1. Gradients and Hessians

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

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

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

$$(\nabla^2 g(\vec{x}))_{ij} = \frac{\partial^2 g}{\partial x_i \partial x_j}(\vec{x}), \quad i = 1, \dots, n, \quad j = 1, \dots, n.$$
 (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{q} with respect to the variables:

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

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

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

4. Gradient of the Cross Entropy Loss (Optional)

Consider the data (\vec{x}_i, y_i) for i = 1, ..., 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 $i \in \{1, ..., n\}$, define the *logistic function* $p_i : \mathbb{R}^d \to \mathbb{R}$ given as

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

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

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

$$H_i(p) \doteq -y_i \log(p) - (1 - y_i) \log(1 - p).$$
 (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 $\ell(\vec{w})$.