y axes on a log scale (of any base), it will appear to have a linear relationship with the slope corresponding to the power b. Below is an illustration of the function $y = 3x^{1/2}$ plotted on a linear-linear scale (left) and a log-log scale (right).



7.6 Connections to physical chemistry

The methods outlined here are common throughout physics and chemistry. For instance, functions of matrices or operators are defined in terms of their series expansions. One example is the quantum mechanical time-evolution operator, which describes how a quantum state evolves until time t. The time-evolution operator is given by:

$$e^{-iHt/\hbar} = 1 - \frac{i}{\hbar}Ht - \frac{1}{2\hbar^2}H^2t^2 - \dots \,, \tag{7.20}$$

where H is the Hamiltonian operator. If you want to evolve a state for a short time so that t is small, you may approximate the time-evolution by truncating the above expansion to first order, so that $e^{-iHt/\hbar} \approx 1 - iHt/\hbar$.

Additionally, Taylor expansions are a framework for thinking about **perturbation theory**, a method often used in the physical sciences to approximate the solution of a difficult problem through the use of a reference problem that is simple to solve. For example, consider the behavior of a particle under the effect of a weak force f. If you already know the equation for how the particle behaves without any force, you can add a term linear in the force (*i.e.* proportional to f) to approximate this more complex problem. Since the force is

weak, terms that are quadratic or higher in the force (*i.e.* proportional to $f^2, f^3, \dots$) can be ignored. This approximation to first order is called **linear response theory**.

The finite difference method for solving differential equations is used frequently, as many differential equations are too difficult or impossible to solve analytically. This method is also often used to numerically propagate an object in time, such as evolving a wavefunction in time according to the Schrödinger equation, its equation of motion.

Plotting can always be an extremely useful tool – when you are trying to understand how a function behaves with a changing parameter, when you are trying to make sense of your experimental data, and more.

7.7 Additional text resources

Mathematical Methods for Physicists (7th Edition) by Arkfen, Weber, and Harris: Sections 1.1, 1.2, 1.3, 1.5, 1.6, 1.8, and 1.9

7.8 Example problem solutions

Example 7.1: *Determine the series expansion for $f(x) = \cos x$ by performing a Taylor expansion around the point $a = 0$.*

To evaluate the Taylor expansion of $\cos(x)$ around the point $a = 0$, we will need to find the first few derivatives of $\cos(x)$ with respect to x and then evaluate them at $a = 0$:

$$\cos(x)\Big|_0 = 1 \tag{7.21}$$

$$\frac{d}{dx}\cos(x)\Big|_0 = -\sin(x)\Big|_0 = 0 \tag{7.22}$$

$$\frac{d^2}{dx^2}\cos(x)\Big|_0 = -\frac{d}{dx}\sin(x)\Big|_0 = -\cos(x)\Big|_0 = -1 \tag{7.23}$$

$$\frac{d^3}{dx^3}\cos(x)\Big|_0 = -\frac{d}{dx}\cos(x)\Big|_0 = \sin(x)\Big|_0 = 0 \tag{7.24}$$

$$\frac{d^4}{dx^4}\cos(x)\Big|_0 = \frac{d}{dx}\sin(x)\Big|_0 = \cos(x)\Big|_0 = 1\,. \tag{7.25}$$

Putting this all together gives

$$\cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} + \dots\,. \tag{7.26}$$

Examining these first few terms and recognizing a pattern, we can write this in summation notation as:

$$\cos(x) = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n}}{(2n)!}\,. \tag{7.27}$$

Example 7.2: *Given the differential equation $f'(x) = 2x$ and the initial condition $f(0) = 1$, use the Euler formula to approximate the function near $x = 0$. Use steps of $\varepsilon = 0.1$ and 0.5. Plot both of those approximations as well as the analytical solution on the same graph.*

We start with plugging in $f'(x) = 2x$ into Eq. (7.12), which gives:

$$f(x + \varepsilon) = f(x) + 2x\varepsilon \,. \tag{7.28}$$

Now, we can use our initial condition $f(x = 0) = 1$ to iteratively evaluate $f(x)$ away from $x = 0$ in steps of ε:

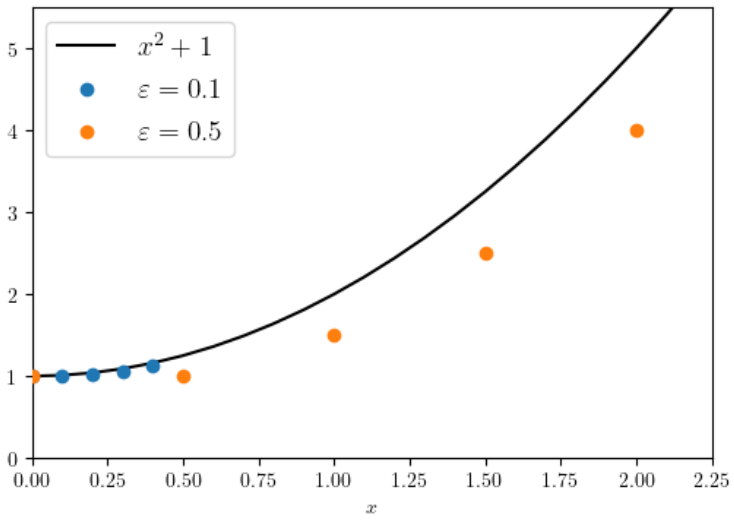
$$f(\varepsilon) = f(0) + 2 \cdot 0 \cdot \varepsilon = 1 \tag{7.29}$$
$$f(2\varepsilon) = f(\varepsilon) + 2 \cdot \varepsilon \cdot \varepsilon = 1 + 2\varepsilon^2 \tag{7.30}$$
$$f(3\varepsilon) = f(2\varepsilon) + 2 \cdot 2\varepsilon \cdot \varepsilon = 1 + 6\varepsilon^2 \tag{7.31}$$
$$f(4\varepsilon) = f(3\varepsilon) + 2 \cdot 3\varepsilon \cdot \varepsilon = 1 + 12\varepsilon^2 \,. \tag{7.32}$$

Analytically, we can directly integrate $f'(x)$ and then use in our initial condition to find $f(x)$:

$$f(x) = \int f'(x)dx = \int 2xdx = x^2 + C \tag{7.33}$$
$$f(0) = C = 1 \tag{7.34}$$
$$f(x) = x^2 + 1 \,. \tag{7.35}$$

We can plot the analytical solution along with our numerical estimates using step sizes of $\varepsilon = 0.1$ and 0.5. We see that, for both numerical estimates, the points closer to our initial condition are more accurate. Additionally, using a smaller step size provides a better estimate of the analytical solution.

If you want to learn how you can use Python as a tool to solve this problem and plot the solutions, see the next section!


$x^2 + 1$
$\varepsilon = 0.1$
$\varepsilon = 0.5$
0
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2
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0.50
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