Gradients, Hessians, and Positive Definiteness

Local Minima and Local Maxima

We want to consider the local minima (or maxima) of a function $f(w_1, w_2) : \mathbb{R}^2 \to \mathbb{R}$. First do a power series expansion and just keep the first three terms to get

$$
\begin{aligned}
f(w_1, w_2) \quad &\approx \quad f(w_{01}, w_{02}) + \begin{bmatrix} \dfrac{\partial f}{\partial w_1} & \dfrac{\partial f}{\partial w_2} \end{bmatrix}_{|(w_{01}, w_{02})} \begin{bmatrix} w_1 - w_{01} \\ w_2 - w_{02} \end{bmatrix} + \\
&\frac{1}{2} \begin{bmatrix} w_1 - w_{01} & w_2 - w_{02} \end{bmatrix} \begin{bmatrix} \dfrac{\partial^2 f}{\partial^2 w_1} & \dfrac{\partial^2 f}{\partial w_1 \partial w_2} \\ \dfrac{\partial^2 f}{\partial w_2 \partial w_1} & \dfrac{\partial^2 f}{\partial^2 w_2} \end{bmatrix}_{|(w_{01}, w_{02})} \begin{bmatrix} w_1 - w_{01} \\ w_2 - w_{02} \end{bmatrix}.
\end{aligned}
$$

If (w_{01}, w_{02}) is a local mimimum or a local maximum then

$$
\begin{bmatrix} \dfrac{\partial f}{\partial w_1} \\ \dfrac{\partial f}{\partial w_2} \end{bmatrix}_{|(w_{01}, w_{02})} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}
$$

and

$$
f(w_1, w_2) \approx f(w_{01}, w_{02}) + \frac{1}{2} \begin{bmatrix} w_1 - w_{01} & w_2 - w_{02} \end{bmatrix} \begin{bmatrix} \dfrac{\partial^2 f}{\partial^2 w_1} & \dfrac{\partial^2 f}{\partial w_1 \partial w_2} \\ \dfrac{\partial^2 f}{\partial w_2 \partial w_1} & \dfrac{\partial^2 f}{\partial^2 w_2} \end{bmatrix}_{|(w_{01}, w_{02})} \begin{bmatrix} w_1 - w_{01} \\ w_2 - w_{02} \end{bmatrix}.
$$

If (w_{01}, w_{02}) is a local mimimum then the Hessian[1] given by

$$
\begin{bmatrix} \dfrac{\partial^2 f}{\partial^2 w_1} & \dfrac{\partial^2 f}{\partial w_1 \partial w_2} \\ \dfrac{\partial^2 f}{\partial w_2 \partial w_1} & \dfrac{\partial^2 f}{\partial^2 w_2} \end{bmatrix}_{|(w_{01}, w_{02})}
$$

is positive definite. Why? On the other hand, if (w_{01}, w_{02}) is a local maximum then the Hessian

$$
\begin{bmatrix} \dfrac{\partial^2 f}{\partial^2 w_1} & \dfrac{\partial^2 f}{\partial w_1 \partial w_2} \\ \dfrac{\partial^2 f}{\partial w_2 \partial w_1} & \dfrac{\partial^2 f}{\partial^2 w_2} \end{bmatrix}_{|(w_{01}, w_{02})}
$$

is negative definite. Why?

[1] Note that the Hessian is always symmetric.

Gradient Descent

For complicated functions such as neural networks, we cannot solve

$$\nabla f = \begin{bmatrix} \dfrac{\partial f}{\partial w_1} \\ \\ \dfrac{\partial f}{\partial w_2} \end{bmatrix}_{|(w_{01}, w_{02})} = \begin{bmatrix} 0 \\ \\ 0 \end{bmatrix}$$

for (w_{01}, w_{02}). Instead, we start at a random point $(w_1^{(1)}, w_2^{(1)})$ and search for where $\nabla f = 0$. To do this we use the approximation

$$f(w_1^{(n+1)}, w_2^{(n+1)}) \approx f(w_1^{(n)}, w_2^{(n)}) + \begin{bmatrix} \dfrac{\partial f}{\partial w_1} & \dfrac{\partial f}{\partial w_2} \end{bmatrix}_{|(w_1^{(n)}, w_2^{(n)})} \begin{bmatrix} w_1^{(n+1)} - w_1^{(n)} \\ w_2^{(n+1)} - w_2^{(n)} \end{bmatrix}.$$

Then set $(w_1^{(n+1)}, w_2^{(n+1)})$ according to $(\eta > 0)$

$$(w_1^{(n+1)}, w_2^{(n+1)}) \triangleq (w_1^{(n)}, w_2^{(n)}) - \eta \nabla f_{|(w_1^{(n)}, w_2^{(n)})} = (w_1^{(n)}, w_2^{(n)}) - \eta \begin{bmatrix} \dfrac{\partial f}{\partial w_1} & \dfrac{\partial f}{\partial w_2} \end{bmatrix}_{|(w_1^{(n)}, w_2^{(n)})}.$$

This forces f to decrease as

$$\begin{aligned} \Delta f = f(w_1^{(n+1)}, w_2^{(n+1)}) - f(w_1^{(n)}, w_2^{(n)}) &= \begin{bmatrix} \dfrac{\partial f}{\partial w_1} & \dfrac{\partial f}{\partial w_2} \end{bmatrix}_{|(w_1^{(n)}, w_2^{(n)})} \begin{bmatrix} w_1^{(n+1)} - w_1^{(n)} \\ w_2^{(n+1)} - w_2^{(n)} \end{bmatrix} \\ &= -\eta \begin{bmatrix} \dfrac{\partial f}{\partial w_1} & \dfrac{\partial f}{\partial w_2} \end{bmatrix}_{|(w_1^{(n)}, w_2^{(n)})} \begin{bmatrix} \dfrac{\partial f}{\partial w_1} \\ \\ \dfrac{\partial f}{\partial w_2} \end{bmatrix}_{|(w_1^{(n)}, w_2^{(n)})} \\ &= -\eta \left(\left(\dfrac{\partial f}{\partial w_1} \right)^2 + \left(\dfrac{\partial f}{\partial w_2} \right)^2 \right) < 0 \end{aligned}$$

showing that f is decreasing in value.

Symmetric and Positive Definite Matrices

Definition 1 *Symmetric Matrix*

A matrix Q is *symmetric* if

$$Q^T = Q.$$

Definition 2 *Positive Semidefinite Matrix*

A symmetric matrix $Q \in \mathbb{R}^{m \times m}$ is *positive semidefinite* if for all $x \in \mathbb{R}^m$,

$$x^T Q x \geq 0.$$

Definition 3 *Positive Definite Matrix*

A symmetric matrix $Q \in \mathbb{R}^{m \times m}$ is *positive definite* if for all $x \in \mathbb{R}^m$

$$x^T Q x \geq 0$$

and

$$x^T Q x = 0$$

if and only if x is the zero vector, i.e., $x = 0_{n \times 1}$.

Example 1 *Positive Definite Matrix*
Let

$$Q_1 = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$$

and note that $Q_1 = Q_1^T$. Then

$$x^T Q_1 x = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^T \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = x_1^2 + 2x_2^2 \geq 0 \text{ for all } x \in \mathbb{R}^2$$

and the only way it can equal zero is if $x_1 = 0$ and $x_2 = 0$. That is, Q_1 is positive definite.

Example 2 *Positive Semidefinite Matrix*
Let

$$Q_2 = \begin{bmatrix} 0 & 0 \\ 0 & 2 \end{bmatrix}$$

and note that $Q_2 = Q_2^T$. Then

$$x^T Q_2 x = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^T \begin{bmatrix} 0 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 2x_2^2 \geq 0 \text{ for all } x \in \mathbb{R}^2.$$

Thus Q_2 is positive semidefinite. However, in this example, $x = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ makes $x^T Q_2 x = 0$, that is, Q_2 is *not* positive definite.

Example 3 *Indefinite Matrix*
Let

$$Q_3 = \begin{bmatrix} -1 & 0 \\ 0 & 2 \end{bmatrix}$$

and note that $Q_3 = Q_3^T$. Then

$$x^T Q_3 x = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^T \begin{bmatrix} -1 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = -x_1^2 + 2x_2^2.$$

In this example, $x^T Q_3 x$ can be positive if $x = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, or negative if $x = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$. Consequently, it is an indefinite matrix.

Check for definiteness matrices

$$Q \triangleq \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{bmatrix} \quad \text{with} \quad Q^T = Q.$$

Q is *positive* definite if and only if

$$q_{11} > 0, \det \begin{bmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{bmatrix} > 0, \text{ and } \det Q > 0.$$

- Equivalently, Q is *positive* definite if and only if all of its eigenvalues are positive.
- Q is *negative* definite if and only $-Q$ is positive definite.