Discussion 4

1. Gradients and Hessians

The *gradient* of a scalar-valued function $g\colon \mathbb{R}^n \to \mathbb{R}$, is the column vector of length n, denoted as ∇g, containing the derivatives of components of g with respect to the variables:

$$(\nabla g(\vec{x}))_i = \frac{\partial g}{\partial x_i}(\vec{x}),\ i = 1, \ldots n. \tag{1}$$

The *Hessian* of a scalar-valued function $g\colon \mathbb{R}^n \to \mathbb{R}$, is the $n \times n$ matrix, denoted as $\nabla^2 g$, containing the second derivatives of components of g with respect to the variables:

$$(\nabla^2 g(\vec{x}))_{ij} = \frac{\partial^2 g}{\partial x_i\, \partial x_j}(\vec{x}),\quad i = 1, \ldots, n,\quad j = 1, \ldots, n. \tag{2}$$

For the remainder of the class, we will repeatedly have to take gradients and Hessians of functions we are trying to optimize. This exercise serves as a warm up for future problems. Compute the gradients and Hessians for the following functions:

(a) Compute the gradient and Hessian (with respect to $\vec{x}$) for $g(\vec{x}) = \vec{y}^\top A\vec{x}$.

Solution: Let $A = \begin{bmatrix}\vec{a}_1 & \vec{a}_2 & \ldots & \vec{a}_n\end{bmatrix}$ where a_i is the i-th column of A. then

$$\begin{aligned}
g(\vec{x}) &= \vec{y}^\top A\vec{x} && (3)\\
&= \vec{y}^\top \begin{bmatrix}\vec{a}_1 & \vec{a}_2 & \ldots & \vec{a}_n\end{bmatrix}\vec{x} && (4)\\
&= \vec{y}^\top(\vec{a}_1 x_1 + \vec{a}_2 x_2 + \ \ldots\ + \vec{a}_n x_n) && (5)\\
&= \sum_{i=1}^{n}(\vec{y}^\top \vec{a}_i)x_i. && (6)
\end{aligned}$$

Thus

$$\frac{\partial g}{\partial x_j}(\vec{x}) = \vec{y}^\top \vec{a}_j = \vec{a}_j^\top \vec{y}, \tag{7}$$

and the gradient $\nabla g(\vec{x}) = A^\top \vec{y}$. Since the gradient does not depend on $\vec{x}$, we then have the Hessian $\nabla^2 g(\vec{x}) = 0$.

(b) Compute the gradient and Hessian of $h(\vec{x}) = \sum_{i=1}^{n}(x_i \log(x_i) - x_i)$ for $\vec{x} \in \mathbb{R}^n_{++}$ and establish that the Hessian is positive semi-definite (as we will see soon in lecture, this establishes that h is a convex function). *NOTE*: In fact, the Hessian is positive definite.

Solution: We have

$$\begin{aligned}
\frac{\partial h(\vec{x})}{\partial x_i} &= \log(x_i)\\
\frac{\partial^2 h(\vec{x})}{\partial x_i^2} &= 1/x_i\\
\frac{\partial^2 h(\vec{x})}{\partial x_i \partial x_j} &= 0, \qquad \text{for } i \neq j.
\end{aligned}$$

Hence the i^{th} entry of $\nabla h(\vec{x})$ is $\log(x_i)$ and the Hessian $\nabla^2 h(\vec{x})$ is a diagonal matrix with the $(i,i)^{th}$ entry is $1/x_i$. As x_i are positive, so is $1/x_i$ and so the diagonal matrix has only positive entries, and hence has positive eigenvalues.

(c) Compute the gradient and Hessian of $g(\vec{x}) = e^{\vec{a}^\top \vec{x}+b}$ for $\vec{a}, \vec{x} \in \mathbb{R}^n, b \in \mathbb{R}$ and establish that the Hessian is positive semi-definite.

Solution: We can either compute the gradient and Hessian directly or we can use the properties of gradient and Hessians under composition with linear functions.

We will first see the former.

$$\frac{\partial g(\vec{x})}{\partial x_i} = e^{\vec{a}^\top \vec{x}+b} a_i$$
$$\frac{\partial^2 g(\vec{x})}{\partial x_i^2} = e^{\vec{a}^\top \vec{x}+b} a_i^2$$
$$\frac{\partial^2 g(\vec{x})}{\partial x_i \partial x_j} = e^{\vec{a}^\top \vec{x}+b} a_i a_j$$

Writing these in matrix form, we get,

$$\nabla g(\vec{x}) = e^{\vec{a}^\top \vec{x}+b} \vec{a}$$
$$\nabla^2 g(\vec{x}) = e^{\vec{a}^\top \vec{x}+b} \vec{a}\vec{a}^\top$$

The Hessian is clearly a rank one positive semi-definite matrix.

To see the second way, we notice that considering $e(x) = e^x$ for a scalar x, the derivative and second derivative of $e(x)$ is just e^x. Since the linear transform we are taking is $a^\top x + b$, we get the same result.

2. Jacobians

The *Jacobian* of a vector-valued function $\vec{g}\colon \mathbb{R}^n \to \mathbb{R}^m$ is the $m \times n$ matrix, denoted as $D\vec{g}$, containing the derivatives of the components of $\vec{g}$ with respect to the variables:

$$(D\vec{g})_{ij} = \frac{\partial g_i}{\partial x_j}, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n. \tag{8}$$

Compute the Jacobian of $\vec{g}\colon \mathbb{R}^n \to \mathbb{R}^n$, where

$$g\left(\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}\right) = \frac{1}{2}\begin{bmatrix} x_1^2 \\ \vdots \\ x_n^2 \end{bmatrix}. \tag{9}$$

Solution: Notice that

$$g_i(\vec{x}) = \frac{1}{2}x_i^2, \qquad \text{so} \qquad \frac{\partial g_i}{\partial x_j}(\vec{x}) = \begin{cases} x_i & i = j \\ 0 & i \neq j \end{cases}. \tag{10}$$

Thus $D\vec{g}(\vec{x}) = \begin{bmatrix} x_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & x_n \end{bmatrix} = \operatorname{diag}(\vec{x})$ where $\operatorname{diag}(\vec{x}) \in \mathbb{R}^{n\times n}$ is the diagonal matrix whose diagonal entries are the entries of $\vec{x}$.

3. Jacobian of Matrix Exponential

Let $\lambda \in \mathbb{R}$, let $\vec{z} \in \mathbb{R}^n$, let $V = \begin{bmatrix} \vec{v}_1 & \cdots & \vec{v}_n \end{bmatrix} \in \mathbb{R}^{n\times n}$ be an orthonormal matrix, and let $\vec{f}\colon \mathbb{R}^n \to \mathbb{R}^n$ be defined as

$$\vec{f}(\vec{x}) = V \begin{bmatrix} \mathrm{e}^{\lambda x_1} & & \\ & \ddots & \\ & & \mathrm{e}^{\lambda x_n} \end{bmatrix} V^\top \vec{z}. \tag{11}$$

Calculate the Jacobian $D\vec{f}(\vec{x})$.

Solution: Writing $\vec{f}(\vec{x})$ out in outer product form, we get

$$\vec{f}(\vec{x}) = V \begin{bmatrix} \mathrm{e}^{\lambda x_1} & & \\ & \ddots & \\ & & \mathrm{e}^{\lambda x_n} \end{bmatrix} V^\top \vec{z} \tag{12}$$

$$= \sum_{i=1}^{n} \mathrm{e}^{\lambda x_i} \vec{v}_i \vec{v}_i^\top \vec{z}. \tag{13}$$

Using linearity of the derivative, we get

$$\frac{\partial \vec{f}}{\partial x_j}(\vec{x}) = \frac{\partial}{\partial x_j} \sum_{i=1}^{n} \mathrm{e}^{\lambda x_i} \vec{v}_i \vec{v}_i^\top \vec{z} \tag{14}$$

$$= \frac{\partial}{\partial x_j} \mathrm{e}^{\lambda x_j} \vec{v}_j \vec{v}_j^\top \vec{z} \tag{15}$$

$$= \lambda \mathrm{e}^{\lambda x_j} \vec{v}_j \vec{v}_j^\top \vec{z}. \tag{16}$$

Therefore, we have

$$D\vec{f}(\vec{x}) = \begin{bmatrix} \frac{\partial \vec{f}}{\partial x_1}(\vec{x}) & \cdots & \frac{\partial \vec{f}}{\partial x_n}(\vec{x}) \end{bmatrix} \tag{17}$$

$$= \lambda \begin{bmatrix} \mathrm{e}^{\lambda x_1} \vec{v}_1 \vec{v}_1^\top \vec{z} & \cdots & \mathrm{e}^{\lambda x_n} \vec{v}_n \vec{v}_n^\top \vec{z} \end{bmatrix} \tag{18}$$

$$= \lambda \begin{bmatrix} \vec{v}_1 \vec{v}_1^\top \vec{z} & \cdots & \vec{v}_n \vec{v}_n^\top \vec{z} \end{bmatrix} \begin{bmatrix} \mathrm{e}^{\lambda x_1} & & \\ & \ddots & \\ & & \mathrm{e}^{\lambda x_n} \end{bmatrix}. \tag{19}$$

4. Gradient of the Cross Entropy Loss

Consider the data $(\vec{x}_i, y_i)$ for $i = 1, \ldots, n$ where $\vec{x} \in \mathbb{R}^d$ and $y_i \in \{0, 1\}$. Consider the parameter vector $\vec{w} \in \mathbb{R}^n$. For each $i \in \{1, \ldots, n\}$, define the *logistic function* $p_i \colon \mathbb{R}^d \mapsto \mathbb{R}$ given as

$$p_i(\vec{w}) = \frac{1}{1 + e^{-\vec{w}^\top \vec{x}_i}}. \tag{20}$$

(a) Find the gradient of the function $p_i(\vec{w})$.

Solution: The gradient is

$$\nabla p_i(\vec{w}) = \begin{bmatrix} \frac{\partial p_i}{\partial w_1}(\vec{w}) \\ \vdots \\ \frac{\partial p_i}{\partial w_d}(\vec{w}) \end{bmatrix}. \tag{21}$$

Here

$$\frac{\partial p_i}{\partial w_j}(\vec{w}) = \frac{(\vec{x}_i)_j e^{-\vec{w}^\top \vec{x}_i}}{\left(1 + e^{-\vec{w}^\top \vec{x}_i}\right)^2}. \tag{22}$$

Thus

$$\nabla p_i(\vec{w}) = \vec{x}_i \cdot \frac{e^{-\vec{w}^\top \vec{x}_i}}{\left(1 + e^{-\vec{w}^\top \vec{x}_i}\right)^2} \tag{23}$$

(b) For $i \in \{1, \ldots, n\}$, the *cross entropy* of $p \in [0, 1]$ against y_i is defined as

$$H_i(p) \doteq -y_i \log(p) - (1 - y_i) \log(1 - p). \tag{24}$$

Find the gradient of the function $\ell_i(\vec{w}) \doteq H(p_i(\vec{w}))$ with respect to $\vec{w}$.

Solution: The gradient is

$$\nabla_{\vec{w}} \ell_i(\vec{w}) = \begin{bmatrix} \frac{\partial \ell_i}{\partial w_1}(\vec{w}) \\ \vdots \\ \frac{\partial \ell_i}{\partial w_d}(\vec{w}) \end{bmatrix}. \tag{25}$$

We can use the chain rule to find each component:

$$\begin{aligned}
\frac{\partial \ell_i}{\partial w_j}(\vec{w}) &= -\left[\frac{\partial H}{\partial p}(p_i(\vec{w}))\right]\left[\frac{\partial p_i}{\partial w_j}(\vec{w})\right] && (26)\\
&= -\left[\frac{y_i}{p_i(\vec{w})} - \frac{1 - y_i}{1 - p_i(\vec{w})}\right]\left[\frac{(\vec{x}_i)_j e^{-\vec{w}^\top \vec{x}_i}}{\left(1 + e^{-\vec{w}^\top \vec{x}_i}\right)^2}\right] && (27)\\
&= -\left[\frac{y_i}{1/(1 + e^{-\vec{w}^\top \vec{x}_i})} - \frac{1 - y_i}{e^{-\vec{w}^\top \vec{x}_i}/(1 + e^{-\vec{w}^\top \vec{x}_i})}\right]\left[\frac{(\vec{x}_i)_j e^{-\vec{w}^\top \vec{x}_i}}{\left(1 + e^{-\vec{w}^\top \vec{x}_i}\right)^2}\right] && (28)\\
&= -\left[y_i(1 + e^{-\vec{w}^\top \vec{x}_i}) - \frac{(1 - y_i)(1 + e^{-\vec{w}^\top \vec{x}_i})}{e^{-\vec{w}^\top \vec{x}_i}}\right]\left[\frac{(\vec{x}_i)_j e^{-\vec{w}^\top \vec{x}_i}}{\left(1 + e^{-\vec{w}^\top \vec{x}_i}\right)^2}\right] && (29)\\
&= -(\vec{x}_i)_j \left[y_i \frac{e^{-\vec{w}^\top \vec{x}_i}}{1 + e^{-\vec{w}^\top \vec{x}_i}} - (1 - y_i)\frac{1}{1 + e^{-\vec{w}^\top \vec{x}_i}}\right] && (30)\\
&= -(\vec{x}_i)_j \left[y_i(1 - p_i(\vec{w})) - (1 - y_i)p_i(\vec{w})\right] && (31)\\
&= -(\vec{x}_i)_j \left[y_i - p_i(\vec{w})\right] && (32)\\
&= (\vec{x}_i)_j \left[p_i(\vec{w}) - y_i\right]. && (33)
\end{aligned}$$

Thus

$$\nabla_{\vec{w}} \ell_i(\vec{w}) = \vec{x}_i \left[p_i(\vec{w}) - y_i\right]. \tag{34}$$

(c) Define the cross-entropy loss function as the sum of the cross entropy functions over the entire data set:

$$\ell(\vec{w}) = \sum_{i=1}^{n} \ell_i(\vec{w}). \tag{35}$$

Find the gradient of the function $\ell(\vec{w})$.

Solution: Using linearity of the derivatives,

$$\begin{aligned}
\nabla \ell(\vec{w}) &= \sum_{i=1}^{n} \nabla \ell_i(\vec{w}) && (36)\\
&= \sum_{i=1}^{n} \vec{x}_i \cdot (p_i(\vec{w}) - y_i) && (37)\\
&= X^\top (\vec{p}(\vec{w}) - \vec{y}). && (38)
\end{aligned}$$

Here

$$X = \begin{bmatrix} \vec{x}_1^\top \\ \vdots \\ \vec{x}_n^\top \end{bmatrix}, \qquad \vec{p}(\vec{w}) = \begin{bmatrix} p_1(\vec{w}) \\ \vdots \\ p_n(\vec{w}) \end{bmatrix}, \qquad \vec{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \tag{39}$$

Notice that this is the same type of gradient as least squares! All it requires is replacing our linear predictors $X\vec{w}$ with our logistic predictors $\vec{p}(\vec{w})$.

