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Problem Set 08, Nov 05, 2020 (Solution to Theory Question)

1 Vanishing Gradient

Note that the overall function $f(x_0)$ is a composition of (L+1) functions, where the first L functions correspond to the L layers of the neural network and the last one corresponds to the output layer. So we have

$$f(\mathbf{x}^{(0)}) = (f_{L+1} \circ \cdots \circ f_2 \circ f_1)(\mathbf{x}^{(0)}).$$

where

$$\mathbf{x}^{(l)} = f_l(\mathbf{x}^{(l-1)}) = \phi((\mathbf{W}^{(l)})^{\top} \mathbf{x}^{(l-1)} + \mathbf{b}^{(l)}).$$
 (1)

Applying the chain rule to calculate $\frac{\partial f}{\partial W_{i,j}^{(1)}}$ we get:

$$\frac{\partial f}{\partial W_{1,1}^{(1)}} = f'_{L+1} \times f'_{L} \times \ldots \times f'_{2} \times \frac{\partial f_{1}}{\partial W_{1,1}^{(1)}}$$

We are interested in showing that this value vanishes exponentially with L, i.e. $\left\|\frac{\partial f}{\partial W_{1,1}^{(1)}}\right\|_2 \leq O(\frac{3}{4}^L)$. We first remark the following definition:

Definition: The 2-operator norm of a matrix can be defined as $\|A\|_2^2 := \max_v \frac{\|Av\|_2^2}{\|v\|_2^2}$ where the maximum is taken over all vectors. Note that the norm in the left side is a operator norm which is different from the norms in the right side corresponding to L2-norm defined in vector space which is also shown by the symbol $\|v\|_2$ but where v is a vector.

Applying $\|Av\|_2 \le \|A\|_2 \|v\|_2$ (which follows from the definition of 2-operator norm) and $\|AB\|_2 \le \|A\|_2 \|B\|_2$ (which can be seen by noting that $\frac{\|ABv\|_2^2}{\|v\|_2^2} = \frac{\|A(Bv)\|_2^2}{\|Bv\|_2^2} \cdot \frac{\|Bv\|_2^2}{\|v\|_2^2}$ and taking the max), we get

$$\left\| \frac{\partial f}{\partial W_{1,1}^{(1)}} \right\|_{2} \le \left\| f'_{L+1} \right\|_{2} \cdot \left\| f'_{L} \right\|_{2} \cdot \dots \cdot \left\| f'_{2} \right\|_{2} \times \left\| \frac{\partial f_{1}}{\partial W_{1,1}^{(1)}} \right\|_{2}. \tag{2}$$

From (1) we can obtain

$$f_l'(\boldsymbol{x}^{(l-1)}) = (\boldsymbol{W}^{(l)})^\top \operatorname{diag}(\phi'((\boldsymbol{W}^{(l)})^\top \boldsymbol{x}^{(l-1)} + \boldsymbol{b}^{(l)})$$

where diag(v) converts a vector to a diagonal matrix with the diagonal entries filled with elements of v. We can now bound the norm as

$$||f'_{l}(\boldsymbol{x}^{(l-1)})|| \leq ||(\boldsymbol{W}^{(l)})^{\top}||_{2} \cdot ||\operatorname{diag}(\phi'((\boldsymbol{W}^{(l)})^{\top}\boldsymbol{x}^{(l-1)} + \boldsymbol{b}^{(l)})||_{2} \leq ||(\boldsymbol{W}^{(l)})^{\top}||_{2} \cdot \max[\phi'((\boldsymbol{W}^{(l)})^{\top}\boldsymbol{x}^{(l-1)})]$$
(3)

where the last inequality follows from the second term being diagonal. Now note that our activation functions are sigmoids and those have a maximal derivative of $\frac{1}{4}$, i.e.,

$$\max_{x} \left(\frac{1}{1 + e^{-x}} \right)' = \max \frac{e^{-x}}{(1 + e^{-x})^2} = \frac{1}{4}.$$

Therefore, the sigmoid term in (3) is upper bounded by $\frac{1}{4}$. Note that by assumption each weight has magnitude at most 1 and we assumed that we have K=3, i.e., we have only three nodes per layer. Now note that for any vector v

$$(\boldsymbol{W}^{(l)}v)_i = \sum_{j=1}^3 (\boldsymbol{W}_{i,j}^{(l)}v_j) \le \sum_{j=1}^3 |\boldsymbol{W}_{i,j}^{(l)}| \cdot |v_j| \le \sum_{j=1}^3 |v_j|$$

Using the inequality $(a+b+c)^2 \le 3(a^2+b^2+c^2)$ (which can be proven using Cauchy-Schwarz inequality), we can write for any vector v,

$$\frac{\left\|\boldsymbol{W}^{(l)}v\right\|_{2}^{2}}{\left\|v\right\|_{2}^{2}} \leq \frac{3(\sum_{j=1}^{3}|v_{j}|)^{2}}{(\sum_{j=1}^{3}|v_{j}|^{2})} \leq 9.$$

Therefore, we get $\|\boldsymbol{W}^{(l)}\|_2 \leq 3$ which means the second term in (3) is bounded by 3. Therefore $\|f_l'(\boldsymbol{x}^{(l-1)})\|_2 \leq \frac{3}{4}$ which in combination with (2) proves our goal.