CS 189 Introduction to Machine Learning
Spring 2018 DIS0

1 Vector Calculus

Below, $\mathbf{x} \in \mathbb{R}^d$ means that $\mathbf{x}$ is a $d \times 1$ (column) vector with real-valued entries. Likewise, $\mathbf{A} \in \mathbb{R}^{d \times d}$ means that $\mathbf{A}$ is a $d \times d$ matrix with real-valued entries. In this course, we will by convention consider vectors to be column vectors.

Consider $\mathbf{x}, \mathbf{w} \in \mathbb{R}^d$ and $\mathbf{A} \in \mathbb{R}^{d \times d}$. In the following questions, $\frac{\partial}{\partial \mathbf{x}}$ denotes the derivative with respect to $\mathbf{x}$, while $\nabla_{\mathbf{x}}$ denote the gradient with respect to $\mathbf{x}$. Compute the following:

(a) $\frac{\partial \mathbf{w}^T \mathbf{x}}{\partial \mathbf{x}}$ and $\nabla_{\mathbf{x}}(\mathbf{w}^T \mathbf{x})$

(b) $\frac{\partial (\mathbf{w}^T \mathbf{A}\mathbf{x})}{\partial \mathbf{x}}$ and $\nabla_{\mathbf{x}}(\mathbf{w}^T \mathbf{A}\mathbf{x})$

(c) $\frac{\partial (\mathbf{w}^T \mathbf{A}\mathbf{x})}{\partial \mathbf{w}}$ and $\nabla_{\mathbf{w}}(\mathbf{w}^T \mathbf{A}\mathbf{x})$

(d) $\frac{\partial (\mathbf{w}^T \mathbf{A}\mathbf{x})}{\partial \mathbf{A}}$ and $\nabla_{\mathbf{A}}(\mathbf{w}^T \mathbf{A}\mathbf{x})$

(e) $\frac{\partial (\mathbf{x}^T \mathbf{A}\mathbf{x})}{\partial \mathbf{x}}$ and $\nabla_{\mathbf{x}}(\mathbf{x}^T \mathbf{A}\mathbf{x})$

(f) $\nabla^2_{\mathbf{x}}(\mathbf{x}^T \mathbf{A}\mathbf{x})$

2 Eigenvalues

(a) Let $\mathbf{A}$ be an invertible matrix. Show that if $\mathbf{v}$ is an eigenvector of $\mathbf{A}$ with eigenvalue λ, then it is also an eigenvector of $\mathbf{A}^{-1}$ with eigenvalue λ^{-1}.

(b) A square and symmetric matrix $\mathbf{A}$ is said to be positive semidefinite (PSD) ($\mathbf{A} \succeq 0$) if $\forall \mathbf{v} \neq 0, \mathbf{v}^T \mathbf{A}\mathbf{v} \geq 0$. Show that $\mathbf{A}$ is PSD if and only if all of its eigenvalues are nonnegative.

Hint: Use the eigendecomposition of the matrix $\mathbf{A}$.

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1 Trace Derivatives

(a) Let $\mathbf{P}$ be a $p \times q$ matrix and $\mathbf{Q}$ be a $q \times p$ matrix. Compute $\frac{\partial \text{trace}(\mathbf{PQ})}{\partial \mathbf{P}}$.

(b) Let $\mathbf{P}$ be a $p \times q$ matrix and $\mathbf{Q}$ be a $q \times q$ matrix. Compute $\frac{\partial \text{trace}(\mathbf{PQP}^\top)}{\partial \mathbf{P}}$ at $\mathbf{P} = \mathbf{U}$.

2 Unitary invariance

(a) Prove that the regular Euclidean norm (also called the ℓ^2-norm) is unitary invariant; in other words, the ℓ^2-norm of a vector is the same, regardless of how you apply a rigid linear transformation to the vector (i.e., rotate or reflect). Note that rigid linear transformation of a vector $\mathbf{v} \in \mathbb{R}^d$ means multiplying by an orthogonal $\mathbf{U} \in \mathbb{R}^{d \times d}$.

(b) Now show that the Frobenius norm of matrix $\mathbf{A}$ is unitary invariant. The Frobenius norm is defined as $\|\mathbf{A}\|_F = \sqrt{\sum_{i,j=1}^n |a_{ij}|^2} = \sqrt{tr(\mathbf{A}^\top \mathbf{A})}$.

3 Least Squares (using vector calculus)

(a) In ordinary least-squares linear regression, we typically have $n > d$ so that there is no $\mathbf{w}$ such that $\mathbf{Xw} = \mathbf{y}$ (these are typically overdetermined systems — too many equations given the number of unknowns). Hence, we need to find an approximate solution to this problem. The residual vector will be $\mathbf{r} = \mathbf{Xw} - \mathbf{y}$ and we want to make it as small as possible. The most common case is to measure the residual error with the standard Euclidean ℓ^2-norm. So the problem becomes:

$$\min_{\mathbf{w}} \|\mathbf{Xw} - \mathbf{y}\|_2^2$$

Where $\mathbf{X} \in \mathbf{R}^{n \times d}, \mathbf{w} \in \mathbf{R}^d, \mathbf{y} \in \mathbf{R}^n$. Derive using vector calculus an expression for an optimal estimate for $\mathbf{w}$ for this problem assuming $\mathbf{X}$ is full rank.

(b) How do we know that $\mathbf{X}^\top \mathbf{X}$ is invertible?

(c) What should we do if $\mathbf{X}$ is not full rank?