Caleb Logemann MATH 565 Continuous Optimization Homework 1

1. Problem 1

Compute the gradient $\nabla f(x)$ and Hessian $\nabla^2 f(x)$ of the Rosenbrock function

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

The gradient of f is defined as $\left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}\right)^T$. The first derivatives of f are stated below.

$$\frac{\partial f}{\partial x_1} = -400x_1 \left(x_2 - x_1^2 \right) - 2(1 - x_1)$$
$$\frac{\partial f}{\partial x_2} = 200 \left(x_2 - x_1^2 \right)$$

So the gradient of f is

$$\nabla f(x) = \begin{bmatrix} -400x_1(x_2 - x_1^2) - 2(1 - x_1) \\ 200(x_2 - x_1^2) \end{bmatrix}$$

The Hessian of f is the matrix

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

The second derivatives are shown below.

$$\frac{\partial^2 f}{\partial x_1^2} = \frac{\partial}{\partial x_1} \left(\frac{\partial f}{\partial x_1} \right)$$

$$= -400 \left(x_2 - x_1^2 \right) + 800 x_1^2 + 2$$

$$= -400 \left(x_2 - 3x_1^2 \right) + 2$$

$$\frac{\partial^2 f}{\partial x_1 \partial x_2} = \frac{\partial}{\partial x_1} \left(\frac{\partial f}{\partial x_2} \right)$$

$$= -400 x_1$$

$$\frac{\partial^2 f}{\partial x_2^2} = \frac{\partial}{\partial x_2} \left(\frac{\partial f}{\partial x_2} \right)$$

$$= -200$$

Note that $\frac{\partial^2 f}{\partial x_2 \partial x_1} = \frac{\partial^2 f}{\partial x_1 \partial x_2}$ as f has continuous second derivatives. Thus the Hessian of f is

$$\nabla^2 f(x) = \begin{bmatrix} -400(x_2 - 3x_1^2) + 2 & -400x_1 \\ -400x_1 & 200 \end{bmatrix}$$

2. Problem 8

Suppose that f is a convex function. Show that the set of global minimizers of f is a convex set.

Proof. Let f be a convex function. This implies that

3. Problem 9

Consider the function $f(x_1, x_2) = (x_1 + x_2^2)^2$. At the point $x^T = (1, 0)$ we consider the search direction $p^T = (-1, 1)$. Show that p is a descent direction and find all minimizers of the problem (2.10).

4. Problem 13

Show that the sequence $x_k = 1/k$ is not Q-linearly convergent, though it does converge to zero.

5. Problem 14

Show that the sequence $x_k = 1 + (0.5)^{2^k}$ is Q-quadractically convergent to 1.

6. Consider the following fixed point iteration scheme:

$$x_{k+1} = x_k - \frac{[g(x_k)]^2}{g(x_k + g(x_k)) - g(x_k)}$$

Prove that if this method is converges to a root x^* of g(x) such that $g'(x^*) \neq 0$ and $g''(x^*) \neq 0$, then the rate of convergence is quadractic: p = 2.

Proof.

7. Implement the method from problem 6 in MATLAB (or PYTHON if you prefer). Use it to solve problems 8 and 9.

The following function implements the method from problem 6.

```
import numpy as np
def problem7(g, x0, TOL, MaxIter):
    x = np.zeros(MaxIter+2)
    x[0] = x0
    nIter = 0
    mstop = 1
    gx = g(x[nIter])
    delta = -np.square(gx)/(g(x[nIter] + gx) + gx)
    while nIter <= MaxIter and mstop:
        nIter +=1
        x[nIter] = x[nIter - 1] + delta
        gx = g(x[nIter])
        if abs(gx) < TOL and abs(delta) < TOL:
            mstop = 0
        else:
            delta = -np.square(gx)/(g(x[nIter] + gx) + gx)
    x = x [: nIter + 1]
    return x
```

8. The van der Waal equation

$$\left(P + \frac{a}{V^2}\right)(V - b) = nRT$$

generalizes the ideal gas law PV = nRT. In each equation, P represents the pressure (atm), V represents the volume (liters), n is the number of moles of gas, and T represents the temperature (K). R is the universal gas constant and has the value

$$R = 0.08205 \frac{\text{liters} \cdot \text{atm}}{\text{mole} \cdot \text{K}}$$

Determine the volume of 1 mole of isobutane at a temperature of T = 313K and a pressure of P = 2 atm, given that, for isobutane, a = 12.87atm · liters² and b = 0.1142 liters. Compare this to the value predicted from the ideal gas law. You may use any one of your methods (make clear in your writeup which one you are using, what initial guesses or intervals you are using, etc...).

The following script uses the method implemented in problem 7 to find the volume that satisfies the van der Waal equation.

```
import numpy as np
import matplotlib.pyplot as plt
execfile ('01 7.pv')
P = 2
a = 12.87
b = 0.1142
n = 1
R = 0.08205
T = 313
g = lambda V: (P + a/np.square(V))*(V - b) - n*R*T
V0 = 12
TOL = 1e-10
MaxIter = 1000
sol = problem7(g, V0, TOL, MaxIter)
print 'The volume of the isobutane is \{0:.10 \text{ f}\}'. format (sol [-1])
x = np. linspace (1, 20, 10000)
plt.plot(x, g(x), '-', sol[-1], g(sol[-1]), 'o')
```

9. According to ArchimedesâĂŹ law, when a solid of density IČ is placed in a liquid of density ρ , it will sink to a depth h that displaces an amount of liquid whose weight equals the weight of the solid. For a sphere of radius r, Archimedes law is

$$\frac{1}{3}\pi \left(3rh^2 - h^3\right)\rho = \frac{4}{3}\pi r^3\sigma$$

Given r = 5, $\rho = 1$, and $\sigma = 0.6$, determine h. You may use any one of your methods (make clear in your writeup which one you are using, what initial guesses or intervals you are using, etc...).

```
sol = problem7(g, h0, TOL, MaxIter)
print 'The_depth_of_the_sphere_is_{{}}{0:.10 f}'.format(sol[-1])

x = np.linspace(1,10,10000)
plt.plot(x, g(x), '-', sol[-1], g(sol[-1]), 'o')
```