Day 4: Linear Classifiers

Summer STEM: Machine Learning

Nikola Janjušević, Akshaj Kumar Veldanda, Jacky Yuan, Tejaishwarya Gagadam

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

July 11, 2019

Outline

Review of Day 3

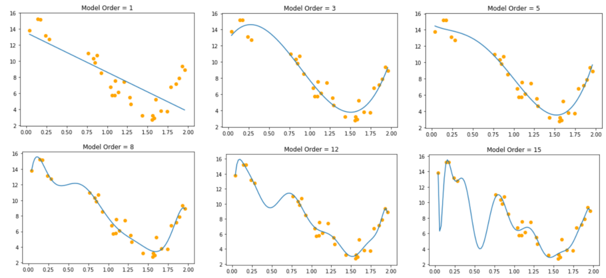
- Yesterday we learned about:
    -
- Polynomial Regression
- Overfitting
- Regularization
- Cross-Validation

Review: Polynomial Regression

- Polynomial Model: $y = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots w_D x^D$
- Design Matrix for Polynomial: $X = \begin{bmatrix} 1 & x_1 & x_2^2 & \cdots & x_1^D \\ 1 & x_2 & x_2^2 & \cdots & x_2^D \\ \vdots & & \ddots & & \vdots \\ 1 & x_N & x_N^2 & \cdots & x_N^D \end{bmatrix}$
- Think of this design matrix as creating new features that are powers of the original single feature
- This is Linear Regression, the process for calculating the weights w's are same
- Python function: sklearn or np.polyfit

Review: Over-fitting

- Train error always decreases as you use higher order models
- A model that is over-fitted on train data is unlikely to work well on new data



Cross-Validation

- Motivation: never determine a hyper-parameter based on training data
- **Hyper-Parameter**: a parameter of the algorithm that is not a model-parameter solved for in optimization.
  - Ex: λ weight regularization value vs. model weights ($\mathbf{w}$)
- Solution: split dataset into three
  - **Training set**: to compute the model-parameters ($\mathbf{w}$)
  - **Validation set**: to tune hyper-parameters (λ)
  - **Test set**: to compute the performance of the algorithm (MSE)

Review: Regularization

- Another method to combat over-fitting
- High weight terms usually lead to over-fitting
- Introduction of a new term in cost function
- $$J = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

Review: Regularization

- Another method to combat over-fitting
- High weight terms usually lead to over-fitting
- Introduction of a new term in cost function
- $$J = \sum_{i=1}^{N}(y_i - \hat{y}_i)^2 + \lambda \sum_{j=1}^{D}(w_j)^2$$
- The new term penalizes the magnitude of weights
- Hyperparameter *lambda* determines how much you regularize: higher lambda $\leftarrow$ more regularization

Outline

Motivation

- Cannot rely on closed form solutions

Motivation

- Cannot rely on closed form solutions
  - Computation efficiency: operations like inverting a matrix is not efficient

Motivation

- Cannot rely on closed form solutions
  - Computation efficiency: operations like inverting a matrix is not efficient
  - For more complex problems, like neural network, a closed form solution is not always available

Motivation

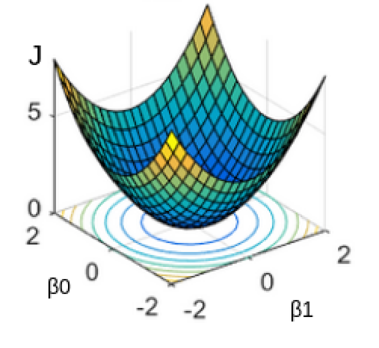
- Cannot rely on closed form solutions
  - Computation efficiency: operations like inverting a matrix is not efficient
  - For more complex problems, like neural network, a closed form solution is not always available
- Need an optimization technique to find an optimal solution

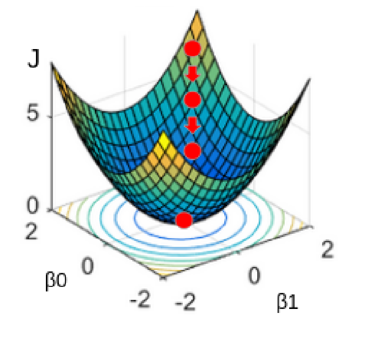
Motivation

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

Understanding Optimization

- *Recap* $\hat{y} = w_0 + w_1 x$
- *Loss*, $J = \Sigma_{i=1}^{N}(y_i - \hat{y}_i)^2 \implies J = \Sigma_{i=1}^{N}(y_i - w_0 - w_1 x_i)^2$
- Want to find $w_0 and w_1$ that minimizes J





Gradient Descent Algorithm

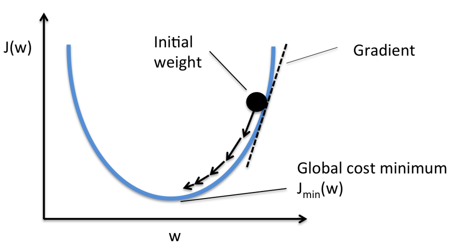
- Update Rule

  Repeat{

  $$w_{new} = w - \alpha \frac{dJ}{dw}$$

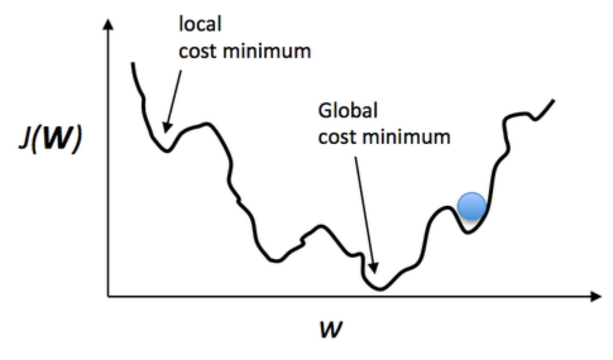
  }

  α is the learning rate

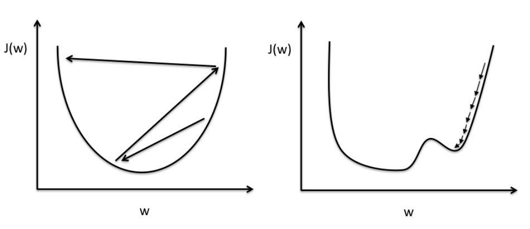


General Loss Function Contours

- 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

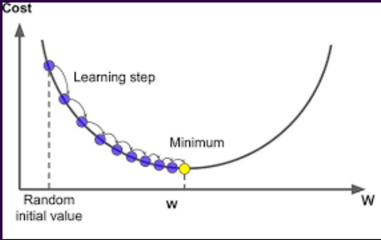


Understanding Learning Rate



Large learning rate: Overshooting.

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



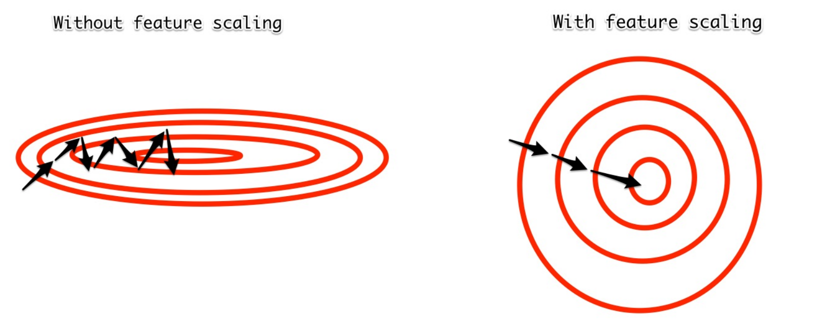
Correct learning rate

Some Animations

- Demonstrate gradient descent animation

Importance of Feature Normalization (Optional)

- Helps improve the performance of gradient based optimization



Some Gradient Based Algorithms

- Gradient descent
  - Stochastic gradient descent
  - Mini-batch gradient descent
- Gradient descent with momentum
- RMSprop
- Adam optimization algorithm

We have many frameworks that help us use these techniques in a single line of code (Eg: TensorFlow, PyTorch, Caffe, etc).

Outline

Demo: 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 linear regression.

Outline

Classification

- One method is to use linear regression
  - Map all predictions ($\hat{y}$) greater than 0 as class 1 and all less than 0 as class 0
  - This method doesn't work well because classification is not actually a linear function
- Classification takes the only discrete values for prediction
  - For binary classification problem, y can only take two values, 0 and 1
  - Ex: If we want to build a spam classifier for email, then x may be some features of the email
    - The $y = 1$ if it is a spam
    - Otherwise, $y = 0$

Hypothesis Representation

- Approach classification as old linear regression problem, ignoring the fact that y is discrete

Hypothesis Representation

- Approach classification as old linear regression problem, ignoring the fact that y is discrete
  - We have seen that this approach performs poorly

Hypothesis Representation

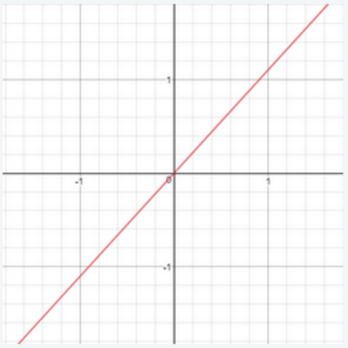
- Approach classification as old linear regression problem, ignoring the fact that y is discrete
  - We have seen that this approach performs poorly
- To fix this, develop an hypothesis such that $0 \leq \hat{y} \leq 1$

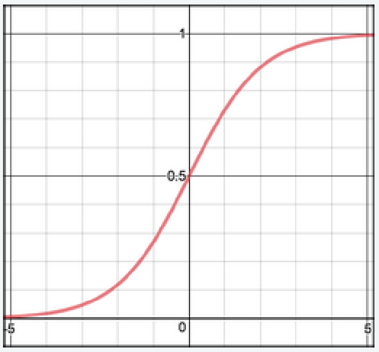
Hypothesis Representation

- Approach classification as old linear regression problem, ignoring the fact that y is discrete
  - We have seen that this approach performs poorly
- To fix this, develop an hypothesis such that $0 \leq \hat{y} \leq 1$
  - This is accomplished by using the Sigmoid function

Sigmoid Function

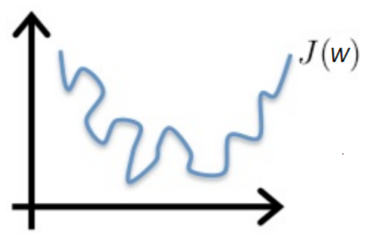
- Recall from linear regression $z = w_0 + w_1 x$
- On application of sigmoid function to z, we force $0 \leq \hat{y} \leq 1$
  - $\hat{y} = sigmoid(z) = \frac{1}{1+e^{-z}}$

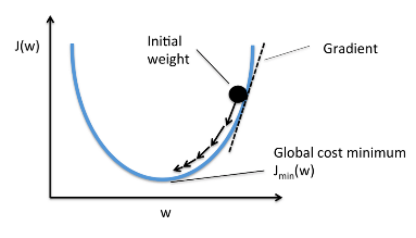




Classification Loss Function

- Cannot use the same cost function that we used for linear regression
  - Logistic function has many local optima
- Logistic cost function is $\frac{1}{m}\Sigma_{i=1}^{m}[-ylog(\hat{y}) - (1-y)log(1-\hat{y})$
  - This loss function is called binary cross entropy loss
  - This loss function has only one optimum point





Outline

Types of Errors in Classification

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

❑ Accuracy of classifier can be measured by:
- $TPR = P(\hat{y} = 1 | y = 1)$
- $FPR = P(\hat{y} = 1 | y = 0)$
- Accuracy=$P(\hat{y} = 1 | y = 1)$+ $P(\hat{y} = 0 | y = 0)$
  - (percentage of correct classification)

predicted→ real↓	*Class_pos*	*Class_neg*
Class_pos	TP	FN
Class_neg	FP	TN

$$\text{TPR (sensitivity)} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{FPR (1-specificity)} = \frac{\text{FP}}{\text{TN} + \text{FP}}$$

NYU TANDON SCHOOL OF ENGINEERING

Different Metrics for Error

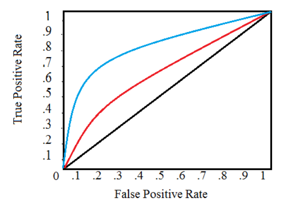
- Metrics to measure the error rate:
  - Recall/Sensitivity/TPR = TP/(TP+FN) (How many positives are detected among all positive?)
  - Precision = TP/(TP+FP) (How many detected positive is actually positive?)
  - Accuracy = (TP+TF)/(TP+FP+TN+FN) (percentage of correct classification)
  - F1-score = $\frac{Precision * Recall}{(Precision + Recall)/2}$
- Why accuracy alone is not a good measure for assessing the model
  - There might be an overwhelming proportion of one class over another
  - 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

Thresholding and ROC

- We can trade-off TPR (sensitivity) and FPR by changing the threshold
- Increasing $t \rightarrow$ Decreases false positives, but also reduces sensitivity
- Decreasing $t \rightarrow$ Increases sensitivity, but also increases false positive
- Why do we want this trade-off?
- Example:
  1. Detection for burglary into a building, need high sensitivity, we can tolerate a few false alarms $\rightarrow$ decrease t
  2. Making decision to buy a stock, making a false positive decision will lose millions $\rightarrow$ increase t

Thresholding and ROC

- ROC (Receiver Operating Characteristics) curve:
- Plot the change between TPR and FPR by varying the threshold
- Allow you to choose the threshold to meet a target TPR/FPR
- A good classifier will have large area under the curve
- A classifier with a higher area under the curve means that under same FPR, it has higher TPR



Outline

Outline

On Board:

- Previous Model: $\hat{y} = \sigma(\mathbf{x}^T w)$

On Board:

- Previous Model: $\hat{y} = \sigma(\mathbf{x}^T w)$
- Representing Multiple Classes:

On Board:

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

On Board:

- Previous Model: $\hat{y} = \sigma(\mathbf{x}^T w)$
- Representing Multiple Classes:
  - One-hot / 1-of-K vectors, ex: Class 2 of 4 $[0, 1, 0, 0]$
- Multiple Outputs:

$$\hat{\mathbf{y}} = softmax(W\mathbf{x})$$

On Board:

- Previous Model: $\hat{y} = \sigma(\mathbf{x}^T w)$
- Representing Multiple Classes:
  - One-hot / 1-of-K vectors, ex: Class 2 of 4 $[0, 1, 0, 0]$
- Multiple Outputs:

$$\hat{\mathbf{y}} = softmax(W\mathbf{x})$$

  - (K,1) = (K,M) x (M,1)

On Board:

- Previous Model: $\hat{y} = \sigma(\mathbf{x}^T w)$
- Representing Multiple Classes:
  - One-hot / 1-of-K vectors, ex: Class 2 of 4 $[0, 1, 0, 0]$
- Multiple Outputs:

$$\hat{\mathbf{y}} = softmax(W\mathbf{x})$$

  - (K,1) = (K,M) x (M,1)

$$softmax(\mathbf{z})_k = \frac{e^{z_k}}{\sum_j e^{z_j}}$$

On Board:

- Previous Model: $\hat{y} = \sigma(\mathbf{x}^T w)$
- Representing Multiple Classes:
  - One-hot / 1-of-K vectors, ex: Class 2 of 4 $[0, 1, 0, 0]$
- Multiple Outputs:

$$\hat{\mathbf{y}} = softmax(W\mathbf{x})$$

  - (K,1) = (K,M) x (M,1)

$$softmax(\mathbf{z})_k = \frac{e^{z_k}}{\sum_j e^{z_j}}$$

- Cross-Entropy: $J = -\sum_{i=1}^{N} \sum_{k=1}^{K} y_{ik} ln(\hat{y}_{ik})$

Outline

Thank You!

- Next Class: Linear Regression
- The real machine learning will begin!