CHEM1047 – Week 2 Lecture 2 – Well-behaved functions

☐ *Chapter I, Sections 3-5 of Demidovich, "Problems in Mathematical Analysis", 2nd edition.*

Not every function is admissible as a solution for a chemical or a physical problem. This lecture is about the restrictions that physical reality places on what functions encountered in natural sciences can and cannot be. Physically admissible functions are informally called *well-behaved*.

1. Discontinuities

At a simplified level, a *discontinuity* is a missing point or an abrupt jump in the function value from one point to the next. Discontinuities are common in mathematics, but rare in chemistry and physics for reasons that we will now discuss.

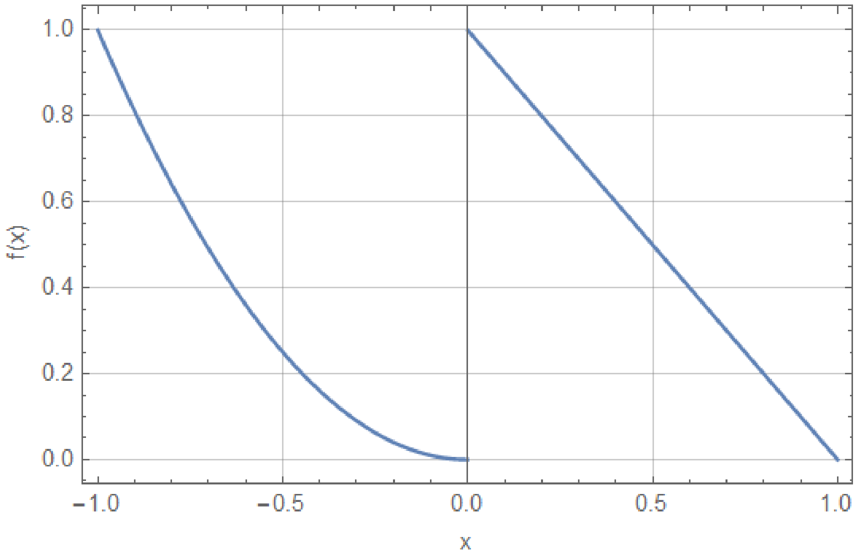

Figure 1. *An example of a discontinuity in a function at the point where x=0.*

Formally, a point of discontinuity of a function $f(x)$ is defined as a point x_0 where there is a difference between the right and the left limit of the function:

$$\lim_{x \to x_0 -} f(x) \neq \lim_{x \to x_0 +} f(x) \tag{1}$$

where the *left limit* $\lim_{x \to x_0 -} f(x)$ is defined as the value that the function approaches when x approaches x_0 from the left, and similarly for the *right limit*.

2. Restrictions imposed by physical reality

Let us calculate the energy required to create a discontinuity in the trajectory $x(t)$ of a particle of mass m. We will make a discontinuous function using the following limit:

$$x(t) = \lim_{k \to \infty} \left[\frac{1}{1 + e^{-kt}} \right] \tag{2}$$

It is clear from Figure 2 that the jump from $x = 0$ to $x = 1$ around $t = 0$ gets sharper and sharper as the value of k increases. In the limit of infinite k the function has a discontinuity.

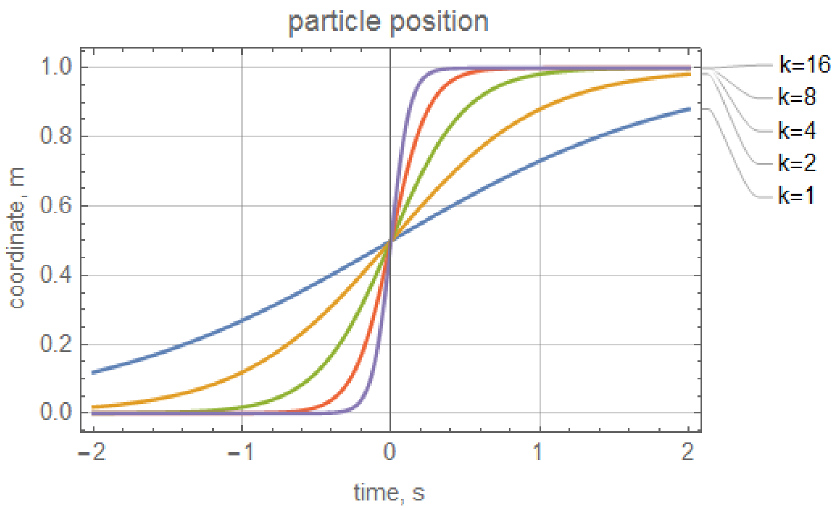

Figure 2. *Time dependence the particle coordinate defined by Equation (2) when the parameter k is increased.*

Let us now consider the velocity and the acceleration of the particle. To obtain the velocity, we must differentiate the coordinate with respect to time:

$$v_x(t) = x'(t) = \left(\frac{1}{1+e^{-kt}}\right)' = \frac{ke^{-kt}}{(1+e^{-kt})^2} \tag{3}$$

The result is plotted in Figure 3. As expected, larger values of k require greater velocities because the particle moves faster.

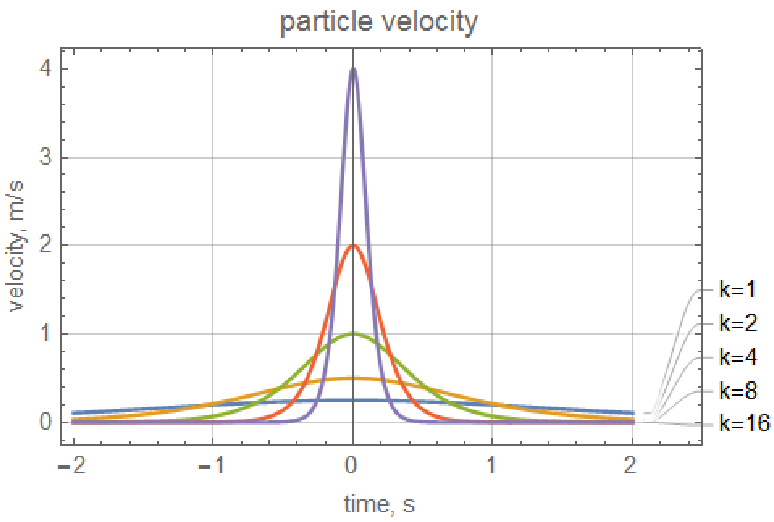

Figure 3. *Time dependence the particle velocity defined by Equation* (3) *when the parameter k is increased.*

After setting time to zero and then calculating the limit of the velocity for $k \to \infty$:

$$v_x(t) = x'(t) = \lim_{k\to\infty}\left[\frac{ke^{-kt}}{\left(1+e^{-kt}\right)^2}\right] \quad \Rightarrow \quad v_x(0) = \lim_{k\to\infty}\left[\frac{k}{4}\right] = \infty$$

we conclude that *infinite velocity* would be required. Because energy is proportional to the square of the velocity, this means that *infinite energy* would have to be supplied to the particle to achieve a discontinuity in its trajectory. This is clearly impossible.

What about a sharp turn? The following function has a sharp corner when $k \to \infty$:

$$y(t) = \frac{1}{k}\ln\left[1+e^{kt}\right] \qquad (4)$$

Its plot for different values of k is shown in Figure 4.

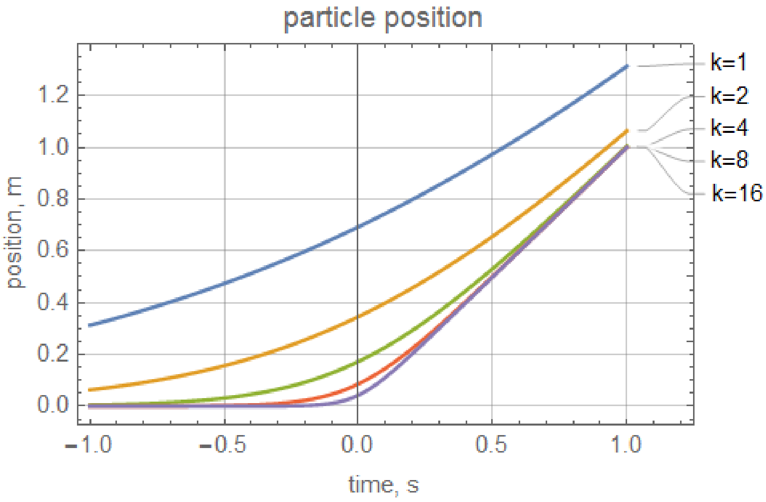

Figure 4. *Time dependence the particle coordinate defined by Equation* (4) *when the parameter k is increased.*

Velocities are realistic here – the first derivative of $y(t)$ never goes to infinity:

$$v_{\mathrm{y}}(t) = y'(t) = \frac{e^{kt}}{1+e^{kt}}$$

However, the *second derivative* (*i.e.* acceleration) now becomes infinite at $t=0$ when $k \to \infty$:

$$a_{\mathrm{y}}(t) = y''(t) = \lim_{k\to\infty}\left[\frac{ke^{kt}}{\left(1+e^{kt}\right)^2}\right] \quad \Rightarrow \quad a_{\mathrm{y}}(0) = \lim_{k\to\infty}\left[\frac{k}{4}\right] = \infty$$

Newton's second law ($F = ma$) then means that *infinite force* would be required to create a sharp corner in the trajectory. That is also impossible.

Deeper inspection indicates that the same problem appears whenever there is a discontinuity in any of the derivatives of the state functions almost anywhere in chemistry and physics. It is therefore reasonable to create a category of functions that are admissible as realistic solutions to physical models. Such functions are called *well-behaved*. This is an informal term; it usually means: (a) finite; (b) continuous derivatives of any order.

In some specific situations conditions may also exist on the integrals: either a positive integral, or a finite integral, or a finite integral of the absolute square. For example, when the function describes concentration across the sample, its integral is the total quantity of the substance present – obviously, it must be positive and cannot be infinite. When the function is a quantum mechanical wavefunction, its absolute square is probability density, which must integrate to 1 to maintain the balance of probabilities:

$$\int_{-\infty}^{\infty} \left|\psi(x,t)\right|^2 dx = 1 \qquad \forall t \qquad (5)$$

3. Formal definition of continuity

A function $f(x)$ defined in an interval (a,b) is called *continuous* in a point $x_0 \in (a,b)$ if

$$\lim_{x \to x_0} f(x) = f(x_0) \tag{6}$$

Sums, products and superpositions of continuous functions are continuous. Any function that is continuous in a particular interval is necessarily finite in that interval. If a function is continuous and monotonic in a certain interval, then its inverse function is also continuous and monotonic.

Examples of discontinuous functions:

1. Heaviside step function:

$$H(x) = \begin{cases} 1 & \text{if} \quad x \ge 0 \\ 0 & \text{if} \quad x < 0 \end{cases}$$

2. Signum function:

$$\operatorname{sign}(x) = \begin{cases} +1 & \text{if} \quad x > 0 \\ 0 & \text{if} \quad x = 0 \\ -1 & \text{if} \quad x < 0 \end{cases}$$

3. Dirichlet function:

$$D(x) = \begin{cases} 0 & \text{if } x \text{ is an irrational number} \\ 1 & \text{if } x \text{ is a rational number} \end{cases}$$

Heaviside and signum functions are discontinuous in just one point; Dirichlet function is discontinuous everywhere because there are irrational numbers around every rational number and *vice versa*.

Example: demonstrate that $y(x) = x+1$ is continuous at $x=3$, but $z(x) = 1/(x-3)$ is not.

Solution: inspecting the $y(x) = x+1$ around $x=3$ reveals no special points; the left and the right limits are both straightforward and equal to the value of the function at that point

$$\lim_{x \to 3-} y(x) = \lim_{x \to 3+} y(x) = 4 \tag{7}$$

Therefore, $y(x) = x+1$ is continuous at $x=3$. However, $z(x) = 1/(x-3)$ is not even defined at $x=3$ because division by zero occurs. The two limits are also different:

$$\lim_{x \to 3-} z(x) = -\infty, \qquad \lim_{x \to 3+} z(x) = +\infty \tag{8}$$

Therefore, $z(x) = 1/(x-3)$ is not continuous at $x=3$.

4. Discontinuities and singularities in physical theories

Note that the discussion above only applies to *solutions* of physical equations of motion. No such restrictions exist on the problem specifications – point particles, infinitely high walls and infinitely large masses are rather common as stage settings. A good example is Coulomb interaction energy between a pair of point charges, which goes to infinity as the inter-particle distance decreases:

$$E(r) = \frac{q_1 q_2}{4\pi\varepsilon_0} \frac{1}{r}$$

This makes the very definition of a point charge problematic because such an object would have an infinite energy. The same applies to the gravitational potential of a point mass. A point at which a continuous function goes to infinity is called a *singularity*; these are quite common in the *equations of motion*.

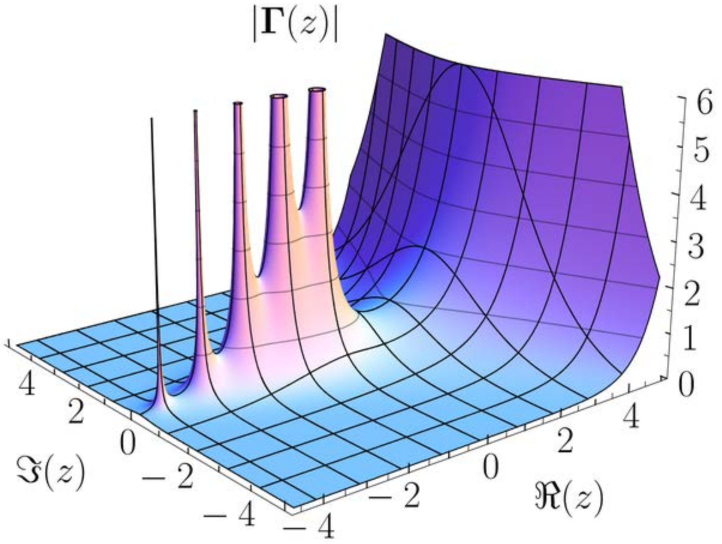

Figure 5. *A plot of the absolute value of the gamma function of a complex argument.*

A few singularities in the gamma function of a complex argument are shown in the figure above. In all cases, however, physically meaningful solutions to the equations of motion must be well-behaved. The only exception that appears to actually exist is black holes.