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 $g(\vec{x}) = \vec{y}^\top A\vec{x}$.

(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.

(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.

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:

$$(D\vec{g})_{ij} = \frac{\partial g_i}{\partial x_j}, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n. \tag{3}$$

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

$$g\left(\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}\right) = \frac{1}{2}\begin{bmatrix} x_1^2 \\ \vdots \\ x_n^2 \end{bmatrix}. \tag{4}$$

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

$$\vec{f}(\vec{x}) = V \begin{bmatrix} \mathrm{e}^{\lambda x_1} & & \\ & \ddots & \\ & & \mathrm{e}^{\lambda x_n} \end{bmatrix} V^\top \vec{z}. \tag{5}$$

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

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

$$p_i(\vec{w}) = \frac{1}{1 + e^{-\vec{w}^\top \vec{x}_i}}. \tag{6}$$

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

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

$$H_i(p) \doteq -y_i \log(p) - (1 - y_i) \log(1 - p). \tag{7}$$

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

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

$$\ell(\vec{w}) = \sum_{i=1}^{n} \ell_i(\vec{w}). \tag{8}$$

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