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: *A hypothesis set is the set of all possible mappings between data and output (i.e. all possible functions that satisfy $f(x) = y$) .*

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

Solution B: *If $x \in \Re$, the hypothesis set is $f(x|w) = w^t x$ for $w \in \Re$.*

Problem C [2 points]: What is overfitting?

Solution C: *Overfitting is when your model fits your training data too well, such that the test error $\gg$ training error. This usually occurs because your model is too complex.*

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

Solution D: *Use a more simple model or include more training data (increase N).*

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: *When building a model your data can be split into training and test (validation) data sets, where the training data is used to train your model and estimate your model parameters and your test data set is used to ensure model accuracy/error. It's important to have separate training and test data set (i.e. not using test data to train your model) because you want to ensure that your model is generalizable when you deploy it using real world data.*

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

Solution F: *Independent and identically distributed from the "true" dataset distribution $P(x, y)$, where x are inputs and y are outputs.*

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: *One possible input X could be a vector of all unique words used in email. The output Y would be "spam" or "not spam"*

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

Solution H: *K-fold cross-validation is when you split your data into k equally sized parts, training your model on the $k-1$ parts, and then testing your model on the other part, repeating this process for each split.*

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: *Filing in the definition of $E_{out}(f_S)$ into the left hand side and expanding the quadratic:*

$$\begin{aligned} &\mathbb{E}_S\left[\mathbb{E}_x\left[\left(f_S(x) - y(x)\right)^2\right]\right] \\ &\mathbb{E}_S\left[\mathbb{E}_x\left[f_S(x)^2 - 2f_S(x)y(x) + y(x)^2\right]\right] \end{aligned}$$

Distributing the expectation signs and simplifying for some convenience

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

Now adding some terms that amount to 0:

$$\mathbb{E}_x\begin{pmatrix} F(x)^2 - 2F(x)y(x) + y(x)^2 + \mathbb{E}_S\left[f_S(x)^2 - 2f_S(x)F(x) + F(x)^2\right] \\ -F(x)^2 + 2\mathbb{E}_S\left[f_S(x)F(x) - F(x)^2\right] \end{pmatrix}$$

We can fill in the $Bias(x)$ and $Var(x)$ terms now and we're left with:

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

Simplifying the extra terms knowing that $\mathbb{E}_S\left[f_S(x)\right] = F(x)$:

$$\begin{aligned} &\mathbb{E}_x\left[Bias(x) + Var(x) - F(x)^2 + 2F(x)^2 - F(x)^2\right] \\ &\mathbb{E}_x\left[Bias(x) + Var(x)\right] \end{aligned}$$

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.

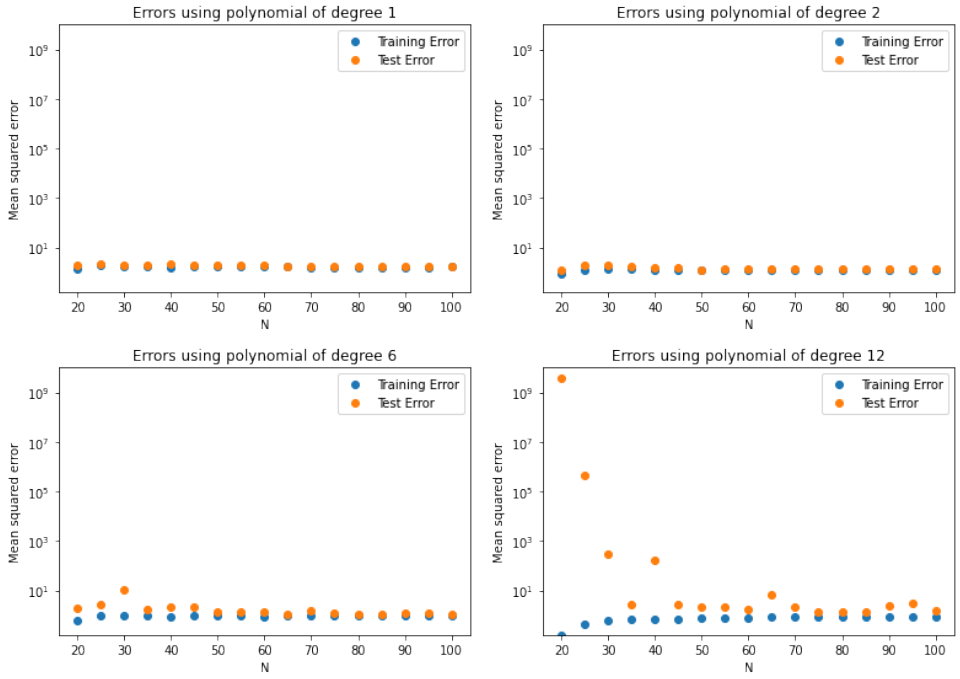
Polynomial regression is a type of regression that models the target y as a degree–d polynomial function of the input x. (The modeler chooses d.) You don't need to know how it works for this problem, just know that it produces a polynomial that attempts to fit the data.

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: *Link to notebook for problem 2B*



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?

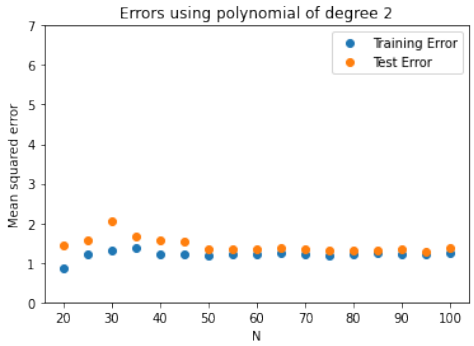
Solution C: *Bias is defined as the mean squared error from the test data, $(F(x) - y(x))^2$. As such, the regression using the 12th degree polynomial has the highest bias since the test error is the greatest.*

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

Solution D: *The model using N=20 has the highest variance because it is an unstable model class, producing a wide range of test errors across the 4 different polynomial degrees.*

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:



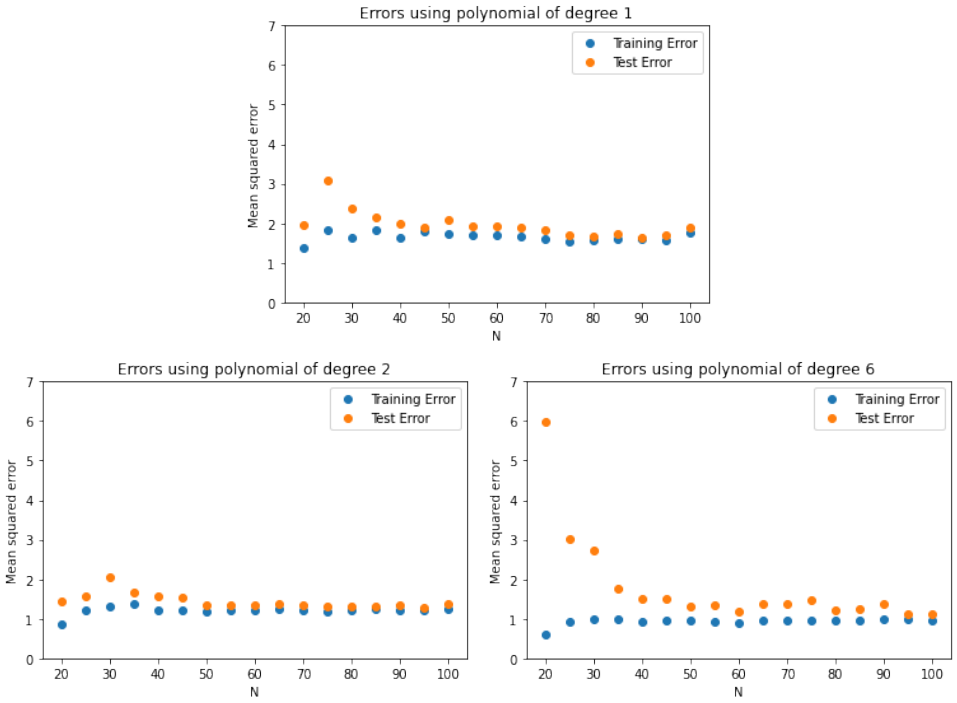
The model appears to stabilize after N=50 (test and training errors are converging to a value), and as such will most likely not improve if we add more training points.

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

Solution F: *Training error is lower than validation error because our model is designed to minimize the error for this data set, and the validation error should be additional data that is not considered. Because is not considered, our model is not optimizing to minimize error in the data points in the validation set.*

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:



I would expect the quadratic (degree 2) to perform the best because it has the lowest test error across a range of different number of points N.

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: *Add an additional element to* $\mathbf{x}$ *that is equal to 1 and a corresponding parameter in* $\mathbf{w}$ *that represents this bias (i.e.* $x_0 = 1$ *corresponding to* w_0*).*

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:

$$\frac{\partial}{\partial w} \left[\sum_{i=1}^{N} (y_i - \boldsymbol{w}^T \boldsymbol{x}_i)^2 \right] =$$
$$-2 \left[\sum_{i=1}^{N} (y_i - \boldsymbol{w}^T \boldsymbol{x}_i) \boldsymbol{x}_i \right]$$

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.

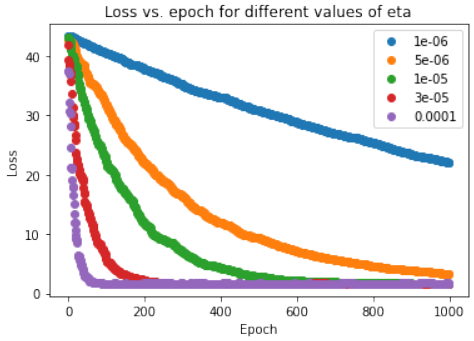
Solution C: *See code. Link to notebook for problem 3C-E*

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: *Starting points with larger losses make larger steps along the parameter space (conversely those with smaller losses take small steps), and interestingly they all converge to the same point in about the same number of epochs. The convergence also appears to go in a straight line, presumably because the trajectory finds the steepest route and stays on the same route. Between the data sets, the behavior is the same, even though the hyperplane takes a different shape and the initial losses of each starting point are different.*

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:



The loss converges faster for larger values of eta.

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.

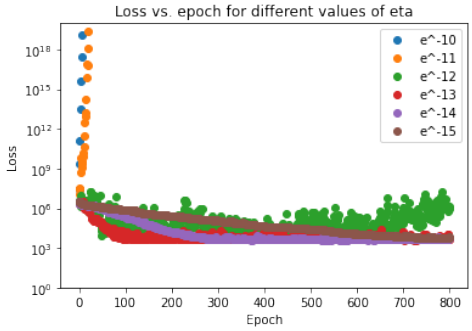
Solution F: *Link to notebook for problem 3F-H*
Final weights (will vary since points are being randomized): $w_0 = -0.28$, $w_1 = -5.93$, $w_2 = 3.95$, $w_3 = -11.66$, $w_4 = 8.81$

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:



For large values of eta (i.e. $\geq \exp -12$) the model becomes unstable, and at later epochs, the weights actually approach infinity.

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 from analytical solution: $w_0 = -0.32$, $w_1 = -5.99$, $w_2 = 4.01$, $w_3 = -11.93$, $w_4 = 8.99$. Yes the solutions between the analaytical and numerical methods are about the same.*

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: *The $\boldsymbol{x}_i \boldsymbol{x}_i^T$ term may not be invertible, so a numerical method may be preferred.*

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: *If the loss deviation appears to be within a certain percentage of previous losses, you can stop the SGD.*

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

Solution K: *The SGD algorithms converge in all cases that we saw here, but in the perceptron algorithm there are certain datasets that will not allow the alogrithm to converge.*

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.

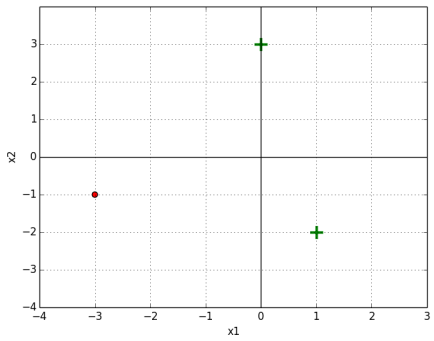


Figure 1: The green $+$ are positive and the red $\circ$ is negative

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.

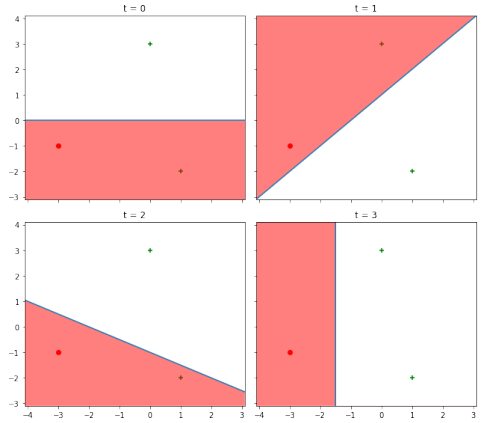
t	b	w_1	w_2	x_1	x_2	y
0	0	0	1	1	-2	+1
1	1	1	-1	0	3	+1
2	2	1	2	1	-2	+1
3	3	2	0			

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: *Link to notebook for problem 4*

```
t=0, b=1, w1=1, w2=-1, x1=1, x2=-2, y=1
t=1, b=2, w1=1, w2=2, x1=0, x2=3, y=1
t=2, b=3, w1=2, w2=0, x1=1, x2=-2, y=1
t=3, b=3, w1=2, w2=0

final w = [2. 0.], final b = 3.0
```



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: *The smallest number of points for a 2D dataset is 4 points. The easiest way to visualize it in the 2D case is to assume that each axis has a finite value, and you place a marker at the extremes of each axis, organized such that each point is collinear with exactly 2 other points. The value of each point that it is collinear with should be opposite. Using this same logic, the smallest number of points for a 3D dataset is 6 points and in the N-dimensional case, there are a minimum of 2N points to make a non-linearly separable set.*

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: *No the algorithm will never converge because the sign of the sum of the points will never become 0 (i.e. the loss function will never hit its objective).*