

Exercise Sheet 5

Exercise 1: Neural Network Regularization (5 × 20 P)

For a neural network to generalize from limited data, it is desirable to make it sufficiently invariant to small local perturbations. This can be done by limiting the gradient norm $\|\partial f / \partial \mathbf{x}\|$ for all \mathbf{x} in the input domain. As the input domain can be high-dimensional, it is impractical to minimize the gradient norm directly. Instead, we can minimize an upper-bound of it that depends only on the model parameters.

We consider a two-layer neural network with d input neurons, h hidden neurons, and one output neuron. Let W be a weight matrix of size $d \times h$, and $(b_j)_{j=1}^h$ a collection of biases. We denote by $W_{i,:}$ the i th row of the weight matrix and by $W_{:,j}$ its j th column. The neural network computes:

$$\begin{aligned} a_j &= \max(0, W_{:,j}^\top \mathbf{x} + b_j) && \text{(layer 1)} \\ f(\mathbf{x}) &= \sum_j a_j && \text{(layer 2)} \end{aligned}$$

The first layer detects patterns of the input data, and the second layer performs a pooling operation over these detected patterns.

(a) *Show that the gradient norm of the network can be upper-bounded as:*

$$\left\| \frac{\partial f}{\partial \mathbf{x}} \right\| \leq \sqrt{h} \cdot \|W\|_F$$

Hint: Use the Cauchy-Schwarz inequality.

(b) *Show that the well-known weight decay procedure $(W^{(t+1)} \leftarrow (1 - \gamma) \cdot W^{(t)})$ for some $\gamma > 0$) can be interpreted as a gradient descent of $\|W\|_F$ or some related quantity.*

(c) Let $\|W\|_{\text{Mix}} = \sqrt{\sum_i \|W_{i,:}\|_1^2}$ be a ℓ_1/ℓ_2 mixed matrix norm. *Show that the gradient norm of the network can be upper-bounded by it as:*

$$\left\| \frac{\partial f}{\partial \mathbf{x}} \right\| \leq \|W\|_{\text{Mix}}$$

(d) *Show that the bound is tighter than the one based on the Frobenius norm, i.e. show that $\|W\|_{\text{Mix}} \leq \sqrt{h} \cdot \|W\|_F$.*

(e) *Show that the gradient of the squared mixed norm is given by*

$$\frac{\partial}{\partial W_{ij}} \|W\|_{\text{Mix}}^2 = 2 \cdot \|W_{i,:}\|_1 \cdot \text{sign}(W_{ij}).$$

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We consider a two-layer neural network with d input neurons, h hidden neurons, and one output neuron. Let W be a weight matrix of size $d \times h$, and $(b_j)_{j=1}^h$ a collection of biases. We denote by $W_{i,:}$ the i th row of the weight matrix and by $W_{:,j}$ its j th column. The neural network computes:

$$a_j = \max(0, W_{:,j}^\top \mathbf{x} + b_j) \quad (\text{layer 1})$$

$$f(\mathbf{x}) = \sum_j a_j \quad (\text{layer 2})$$

The first layer detects patterns of the input data, and the second layer performs a pooling operation over these detected patterns.

(a) Show that the gradient norm of the network can be upper-bounded as:

$$\left\| \frac{\partial f}{\partial \mathbf{x}} \right\| \leq \sqrt{h} \cdot \|W\|_F$$

Hint: Use the Cauchy-Schwarz inequality.

$$\begin{aligned} \frac{\partial f}{\partial x_i} &= \sum_{j=1}^h \frac{\partial f}{\partial a_j} \cdot \frac{\partial a_j}{\partial x_i} = \sum_{j=1}^h \mathbb{1}_{a_j > 0} \cdot \frac{\partial (W_{i,:}^\top \mathbf{x} + b_j)}{\partial x_i} \\ &= \sum_{j=1}^h \mathbb{1}_{a_j > 0} \cdot \frac{\partial \sum_{i=1}^d W_{i,j} \cdot x_i}{\partial x_i} \\ &= \sum_{j=1}^h \mathbb{1}_{a_j > 0} \cdot W_{i,j} \end{aligned}$$

$$(\sum a_i b_i)^2 \leq (\sum a_i^2) (\sum b_i^2)$$

$$\begin{aligned} \left\| \frac{\partial f}{\partial \mathbf{x}} \right\| &= \sqrt{\sum_{i=1}^d \left(\frac{\partial f}{\partial x_i} \right)^2} = \sqrt{\sum_{i=1}^d \left(\sum_{j=1}^h \mathbb{1}_{a_j > 0} \cdot W_{i,j} \right)^2} \\ &\leq \sqrt{\sum_{i=1}^d \left(\sum_{j=1}^h \mathbb{1}_{a_j > 0}^2 \right) \left(\sum_{j=1}^h W_{i,j}^2 \right)} \\ &\leq \sqrt{\sum_{i=1}^d h \cdot \left(\sum_{j=1}^h W_{i,j}^2 \right)} \\ &= \sqrt{h} \sqrt{\sum_{i=1}^d \sum_{j=1}^h W_{i,j}^2} \\ &= \sqrt{h} \cdot \|W\| \end{aligned}$$

(b) Show that the well-known weight decay procedure $W^{(t+1)} \leftarrow (1 - \gamma) \cdot W^{(t)}$ for some $\gamma > 0$ can be interpreted as a gradient descent of $\|W\|_F$ or some related quantity.

$$\begin{aligned} W^{(t+1)} &\leftarrow (1 - \gamma) W^{(t)} = W^{(t)} - \gamma W^{(t)} \\ &= W^{(t)} - \frac{\gamma}{2} \cdot 2 W^{(t)} \\ &= W^{(t)} - \frac{\gamma}{2} \cdot \frac{\partial \|W^{(t)}\|^2}{\partial W^{(t)}} \end{aligned} \quad \text{Descending } \|W\|_F^2 \text{ with a learning rate } \frac{\gamma}{2}$$

(c) Let $\|W\|_{\text{Mix}} = \sqrt{\sum_i \|W_{i,:}\|_1^2}$ be a ℓ_1/ℓ_2 mixed matrix norm. Show that the gradient norm of the network can be upper-bounded by it as:

$$\left\| \frac{\partial f}{\partial x} \right\| \leq \|W\|_{\text{Mix}}$$

from 1.a) we have showed: $\left\| \frac{\partial f}{\partial x} \right\| = \sqrt{\sum_{i=1}^d \left(\sum_{j=1}^h 1_{a_j > 0} \cdot W_{i,j} \right)^2}$

then we have:

$$\begin{aligned} &\leq \sqrt{\sum_{i=1}^d \left(\sum_{j=1}^h |W_{i,j}| \right)^2} \\ &= \sqrt{\sum_{i=1}^d \|W_{i,:}\|_1^2} \\ &= \|W\|_{\text{Mix}} \end{aligned}$$

(d) Show that the bound is tighter than the one based on the Frobenius norm, i.e. show that $\|W\|_{\text{Mix}} \leq \sqrt{h} \cdot \|W\|_F$.

$$\begin{aligned} \|W\|_{\text{Mix}} &= \sqrt{\sum_{i=1}^d \left(\sum_{j=1}^h W_{i,j} \right)^2} \\ &\leq \sqrt{\sum_{i=1}^d \left(\sum_{j=1}^h 1^2 \cdot \sum_{j=1}^h W_{i,j} \right)} \quad \text{Cauchy-Schwarz inequality} \\ &\leq \sqrt{\sum_{i=1}^d h \cdot \sum_{j=1}^h W_{i,j}} \\ &= \sqrt{h} \cdot \|W\|_F \end{aligned}$$

(e) Show that the gradient of the squared mixed norm is given by

$$\frac{\partial}{\partial W_{ij}} \|W\|_{\text{Mix}}^2 = 2 \cdot \|W_{i,:}\|_1 \cdot \text{sign}(W_{ij}).$$

$$\|W\|_{\text{Mix}}^2 = \sum_{i=1}^d \|W_{i,:}\|_1^2$$

$$\begin{aligned} \frac{\partial}{\partial W_{ij}} \|W\|_{\text{Mix}}^2 &= \frac{\partial \|W\|_{\text{Mix}}^2}{\partial \|W_{i,:}\|_1} \cdot \frac{\partial \|W_{i,:}\|_1}{\partial W_{ij}} \\ &= 2 \|W_{i,:}\|_1 \cdot \frac{\partial}{\partial W_{ij}} \left(\sqrt{\sum_{j=1}^h |W_{i,j}|} \right) = 2 \|W_{i,:}\|_1 \cdot \frac{\partial}{\partial W_{ij}} \left(\sum_{j=1}^h |W_{i,j}| \right) \\ &= 2 \|W_{i,:}\|_1 \cdot \text{sign}(W_{i,j}) \end{aligned}$$