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.:

We notice that the second network initializes all weights to 0 and as a result over the 250 iterations, no changes are made to the weights upon backpropogation and the network does not converge on a loss reduction instead performing as well as randomly guessing (50% *error), while the random initialization of the first network to non-zero weights leads to the network learning well and performing at* $< 1\%$ *test and training error. The mathematical justification for this is that the gradient of the loss function with respect to the weights (*$\frac{\partial L}{\partial W}$*) will be zero since the ReLU activatin function at input weight* $w = 0$ *results in ReLU function outputting zero and the input of the next layer being zero as well, meaning the gradien with respect to the weights at that layer and by the same logic for all other layers will be zero. Thus the gradient descent step* $W = W - \eta * \frac{\partial L}{\partial W} = W$ *and thus no learning takes place and all weights remain 0, resulting in the second network not learning at all and not performing well.*

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.:

The first network trains well to the data but takes considerably longer for the sigmoid activation function compared to the ReLU activation function. This occurs likely because the ReLU function does not saturate compared to the sigmoid function, meaning that the sigmoid function has many points where derivatives have magnitude close to zero and as a result learning is much slower, versus the constant derivative of the ReLU function with positive inputs and the zero-ing gradient in the negative inputs results in faster learning moves in the model and faster overall fitting to the data. For the seocnd network, we again see no change in the model performance because even though the sigmoid and its gradient at initialization 0 are non-zero the issue arises that all weights are equal to one another so all activation outputs are the same meaning each weight will learn the exact same thing over the same input at each layer and as a result all weights will move in the same direction. This seriously limits the space the model can expand to given all weights are equal and thus results in poor learning as witnessed in the demo.

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:

Looping through the negative valued training data first, the model will learning weights to fit the negative output, likely setting many of the weights to highly negative numbers during learning. This is problematic because the negative weights will result in negative output/ input to the activation function which for ReLU, negative inputs are set to zero and largely negative inputs will have derivative zero, essentially then becoming dead weights in that their derivatives being pushed to zero by the many negative weights will result in no updates being made to those weights. Thus, when all the negative weights are looped through first the model will learn many negative weights which will result in negative value input to the activation function at many/ all layers of the network even when the positive values are looped through meaning even for the positive values the derivative will be zero due to its negative input to the ReLU activation function and no learning will occur. Basically the initial negative points will train weights too far negative such that taking the gradient once the positive points are iterated will still result in taking the gradient on the negative side of the ReLU function (since all positive inputs will be made negative by the weights before being plugged into the ReLU) meaning gradient is zero and no learning will happen (weights are dead).

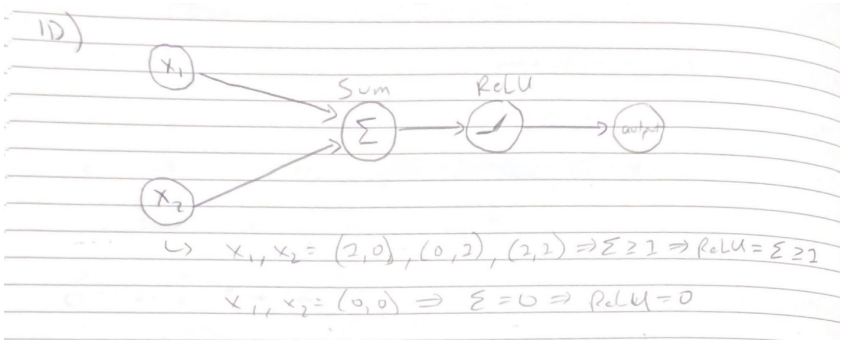
Problem D: Approximating Functions Part 1 **[7 Points]**

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:

$$\text{OR}(1,0) \geq 1$$
$$\text{OR}(0,1) \geq 1$$
$$\text{OR}(1,1) \geq 1$$
$$\text{OR}(0,0) = 0$$

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]**

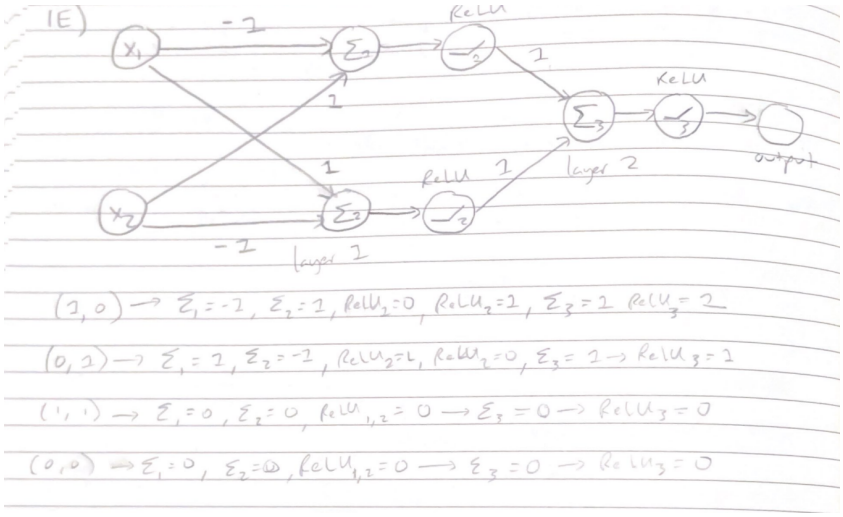
What is the minimum number of fully-connected layers (with ReLU units) needed to implement an XOR of two 0/1-valued inputs x_1, x_2? Recall that the XOR function is defined as:

$$\text{XOR}(1,0) \geq 1$$
$$\text{XOR}(0,1) \geq 1$$
$$\text{XOR}(0,0) = \text{XOR}(1,1) = 0$$

For the purposes of this problem, we say that a network f computes the XOR function if $f(x_1, x_2) = \text{XOR}(x_1, x_2)$ 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 following network implements the ReLU activation to implement the XOR function by using the first layer to determine two activations based on if X_1 and X_2 are different and the second for setting the activation output to ≥ 1 if the two inputs are different. Considering this is two layers, we notice that the same operation cannot be done in 1 layer because we cannot determine both decisions if $X_1 \neq X_2$ and forcing that operation output to be positive and ≥ 1 independent of what X_1, X_2 values are, so we must require more than 1 layer, and the solution provided uses 2 so it must thus be the solution using the minimum amount of layers required.

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

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.

To install both packages, 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.

Once you have finished installing, write down the version numbers for both **torch** and **torchvision** that you have installed.

Solution A:

Not sure if this is correct, I already have both installed so running torch/ torchvision .__version__ output the following:

torch: 2.1.0+cu121

torchvision: 0.16.0+cu121

Problem B: The Data [3 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.:

The height and width of the images are 28 x 28 pixels. The values at each array index correspond to the whiteness of the pixel at that index of the image, with values of 0 being black and values closer to 1 getting progressively lighter towards white. There are 60000 images in the training set and 10000 images in the test set.

Problem C: Modeling Part 1 [8 Points]

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

- **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: 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. PyTorch should make it very easy to tinker with your network architecture.

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.

Hint: for best results on this problem and the two following problems, normalize the input vectors by dividing the values by 255 (as the pixel values range from 0 to 255).

Solution C:

Code for solution

Maximum accuracy achieved: .9777

Problem D: Modeling Part 2 [6 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:

Code for solution

Maximum accuracy achieved: .9824

Problem E: Modeling Part 3 [6 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:

Code for solution

Maximum accuracy achieved: .9836

3 Convolutional Neural Networks [40 Points]

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:

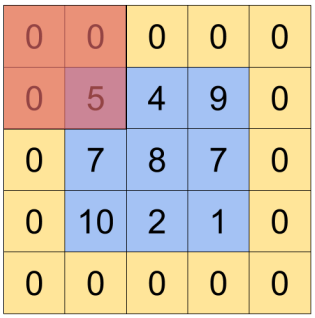


Figure: A convolution being applied to a 2×2 patch (the red square) of a 3×3 image that has been zero-padded to allow convolutions past the edges of the image.

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 the zero-padding scheme is the preservation of spatial size through the padded layer. Padding allows for the moving patch to iterate over a larger space and thus creates more outputs and a larger image output from that layer. This is a benefit since it allows for information at the edge pixels to be put through the layer with increased presence compared to without padding where edge pixels have much less presence than middle pixels. A drawback to this zero-padding scheme is the higher computational cost as the increased nodes and convolutions makes the hidden layers larger and thus the computation for optimizing the network a more difficult problem.

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: 1
- No zero-padding

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

Solution B.:

*The size of each filter is equal to the size of each convolution as the filters are applied to the convolutions so there are 5x5x3 = 75 + 1 (for bias term) = 76 weights per filter and 8 filters so there are 76 * 8 = 608 total weights in this layer.*

Problem C [3 points]: What is the shape of the output tensor?

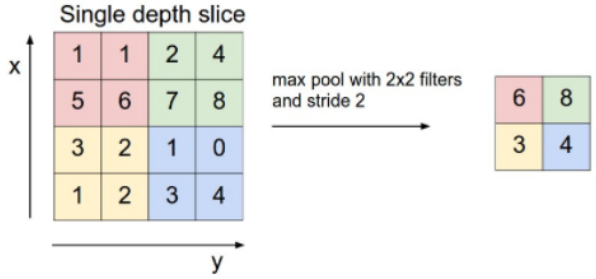
Solution C.:

The number of filters is equal to the number of channels in the output layer, and with a 5x5x3 convolution on a 32x32x3 image there will be 28x28 convolutions so the shape of the output feature is 28x28x8.

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):



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

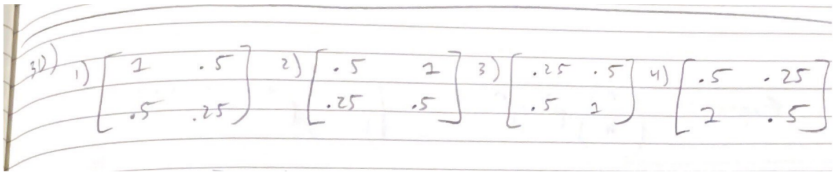
Consider the following 4 matrices:

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

Problem D [3 points]:

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

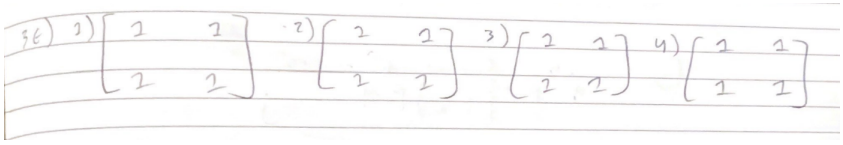
Solution D.:



Problem E [3 points]:

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

Solution E.:



Problem F [4 points]:

Consider a scenario in which we wish to classify a dataset of images of various animals, taken at various angles/locations and containing small amounts of noise (e.g. some pixels may be missing). Why might pooling be advantageous given these distortions in our dataset?

Solution F.:

We do not want weights to be trained on missing/ noisy pixels, instead taking the average/ max of a small patches across the image will better generalize the information provided by the image and remove the noise as operations such as averaging aim to best capture the general values of data and thus represent values that are less affected by noise. This would help with learning beyond the pooling layer as the removal of noise/ weights on missing pixels should lead to better learning as the model is not thrown off by bad quality data.

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 non-linearities (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 (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 probabil-

ities) 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 large-scale 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.:

Code for solution

The final errors on the last epoch gave accuracy of .9855 but a max of 98.95 was achieved at epoch 6. Some effective strategies that I test in building the network were padding, and moving MaxPool2D to later layers so the reduction of information takes place after multiple convolutions rather than after the first one. Reading the following article: link I also tested using bigger kernel sizes initially to generalize larger signals in initial layers and smaller kernel sizes in deeper layers to learn on finer portions of the images, I also added 2 layers following the idea of deeper networks outperforming wider ones. A BatchNorm layer after convolutions and before activation layers also helped when testing. In terms of regularization, smaller dropout probabilities seemed to work well, specifically when testing for $p \in [0, 1]$, the error minimizing p value was $p = 1/9$. The problemsI foresee with this type of hyperparameter validation is that it is computationally very long and the space of parameters to test over is very large. The test over the dropout probabilities can easily be replicated over larger spaced parameters

such as kernel size, channel quantities, etc. all which combine for a very rigorous but very long testing process. Additionally with only 1 epoch of testing it is difficult to determine trends of over/ underfitting as cannot deduce any movements in test error in relation to movements in training error as there are no movements over a singular example.