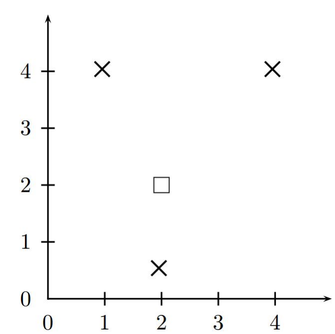
CM146, Winter 2022
Problem Set 3: Deep learning, Learning theory, Kernels
Due February 28,2022, 11:59pm PST

1 VC-Dimension [8 pts]

(a) **(4 pts)** Consider the space of instances X corresponding to all points in the x, y plane. What is the VC-dimension of the hypothesis space defined by H_c = circles in the x, y plane, with points inside the circle are classified as positive examples? Justify your answer (e.g. with one or more diagrams). **Solution:** VC-dim = 3. It is easy to see the VC-dimension is at least 3 since any 3 points that make up a non-degenerate triangle can be shattered. It is a bit trickier to prove that the VC-dimension is less than 4. Given 4 points, the easy case is when one is inside the convex hull of the others. In that case, because circles are convex, it is not possible to label the inside point and the outside points $+$. Otherwise, it is not possible to label them in alternating $+, -, +, -$ order.

Pictorial solution for $VC < 4$: We will only show that some 4 points cannot be shattered. For instance, you cannot find a circle which covers all the crosses below but not the square.



(b) **(4 pts)** This problem investigates a few properties of the VC dimension, mostly relating to how $VC(H)$ increases as the set H increases. For each part of this problem, you should state whether the given statement is true, and justify your answer with either a formal proof or a counter-example. **Solution:** [for each: 1 pt True/False, 1 pt justification]

i. **(2 pts)** Let two hypothesis classes H_1 and H_2 satisfy $H_1 \subseteq H_2$. Prove or disprove: $VC(H_1) \leq VC(H_2)$. **Solution:** True. Suppose that $VC(H_1) = d$. Then there exists a set of d points that is shattered by H_1 (i.e., for each possible labeling of the d points, there exists a hypothesis $h \in H_1$ which realizes that labeling). Now, since H_2 contains all hypotheses in H_1, then H_2 shatters the same set, and thus we have $VC(H_2) \geq d = VC(H_1)$.

ii. **(2 pts)** Let $H_1 = H_2 \cup H_3$. Prove or disprove: $VC(H_1) \leq VC(H_2) + VC(H_3)$. **Solution:** False. Counterexample: let $H_1 = \{h_1\}$, $H_2 = \{h_2\}$, and $\forall x, h_1(x) = 0, h_2(x) = 1$. Then we have $VC(H_1) = VC(H_2) = 0$, but $VC(H_1 \cup H_2) = 1$.

Parts of this assignment are adapted from course material by Tommi Jaakola (MIT), and Andrew Ng (Stanford), and Jenna Wiens (UMich).

2 Kernels [8 pts]

(a) **(2 pts)** For any two documents $\boldsymbol{x}$ and $\boldsymbol{z}$, define $k(\boldsymbol{x}, \boldsymbol{z})$ to equal the number of unique words that occur in both $\boldsymbol{x}$ and $\boldsymbol{z}$ (i.e., the size of the intersection of the sets of words in the two documents). Is this function a kernel? Give justification for your answer. **Solution:** We can show that $K(\boldsymbol{x}, \boldsymbol{z})$ is a kernel by explicitly constructing feature vectors $\phi(\boldsymbol{x})$ and $\phi(\boldsymbol{z})$ such that $k(\boldsymbol{x}, \boldsymbol{z}) = \phi(\boldsymbol{x}) \cdot \phi(\boldsymbol{z})$. For any set of documents, we can always construct a vocabulary $\mathcal{V}$ with finite size for the words in the document set. Given the vocabulary $\mathcal{V}$, we can construct a feature mapping $\phi(\boldsymbol{x})$ for $\boldsymbol{x}$ by the following: For the ℓ^{th} word w_ℓ in $\mathcal{V}$, if w_ℓ appears in document $\boldsymbol{x}$, assign $\phi(\boldsymbol{x})_\ell$ (the ℓ^{th} element of $\phi(\boldsymbol{x})$) to be 1; otherwise set the element $\phi(\boldsymbol{x})_\ell$ to 0. Then the number of unique words common in $\boldsymbol{x}$ and $\boldsymbol{z}$ is $\phi(\boldsymbol{x}) \cdot \phi(\boldsymbol{z})$, giving us the kernel.

(b) **(3 pts)** One way to construct kernels is to build them from simpler ones. We have seen various "construction rules", including the following: Assuming $k_1(\boldsymbol{x}, \boldsymbol{z})$ and $k_2(\boldsymbol{x}, \boldsymbol{z})$ are kernels, then so are

- (scaling) $f(\boldsymbol{x})k_1(\boldsymbol{x}, \boldsymbol{z})f(\boldsymbol{z})$ for any function $f(\boldsymbol{x}) \in \mathbb{R}$
- (sum) $k(\boldsymbol{x}, \boldsymbol{z}) = k_1(\boldsymbol{x}, \boldsymbol{z}) + k_2(\boldsymbol{x}, \boldsymbol{z})$
- (product) $k(\boldsymbol{x}, \boldsymbol{z}) = k_1(\boldsymbol{x}, \boldsymbol{z})k_2(\boldsymbol{x}, \boldsymbol{z})$

Using the above rules and the fact that $k(\boldsymbol{x}, \boldsymbol{z}) = \boldsymbol{x} \cdot \boldsymbol{z}$ is (clearly) a kernel, show that the following is also a kernel:

$$\left(1 + \left(\frac{\boldsymbol{x}}{||\boldsymbol{x}||}\right) \cdot \left(\frac{\boldsymbol{z}}{||\boldsymbol{z}||}\right)\right)^3$$

Solution: We can construct the kernel in the following steps.

i. scaling. $k_1(\boldsymbol{x}, \boldsymbol{z}) = \frac{1}{||\boldsymbol{x}||}\frac{1}{||\boldsymbol{z}||}k(\boldsymbol{x}, \boldsymbol{z}) = \left(\frac{\boldsymbol{x}}{||\boldsymbol{x}||}\right) \cdot \left(\frac{\boldsymbol{z}}{||\boldsymbol{z}||}\right)$

ii. sum. $k_2(\boldsymbol{x}, \boldsymbol{z}) = 1 + k_1(\boldsymbol{x}, \boldsymbol{z}) = 1 + \left(\frac{\boldsymbol{x}}{||\boldsymbol{x}||}\right) \cdot \left(\frac{\boldsymbol{z}}{||\boldsymbol{z}||}\right)$

iii. product. $k_3(\boldsymbol{x}, \boldsymbol{z}) = k_2(\boldsymbol{x}, \boldsymbol{z})k_2(\boldsymbol{x}, \boldsymbol{z}) = \left(1 + \left(\frac{\boldsymbol{x}}{||\boldsymbol{x}||}\right) \cdot \left(\frac{\boldsymbol{z}}{||\boldsymbol{z}||}\right)\right)^2$

iv. product. $k_4(\boldsymbol{x}, \boldsymbol{z}) = k_3(\boldsymbol{x}, \boldsymbol{z})k_2(\boldsymbol{x}, \boldsymbol{z}) = \left(1 + \left(\frac{\boldsymbol{x}}{||\boldsymbol{x}||}\right) \cdot \left(\frac{\boldsymbol{z}}{||\boldsymbol{z}||}\right)\right)^3$

For step 2, note that $k(\boldsymbol{x}, \boldsymbol{z}) = 1$ is a valid kernel given by the constant feature mapping $\phi(\boldsymbol{x}) = 1$.

(c) **(3 pts)** Given vectors $\boldsymbol{x}$ and $\boldsymbol{z}$ in $\mathbb{R}^2$, define the kernel $k_\beta(\boldsymbol{x}, \boldsymbol{z}) = (1 + \beta\boldsymbol{x} \cdot \boldsymbol{z})^3$ for any value $\beta > 0$. Find the corresponding feature map $\phi_\beta(\cdot)$[1]. What are the similarities/differences from the kernel $k(\boldsymbol{x}, \boldsymbol{z}) = (1 + \boldsymbol{x} \cdot \boldsymbol{z})^3$, and what role does the parameter β play? **Solution:** To show that k_β is a kernel, simply use the same feature mapping as used by the polynomial kernel of degree 3, but first scale $\boldsymbol{x}$ by $\sqrt{\beta}$. So, in effect they are both polynomial kernels of degree 3. If you look at the resulting feature vector, the offset term 1 is unchanged, the linear terms are scaled by $\sqrt{\beta}$, the quadratic terms are scaled by β, and the cubic terms are scaled by $\beta^{1.5}$. Although the model class remains unchanged, this changes how we penalize the features during learning (from the $||\boldsymbol{\theta}||^2$ in the objective). In particular, higher-order features will become more costly to use, so this will bias more towards a lower-order polynomial.

[1] You may use any external program to expand the cubic.

That is,

$$\begin{aligned}
k_\beta(\boldsymbol{x}, \boldsymbol{z}) &= (1 + \beta \boldsymbol{x} \cdot \boldsymbol{z})^3 \\
&= (1 + \beta (x_1 z_1 + x_2 z_2))^3 \\
&= 1 + 3\beta (x_1 z_1 + x_2 z_2) + 3\beta^2 \left(x_1^2 z_1^2 + 2 x_1 z_1 x_2 z_2 + x_2^2 z_2^2\right) \\
&\qquad + \beta^3 \left(x_1^3 z_1^3 + 3 x_1^2 z_1^2 x_2 z_2 + 3 x_1 z_1 x_2^2 z_2^2 + x_2^3 z_2^3\right)
\end{aligned}$$

so that

$$\phi_\beta(\boldsymbol{x}) = (1, \sqrt{3\beta} x_1, \sqrt{3\beta} x_2, \sqrt{3}\beta x_1^2, \sqrt{6}\beta x_1 x_2, \sqrt{3}\beta x_2^2, \sqrt{\beta^3} x_1^3, \sqrt{3\beta^3} x_1^2 x_2, \sqrt{3\beta^3} x_1 x_2^2, \sqrt{\beta^3} x_2^3)^T$$

The m^{th}-order terms in $\phi_\beta(\cdot)$ are scaled by $\beta^{m/2}$, so β trades off the influence of the higher-order versus lower-order terms in the polynomial. If $\beta = 1$, then $\beta^{1/2} = \beta = \beta^{3/2}$ so that $k_\beta = k$. If $0 < \beta < 1$, then $\beta^{1/2} > \beta > \beta^{3/2}$ so that lower-order terms have more weight and higher-order terms less weight; as $\beta \to 0$, k_β approaches $1 + 3\beta \boldsymbol{x} \cdot \boldsymbol{z}$ (a linear separator). If $\beta > 1$, the trade-off is reversed; as $\beta \to \infty$, only the constant and cubic terms in k_β remain.

3 SVM [8 pts]

Suppose we are looking for a maximum-margin linear classifier *through the origin*, i.e. $b = 0$ (also hard margin, i.e., no slack variables). In other words, we minimize $\frac{1}{2}||\boldsymbol{\theta}||^2$ subject to $y_n \boldsymbol{\theta}^T \boldsymbol{x}_n \geq 1, n = 1, \ldots, N$.

(a) **(2 pts)** Given a single training vector $\boldsymbol{x} = (a, e)^T$ with label $y = -1$, what is the $\boldsymbol{\theta}^*$ that satisfies the above constrained minimization? **Solution:** The SVM with one negative data point orients $\boldsymbol{\theta}$ in the opposite direction of the single data point $\boldsymbol{x}$ in order to minimize the objective function while satisfying the constraint $y_n \boldsymbol{\theta}^T \boldsymbol{x}_n = 1$. The corresponding $\boldsymbol{\theta}$ is

$$\boldsymbol{\theta}^* = -\frac{\boldsymbol{x}}{||\boldsymbol{x}||^2}.$$

(b) **(2 pts)** Suppose we have two training examples, $\boldsymbol{x}_1 = (1, 1)^T$ and $\boldsymbol{x}_2 = (1, 0)^T$ with labels $y_1 = 1$ and $y_2 = -1$. What is $\boldsymbol{\theta}^*$ in this case, and what is the margin γ? **Solution:** In this case, the SVM uses both data points as support vectors such that $y_1 \boldsymbol{\theta}^T \boldsymbol{x}_1 = 1$ and $y_2 \boldsymbol{\theta}^T \boldsymbol{x}_2 = 1$. The corresponding $\boldsymbol{\theta}$ and γ are

$$\boldsymbol{\theta}^* = [-1, 2]^T, \gamma = \frac{1}{\sqrt{5}}.$$

(c) **(4 pts)** Suppose we now allow the offset parameter b to be non-zero. How would the classifier and the margin change in the previous question? What are $(\boldsymbol{\theta}^*, b^*)$ and γ? Compare your solutions with and without offset. **Solution:** In this case, the SVM uses both data points as support vectors such that $y_1 \boldsymbol{\theta}^T \boldsymbol{x}_1 + b = 1$ and $y_2 \boldsymbol{\theta}^T \boldsymbol{x}_2 + b = 1$. The corresponding $\boldsymbol{\theta}$, b, and γ are

$$\boldsymbol{\theta}^* = [0, 2]^T, b^* = -1, \gamma = \frac{1}{2}$$

The margin for the classifier with offset is larger than the margin for the classifier without offset.

4 Implementation: Digit Recognizer [48 pts]

In this exercise, you will implement a digit recognizer in pytorch. Our data contains pairs of 28×28 images $\mathbf{x}_n$ and the corresponding digit labels $y_n \in \{0, 1, 2\}$. For simplicity, we view a 28×28 image $\mathbf{x}_n$ as a 784-dimensional vector by concatenating the row pixels. In other words, $\mathbf{x}_n \in \mathbb{R}^{784}$. Your goal is to implement two digit recognizers (`OneLayerNetwork` and `TwoLayerNetwork`) and compare their performances.

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code and data

- code : `CS146-Winter2022-PS3.ipynb`
- data : `ps3_train.csv`, `ps3_valid.csv`, `ps3_test.csv`

Please use your *@g.ucla.edu* email id to access the code and data. Similar to *PS1*, copy the colab notebook to your drive and make the changes. Mount the drive appropriately and copy the shared data folder to your drive to access via colab. The notebook has marked blocks where you need to code.

$\#\#\# ========= TODO : START ========= \#\#\#$

$\#\#\# ========= TODO : END ========== \#\#\#$

Note: For the questions requiring you to complete a piece of code, you are expected to copy-paste your code as a part of the solution in the submission pdf. Tip: If you are using LaTeX, check out the Minted package (example) for code highlighting.

Data Visualization and Preparation [10 pts]

(a) Randomly select three training examples with *different labels* and print out the images by using `plot_img` function. Include those images in your report. [2 pts]

Solution:

(b) The loaded examples are numpy arrays. Convert the numpy arrays to tensors. You do not need to submit anything for this part.[3 pts]

Solution:

(c) Prepare `train_loader`, `valid_loader`, and `test_loader` by using `TensorDataset` and `DataLoader`. We expect to get a batch of pairs $(\mathbf{x}_n, y_n)$ from the dataloader. Please set the batch size to 10. [5 pts]

You can refer `https://pytorch.org/docs/stable/data.html` for more information about `TensorDataset` and `DataLoader`.

Solution:

One-Layer Network [15 pts]

For one-layer network, we consider a *784–3* network. In other words, we learn a 784×3 weight matrix $\mathbf{W}$ (you can ignore the bias term). Given a $\mathbf{x}_n$, we can compute the probability vector

$\mathbf{p}_n = \sigma(\mathbf{W}^\top \mathbf{x}_n)$, where $\sigma(.)$ is the element-wise sigmoid function and $\mathbf{p}_{n,c}$ denotes the probability of class c. Then, we focus on the *cross entropy loss*

$$-\sum_{n=0}^{N}\sum_{c=0}^{C}\mathbf{1}(c = y_n)\log(\mathbf{p}_{n,c})$$

where N is the number of examples, C is the number of classes, and $\mathbf{1}$ is the indicator function.

(d) Implement the constructor of `OneLayerNetwork` with `torch.nn.Linear` and implement the `forward` function to compute the outputs of the single fully connected layer i.e. $\mathbf{W}^\top \mathbf{x}_n$. Notice that we do not compute the sigmoid function here since we will use `torch.nn.CrossEntropyLoss` later. [5 pts]

You can refer to https://pytorch.org/docs/stable/generated/torch.nn.Linear.html for more information about `torch.nn.Linear` and refer to https://pytorch.org/docs/stable/generated/torch.nn.CrossEntropyLoss.html for more information about using `torch.nn.CrossEntropyLoss`.

Solution:

(e) Create an instance of `OneLayerNetwork`, set up a criterion with `torch.nn.CrossEntropyLoss`, and set up a SGD optimizer with learning rate 0.0005 by using `torch.optim.SGD` [2 pts]

Solution:

You can refer to https://pytorch.org/docs/stable/optim.html for more information about `torch.optim.SGD`.

(f) Implement the training process. This includes forward pass, initializing gradients to zeros, computing loss, loss.backward, and updating model parameters. If you implement everything correctly, after running the `train` function in main, you should get results similar to the following. [8 pts]

```
Start training OneLayerNetwork...
| epoch  1 | train loss 1.075387 | train acc 0.453333 | valid loss ...
| epoch  2 | train loss 1.021301 | train acc 0.563333 | valid loss ...
| epoch  3 | train loss 0.972599 | train acc 0.630000 | valid loss ...
| epoch  4 | train loss 0.928335 | train acc 0.710000 | valid loss ...
...
```

Solution:

Two-Layer Network [7 pts]

For two-layer network, we consider a *784–400–3* network. In other words, the first layer will consist of a fully connected layer with 784×400 weight matrix $\mathbf{W}_1$ and a second layer consisting of 400×3 weight matrix $\mathbf{W}_2$ (you can ignore the bias term). Given a $\mathbf{x}_n$, we can compute the probability vector $\mathbf{p}_n = \sigma(\mathbf{W}_2^\top \sigma(\mathbf{W}_1^\top \mathbf{x}_n))$, where $\sigma(.)$ is the element-wise sigmoid function. Again, we focus on the *cross entropy loss*, hence the network will impelement $\mathbf{W}_2^\top \sigma(\mathbf{W}_1^\top \mathbf{x}_n)$ (note the outer sigmoid will be taken care of implicitly in our loss).

(g) Implement the constructor of `TwoLayerNetwork` with `torch.nn.Linear` and implement the `forward` function to compute $\mathbf{W}_2^\top \sigma(\mathbf{W}_1^\top \mathbf{x}_n)$. [5 pts]

Solution:

(h) Create an instance of `TwoLayerNetwork`, set up a criterion with `torch.nn.CrossEntropyLoss`, and set up a SGD optimizer with learning rate 0.0005 by using `torch.optim.SGD`. Then train `TwoLayerNetwork`. [2 pts]

Solution:

Performance Comparison [16 pts]

(i) Generate a plot depicting how `one_train_loss`, `one_valid_loss`, `two_train_loss`, `two_valid_loss` varies with epochs. Include the plot in the report and describe your findings. [3 pts]

Solution:

(j) Generate a plot depicting how `one_train_acc`, `one_valid_acc`, `two_train_acc`, `two_valid_acc` varies with epochs. Include the plot in the report and describe your findings. [3 pts]

Solution:

(k) Calculate and report the test accuracy of both the one-layer network and the two-layer network. How can you improve the performance of the two-layer network ? [3 pts]

Solution:

(l) Replace the SGD optimizer with the Adam optimizer and do the experiments again. Show the loss figure, the accuracy figure, and the test accuracy. Include the figures in the report and describe your findings. [7 pts]

You can refer to https://pytorch.org/docs/stable/optim.html for more information about `torch.optim.Adam`.

Solution: