How r u guys?
Let's talk about the classification today!

Day 4: Classification

Summer STEM: Machine Learning

Department of Electrical and Computer Engineering
NYU Tandon School of Engineering
Brooklyn, New York

July 15, 2021

Outline

1 Review

2 Non-linear Optimization

3 Logistic Regression

4 Lab: Diagnosing Breast Cancer

5 Multiclass Classificaiton

6 Lab: Iris Dataset

Review

First, recall that

- Machine learning pipeline:
  - Process Data
  - Train on training data
  - Test on testing data
- Is it possible have a high accuracy for the training data and a low accuracy for the testing data? What should we do?

Review

- Imagine you are preparing for the SATs and you come across a book full of practice questions you did not understand how to solve any of the problems. However, you memorized all of the answers.
- What do you think will happen if you try to solve practice questions in a different book.

The other way is that you can

- Why are you studying actual problem solving techniques instead of just memorizing solutions from practice questions?
- Assuming you have an eidetic memory will memorizing solutions from practice questions be a good strategy?

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Review

2. Also recall that the loss function J(w), one way we could handle the overfitting problem is using the regularization term, which is this term here. By doing this, we panelize the lost function in a way that we want the penalty as small as possible so that the lost function would be small, which means we force the model to learn less on the training dataset.

- $J(w) = \frac{1}{N}\|Y - Xw\|^2 + \lambda\|w\|^2$
- $w = [10000, 20000, 30000, 10000]$ does this look good?

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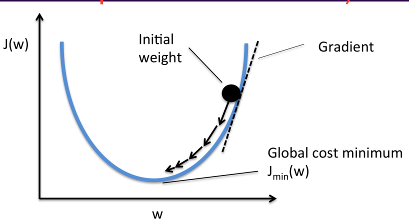
~~Motivation~~

- Cannot rely on closed form solutions
  - Computation efficiency: operations like inverting a matrix is not efficient
  - For more complex problems such as neural networks, a closed-form solution is not always available
- Need an optimization technique to find an optimal solution
  - Machine learning practitioners use **gradient**-based methods

Gradient Descent Algorithm

So let me introduce a solution here,
which is called gradient descent. Our goal here is to minimize the cost function J(w), we want to find its minimum point (cost function/plot on whiteboard)

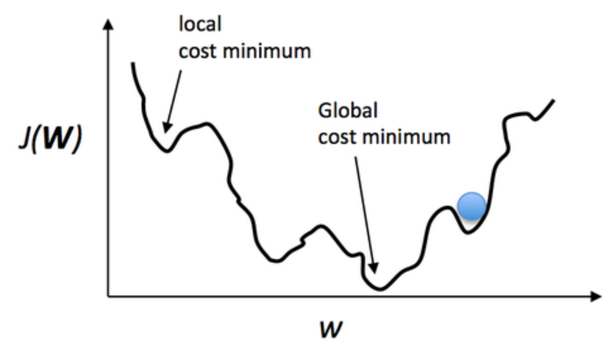
- Update Rule
  Repeat{
  $$\mathbf{w}_{new} = \mathbf{w} - \alpha \nabla J(\mathbf{w})$$
  }
  α is the learning rate



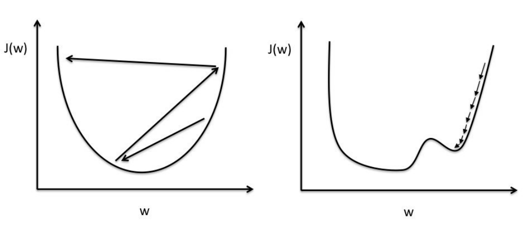
whiteboard

General Loss Function Contours

- Most loss function contours are not perfectly parabolic
- Our goal is to find a solution that is very close to global minimum by the right choice of hyper-parameters

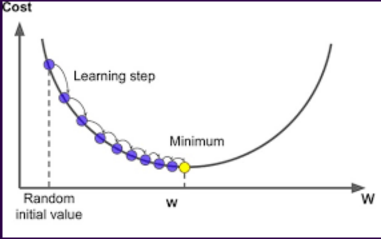


Understanding Learning Rate



Large learning rate: Overshooting.

Small learning rate: Many iterations until convergence and trapping in local minima.



Correct learning rate

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BREAK!

Classification Vs. Regression

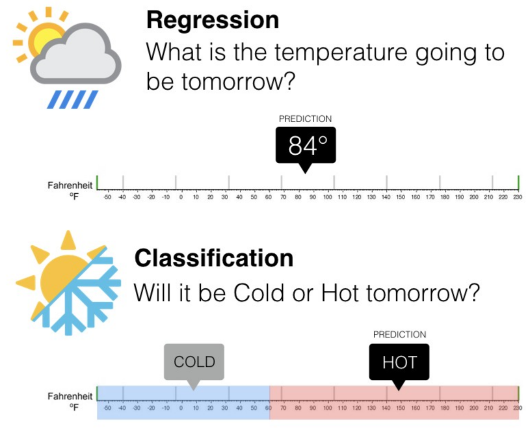
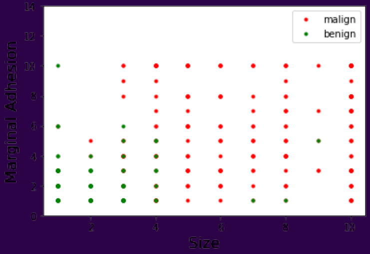


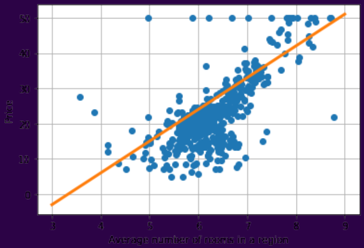
Figure: https://www.pinterest.com/pin/672232681855858622/?lp=true

Classification Vs. Regression

There will be two datasets you need to handle as demo



(a) Breast cancer dataset

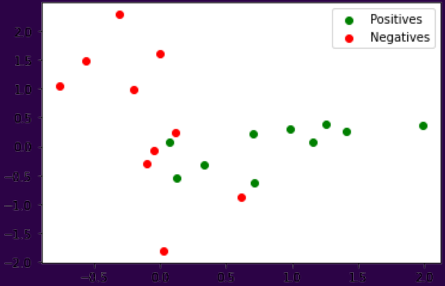


(b) Boston Housing dataset

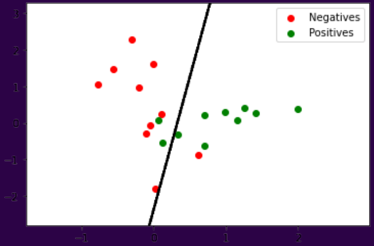
Classification

Given the dataset (x_i, y_i) for $i = 1, 2, \ldots, N$, find a function $f(x)$ (model) so that it can predict the label $\hat{y}$ for some input x, even if it is not in the dataset, i.e. $\hat{y} = f(x)$.

- Positive : $y = 1$
- Negative : $y = 0$

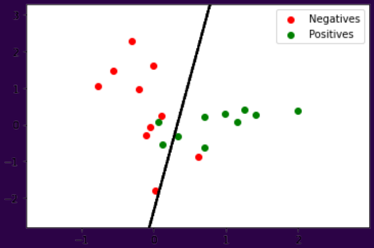


Decision Boundary



The decision boundary is the black line in the plane, which seperates the datapoints into two groups. On the left of the boundary, we say the data is negatives, while on the right, the data is positives

Decision Boundary

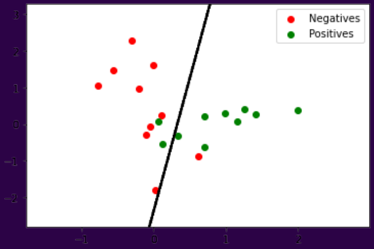


- Evaluation metric :

is calculated as

$$\text{Accuracy} = \frac{\text{Number of correct prediction}}{\text{Total number of prediction}}$$

- What is the accuracy in this example ?



- Evaluation metric :

$$\text{Accuracy} = \frac{\text{Number of correct prediction}}{\text{Total number of prediction}} = \frac{17}{20} = 0.85 = 85\%$$

Need for a new model

- What would happen if we used the linear regression model :

$$\hat{y} = w_0 + w_1 x$$

Need for a new model

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- y is 0 or 1
- $\hat{y}$ will take any value between $-\infty$ and ∞

Need for a new model

- What would happen if we used the linear regression model :

$$\hat{y} = w_0 + w_1 x$$

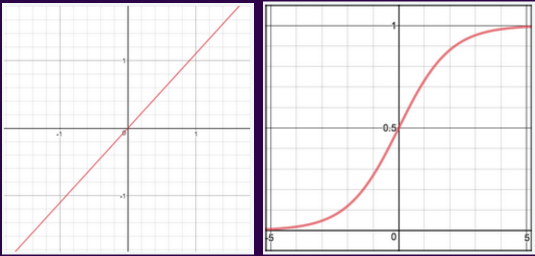
- y is 0 or 1
- $\hat{y}$ will take any value between $-\infty$ and ∞
- It will be hard to find w_0 and w_1 that make the prediction $\hat{y}$ match the label y.

Sigmoid Function

range of y hat to be in [0,1]

- By applying the sigmoid function, we enforce $0 \leq \hat{y} \leq 1$

$$\hat{y} = \text{sigmoid}(w_0 + w_1 x) = \frac{1}{1 + e^{-(w_0 + w_1 x)}}$$



(a) Linear model (b) Sigmoid model

A new loss function

- Binary cross entropy loss :

$$\text{Loss} = \frac{1}{N}\sum_{i=1}^{N}\Big[-y_i\log(\hat{y}_i) - (1-y_i)\log(1-\hat{y}_i)\Big]$$

pause

- What happens if $y_i = 0$:

$$\Big[-y_i\log(\hat{y}_i) - (1-y_i)\log(1-\hat{y}_i)\Big] = ?$$

A new loss function

- Binary cross entropy loss :

$$\text{Loss} = \frac{1}{N}\sum_{i=1}^{N}\Big[-y_i\log(\hat{y}_i) - (1-y_i)\log(1-\hat{y}_i)\Big]$$

- If $y_i = 0$:

$$\Big[-y_i\log(\hat{y}_i) - (1-y_i)\log(1-\hat{y}_i)\Big] = -\log(1-\hat{y}_i)$$

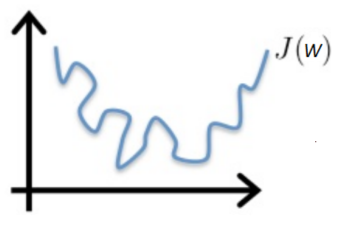
A new loss function

- Binary cross entropy loss :
$$\text{Loss} = \frac{1}{N}\sum_{i=1}^{N}\Big[-y_i\log(\hat{y}_i) - (1-y_i)\log(1-\hat{y}_i)\Big]$$
- If $y_i = 0$:
$$\Big[-y_i\log(\hat{y}_i) - (1-y_i)\log(1-\hat{y}_i)\Big] = -\log(1-\hat{y}_i)$$
- If $y_i = 1$:
$$\Big[-y_i\log(\hat{y}_i) - (1-y_i)\log(1-\hat{y}_i)\Big] = -\log(\hat{y}_i)$$

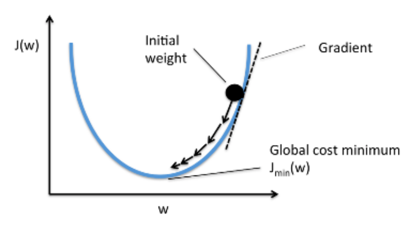
MSE vs Binary cross entropy loss

One good point about the binary cross entropy loss is

- MSE of a logistic function has many local minima.
- The Binary cross entropy loss has only one minimum.



(a) MSE



(b) Binary cross entropy loss

which means we could do optimization mcuh easier, right? We do not have to worry about the case we reaches at a local minimum here and get stuck at that point.

Classifier

$$\hat{y} = \text{sigmoid}(w_0 + w_1 x) = \frac{1}{1 + e^{-(w_0 + w_1 x)}}$$

- How to deal with uncertainty ?
  - Thanks to the sigmoid, $\hat{y} = f(x)$ is between 0 and 1.

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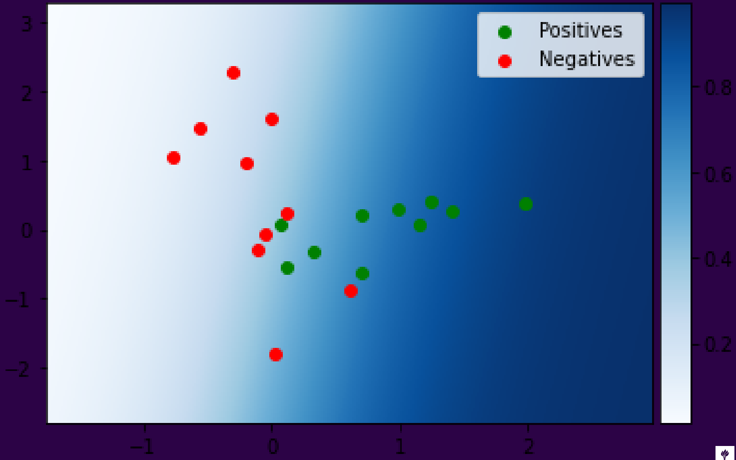
Classifier

$$\hat{y} = \text{sigmoid}(w_0 + w_1 x) = \frac{1}{1 + e^{-(w_0 + w_1 x)}}$$

- How to deal with uncertainty ?
  - Thanks to the sigmoid, $\hat{y} = f(x)$ is between 0 and 1.
- If $\hat{y}$ is close to 0, the data is probably negative
- If $\hat{y}$ is close to 1, the data is probably positive
- If $\hat{y}$ is around 0.5, we are not sure.

Classifier



Decision Boundary

- Once, we have a classifier outputting a score $0 < \hat{y} < 1$, we need to create a decision rule.

Decision Boundary

- Once, we have a classifier outputting a score $0 < \hat{y} < 1$, we need to create a decision rule. threshold
- Let $0 < t < 1$ be a Threshold :
  - If $\hat{y} > t$, $\hat{y}$ is classified as positive.
  - If $\hat{y} < t$, $\hat{y}$ is classified as negative.

Decision Boundary

- Once, we have a classifier outputting a score $0 < \hat{y} < 1$, we need to create a decision rule.
- Let $0 < t < 1$ be a Threshold :
  - If $\hat{y} > t$, $\hat{y}$ is classified as positive.
  - If $\hat{y} < t$, $\hat{y}$ is classified as negative.
- How to choose t ?

Impact of the threshold

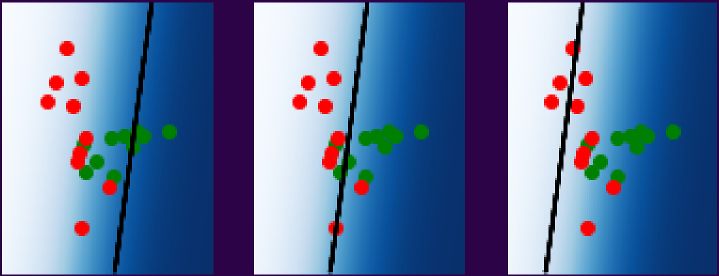


Figure: $t = 0.2, 0.5, 0.8$

Performance metrics for a classifier

- Accuracy of a classifier: percentage of correct classification
- Why accuracy alone is not a good measure for assessing the model ?

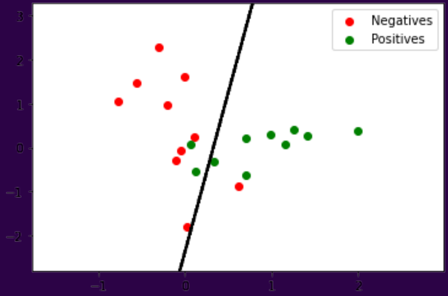
Performance metrics for a classifier

- Accuracy of a classifier: percentage of correct classification
- Why accuracy alone is not a good measure for assessing the model ?
  - Example: A rare disease occurs 1 in ten thousand people
  - A test that classifies everyone as free of the disease can achieve 99.999% accuracy when tested with people drawn randomly from the entire population

Types of Errors in Classification

- Correct predictions:
  - True Positive (TP) : Predict $\hat{y} = 1$ when $y = 1$
  - True Negative (TN) : Predict $\hat{y} = 0$ when $y = 0$
- Two types of errors:
  - False Positive/ False Alarm (FP): $\hat{y} = 1$ when $y = 0$
  - False Negative/ Missed Detection (FN): $\hat{y} = 0$ when $y = 1$

Example



- How many True Positive (TP) are there ?
- How many True Negative (TN) are there ?
- How many False Positive (FP) are there ?
- How many False Negative (FN) are there ?

Other metrics

- Sensitivity/Recall/TPR (How many positives are detected among all positive?)

$$\frac{\text{TP}}{\text{TP} + \text{FN}}$$

- Precision (How many detected positives are actually positive?)

$$\frac{\text{TP}}{\text{TP} + \text{FP}}$$

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Lab: Diagnosing Breast Cancer

- We're going to use the breast cancer dataset to predict whether the patients' scans show a malignant tumour or a benign tumour.
- Let's try to find the best linear classifier using logistic regression.

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Multiclass Classificaiton

- Previous model: $f(\mathbf{x}) = \sigma(\phi(\mathbf{x})w)$
- Representing Multiple Classes:
  - One-hot / 1-of-K vectors, ex : 4 Class
  - Class 1 : $\mathbf{y} = [1, 0, 0, 0]$
  - Class 2 : $\mathbf{y} = [0, 1, 0, 0]$
  - Class 3 : $\mathbf{y} = [0, 0, 1, 0]$
  - Class 4 : $\mathbf{y} = [0, 0, 0, 1]$

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  - Class 1 : $\mathbf{y} = [1, 0, 0, 0]$
  - Class 2 : $\mathbf{y} = [0, 1, 0, 0]$
  - Class 3 : $\mathbf{y} = [0, 0, 1, 0]$
  - Class 4 : $\mathbf{y} = [0, 0, 0, 1]$
- Multiple outputs: $f(\mathbf{x}) = \text{softmax}(\phi(\mathbf{x})W)$
- Shape of $\phi(\mathbf{x})W$: $(N, K) = (N, D) \times (D, K)$
- $\text{softmax}(\mathbf{z})_k = \dfrac{e^{z_k}}{\sum_j e^{z_j}}$

Multiclass Classificaiton

- Multiple outputs: $f(\mathbf{x}) = \text{softmax}(\mathbf{z})$ with $\mathbf{z} = \phi(\mathbf{x})W$
- $\text{softmax}(\mathbf{z})_k = \dfrac{e^{\mathbf{z}_k}}{\sum_j e^{\mathbf{z}_j}}$
- Softmax example: If $\mathbf{z} = \begin{bmatrix} -1 \\ 2 \\ 1 \\ -4 \end{bmatrix}$ then,

$$\text{softmax}(z) = \begin{bmatrix} \frac{e^{-1}}{e^{-1}+e^{2}+e^{1}+e^{-4}} \\ \frac{e^{2}}{e^{-1}+e^{2}+e^{1}+e^{-4}} \\ \frac{e^{1}}{e^{-1}+e^{2}+e^{1}+e^{-4}} \\ \frac{e^{-4}}{e^{-1}+e^{2}+e^{1}+e^{-4}} \end{bmatrix} \approx \begin{bmatrix} 0.035 \\ 0.704 \\ 0.259 \\ 0.002 \end{bmatrix}$$

Cross-entropy

- Multiple outputs: $\hat{\mathbf{y}}_{\mathbf{i}} = \text{softmax}(\phi(\mathbf{x}_i)W)$
- Cross-Entropy: $J(W) = -\sum_{i=1}^{N}\sum_{k=1}^{K} \mathbf{y}_{ik} log(\hat{\mathbf{y}}_{ik})$
- Example : K = 4

$$\text{If, } \mathbf{y}_i = [0, 0, 1, 0] \text{ then, } \sum_{k=1}^{K} \mathbf{y}_{ik} log(\hat{\mathbf{y}}_{ik}) = log(\hat{\mathbf{y}}_{i3})$$

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- Open demo_iris.ipynb