CSC413: Homework 1

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1 Hard-Coding Networks

1.1 Verify Sort

Soln. The first layer performs pairwise comparison to construct indicators $\mathbb{1}\{x_1 \leq x_2\}$, $\mathbb{1}\{x_2 \leq x_3\}$, and $\mathbb{1}\{x_3 \leq x_4\}$. The second layer performs an `all()` operation on indicators from the previous layer.

$$\mathbf{W}^{(1)} = \begin{pmatrix} -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix} \tag{1.1}$$

$$\mathbf{b}^{(1)} = \begin{pmatrix} 0 & 0 & 0 \end{pmatrix} \tag{1.2}$$

So that

$$\varphi(\mathbf{h}) = \varphi(\mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)}) = \varphi\begin{pmatrix} x_2 - x_1 \\ x_3 - x_2 \\ x_4 - x_3 \end{pmatrix} = \begin{pmatrix} \mathbb{1}\{x_2 \geq x_1\} \\ \mathbb{1}\{x_3 \geq x_2\} \\ \mathbb{1}\{x_4 \geq x_3\} \end{pmatrix} \tag{1.3}$$

$$\mathbf{w}^{(2)} = \begin{pmatrix} 1 & 1 & 1 \end{pmatrix} \tag{1.4}$$

$$b^{(2)} = -2.5 \tag{1.5}$$

Such that $y = 1$ if and only if all components of $\mathbf{h}$ are ones, i.e., the list is sorted. ■

1.2 Perform Sort

Proof. For this section, I am implementing a feedforward neural network performing bubble sort.
Note that given $\mathbf{x} = (x_1, x_2, x_3, x_4)$, the **swapping** operation can be conducted by multiplying $\mathbf{x}$ by a matrix.

For instance, the following $\mathbf{W}^{(12)}$ swaps the first and second elements.

$$\underbrace{\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}}_{\mathbf{W}^{(12)}} (x_1, x_2, x_3, x_4)^T = (x_2, x_1, x_3, x_4)^T \tag{1.6}$$

Let $\mathbf{I}_4$ denote the identity matrix. Define the following neural network:

$$\mathbf{h}_1 := \mathbb{1}\{x_1 \leq x_2\} \mathbf{I}_4 \mathbf{x} + \mathbb{1}\{x_1 > x_2\} \mathbf{W}^{(12)} \mathbf{x} \tag{1.7}$$
$$\mathbf{h}_2 = \mathbb{1}\{x_2 \leq x_3\} \mathbf{I}_4 \mathbf{h}_1 + \mathbb{1}\{x_2 > x_3\} \mathbf{W}^{(23)} \mathbf{h}_1 \tag{1.8}$$
$$\mathbf{h}_3 = \mathbb{1}\{x_3 \leq x_4\} \mathbf{I}_4 \mathbf{h}_2 + \mathbb{1}\{x_3 > x_4\} \mathbf{W}^{(34)} \mathbf{h}_2 \tag{1.9}$$
$$\mathbf{h}_4 = \mathbb{1}\{x_1 \leq x_2\} \mathbf{I}_4 \mathbf{h}_3 + \mathbb{1}\{x_1 > x_2\} \mathbf{W}^{(12)} \mathbf{h}_3 \tag{1.10}$$
$$\mathbf{h}_5 = \mathbb{1}\{x_2 \leq x_3\} \mathbf{I}_4 \mathbf{h}_4 + \mathbb{1}\{x_2 > x_3\} \mathbf{W}^{(23)} \mathbf{h}_4 \tag{1.11}$$
$$\mathbf{y}(\mathbf{x}) = \mathbb{1}\{x_1 \leq x_2\} \mathbf{I}_4 \mathbf{h}_5 + \mathbb{1}\{x_1 > x_2\} \mathbf{W}^{(12)} \mathbf{h}_5 \tag{1.12}$$

Note: x_is in different equations have potentially different values. For instance, the x_2 in equations (1.7) and (1.8) are potentially different, in 1.7, it represents the second component of $\mathbf{x}$ and in 1.8 it represents the second component of $\mathbf{h}_1$.
The above neural network can also be implemented using a recurrent structure, in which hidden states record the number of pairwise comparisons made. ■

1.3 Universal Approximation Theorem

1.3.1

Soln. To avoid over-using of notations, let $\varphi(y) := \mathbb{1}\{y \geq 0\}$ denote the activation function.

$$n = 2 \tag{1.13}$$
$$\mathbf{W}_0 = (1, -1) \tag{1.14}$$
$$\mathbf{b}_0 = (-a, b) \tag{1.15}$$
$$\mathbf{W}_1 = (h, h) \tag{1.16}$$
$$\mathbf{b}_1 = -h \tag{1.17}$$

Justification:

$$\varphi(\mathbf{h}) = \varphi((x - a, b - x)) \tag{1.18}$$
$$= (\mathbb{1}\{x - a \geq 0\}, \mathbb{1}\{b - x \geq 0\}) \tag{1.19}$$
$$= (\mathbb{1}\{x \geq a\}, \mathbb{1}\{x \leq b\}) \tag{1.20}$$
$$\mathbf{W}_1 \varphi(\mathbf{h}) + \mathbf{b}_1 = \mathbb{1}\{x \geq a\} h + \mathbb{1}\{x \leq b\} h - h \tag{1.21}$$
$$= \mathbb{1}\{a \leq x \leq b\} h \tag{1.22}$$

■

1.3.2

Soln. Let $\delta \in (0,1)$ denote the ratio parameter, a higher value of δ results in a finer approximation is. In this example, take $\delta = \frac{9}{10}$.
Without loss of generality, assume the region I on which function f is defined on to be symmetric across zero.
Let $I = [-1,1]$, given f is symmetric, $f(-\delta) = f(\delta)$.
Define:

$$\hat{f}_1(x) = \hat{f}_0(x) + g(f(\delta), -\delta, \delta, x) \tag{1.23}$$

Note that

$$||f - \hat{f}_1|| = \int_{-1}^{1} \left| f(x) - \hat{f}_1(x) \right| \, dx \tag{1.24}$$

$$= \int_{-1}^{-\delta} |f(x)| \, dx + \int_{-\delta}^{\delta} \left| f(x) - \hat{f}_1(x) \right| \, dx + \int_{\delta}^{1} |f(x)| \, dx \tag{1.25}$$

Given that $\forall x \in (-\delta, \delta), \; f(x) > f(-\delta) = f(\delta) > 0$, it follows

$$\int_{-\delta}^{\delta} \left| f(x) - \hat{f}_1(x) \right| \, dx = \int_{-\delta}^{\delta} f(x) - \hat{f}_1(x) \, dx \tag{1.26}$$

$$= \int_{-\delta}^{\delta} f(x) \, dx - \int_{-\delta}^{\delta} \hat{f}_1(x) \, dx \tag{1.27}$$

Also, $\int_{-\delta}^{\delta} \hat{f}_1(x) \, dx > 0$ provided $\delta \neq 0$. Therefore,

$$\int_{-\delta}^{\delta} \left| f(x) - \hat{f}_1(x) \right| \, dx < \int_{-\delta}^{\delta} f(x) \, dx \tag{1.28}$$

$$= \int_{-\delta}^{\delta} |f(x)| \, dx \tag{1.29}$$

Therefore,

$$||f - \hat{f}_1|| = \int_{-1}^{-\delta} |f(x)| \, dx + \int_{-\delta}^{\delta} \left| f(x) - \hat{f}_1(x) \right| \, dx + \int_{\delta}^{1} |f(x)| \, dx \tag{1.30}$$

$$< \int_{-1}^{-\delta} |f(x)| \, dx + \int_{-\delta}^{\delta} |f(x)| \, dx + \int_{\delta}^{1} |f(x)| \, dx \tag{1.31}$$

$$= \int_{-1}^{1} |f(x) - 0| \, dx \tag{1.32}$$

$$= \int_{-1}^{1} \left| f(x) - \hat{f}_0(x) \right| \, dx \tag{1.33}$$

$$= ||f(x) - \hat{f}_0(x)|| \tag{1.34}$$

Therefore,

$$||f(x) - \hat{f}_1(x)|| < ||f(x) - \hat{f}_0(x)|| \tag{1.35}$$

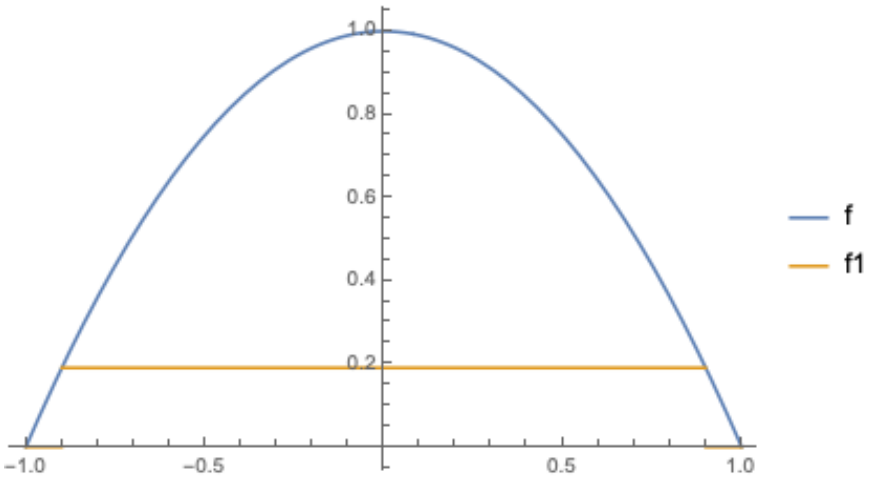

Figure 1.1: Approximated Result

■

1.3.3

Soln. **Algorithm:**

(i) Divide $I = [-1, 1]$ into $N + 2$ sub-intervals with equal length, such that

$$I_i := \left[-1 + \frac{i}{N+2}, -1 + \frac{i+1}{N+2}\right] \quad \forall\, i \in \{1, 2, \cdots, N\} \tag{1.36}$$

Note that the first and last sub-intervals are not used to construct g_i.

(ii) For each i, define

$$h_i := \min_{x \in I_i} f(x) \tag{1.37}$$

$$a_i := -1 + \frac{i}{N+2} \tag{1.38}$$

$$b_i := -1 + \frac{i+1}{N+2} \tag{1.39}$$

Because $f(x) \geq 0\ \forall x \in I$.
By the definition of $g_i(x)$, it can be shown that[1]

$$f(x) \geq f_i(x)\ \forall i \in \{1, 2, \cdots, N\}\ \forall x \in \bigcup_{i=1}^{N} (a_i, b_i) \tag{1.40}$$

Further,

$$f(x) = f_i(x) \quad \forall i \in \{1, 2, \cdots, N\}\ \forall x \in \left[-1, -1 + \frac{1}{N+2}\right) \bigcup \left(1 - \frac{1}{N+2}, 1\right] \tag{1.41}$$

[1] I am excluding those boundary points between consecutive sub-intervals, because at those points, the value of f_i spikes due to duplicate counts of indicator functions. However, while doing integral, this does not matter as the set of boundary points has measure zero.

Define

$$\mathcal{K} := \left[-1, -1 + \frac{1}{N+2}\right) \bigcup \left(1 - \frac{1}{N+2}, 1\right] \bigcup \left(\bigcup_{i=1}^{N} (a_i, b_i)\right) \tag{1.42}$$

Note that the set $I \backslash \mathcal{K}$ consists of all boundary points between consecutive sub-intervals. There are only finitely many such points, therefore $I \backslash \mathcal{K}$ has measure zero, and

$$\int_I \left| f(x) - \hat{f}_i(x) \right| \, dx = \int_{\mathcal{K}} \left| f(x) - \hat{f}_i(x) \right| \, dx \tag{1.43}$$

And I've shown that for every i and every $x \in \mathcal{K}$, $f(x) \geq f_i(x)$. Consequently,

$$\int_I \left| f(x) - \hat{f}_i(x) \right| \, dx = \int_{\mathcal{K}} \left| f(x) - \hat{f}_i(x) \right| \, dx \text{ (removing measure zero set.)} \tag{1.44}$$

$$= \int_{\mathcal{K}} f(x) - \hat{f}_i(x) \, dx \tag{1.45}$$

$$= \int_I f(x) - \hat{f}_i(x) \, dx \text{ (adding back the measure zero set.)} \quad (\dagger) \tag{1.46}$$

Define $\hat{f}_0(x) = 0$ and let $i \in \{1, 2, \cdots, N\}$,

$$||f - \hat{f}_{i+1}|| = \int_{-1}^{1} \left| f(x) - \hat{f}_{i+1}(x) \right| \, dx \tag{1.47}$$

$$= \int_{-1}^{1} f(x) - \hat{f}_{i+1}(x) \, dx \text{ by } (\dagger) \tag{1.48}$$

$$= \int_{-1}^{-1 \frac{i+1}{N}} f(x) - \hat{f}_{i+1}(x) \, dx + \int_{-1+\frac{i+1}{N}}^{-1+\frac{i+2}{N}} f(x) - \hat{f}_{i+1}(x) \, dx + \int_{-1+\frac{i+2}{N}}^{1} f(x) - \hat{f}_{i+1}(x) \, dx \tag{1.49}$$

Further, by construction, $\hat{f}_{i+1}(x) = \hat{f}_i(x) \; \forall x \notin [a_{i+1}, b_{i+1}]$. Therefore,

$$||f - \hat{f}_{i+1}|| = \int_{-1}^{a_{i+1}} f(x) - \hat{f}_i(x) \, dx + \int_{a_{i+1}}^{b_{i+1}} f(x) - \hat{f}_{i+1}(x) \, dx + \int_{b_{i+1}}^{1} f(x) - \hat{f}_i(x) \, dx \tag{1.50}$$

$$= \int_{-1}^{a_{i+1}} f(x) - \hat{f}_i(x) \, dx + \int_{a_{i+1}}^{b_{i+1}} f(x) - \hat{f}_i(x) - g(h_{i+1}, a_{i+1}, b_{i+1}, x) \, dx + \int_{b_i}^{1} f(x) - \hat{f}_i(x) \, dx \tag{1.51}$$

$$= \int_{-1}^{a_{i+1}} f(x) - \hat{f}_i(x) \, dx + \int_{a_{i+1}}^{b_{i+1}} f(x) - \hat{f}_i(x) \, dx + \int_{b_{i+1}}^{1} f(x) - \hat{f}_i(x) \, dx - \int_{a_{i+1}}^{b_{i+1}} g(h_{i+1}, a_{i+1}, b_{i+1}, x) \, dx \tag{1.52}$$

$$= \int_{-1}^{1} f(x) - \hat{f}_i(x) \, dx - \int_{a_{i+1}}^{b_{i+1}} g(h_{i+1}, a_{i+1}, b_{i+1}, x) \, dx \tag{1.53}$$

$$= ||f - \hat{f}_i|| - \int_{a_{i+1}}^{b_{i+1}} g(h_{i+1}, a_{i+1}, b_{i+1}, x) \, dx \tag{1.54}$$

Note that for every i, for every $x \in [a_i, b_i]$, $g(h_i, a_i, b_i, x) > 0$. Therefore, $\int_{a_i}^{b_i} g(h_i, a_i, b_i, x)\ dx > 0$. Hence,

$$||f - \hat{f}_{i+1}|| = ||f - \hat{f}_i|| - \int_{a_{i+1}}^{b_{i+1}} g(h_{i+1}, a_{i+1}, b_{i+1}, x)\ dx \tag{1.55}$$

$$> ||f - \hat{f}_i|| \tag{1.56}$$

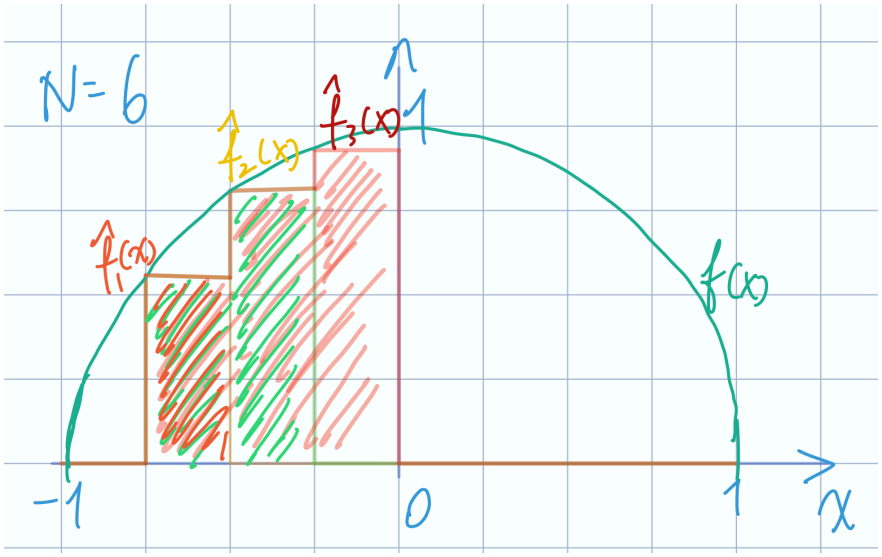

Figure 1.2: Approximated Results for $N = 6$

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1.3.4

Soln. Not required. ■

2 Backprop

2.1 Computational Graph

2.1.1

Soln. The computational graph can be drawn as:

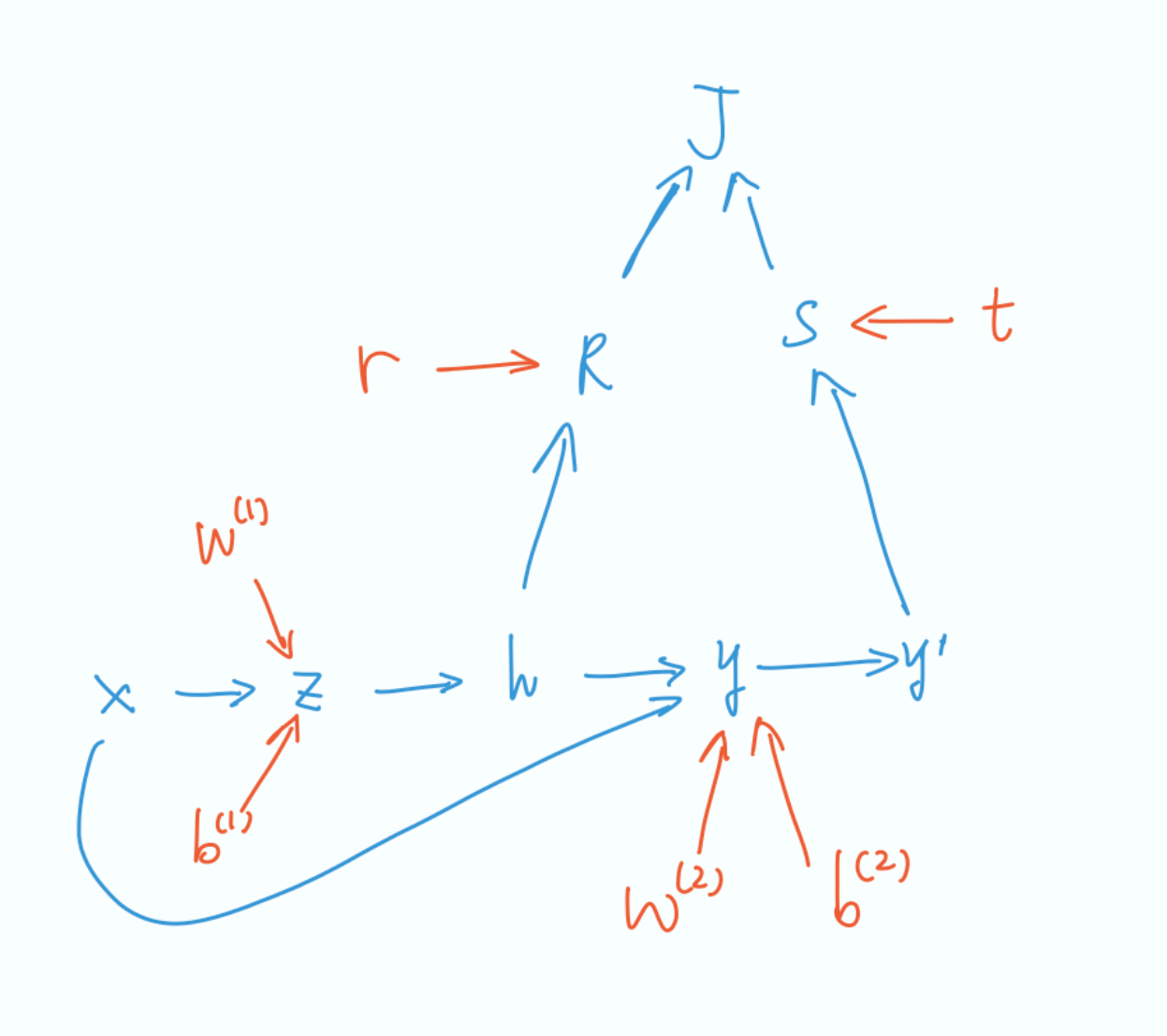


Figure 2.1: Computational Graph

■

2.1.2

Soln. For individual derivatives:

$$\overline{\mathcal{J}} = \frac{\partial \mathcal{J}}{\partial \mathcal{J}} = 1 \tag{2.1}$$

$$\overline{\mathcal{R}} = \frac{\partial \mathcal{J}}{\partial \mathcal{R}} = \overline{\mathcal{J}} 1 = 1 \tag{2.2}$$

$$\overline{\mathcal{S}} = \overline{\mathcal{J}}(-1) = -1 \tag{2.3}$$

$$\overline{\mathbf{r}} = \overline{\mathcal{R}} \frac{\partial \mathcal{R}}{\partial \mathbf{r}} = \mathbf{h}^T \overline{\mathcal{R}} \tag{2.4}$$

$$\overline{\mathbf{y}'} = \overline{\mathcal{S}} \frac{\partial \mathcal{S}}{\partial \mathbf{y}'} = \mathbf{e}_t^T \overline{\mathcal{S}} \tag{2.5}$$

$$\overline{\mathbf{y}} = \overline{\mathbf{y}'} \frac{\partial \mathbf{y}'}{\partial \mathbf{y}} = \texttt{softmax}'(\mathbf{y})^T \overline{\mathbf{y}'} \tag{2.6}$$

$$\overline{\mathbf{h}} = \overline{\mathcal{R}} \frac{\partial \mathcal{R}}{\partial \mathbf{h}} + \overline{\mathbf{y}} \frac{\partial \mathbf{y}}{\partial \mathbf{h}} = \overline{\mathcal{R}} \mathbf{r} + \mathbf{W}^{(2)T} \overline{\mathbf{y}} \tag{2.7}$$

$$\overline{\mathbf{b}^{(2)}} = \overline{\mathbf{y}} \tag{2.8}$$

$$\overline{\mathbf{W}^{(2)}} = \overline{\mathbf{y}} \mathbf{h}^T \in \mathbb{R}^{N \times N} \tag{2.9}$$

$$\overline{\mathbf{z}} = \overline{\mathbf{h}} \mathbb{1} \{\mathbf{z} \geq 0\} \tag{2.10}$$

$$\overline{\mathbf{W}^{(1)}} = \overline{\mathbf{z}} \mathbf{x}^T \in \mathbb{R}^{N \times N} \tag{2.11}$$

$$\overline{\mathbf{b}^{(1)}} = \overline{\mathbf{z}} \tag{2.12}$$

$$\overline{\mathbf{x}} = \mathbf{W}^{(1)T} \overline{\mathbf{z}} + \overline{\mathbf{y}} \tag{2.13}$$

where $\mathbf{e}_t$ denotes the one-hot vector in $\mathbb{R}^N$ in which the t^{th} element is one. ■

2.2 Vector-Jacobean Product (VJPs)

2.2.1

Soln.

$$\mathbf{f}(\mathbf{x}) := \mathbf{v}\mathbf{v}^T \mathbf{x} \tag{2.14}$$

$$\implies J = \frac{d}{d\mathbf{x}} \mathbf{f}(\mathbf{x}) = \mathbf{v}\mathbf{v}^T \tag{2.15}$$

$$\implies J = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 6 \\ 3 & 6 & 9 \end{pmatrix} \tag{2.16}$$

■

2.2.2

Soln. Time cost: n^2. Memory cost: $\frac{(n+1)n}{2}$ (only need to store elements above the diagonal (including the diagonal), because J is symmetric). Therefore, both time and memory cost are $\mathcal{O}(n^2)$. ■

2.2.3

Soln.

$$J^T\mathbf{y} = \mathbf{v}\mathbf{v}^T\mathbf{y} \tag{2.17}$$
$$= \mathbf{v}(\mathbf{v}^T\mathbf{y}) \tag{2.18}$$
$$= \underbrace{\mathbf{v}\overbrace{\langle \mathbf{v}, \mathbf{y}\rangle}^{\text{step 1}}}_{\text{step 2}} \quad (\dagger) \tag{2.19}$$
$$\implies \mathbf{z}\mathbf{v}\sum_{i=1}^{3} v_i y_i \tag{2.20}$$
$$\implies \mathbf{z}^T = 6\mathbf{v}^T \tag{2.21}$$
$$\implies \mathbf{z}^T = [6, 12, 18] \tag{2.22}$$

where the inner product operation has time cost n and its output takes memory cost 1. Let $\alpha = \langle \mathbf{v}, \mathbf{y}\rangle \in \mathbb{R}$, the vector scaler multiplication operation $\mathbf{v}\alpha$ has time cost n and its output has memory cost n.
The overall time cost for $(\dagger)$ is therefore $2n$ and memory cost is $n + 1$.
So that both the memory and time costs are in $\mathcal{O}(n)$. ■

3 Linear Regression

3.1 Driving the Gradient

Soln.

$$\frac{d}{d\hat{\mathbf{w}}}\frac{1}{n}(X\hat{\mathbf{w}} - \mathbf{t})^2 = \frac{d}{d\hat{\mathbf{w}}}\frac{1}{n}||X\hat{\mathbf{w}} - \mathbf{t}||_2^2 \tag{3.1}$$
$$= \frac{2}{n}(X\hat{\mathbf{w}} - \mathbf{t})^T X \tag{3.2}$$
$$\implies \nabla_{\mathbf{w}}\mathcal{J} = \frac{2}{n}X^T(X\hat{\mathbf{w}} - \mathbf{t}) \tag{3.3}$$

■

3.2 Under-parameterized Model

3.2.1

Soln. Assume $d < n$ so that X^TX is invertible. The gradient descent algorithm converges when the gradient equals zero:

$$\frac{2}{n}(X\hat{\mathbf{w}} - \mathbf{t})^T X = 0 \tag{3.4}$$
$$\implies (X\hat{\mathbf{w}} - \mathbf{t})^T X = 0 \tag{3.5}$$
$$\implies X^T(X\hat{\mathbf{w}} - \mathbf{t}) = 0^T \tag{3.6}$$
$$\implies X^TX\hat{\mathbf{w}} - X^T\mathbf{t} = 0^T \tag{3.7}$$
$$\implies X^TX\hat{\mathbf{w}} = X^T\mathbf{t} \tag{3.8}$$
$$\implies \hat{\mathbf{w}} = (X^TX)^{-1}X^T\mathbf{t} \tag{3.9}$$

■

3.2.2

Soln. Let $\mathbf{x} \in \mathbb{R}^d$, note that $(X^TX)^{-1}$ is symmetric. Assuming target $\mathbf{t}$ is generated by a linear process, then $\mathbf{t} = X\mathbf{w}^*$. Immediately, $\mathbf{t}^T = \mathbf{w}^{*T}X^T$.

$$
\begin{aligned}
(\mathbf{w}^{*T}\mathbf{x} - \hat{\mathbf{w}}^T\mathbf{x})^2 &= (\mathbf{w}^{*T}\mathbf{x} - [(X^TX)^{-1}X^T\mathbf{t}]^T\mathbf{x})^2 && (3.10)\\
&= (\mathbf{w}^{*T}\mathbf{x} - \mathbf{t}^TX(X^TX)^{-1}\mathbf{x})^2 && (3.11)\\
&= (\mathbf{w}^{*T}\mathbf{x} - \mathbf{w}^{*T}X^TX(X^TX)^{-1}\mathbf{x})^2 && (3.12)\\
&= (\mathbf{w}^{*T}\mathbf{x} - \mathbf{w}^{*T}\mathbf{x})^2 && (3.13)\\
&= 0 && (3.14)
\end{aligned}
$$

■

3.3 Over-parameterized Model: 2D Example

3.3.1

Soln. To minimize the empirical risk minimizer,

$$\min_{w_1,w_2} (w_1x_1 + w_2x_2 - t_1)^2 \tag{3.15}$$

$$\text{equivalently, } \min_{w_1,w_2} (2w_1 + w_2 - 2)^2 \tag{3.16}$$

Any pair of (w_1, w_2) satisfying

$$2w_1 + w_2 - 2 = 0 \quad (\dagger) \tag{3.17}$$

attains the minimum level of empirical risk (zero). Equivalently, any $\hat{\mathbf{w}}$ on the line

$$\hat{\mathbf{w}} = \begin{pmatrix} 0 \\ 2 \end{pmatrix} + t \begin{pmatrix} 1 \\ -2 \end{pmatrix} \text{ for } t \in \mathbb{R} \tag{3.18}$$

satisfies (†). Therefore, there are infinitely many empirical risk minimizers.
Equivalently, the collection of solution is

$$w_2 = -2w_1 + 2 \tag{3.19}$$

■

3.3.2

Soln. From the fist part of this question we know that

$$\nabla_{\mathbf{w}}\mathcal{J} = \frac{2}{n}(X\hat{\mathbf{w}} - \mathbf{t})^T X \tag{3.20}$$

$$= \frac{2}{1}\left[\begin{pmatrix}2\\1\end{pmatrix}\cdot\begin{pmatrix}0\\0\end{pmatrix} - 2\right]\begin{pmatrix}2\\1\end{pmatrix} \tag{3.21}$$

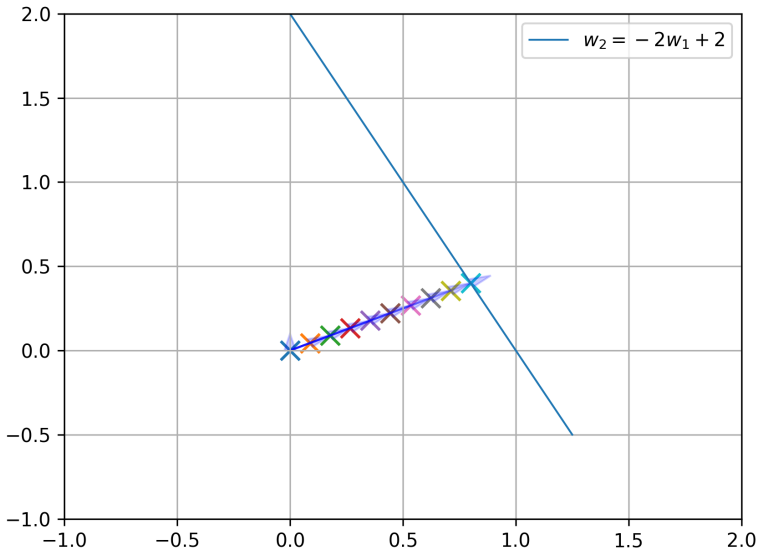
$$= \begin{pmatrix}-4\\-2\end{pmatrix} \tag{3.22}$$

The unit-norm gradient is

$$\widehat{\nabla_{\mathbf{w}}\mathcal{J}} = \begin{pmatrix}-\frac{2\sqrt{5}}{5}\\-\frac{\sqrt{5}}{5}\end{pmatrix} \tag{3.23}$$

The direction (gradient) does not change along the trajectory. Ultimately, the gradient descend algorithm converges to

$$\hat{\mathbf{w}}^* = \left(\frac{4}{5}, \frac{2}{5}\right) \tag{3.24}$$



■

3.3.3

Soln. Let $\hat{\mathbf{w}}^*$ denote the solution found using gradient descent. Note that the line of solution can be written parametrically as

$$\hat{\mathbf{w}}(t) = \begin{pmatrix} 0 \\ 2 \end{pmatrix} + t \begin{pmatrix} 1 \\ -2 \end{pmatrix} \tag{3.25}$$

The path of gradient descent starts from $\mathcal{S} = \mathbf{0}$ and the path is perpendicular to the line of solutions $\{\hat{\mathbf{w}}(t) : t \in \mathbb{R}\}$. By Pythagorean theorem, we know that the shortest path from a fixed point x to a line ℓ is the perpendicular line x and some point y on ℓ. Meanwhile, y is the point on ℓ nearest to x. The path of gradient descent is exactly such a shortest path. Therefore, $\hat{\mathbf{w}}^*$ is the solution nearest to $\mathbf{0}$. In another word, $\hat{\mathbf{w}}$ is solution with smallest Euclidean among all solutions in $\mathcal{S}$.
Note: this proof is rough and relies on geometric intuition, for a more formal and general proof, please refer to 3.4.2. ■

3.4 Overparameterized Model: General Case

3.4.1

Proof. Note that the solution reached by gradient descent $\mathbf{w}^*$ can be written as a linear combination of rows of X:

$$X = \begin{pmatrix} x_{11} & \cdots & x_{1d} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nd} \end{pmatrix} \tag{3.26}$$

$$\mathbf{w}^* = r_1 \begin{pmatrix} x_{11} \\ \vdots \\ x_{1d} \end{pmatrix} + \cdots + r_n \begin{pmatrix} x_{n1} \\ \vdots \\ x_{nd} \end{pmatrix} \tag{3.27}$$

$$= \begin{pmatrix} x_{11} & \cdots & x_{1d} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nd} \end{pmatrix}^T \begin{pmatrix} r_1 \\ \vdots \\ r_n \end{pmatrix} \tag{3.28}$$

$$= X^T \mathbf{r} \tag{3.29}$$

The original minimization problem in $\mathbb{R}^d$ (choosing the optimal $\mathbf{w} \in \mathbb{R}^d$) can be reduced to a minimization problem in $\mathbb{R}^n$ (choosing the optimal $\mathbf{r} \in \mathbb{R}^n$).
The gradient descent algorithm converges if and only if zero gradient is encountered, which is characterized by the following condition:

$$\frac{d}{d\mathbf{r}} \frac{1}{n} ||XX^T\mathbf{r} - \mathbf{t}||_2^2 = 0 \tag{3.30}$$

$$\implies \frac{2}{n}(XX^T\mathbf{r} - \mathbf{t})^T XX^T = 0 \tag{3.31}$$

$$\implies XX^T(XX^T\mathbf{r} - \mathbf{t}) = 0 \text{ (take transpose on both sides)} \tag{3.32}$$

$$\implies XX^TXX^T\mathbf{r} = XX^T\mathbf{t} \tag{3.33}$$

Because $d > n$, so $rank(XX^T) = n$ and it is invertible. Therefore,

$$(XX^T)^{-1}XX^TXX^T\mathbf{r} = (XX^T)^{-1}XX^T\mathbf{t} \tag{3.34}$$
$$\implies XX^T\mathbf{r} = \mathbf{t} \tag{3.35}$$
$$\implies \mathbf{r}^* = (XX^T)^{-1}\mathbf{t} \tag{3.36}$$
$$\implies \mathbf{w}^* = X^T(XX^T)^{-1}\mathbf{t} \tag{3.37}$$

where the solution is uniquely determined. ■

3.4.2

Proof. Let $\hat{\mathbf{w}}_1$ be another zero loss weight, then

$$X\hat{\mathbf{w}}_1 = \mathbf{t} \tag{3.38}$$

Immediately,

$$\hat{\mathbf{w}}_1^T X^T = \mathbf{t}^T \tag{3.39}$$

Evaluating

$$(\hat{\mathbf{w}} - \hat{\mathbf{w}}_1)^T\hat{\mathbf{w}} = ||\hat{\mathbf{w}}||_2^2 - \hat{\mathbf{w}}_1^T\hat{\mathbf{w}} \tag{3.40}$$
$$= (X^T(XX^T)^{-1}\mathbf{t})^T(X^T(XX^T)^{-1}\mathbf{t}) - \hat{\mathbf{w}}_1^T\hat{\mathbf{w}} \tag{3.41}$$
$$= \mathbf{t}^T(XX^T)^{-1}X(X^T(XX^T)^{-1}\mathbf{t}) - \hat{\mathbf{w}}_1^T\hat{\mathbf{w}} \tag{3.42}$$
$$= \mathbf{t}^T(XX^T)^{-1}\mathbf{t} - \hat{\mathbf{w}}_1^TX^T(XX^T)^{-1}\mathbf{t} \tag{3.43}$$
$$= \mathbf{t}^T(XX^T)^{-1}\mathbf{t} - \mathbf{t}^T(XX^T)^{-1}\mathbf{t} \tag{3.44}$$
$$= 0 \quad (\dagger) \tag{3.45}$$

Because $\hat{\mathbf{w}}_1$ is chosen arbitrarily, let $\mathcal{S}$ denote the space of zero-loss weights. (†) suggests the optimal solution found by gradient descent $\hat{\mathbf{w}} \perp \mathcal{S}$.
Let $\hat{\mathbf{w}}$ denote the solution found by gradient descent.
Let $\hat{\mathbf{w}}_\alpha \in \mathcal{S}$ and $\mathbf{v} = \hat{\mathbf{w}}_\alpha - \hat{\mathbf{w}}$.

$$||\hat{\mathbf{w}}_\alpha||_2^2 = ||\hat{\mathbf{w}} + \mathbf{v}||_2^2 \tag{3.46}$$
$$= ||\hat{\mathbf{w}}||_2^2 + 2\mathbf{v}\cdot\hat{\mathbf{w}} + ||\mathbf{v}||_2^2 \tag{3.47}$$
$$= ||\hat{\mathbf{w}}||_2^2 + 2(\hat{\mathbf{w}}_\alpha - \hat{\mathbf{w}})\cdot\hat{\mathbf{w}} + ||\mathbf{v}||_2^2 \tag{3.48}$$
$$= ||\hat{\mathbf{w}}||_2^2 + ||\mathbf{v}||_2^2 \text{ by } (\dagger) \tag{3.49}$$
$$\geq ||\hat{\mathbf{w}}||_2^2 \tag{3.50}$$

Therefore,

$$||\hat{\mathbf{w}}_\alpha||_2^2 \geq ||\hat{\mathbf{w}}||_2^2 \quad \forall\ \hat{\mathbf{w}}_\alpha \in \mathcal{S} \tag{3.51}$$

And $\hat{\mathbf{w}}$ is the element with smallest Euclidean norm among all zero-loss solutions in $\mathcal{S}$. ■

3.5 Benefit of Overparameterization

3.5.1

Soln. Fitting function implementation:

```
def fit_poly(X, d,):
    X_expand = poly_expand(X, d=d, poly_type = poly_type)
    if d > n: # Over-parameterized case
        W = X_expand.T @ np.linalg.inv(X_expand @ X_expand.T) @ t
    else:  # Under parameterized case.
        W = np.linalg.inv(X_expand.T @ X_expand) @ X_expand.T @ t
    return W

```

Lines fitted and the corresponding losses using both legendre and chebyshev polynomials are presented in figures below. In both experiments, over-parameterization does **not** always lead to overfitting. In fact, models with a super high degree (say 100) models resulted similar performances compared with low degrees (In the Legendre case, high degree models actually outperformed low degree models).

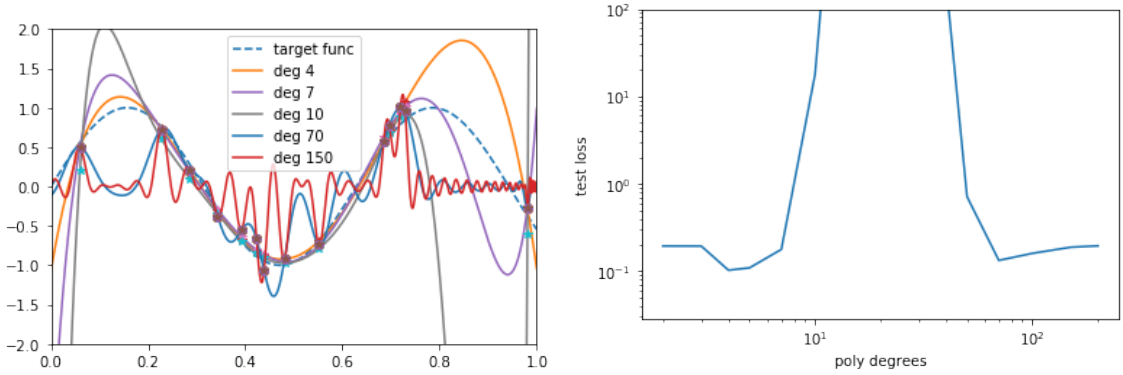


Figure 3.1: chebyshev results

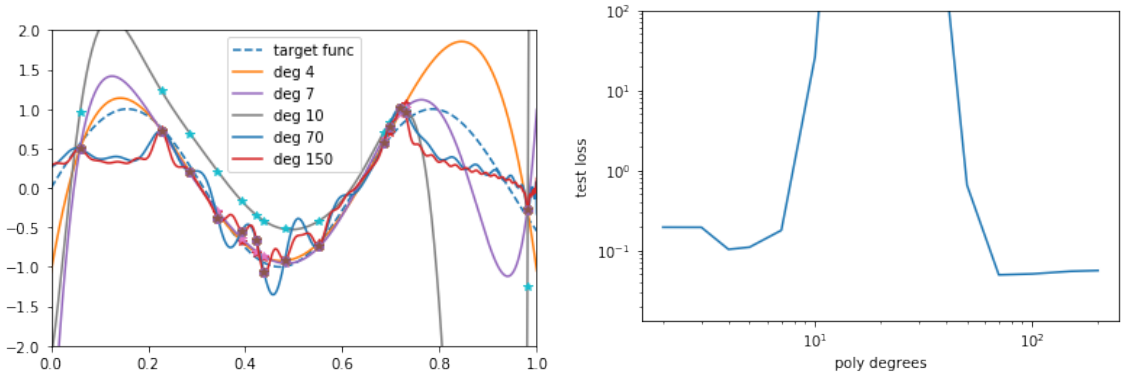


Figure 3.2: legendre results

■

3.5.2

Soln. Not required. ■