Machine Learning & Data Mining
Set 1

Caltech CS/CNS/EE 155
January 4^{th}, 2022

Policies

- Due 9 PM PST, January 12^{th} on Gradescope.
- You are free to collaborate on all of the problems, subject to the collaboration policy stated in the syllabus.
- If you have trouble with this homework, it may be an indication that you should drop the class.
- In this course, we will be using Google Colab for code submissions. You will need a Google account.

Submission Instructions

- Submit your report as a single .pdf file to Gradescope (entry code 7426YK), under "Set 1 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_originaltitle", e.g."yue_yisong_3_notebook_part1.ipynb"

1 Basics [16 Points]

Relevant materials: lecture 1

Answer each of the following problems with 1-2 short sentences.

Problem A [2 points]: What is a hypothesis set?

Solution A: *In short, the hypothesis set consists of all models and model parameters that are under exploration to learn a supervised relationship.*

Problem B [2 points]: What is the hypothesis set of a linear model?

Solution B: *The space of all functions given by $w * \phi(x)$ where w is a weight matrix and $\phi(x)$ is a polynomial function of x.*

Problem C [2 points]: What is overfitting?

Solution C: *Overfitting occurs when a model learns too closely to the data given to it but does not generalize well to the underlying distribution of all the data. In practice, this occurs when the training error is low but the validation error is high.*

Problem D [2 points]: What are two ways to prevent overfitting?

Solution D: *(1) cross-validation, which means checking the error on a validation set and making sure that the validation error decreases during training. (2) early stopping, or stopping training after fewer epochs.*

Problem E [2 points]: What are training data and test data, and how are they used differently? Why should you never change your model based on information from test data?

Solution E: *The training data is seen by the model to learn parameters, while the test data is also used to verify that the model is actually performing well. The model should never see the test data because they it could overfit to the distriubtion of the test data at the expense of generalizability to the underlying true distribution.*

Problem F [2 points]: What are the two assumptions we make about how our dataset is sampled?

Solution F: *(1) the X inputs and (2) the Y labels are sampled uniformly independently from their respective underlying true distributions.*

Problem G [2 points]: Consider the machine learning problem of deciding whether or not an email is spam. What could X, the input space, be? What could Y, the output space, be?

Solution G: *Each entry in X could be a numerical embedding of all the words in the email. Each entry in Y could be a 0 or 1 classification of whether or not the email is spam.*

Problem H [2 points]: What is the k-fold cross-validation procedure?

Solution H: *1. Shuffle the data and split it into k equal partitions. 2. Selecting one of the partitions at a time, train the model on the remaining k-1 partitions and calculate the validation error on the selected partition. 3. Repeat for each of the partitions and average together all of the validation errors.*

2 Bias-Variance Tradeoff [34 Points]

Relevant materials: lecture 1

Problem A [5 points]: Derive the bias-variance decomposition for the squared error loss function. That is, show that for a model f_S trained on a dataset S to predict a target $y(x)$ for each x,

$$\mathbb{E}_S\left[E_{\text{out}}\left(f_S\right)\right] = \mathbb{E}_x[\text{Bias}(x) + \text{Var}(x)]$$

given the following definitions:

$$\begin{aligned} F(x) &= \mathbb{E}_S\left[f_S(x)\right] \\ E_{\text{out}}(f_S) &= \mathbb{E}_x\left[\left(f_S(x) - y(x)\right)^2\right] \\ \text{Bias}(x) &= \left(F(x) - y(x)\right)^2 \\ \text{Var}(x) &= \mathbb{E}_S\left[\left(f_S(x) - F(x)\right)^2\right] \end{aligned}$$

Solution A:

$$\mathbb{E}_S[E_{out}(f_S)] = \mathbb{E}_S[\mathbb{E}_x\left[\left(f_S(x) - y(x)\right)^2\right]] \tag{1}$$

$$\mathbb{E}_S[E_{out}(f_S)] = \mathbb{E}_S\left[\mathbb{E}_x\left[\left(f_S(x) - F(x) + F(x) - y(x)\right)^2\right]\right] \tag{2}$$

$$\mathbb{E}_S[E_{out}(f_S)] = \mathbb{E}_S\left[\mathbb{E}_x\left[\left(f_S(x) - F(x)\right)^2 + \left(F(x) - y(x)\right)^2 + 2\left(f_S(x) - F(x)\right)\left(F(x) - y(x)\right)\right]\right] \tag{3}$$

$$\mathbb{E}_S[E_{out}(f_S)] = \mathbb{E}_x\left[\mathbb{E}_S\left[\left(f_S(x) - F(x)\right)^2\right] + \mathbb{E}_S\left[\left(F(x) - y(x)\right)^2\right] + 2\mathbb{E}_S\left[\left(f_S(x) - F(x)\right)\left(F(x) - y(x)\right)\right]\right] \tag{4}$$

$$\mathbb{E}_S[E_{out}(f_S)] = \mathbb{E}_x\left[\mathbb{E}_S\left[\left(f_S(x) - F(x)\right)^2\right] + \mathbb{E}_S\left[\left(F(x) - y(x)\right)^2\right]\right] \tag{5}$$

$$\mathbb{E}_S[E_{out}(f_S)] = \mathbb{E}_x\left[\mathbb{E}_S\left[\left(f_S(x) - F(x)\right)^2\right] + \left(F(x) - y(x)\right)^2\right] \tag{6}$$

$$\mathbb{E}_S\left[E_{out}\left(f_S\right)\right] = \mathbb{E}_x[\text{Bias}(x) + \text{Var}(x)] \tag{7}$$

In the following problems you will explore the bias-variance tradeoff by producing learning curves for polynomial regression models.

A *learning curve* for a model is a plot showing both the training error and the cross-validation error as a function of the number of points in the training set. These plots provide valuable information regarding the bias and variance of a model and can help determine whether a model is over– or under–fitting.

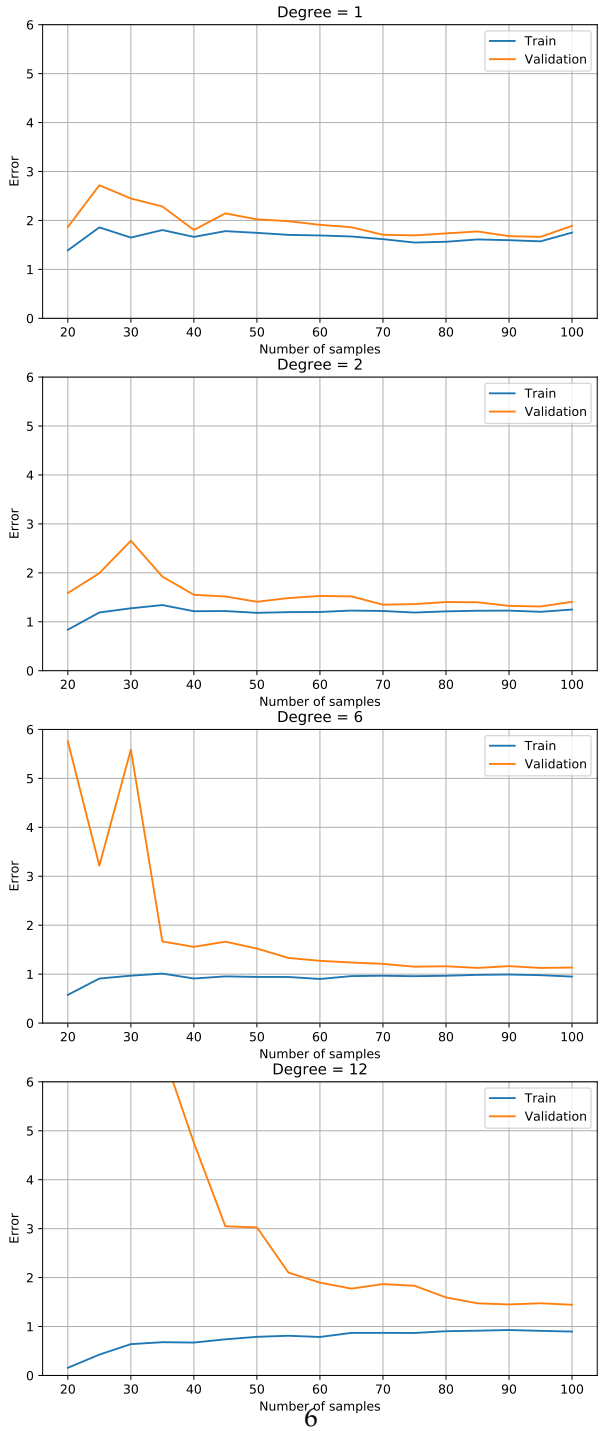
Polynomial regression is a type of regression that models the target y as a degree–d polynomial function of the input x. (The modeler chooses d.) You don't need to know how it works for this problem, just know that it produces a polynomial that attempts to fit the data.

Problem B [14 points]: Use the provided `2_notebook.ipynb` Jupyter notebook to enter your code for this question. This notebook contains examples of using NumPy's polyfit and polyval methods, and scikit-learn's KFold method; you may find it helpful to read through and run this example code prior to continuing with this problem. Additionally, you may find it helpful to look at the documentation for scikit-learn's learning_curve method for some guidance.

The dataset `bv_data.csv` is provided and has a header denoting which columns correspond to which values. Using this dataset, plot learning curves for 1st–, 2nd–, 6th–, and 12th–degree polynomial regression (4 separate plots) by following these steps for each degree $d \in \{1, 2, 6, 12\}$:

1. For each $N \in \{20, 25, 30, 35, \cdots, 100\}$:
   i. Perform 5-fold cross-validation on the first N points in the dataset (setting aside the other points), computing the both the training and validation error for each fold.
      - Use the mean squared error loss as the error function.
      - Use NumPy's polyfit method to perform the degree–d polynomial regression and NumPy's polyval method to help compute the errors. (See the example code and NumPy documentation for details.)
      - When partitioning your data into folds, although in practice you should randomize your partitions, for the purposes of this set, simply divide the data into K contiguous blocks.
   ii. Compute the average of the training and validation errors from the 5 folds.
2. Create a learning curve by plotting both the average training and validation error as functions of N. *Hint: Have same y-axis scale for all degrees d.*

Solution B: *See Code.*


Degree = 1
Train
Validation
Error
Number of samples
Degree = 2
Train
Validation
Error
Number of samples
Degree = 6
Train
Validation
Error
Number of samples
Degree = 12
Train
Validation
Error
Number of samples

Problem C [3 points]: Based on the learning curves, which polynomial regression model (i.e. which degree polynomial) has the highest bias? How can you tell?

Solution C: *The degree 1 polynomial has the highest bias. It converges to the highest error on the training and validation sets (when 100 samples are considered).*

Problem D [3 points]: Which model has the highest variance? How can you tell?

Solution D: *The gdegree 12 polynomial has the highest variance. On the training and validation sets, it has the highest range in errors given different numbers of samples.*

Problem E [3 points]: What does the learning curve of the quadratic model tell you about how much the model will improve if we had additional training points?

Solution E: *The training and validation errors have largely converged to a constant value as a function of training pts, thus adding additional training pts would likely not improve performance any further.*

Problem F [3 points]: Why is training error generally lower than validation error?

Solution F: *The model sees the training set when it is learning, thus it will be biased to do better on this distribution. On the other hand, the validation error is an approximation to how well the model performs on the underlying true distribution of the data, which is different from the training distribution and unseen.*

Problem G [3 points]: Based on the learning curves, which model would you expect to perform best on some unseen data drawn from the same distribution as the training data, and why?

Solution G: *The degree 6 model would likely have the best performance on unseen data because it has the lowest validation error, which is an estimate of the model's performance on generalized unseen data drawn from the same distribution.*

3 Stochastic Gradient Descent [36 Points]

Relevant materials: lecture 2

Stochastic gradient descent (SGD) is an important optimization method in machine learning, used everywhere from logistic regression to training neural networks. In this problem, you will be asked to first implement SGD for linear regression using the squared loss function. Then, you will analyze how several parameters affect the learning process.

Linear regression learns a model of the form:

$$f(x_1, x_2, \cdots, x_d) = \left(\sum_{i=1}^{d} w_i x_i \right) + b$$

Problem A [2 points]: We can make our algebra and coding simpler by writing $f(x_1, x_2, \cdots, x_d) = \mathbf{w}^T \mathbf{x}$ for vectors $\mathbf{w}$ and $\mathbf{x}$. But at first glance, this formulation seems to be missing the bias term b from the equation above. How should we define $\mathbf{x}$ and $\mathbf{w}$ such that the model includes the bias term?

Hint: *Include an additional element in* $\mathbf{w}$ *and* $\mathbf{x}$.

Solution A: *Append a column of 1s to the right of* $\mathbf{w}$ *and append* b *to the end of* $\mathbf{x}$.

Linear regression learns a model by minimizing the squared loss function L, which is the sum across all training data $\{(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_N, y_N)\}$ of the squared difference between actual and predicted output values:

$$L(f) = \sum_{i=1}^{N} (y_i - \mathbf{w}^T \mathbf{x}_i)^2$$

Problem B [2 points]: SGD uses the gradient of the loss function to make incremental adjustments to the weight vector $\mathbf{w}$. Derive the gradient of the squared loss function with respect to $\mathbf{w}$ for linear regression.

Solution B: *gradient* $= -2 \sum_{i=1}^{N} (y_i - \mathbf{w}^T \mathbf{x}_i) \mathbf{x}_i$

The following few problems ask you to work with the first of two provided Jupyter notebooks for this problem, `3_notebook_part1.ipynb`, which includes tools for gradient descent visualization. This notebook utilizes the files `sgd_helper.py` and `multiopt.mp4`, but you should not need to modify either of these files.

For your implementation of problems C-E, **do not** consider the bias term.

Problem C [8 points]: Implement the `loss`, `gradient`, and `SGD` functions, defined in the notebook, to perform SGD, using the guidelines below:

- Use a squared loss function.
- Terminate the SGD process after a specified number of epochs, where each epoch performs one SGD iteration for each point in the dataset.
- It is recommended, but not required, that you shuffle the order of the points before each epoch such that you go through the points in a random order. You can use `numpy.random.permutation`.
- Measure the loss after each epoch. Your `SGD` function should output a vector with the loss after each epoch, and a matrix of the weights after each epoch (one row per epoch). Note that the weights from all epochs are stored in order to run subsequent visualization code to illustrate SGD.

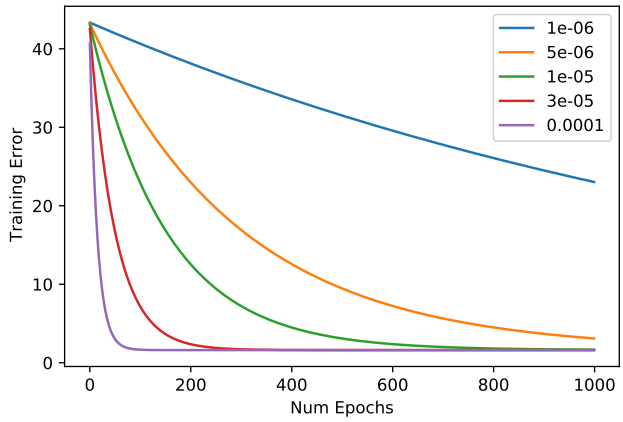
Solution C: *See Code.*

Problem D [2 points]: Run the visualization code in the notebook corresponding to problem D. How does the convergence behavior of SGD change as the starting point varies? How does this differ between datasets 1 and 2? Please answer in 2-3 sentences.

Solution D: *The starting point does not seem to have a signficiant effect on the convergence behavior. After 1000 epochs, the algorithm has basically converged to the same minimum, independent of the starting point. Even though the loss landscape is different for datasets 1 and 2, this observed behavior is the same.*

Problem E [6 points]: Run the visualization code in the notebook corresponding to problem E. One of the cells—titled "Plotting SGD Convergence"—must be filled in as follows. Perform SGD on dataset 1 for each of the learning rates $\eta \in \{$1e-6, 5e-6, 1e-5, 3e-5, 1e-4$\}$. On a single plot, show the training error vs. number of epochs trained for each of these values of η. What happens as η changes?

Solution E: *For these learning rates, increasing the step size increases the rate at which the training error decreases.*



The following problems consider SGD with the larger, higher-dimensional dataset, `sgd_data.csv`. The file has a header denoting which columns correspond to which values. For these problems, use the Jupyter notebook `3_notebook_part2.ipynb`.

For your implementation of problems F-H, **do** consider the bias term using your answer to problem A.

Problem F [6 points]: Use your SGD code with the given dataset, and report your final weights. Follow the guidelines below for your implementation:

- Use $\eta = e^{-15}$ as the step size.
- Use $\mathbf{w} = [0.001, 0.001, 0.001, 0.001]$ as the initial weight vector and $b = 0.001$ as the initial bias.
- Use at least 800 epochs.
- You should incorporate the bias term in your implementation of SGD and do so in the vector style of problem A.
- Note that for these problems, it is no longer necessary for the `SGD` function to store the weights after all epochs; you may change your code to only return the final weights.

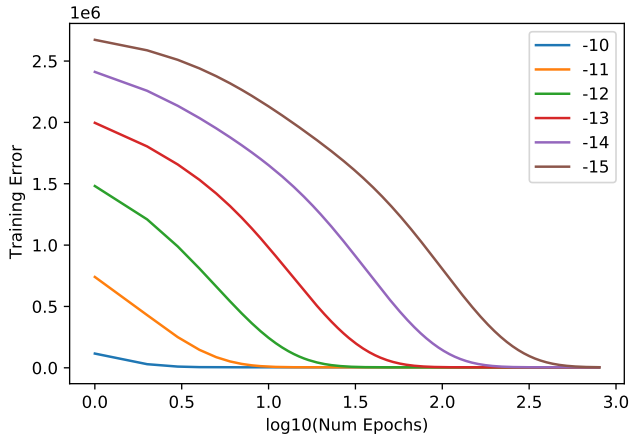
Solution F: *See Code. Final weights (bias is the final term):*
[-5.94229011, 3.94369494, -11.72402388, 8.78549375, -0.22720591]

Problem G [2 points]: Perform SGD as in the previous problem for each learning rate η in

$$\{e^{-10}, e^{-11}, e^{-12}, e^{-13}, e^{-14}, e^{-15}\},$$

and calculate the training error at the beginning of each epoch during training. On a single plot, show training error vs. number of epochs trained for each of these values of η. Explain what is happening.

Solution G:



The training error decreases faster for a higher learning rate.

Problem H [2 points]: The closed form solution for linear regression with least squares is

$$\mathbf{w} = \left(\sum_{i=1}^{N} \mathbf{x_i} \mathbf{x_i}^T \right)^{-1} \left(\sum_{i=1}^{N} \mathbf{x_i} y_i \right).$$

Compute this analytical solution. Does the result match up with what you got from SGD?

Solution H: *Final weights (bias is the final term):*
[-5.99157048, 4.01509955, -11.93325972, 8.99061096, -0.31644251]. The analytcal solution matches up well with the results from SGD (error less than 10%).

Answer the remaining questions in 1-2 short sentences.

Problem I [2 points]: Is there any reason to use SGD when a closed form solution exists?

Solution I: *Both the computational cost of computing the analytical solution and the process of SGD scale as $O(D^2 n)$, where D is the dimension of the input data and n is the number of training samples for n greater than D. Thus, there is not necessarily a computational benefit to either method. However, SGD may be beneficial if*

there the matrix is not invertible in the analytical solution.

Problem J [2 points]: Based on the SGD convergence plots that you generated earlier, describe a stopping condition that is more sophisticated than a pre-defined number of epochs.

Solution J: *One could lower the step size every time that the validation error no longer decreases and terminate training if the validation error fails to decrease after a certain number of epochs.*

Problem K [2 points]: How does the convergence behavior of the weight vector differ between the perceptron and SGD algorithms?

Solution K: *It is generally always possible for an SGD algorithm to converge to a local minimum, given properly tuned training hyperparameters. On the other hand, the perceptron will not necessarily converge if the data is not linearly separable.*

4 The Perceptron [14 Points]

Relevant materials: lecture 2

The perceptron is a simple linear model used for binary classification. For an input vector $\mathbf{x} \in \mathbb{R}^d$, weights $\mathbf{w} \in \mathbb{R}^d$, and bias $b \in \mathbb{R}$, a perceptron $f : \mathbb{R}^d \to \{-1, 1\}$ takes the form

$$f(\mathbf{x}) = \text{sign}\left(\left(\sum_{i=1}^{d} w_i x_i\right) + b\right)$$

The weights and bias of a perceptron can be thought of as defining a hyperplane that divides $\mathbb{R}^d$ such that each side represents an output class. For example, for a two dimensional dataset, a perceptron could be drawn as a line that separates all points of class $+1$ from all points of class -1.

The PLA (or the Perceptron Learning Algorithm) is a simple method of training a perceptron. First, an initial guess is made for the weight vector $\mathbf{w}$. Then, one misclassified point is chosen arbitrarily and the $\mathbf{w}$ vector is updated by

$$\mathbf{w}_{t+1} = \mathbf{w}_t + y(t)\mathbf{x}(t)$$
$$b_{t+1} = b_t + y(t),$$

where $\mathbf{x}(t)$ and $y(t)$ correspond to the misclassified point selected at the t^{th} iteration. This process continues until all points are classified correctly.

The following few problems ask you to work with the provided Jupyter notebook for this problem, titled `4_notebook.ipynb`. This notebook utilizes the file `perceptron_helper.py`, but you should not need to modify this file.

Problem A [8 points]: The graph below shows an example 2D dataset. The $+$ points are in the $+1$ class and the $\circ$ point is in the -1 class.

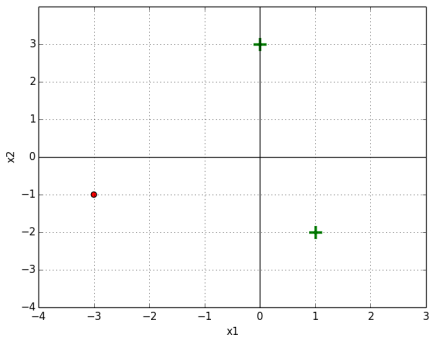


Figure 1: The green $+$ are positive and the red $\circ$ is negative

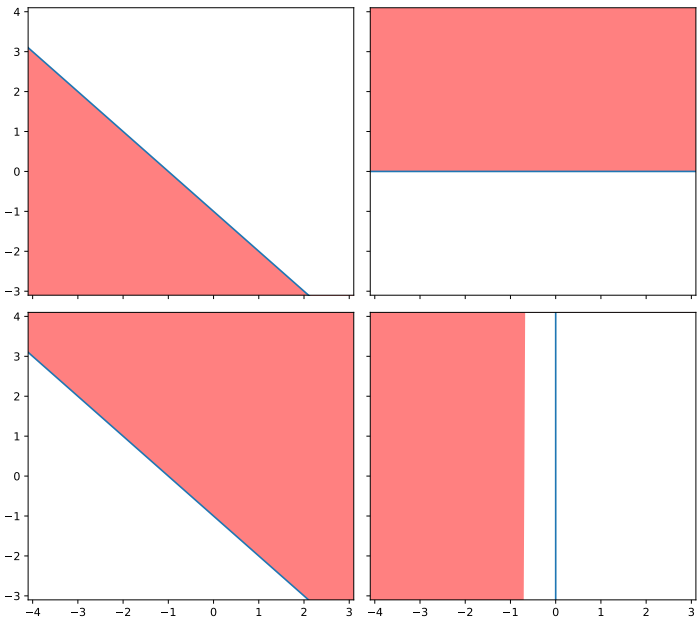
Implement the `update_perceptron` and `run_perceptron` methods in the notebook, and perform the perceptron algorithm with initial weights $w_1 = 0, w_2 = 1, b = 0$.

Give your solution in the form a table showing the weights and bias at each timestep and the misclassified point $([x_1, x_2], y)$ that is chosen for the next iteration's update. You can iterate through the three points in any order. Your code should output the values in the table below; cross-check your answer with the table to confirm that your perceptron code is operating correctly.

t	b	w_1	w_2	x_1	x_2	y
0	0	0	1	1	-2	+1
1	1	1	-1	0	3	+1
2	2	1	2	1	-2	+1
3	3	2	0			

Include in your report both: the table that your code outputs, as well as the plots showing the perceptron's classifier at each step (see notebook for more detail).

Solution A: *See Code.*
Table:
b = 1.0, w = [1. -1.], missclassifed = [1 -2], y = 1
b = 2.0, w = [1. 2.], missclassifed = [0 3], y = 1
b = 3.0, w = [2. 0.], missclassifed = [1 -2], y = 1



Problem B [4 points]: A dataset $S = \{(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_N, y_N)\} \subset \mathbb{R}^d \times \mathbb{R}$ is *linearly separable* if there exists a perceptron that correctly classifies all data points in the set. In other words, there exists a hyperplane that separates positive data points and negative data points.

In a 2D dataset, how many data points are in the smallest dataset that is not linearly separable, such that no three points are collinear? How about for a 3D dataset such that no four points are coplanar? Please limit your solution to a few lines - you should justify but not prove your answer.

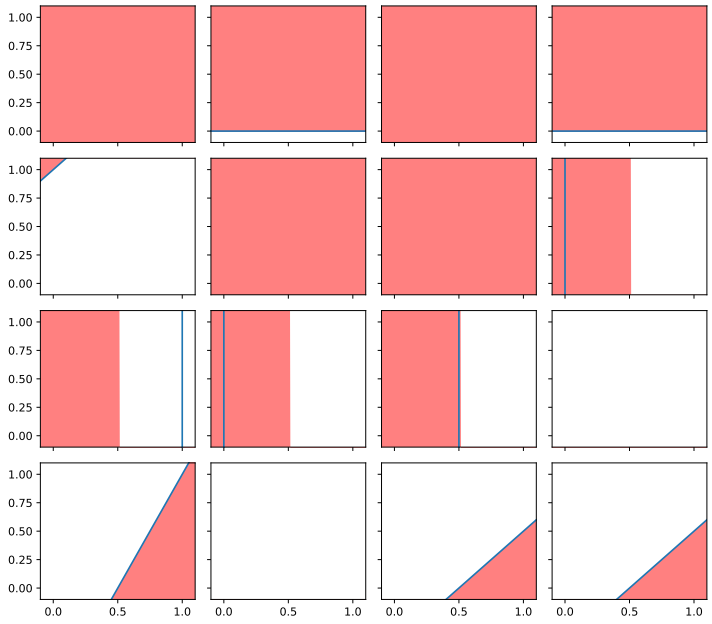
Finally, how does this generalize for an N-dimensional set, in which **no** $<N$-dimensional hyperplane contains a non-linearly-separable subset? For the N-dimensional case, you may state your answer without proof or justification.

Solution B: *For a 2D dataset, 4 data points can form the smallest dataset that is not linearly separable. For a 3D dataset, 5 pts will form the smallest dataset that is not linearly separable. Justification that N+2 pts form a dataset that is not linearly separable in N dimensions:*

Assume all of the pts have the same classification. Choose a hyperplane that goes through N of the pts and shift this plane slightly up so that those N points lie on one side of the hyperplane. Since N+1 of the points are not coplanar, one of the other points must lie on this side of the classification. Now, choose the remaining pt to be on the other side of the hyperplane. We have constructed a dataset that is not linearly separable.

Problem C [2 points]: Run the visualization code in the Jupyter notebook section corresponding to question C (report your plots). Assume a dataset is *not* linearly separable. Will the Perceptron Learning Algorithm ever converge? Why or why not?

Solution C:



The perceptron learning algorithm will not converge because it's not linearly separable. It will oscillate between various subpar solutions.