MAT-2201: Third mandatory assignment

October 24, 2023

The assignment consists of 2 main problems, divided into 10 subproblems in total. Each subproblem is worth 10 points.

Problem 1

Solve Problem 4 in the MAT-2201 exam from December 4, 2019.

Problem 2

The Gauss error function[1] is given by

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt.$$

It turns out that this function can not be written in terms of elementary functions (polynomials, trigonometric and exponential functions etc.). Our goal is to use elementary functions to approximate $\operatorname{erf}(x)$ on the interval $[0, 2]$ in three different ways. The motivation is the following: If we can find a good approximation, we don't have to compute (a numerical approximation of) an integral every time we need to compute $\operatorname{erf}(x_0)$ for some $x_0 \in [0, 2]$.

(a) Compute the 5 first derivatives of $\operatorname{erf}(x)$ and their values at $x = 0$:

$$\operatorname{erf}(0), \quad \operatorname{erf}'(0), \quad \ldots, \quad \operatorname{erf}^{(5)}(0).$$

Write down the 5th-degree Taylor polynomial of $\operatorname{erf}(x)$ around $x = 0$ and denote it by $T_5(x)$. What is the multiplicity of the root $x = 0$ of $\operatorname{erf}(x)$? (The fundamental theorem of calculus may be useful in this exercise.)

[1] See for example `https://en.wikipedia.org/wiki/Error_function`.

(b) Consider the points $(x_1, y_1), \ldots, (x_5, y_5)$ given by

$$x_1 = 0, \quad x_2 = 1/2, \quad x_3 = 1, \quad x_4 = 3/2, \quad x_5 = 2$$

and $y_i = e^{-x_i^2}$ for $i = 1, \ldots, 5$. Find the 4th-degree interpolating polynomial $P_4(x)$ of these points, and compute its anti-derivative. Find the polynomial $P_5(x) = \int_0^x P_4(t)dt$. Do you expect $P_5(x)$ to be a good approximation to $\mathrm{erf}(x)$?

(c) Consider the function

$$f(x) = 1 - \left(\frac{c_1}{1 + 0.47047x} + \frac{c_2}{(1 + 0.47047x)^2} + \frac{c_3}{(1 + 0.47047x)^3} \right) e^{-x^2}$$

which depends on 3 parameters c_1, c_2, c_3. Let now $x_1, \ldots, x_4$ be 4 ordered and equally spaced points on the interval $[0, 2]$, with $x_1 = 0$ and $x_4 = 2$ and let $y_i = \mathrm{erf}(x_i)$ for $i = 1, 2, 3, 4$. You can use the approximate numerical values

$$y_1 = 0.0, \quad y_2 = 0.65422141, \quad y_3 = 0.94065356, \quad y_4 = 0.99532227.$$

(These can be found by numerical integration, but we'll save you the time of doing it yourself. You will get to try numerical integration in (d).)

Explain that the conditions $y_1 = f(x_1), \ldots, y_4 = f(x_4)$ can be interpreted as a linear system of equations on the variables c_1, c_2, c_3. Is this system consistent (does it have a solution)? Find the least squares solution of the system and explain in which sense it determines the best approximation to $\mathrm{erf}(x)$.

Choose the values for c_1, c_2, c_3 found above and plot the graph of $f(x)$ in a coordinate system together with the graphs of $T_5(x)$ and $P_5(x)$.

See if you can find an approximation similar to your function $f(x)$ on the webpage in Footnote 1.

We are going to do a rough test of our 3 approximations $T_5(x)$, $P_5(x)$ and $f(x)$ of $\mathrm{erf}(x)$ that we found in (a)-(c). For this we need to know a sufficiently precise approximation of $\mathrm{erf}(x_0)$ for some $x_0 \in [0, 2]$. Take for example $x_0 = 2$.

The composite trapezoid rule says that the integral $\int_a^b e^{-t^2} dt$ can be approximated by considering an evenly spaced grid of points

$$t_0 = a < t_1 < \cdots < t_N = b$$

and computing

$$I_h = \frac{h}{2}\left(e^{-a^2} + e^{-b^2} + 2\sum_{i=1}^{N-1} e^{-t_i^2}\right)$$

where $h = x_i - x_{i-1}$. This is what you get by applying the trapezoid rule to each subinterval $[x_i, x_{i+1}]$ and adding all the results together.

(d) Split $[0, 2]$ into 2000 subintervals,

$$[0, 10^{-3}], \quad [10^{-3}, 2\cdot 10^{-3}], \quad [2\cdot 10^{-3}, 3\cdot 10^{-3}], \quad \dots, \quad [1999\cdot 10^{-3}, 2],$$

and find an approximation of $\operatorname{erf}(2)$ by applying the composite trapezoid rule for the corresponding grid of points. You are not allowed to do this by hand.

(e) Use a result from the textbook to explain that

$$I_h - \int_a^b e^{-t^2}\,dt = \frac{(b-a)h^2}{12}(4c^2 - 2)e^{-c^2}$$

for some c between a and b. Use this to show that the approximation of $\operatorname{erf}(2)$ that you found using the composite trapezoid rule is correct within at least 5 decimal places. This is a relatively coarse estimate of the error. The real error is somewhat smaller than this. (Hint: Remember that $e^{-C} \le 1$ for $C \ge 0$.)

(f) Assess the accuracy of each of your estimates $T_5(x), P_5(x), f(x)$ by evaluating these functions at $x = 2$ and comparing to your answer in (d). Which approximation looks like the best one?