Numerical Optimization Re-exam Handin 1

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1 Introduction

This submission based on the group handin by myself, Michael Emil Rosenstrøm (kfg364), Magnus Fellenius-Blædel (gwm418), and Xuening He (pcr980). In this assignment we will implement five case functions including their gradients and hessians. The case functions are used to test optimisation algorithms. We discuss how to test the case functions and show results needed to perform an implementation of the functions.

2 Analysis

2.1 Testing of the case functions

We can never test too much, so we we need to prioritize what to test. Finding the local minima of a function is essential in minimisation problems. The five case functions presented in this assignment are created to test optimization algorithms. Therefore it is essential that implementations of the case function are implemented correctly and especially that they have correct local minimum.

2.2 Proof for the Diagonal Hessian Matrix

For functions on the form $f(x) = \sum_{i=1}^{N} g_i(x_i), x \in \mathbb{R}^N$ we have $(Hf(x))_{ii} = g_i''(x_i)$ we can spare some time later in computing the Hessian of functions like the ellipsoid function and the attractive sector functions.

 $\frac{\partial f(x)}{\partial x_i}=g_i'(x_i)$ because all $\frac{\partial g_j(x_j)}{\partial x_i}=0, j\neq i$ as they do not depend on x_i and

$$\frac{\partial f(x)}{\partial x_i \partial x_j} = \begin{cases} g_i''(x_i) & i = j \\ 0 & i \neq j \end{cases}$$

as all $\frac{\partial g_i(x_i)}{\partial x_i \partial x_j} = 0, j \neq i$ as they do not depend on x_j .

3 The Ellipsoid function

The Ellipsoid function is defined as

$$f_1(x) = \sum_{i=1}^d \alpha^{\frac{i-1}{d-1}} x_i^2$$

and has gradient

$$(\nabla f_1(x))_i = 2\alpha^{\frac{i-1}{d-1}} x_i$$

and Hessian

$$(Hf_1(x))_{ij} = \begin{cases} 2\alpha^{\frac{i-1}{d-1}} & i = j\\ 0 & i \neq j \end{cases}$$

The following 3d plot and contour plot gives an idea of the shape of the Ellipsoid funtion. The gradient at (0,0) is given by

$$(\nabla f_1(0,0))_i = 2\alpha^{\frac{i-1}{d-1}}0 = 0$$

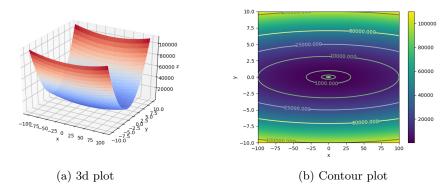


Figure 1: These two figures of the ellipsoid function demonstrates the local minimum of the function

as f_1 is continuously differentiable in a neighborhood of (0,0) and $(\nabla f_1(0,0))_i = \mathbf{0}$, (0,0) is a local minimizer according to theorem 2.2. The Hessian in (0,0) is given by

$$(Hf_1(0,0))_{ij} = \begin{cases} 2\alpha^{\frac{i-1}{d-1}} & i=j\\ 0 & i\neq j \end{cases}$$

and we can clearly see without computation that both $\det(Hf_1(0,0)) > 0$ and $\operatorname{trace}(Hf_1(0,0)) > 0$ and thus $Hf_1(0,0)$ is positive definite. Since $(\nabla^2 f_2(x))_i$ is continous and we just found that $(\nabla f_1((0,0)))_i = \mathbf{0}$ we have according to 2.4 that (0,0) is a strict local minimizer, which is in good accordance with the ellipsoid plot.

4 The Rosenbrock Banana Function

The Rosenbrock banana function is defined as

$$f_2(x) = (1 - x_1)^2 + 100(x_2 - x_1^2)^2$$

and has gradient

$$(\nabla f_2(x))_i = \begin{pmatrix} -2(1-x_1) - 400x_1(x_2 - x_1^2) \\ 200(x_2 - x_1^2) \end{pmatrix}$$

and Hessian

$$(Hf_2(x)) = \begin{pmatrix} 2 - 400x_2 + 1200x_1^2 & -400x_1 \\ -400x_1 & 200 \end{pmatrix}$$

The following 3d plot and contour plot gives an idea of the shape of the Rosenbrock banana funtion

The gradient in (1,1) is given by

$$(\nabla f_2((1,1)))_i = \begin{pmatrix} -2(1-1) - 400(1-1^2) \\ 200(1-1^2) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

as f_2 is continuously differentiable in a neighborhood of (1,1) and $(\nabla f_2((1,1)))_i = \mathbf{0}$, (1,1) is a local minimizer according to theorem 2.2. The Hessian in (1,1) is given by

$$(Hf_2(1,1)) = \begin{pmatrix} 2 - 400 + 1200 & -400 \\ -400 & 200 \end{pmatrix} = \begin{pmatrix} 802 & -400 \\ -400 & 200 \end{pmatrix}$$

with $\det((Hf_2(1,1))) = 400$ and $\operatorname{trace}((Hf_2(1,1))) = 1002$. Since $\det((Hf_2(1,1))) > 0$ and $\operatorname{trace}((Hf_2(1,1))) > 0$ we know that $(Hf_2(1,1))$ is positive definite and as $(\nabla^2 f_2(x))_i$ is clearly continuous in an open interval of (1,1) and we found before that $(\nabla f_2((1,1)))_i = \mathbf{0}$, (1,1) is a strict local minimizer according to theorem 2.4.

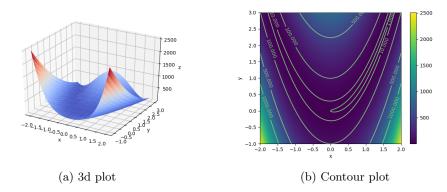


Figure 2: The plots show the Rosenbrock banana function. The point (1,1) is a strict local minimizer of the function. On plot b the point (1,1) can be seen in the lowest level.

5 The Log-Ellipsoid function

The log-Ellipsoid function is defined as

$$f_3(x) = \log(\epsilon - f_1(x)), \qquad \epsilon = 10^{-16}$$

and has gradient

$$(\nabla f_3(x))_i = \frac{2\alpha^{\frac{i-1}{d-1}} x_i}{\epsilon + \sum_{i=1}^d \alpha^{\frac{i-1}{d-1}} x_i^2}$$

and Hessian

$$(Hf_3(x))_{ij} = -\frac{4\alpha^{\frac{i-1}{d-1}}\alpha^{\frac{j-1}{d-1}}x_ix_j}{(\epsilon + \sum_{i=1}^d \alpha^{\frac{i-1}{d-1}}x_i^2)^2}$$

The following plot gives in idea of the shape of the Log-ellipsoid function

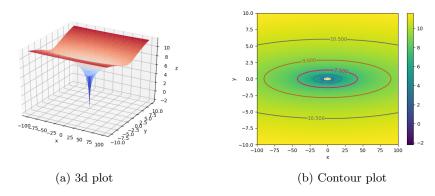


Figure 3: The plots show that the point (0,0) is a strict local minimizer for the log-Ellipsoid function

6 The Attractive-Sector Functions

The Attractive-Sector planar function is defined as

$$f_4(x) = \sum_{i=1}^{d} h(x_i) + 100h(-x_i), \qquad h(x) = \frac{\log(1 + \exp(qx))}{q}, \ q = 10^8$$

and it has gradient

$$(\nabla f_4(x))_i = \frac{\exp(qx_i)}{1 + \exp(qx_i)} - 100 \frac{\exp(-qx_i)}{1 + \exp(-qx_i)}$$

and Hessian

$$(Hf_4(x))_{ij} = \begin{cases} \frac{\exp(qx_i)}{(1+\exp(qx_i))^2} + 100 \frac{\exp(-qx_i)}{(1+\exp(-qx_i))^2} & i=j\\ 0 & i\neq j \end{cases}$$

Before we start programming and ploting it is worth noting that

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

since:

$$\begin{array}{lll} & \text{for } x < 0: \\ & \log(1 + \exp(-x)) & = & \log(1 + \exp(-|-x|)) + \max(-x, 0) \\ & = & \log(1 + \exp(-x)) + 0 \\ & = & \log(1 + \exp(-x)) \\ & \text{for } x \geq 0: \\ & \log(1 + \exp(x)) & = & \log(1 + \exp(-x)) + \max(x, 0) \\ & = & \log(1 + \exp(-x)) + x \\ & = & \log(1 + \exp(-x)) + \log(\exp(x)) \\ & = & \log((1 + \exp(-x)) \exp(x)) \\ \end{array}$$

This formulation is beneficial in a context of a computer implementation, since when x is a large number, such as 10^8 in the Attractive-Sector function. The value of e x would be a huge number that is much larger than 10^{32} or even 10^{64} . Therefore, it can not fit in any type of CPU registers and would result in a overflow. |x| > 0 for all real values of x, hence $e^{-|x|}$ would become a very small number for high values of x and would be rounded to zero, which would eliminate the overflow problem.

The Attractive-Sector quadratic function is defined as

$$f_5(x) = \sum_{i=1}^d h(x_i)^2 + 100h(-x_i)^2, \qquad h(x) = \frac{\log(1 + \exp(qx))}{q}, \ q = 10^8$$

and it has gradient

$$(\nabla f_5(x))_i = \frac{2\log(1 + \exp(qx_i))\exp(qx_i)}{q(1 + \exp(qx_i))} - \frac{2\log(1 + \exp(-qx_i))\exp(-qx_i)}{q(1 + \exp(-qx_i))}$$

and Hessian

$$(Hf_5(x))_{ij} = \begin{cases} \frac{2\exp(qx_i)(\log(1+\exp(qx_i))+\exp(qx_i))}{(1+\exp(qx_i))^2} + \frac{2\exp(-qx_i)(\log(1+\exp(-qx_i))+\exp(-qx_i))}{(1+\exp(-qx_i)^2)} & i = 3i \\ 0 & i \neq 3i \end{cases}$$

The following 3d and contour plot gives an idea of the shape of the attractive sector quadratic function, which looks a lot like f_4 but but is curved where f_4 seems to have sharp edges.

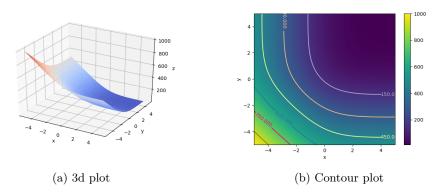


Figure 4: The plots show the surface of the Attractive Sector planar function

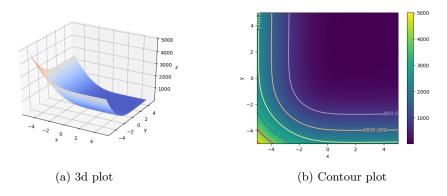


Figure 5: The plots show the surface of the Attractive-Sector quadratic function

7 Testing Protocol

In order to test if our calculation of gradient is correct, we can test if it equals 0 at the optima of the functions, which is (1,1) for the Rosenbrock function and (0,0) for the others.

8 Conclusion

In this assignment we have implemented the five case functions and their gradient and hessian. We have tested that our implementations performs correct in local minimas of the functions. Our tests show that the five case functions are implemented correctly.