Homework II

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Abstract

This is Daniel's homework of "Numerical Algorithms with Case Studies II".

1 Problems

Q1 First of all, we have to embed the four chemistry equations into mathematical equations, where $(x_1, x_2, x_3, x_4) = (ln([H^+]), ln([OH^-]), ln([HCO_3^-]), ln([CO_3^{2-}]))$,

$$\begin{cases} f_1(x) = x_1 + x_2 - lg(10^{-14}) = 0 \\ f_2(x) = x_1 + x_3 - lg(10^{-13.76}) = 0 \\ f_3(x) = x_1 - x_3 + x_4 \\ f_4(x) = lg(e^{x_1}) - lg(e^{x_2} + e^(x_3) + 2e^{x_4}) \end{cases} \tag{1}$$

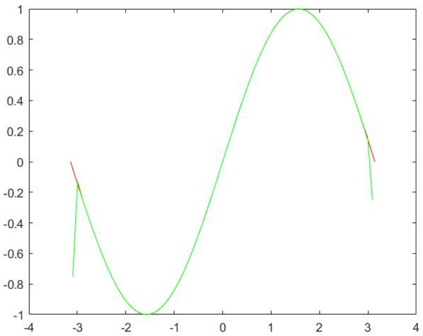
Then, in order to use Newton method $x_{k+1} = -J^{-1}f(x_k) + x_k$, we need to compute the Jacobian matrix.

$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} & \frac{\partial f_1}{\partial x_4} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} & \frac{\partial f_2}{\partial x_4} \\ \frac{\partial f_3}{\partial x_1} & \frac{\partial f_3}{\partial x_2} & \frac{\partial f_3}{\partial x_3} & \frac{\partial f_3}{\partial x_4} \\ \frac{\partial f_4}{\partial x_1} & \frac{\partial f_4}{\partial x_2} & \frac{\partial f_4}{\partial x_3} & \frac{\partial f_4}{\partial x_4} \end{pmatrix} \tag{2}$$

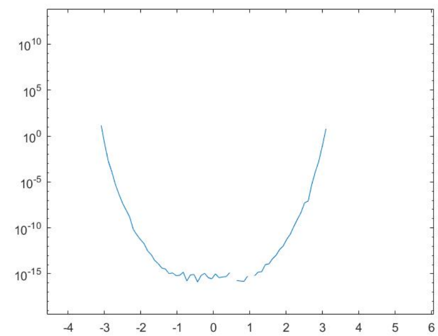
$$= \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & -1 & 1 \\ 1 & -\frac{e^{x_2}}{e^{x_2}+e^{x_3}+2e^{x_4}} & -\frac{e^{x_3}}{e^{x_2}+e^{x_3}+2e^{x_4}} & -\frac{2e^{x_4}}{e^{x_2}+e^{x_3}+2e^{x_4}} \end{pmatrix} \tag{3}$$

After several iteration, we finally find the pH of the rainwater, which is approximately 5.592643.

Q2 Sine function is perfectly interpolated with Lagrange method if x is not too faraway from our taken points of $sin(x)$.



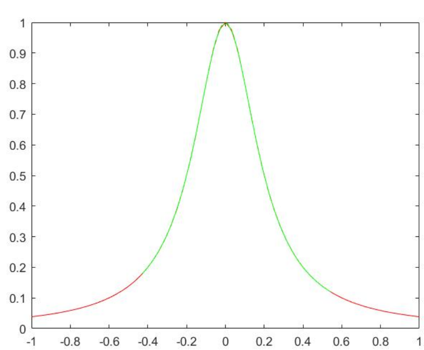
(a) interpolation of sin(x)



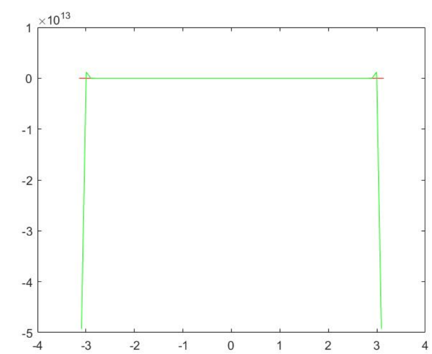
(b) relative error

As we can see, the marginal points seem fit poorly, but the rest of them fits in fairly well.

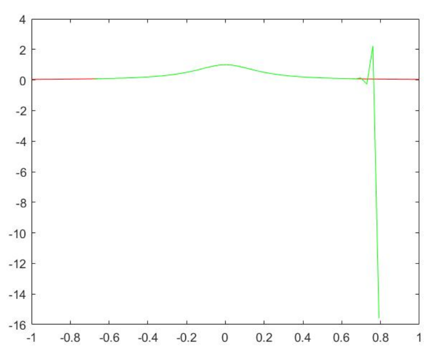
Secondly, we apply similar method to $f(x) = (1 + 25x^2)^{-1}$, the result remains good on limited range of points with the polynomial. While we start to estimate x on marginal points, the result is terribly disappointing.



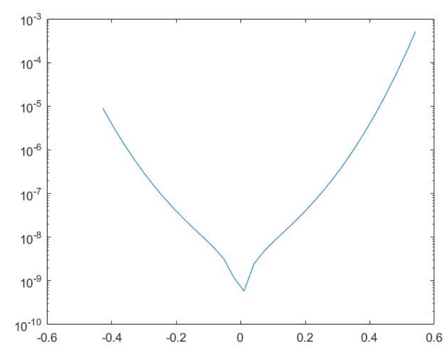
(c) interpolation of f(x)



(d) bad estimation



(e) bad estimation



(f) relative error

Q3 We can determine an n-degree polynomial with at least n+1 given points, and for n+1 consecutive integer points $(i, f(i)), (i+1, f(i+1)), \cdots, (i+n, f(i+n)) \in \mathbb{Z}$, we construct our lagrange polynomial as follows,

$$p(x) = f(i)\frac{\prod_{j\neq i}(x-x_j)}{\prod_{j\neq k}(x_j-x_k)} + \cdots + f(i+n)\frac{\prod_{j\neq i+n}(x-x_j)}{\prod_{j\neq k}(x_j-x_k)} \tag{4}$$

$$= \sum_{k=0}^{n}(f(n+k)\cdot\frac{\prod_{j=i}^{n}(x-x_j)}{x-x_k}\cdot\frac{(-1)^{n-k}}{k!(n-k)!}) \tag{5}$$

Put in $x = i+n+1$, we have,

$$p(i+n+1) = \sum_{k=0}^{n}(f(n+k)\cdot\frac{(n+1)!}{n-k+1}\cdot\frac{(-1)^{n-k}}{k!(n-k)!}) \tag{6}$$

$$= \sum_{k=0}^{n}((-1)^{n-k}f(n+k)\cdot\frac{(n+1)!}{k!(n-k+1)!}) \tag{7}$$

$$= \sum_{k=0}^{n}(-1)^{n-k}\binom{n+1}{k}f(n+k) \tag{8}$$

Since $\forall k$, $\binom{n+1}{k}\in\mathbb{Z}$ is a combinatorial number, we have the aggregate of integers,

$$p(i+n+1) = \sum_{k=0}^{n}(-1)^{n-k}\binom{n+1}{k}f(n+k)\in\mathbb{Z} \tag{9}$$

Similarly, we can prove that $p(i+n+2), p(i+n+3)\cdots\in\mathbb{Z}$ through mathematical induction (i.e. given that we have been convinced already $(j, f(j)), (j+1, f(j+1)), \cdots, (j+n, f(j+n))\in\mathbb{Z}$ for some $j>i$). And likewise, $\forall j<i$, we could still prove $p(j)\in\mathbb{Z}$ with the same method.