HOMEWORK SET 1

CSCI5527 Deep Learning (Fall 2023)

Due 11:59 pm, Oct 19 2023

Instruction Your writeup, either typeset or scanned, should be a single PDF file. For problems requiring coding, organize all codes for each problem into a separate Jupyter notebook file (i.e., `.ipynb` file). Your submission to Gradescope should include the single PDF and all notebook files—**please DO NOT zip them**! No late submission will be accepted. For each problem, you should acknowledge your collaborators—**including AI tools**, if any.

About the use of AI tools You are strongly encouraged to use AI tools—they are becoming our workspace friends, such as ChatGPT (`https://chat.openai.com/`, which does not yet accept PDFs, but we provide the LaTeX source codes for our problems that you can copy and enter), Claude (`https://claude.ai/chats`, which accepts numerous forms of inputs, including PDFs), and Github Copilot (`https://github.com/features/copilot`), to help you when trying to solve problems. It takes a bit of practice to ask the right and effective questions/prompts to these tools; we highly recommend that you go through this popular free short course **ChatGPT Prompt Engineering for Developers** offered by `https://learn.deeplearning.ai/` to get started.

If you use any AI tools for any of the problems, you should include screenshots of your prompting questions and their answers in your writeup. The answers provided by such AI tools often contain factual errors and reasoning gaps. **So, if you only submit an AI answer with such bugs for any problem, you will obtain a zero score for that problem**. You obtain the scores only when you explain the bugs and also correct them in your own writing. You can also choose not to use any of these AI tools, in which case we will grade based on the efforts you have made.

Notation We will use small letters (e.g., u) for scalars, small boldface letters (e.g., $\boldsymbol{a}$) for vectors, and capital boldface letters (e.g., $\boldsymbol{A}$) for matrices. $\mathbb{R}$ is the set of real numbers. $\mathbb{R}^n$ is the space of n-dimensional real vectors, and similarly $\mathbb{R}^{m \times n}$ is the space of $m \times n$ real matrices. The dotted equal sign $\doteq$ means defining.

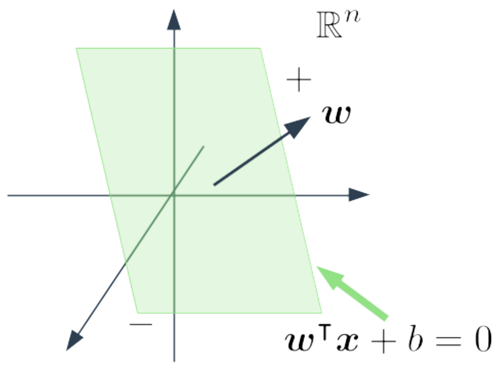
Problem 1 (Neural networks can represent all Boolean functions; $5/15$) The standard perceptron is a single-layer, single-output neural network with the step function as the activation, i.e.,

$$f(\boldsymbol{x}) = \mathrm{step}(\boldsymbol{w}^\intercal \boldsymbol{x} + b),$$

where $\mathrm{step}(z) = 1$ if $z \geq 0$ and 0 otherwise. Geometrically, f is a $\{0, 1\}$-valued function with the hyperplane $\{\boldsymbol{x} : \boldsymbol{w}^\intercal \boldsymbol{x} + b = 0\}$ as the separating boundary between the 0- and the 1-region; see Fig. 1 (left). Consider Boolean functions $\{0, 1\}^n \to \{0, 1\}$. We will work out how arbitrary Boolean functions can be represented by two-layer or deep neural networks.

(a) Consider $n = 1$ first. Show that the `NOT` function can be implemented using a single-input perceptron by setting the weight w and the bias b appropriately; **please write down the set of all possible pairs of** (w, b). $(0.5/15)$

(b) Now consider the case $n = 2$. Show that the two-input `AND`, `OR` functions can be implemented using a two-input perceptron; **please write down the set of all possible such** $(\boldsymbol{w}, b)$ **pairs**. Hint: the geometric view might help. For example, for the `AND` function, we are effectively trying to separate the point $(1, 1)$ from $(1, 0)$, $(0, 1)$ and $(0, 0)$. The hint applies to all subsequent subproblems of **Problem 1**. $(1/15)$



X_1	X_2	X_3	X_4	X_5	Y
0	0	1	1	0	1
0	1	0	1	1	1
0	1	1	0	0	1
1	0	0	0	1	1
1	0	1	1	1	1
1	1	0	0	1	1

Figure 1: (left) Geometric illustration of the perceptron. (right) An example truth table.

(c) Can we encode the `XOR` function (https://en.wikipedia.org/wiki/Exclusive_or) using a two-input perceptron? How if yes? Why if not? $(1/15)$

(d) For general $n \geq 2$, we consider general `AND` functions that take n inputs, where each input is either x_i or $\overline{x_i}$. A typical such function looks like $x_1 \cdot \overline{x_2} \cdot \overline{x_3} \cdot x_{n-1} \cdot x_n$. Show that all general n-input `AND` function can be implemented using an n-input perceptron. Similarly, show that all n-input general `OR` function can be implemented using an n-input perceptron. **Please write down the set of all possible such $(\boldsymbol{w}, b)$ pairs for both cases.** $(1/15)$

(e) Any Boolean function is fully specified by a list of all variable combinations that are evaluated to 1. Such a list is often tabulated, and the resulting table is called the truth table. For example, in the truth table of Fig. 1 (right), the Boolean function represented reads (i.e., "1" position we put the variable itself, and "0" position we put the vaiable negated, and each summand below corresponds to a row of the table)

$$\overline{x_1}\,\overline{x_2}x_3x_4\overline{x_5} + \overline{x_1}x_2\overline{x_3}x_4x_5 + \overline{x_1}x_2x_3\overline{x_4}\,\overline{x_5} + x_1\overline{x_2}\,\overline{x_3}\,\overline{x_4}\,x_5 + x_1\overline{x_2}x_3x_4x_5 + x_1x_2\overline{x_3}\,\overline{x_4}x_5,$$

where product $\cdot$ (which is omitted) means `AND` and summation $+$ means `OR`. In Boolean logic, this is called the disjunctive normal form (https://en.wikipedia.org/wiki/Disjunctive_normal_form). All Boolean functions can be represented in the disjunctive normal form.

Based on these, show that all n-input Boolean functions can be represented by a two-layer neural network. In the worst case, how many hidden nodes are needed? $(1.5/15)$

Problem 2 (Universal approximation property of ABS networks; $2/15$) Recall how we argued that two-layer neural networks with the sigmoid activation function (i.e., $\sigma(z) = \frac{1}{1+e^{-z}}$) can approximate any functions that map $\mathbb{R}$ to $\mathbb{R}$. We constructed the step function and then the bump function, and finally we sum up the bumps to form the approximation. We also briefly discussed in class how to use two ReLU functions ($h(z) = \max(0, z)$) to approximate a step function.

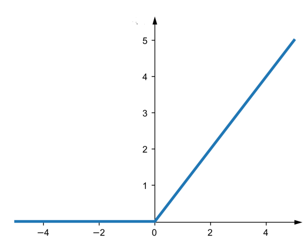


Figure 2: ReLU function

(a) Obviously, we can directly choose σ as the step function or even the bump function. This not only makes the approximation much more accurate, but also simplifies the neural network we need. Is this good for computation? And why? $(1/15)$

(b) Sketch the main steps of using ReLU networks for approximating an arbitrary function that maps from $\mathbb{R}$ to $\mathbb{R}$, i.e., ReLU $\to$ step function $\to$ bump function $\to$ approximating the original function. $(1/15)$

Problem 3 (Jacobian, gradient and Hessian from expansions, or chain rule; optimality conditions; $4/15$) To derive Jacobian, gradient, and Hessian below, you can choose applying the chain rule, the Taylor expansion trick, or any mixture of them. But you may find that the Taylor trick mixed together with basic gradient rules (sum, product, quotient, and sometime chain rule) is much easier and quicker than applying the chain rule alone. **When you deriving gradients and Hessians, feel free to use AI or online tools to validate your calculation**.

(a) Derive the gradient and Hessian of the quadratic function $h(\boldsymbol{x}) = \boldsymbol{x}^\intercal \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}^\intercal \boldsymbol{x}$ and remember to include the detailed steps. Here, $\boldsymbol{A}$ is square but **not necessarily symmetric**. $(1/15)$

(b) We talk about the algebraic and geometric definitions of convex functions in class. But it is often a tedious process to tell convex functions using the definition. To simplify the job, we rely on additional properties and characterizations. A twice-differentiable function $f(\boldsymbol{x})$ is convex if and only if its Hessian is positive semidefinite, i.e., $\nabla^2 f \succeq \mathbf{0}$ for all $\boldsymbol{x}$. Apply this to $h(\boldsymbol{x})$ in (a) and state the condition for $h(\boldsymbol{x})$ being convex. Do we have a unique *minimizer* or not for $h(\boldsymbol{x})$, and why? $(1/15)$

(c) We talked of the first- and second-order optimality conditions for $\min_{\boldsymbol{x}} \; f(\boldsymbol{x})$ for a generic differentiable function f. What are the first- and second-order optimality conditions for $\max_{\boldsymbol{x}} \; f(\boldsymbol{x})$, i.e., conditions for locating local maximizers? And why? $(1/15)$

(d) In this course, we will not think much about constrained optimization. But let's play with a simple yet important one here. Consider constrained optimization problems of the form

$$\min_{\boldsymbol{x}} \; f(\boldsymbol{x}) \quad \text{s.t.} \; g(\boldsymbol{x}) = \mathbf{0},$$

where $g(\boldsymbol{x})$ is a vector-to-vector function and conveniently collects together all the single scalar constraints. Introduce a Lagrangian multipler vector $\boldsymbol{\lambda}$ and form the Lagrangian function

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) + \langle \boldsymbol{\lambda}, g(\boldsymbol{x}) \rangle .$$

The first-order optimality condition says that there exists a $\boldsymbol{\lambda}$ so that $\nabla_{\boldsymbol{x}} \mathcal{L} = \mathbf{0}$ ($\nabla_{\boldsymbol{\lambda}} \mathcal{L} = g(\boldsymbol{x}) = \mathbf{0}$ for obvious reasons).

Now consider a constrained optimization problem

$$\max_{\boldsymbol{x}} \boldsymbol{x}^\intercal \boldsymbol{A}\boldsymbol{x} \quad \text{s.t.} \; \|\boldsymbol{x}\|_2^2 = 1,$$

where $\boldsymbol{A}$ is a square but **not necessarily symmetric** matrix. Write down the first-order optimality condition and what can you say about the solution $(1/15$; Hint: think of eigenvalues and eigenvectors)?

For those familiar with the second-order condition (https://en.wikipedia.org/wiki/Karush%E2%80%93Kuhn%E2%80%93Tucker_conditions#Necessary_conditions), you're encouraged to dig in and find the exact solution to the problem, but this is optional. This problem is closely connected to the famous Rayleigh quotient (https://en.wikipedia.org/wiki/Rayleigh_quotient).

Problem 4 (Deep learning problems are typically non-convex; 4/15) Convex analysis and optimization has dominated classical machine learning (e.g., the famous support vector machines, and lasso for variable selection), as with convexity most of the time we can focus on the modeling part and worry little about the possibility of finding a bad local solution for the resulting optimization problem. In deep learning, the optimization problems involved are almost always non-convex. Let's try to convince ourselves using two different arguments. **When you deriving gradients and Hessians, feel free to use AI or online tools to validate your calculation**.

(a) Consider a simplistic two-layer, single-hidden-node network with identity activation, i.e., $f(x) = w_2 w_1 x$. For a training set $\{(x_i, y_i)\}_{i=1,\dots,N}$, let's take the mean squared loss and set up a supervised learning objective

$$L(w_1, w_2) = \frac{1}{N} \sum_{i=1}^{N} (y_i - f(x_i))^2.$$

Show that $L(w_1, w_2)$ is non-convex by checking its Hessian. (Hint: recall how to check convexity from Problem 3(b) above; also, when a 2×2 matrix is positive semidefinite, both its trace and determinant are nonnegative. 1/15)

(b) An alternative way to see L is non-convex is to prove by contradiction. Let's assume that L is indeed convex. In class, we recognized that for any (w_1, w_2), $L(w_1, w_2) = L(-w_1, -w_2)$. If a particular pair (w_1^*, w_2^*) is a global minimizer of L, what can we say about $(0, 0)$? Then conclude that L being convex will lead to trivial learning. (Hint: $(0, 0)$ is a convex combination of (w_1^*, w_2^*) and $(-w_1^*, -w_2^*)$, i.e., lying on the line segment connecting (w_1^*, w_2^*) and $(-w_1^*, -w_2^*)$.) (1/15)

(c) Is L convex if $f(x) = w_k w_{k-1} \dots w_2 w_1 x$, i.e., when the network is k-layer with $k \geq 3$? What happens when we replace the mean squared loss by the mean absolute error, i.e.,

$$L(w_1, w_2, \dots, w_{k-1}, w_k) = \frac{1}{N} \sum_{i=1}^{N} |y_i - f(x_i)|?$$

(1/15)

(d) Now let's move to realistic multi-layer perceptrons with multi-neuron hidden layers. To fix the notation, assume that the input dimension is n_0, and we have L hidden layers with $n_1, \dots, n_L$ hidden neurons, respectively, and n_f outputs, that is,

$$f(\boldsymbol{x}) = \boldsymbol{W}_{L+1} \circ \sigma \circ \boldsymbol{W}_L \circ \sigma \cdots \circ \boldsymbol{W}_1 \circ \sigma \circ \boldsymbol{W}_0 \boldsymbol{x},$$

where $\circ$ means the composition of the function (https://en.wikipedia.org/wiki/Function_composition; we use this neat notation to avoid nesting many parentheses), and activation σ is always applied elementwise. Suppose that we take the mean squared loss, i.e.,

$$L(\boldsymbol{W}_1, \dots, \boldsymbol{W}_{L+1}) = \frac{1}{N} \sum_{i=1}^{N} \|y_i - f(\boldsymbol{x}_i)\|_2^2,$$

argue that L is in general nonconvex to achieve nontrivial learning. (Hint: Assume σ is the identity for simplicity. We have that $\boldsymbol{W}_1 \boldsymbol{W}_0 \boldsymbol{x} = (\boldsymbol{W}_1 \boldsymbol{\Pi})(\boldsymbol{\Pi}^\intercal \boldsymbol{W}_0) \boldsymbol{x}$ for any permutation matrix $\boldsymbol{\Pi} \in \mathbb{R}^{n_1 \times n_1}$. What is the average of all permutation matrices?) (1/15)