Mathematical Fundamentals for Electrochemical Energy Storage Systems

Exercise 1

Task 1: Least squares fitting

a. Write a program in python that plots the following functions. List some of the maxima, minima and saddle points (if they exist)
   i. $f(x,y) = \cos(x)\cos(y)\, e^{-x^2} e^{-y^2}$
   ii. $f(x,y) = (x^2 - y^2)$
   iii. $f(x) = \frac{\sin\left(10(x^2+y^2)\right)}{10}$

b. Write a program in python that utilizes iterative method to identify the minima of the functions given above using their gradients (Note: This is also called as gradient descent, which is a popular algorithm in machine learning)

c. (Bonus) As an engineer at Tesla, you decide to collect 10 cells from the production line and cycle (charge and discharge) these cells at high temperatures until they stop working. Finally, you collect the following information about the cells that you tested. You are confident that the initial internal resistance and coulombic efficiency of the cell immediately after manufacturing is directly correlated to the lifetime

Cell ID	Initial internal resistance ($m\Omega$)	Coulombic efficiency (CE)	Cycle life (Days)
A1	42.3	0.870	599
A2	43.1	0.823	520
A3	41.6	0.861	420
A4	53.2	0.880	380
A5	49.8	0.875	350
A6	46.3	0.862	420
A7	43.8	0.848	490
A8	46.1	0.861	390
A9	52.8	0.9	370
A10	44.2	0.871	510

i) Make the following plots using python

a. IR vs Cycle life (2D)

b. CE vs Cycle life (2D)

c. IR & CE vs cycle life (3D)

ii) Implement a least square regression fit in python and use it to identify a good model that can predict the cycle life from the initial characterization data.