CSC 311: Introduction to Machine Learning

Tutorial 9 - Math Review

Fall 2023

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Outline

- Gradients of multivariate functions
- Matrix decomposition

Gradients of vector-valued functions

Vector-valued functions

For a function $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$ and a vector $\mathbf{x} = [x_1, \cdots, x_n]^T \in \mathbb{R}^n$, the corresponding vector of function values is given as:

$$\mathbf{f}(\mathbf{x}) = [f_1(\mathbf{x}) \cdots f_m(\mathbf{x})] \in \mathbb{R}^m$$

where $f_i : \mathbb{R}^n \to \mathbb{R}$.

Partial derivatives

The partial derivative of a vector-valued function $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$ with respect to $x_i \in \mathbb{R}$ is given as:

$$\frac{\partial \mathbf{f}}{\partial x_i} = [\frac{\partial f_1}{\partial x_i} \cdots \frac{\partial f_m}{\partial x_i}] \in \mathbb{R}^m$$

Jacobian

The collection of all first-order partial derivatives of a vector-valued function $\mathbf{f} : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is called the *Jacobian*. The Jacobian $\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}}$ is an $m \times n$ matrix, which is defined as:

$$\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} = [\frac{\partial \mathbf{f}(\mathbf{x})}{\partial x_1} \cdots \frac{\partial \mathbf{f}(\mathbf{x})}{\partial x_n}]$$

$$= \begin{bmatrix} \frac{\partial f_1(\mathbf{x})}{\partial x_1} & \dots & \frac{\partial f_1(\mathbf{x})}{\partial x_n} \\ \vdots & \vdots & \vdots \\ \frac{\partial f_m(\mathbf{x})}{\partial x_1} & \dots & \frac{\partial f_m(\mathbf{x})}{\partial x_n} \end{bmatrix}$$

Example

Given $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{A} \in \mathbb{R}^{m \times n}$, we define the linear vector-valued function $\mathbf{f}$ as:

$$\mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x}$$

- Q_1: What is the dimension of $\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}}$?
- Q_2: Compute $\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}}$.

Answer

- Since $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$, its follows that $\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} \in \mathbb{R}^{m \times n}$.
- The first step is to compute each entry of the Jacobian matrix, $\frac{\partial f_i}{\partial x_j}$. From the definition of the matrix decomposition, we know:

$$f_i(\mathbf{x}) = \sum_{j=1}^{N} A_{ij} x_j$$

Then each entry $\frac{\partial f_i}{\partial x_j} = A_{ij}$. It follows that:

$$\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial f_1(\mathbf{x})}{\partial x_1} & \dots & \frac{\partial f_1(\mathbf{x})}{\partial x_n} \\ \vdots & \vdots & \vdots \\ \frac{\partial f_m(\mathbf{x})}{\partial x_1} & \dots & \frac{\partial f_m(\mathbf{x})}{\partial x_n} \end{bmatrix} = \begin{bmatrix} A_{11} & \dots & A_{1N} \\ \vdots & \vdots & \vdots \\ A_{M1} & \dots & A_{MN} \end{bmatrix} = \mathbf{A}$$

Gradients with respect to the matrix

- Often in machine learning, we need to take gradients of matrices with respect to other matrices. The Jacobian in this case will be a multi-dimension tensor.
- For example, if we compute the gradient of an $m \times n$ matrix $\mathbf{A}$ with respect to a $p \times q$ matrix $\mathbf{B}$, the resulting Jacobian $\mathbf{J}$ is a four-dimensional tensor $m \times n \times p \times q$. Each entry $\mathbf{J}_{ijkl} = \frac{\partial \mathbf{A}_{ij}}{\partial \mathbf{B}_{kl}}$.

Exercise

Given a matrix $\mathbf{R} \in \mathbb{R}^{m\times n}$. We define:

$$\mathbf{f}(\mathbf{R}) = \mathbf{R}^T\mathbf{R}$$

- Q_1: What is the diminsion of $\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}}$?
- Q_2: Compute $\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}}$.

Recommended resources

Petersen, Kaare Brandt, and Michael Syskind Pedersen. ”The matrix cookbook.” Technical University of Denmark 7, no. 15 (2008): 510.

Matrix decomposition

Introduction

- We can decompose an integer into its prime factors, e.g., $12 = 2 \times 2 \times 3$.
- Similarly, matrices can be decomposed into product of other matrices.
- Examples are Eigendecomposition, SVD, Schur decomposition, LU decomposition, ...

Eigenvector

- An eigenvector of a square matrix A is a nonzero vector v such that multiplication by A only changes the scale of v:

$$Av = \lambda v$$

- The scalar λ is known as the eigenvalue.
- If v is an eigenvector of A, so is any rescaled vector sv. Moreover, sv still has the same eigenvalue. Thus, we constrain the eigenvector to be of unit length.

Compute eigenvalues - characteristic polynomial

- Eigenvalue equation of matrix A:

$$\begin{aligned} Av &= \lambda v \\ \lambda v - Av &= 0 \\ (\lambda I - A)v &= 0 \end{aligned}$$

- If nonzero solution for v exists, then it must be the case that:

$$det(\lambda I - A) = 0$$

- Unpacking the determinant as a function of λ , we get a polynomial, called the characteristic polynomial:

$$P_A(\lambda) = det(\lambda I - A) = \lambda^n + c_{n-1}\lambda^{n-1} + \lambda + c_0$$

- Compute eigenvalues of $A \rightarrow$ solve $P_A(\lambda) = 0$

Exercise

Consider the matrix:

$$A = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

- What is the characteristic polynomial of A?
- What are the eigenvalues of A?
- What are the associated eigenvectors?

Eigendecomposition

- Every symmetric (hermitian) matrix of dimension n has a set of (not necessarily unique) n orthogonal eigenvectors. Furthermore, all eigenvalues are real.
- Every real symmetric matrix A can be decomposed into real-valued eigenvectors and eigenvalues:

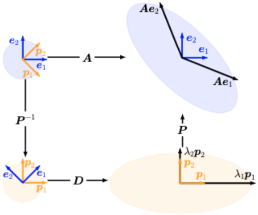
$$A = PDP^{-1}$$

- P is an orthogonal matrix of the eigenvectors of A, and D is a diagonal matrix of eigenvalues.

Intuitions of Eigendecomposition

- Diagonal matrix allows fast computations of their determinants, powers and inverses.
- Eigendecomposition transforms a matrix into a diagonal form by changing the basis.

Geometric intuitions of eigendecomposition



- Top-left to bottom-left: P^{-1} performs a basis change.
- Bottom-left to bottom-right: D performs a scaling.
- Bottom-right to top-right: P undoes the basis change.

Singular Value Decomposition (SVD)

- If A is not square, eigendecomposition is undefined.
- SVD is a decomposition of the form $A = UDV^T$.
- SVD is more general than eigendecomposition.
- Every real matrix has a SVD.

SVD

- If A is $m \times n$, then U is $m \times m$, D is $m \times n$, and V is $n \times n$.
- U and V are orthogonal matrices, and D is a diagonal matrix (not necessarily square).
- Diagonal entries of D are called singular values of A.
- Columns of U are the left singular vectors, and columns of V are the right singular vectors.

SVD and eigendecomposition

- SVD can be interpreted in terms of eigendecompostion.
- Left singular vectors of A are the eigenvectors of AA^T.
- Right singular vectors of A are the eigenvectors of A^TA
- Nonzero singular values of A are square roots of eigenvalues of A^TA and AA^T. (A^TA and AA^T are semipositive definite, thus their eigenvalues are positive)

Exercise

Compute SVD of the matrix:

$$A = \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{bmatrix}$$

Exercise

Compute SVD of the matrix:

$$A = \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{bmatrix}$$

- What is AA^T and $A^T A$?
- Apply eigendecomposition on AA^T and $A^T A$

Rank-r approximation

- Given a matrix A, SVD allows us to find its "best" (to be defined) rank-r approximation A_r.
- We can write $A = UDV^T$ as $A = \sum_{i=1}^{n} d_i u_i v_i^T$, where d_i are sorted from the largest to the smallest.
- The rank-r approximation A_r is defined as:

$$A = \sum_{i=1}^{r} d_i u_i v_i^T$$

- A_r is the best approximation of rank r by many norms, such as, L_2 norm. It means that $||A - A_r||_2 \leq ||A - B||_2$ for any rank r matrix B.

Exercise

Fine the rank-1 approximation and rank-2 approximation of the matrix:

$$A = \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{bmatrix}$$