Homework 1 - Version 1.3

Deadline: Monday, Jan.27, at 11:59pm.

Submission: You must submit your solutions as a PDF file through MarkUs[1]. You can produce the file however you like (e.g. LaTeX, Microsoft Word, scanner), as long as it is readable.

See the syllabus on the course website[2] for detailed policies. You may ask questions about the assignment on Piazza[3]. *Note that 10% of the homework mark (worth 1 pt) may be removed for a lack of neatness.*

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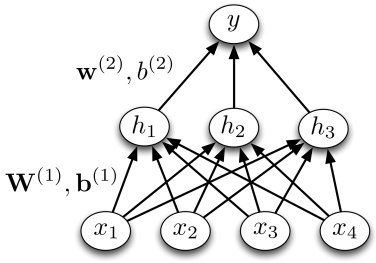
1 Hard-Coding Networks

The reading on multilayer perceptrons located at `https://csc413-2020.github.io/assets/readings/L02a.pdf` may be useful for this question.

1.1 Verify Sort [1pt]

In this problem, you need to find a set of weights and biases for a multilayer perceptron which determines if a list of length 4 is in sorted order. More specifically, you receive four inputs $x_1, \ldots, x_4$, where $x_i \in \mathbb{R}$, and the network must output 1 if $x_1 \leq x_2 \leq x_3 \leq x_4$, and 0 otherwise. You will use the following architecture:



All of the hidden units and the output unit use a hard threshold activation function:

$$\phi(z) = \mathbb{I}(z \geq 0) = \begin{cases} 1 & \text{if } z \geq 0 \\ 0 & \text{if } z < 0 \end{cases}$$

Please give a set of weights and biases for the network which correctly implements this function (including cases where some of the inputs are equal). Your answer should include:

- A 3×4 weight matrix $\mathbf{W}^{(1)}$ for the hidden layer
- A 3-dimensional vector of biases $\mathbf{b}^{(1)}$ for the hidden layer
- A 3-dimensional weight vector $\mathbf{w}^{(2)}$ for the output layer

[1] `https://markus.teach.cs.toronto.edu/csc413-2020-01`
[2] `https://csc413-2020.github.io/assets/misc/syllabus.pdf`
[3] `https://piazza.com/class/k58ktbdnt0h1wx?cid=1`

- A scalar bias $b^{(2)}$ for the output layer

You do not need to show your work.

1.2 Perform Sort [1pt]

Describe how to implement a sorting function $\hat{f} : \mathbb{R}^4 \to \mathbb{R}^4$ where $\hat{f}(x_1, x_2, x_3, x_4) = (\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{x}_4)$ where $(\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{x}_4)$ is (x_1, x_2, x_3, x_4) in sorted order. In other words, $\hat{x}_1 \leq \hat{x}_2 \leq \hat{x}_3 \leq \hat{x}_4$, and each $\hat{x}_i$ is a distinct x_j. Implement $\hat{f}$ using a feedforward or recurrent neural network with elementwise activations. Do not explicitly give the weight matrices or biases for the entire function. Instead, describe how to compose smaller, modular networks.

Hint: There are multiple solutions. You could brute-force the answer by using copies of *Verify Sort* on permutations of the input, or you could implement a more scalable sorting algorithm where each hidden layer i is the algorithms state at step i.

1.3 Universal Approximation Theorem [1pt]

We are going to build an intuition behind a simple Universal Approximation theorem, which shows that some class of function approximators can approximate a particular class of functions arbitrarily well.

In the reading we saw that neural networks can be universal approximators on binary functions, because with fixed input dimension there is a finite number of potential inputs and a network can memorize a different output for each input. But, what can we do if we have an uncountably infinite set of potential inputs like $\mathbb{R}$? Here, our class of function approximators will be neural networks with a single hidden layer with a threshold function as the activation, and fixed choice of some concave f.

Suppose $f : I \to \mathbb{R}$, where $I = [a, b] \subset \mathbb{R}$ and $a \leq b$ is a closed interval. Also, let $\hat{f}_\tau : I \to \mathbb{R}$ be some function approximator from our network where τ is a description of our networks architecture and weights. Here, τ is a tuple of $(n, \mathbf{W}_0 \in \mathbb{R}^{n\times 1}, \mathbf{b}_0 \in \mathbb{R}^n, \mathbf{W}^1 \in \mathbb{R}^{1\times n}, \mathbf{b}^1 \in \mathbb{R})$, where n is the hidden layer size, $\mathbf{W}_0$ & $\mathbf{b}_0$ describe the input to hidden parameters, and $\mathbf{W}_1$ & $\mathbf{b}_1$ describe the hidden to output parameters. This is visualized in Figure 1.

The difference between our functions is defined as $\|f - \hat{f}_\tau\| = \int_I |f(x) - \hat{f}_\tau(x)|\, dx$. Our activation is an indicator function $a(y) = \mathbb{I}(y \geq 0)$, where $\mathbb{I}(s)$ is 1 when the boolean value s is true and 0 otherwise. The output is computed as $\hat{f}_\tau(x) = \mathbf{W}_1 a(\mathbf{W}_0 x + \mathbf{b}_0) + \mathbf{b}_1$.

We want to show that there exist a series of neural networks $\{\tau_i\}_{i=1}^N$ such that:

$$\forall \epsilon > 0, \exists M : \forall m > M, \|f - \hat{f}_{\tau_m}\| < \epsilon \tag{1}$$

1.3.1

Consider a bump function $g(h, a, b, x) = h \cdot \mathbb{I}(a \leq x \leq b)$ visualized in Figure 2. Given some (h, a, b) show $\exists \tau : \hat{f}_\tau(x) = g(h, a, b, x)$. You answer should be a specific choice of n, $\mathbf{W}_0$, $\mathbf{b}_0$, $\mathbf{W}_1$, and $\mathbf{b}_1$, which will be functions of the selected (h, a, b).

1.3.2

Given $f(x) = -x^2 + 1$ where $I = [-1, 1]$ and some initial function $\hat{f}_0(x) = 0$ which is identically 0, construct a new function $\hat{f}_1(x) = \hat{f}_0(x) + g(h_1, a_1, b_1, x)$ such that $\|f - \hat{f}_1\| < \|f - \hat{f}_0\|$, with the g defined in 1.3.1. Note that h_1, a_1, and b_1 are going to depend on our choice of f, $\hat{f}_0$ and I. Plot f & $\hat{f}_1$, write down h_1, a_1, and b_1, and justify why $\|f - \hat{f}_1\| < \|f - \hat{f}_0\|$.

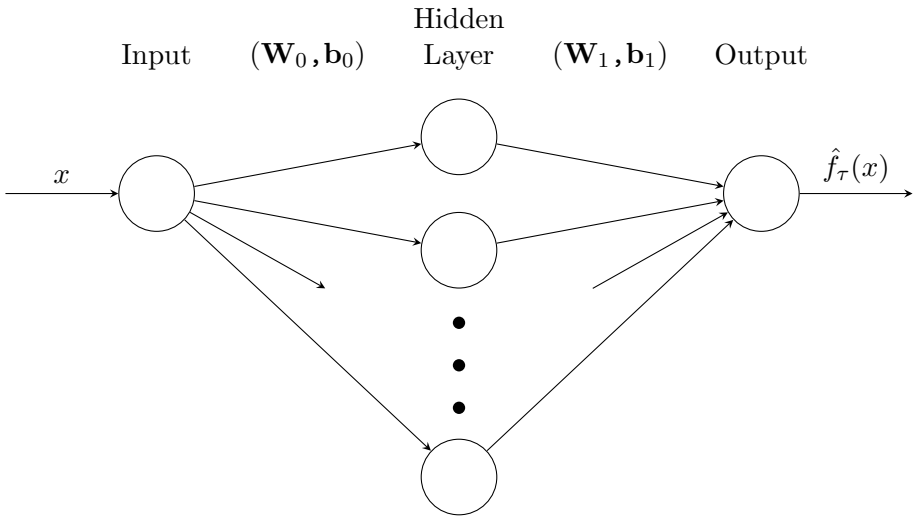


Figure 1: A neural network that has an input $x \in \mathbb{R}$ with a single hidden layer that has n units, and an output $\hat{f}_\tau(x) \in \mathbb{R}$. The network description is $\tau = (n, \mathbf{W}_0 \in \mathbb{R}^{n \times 1}, \mathbf{b}_0 \in \mathbb{R}^n, \mathbf{W}^1 \in \mathbb{R}^{1 \times n}, \mathbf{b}^1 \in \mathbb{R})$.

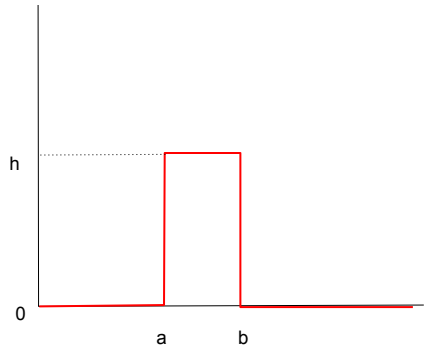


Figure 2: A bump function $g(h, a, b, x)$ is shown in red.

1.3.3

Describe a procedure which starts with $\hat{f}_0(x) = 0$ and a fixed N then construct a series $\{\hat{f}_i\}_{i=0}^N$ where $\hat{f}_{i+1}(x) = \hat{f}_i(x) + g(h_{i+1}, a_{i+1}, b_{i+1}, x)$ which satisfies $\|f - \hat{f}_{i+1}\| < \|f - \hat{f}_i\|$. Use the definition of g from 1.3.1 and the choice of f from 1.3.2. Plot $f, \hat{f}_1, \hat{f}_2$, & $\hat{f}_3$, write down how to generate $h_{i+1}, a_{i+1}, b_{i+1}$, and justify why $\|f - \hat{f}_{i+1}\| < \|f - \hat{f}_i\|$.

1.3.4

Not for marks - do not submit. Describe how to recover τ_i from your $\hat{f}_i$. Generalize your series to work for $\{\hat{f}_i\}_{i=0}^\infty$, and show that $\lim_{m \to \infty} \|f - \hat{f}_{\tau_m}\| = c$. We need $c = 0$ for arbitrarily good approximations - does your solution for $\{\hat{f}_i\}_{i=0}^\infty$ force $c = 0$? Can you generalize your procedure to work for any concave f? What about an f which isn't unimodal, like a piecewise continuous f?

2 Backprop

The reading on backpropagation located at `https://csc413-2020.github.io/assets/readings/L02b.pdf` may be useful for this question.

2.1 Computational Graph [1pt]

Consider a neural network with N input units, N output units, and K hidden units. The activations are computed as follows:

$$\begin{aligned}\mathbf{z} &= \mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)} \\ \mathbf{h} &= \text{ReLU}(\mathbf{z}) \\ \mathbf{y} &= \mathbf{x} + \mathbf{W}^{(2)}\mathbf{h} + \mathbf{b}^{(2)}, \\ \mathbf{y}' &= \text{softmax}(\mathbf{y}),\end{aligned}$$

where $\text{ReLU}(\mathbf{z}) = \max(\mathbf{z}, 0)$ denotes the ReLU activation function, applied elementwise, and $\text{softmax}(\mathbf{y}) = \frac{\exp(\mathbf{y})}{\sum_{i=1}^{M}\exp(\mathbf{y}_i)}$.

The cost will involve both $\mathbf{h}$ and $\mathbf{y}'$:

$$\begin{aligned}\mathcal{J} &= \mathcal{R} - \mathcal{S} \\ \mathcal{R} &= \mathbf{r}^\top \mathbf{h} \\ \mathcal{S} &= \sum_{k=1}^{N} \mathbb{I}(t = k)\mathbf{y}'_k\end{aligned}$$

for given vectors $\mathbf{r}$ and class label t with input x.

2.1.1

Draw the computation graph relating $\mathbf{x}$, t, $\mathbf{z}$, $\mathbf{h}$, $\mathbf{y}$, $\mathbf{y}'$, $\mathbf{r}$, $\mathcal{R}$, $\mathcal{S}$, and $\mathcal{J}$.

2.1.2

Derive the backprop equations for computing $\bar{\mathbf{x}} = \frac{\partial \mathcal{J}}{\partial \mathbf{x}}$. You may use softmax$'$ to denote the derivative of the softmax function (so you don't need to write it out explicitly).

2.2 Vector-Jacobian Products (VJPs) [1pt]

Consider the function $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n$ where $\mathbf{f}(\mathbf{x}) = \mathbf{v}\mathbf{v}^T\mathbf{x}$, and $\mathbf{v} \in \mathbb{R}^{n\times 1}$ and $\mathbf{x} \in \mathbb{R}^{n\times 1}$. Here, we will explore the relative costs of evaluating Jacobians and vector-Jacobian products. We denote the Jacobian of $\mathbf{f}$ with respect to $\mathbf{x}$ as J.

2.2.1

Compute $J \in \mathbb{R}^{n\times n}$ for $n = 3$ and $\mathbf{v}^T = [1, 2, 3]$ - i.e, write down the values in $J = \begin{pmatrix} j_{1,1} & j_{1,2} & \cdots & j_{1,n} \\ j_{2,1} & j_{2,2} & \cdots & j_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ j_{n,1} & j_{n,2} & \cdots & j_{n,n} \end{pmatrix}$.

2.2.2

What is the time and memory cost of evaluating the Jacobian of function $\mathbf{f}$ in terms of n?

2.2.3

Describe how to evaluate $J^T\mathbf{y}$ with a time and memory cost that is linear in n. Then, compute $\mathbf{z} = J^T\mathbf{y}$ where $\mathbf{v}^T = [1, 2, 3]$ and $\mathbf{y}^T = [1, 1, 1]$ - i.e., write down the entries in $\mathbf{z}^T = [z_1, \ldots, z_n]$.

3 Linear Regression

The reading on linear regression located at `https://csc413-2020.github.io/assets/readings/L01a.pdf` may be useful for this question.

Given n pairs of input data with d features and scalar label $(\mathbf{x}_i, t_i) \in \mathbb{R}^d \times \mathbb{R}$, we wish to find a linear model $f(\mathbf{x}) = \hat{\mathbf{w}}^\top \mathbf{x}$ with $\hat{\mathbf{w}} \in \mathbb{R}^d$ that minimizes the squared error of prediction on the training samples defined below. This is known as an empirical risk minimizer. For concise notation, denote the data matrix $X \in \mathbb{R}^{n\times d}$ and the corresponding label vector $\mathbf{t} \in \mathbb{R}^n$. The training objective is to minimize the following loss:

$$\min_{\hat{\mathbf{w}}} \frac{1}{n}\sum_{i=1}^{n}(\hat{\mathbf{w}}^\top \mathbf{x}_i - t_i)^2 = \min_{\hat{\mathbf{w}}} \frac{1}{n}\|X\hat{\mathbf{w}} - \mathbf{t}\|_2^2.$$

We assume X is full rank: $X^\top X$ is invertible when $n > d$, and $XX^\top$ is invertible otherwise. Note that when $d > n$, the problem is *underdetermined*, i.e. there are less training samples than parameters to be learned. This is analogous to learning an *overparameterized* model, which is common when training of deep neural networks.

3.1 Deriving the Gradient [1pt]

Write down the gradient of the loss w.r.t. the learned parameter vector $\hat{\mathbf{w}}$.

3.2 Underparameterized Model [1pt]

3.2.1

First consider the underparameterized $d < n$ case. Write down the solution obtained by gradient descent assuming training converges. Show your work. Is the solution unique?

Hint: Set the gradient derived in part 3.1 to 0 and manipulate the equality.

3.2.2

Assume that ground truth labels are generated by a linear target: $t_i = \mathbf{w}^{*\top}\mathbf{x}_i$. Show that the solution in part 3.2.1 achieves perfect generalization when $d < n$, i.e. $\forall \mathbf{x} \in \mathbb{R}^d$, $(\mathbf{w}^{*\top}\mathbf{x} - \hat{\mathbf{w}}^\top \mathbf{x})^2 = 0$.

3.3 Overparameterized Model: 2D Example [1pt]

3.3.1

Now consider the overparameterized $d > n$ case. We first illustrate that there exist multiple empirical risk minimizers. For simplicity we let $n = 1$ and $d = 2$. Choose $\mathbf{x}_1 = [2, 1]$ and $t_1 = 2$, i.e. the one data point and all possible $\hat{\mathbf{w}}$ lie on a 2D plane. Show that there exists infinitely many $\hat{\mathbf{w}}$ satisfying $\hat{\mathbf{w}}^\top \mathbf{x}_1 = y_1$ on a real line. Write down the equation of the line.

3.3.2

We know that multiple empirical risk minimizers exist in overparameterized linear regression and there is only one true solution. Thus, it seems unlikely that gradient descent will generalize if it returns an arbitrary minimizer. However, we will show that gradient descent tends to find certain solution with good properties. This phenomenon, know as *implicit regularization*, helps explain the success in using gradient-based methods to train overparameterized models, like deep neural networks.

First consider the 2-dimensional example in the previous part: starting from zero initialization i.e. $\hat{\mathbf{w}}(0) = 0$, what is the direction of the gradient? You should write down a unit-norm vector. Does the direction change along the trajectory? Based on this geometric intuition, which solution - along the line of solutions - does gradient descent find? Provide a pictorial sketch or a short description of your reasoning.

3.3.3

Give a geometric argument that among all the solutions on the line, the gradient descent solution from the previous part has the smallest Euclidean norm.

Hint: Use the Pythagorean Theorem.

3.4 Overparameterized Model: General Case [1pt]

3.4.1

Now we generalize the previous geometric insight developed to general $d > n$. Show that gradient descent from zero initialization i.e. $\hat{\mathbf{w}}(0) = 0$ finds a unique minimizer if it converges. Write down the solution and show your work.

Hint: Recall the result on the direction of the gradient in the previous 2D example, which suggests that the gradient vector is always spanned by the rows of X. What does this tell you about the gradient descent solution?

3.4.2

Given the gradient descent solution from the previous part $\hat{\mathbf{w}}$ and another zero-loss solution $\hat{\mathbf{w}}_1$, evaluate $(\hat{\mathbf{w}} - \hat{\mathbf{w}}_1)^\top \hat{\mathbf{w}}$. Use this quantity to show that among all the empirical risk minimizers for $d > n$, the gradient descent solution has the smallest Euclidean norm.

3.5 Benefit of Overparameterization

3.5.1

Visualize and compare underparameterized with overparameterized polynomial regression: `https://colab.research.google.com/drive/1NCSHp-gkh1kGhcySImbJo6AqeKoz-HcR`. Include your code snippets for the `fit_poly` function in the write-up. Does overparameterization (higher degree polynomial) always lead to overfitting, i.e. larger test error?

3.5.2

Not for marks. What are some potential benefits of the minimum-norm solution?

Hint: readings on SVM might be helpful: `https://www.cs.toronto.edu/~urtasun/courses/CSC411_Fall16/15_svm.pdf`.