Review Assignment 2

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Machine Learning

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1 Calculus review

Recall that the Jacobian of a function $f : \mathbb{R}^n \to \mathbb{R}^m$ is an $m \times n$ matrix of partial derivatives

$$
Df(x) = \begin{bmatrix}
\frac{\partial f_1(x)}{\partial x_1} & \frac{\partial f_1(x)}{\partial x_2} & \cdots & \frac{\partial f_1(x)}{\partial x_n} \\
\frac{\partial f_2(x)}{\partial x_1} & \frac{\partial f_2(x)}{\partial x_2} & \cdots & \frac{\partial f_2(x)}{\partial x_3} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial f_m(x)}{\partial x_1} & \frac{\partial f_m(x)}{\partial x_2} & \cdots & \frac{\partial f_m(x)}{\partial x_n}
\end{bmatrix}
$$

where $x = [x_1 x_2 \dots x_n]^\intercal$, $f(x) = [f_1(x) f_2(x) \dots f_m(x)]^\intercal$ and $\frac{\partial f_i(x)}{\partial x_j}$ is the partial derivative of the i-th output with respect to the j-th input. When f is a scalar-valued function (i.e., when $f : \mathbb{R}^n \to \mathbb{R}$), the Jacobian $Df(x)$ is a $1 \times n$ matrix, i.e., it is a row vector. Its transpose is called the *gradient* of the function

$$
\nabla f(x) = Df(x)^\intercal \begin{bmatrix}
\frac{\partial f_1(x)}{\partial x_1} \\
\frac{\partial f(x)}{\partial x_2} \\
\vdots \\
\frac{\partial f(x)}{\partial x_n}
\end{bmatrix} \tag{1}
$$

Also, recall that the **chain rule** is a tool to calculate gradients of function compositions. Suppose $f : \mathbb{R}^n \to \mathbb{R}^m$ is differentiable at x and $g : \mathbb{R}^m \to \mathbb{R}^p$ is differentiable at $f(x)$. Define the composition $h : \mathbb{R}^m \to \mathbb{R}^p$ by $h(z) = g(f(z))$. Then h is differentiable at x, with Jacobian

$$
Dh(x) = Dg(z)\Big|_{z=f(x)} Df(x). \tag{2}
$$

1. Consider the function $g : \mathbb{R}^m \to \mathbb{R}$ with $g(x) = x^\intercal x$. We can readily calculate the gradient $\nabla g(x) = 2x$ by noticing that

$$
\forall j = 1, \dots, n \qquad \frac{\partial x^\intercal x}{\partial x_j} = \frac{\partial x^2 j}{\partial x_j} = 2x_j \to \nabla g(x) = 2x \tag{3}
$$

Consider also the function $a : \mathbb{R}^n \to \mathbb{R}^m$ with $a(x) = Ax$, and $A \in \mathbb{R}^{m \times n}$. The Jacobian of $a(x)$ is $Da(x) = A$. Given this, answer the following questions by using the above definitions (show all the steps of your working)

(a) Consider the function $h : \mathbb{R}^n \to \mathbb{R}$ and $h(x) = x^\mathsf{T} Q x$, where $Q \in \mathbb{R}^{n \times n}$ is a symmetric matrix. Calculate $\nabla h(x)$ by using the product rule, the gradient of g in eq. (3), and the Jacobian of the linear function $a(x)$.

We notice that $\nabla g(x) = 2x$, therefore

$$\nabla h(x) = \frac{\partial x^\mathsf{T} Q x^\mathsf{T}}{\partial x}$$
$$= 2Qx$$

(b) Consider the function $f : \mathbb{R}^n \to \mathbb{R}$, where $f(x) = \|Ax - b\|^2$, $A \in \mathbb{R}^{m \times n}$, and $b \in \mathbb{R}^m$. Calculate $\nabla h(x)$ by using the chain rule in eq. (2), the gradient of g in eq. (3), and the Jacobian of the linear function $a(x)$.

$$\|Ax - b\|^2 = (Ax - b)^\mathsf{T}(Ax - b)$$
$$= x^\mathsf{T} A^\mathsf{T} A x - 2b^\mathsf{T} A x + b^\mathsf{T} b$$

From that we can use the steps like in (a)

$$\nabla h(x) = 2A^\mathsf{T} A x - 2A^\mathsf{T} b$$

(c) Consider a function $f : \mathbb{R}^n \to \mathbb{R}$. Suppose we have a matrix $A \in \mathbb{R}^{n \times m}$ and a vector $x \in \mathbb{R}^m$. Calculate $\nabla x f(Ax)$ as a function of $\nabla x f(x)$.

(d) Show that

$$\frac{\partial}{\partial X} \sum_{i=1}^{n} n\lambda_i = 1$$

where $X \in \mathbb{R}^{m \times n}$ and has eigenvalues $\lambda_1 \ldots \lambda_n$

We know form theory $f(x) = \sum_{i=1}^{n} n\lambda_i = \sum_{i=1}^{n} x_{ii}$

$$\frac{\partial}{\partial x} f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_{11}} & \frac{\partial f(x)}{\partial x_{1n}} \\ \frac{\partial f(x)}{\partial x_{n1}} & \frac{\partial f(x)}{\partial x_{nn}} \end{bmatrix}$$

(e) Show that

$$\frac{\partial}{\partial X} \prod_{i=1}^{} n\lambda_i = (det)(X)X^{-\intercal}$$

where $X \in \mathbb{R}^{m \times n}$ and has eigenvalues $\lambda_1 \dots \lambda_n$

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2. Assume $A \in \mathbb{R}^{m \times n}$, $X \in \mathbb{R}^{m \times n}$, and $B \in \mathbb{R}^{m \times m}$. Show that $\nabla X \text{tr}(AX^\intercal B) = BA$

$$
\begin{aligned}
BA &= \nabla X \text{tr}(AX^\intercal B) \\
&= \nabla X \text{tr}(X^\intercal BA) && \text{we can get rid of the trace} \\
&= ((BA)^\intercal)^\intercal && \text{transpose of transpose eliminate each other} \\
&= BA
\end{aligned}
$$

3. Solve the following equality constrained optimization problem

$$\max_{x \in \mathbb{R}^n} x^\intercal A x \qquad \text{subject to } b^\intercal x = 1$$

for a symmetric matrix $A \in \mathbb{S}^n$. Assume that A is invertible and $b \neq 0$.

A standard way of solving optimization problems with equality constraints is by forming the Lagrangian, an objective function that includes the equality constraints. The Lagrangian in this case is be given by

$$\mathcal{L}(x, \lambda) = x^\intercal A x - \lambda(b^\intercal x - 1).$$

The parameter λ is called the Lagrangian multiplier associated with the equality constraint. It can be shown that for x_* to be an optimal solution to the problem, the gradient of the Lagrangian w.r.t. x has to be zero at x_*. That is,

$$\nabla_x(\mathcal{L}(x, \lambda)) = \nabla_x(x^\intercal A x - \lambda b^\intercal x) = 2Ax - \lambda b \overset{!}{=} 0$$

$$Ax = \frac{1}{2}\lambda b$$

This shows that the only points which can be possibly maximize (or minimize) $b^\intercal A x$ assuming $x^\intercal b = 1$ are the eigenvectors of A.

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