18s1: COMP9417 Machine Learning and Data Mining

Lectures: Linear Models for Regression
Topic: Questions from lecture topics
Version: review answers

Review

How to solve the partial derivatives with respect to one value?
when

$$f(x, y) = a_1x^2y^2 + a_4xy + a_5x + a_7$$

$$\frac{\partial f(x, y)}{\partial x} = 2x(a_1y^2) + a_4y + a_5$$

$$\frac{\partial f(x, y)}{\partial y} = 2y(a_1x^2) + a_4x$$

when

$$f(x, y) = a_1x^2y^2 + a_2x^2y + a_3xy^2 + a_4xy + a_5x + a_6y + a_7$$

what $\frac{\partial f(x,y)}{\partial x}$ will be?

$$\frac{\partial f(x, y)}{\partial x} = 2a_1xy^2 + 2a_2xy + a_3y^2 + a_4x + a_5$$

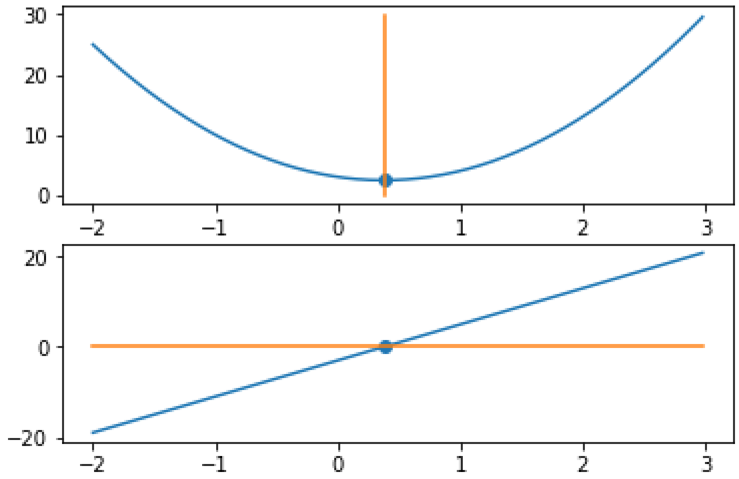
what $\frac{\partial f(x,y)}{\partial y}$ will be?

$$\frac{\partial f(x, y)}{\partial x} = 2a_1x^2y + a_2x^2 + 2a_3xy2 + a_4x + a_6$$

How to solve optimization problems for Quadratic function? For example, $y = -4x^2 + 3x + 3$. The solution is minimum or maximum?

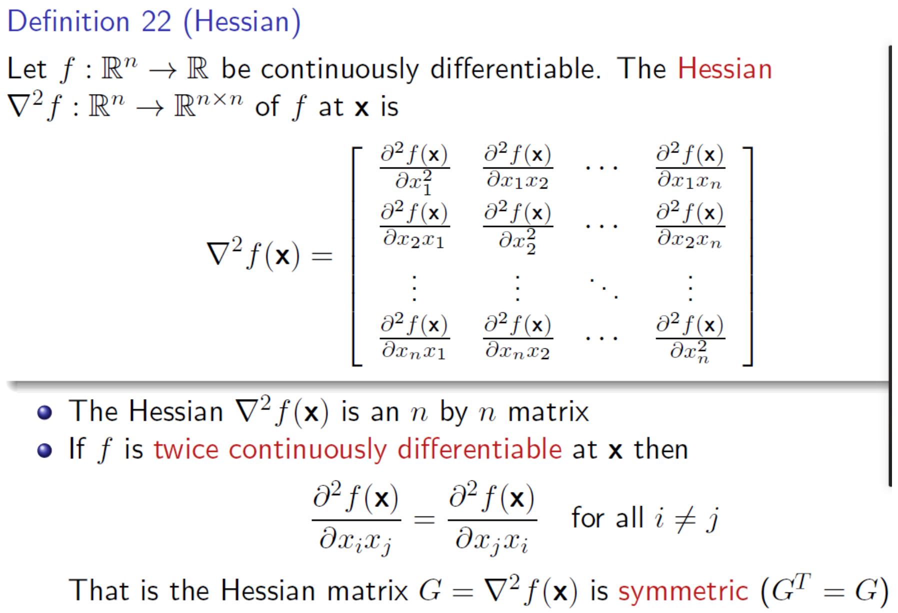
$$\frac{\partial y}{\partial x} = -8x + 3$$

when $x = \frac{8}{3}, \frac{\partial y}{\partial x} = 0$ and y is minimum.



When f(x,y) is Quadratic function, how to solve optimization problems?

Solving optimization problems is not easy. There are some cases without solution and some have many solution. But in our cases, it is easy as the derivatives of the loss function is linear.



Definition 22 (Hessian)

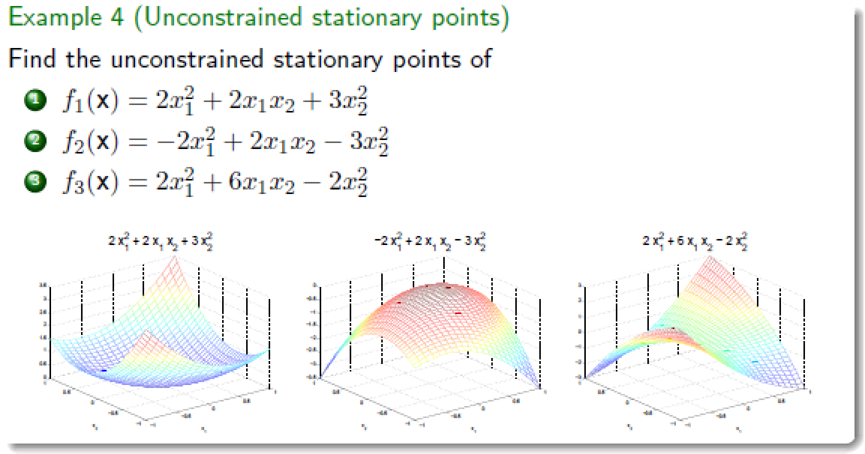
Let $f : \mathbb{R}^n \to \mathbb{R}$ be continuously differentiable. The Hessian $\nabla^2 f : \mathbb{R}^n \to \mathbb{R}^{n \times n}$ of f at $\mathbf{x}$ is

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

- The Hessian $\nabla^2 f(\mathbf{x})$ is an n by n matrix
- If f is twice continuously differentiable at $\mathbf{x}$ then

$$\frac{\partial^2 f(\mathbf{x})}{\partial x_i x_j} = \frac{\partial^2 f(\mathbf{x})}{\partial x_j x_i} \quad \text{for all } i \neq j$$

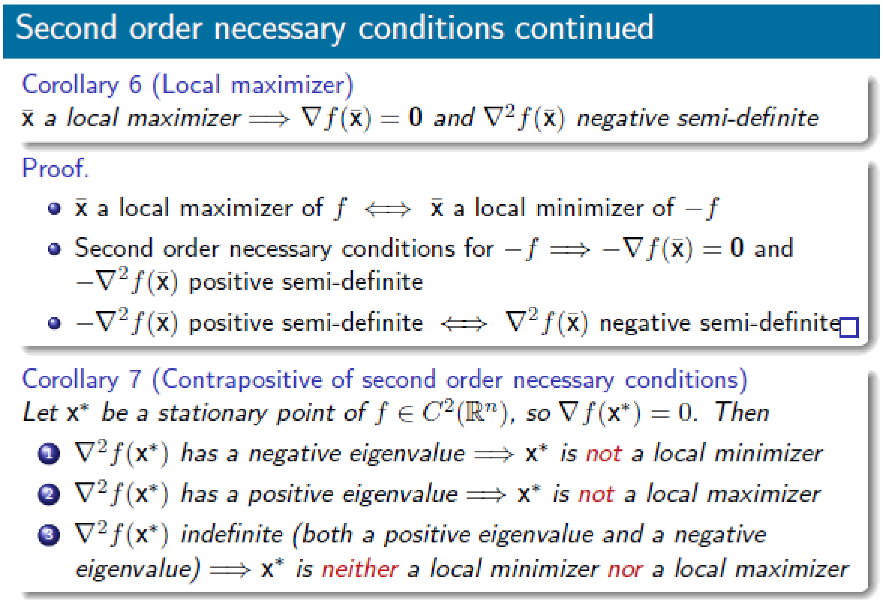
That is the Hessian matrix $G = \nabla^2 f(\mathbf{x})$ is symmetric $(G^T = G)$



Example 4 (Unconstrained stationary points)

Find the unconstrained stationary points of

1. $f_1(\mathbf{x}) = 2x_1^2 + 2x_1x_2 + 3x_2^2$
2. $f_2(\mathbf{x}) = -2x_1^2 + 2x_1x_2 - 3x_2^2$
3. $f_3(\mathbf{x}) = 2x_1^2 + 6x_1x_2 - 2x_2^2$



Second order necessary conditions continued

Corollary 6 (Local maximizer)

$\bar{\mathbf{x}}$ a local maximizer $\Longrightarrow \nabla f(\bar{\mathbf{x}}) = \mathbf{0}$ and $\nabla^2 f(\bar{\mathbf{x}})$ negative semi-definite

Proof.

- $\bar{\mathbf{x}}$ a local maximizer of $f \iff \bar{\mathbf{x}}$ a local minimizer of $-f$
- Second order necessary conditions for $-f \Longrightarrow -\nabla f(\bar{\mathbf{x}}) = \mathbf{0}$ and $-\nabla^2 f(\bar{\mathbf{x}})$ positive semi-definite
- $-\nabla^2 f(\bar{\mathbf{x}})$ positive semi-definite $\iff \nabla^2 f(\bar{\mathbf{x}})$ negative semi-definite □

Corollary 7 (Contrapositive of second order necessary conditions)

Let $\mathbf{x}^*$ be a stationary point of $f \in C^2(\mathbb{R}^n)$, so $\nabla f(\mathbf{x}^*) = 0$. Then

1. *$\nabla^2 f(\mathbf{x}^*)$ has a negative eigenvalue $\Longrightarrow \mathbf{x}^*$ is not a local minimizer*
2. *$\nabla^2 f(\mathbf{x}^*)$ has a positive eigenvalue $\Longrightarrow \mathbf{x}^*$ is not a local maximizer*
3. *$\nabla^2 f(\mathbf{x}^*)$ indefinite (both a positive eigenvalue and a negative eigenvalue) $\Longrightarrow \mathbf{x}^*$ is neither a local minimizer nor a local maximizer*

What is the loss function of linear regression?

$$\mathcal{L} = \frac{1}{N}\sum_{i=1}^{n}(y_i - (w_0 + w_1 x_i))^2$$

.

Q1

A *univariate linear regression model* is a linear equation $y = a + bx$. Learning such a model requires fitting it to a sample of training data so as to minimize the error function $\mathcal{L} = \sum_{i=1}^{n}(y_i - (w_0 + w_1 x_i))^2$. To find the best parameters a and b that minimize this error function we need to find the error *gradients* $\frac{\partial \mathcal{L}}{\partial w_0}$ and $\frac{\partial \mathcal{L}}{\partial w_1}$. So we need to derive these expressions by taking partial derivatives, set them to zero, and solve for w_0 and w_1.

First we write the loss function for the univariate linear regression $y = w_0 + w_1 x$ as

$$\begin{aligned}
\mathcal{L} &= \frac{1}{N}\sum_{n=1}^{N}(y_n - (w_0 + w_1 x_n))^2 \\
&= \frac{1}{N}\sum_{n=1}^{N}(y_n - (w_0 + w_1 x_n))(y_n - (w_0 + w_1 x_n)) \\
&= \dots \\
&= \frac{1}{N}\sum_{n=1}^{N}[w_1^2 x_n^2 + 2w_1 x_n(w_0 - y_n) + w_0^2 - 2w_0 y_n + y_n^2]
\end{aligned}$$

At a minimum of $\mathcal{L}$ the partial derivatives with respect to w_0, w_1 should be zero. We will start with w_0, so first we remove from the above expression all terms not including w_0.

$$\frac{1}{N}\sum_{n=1}^{N}[w_0^2 + 2w_1 x_n w_0 - 2w_0 y_n]$$

Rearrange, taking terms not indexed by n outside:

$$w_0^2 + 2w_0 w_1 \frac{1}{N}(\sum_{n=1}^{N} x_n) - 2w_0 \frac{1}{N}(\sum_{n=1}^{N} y_n)$$

Taking the partial derivative with respect to w_0 we get:

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial w_0} &= 2w_0 + 2w_1 \frac{1}{N}(\sum_{n=1}^{N} x_n) - \frac{2}{N}(\sum_{n=1}^{N} y_n) \\
E(y) &= \frac{\sum_{n=1}^{N} y_n}{N} \\
E(x) &= \frac{\sum_{n=1}^{N} x_n}{N} \\
\widehat{w_0} &= E(y) - w_1 E(x)
\end{aligned}$$

Now we do the same for w_1, first removing all terms not including w_1:

$$\frac{1}{N}\sum_{n=1}^{N}[w_1^2 x_n^2 + 2w_1 x_n w_0 - 2w_1 x_n y_n]$$

Rearrange, taking terms not indexed by n outside:

$$w_1^2\frac{1}{N}(\sum_{n=1}^{N}x_n^2) + 2w_1\frac{1}{N}(\sum_{n=1}^{N}x_n(w_0 - y_n))$$

Taking the partial derivative with respect to w_1 we get:

$$\begin{aligned}
\frac{\partial\mathcal{L}}{\partial w_1} &= 2w_1\frac{1}{N}(\sum_{n=1}^{N}x_n^2) + \frac{2}{N}(\sum_{n=1}^{N}x_n(w_0 - y_n)) \\
&= w_1\frac{2}{N}(\sum_{n=1}^{N}x_n^2) + \frac{2}{N}(\sum_{n=1}^{N}x_n(\widehat{w_0} - y_n)) \\
&= w_1\frac{2}{N}(\sum_{n=1}^{N}x_n^2) + \frac{2}{N}(\sum_{n=1}^{N}x_n(E(y) - w_1E(x) - y_n)) \\
&= \ldots \\
&= 2w_1[\frac{1}{N}(\sum_{n=1}^{N}x_n^2) - E(x)E(x)] + 2E(y)E(x) - 2\frac{1}{N}(\sum_{n=1}^{N}x_ny_n) \\
&= 2w_1E(x^2) - w_1(E(x))^2 + 2E(y)E(x) - 2E(xy)
\end{aligned}$$

$$\frac{\partial\mathcal{L}}{\partial w_1} = 0$$

$$w_1(E(x^2) - (E(x))^2) = E(xy) - E(y)E(x)$$

$$\begin{aligned}
\widehat{w_1} &= \frac{E(xy) - E(x)E(y)}{E(x^2) - (E(x))^2} \\
&= \frac{E(xy) - E(x)E(y)}{Var(x)} \\
&= \frac{COV(x,y)}{Var(x)} \\
\widehat{w_0} &= E(y) - w_1E(x)
\end{aligned}$$

To make sure you know the process, you could try to solve the following loss function for linear regression with L-2 normalization. The result is similar.

$$\begin{aligned}
\mathcal{L} &= \frac{1}{N}\sum_n (y_n - (w_0 + w_1 x_n))^2 + \frac{\lambda (w_1)^2}{2} \\
\widehat{w_0} &= E(y) - w_1 E(x) \\
\widehat{w_1} &= \frac{E(xy) - E(x)E(y)}{E(x^2) - (E(x))^2 + \lambda}
\end{aligned}$$