Lesson #13
Logistic Regression

notas

- Classification
- Binary Classification
- Decision Boundary
- Cost Function
- Multiclass Classification
- Regularization (L1, L2)
- Hands on Scikit-Learn

notas

Classification Problem

MEDICAL MODEL

HEALTHY

SICK

SPAM CLASSIFIER MODEL

NOT SPAM

SPAM

Test

Grades

Student 1
Test: 9/10
Grades: 8/10

Student 2
Test: 3/10
Grades: 4/10

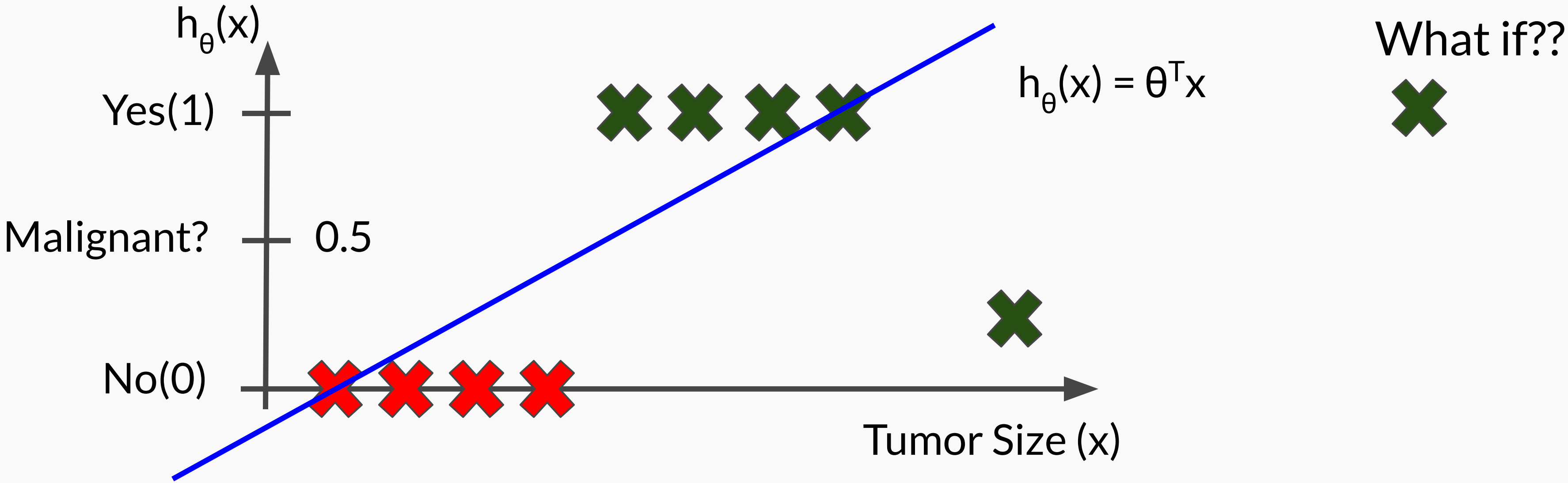
Student 3
Test: 7/10
Grades: 6/10

Binary Classification Problem

- Email = {spam, not spam}
- Medical model = {healthy, sick}
- Fraudulent operation = {yes, not}
- Academic acceptance = {success, fail}
- Movie review = {good, bad}

$Y \in \{0,1\} \longrightarrow$ 0: negative class
1: positive class

Binary Classification Problem (observation #1)



Threshold classifier output as $h_\theta(x)$:

- If $h_\theta(x) \geq 0.5$, predict $y = 1$
- If $h_\theta(x) < 0.5$, predict $y = 0$

Binary Classification Problem (observation #2)

- Y assume only two values: 0 or 1.
- In linear case, $h_\theta(x) \geq 1$ and $h_\theta(x) \leq 0$ can occur.

→ Logistic Regression

$$0 \leq h_\theta(x) \leq 1$$

Logistic Regression - Hypothesis Representation

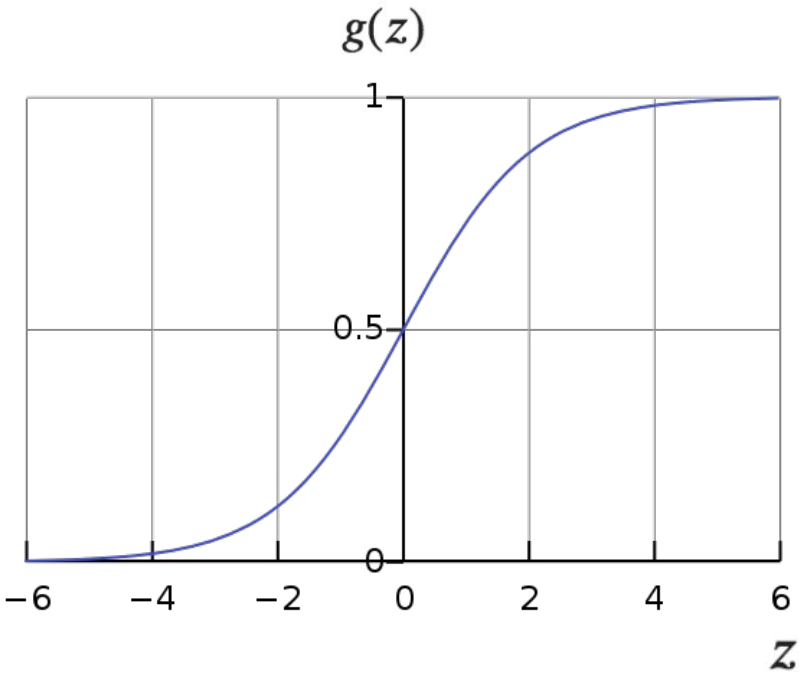
Target → $0 \leq h_\theta(x) \leq 1$

$h_\theta(x) = \theta^T x$ (doesn't work)

$h_\theta(x) = g(z)$,where $z = \theta^T x$

$$g(z) = \frac{1}{1+e^{-z}}$$

Sigmoid function or
Logistic function



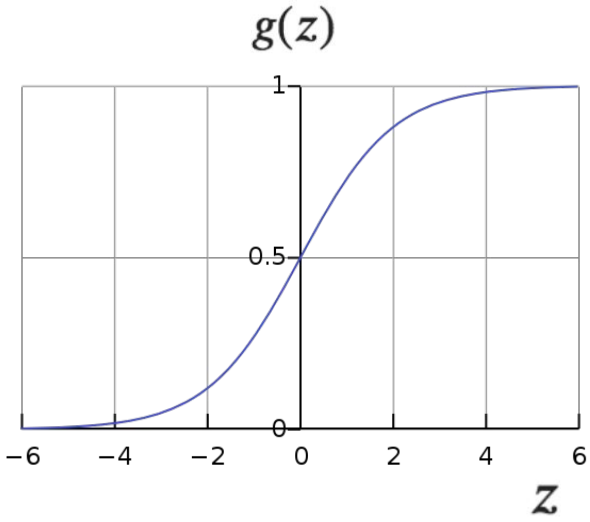
Logistic Regression - Decision Boundary

Suppose:
Predict y = 1 if $h_\theta(x) \geq 0.5$

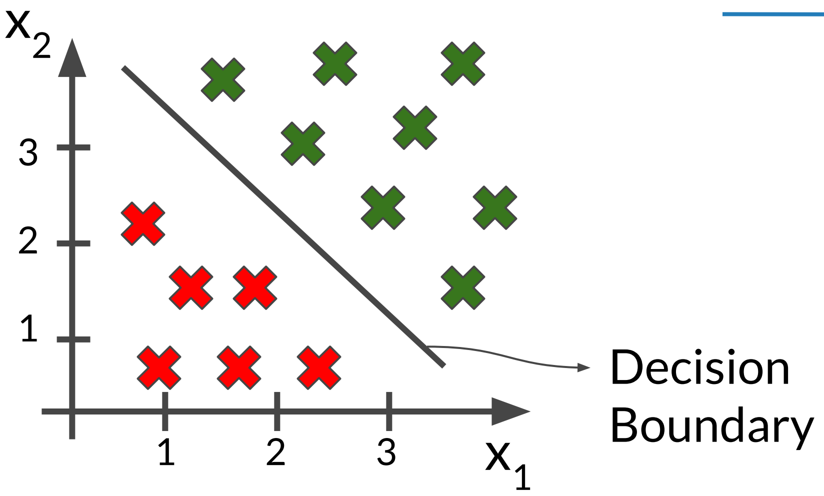
$$g(z) \geq 0.5 \text{ when } z \geq 0$$

Suppose:
Predict y = 0 if $h_\theta(x) < 0.5$

$$g(z) < 0.5 \text{ when } z < 0$$



Logistic Regression - Decision Boundary



$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

$$\theta = \begin{bmatrix} -3 \\ 1 \\ 1 \end{bmatrix}$$

$$z = -3 + x_1 + x_2$$

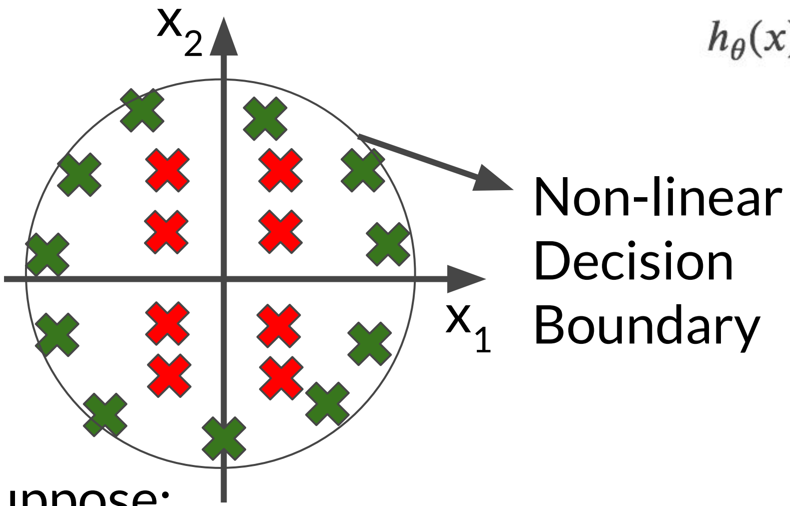
Suppose:
Predict y = 1 if $z \geq 0$

$$-3 + x_1 + x_2 \geq 0$$
$$x_1 + x_2 \geq 3$$

Suppose:
Predict y = 0 if $z < 0$

$$-3 + x_1 + x_2 < 0$$
$$x_1 + x_2 < 3$$

Logistic Regression - Decision Boundary



$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2)$$

$$\theta = \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$$

$$z = -1 + x_1^2 + x_2^2$$

Suppose:

Predict y = 1 if $z \geq 0$

$$-1 + x_1^2 + x_2^2 \geq 0$$

$$x_1^2 + x_2^2 \geq 1$$

Suppose:

Predict y = 0 if $z < 0$

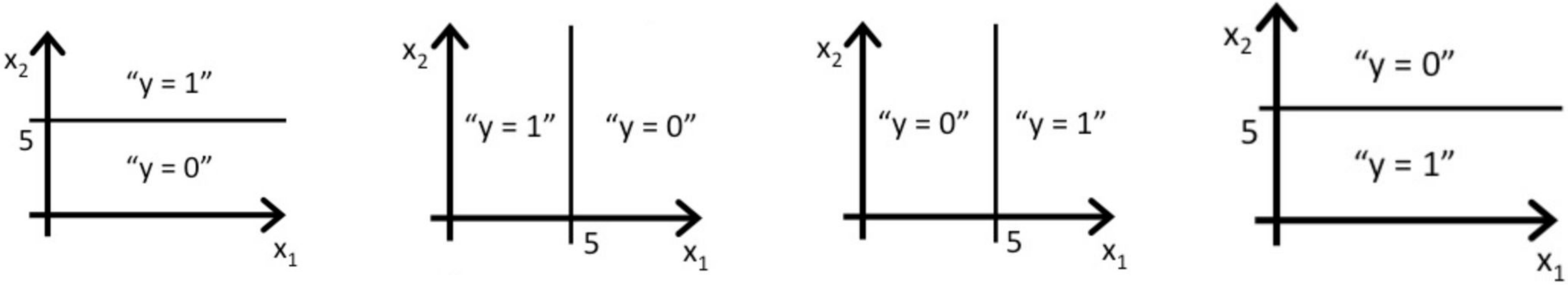
$$-1 + x_1^2 + x_2^2 < 0$$

$$x_1^2 + x_2^2 < 1$$

Logistic Regression - Decision Boundary

Consider logistic regression with two features x_1 and x_2. Suppose $\Theta_0 = 5$, $\Theta_1 = -1$ and $\Theta_2 = 0$, so that $h_\Theta(x) = g(5 - x_1)$.

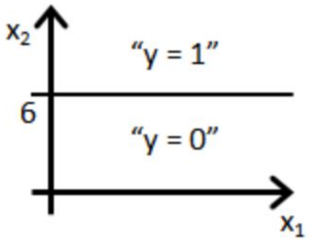
Which of these shows the decision boundary of $h_\Theta(x)$?

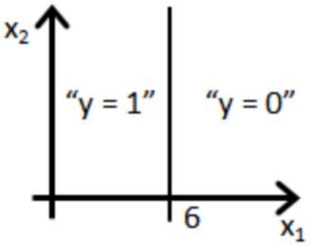


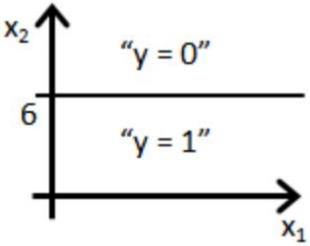
Logistic Regression - Decision Boundary

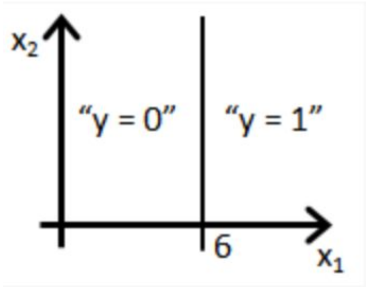
Consider logistic regression with two features x_1 and x_2. Suppose $\Theta_0 = 6$, $\Theta_1 = 0$ and $\Theta_2 = -1$, so that $h_\Theta(x) = g(\Theta_0 + \Theta_1 x_1 + \Theta_2 x_2)$.

Which of these shows the decision boundary of $h_\Theta(x)$?









Logistic Regression - Decision Boundary

Suppose that you have trained a logistic regression classifier, and it outputs on a new example x a prediction $h_\theta(x)$ = 0.4. This means (check all that apply):

Our estimate for $P(y = 0|x;\theta)$ is 0.4.

Our estimate for $P(y = 0|x;\theta)$ is 0.6.

Our estimate for $P(y = 1|x;\theta)$ is 0.4.

Our estimate for $P(y = 1|x;\theta)$ is 0.6.

RECAP

$f(x)$ cost function

Training Set: $\{(x^1, y^1), (x^2, y^2), \ldots, (x^m, y^m)\}$

m examples

<n+1 elements>

$$x \in \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}, x_0 = 1, y \in \{0, 1\}$$

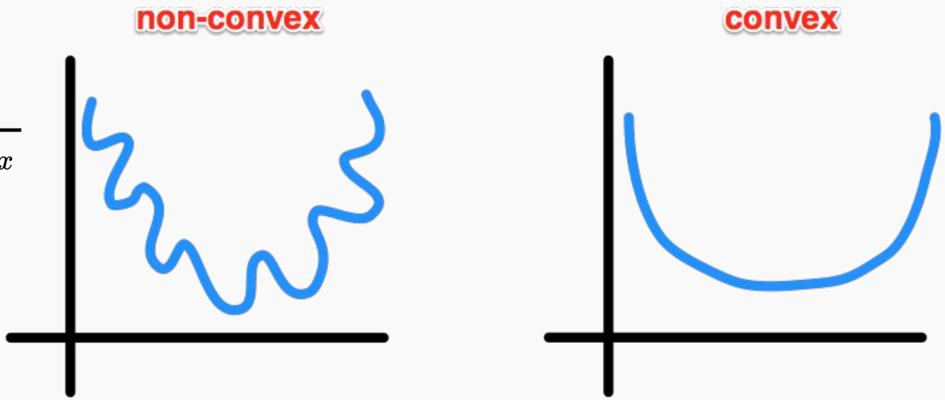
$$h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$$

How to fit the parameter θ?

Cost Function

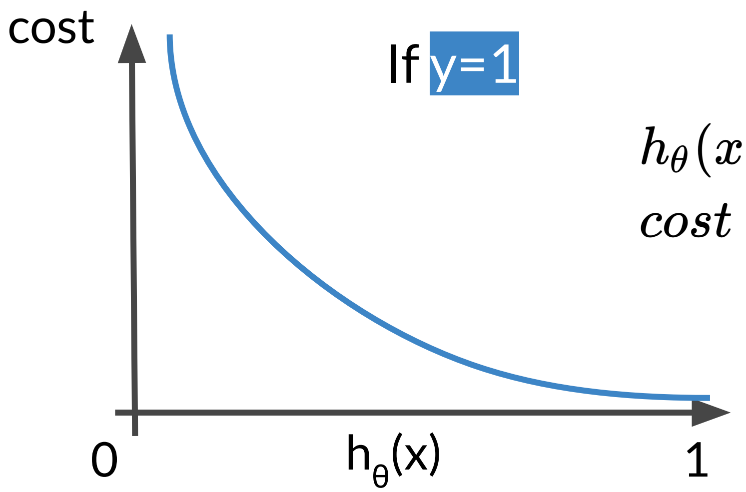
$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \frac{1}{2}\left(h_\theta(x^i) - y^i\right)^2 \longrightarrow cost(h_\theta(x), y)$$

$$h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$$



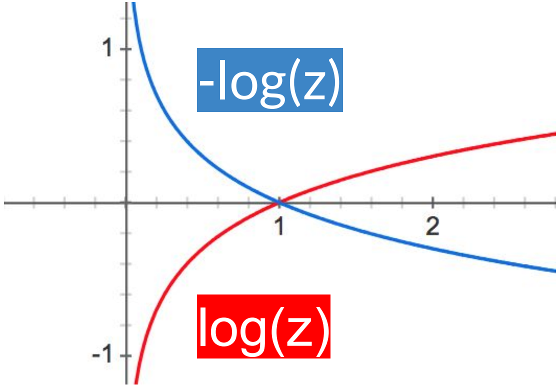
Logistic Regression Cost Function

$$cost(h_\theta(x), y) = \begin{cases} -log(h_\theta(x)) & \text{if y=1} \\ -log(1 - h_\theta(x)) & \text{if y=0} \end{cases}$$



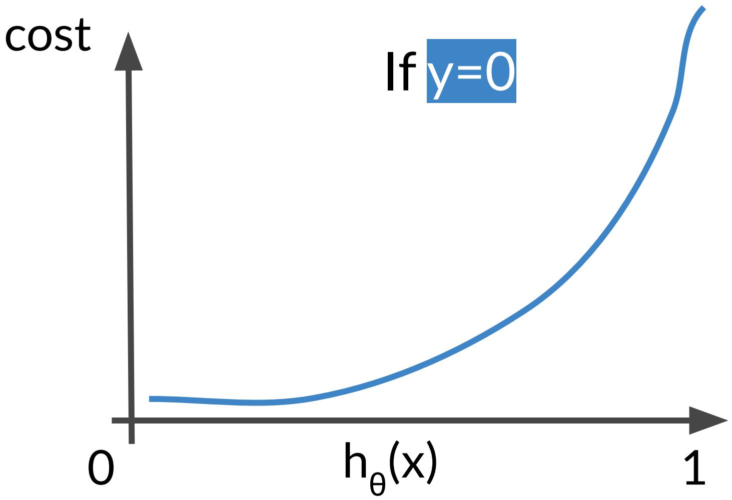
$h_\theta(x) \rightarrow 1$ $\quad$ $h_\theta(x) \rightarrow 0$

$cost \rightarrow 0$ $\quad$ $cost \rightarrow \infty$



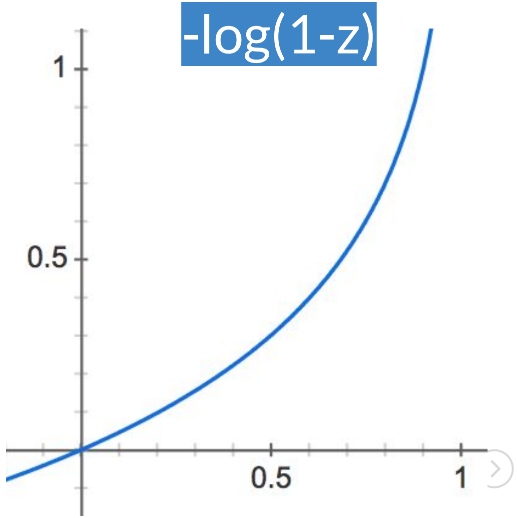
Logistic Regression Cost Function

$$cost(h_\theta(x), y) = \begin{cases} -log(h_\theta(x)) & \text{if y=1} \\ -log(1 - h_\theta(x)) & \text{if y=0} \end{cases}$$



$$h_\theta(x) \to 1$$
$$cost \to \infty$$

$$h_\theta(x) \to 0$$
$$cost \to 0$$



Simplified Cost Function & Gradient Descent

Logistic Regression Cost Function

$$cost(h_\theta(x), y) = \begin{cases} -log(h_\theta(x)) & \text{if y=1} \\ -log(1 - h_\theta(x)) & \text{if y=0} \end{cases}$$

$$cost(h_\theta(x), y) = -y\, log(h_\theta(x)) - (1 - y)log(1 - h_\theta(x))$$

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^{m} [y^{(i)} \log(h_\theta(x^{(i)})) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))]$$

Cost Function - Vectorized Implementation

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}[y^{(i)}\log(h_\theta(x^{(i)})) + (1-y^{(i)})\log(1-h_\theta(x^{(i)}))]$$

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_k \end{bmatrix}$$

[m; k+1] x [k+1;1] = [m;1]

$$h = g(X\theta)$$

$$J(\theta) = \frac{1}{m}\cdot\left(-y^T\log(h) - (1-y)^T\log(1-h)\right)$$

[1;m] x [m;1] = scalar

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log(h_\theta(x^{(i)})) + (1-y)(\log(1-h_\theta(x^{(i)}))\right]$$

```
def cost_function(theta, X, y):
  thetaX = logistic(np.matmul(X, theta))
  return -1/len(y) * np.sum(y*np.log(thetaX) + (1-y)*np.log(1 - thetaX))
```

General Form of Gradient Descent

$$
\begin{aligned}
&Repeat\ \{ \\
&\quad \theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \\
&\}
\end{aligned}
$$

$$
\begin{aligned}
&Repeat\ \{ \\
&\quad \theta_j := \theta_j - \frac{\alpha}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} \\
&\}
\end{aligned}
$$

Vectorized Implementation

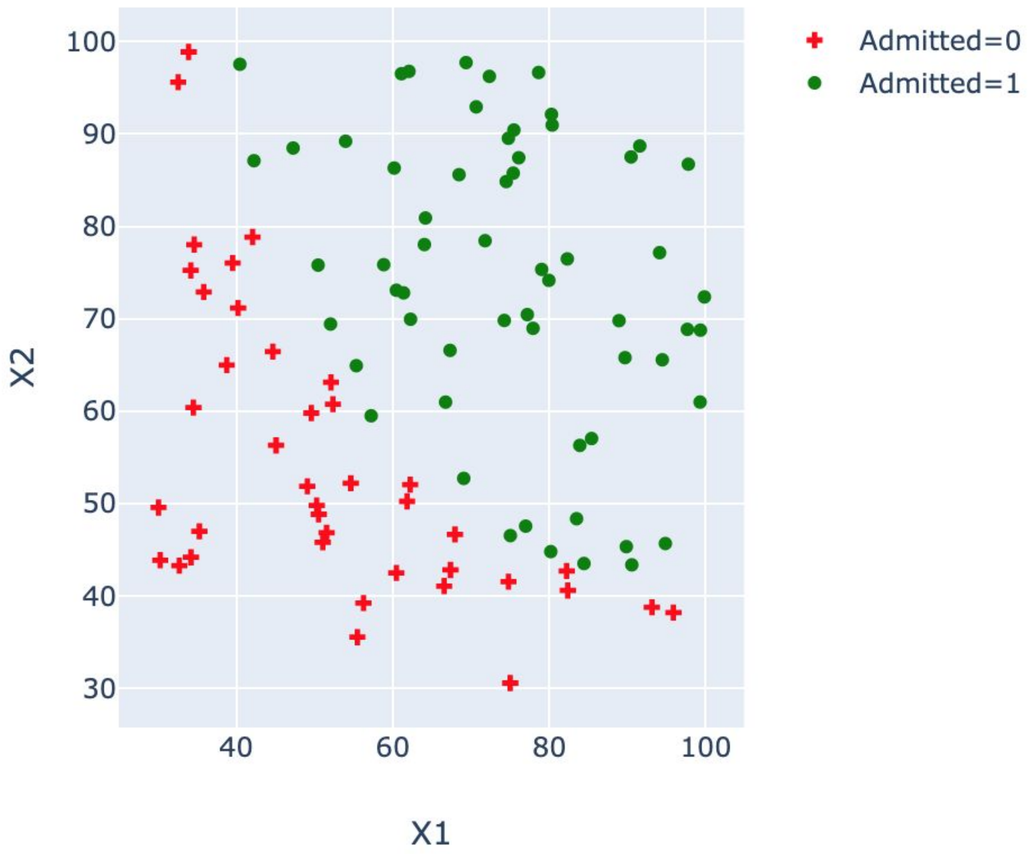
$$\theta := \theta - \frac{\alpha}{m} X^T (g(X\theta) - \vec{y})$$

gradient

$$\theta := \theta - \frac{\alpha}{m} X^T (g(X\theta) - \vec{y})$$

```
def gradient_descent_multi(theta_, X, y, alpha, iterations):
    m = len(X)
    theta = theta_.copy()
    cost_history = []
    for i in range(iterations):
        gradient = (1/m) * np.dot(X.T, logistic(np.dot(X, theta)) - y)
        theta = theta - (alpha * gradient)
        cost_history.append(cost_function(theta,X, y))
    return theta, cost_history
```

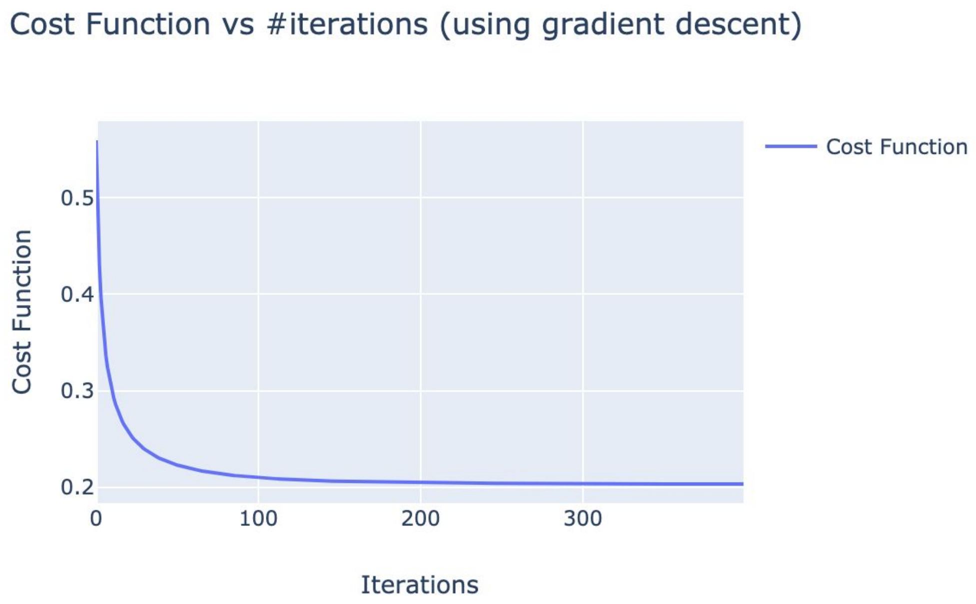
Admitted vs not Admitted

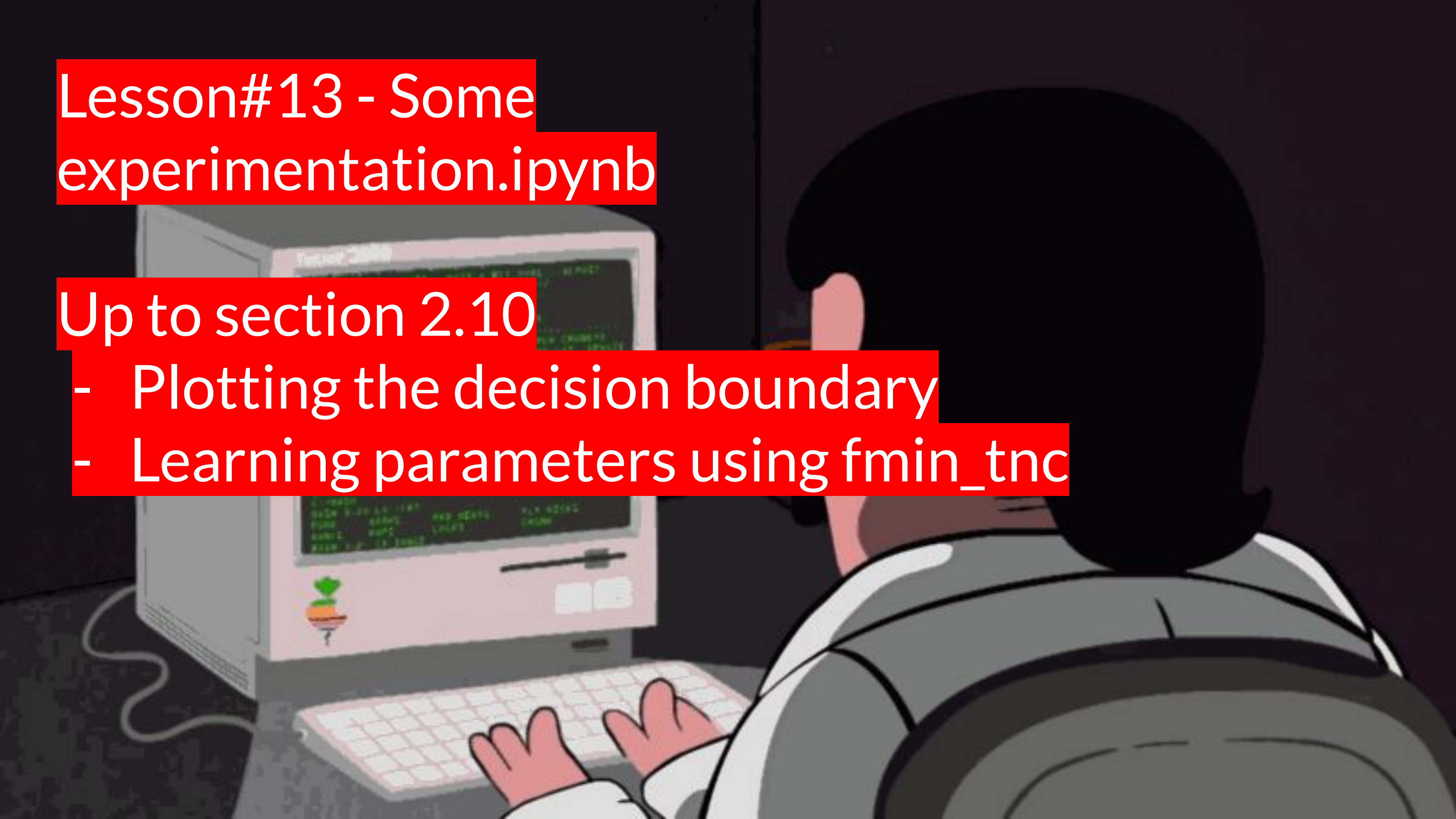


```python
# define X and y
X = np.column_stack((np.ones(data.shape[0]),
                          data[["X1_scaled","X2_scaled"]]))
y = data.Admitted.astype(np.int64).values.reshape(-1,1)

# define m and n
m,n = X.shape

# guess an initial value for theta
theta = np.zeros((n,1))
```

```
# using gradient descent
# theta, X, y, alpha, iterations
theta_batch, cost_history = gradient_descent_multi(theta,X,y,1,400)
```

```
array([[1.65947664],
       [3.8670477 ],
       [3.60347302]])
```





Lesson#13 - Some experimentation.ipynb

Up to section 2.10

- Plotting the decision boundary
- Learning parameters using fmin_tnc

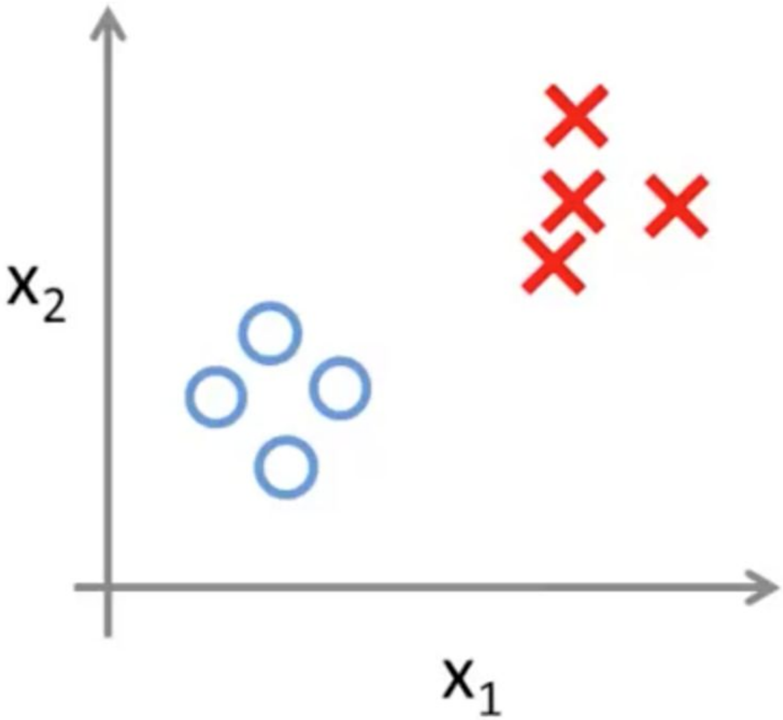
Multiclass Classification:

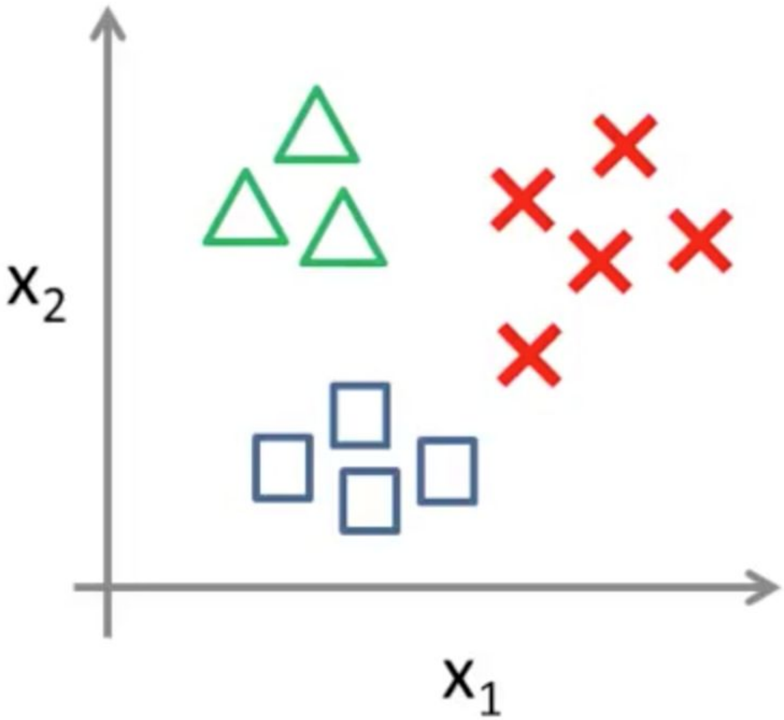
One vs All

Multiclass Classification

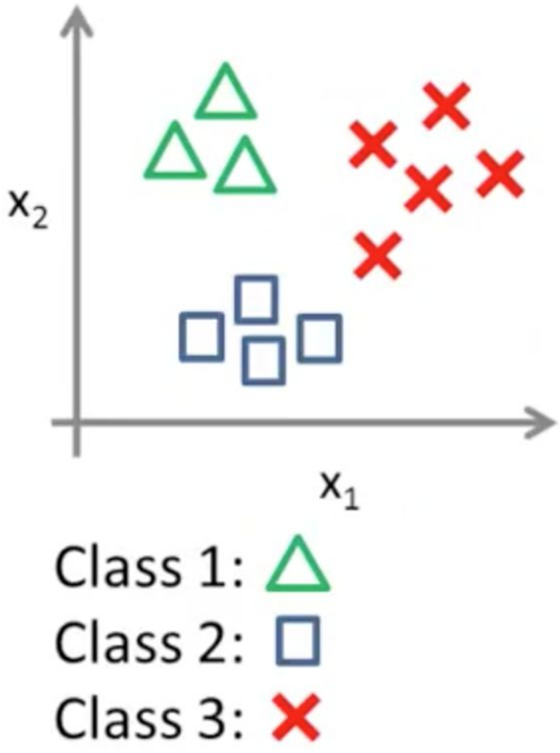
- Email foldering/tagging: work, ad, family, friends, hobby
- Medical diagrams: not ill, cold, flu
- Weather: sunny, cloudy, rain, snow

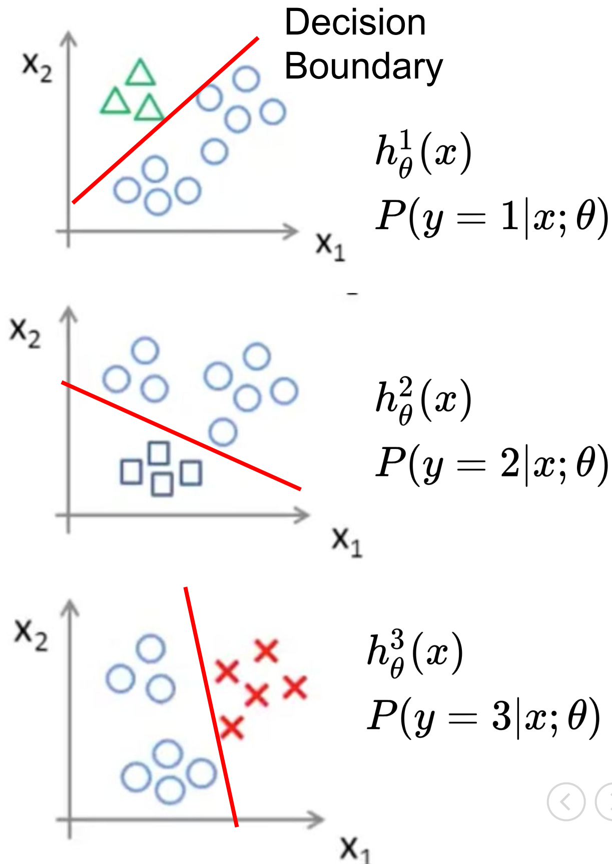
Binary vs Multiclass Classification





Multiclass Classification (One vs All)





Multiclass Classification (One vs All)

Train a logistic regression classifier $h_\theta^{(i)}(x)$ for each class i:

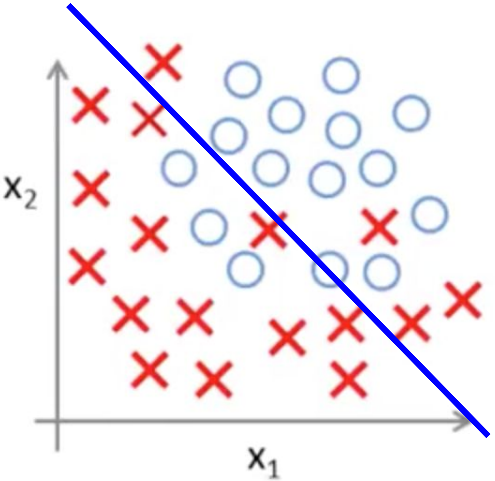
$$h_\theta^i(x) = P(y = i|x;\theta)$$

On a new input x, to make a prediction, pick the class i that maximizes:

$$\max_i h_\theta^{(i)}(x)$$

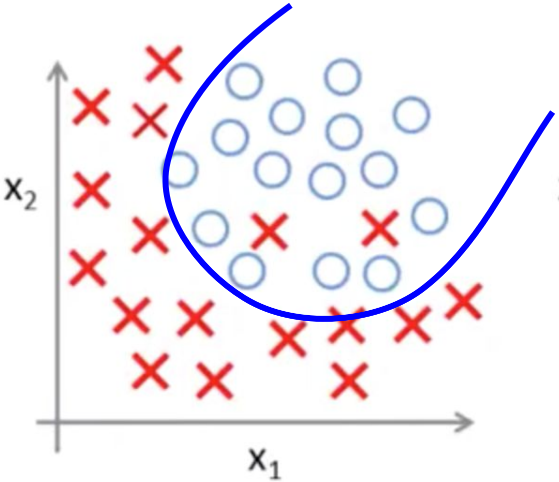
overfitting problem

Logistic Regression

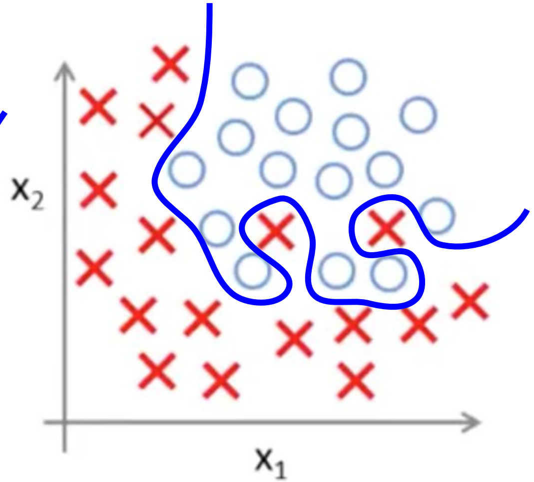


$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

(g = sigmoid function)



$$g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 \\ +\theta_3 x_1^2 + \theta_4 x_2^2 \\ +\theta_5 x_1 x_2)$$



$$g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 \\ +\theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 \\ +\theta_5 x_1^2 x_2^3 + \theta_6 x_1^3 x_2 + \dots)$$

Underfit

Overfit

```python
import numpy as np
from sklearn.preprocessing import PolynomialFeatures

a = np.arange(6).reshape(3, 2)
print(a)
[[0 1]
 [2 3]
 [4 5]]
```

```python
poly = PolynomialFeatures(2)
poly.fit_transform(a)

array([[ 1.,  0.,  1.,  0.,  0.,  1.],
       [ 1.,  2.,  3.,  4.,  6.,  9.],
       [ 1.,  4.,  5., 16., 20., 25.]])
```

$$terms = \binom{n+d}{d} = \binom{2+2}{2} = 6$$

$$[1, x_1, x_2, x_1^2, x_1 x_2, x_2^2]$$

$$\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_1 x_2 + \theta_5 x_2^2$$

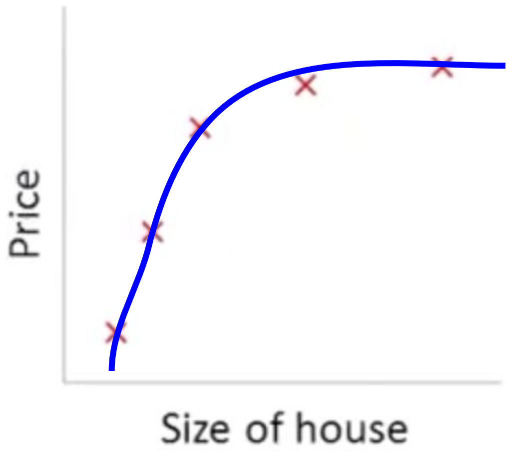
Addressing Overfitting

1. Reduce number of features
   a. Manually select which feature to keep
2. Regularization
   a. Keep all the features, but reduce magnitude/values of parameters Θ_j
   b. Works well when we have a lot of features, each of which contributes a bit to predicting y.

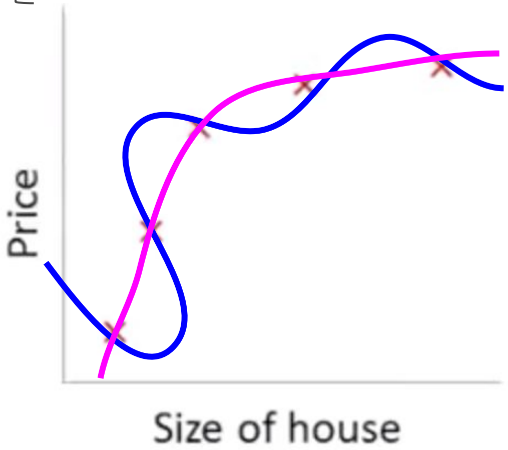
Intuition - Regularized Linear Regression

$$min_\theta \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n}\theta_j^2\right]$$

Regularization Parameter



$$\theta_0 + \theta_1 x + \theta_2 x^2$$



$$\theta_0 + \theta_1 x + \theta_2 x^2 + \cancel{\theta_3 x^3} + \cancel{\theta_4 x^4}$$

Suppose we penalize and make Θ_3 and Θ_4 very small

$$min_\theta \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + 1000 \cdot \theta_3^2 + 1000 \cdot \theta_4^2$$

Intuition - Gradient Descent (L2 - Ridge)

Repeat {

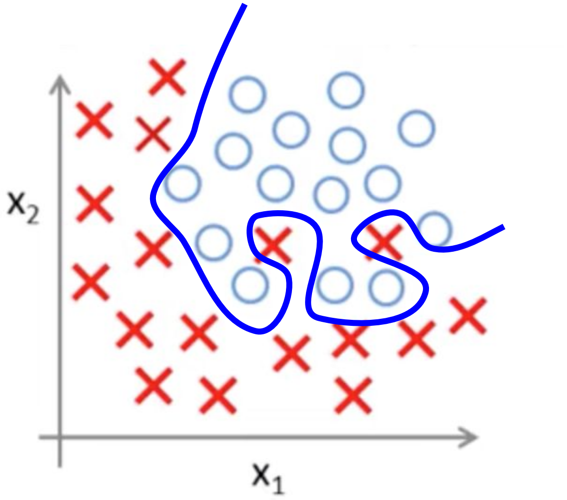
$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \left[\left(\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)} \right) + \frac{\lambda}{m} \theta_j \right] \qquad j \in \{1, 2 \ldots n\}$$

}

$$\theta_j := \theta_j (1 - \alpha \frac{\lambda}{m}) - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

Intuition - Regularized Logistic Regression

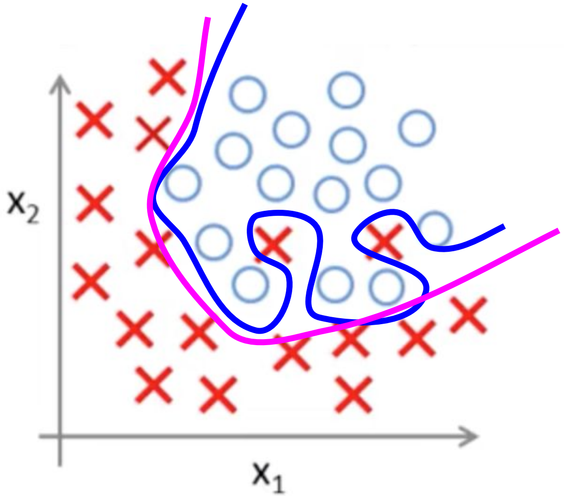


$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 + \theta_5 x_1^2 x_2^3 + \dots)$$

Cost function:

$$J(\theta) = -\left[\frac{1}{m}\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log\left(1 - h_\theta(x^{(i)})\right)\right]$$

Intuition - Regularized Logistic Regression (L2)



$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 + \theta_5 x_1^2 x_2^3 + \dots)$$

Cost function:

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\ \log(h_\theta(x^{(i)})) + (1-y^{(i)})\ \log(1-h_\theta(x^{(i)}))\right] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

L2 - Ridge Regression

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log(h_\theta(x^{(i)})) + (1-y)(\log(1-h_\theta(x^{(i)})\right] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

$$\theta_i \,:\, i = 0 \ldots n$$

```
def cost_function_reg_l2(theta, X, y, lambda_):
  m = len(y)
  thetaX = logistic(np.matmul(X, theta))
  regularization = lambda_/(2*m) * np.sum(theta[1:]**2)
  return -1/m * np.sum(y*np.log(thetaX) + (1-y)*np.log(1 - thetaX)) + regularization
```

L1 - Lasso Regression

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log(h_\theta(x^{(i)})) + (1-y)(\log(1-h_\theta(x^{(i)})\right] + \frac{\lambda}{2m}\sum_{j=1}^{n}|\theta_j|$$

$$\theta_i \; : i = 0 \ldots n$$

```
def cost_function_reg_l1(theta, X, y, lambda_):
  m = len(y)
  thetaX = logistic(np.matmul(X, theta))
  regularization = lambda_/(2*m) * np.sum(np.absolute(theta[1:]))
  return -1/m * np.sum(y*np.log(thetaX) + (1-y)*np.log(1 - thetaX)) + regularization
```

Intuition - Gradient Descent (L2)

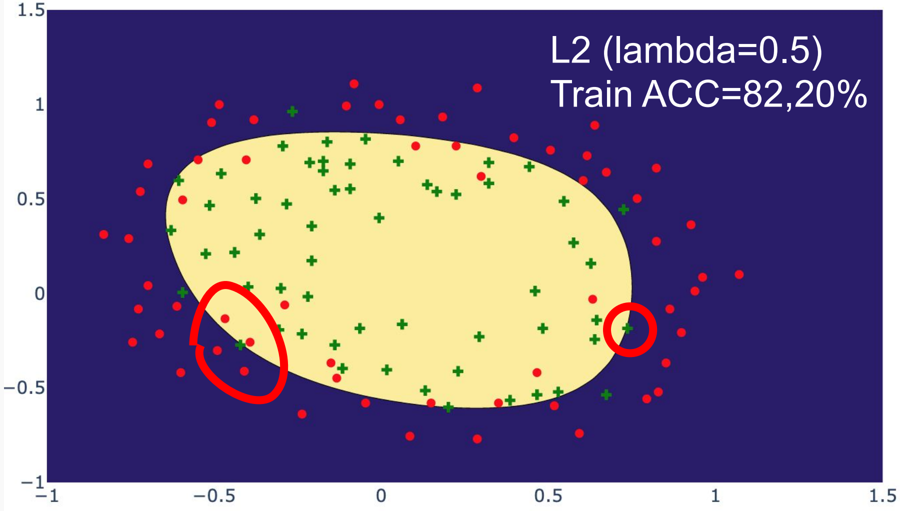
Repeat {

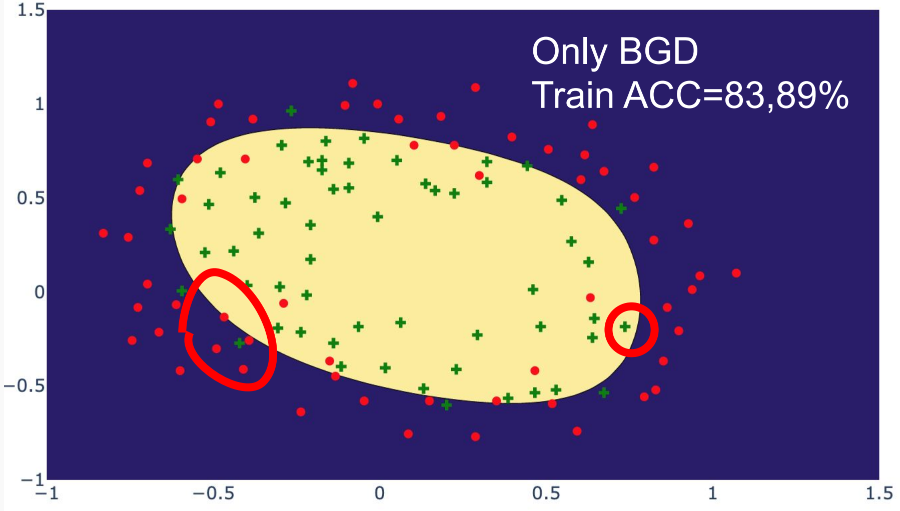
$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})x_0^{(i)}$$

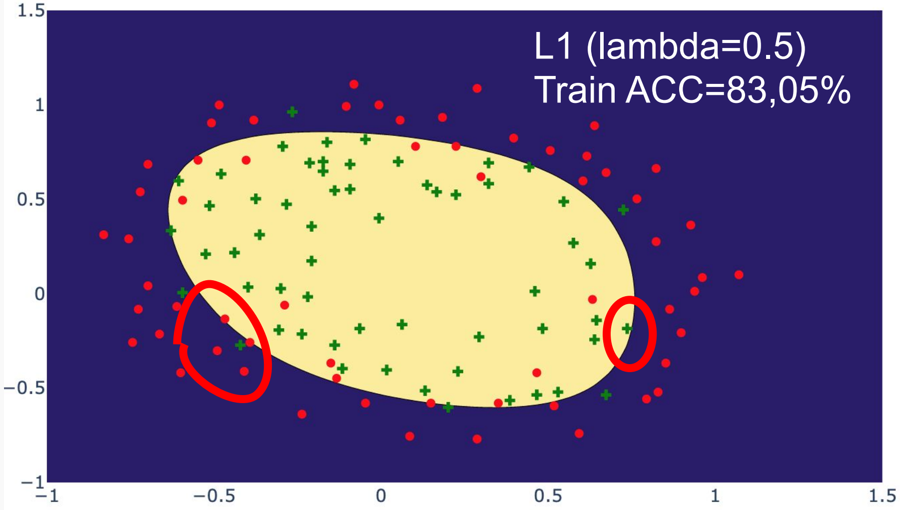
$$\theta_j := \theta_j - \alpha \left[\left(\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)} \right) + \frac{\lambda}{m} \theta_j \right] \qquad j \in \{1, 2 \ldots n\}$$

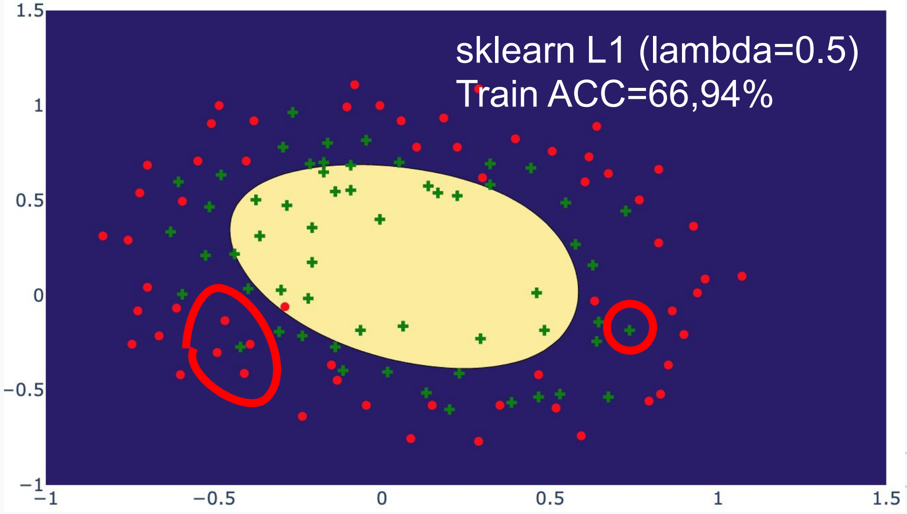
}

$$\theta_j := \theta_j(1 - \alpha\frac{\lambda}{m}) - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$$

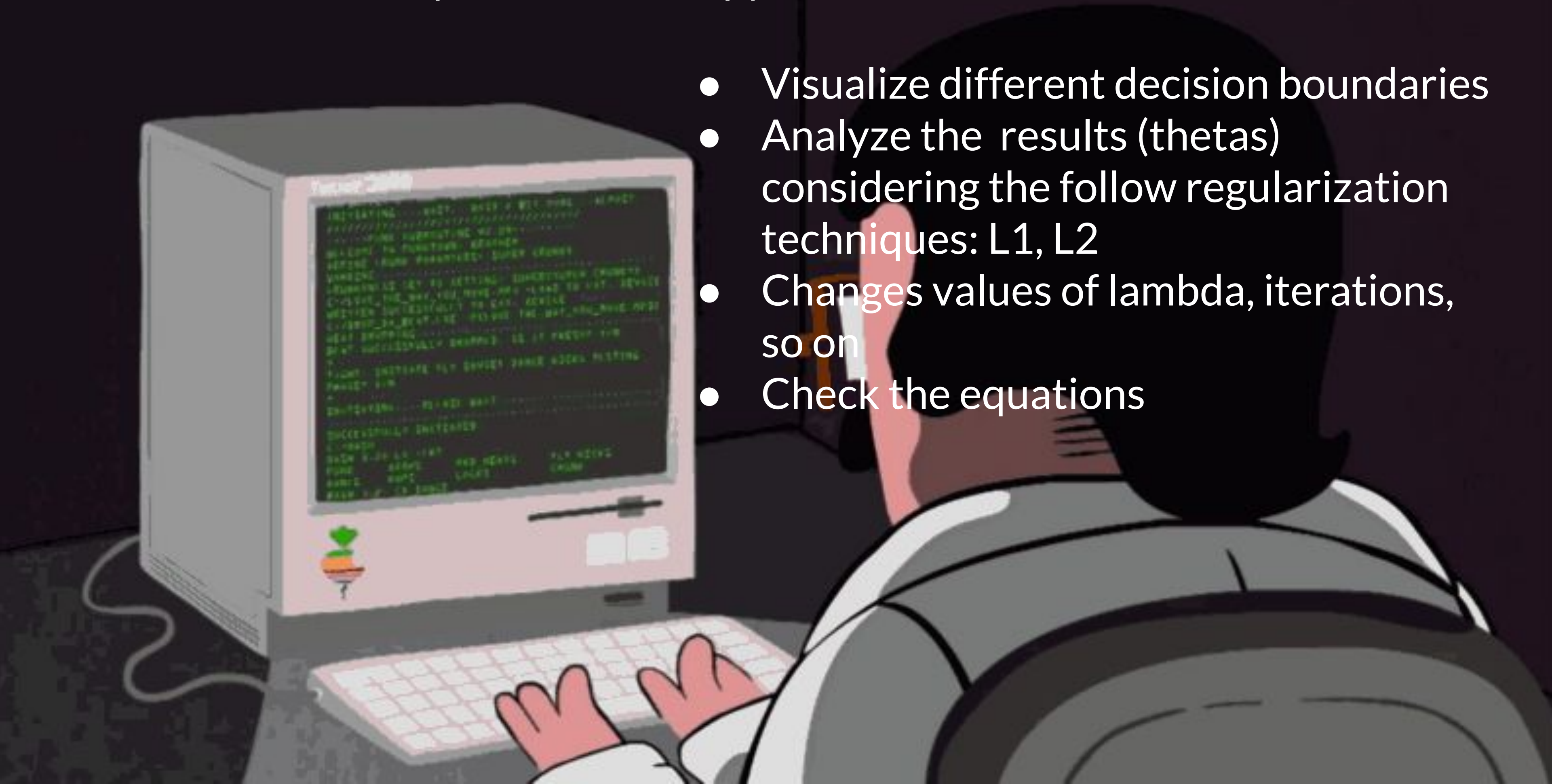

L2 (lambda=0.5)
Train ACC=82,20%
1.5
1
0.5
0
−0.5
−1
−1
−0.5
0
0.5
1
1.5


Only BGD
Train ACC=83,89%
1.5
1
0.5
0
−0.5
−1
−1
−0.5
0
0.5
1
1.5


L1 (lambda=0.5)
Train ACC=83,05%
1.5
1
0.5
0
−0.5
−1
−1
−0.5
0
0.5
1
1.5


sklearn L1 (lambda=0.5)
Train ACC=66,94%
1.5
1
0.5
0
−0.5
−1
−1
−0.5
0
0.5
1
1.5

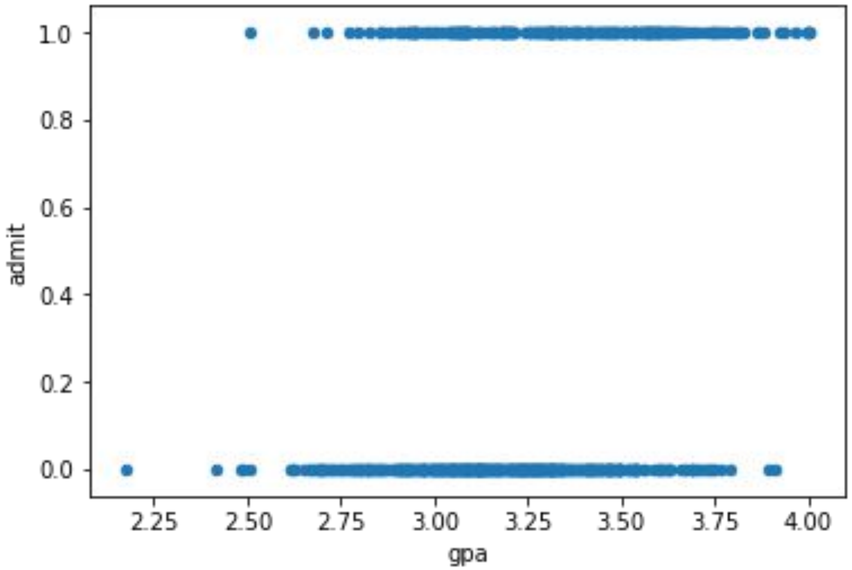
Lesson#13 - Some experimentation.ipynb



- Visualize different decision boundaries
- Analyze the results (thetas) considering the follow regularization techniques: L1, L2
- Changes values of lambda, iterations, so on
- Check the equations

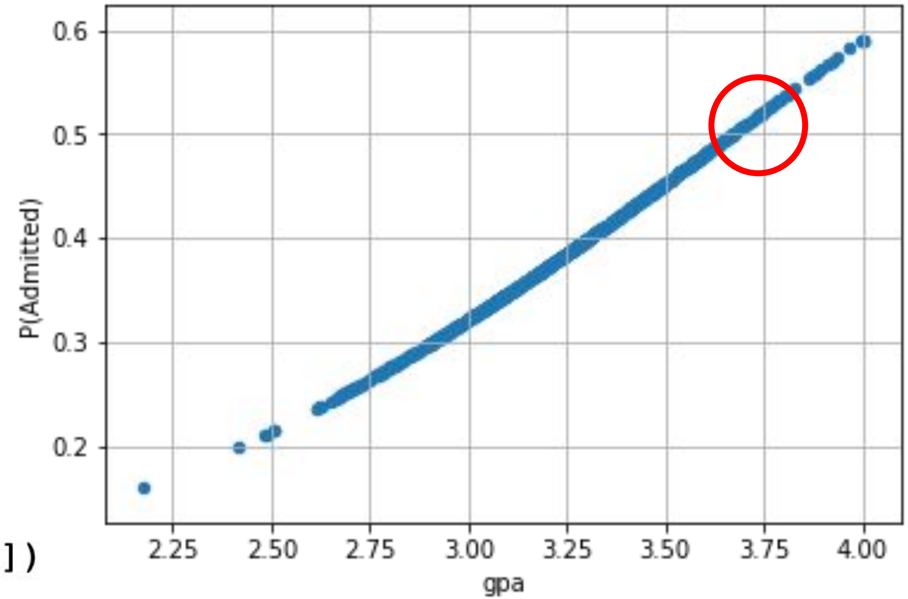
Binary Classification

admit	gpa	gre
0	3.177277	594.102992
0	3.412655	631.528607
0	2.728097	553.714399
0	3.093559	551.089985
0	3.141923	537.184894

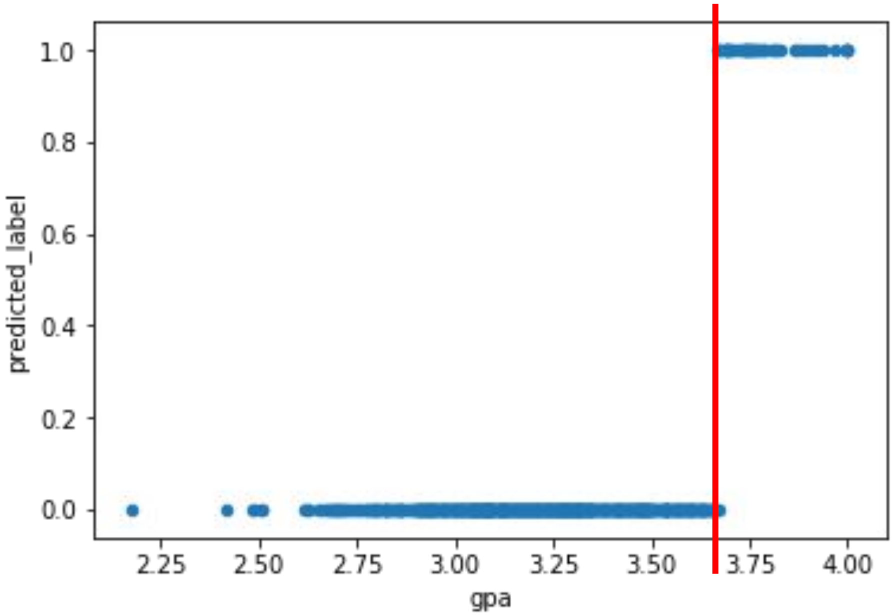


Logistic Regression Model (fit, predict prob.)

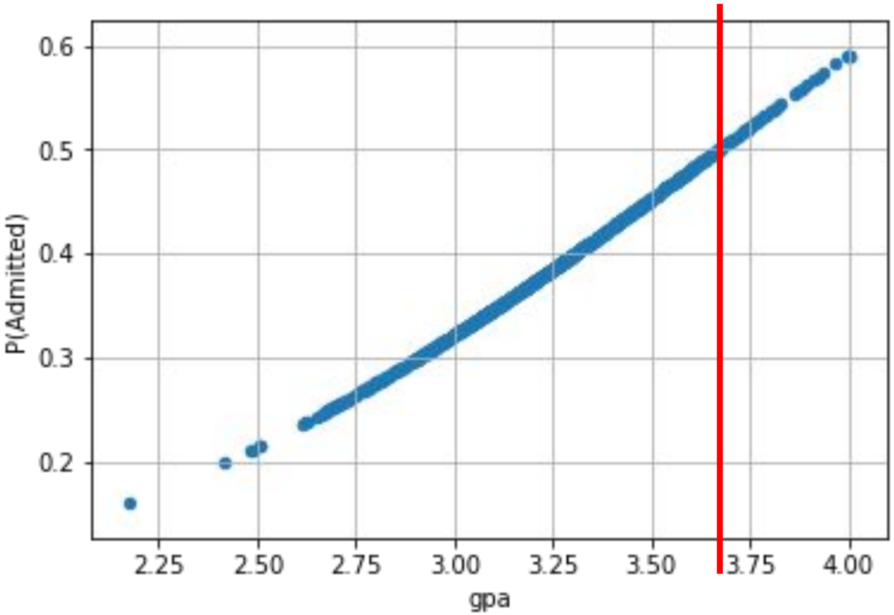
```
# create a model
model = LogisticRegression()
# training
model.fit(data[["gpa"]],data["admit"])
# predict
prob = model.predict_proba(data[["gpa"]])
# store in a dataframe
data["P(Admitted)"] = prob[:,1]
```



Logistic Regression Model (fit, predict class)



`model.predict(data[["gpa"]])`



`model.predict_proba(data[["gpa"]])[:,1]`

Evaluating Binary Classifiers

Prediction	Observation	
	Admitted (1)	Rejected (0)
Admitted (1)	True Positive (TP)	False Positive (FP)
Rejected (0)	False Negative (FN)	True Negative (TN)

```
from sklearn.metrics import confusion_matrix

tn, fp, fn, tp = confusion_matrix(data.admit,
                                  data.predicted_label).ravel()
```

Evaluating Binary Classifiers

Prediction	Observation	
	Admitted (1)	Rejected (0)
Admitted (1)	True Positive (TP)	False Positive (FP)
Rejected (0)	False Negative (FN)	True Negative (TN)

$$Accuracy = \frac{\#\text{correct predictions}}{\#\text{observations}}$$

$$Accuracy = \frac{TP + TN}{TP + TN + FN + FP}$$

$$TPR = \frac{\#\text{true positives}}{\#\text{true positives} + \#\text{false negatives}}$$

Recall

$$TNR = \frac{\#\text{true negatives}}{\#\text{true negatives} + \#\text{false positives}}$$

Evaluating Binary Classifiers

Prediction	Observation	
	Admitted (1)	Rejected (0)
Admitted (1)	True Positive (TP)	False Positive (FP)
Rejected (0)	False Negative (FN)	True Negative (TN)

$$precision = \frac{TP}{(TP + FP)}$$

$$precision = \frac{TN}{(TN + FN)}$$

$$F_1 = 2 \times \frac{Precision \times Recall}{Precision + Recall}$$

```python
from sklearn.metrics import classification_report

print(classification_report(data[["admit"]],
                            data[["predicted_label"]],
                            target_names=['0','1']))
```

```
              precision    recall  f1-score   support

           0       0.64      0.96      0.77       400
           1       0.67      0.13      0.21       244

    accuracy                           0.65       644
   macro avg       0.66      0.54      0.49       644
weighted avg       0.66      0.65      0.56       644
```

Multiclass Classification

	mpg	cylinders	displacement	horsepower	weight	acceleration	year	origin
0	18.0	8	307.0	130.0	3504.0	12.0	70	1
1	15.0	8	350.0	165.0	3693.0	11.5	70	1
2	18.0	8	318.0	150.0	3436.0	11.0	70	1
3	16.0	8	304.0	150.0	3433.0	12.0	70	1
4	17.0	8	302.0	140.0	3449.0	10.5	70	1

origin -- Integer and Categorical. 1: North America, 2: Europe, 3: Asia.

Dummy Variables

cyl_3	cyl_4	cyl_5	cyl_6	cyl_8
0	0	0	0	1
0	0	0	0	1
0	0	0	0	1
0	0	0	0	1
0	0	0	0	1

```
dummy_cylinders = pd.get_dummies(
    cars["cylinders"],prefix="cyl")
cars = pd.concat([cars, dummy_cylinders],
                 axis=1)
cars.head()
```

year_70	year_71	year_72	year_73	year_74	year_75	year_76	year_77	year_78	year_79	year_80	year_81	year_82
1	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0	0	0

Training a Multiclass Logistic Regression Model

```
from sklearn.linear_model import LogisticRegression

unique_origins = cars["origin"].unique()
unique_origins.sort()

models = {}
features = [c for c in train.columns
            if c.startswith("cyl") or c.startswith("year")]

for origin in unique_origins:
    model = LogisticRegression()

    X_train = train[features]
    y_train = train["origin"] == origin

    model.fit(X_train, y_train)
    models[origin] = model
```

Testing (One vs All)

	1	2	3
0	0.613723	0.131164	0.262305
1	0.536781	0.226177	0.236130
2	0.613723	0.131164	0.262305
3	0.678392	0.174871	0.154612
4	0.616443	0.226177	0.162931