Policies

- Due 9 PM, February 2nd, via Gradescope.
- You are free to collaborate on all of the problems, subject to the collaboration policy stated in the syllabus.
- In this course, we will be using Google Colab for code submissions. You will need a Google account.
- This set uses PyTorch, a Python package for neural networks. We recommend using Google Colab, which comes with PyTorch already installed. There will be a PyTorch recitation to help you get started.

Submission Instructions

- Submit your report as a single .pdf file to Gradescope (entry code 7426YK), under "Set 4 Report".
- In the report, include any images generated by your code along with your answers to the questions.
- Submit your code by **sharing a link in your report** to your Google Colab notebook for each problem (see naming instructions below). Make sure to set sharing permissions to at least "Anyone with the link can view". **Links that can not be run by TAs will not be counted as turned in.** Check your links in an incognito window before submitting to be sure.
- For instructions specifically pertaining to the Gradescope submission process, see https://www.gradescope.com/get_started#student-submission.

Google Colab Instructions

For each notebook, you need to save a copy to your drive.

- 1. Open the github preview of the notebook, and click the icon to open the colab preview.
- 2. On the colab preview, go to File \rightarrow Save a copy in Drive.
- 3. Edit your file name to "lastname_firstname_set_problem", e.g. "yue_yisong_set4_prob2.ipynb"

TA Office Hours

- Megan Tjandrasuwita [Question 1 and Question 2]
 - Monday 1/31: 3:00 pm 4:00 pm (Annenberg North Lawn Tent), Tuesday, 2/1: 5:00 pm 6:00 pm (Zoom)
- Pantelis Vafidis [Question 3]
 - Monday, 1/31: 6:00 pm 8:00 pm (Zoom)

1 Deep Learning Principles [35 Points]

Relevant materials: lectures on deep learning

For problems A and B, we'll be utilizing the Tensorflow Playground to visualize/fit a neural network.

Problem A [5 points]: Backpropagation and Weight Initialization Part 1

Fit the neural network at this link for about 250 iterations, and then do the same for the neural network at this link. Both networks have the same architecture and use ReLU activations. The only difference between the two is how the layer weights were initialized – you can examine the layer weights by hovering over the edges between neurons.

Give a mathematical justification, based on what you know about the backpropagation algorithm and the ReLU function, for the difference in the performance of the two networks.

Solution A.: The first network decreases the training and test loss with more iterations, while the second network has the same error throughout fitting. The first network was initialized with non-zero layer weights while the second network's layer weights were all 0. We know ReLU(S) = max(0,S), so the second network will have sums of 0 for each layer. As a result, the gradient of ReLU and $\mathbf{W}^l = \frac{\delta \mathbf{s}^l}{\delta \mathbf{x}^{l-1}}$ both vanish. All the gradients vanish and the backpropagation algorithm will propagate 0 throughout the network. Thus, the network will never update its weights and the model will not change. With non-zero layer weights, we will not have vanishing gradients because ReLU(S) will be nonzero. Thus the backpropagation algorithm will be able to update the weights with each iteration and reduce the loss function.

Problem B [5 points]: Backpropagation and Weight Initialization Part 2

Reset the two demos from part i (there is a reset button to the left of the "Run" button), change the activation functions of the neurons to sigmoid instead of ReLU, and train each of them for 4000 iterations.

Explain the differences in the models learned, and the speed at which they were learned, from those of part i in terms of the backpropagation algorithm and the sigmoid function.

Solution B.: In terms of the first network, the sigmoid function resulted in a much smoother decision boundary than the one given by the ReLU function. The sigmoid function uses a soft threshold and is differentiable for all sums, compared to the ReLU function which is not differentiable at 0. The model with the ReLU function learned a lot faster than the model with the sigmoid function. The network trained with the ReLU function decreased the training and test loss to 0.001 in about 200 iterations, while the sigmoid function took around 4000 iterations to decrease the loss to 0.001. The sigmoid function is saturating while the ReLU function is nonsaturating. As a result, the sigmoid function has small gradients in many places. The backpropagation algorithm will propagate these small gradients throughout the network and since the gradients of sigmoid are small, the gradients become smaller as the algorithm propagates back more. Thus, the weights are updated slower with the sigmoid function compared to the ReLU function.

For the second network, the sigmoid function changed the weights and decreased losses to ≈ 0.4 at the end of the 4000 iterations even with initial weights of 0. On the other hand, the model with ReLU did not change weights or decrease losses at all. With the sigmoid, the gradient can be very small but will never be exactly 0. As a result, the weights will be slowly updated with back propagation.

Problem C: [10 Points]

When training any model using SGD, it's important to shuffle your data to avoid correlated samples. To illustrate one reason for this that is particularly important for ReLU networks, consider a dataset of 1000 points, 500 of which have positive (+1) labels, and 500 of which have negative (-1) labels. What happens if we train a fully-connected network with ReLU activations using SGD, looping through all the negative examples before any of the positive examples? (Hint: this is called the "dying ReLU" problem.)

Solution C: If we loop through all the negative examples before the positive examples, the SGD will update the weights based on all the negative examples first. As a result, the weights will develop a negative bias term so all the negative examples are classified correctly. As a result, all the sums that ReLU takes as inputs will be negative, and ReLU will output 0. As a result, the gradients will be 0 so the backpropagation algorithm will never update the weights and the neurons "die". Thus, even if we use SGD on positive examples later, the model will not be able to learn.

Problem D: Approximating Functions Part 1 [7 Points]

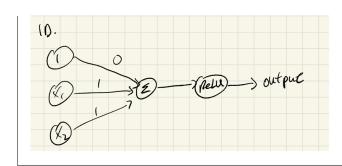
Draw or describe a fully-connected network with ReLU units that implements the OR function on two 0/1-valued inputs, x_1 and x_2 . Your networks should contain the minimum number of hidden units possible. The OR function $OR(x_1, x_2)$ is defined as:

$$OR(1,0) \ge 1$$

 $OR(0,1) \ge 1$
 $OR(1,1) \ge 1$
 $OR(0,0) = 0$

Your network need only produce the correct output when $x_1 \in \{0,1\}$ and $x_2 \in \{0,1\}$ (as described in the examples above).

Solution D.:



Problem E: Approximating Functions Part 2 [8 Points]

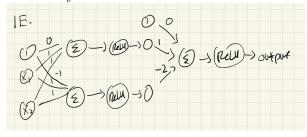
What is the minimum number of fully-connected layers (with ReLU units) needed to implement an XOR of two 0/1-valued inputs x_1, x_2 ? Recall that the XOR function is defined as:

$$\begin{aligned} \mathsf{XOR}(1,0) &\geq 1 \\ \mathsf{XOR}(0,1) &\geq 1 \\ \mathsf{XOR}(0,0) &= \mathsf{XOR}(1,1) = 0 \end{aligned}$$

For the purposes of this problem, we say that a network f computes the XOR function if $f(x_1, x_2) = XOR(x_1, x_2)$ when $x_1 \in \{0, 1\}$ and $x_2 \in \{0, 1\}$ (as described in the examples above).

Explain why a network with fewer layers than the number you specified cannot compute XOR.

Solution E.: The minimum number of fully-connected layers is 2 in order to implement XOR. The XOR dataset, $\{(0,1,y=1),(1,0,y=1),(0,0,y=0),(1,1,y=0)\}$, is not linearly separable. A fully-connected one layer network is just a perceptron, thus it can only compute linear functions. Thus, we need at least two layers to implement XOR correctly. We can decompose the XOR function into OR and NOT AND and implement XOR with two layers:



2 Depth vs Width on the MNIST Dataset [25 Points, 6 EC Points]

Relevant Materials: Lectures on Deep Learning

MNIST is a classic dataset in computer vision. It consists of images of handwritten digits (0 - 9) and the correct digit classification. In this problem you will implement a deep network using PyTorch to classify MNIST digits. Specifically, you will explore what it really means for a network to be "deep", and how depth vs. width impacts the classification accuracy of a model. You will be allowed at most N hidden units, and will be expected to design and implement a deep network that meets some performance baseline on the MNIST dataset.

Problem A: Installation [2 Points]

Before any modeling can begin, PyTorch must be installed. PyTorch is an automatic differentiation framework that is widely used in machine learning research. We will also need the **torchvision** package, which will make downloading the MNIST dataset much easier.

If you use Google Colab (recommended), you won't need to install anything.

If you want to run PyTorch locally, follow the steps on

https://pytorch.org/get-started/locally/#start-locally. Select the 'Stable' build and your system information. We highly recommend using Python 3.6+. CUDA is not required for this class, but it is necessary if you want to do GPU-accelerated deep learning in the future.

Write down the version numbers for both **torch** and **torchvision** that you have installed. On Google Colab, you can find version numbers by running:

!pip list | grep torch

Solution A: *torch:* 1.10.0+*cu*111, *torchvision:* 0.11.1+*cu*111.

Problem B: The Data [5 Points]

Load the MNIST dataset using torchvision; see the problem 2 sample code for how.

Image inputs in PyTorch are generally 3D tensors with the shape (no. of channels, height, width). Examine the input data. What are the height and width of the images? What do the values in each array index represent? How many images are in the training set? How many are in the testing set? You can use the **imshow** function in matplotlib if you'd like to see the actual pictures (see the sample code).

Solution B.: There are 60000 images in the training set and 10000 in the testing set. The height and width of the images are 28 x 28. The values in each array index represent the intensity of each pixel (greyscale).

Problem C: Modeling Part 1 [10 Points]

Using PyTorch's "Sequential" model class, build a deep network to classify the handwritten digits. You may **only** use the following layers:

- Flatten: Flattens any tensor into a single vector
- Linear: A fully-connected layer
- **ReLU** (activation): Sets negative inputs to 0
- **Softmax (activation):** Rescales input so that it can be interpreted as a (discrete) probability distribution.
- **Dropout:** Takes some probability and at every iteration sets weights to zero at random with that probability (effectively regularization)

A sample network with 20 hidden units is in the sample code file. (Note: You may use multiple layers as long as the total number of hidden units are within the limit. Activations, Dropout, and your last Linear layer do not count toward your hidden unit count, because the final layer is "observed" and not hidden.)

Use categorical cross entropy as your loss function. There are also a number of optimizers you can use (an optimizer is just a fancier version of SGD), and feel free to play around with them, but RMSprop and Adam are the most popular and will probably work best. You also should find the batch size and number of epochs that give you the best results (default is batch size = 32, epochs=10).

Look at the sample code to see how to train your model. You can tinker with the network architecture by swapping around layers and parameters.

Your task. Using at most 100 hidden units, build a network using only the allowed layers that achieves test accuracy of at least 0.975. Turn in the code of your model as well as the best test accuracy that it achieved.

Problem D: Modeling Part 2 [8 Points]

Repeat problem C, except that now you may use 200 hidden units and must build a model with at least 2 hidden layers that achieves test accuracy of at least 0.98.

```
Solution D:
Model:
model = nn.Sequential(
    nn.Flatten(),
    nn.Linear(784, 150),
    nn.Dropout(0.25),
    nn.ReLU(),
    nn.Linear(150, 50),
    nn.Dropout(0.25),
    nn.ReLU(),
    nn.Linear(50, 10)
)
Test set: Average loss: 0.0003, Accuracy: 9822/10000 (98.2200).
```

Problem E: Modeling Part 3 [6 EC Points]

Repeat problem C, except that now you may use 1000 hidden units and must build a model with at least 3 hidden layers that achieves test accuracy of at least 0.983.

```
Solution E:
Model:
model = nn.Sequential(
     nn.Flatten(),
     nn.Linear(784, 400),
     nn.Dropout(0.28),
     nn.ReLU(),
     nn.Linear(400, 300),
     nn.Dropout(0.30),
     nn.ReLU(),
     nn.Linear(300, 200),
     nn.Dropout(0.30),
     nn.ReLU(),
     nn.Linear(200, 50),
     nn.Dropout(0.32),
     nn.ReLU(),
     nn.Linear(50, 10)
 )
Test set: Average loss: 0.0005, Accuracy: 9853/10000 (98.5300).
```

3 Convolutional Neural Networks [40 Points]

Relevant Materials: Lecture on CNNs

Problem A: Zero Padding [5 Points]

Consider a convolutional network in which we perform a convolution over each 8×8 patch of a 20×20 input image. It is common to zero-pad input images to allow for convolutions past the edges of the images. An example of zero-padding is shown below:

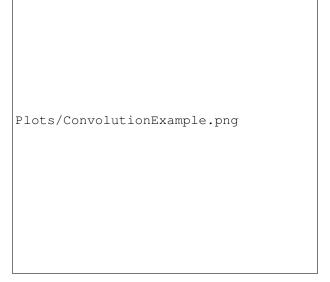


Figure: A convolution being applied to a 2×2 patch (the red square) of a 3×3 image that has been zero-padded to allow convolutions past the edges of the image.

What is one benefit and one drawback to this zero-padding scheme (in contrast to an approach in which we only perform convolutions over patches entirely contained within an image)?

Solution A: One benefit of zero-padding is that the output has the same dimensions as the input. With zero-padding, we get a 3x3 output as opposed to without zero-padding, we get a 2x2 output with the same convolution. One drawback of zero-padding is that we waste computational resources from processing the zero elements from padding.

5 x 5 Convolutions

Consider a single convolutional layer, where your input is a 32×32 pixel, RGB image. In other words, the input is a $32 \times 32 \times 3$ tensor. Your convolution has:

- Size: $5 \times 5 \times 3$
- Filters: 8
- Stride (i.e. how much the filter is displaced after each application): 1
- No zero-padding

Problem B [2 points]: What is the number of parameters (weights) in this layer, including a bias term for each filter?

Solution B.: There are 608 parameters: $[5 \times 5 \times 3 + 1 \text{ (bias term)}] * 8 \text{ filters.}$

Problem C [3 points]: What is the shape of the output tensor? Remember that convolution is performed over the first two dimensions of the input only, and that a filter is applied to all channels.

Solution C.: Shape of output tensor = $(28 \times 28 \times 8)$: (5×5) convolution over (32×32) with stride 1 and no zero padding gives $(32 - 5 + 1) \times (32 - 5 + 1) \times 8$ (for each filter).

Max/Average Pooling

Pooling is a downsampling technique for reducing the dimensionality of a layer's output. Pooling iterates across patches of an image similarly to a convolution, but pooling and convolutional layers compute their outputs differently: given a pooling layer B with preceding layer A, the output of B is some function (such as the max or average functions) applied to patches of A's output.

Below is an example of max-pooling on a 2-D input space with a 2×2 filter (the max function is applied to 2×2 patches of the input) and a stride of 2 (so that the sampled patches do not overlap):

Plots/MaxPool.png

Average pooling is similar except that you would take the average of each patch as its output instead of the maximum.

Consider the following 4 matrices:

$$\begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$

Problem D [3 points]:

Apply 2×2 average pooling with a stride of 2 to each of the above images.

Solution D.:
$$\begin{bmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{4} \end{bmatrix}, \begin{bmatrix} \frac{1}{2} & 1 \\ \frac{1}{4} & \frac{1}{2} \end{bmatrix}, \begin{bmatrix} \frac{1}{4} & \frac{1}{2} \\ \frac{1}{2} & 1 \end{bmatrix}, \begin{bmatrix} \frac{1}{2} & \frac{1}{4} \\ 1 & \frac{1}{2} \end{bmatrix}$$

Problem E [3 points]:

Apply 2×2 max pooling with a stride of 2 to each of the above images.

Solution E.: All matrices have the same 2 x 2 max pooling with stride 2:

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

Problem F [4 points]:

Consider a scenario in which we wish to classify a dataset of images of various animals, where an animal may appear at various angles/locations of the image, and the image contains small amounts of noise (e.g. some pixels may be missing). Why might pooling be advantageous given these properties of our dataset?

Solution F.: The affect of individual pixels are lessened with pooling. As a result, even if there some missing pixels, the noise will not greatly impact the results of the pooling. If we take different angles/locations of the same animal, as long as the images are not distorted too much (max and average of pools are similar as before), the effects of missing pixels will be mitigated by the surrounding pixels of the animal. Thus, fitting the model to noise can be reduced.

PyTorch implementation

Problem G [20 points]:

Using PyTorch "Sequential" model class as you did in 2C, build a deep *convolutional* network to classify the handwritten digits in MNIST. You are now allowed to use the following layers (but **only** the following):

- Linear: A fully-connected layer
 - In convolutional networks, Linear (also called dense) layers are typically used to knit together higher-level feature representations.
 - Particularly useful to map the 2D features resulting from the last convolutional layer to categories for classification (like the 1000 categories of ImageNet or the 10 categories of MNIST).
 - Inefficient use of parameters and often overkill: for A input activations and B output activations, number of parameters needed scales as O(AB).
- Conv2d: A 2-dimensional convolutional layer
 - The bread and butter of convolutional networks, conv layers impose a translational-invariance prior on a fully-connected network. By sliding filters across the image to form another image, conv layers perform "coarse-graining" of the image.

- Networking several convolutional layers in succession helps the convolutional network knit together more abstract representations of the input. As you go higher in a convolutional network, activations represent pixels, then edges, colors, and finally objects.
- More efficient use of parameters. For N filters of $K \times K$ size on an input of size $L \times L$, the number of parameters needed scales as $O(NK^2)$. When N, K are small, this can often beat the $O(L^4)$ scaling of a Linear layer applied to the L^2 pixels in the image.
- MaxPool2d: A 2-dimensional max-pooling layer
 - Another way of performing "coarse-graining" of images, max-pool layers are another way of ignoring finer-grained details by only considering maximum activations over small patches of the input.
 - Drastically reduces the input size. Useful for reducing the number of parameters in your model.
 - Typically used immediately following a series of convolutional-activation layers.
- **BatchNorm2d:** Performs batch normalization (Ioffe and Szegedy, 2014). Normalizes the activations of previous layer to standard normal (mean 0, standard deviation 1).
 - Accelerates convergence and improves performance of model, especially when saturating nonlinearities (sigmoid) are used.
 - Makes model less sensitive to higher learning rates and initialization, and also acts as a form of regularization.
 - Typically used immediately before nonlinearity (Activation) layers.
- **Dropout:** Takes some probability and at every iteration sets weights to zero at random with that probability
 - An effective form of regularization. During training, randomly selecting activations to shut off forces network to build in redundancies in the feature representation, so it does not rely on any single activation to perform classification.
- **ReLU (activation):** Sets negative inputs to 0
- Softmax (activation): Rescales input so that it can be interpreted as a (discrete) probability distribution.
- **Flatten:** Flattens any tensor into a single vector (required in order to pass a 2D tensor output from a convolutional layer as input into Linear layers)

Your tasks. Build a network with only the allowed layers that achieves test accuracy of at least 0.985. You are required to use categorical cross entropy as your loss function and to train for 10 epochs with a batch size of 32. Note: your model must have fewer than 1 million parameters, as measured by the method given in the sample code. Everything else can change: optimizer (e.g., RMSProp, Adam), initial learning rates, dropout probabilities, layerwise regularizer strengths, etc. You are not required to use all of the layers, but

you must have at least one dropout layer and one batch normalization layer in your final model. Try to figure out the best possible architecture and hyperparameters given these building blocks!

In order to design your model, you should train your model for 1 epoch (batch size 32) and look at the final **test accuracy** after training. This should take no more than 10 minutes, and should give you an immediate sense for how fast your network converges and how good it is.

Set the probabilities of your dropout layers to 10 equally-spaced values $p \in [0,1]$, train for 1 epoch, and report the final model accuracies for each.

You can perform all of your hyperparameter validation in this way: vary your parameters and train for an epoch. After you're satisfied with the model design, you should train your model for the full 10 epochs.

In your submission. Turn in the code of your model, the test accuracy for the 10 dropout probabilities $p \in [0,1]$, and the final test accuracy when your model is trained for 10 epochs. We should have everything needed to reproduce your results.

Discuss what you found to be the most effective strategies in designing a convolutional network. Which regularization method was most effective (dropout, layerwise regularization, batch norm)?

Do you foresee any problem with this way of validating our hyperparameters? If so, why?

Hints:

- You are provided with a sample network that achieves a high accuracy. Starting with this network, modify some of the regularization parameters (layerwise regularization strength, dropout probabilities) to see if you can maximize the test accuracy. You can also add layers or modify layers (e.g. changing the convolutional kernel sizes, number of filters, stride, dilation, etc.) so long as the total number of parameters remains under the cap of 1 million.
- You may want to read up on successful convolutional architectures, and emulate some of their design principles. Please cite any idea you use that is not your own.
- To better understand the function of each layer, check the PyTorch documentation.
- Linear layers take in single vector inputs (ex: (784,)) but Conv2D layers take in tensor inputs (ex: (28, 28, 1)): width, height, and channels. Using the transformation transforms. ToTensor() when loading the dataset will reshape the training/test X to a 4-dimensional tensor (ex: (num_examples, width, height, channels)) and normalize values. For the MNIST dataset, channels=1. Typical color images have 3 color channels, 1 for each color in RGB.
- If your model is running slowly on your CPU, try making each layer smaller and stacking more layers so you can leverage deeper representations.
- Other useful CNN design principles:
 - CNNs perform well with many stacked convolutional layers, which develop increasingly largescale representations of the input image.

- Dropout ensures that the learned representations are robust to some amount of noise.
- Batch norm is done after a convolutional or dense layer and immediately prior to an activation/nonlinearity layer.
- Max-pooling is typically done after a series of convolutions, in order to gradually reduce the size of the representation.
- Finally, the learned representation is passed into a dense layer (or two), and then filtered down to the final softmax layer.

```
Solution G: Model:
 model = nn.Sequential(
    nn.Conv2d(1, 16, kernel_size=(3,3)),
nn.BatchNorm2d(16),
    nn.ReLU().
    nn.MaxPool2d(2),
    nn.Dropout(p=0.1),
    nn.Conv2d(16, 8, kernel_size=(3,3)),
nn.BatchNorm2d(8),
    nn.ReLU(),
nn.MaxPool2d(2),
    nn.Dropout(p=0.1),
    nn.Flatten(),
    nn.Linear(25*8, 64)
    nn.Linear(64, 10)
# PyTorch implementation of cross-entropy loss includes softmax layer
          test accuracy
  0.1
              0.9816
  0.2
              0.9684
  0.3
              0.9678
  0.4
              0.9686
  0.5
              0.9568
  0.6
              0.9541
  0.7
              0.9327
  0.8
              0.8740
  0.9
              0.8033
  1.0
              0.0971
```

Final test accuracy = 0.9856.

The most effective strategies in designing a convolutional network was following the CNN design principles provided above, such as adding batch normalization after convolutional layers, using max-pooling after convolutions, and having some dropout. The regularization method that was most effective was batch normalization. From the table, the test accuracy after 1 epoch was highest with p = 0.1, which was the lowest amount of dropout. Layerwise regularization was also not very effective in reducing overfitting. After training my first model with p = 0.1 for dropout, the training accuracy was high but the test accuracy was low. After I added batch normalization to the two convolutional layers, training error stayed about the same, but test accuracy significantly increased. One problem of validating our hyperparameters this way is that we tune our hyperparameters based on the validation accuracy. Thus, our model might be biased towards the validation data, which is not desirable

Machine Learning & Data Mining Derek Ing Set 4

Caltech CS/CNS/EE 155 January 26th, 2022

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Code Links:

Problem 2

Problem 3