Numerical Optimization
Week 1 Assignment

CHM564

Contents

1 Introduction

In this report, our first task is to find the optimum of function 4:

$$f_4(x) = \sum_{i=1}^{d} h(x_i) + 100 \cdot h(-x_i) \qquad h(x) = \frac{\log(1+\exp(q \cdot x))}{q}$$

However, the optimum of this function is roughly at 0 and if x-values is smaller than 0,it will incur a large penalty. So, How can we improve the function to reduce the influence of overflow by machine is our next task.

2 Find the optimum

2.1 Theory analysis

As we all know, if we want to have the optimum of f, we should make gradient equal to 0. So, firstly we will solve the gradient.

gradient matrix:

$$\bigtriangledown f(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \cdot \\ \cdot \\ \cdot \\ \frac{\partial f}{\partial x_d} \end{bmatrix} = 0$$

But, it's not a sufficient condition. It just tells us where the extreme points of the function may appear. Then we should calculate the Hessian which is a matrix of second partial derivatives of f.

$$\bigtriangledown^2 f(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_d} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_d} \\ \cdots & \cdots & & \cdots \\ \frac{\partial^2 f}{\partial x_d \partial x_1} & \frac{\partial^2 f}{\partial x_1 \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_d^2} \end{bmatrix}$$

If the Hessian is a positive definite matrix, there is a local minimum point.
If the Hessian is a negative definite matrix, there is a local maximum point.
If the Hessian is an indefinite matrix, it is not an extreme value at the point.

2.2 Implement the function

We calculate the first and second derivative of f:

$$\frac{\partial f}{\partial x_i} = \frac{\exp(qx_i)}{1+\exp(qx_i)} - 100 \cdot \frac{\exp(qx_i)}{1+\exp(qx_i)} \qquad i \leq d \tag{1}$$

$$\frac{\partial^2 f}{\partial x_i^2} = \frac{\exp(qx_i)\cdot q}{(1+\exp(qx_i))^2} + 100 \cdot \frac{\exp(qx_i)\cdot q}{(1+\exp(qx_i))^2} \qquad i \leq d \tag{2}$$

Then, we can easily get gradient and Hessian matrix. But we can simplify Hessian ,because when $f(x) = \sum_{i=1}^{N} g_i(x_i)$, Hessian is a diagonal matrix with $(Hf(x))_{ii} = g_i''(x_i)$.
Proof: if $i \neq j$

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 \sum_{i=1}^{N} g_i(x_i)}{\partial x_i \partial x_j} = \frac{\partial g_i'(x_i)}{\partial x_j} = 0$$

if $i = j$

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 \sum_{i=1}^{N} g_i(x_i)}{\partial^2 x_i} = g_i''(x_i)$$

Thus, we can find the gradient and Hessian matrix:

$$gradient: \bigtriangledown f_4(x) = \begin{bmatrix} \frac{\partial f_4}{\partial x_1} \\ \cdot \\ \cdot \\ \cdot \\ \frac{\partial f_4}{\partial x_d} \end{bmatrix} \qquad Hessian: \bigtriangledown^2 f_4(x) = \begin{bmatrix} \frac{\partial^2 f_4}{\partial x_1^2} & 0 & \cdots & 0 \\ 0 & \frac{\partial^2 f_4}{\partial x_2^2} & \cdots & 0 \\ \cdots & \cdots & & \cdots \\ 0 & 0 & \cdots & \frac{\partial^2 f_4}{\partial x_d^2} \end{bmatrix}$$

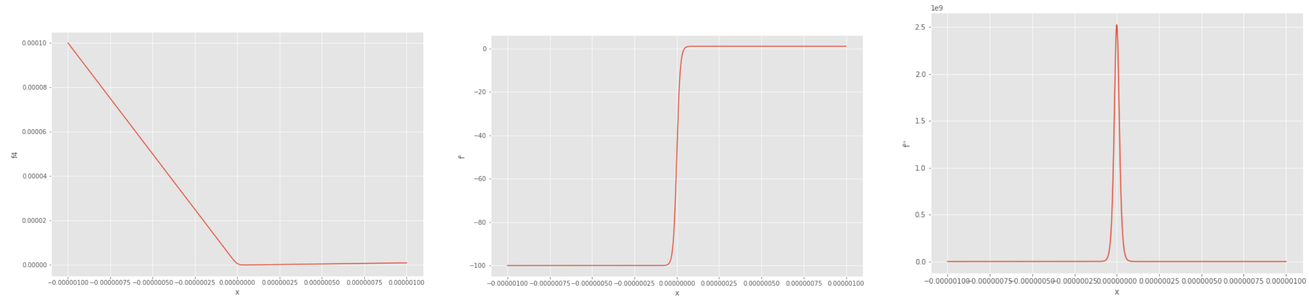
We can see that (2) is always positive, so Hessian always be positive definite. Function exists minimum value. We assume $d = 1, q = 10^8$,

$$f'(x) = 0 \Rightarrow \frac{e^{qx}}{1+e^{qx}} - 100 \cdot \frac{e^{-qx}}{1+e^{-qx}} = 0$$
$$\Rightarrow \frac{e^{qx}}{1+e^{qx}} \cdot \frac{1+e^{-qx}}{e^{-qx}} = 100$$
$$\Rightarrow e^{qx} = 100 \Rightarrow x \approx 4.605 \times 10^{-8}$$

Thus, when$x \approx 4.605 \times 10^{-8}$,$f_4$ has the minimum value.

2.3 Test implementation

We want to test our results, so we plot the functions. Figure (c) shows the second derivative

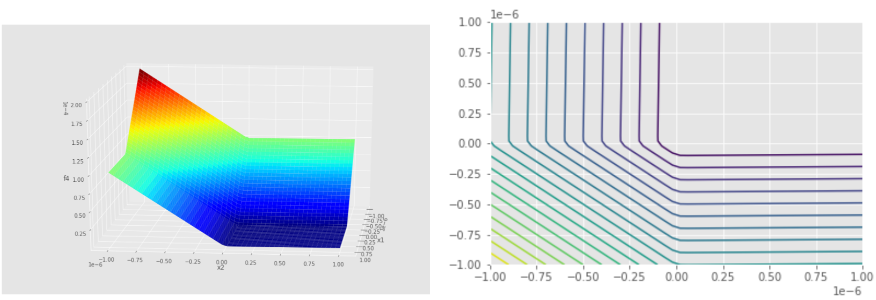


(a) Function4 with d=1 (b) Function of the first derivative (c) Function of the second derivative

Figure 1: Figures with d=1

always positive and the slope of the function of the first derivative will stabilize, then rise rapidly and tabilize again. Figure (b) confirms fig.(c). Also fig.(b) shows the slope of fig.(a). From Figure(a), we can see that the x-value of the minimum f_4 is very close to 0. If x is smaller than 0, it will incur a large penalty.

For further verification, we drew 3d images:



(a) Function4 with d=2 (b) Contour Map

Figure 2: Figures with d=2

From (a), we can intuitively see that x-values are roughly at 0. From (b), gradient drops to 0.

3 Improve the function

From above, x-value is really small. Function and x-values are easily overflow because of exponential function. So, can we improve the formula to reduce the penalty? (In the following discussion, we default d = 1)

3.1 Theory analysis

We use the equation:

$$\log\left(1+\exp\left(x\right)\right) = \log(1+\exp(-|x|)) + \max(x,0)$$

Proof:if $x \geq 0$

$$\begin{aligned}
\log\left(1+\exp\left(x\right)\right) &= \log\left(1+\exp\left(x\right)\right) - x + x \\
&= \log\left(1+\exp\left(x\right)\right) - \log(\exp(x)) + x \\
&= \log\left(\frac{1+\exp(x)}{\exp(x)}\right) + x \\
&= \log(1+\exp(-x)) + x \\
&= \log(1+\exp(-|x|)) + \max(x,0)
\end{aligned}$$

if $x < 0$

$$\begin{aligned}
\log\left(1+\exp\left(x\right)\right) &= \log(1+\exp(-|x|)) + 0 \\
&= \log(1+\exp(-|x|)) + \max(x,0)
\end{aligned}$$

Thus, we can have two forms of f_4:

$$\begin{aligned}
f_1 &= \frac{\log(\exp(qx)+1)}{q} + 100 \cdot \frac{\log(\exp(-qx)+1)}{q} \\
f_2 &= \frac{\log(\exp(-|qx|)+1) + \max(|qx|,0)}{q} + 100 \cdot \frac{\log(\exp(-|-qx|)+1) + \max(|-qx|,0)}{q} \\
&= 101 \cdot \frac{\log(\exp(-|qx|)+1)}{q} + \max(|x|,0)
\end{aligned}$$

3.2 Test by error bound

As we all know, the machine truncation error can be written as $x' = x(1+\epsilon)$, we can calculate residual $r = f(x')(1+\epsilon)$.

Next, we will calculate the residuals r_1, r_2 of f_1', f_2' respectively, and then analyze their error bound.(assume $a = qx(1+\epsilon)$)

$$\begin{aligned}
f_1' &= \frac{\exp(qx)}{1+\exp(qx)} - 100\frac{\exp(-qx)}{1+\exp(-qx)} \\
f_2' &= -101 \cdot \frac{\exp(-|qx|)}{1+\exp(-|qx|)} + 1
\end{aligned}$$

if $x \geq 0 : r_1 = r_2$

$$\begin{aligned} r_1 &= (\frac{\exp(a)}{1+\exp(a)} - 100\frac{\exp(-a)}{1+\exp(-a)})(1+\epsilon) \\ &= \frac{\exp(a)-100}{1+\exp(a)}(1+\epsilon) \end{aligned}$$

$$\begin{aligned} r_2 &= (-101 \cdot \frac{\exp(-a)}{1+\exp(-a)} + 1)(1+\epsilon) \\ &= \frac{\exp(a)-100}{1+\exp(a)}(1+\epsilon) \end{aligned}$$

if $x < 0 : r_1 > r_2$

$$\begin{aligned} r_1 &= (\frac{\exp(-|a|)}{1+\exp(-|a|)} - 100\frac{\exp(|a|)}{1+\exp(|a|)})(1+\epsilon) \\ &= \frac{1-100\exp(|a|)}{1+\exp(|a|}(1+\epsilon) \end{aligned}$$

$$\begin{aligned} r_2 &= (-101 \cdot \frac{\exp(-|a|)}{1+\exp(-|a|)} + 1)(1+\epsilon) \\ &= \frac{\exp(|a|)-100}{1+\exp(|a|)}(1+\epsilon) \end{aligned}$$

from above, we know that $\exp(qx) = 100$, then $\exp(qx(1+\epsilon)) \approx 100$. r_1 is much bigger than r_2. Thus, the f_2 error bound is tighter than f_1's. Also, we can find that, for f_2, residual always same. But for f_1, residual of $x < 0$ is much bigger than $x \geq 0$. For this function, when $x < 0$ always incur a large penalty. So,f_2 is better.

4 Summary

This report disscussed the extreme value of Function4 and tested it with different plots. We get optimal x-value is roughly at 0. And the gradient'absolute value of $x < 0$ is so big that means its easily incur a large influnce.
So, the next step, we pay attention to improve the results. We change initial function to another form, and test these error bound to make sure the other is better.