Exercises week 2

October 5, 2017

Please submit your work before the following class (name the script file as `your_name_problems-week2.m`) at the following e-mail address `francesca.marchetti@uam.es`.

1 Exercise:

Study the function $f(x) = g_1(x)g_2(x)$, where

$$g_1(x) = \frac{x^3 - x + 1}{x^3 - 1} \qquad\qquad g_2(x) = e^{-x/5} \ .$$

1. Plot the function and establish its asymptotic behaviour;
2. Plot the first derivative $\frac{df(x)}{dx}$ evaluated both numerically and analytically and estimate the location of the maximum and minimum of $f(x)$;
3. Make a Taylor expansion of $f(x)$ at $x_0 = 0$ up to third order and plot the polynomial $P_3(x)$ you obtain togher with the original function $f(x)$.
4. Evaluate analytical the maximum and minimum of $P_3(x)$ and compare them with the ones of $f(x)$.

2 Exercise:

Taylor expand analytically the function $f(x) = e^x$ around $x_0 = 0$ up to the first, second, and third order; plot the original function and the various Taylor polynomial you have obtained, $P_n(x)$, in the interval $x \in [-2, 2]$ and discuss the result you get. Repeat the exercise by expanding around the point $x_0 = 1$.
Do the same exercise for the following functions and expansion points (and plot the results in the interval indicated):

$f(x) = \sin(x)$	$x_0 = 0$	$x \in [0, 2\pi]$
$f(x) = \sin(x)$	$x_0 = \pi/2$	$x \in [0, 2\pi]$
$f(x) = \dfrac{1}{1-x}$	$x_0 = 0$	$x \in [-1, 1)$
$f(x) = \log(1 + x)$	$x_0 = 0$	$x \in (-1, 1]$

N.B. you can get acquainted with the build-in function `taylor()`, but, for your own benefit, first always do the expansions analytically.

3 Exercise:

A one-dimensional energy potential landscape is given by $U(x) = x^4 - 2x^2 - 1$. Find the two minima of the potential and do a Taylor expansion around one of them to second order. Show the original function and the approximated one.

4 Exercise: Lennard-Jones potential

The Lennard-Jones potential

$$V(r) = \frac{a}{r^{12}} - \frac{b}{r^6} , \tag{1}$$

is a model potential describing the interaction between a pair of neutral atoms or molecules. Assuming that the typical bond energy $V_0 \sim 150\, k_B T \simeq 6 \times 10^{-19}$ J corresponds to the depth of the potential and that the typical bond length $r_0 \sim 0.15$ nm corresponds to its equilibrium position:

1. Derive the expressions and values of the parameters a and b.
2. For these values of a and b, plot the dimensionless expression of the potential
$$\frac{r_0^{12}}{a} V(\tilde{r} r_0) ,$$
in the interval $\tilde{r} \in [0.8, 2]$.
3. Apply a Taylor expansion around the equilibrium position and determine the effective spring constant $k = \left.\frac{d^2 V(r)}{dr^2}\right|_{r=r_0}$.

5 Exercise: "Achilles and the Tortoise" (Zeno's paradox)

"In a race, the quickest runner can never overtake the slowest, since the pursuer must first reach the point whence the pursued started, so that the slower must always hold a lead."

Zeno's paradox about "Achilles and the Tortoise" can be formulated in the following way: Achilles and the Tortoise compete in a race. The Tortoise (which position as a function of time is plotted as an orange line in Fig. 1) starts (at a lower speed) 20 m ahead of Achilles (who will run at a higher speed). Achilles reaches the 20 m distance after 4 s, but at that time the Tortoise is at a $30(= 20 + 10)$ m distance; Achilles reaches the 30 m distance after $6(= 4+2)$ s, when the Tortoise reaches the $35(= 20+10+5)$ m distance. Will Achilles and the Tortoise ever meet? According how the problem is formulated the answer is paradoxically no.

1. Formulate mathematically the problem above, complete the (geometrical) series and find an estimate of time and distance at which Achilles finally meets the Tortoise;
2. evaluate the velocity at which Achilles and Tortoise respectively run (not very realistic for the Tortoise!);
3. create a plot similar to Fig. 1 and find graphically the point at which the two trajectories meet and compare it with your numerical estimate.

Moral: paradoxes might be solved by introducing the concept of limit.

6 Exercise:

Evaluate numerically (and analytically, when possible)the following integrals

$$I = \int_{-2}^{1} dx(x^2 - 5x^6) \tag{2}$$

$$I = \int_{-5}^{2} dx e^{x^2} x \tag{3}$$

$$I = \int_{2}^{6} dx \log(x) \frac{\sin(x)}{x} \tag{4}$$

with the various approximation schemes introduced in the class. Estimate the numerical error for each approximation scheme for the cases you can integrate analytically and describe how the error evolves when you choose smaller integration subintervals δx.

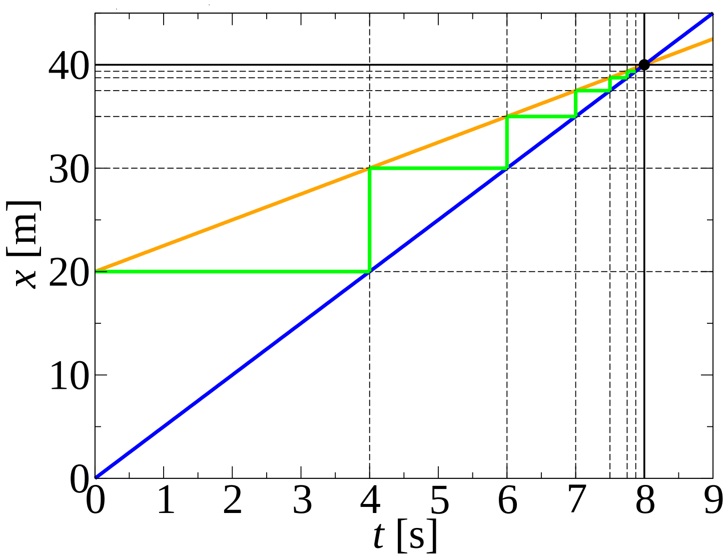

Figure 1: Graphical representation of Zeno's paradox of "Achilles and the Tortoise". Achilles trajectory is plotted in blue and the tortoise one is plotted in orange.

7 Exercise:

Consider the following function

$$f(x) = \int_0^x ds \sin(2s) e^{-s} \; , \tag{5}$$

evaluate it numerically and plot it as a function of x in the interval $x \in [0, 4\pi]$. Compare the numerical result with the exact one $f(x) = \frac{2}{5} - \frac{1}{5} e^{-x} [2\cos(2x) + \sin(2x)]$ — check that $f'(x) = \sin(2x) e^{-x}$.

8 Exercise:

Consider the following function

$$f(x) = \int_0^x ds \frac{\sin(s)}{s} \; ,$$

evaluate it and plot it in the following interval $x \in [0, 6\pi]$. By choosing larger and larger intervals, can you guess the value of the integral $\int_0^\infty ds \frac{\sin(s)}{s} (= \frac{\pi}{2})$?