ECBM E6040 Neural Networks and Deep Learning

Lecture #3: Elements of Probability and Information Theory, and Numerical Computation

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Outline of Part I

Outline of Part II

3. Probability Spaces and Random Variables
   - Probability Spaces
   - Random Variables and Stochastic Processes
   - Conditional Probability

4. Elements of Information Theory
   - Measures of Information

Outline of Part III

5. Gradient-Based Optimization

6. Constraint Optimization
   - Karush-Kuhn-Tucker Approach

7. Linear Least Squares

Part I

Review of Previous Lecture

Topics Covered

Elements of Linear Algebra

- Finite Dimensional Vector Spaces
- Eigendecomposition and SVD
- Principal Component Analysis

Learning Objectives

- Reviewing key elements of Singular Value Decomposition
- Definition of the Psedo-Inverse and characterizing its properties
- Formulating and deriving Principal Component Analysis

Part II

Elements of Probability and Information Theory

Basic Overview

Probability theory is an axiomatic branch of measure theory that provides

- means of quantifying uncertainty,
- a formal calculus to derive statements about uncertain events.

The theory of probability constitutes a formidable body of knowledge that provides a set of tools indispensable in machine learning.

The Notion of Probability

The basic notion in probability theory is that of a random experiment whose outcome cannot be determined in advance. A set of all possible outcomes of an experiment is called a sample space and it is usually denoted by Ω.

An event is a subset of a sample space. An event $A \in \Omega$ is set to occur iff the observed outcome ω is an element of the set A.

Example

Consider an experiment that consists of counting the number of traffic accidents at an intersection during rush hour. Here $\Omega = \{0, 1, 2, ...\}$ and $A = \{0, 1, ..., 7\}$ is the event describing that the number of accidents is less than or equal to 7. The event $A = \{5, 6, 7, ...\}$ occurs iff the number of accidents is 5 or 6 or ...

Frequently Encountered Events

Given $A \in \Omega$, the complement A^c of A is defined to be the event which occurs iff A does not occur, that is,

$$A^c = \{\omega \in \Omega \mid \omega \notin A\}.$$

Given two events A and B, their union is the event which occurs iff either A or B (or both) occurs, that is

$$A \cup B = \{\omega \in \Omega \mid \omega \in A \text{ or } \omega \in B\}.$$

The intersection of A and B is the event which occurs iff both A and B occur, that is

$$A \cap B = \{\omega \in \Omega \mid \omega \in A \text{ and } \omega \in B\}.$$

Frequently Encountered Events (cont'd)

The operations of taking unions, intersections, and complements can be combined to obtain new events.For example,

$$(A \cup B)^c = A^c \cap B^c, \qquad (A \cap B)^c = A^c \cup B^c.$$

Two events are set to be disjoint if they have no element in common, that is

$$A \cup B = \emptyset.$$

If two events are disjoint, the occurrence of one implies that the other has not occurred. A family of events is called disjoint if every pair of them are disjoint.

Definition

Let Ω be a sample space and $\mathbb{P}$ a function which associates a number with each event. Then $\mathbb{P}$ is called a probability measure provided that

(i) for every event A, $0 \leq \mathbb{P}(A) \leq 1$;

(ii) $\mathbb{P}(\Omega) = 1$;

(iii) for any sequence $A_1, A_2, \ldots$ of disjoint events

$$\mathbb{P}(\cup_{i \in \mathbb{N}} A_i) = \sum_{i \in \mathbb{N}} \mathbb{P}(A_i).$$

Remark

It might not be practically possible to assign a probability to each event in an explicit fashion. Often, therefore, the probabilities of only a few key events are specified. The remaining probabilities are computed from the axioms above.

Computing Event Probabilities

Here are a some of the key results that can be directly obtained from the three axioms.

If $A_1, ..., A_n$ are disjoint events

$$\mathbb{P}(A_1 \cup ... \cup A_n) = \mathbb{P}(A_1) + ... + \mathbb{P}(A_n).$$

If $A \subset B$, then $\mathbb{P}(A) \leq \mathbb{P}(B)$.

For any event A, $\mathbb{P}(A) + \mathbb{P}(A^c) = 1$.

If $B_1, B_2, ...$ are disjoint events with $\cup_{i \in \mathbb{N}} B_i = \Omega$, then for any event A,

$$\mathbb{P}(A) = \sum_{i \in \mathbb{N}} \mathbb{P}(A \cap B_i).$$

Random Variables

Definition

A random variable $\mathbf{x}$ with values in a set E is a function which assigns a value $\mathbf{x}(\omega)$ in E to each outcome $\omega \in \Omega$.

Definition

A stochastic process with state space E is a collection $\mathbf{x}_t$, $t \in \mathbb{R}$, defined on the same probability space space and taking values in E.

Independence and Conditional Probability

Definition

The dicrete random variables $\mathbf{x}_1, ..., \mathbf{x}_n$ are said to be independent if

$$\mathbb{P}(\mathbf{x}_1 = a_1, ..., \mathbf{x}_n = a_n) = \mathbb{P}(\mathbf{x}_1 = a_1) \cdots \mathbb{P}(\mathbf{x}_n = a_n)$$

Definition

Let A and B be two events. The conditional probability of A given B, written $\mathbb{P}(A \mid B)$, is a number satisfying

(i) $0 \leq \mathbb{P}(A \mid B) \leq 1$,

(ii) $\mathbb{P}(A \cap B) = \mathbb{P}(A \mid B)\mathbb{P}(B)$.

Entropy and Kullback-Leibler Divergence

To be discussed in class (no slides).

Part III

Elements of Numerical Computation

Optimization in Deep Learning

Most deep learning algorithms involve the minimization of maximization of a function called objective function or criterion. In minimization, these functions are also called cost functions, loss functions or error functions.

The value that minimizes or maximizes a function is denoted by a superscript $*$:

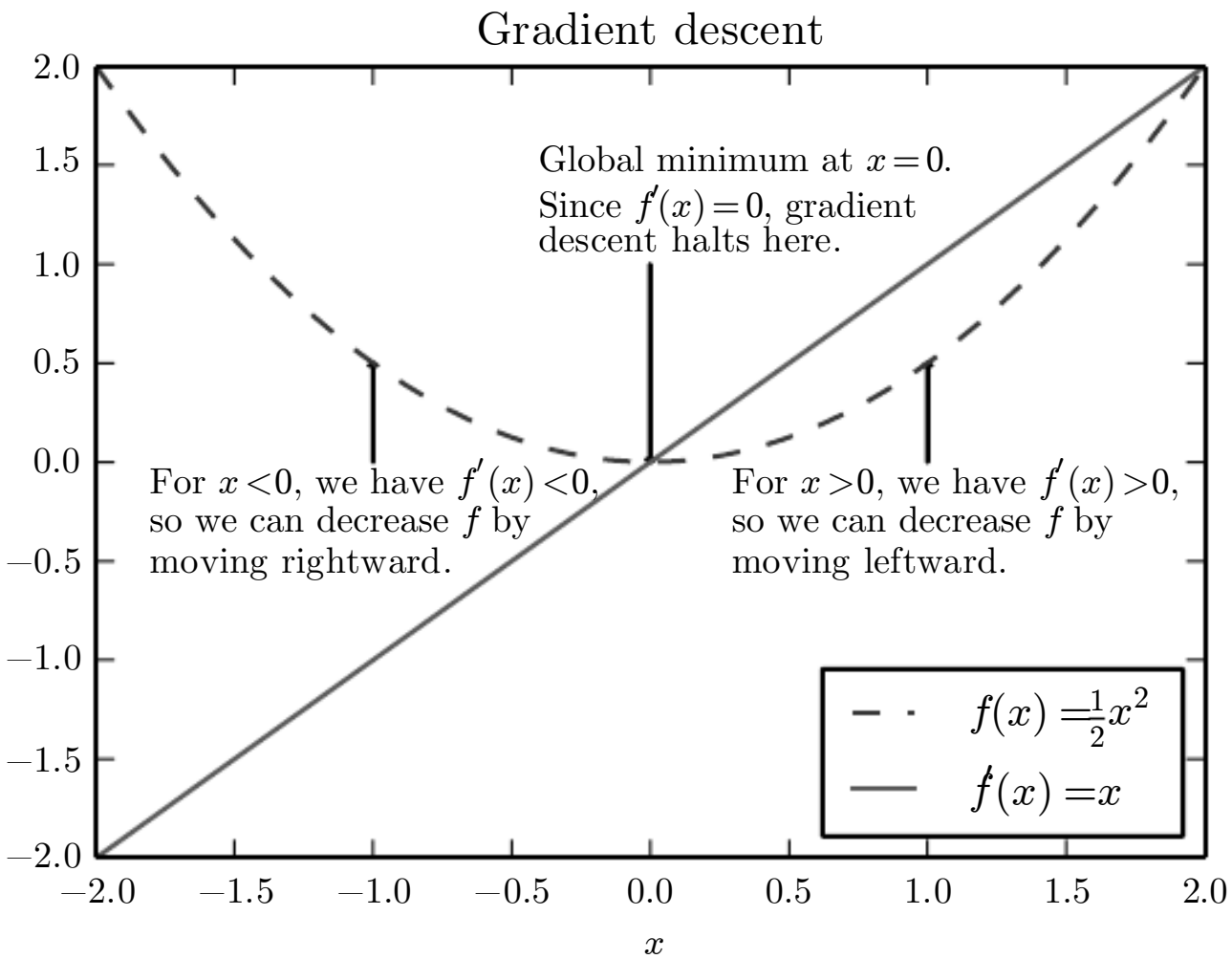
$$\mathbf{x}^* = \arg\min_{\mathbf{x}} f(\mathbf{x}).$$

Assume that $y = f(x)$ with $x, y \in \mathbb{R}$. Points were

$$\frac{df(x)}{dx} = 0$$

are called critical or stationary points. These can be local minima, local maxima, saddle points, or global minima/maxima.

The Intuition Behind the Gradient Descent



The derivative of the function can be used to follow the function downhill to a minimum. This technique is called gradient descent.

Gradient Descent for Functions with Multiple Inputs

Here we consider functions of the form $f : \mathbb{R}^n \to \mathbb{R}$. The partial derivative $\frac{\partial}{\partial x_i} f(\mathbf{x})$ measures how f changes as a function of x_i at point $\mathbf{x}$. The gradient generalizes to the notion of derivative with respect to a vector: the gradient of f is the vector containing all the partial derivatives, denoted by $\nabla f(\mathbf{x})$.

The directional derivative in direction $\mathbf{u}$ (a unit vector) is the slope of the function f in direction $\mathbf{u}$, i.e., the derivative of the function $f(\mathbf{x} + \alpha\mathbf{u})$ with respect to α, evaluated at $\alpha = 0$.

Using the chain rule, the directional derivative amounts to

$$\mathbf{u}^T \nabla f(\mathbf{x}).$$

Gradient Descent: Functions with Multiple Inputs (cont'd)

To minimize f, we have to find the direction in which f decreases the fastest. Using the directional derivative we have

$$\min_{\mathbf{u},\mathbf{u}^T\mathbf{u}=1} \mathbf{u}^T \nabla f(\mathbf{x}) = \min_{\mathbf{u},\mathbf{u}^T\mathbf{u}=1} ||\mathbf{u}||_2 ||\nabla f(\mathbf{x})||_2 \cos\theta,$$

where θ is the angle between $\mathbf{u}$ and the gradient. Since $||\mathbf{u}||_2 = 1$ the minimization above can be reduced to

$$\min_{\mathbf{u}} \cos\theta.$$

The minimum of the cos function above is -1 and is achieved when $\mathbf{u}$ points in the opposite direction of the gradient.

Gradient Descent: Functions with Multiple Inputs (cont'd)

The Method of Steepest Descent

Steepest descent chooses a new point

$$\mathbf{x}^{'} = \mathbf{x} - \varepsilon \, \nabla f(\mathbf{x}),$$

where ε is the size of the step. There are many ways to choose ε (it is an art ...).

Problem Formulation and the KKT Approach

Often, we may wish to find the maximal or minimal value of $f(\mathbf{x})$ for values of $\mathbf{x}$ in some set $\mathbb{S}$. This is known as constrained optimization. Points $\mathbf{x}$ that lie within the set $\mathbb{S}$ are called feasible points in constrained optimization terminology.

A very general solution to constrained optimization problem above is provided by the KarushKuhnTucker (KKT) approach. The KKT approach, is based on introducing a new function called the generalized Lagrangian or generalized Lagrange function.

To define the Lagrangian, we'll first describe $\mathbb{S}$ in terms of equations and inequalities. We want a description of $\mathbb{S}$ in terms of m functions g_i and n functions h_j so that

$$\mathbb{S} = \{\mathbf{x} | \forall i, g_i(\mathbf{x}) = 0 \text{ and } \forall j, h_j(\mathbf{x}) \leq 0\}.$$

The equations involving g_i are called the equality constraints and the inequalities involving h_j are called inequality constraints.

Problem Formulation and the KKT Approach

The generalized Lagrangian is then defined as

$$L(\mathbf{x}, \lambda, \alpha) = f(\mathbf{x}) + \sum_i \lambda_i g_i(\mathbf{x}) + \sum_j \alpha_j h_j(\mathbf{x}).$$

We solve the constrained minimization problem using unconstrained optimization of the generalized Lagrangian. Observe that, so long as at least one feasible point exists and $f(\mathbf{x})$ is not permitted to have the value ∞, then

$$\min_{\mathbf{x}} \max_{\lambda} \max_{\alpha, \alpha \geq 0} L(\mathbf{x}, \lambda, \alpha),$$

has the same optimal objective function value and set of optimal points $\mathbf{x}$ as

$$\min_{\mathbf{x} \in \mathbb{S}} f(\mathbf{x}).$$

Problem Formulation and the KKT Approach

The above follows because any time the constraints are satisfied,

$$\max_{\lambda} \max_{\alpha,\alpha\geq 0} L(\mathbf{x},\lambda,\alpha) = f(\mathbf{x}),$$

while any time a constraint is violated,

$$\max_{\lambda} \max_{\alpha,\alpha\geq 0} L(\mathbf{x},\lambda,\alpha) = \infty,$$

These properties guarantee that no infeasible point will ever be optimal, and that the optimum within the feasible points is unchanged.

Unconstrained Linear Least Squares

Find the value of $\mathbf{x}$ that minimizes

$$f(\mathbf{x}) = \frac{1}{2}||\mathbf{A}\mathbf{x} - \mathbf{b}||_2^2.$$

To apply the gradient-based optimization, we derive the gradient

$$\nabla f(\mathbf{x}) = \mathbf{A}^T(\mathbf{A}\mathbf{x} - \mathbf{b}) = \mathbf{A}^T\mathbf{A}\mathbf{x} - \mathbf{A}^T\mathbf{b}.$$

We now just apply the standard steepest decent algorithm

$$\mathbf{x}^{'} = \mathbf{x} - \varepsilon(\mathbf{A}^T\mathbf{A}\mathbf{x} - \mathbf{A}^T\mathbf{b}).$$

Constrained Linear Least Squares

An Example

We will minimize the same function $f(\mathbf{x})$, but subject to the constraint $\mathbf{x}^T\mathbf{x} \leq 1$. We introduce the Lagrangian

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) + \lambda(\mathbf{x}^T\mathbf{x} - 1).$$

We can now solve the problem

$$\min_{\mathbf{x}} \max_{\lambda, \lambda \geq 0} L(\mathbf{x}, \lambda).$$

The solution to the unconstrained least squares problem is given by $\mathbf{x} = \mathbf{A}^+\mathbf{b}$. If this point is feasible, then it is the solution to the constrained problem. Otherwise, we must find a solution where the constraint is active. By differentiating the Lagrangian with respect to $\mathbf{x}$, we obtain the equation

$$\mathbf{A}^T\mathbf{A}\mathbf{x} - \mathbf{A}^T\mathbf{b} + 2\lambda\mathbf{x} = 0.$$

Constrained Linear Least Squares (cont'd)

An Example

This tells us that the solution will take the form

$$\mathbf{x} = (\mathbf{A}^T\mathbf{A} + 2\lambda\mathbf{I})^{-1}\mathbf{A}^T\mathbf{b}.$$

The magnitude of λ must be chosen such that the result obeys the constraint. We can find this value by performing gradient ascent on λ. To do so, observe that

$$\frac{\partial}{\partial\lambda}L(\mathbf{x},\lambda) = \mathbf{x}^T\mathbf{x} - 1.$$

When the norm of $\mathbf{x}$ exceeds 1, this derivative is positive, so to ascend the gradient and increase the Lagrangian with respect to λ, we increase λ. This will in turn shrink the optimal $\mathbf{x}$. The process continues until $\mathbf{x}$ has the correct norm and the derivative on λ is 0.