

# Nonlinear Optimization - Assignment 1

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## 1 Characterization of Functions

a)  $f(\mathbf{x}) = (\mathbf{a}^T \mathbf{x} - d)^2$  where  $\mathbf{a} = (-1, 3)^T$ ,  $d = 2.5$

Because  $\mathbf{a}$  and  $d$  are constant, we can rewrite  $f$  as  $f(\mathbf{x}) = (-x_1 + 3x_2 - 2.5)^2$ , for which we then compute partial derivatives with respect to  $x_1$  and  $x_2$ :

$$\frac{\partial f(\mathbf{x})}{\partial x_1} = -2(-x_1 + 3x_2 - 2.5)$$

$$\frac{\partial f(\mathbf{x})}{\partial x_2} = 6(-x_1 + 3x_2 - 2.5)$$

Simplifying the brackets, we get the gradient:

$$\nabla f(\mathbf{x}) = \begin{bmatrix} 2x_1 - 6x_2 + 5 \\ -6x_1 + 18x_2 - 15 \end{bmatrix}$$

Next we compute partial derivatives of the gradient with respect to  $x_1$  and  $x_2$ :

$$\frac{\partial \nabla f(\mathbf{x})}{\partial x_1} = \begin{bmatrix} 2 \\ -6 \end{bmatrix}$$

$$\frac{\partial \nabla f(\mathbf{x})}{\partial x_2} = \begin{bmatrix} -6 \\ 18 \end{bmatrix}$$

which gives us the Hessian matrix:

$$\nabla^2 f(\mathbf{x}) = \begin{bmatrix} 2 & -6 \\ -6 & 18 \end{bmatrix}$$

To find the eigenvalues of the Hessian matrix, we need to solve  $\det(\nabla^2 f(\mathbf{x}) - \lambda I_2) = 0$ :

$$\begin{aligned} \det(\nabla^2 f(\mathbf{x}) - \lambda I_2) &= \det\left(\begin{bmatrix} 2 - \lambda & -6 \\ -6 & 18 - \lambda \end{bmatrix}\right) = (2 - \lambda)(18 - \lambda) - ((-6) * (-6)) = \\ &= 36 - 20\lambda + \lambda^2 - 36 = \lambda^2 - 20\lambda = \lambda(\lambda - 20) \end{aligned}$$

Setting  $\lambda(\lambda - 20)$  to 0, we get  $\lambda_1 = 20$  and  $\lambda_2 = 0$ , which implies that the Hessian matrix is positive semi-definite, because  $\lambda_i \geq 0 \quad \forall i \in 1, \dots, n$ , where  $n$  is the dimension of the gradient.

To find the stationary points we have to equate the gradient with a zero vector, i.e.  $\nabla f(\mathbf{x}) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ , which gives us the following system of equations:

$$2x_1 - 6x_2 + 5 = 0$$

$$-6x_1 + 18x_2 - 15 = 0$$

We immediately see that if we multiply the first equation with 3 and equate the two equations, we get  $6x_1 - 18x_2 + 15 = -6x_1 + 18x_2 - 15$ , where both  $x_1$  and  $x_2$  terms cancel out, which implies that the equality holds for any  $x_1, x_2 \in \mathbb{R}$ . In terms of optimization this means that the entire hyperplane defined by  $2x_1 - 6x_2 + 5 = 0$  is a valid solution. And due to the established positive-semidefiniteness of the Hessian matrix, the entire hyperplane is a strict local minimum.

**b)**  $f(\mathbf{x}) = (x_1 - 2)^2 + x_1 x_2^2 - 2$

Computing the partial derivatives of  $f$  with respect to  $x_1$  and  $x_2$  we get:

$$\frac{\partial f(\mathbf{x})}{\partial x_1} = 2(x_1 - 2) + x_2^2 = 2x_1 + x_2^2 - 4$$

$$\frac{\partial f(\mathbf{x})}{\partial x_2} = 2x_1 x_2$$

which gives us the gradient:

$$\nabla f(\mathbf{x}) = \begin{bmatrix} 2x_1 + x_2^2 - 4 \\ 2x_1 x_2 \end{bmatrix}$$

Next we compute the partial derivatives of the gradient with respect to  $x_1$  and  $x_2$ :

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

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

which gives us the Hessian matrix:

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

To find stationary points we have to equate the gradient with the zero vector, i.e.  $\nabla f(\mathbf{x}) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ , which gives us a system of equations:

$$2x_1 + x_2^2 - 4 = 0$$

$$2x_1 x_2 = 0$$

Rearranging the first equation we get  $x_2 = \sqrt{-2x_1 + 4}$ , which we plug into the second equation to get  $2x_1 \sqrt{-2x_1 + 4} = 0$ . Squaring both sides of the equations and then multiplying with  $-\frac{1}{8}$ , we get:

$$4x_1^2(-2x_1 + 4) = 0$$

$$-8x_1^3 + 16x_1^2 = 0$$

$$x_1^3 - 2x_1^2 = 0$$

$$x_1^2(x_1 - 2) = 0$$

from which we get three candidate x-values:  $x_{1,1} = x_{1,2} = 0$  and  $x_{1,3} = 2$ . Plugging these three values into the first equation we get:

$$2 \cdot 0 + x_2^2 - 4 = 0$$

$$x_2^2 = \sqrt{4}$$

which gives us  $x_{2,1} = 2$ ,  $x_{2,2} = -2$ . And

$$2 \cdot 2 + x_2^2 - 4 = 0$$

$$x_2^2 = 0$$

which gives us  $x_{2,3} = 0$ . Therefore we have obtained three candidate points for local extrema:  $\begin{bmatrix} 0 \\ 2 \end{bmatrix}$ ,  $\begin{bmatrix} 0 \\ -2 \end{bmatrix}$  and  $\begin{bmatrix} 2 \\ 0 \end{bmatrix}$ .

To check whether these points are minima, maxima or saddle points, we plug each of them into the Hessian matrix and determine the definiteness of the obtained matrix:

- $\mathbf{x} = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$ :

$$\nabla^2 f(\begin{bmatrix} 2 \\ 0 \end{bmatrix}) = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

The matrix is diagonal, so the eigenvalues are  $\lambda_1 = 2 > 0$  and  $\lambda_2 = 2 > 0$ , therefore the matrix is positive definite, and the point  $\begin{bmatrix} 2 \\ 0 \end{bmatrix}$  is a strict local minimum.

- $\mathbf{x} = \begin{bmatrix} 0 \\ 2 \end{bmatrix}$ :

$$\nabla^2 f(\begin{bmatrix} 0 \\ 2 \end{bmatrix}) = \begin{bmatrix} 2 & 4 \\ 4 & 0 \end{bmatrix}$$

TODO

- $\mathbf{x} = \begin{bmatrix} 0 \\ -2 \end{bmatrix}$ :

$$\nabla^2 f(\begin{bmatrix} 0 \\ -2 \end{bmatrix}) = \begin{bmatrix} 2 & -4 \\ -4 & 0 \end{bmatrix}$$

TODO

c)  $f(\mathbf{x}) = x_1^2 + x_1\|\mathbf{x}\|^2 + \|\mathbf{x}\|^2$

Using the property  $\|\mathbf{x}\|^2 = (\sqrt{x_1^2 + x_2^2})^2 = x_1^2 + x_2^2$ , we simplify the function  $f$  as follows:

$$f(\mathbf{x}) = x_1^2 + x_1(x_1^2 + x_2^2) + x_1^2 + x_2^2 = x_1^3 + 2x_1^2 + x_2^2 + x_1x_2^2$$

Next we compute the partial derivatives of  $f$  with respect to  $x_1$  and  $x_2$ :

$$\frac{\partial f(\mathbf{x})}{\partial x_1} = 3x_1^2 + 4x_1 + x_2^2$$

$$\frac{\partial f(\mathbf{x})}{\partial x_2} = 2x_2 + 2x_1x_2$$

which gives us the gradient:

$$\nabla f(\mathbf{x}) = \begin{bmatrix} 3x_1^2 + 4x_1 + x_2^2 \\ 2x_2 + 2x_1x_2 \end{bmatrix}$$

Computing the partial derivatives of the gradient with respect to  $x_1$  and  $x_2$  we get:

$$\frac{\partial \nabla f(\mathbf{x})}{\partial x_1} = \begin{bmatrix} 6x_1 + 4 \\ 2x_2 \end{bmatrix}$$

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

which gives us the Hessian matrix:

$$\nabla^2 f(x) = \begin{bmatrix} 6x_1 + 4 & 2x_2 \\ 2x_2 & 2x_1 + 2 \end{bmatrix}$$

To get the stationary points, we need  $\nabla f(\mathbf{x}) = \begin{bmatrix} 3x_1^2 + 4x_1 + x_2^2 \\ 2x_2 + 2x_1x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ , which gives us the following system of equations:

$$3x_1^2 + 4x_1 + x_2^2 = 0$$

$$2x_2 + 2x_1x_2 = 0$$

From the second equation we get:

$$x_2(2x_1 + 2) = 0$$

which gives us  $x_2 = 0$  and  $2x_1 + 2 = 0 \rightarrow x_1 = -1$ . Plugging these two values into the first equation we get:

$$3x_1^2 + 4x_1 + 0^2 = 0$$

$$x_1(3x_1 + 4) = 0$$

therefore  $x_{1,1} = 0$  and  $x_{1,2} = -\frac{4}{3}$ . And

$$3(-1)^2 + 4(-1) + x_2^2 = 0$$

$$x_2^2 = 1$$

therefore  $x_{2,1} = -1$  and  $x_{2,2} = 1$ . In total we have thus obtained four candidate points:  $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$ ,  $\begin{bmatrix} -\frac{4}{3} \\ 0 \end{bmatrix}$ ,  $\begin{bmatrix} -1 \\ -1 \end{bmatrix}$  and  $\begin{bmatrix} -1 \\ 1 \end{bmatrix}$ .

Next we need to determine the definiteness of the Hessian matrix in these points:

- $\mathbf{x} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ :

$$\nabla^2 f(\begin{bmatrix} 0 \\ 0 \end{bmatrix}) = \begin{bmatrix} 4 & 0 \\ 0 & 2 \end{bmatrix}$$

Because the matrix is diagonal, the eigenvalues are  $\lambda_1 = 4 > 0$  and  $\lambda_2 = 2 > 0$ , therefore the matrix is positive definite, and the point  $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$  is a strict local minimum.

- $\mathbf{x} = \begin{bmatrix} -\frac{4}{3} \\ 0 \end{bmatrix}$ :

$$\nabla^2 f(\begin{bmatrix} -\frac{4}{3} \\ 0 \end{bmatrix}) = \begin{bmatrix} -4 & 0 \\ 0 & -\frac{2}{3} \end{bmatrix}$$

Again we have a diagonal matrix, where the eigenvalues are  $\lambda_1 = -4 < 0$  and  $\lambda_2 = -\frac{2}{3} < 0$ , therefore the matrix is negative definite, and the point  $\begin{bmatrix} -\frac{4}{3} \\ 0 \end{bmatrix}$  is a strict local maximum.

- $\mathbf{x} = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$ :

$$\nabla^2 f(\begin{bmatrix} -1 \\ -1 \end{bmatrix}) = \begin{bmatrix} -2 & -2 \\ -2 & 0 \end{bmatrix}$$

TODO

- $\mathbf{x} = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$ :

$$\nabla^2 f(\begin{bmatrix} 0 \\ 0 \end{bmatrix}) = \begin{bmatrix} -2 & 2 \\ 2 & 0 \end{bmatrix}$$

TODO

d)  $f(\mathbf{x}) = \alpha x_1^2 - 2x_1 + \beta x_2^2$

Computing the partial derivatives of  $f$  with respect to  $x_1$  and  $x_2$  we get:

$$\frac{\partial f(\mathbf{x})}{\partial x_1} = 2\alpha x_1 - 2$$

$$\frac{\partial f(\mathbf{x})}{\partial x_2} = 2\beta x_2$$

which gives us the gradient:

$$\nabla f(\mathbf{x}) = \begin{bmatrix} 2\alpha x_1 - 2 \\ 2\beta x_2 \end{bmatrix}$$

Next we compute the partial derivatives of the gradient with respect to  $x_1$  and  $x_2$ :

$$\frac{\partial \nabla f(\mathbf{x})}{\partial x_1} = \begin{bmatrix} 2\alpha \\ 0 \end{bmatrix}$$

which gives us the Hessian matrix:

$$\nabla^2 f(\mathbf{x}) = \begin{bmatrix} 2\alpha & 0 \\ 0 & 2\beta \end{bmatrix}$$

To get the stationary points, we need  $\nabla f(\mathbf{x}) = \begin{bmatrix} 2\alpha x_1 - 2 \\ 2\beta x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ , which gives us the following system of equations:

$$2\alpha x_1 - 2 = 0$$

$$2\beta x_2 = 0$$

Rearranging the first equation, we get

$$\alpha x_1 = 1 \rightarrow x_1 = \frac{1}{\alpha}, \quad \alpha \neq 0$$

We clearly see that if  $\alpha = 0$  we have no stationary points because  $0x_1 = 1$  is not satisfied for any  $x_1 \in \mathbb{R}$ .

For the second equation we get:

$$x_2 = \begin{cases} c \in \mathbb{R}, & \text{if } \beta = 0 \\ 0, & \text{if } \beta \neq 0 \end{cases}$$

Because the Hessian matrix is diagonal, we know the eigenvalues are  $\lambda_1 = 2\alpha$  and  $\lambda_2 = 2\beta$ . Therefore  $\alpha$  and  $\beta$  are the only parameters that determine whether a candidate point is a minima, maxima or a saddle point. More specifically:

- minima: positive definiteness of the Hessian matrix is a sufficient condition, in other words all eigenvalues have to be strictly positive, so it is necessary that  $\alpha > 0$  and  $\beta > 0$ .
- maxima: negative definiteness of the Hessian matrix is a sufficient condition, in other words all eigenvalues have to be strictly negative, so it is necessary that  $\alpha < 0$  and  $\beta < 0$ .
- saddle point: indefiniteness of the Hessian matrix is a sufficient condition, in other words at least one eigenvalue has to be strictly positive and at least one eigenvalue has to be strictly negative, so either  $\alpha > 0$  and  $\beta < 0$ , or  $\alpha < 0$  and  $\beta > 0$ .

TODO what if beta is 0? I assume you can't do anything unless you know the specific point  $(x_1, x_2)$ .

- 2 Matrix Calculus**
- 3 Numerical Gradient Verification**
- 7 Computing Gradient using Automatic Differentiation**
- 8 Training the Neural Network**
- 9 Inference**