Data Science & ML Course

Lesson #19 Logistic Regression

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Update from repository

```
git clone https://github.com/ivanovitchm/datascience2machinelearning.git
```

Or ….

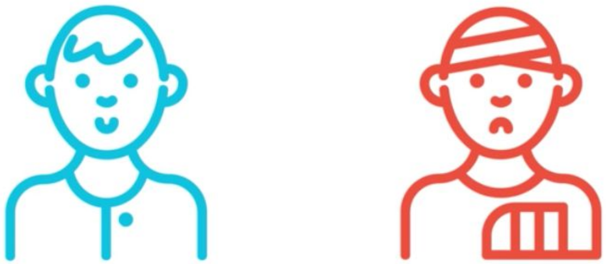
```
git pull
```

Agenda

1. Classification
2. Binary Classification
3. Decision Boundary
4. Cost Function
5. Multiclass Classification
6. Regularization
7. Hands on Scikit

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

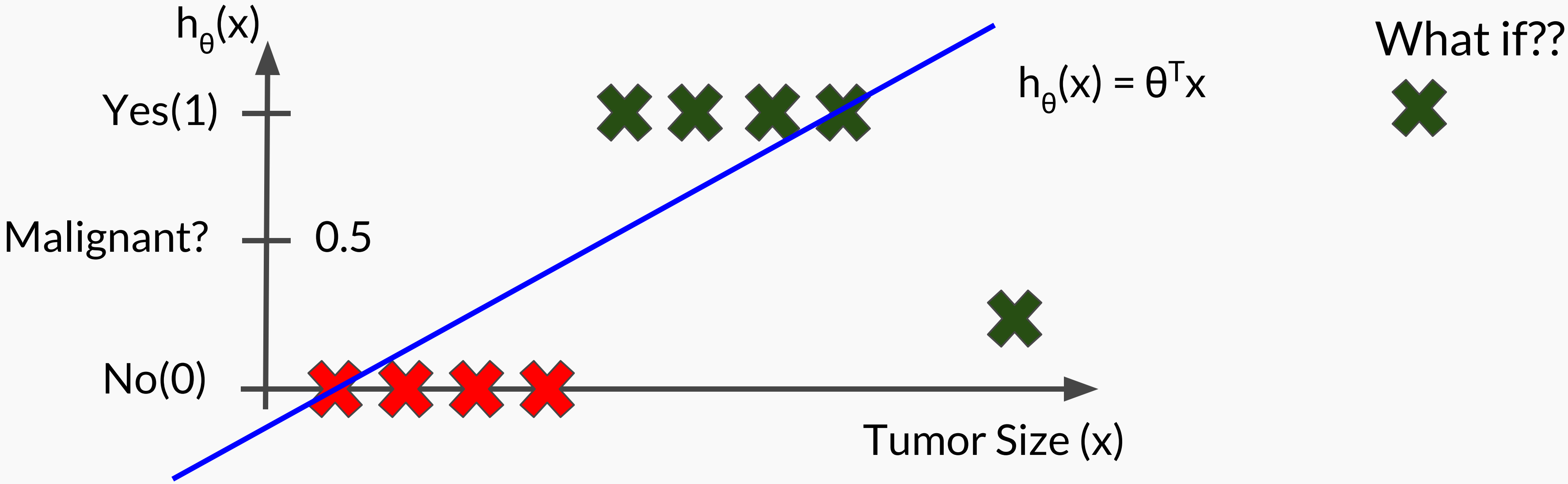
Binary Classification Problem

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

$Y \in \{0,1\}$

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, $h_\theta(x) > 1$ and $h_\theta(x) < 0$ can occur.

Logistic Regression

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

Logistic Regression - Hypothesis Representation

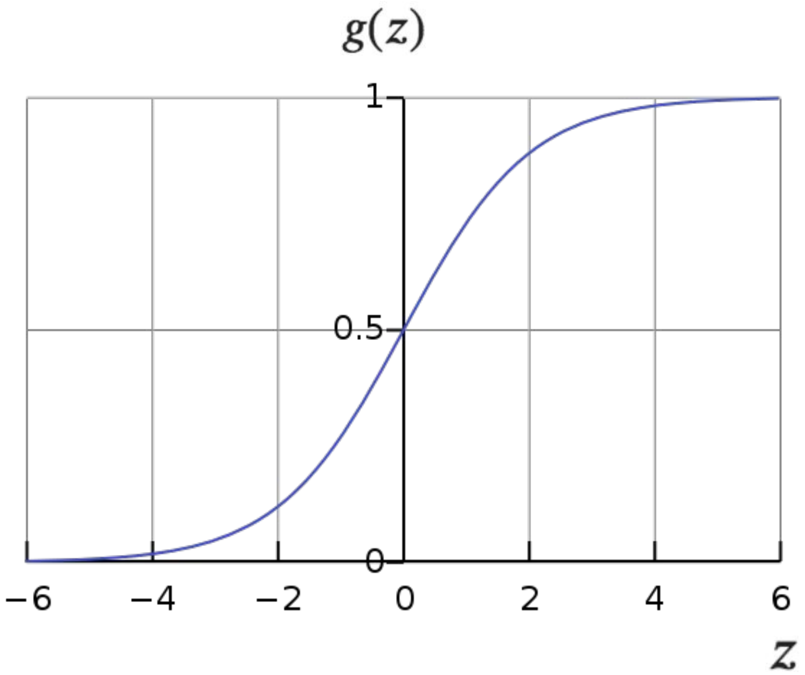
Target → $0 \le h_\theta(x) \le 1$

$$h_\theta(x) = \theta^T x \quad \text{(doesn't work)}$$

$$h_\theta(x) = g(z) \quad \text{,where } z = \theta^T x$$

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

Sigmoid function or logistic function



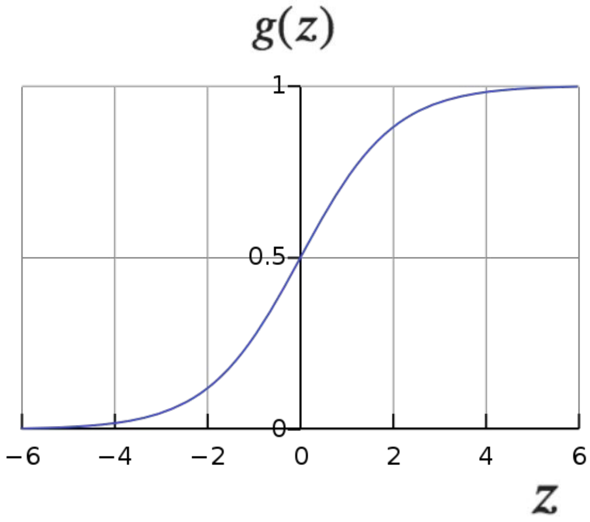
Logistic Regression - Decision Boundary

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

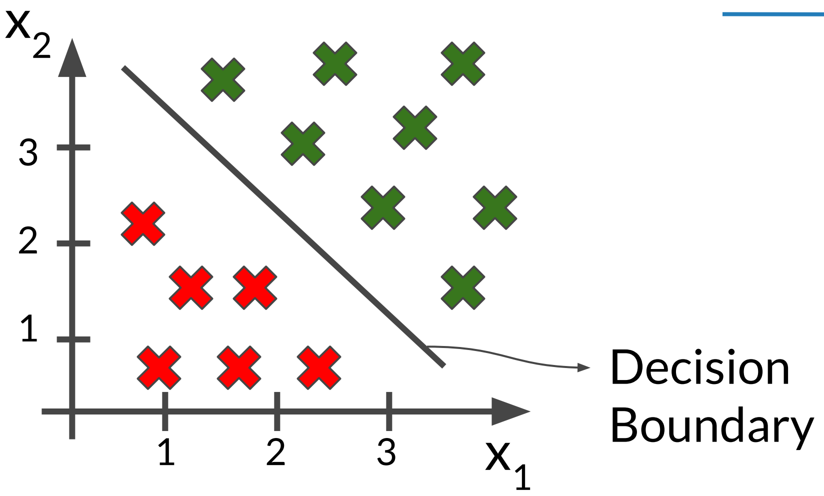
$$g(z) \geq 0.5 \text{ when } z \geq 0$$

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

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



Logistic Regression - Decision Boundary



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

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

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

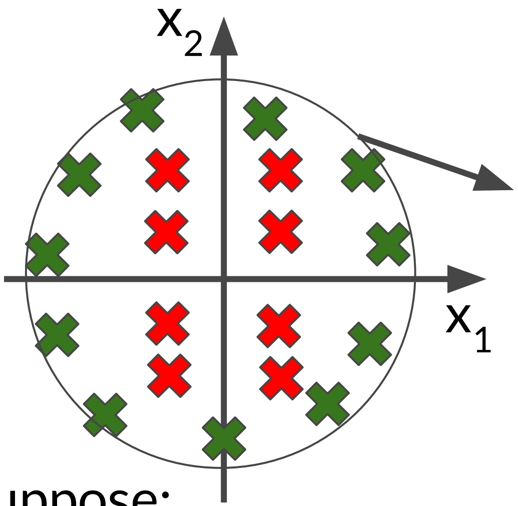
Suppose:
Predict y = 1 if $h_\theta(x) \geq 0.5$

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

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

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

Logistic Regression - Decision Boundary



Non-linear 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 $h_\theta(x) \geq 0.5$

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

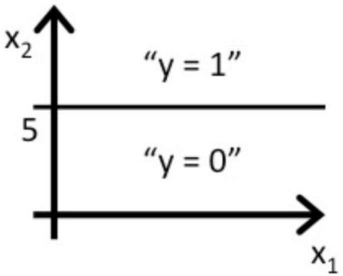
Suppose:
Predict y = 0 if $h_\theta(x) < 0.5$

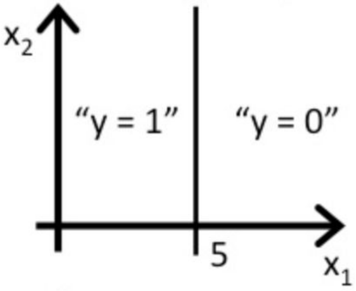
$$-1 + x_1^2 + x_2^2 < 0$$
$$x_1^2 + x_2^2 < 1$$

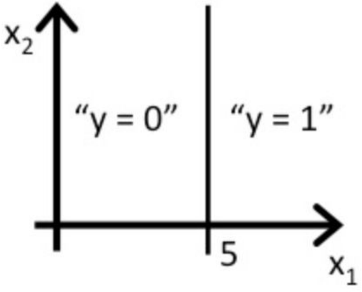
Logistic Regression - Decision Boundary

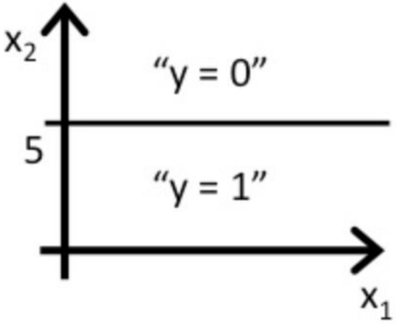
Consider logistic regression with two features x_1 and x_2. Suppose $\Theta_0 = 5$, $\Theta_1 = -1$ and $\Theta_2 = 0$, so that $h_\Theta(x) = g(5 - x_1)$.

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





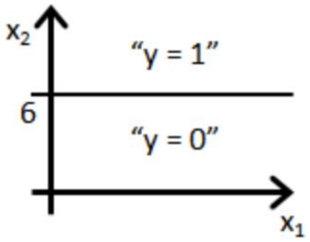


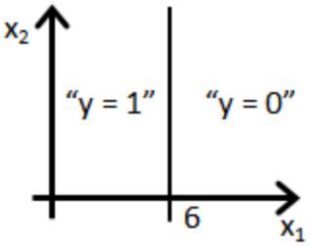


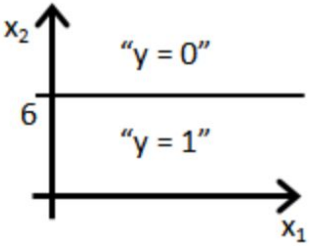
Logistic Regression - Decision Boundary

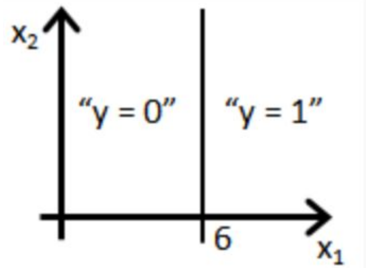
Consider logistic regression with two features x_1 and x_2. Suppose $\Theta_0 = 6$, $\Theta_1 = 0$ and $\Theta_2 = -1$, so that $h_\Theta(x) = g(\Theta_0 + \Theta_1 x_1 + \Theta_2 x_2)$.

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>

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

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

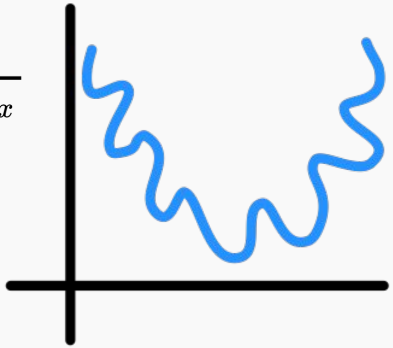
How to fit the parameter θ?

Cost Function

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

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

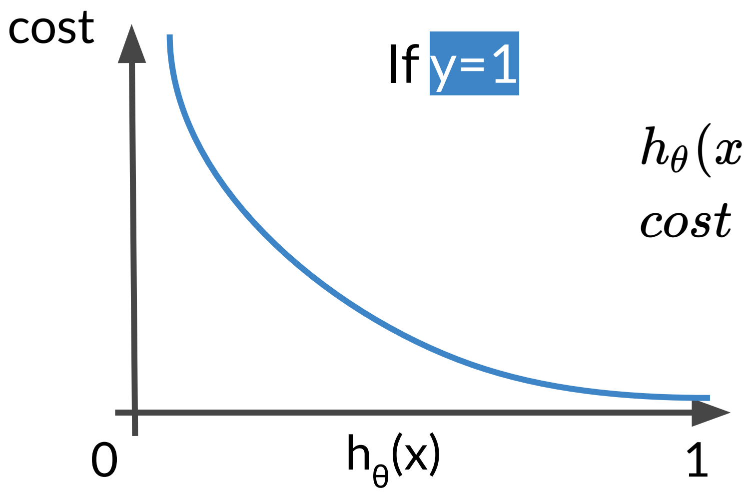
non-convex



convex

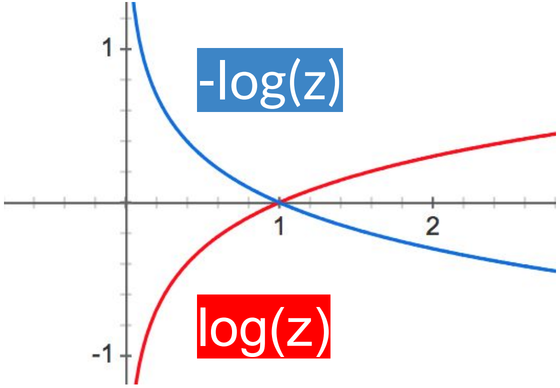
Logistic Regression Cost Function

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



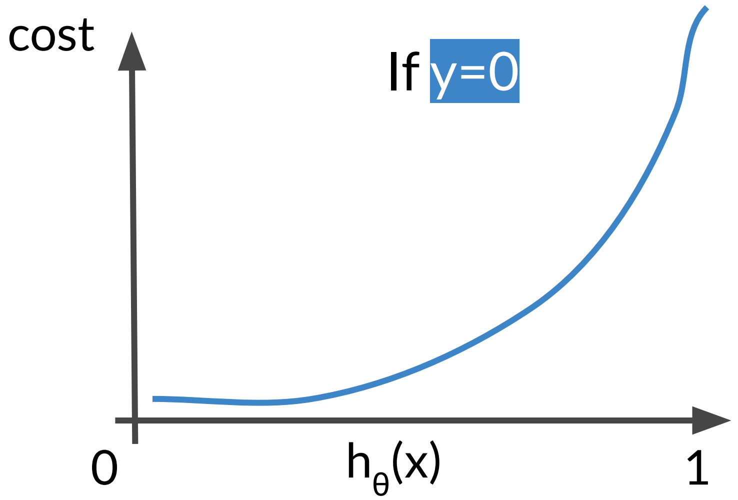
$h_\theta(x) \to 1$ $\quad$ $h_\theta(x) \to 0$

$cost \to 0$ $\quad$ $cost \to \infty$



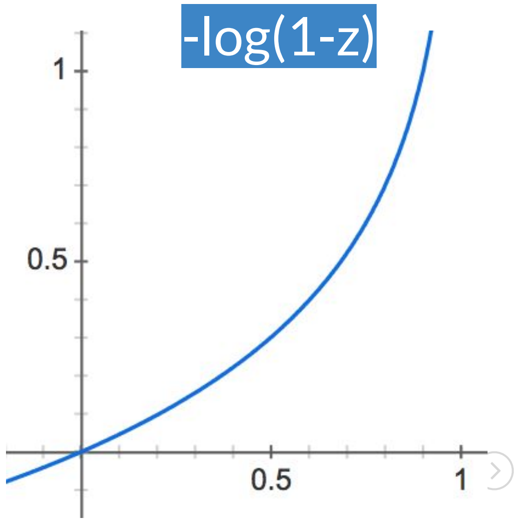
Logistic Regression Cost Function

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



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

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



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

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

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

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_k \end{bmatrix} \qquad h = g(X\theta)$$

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

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

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

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

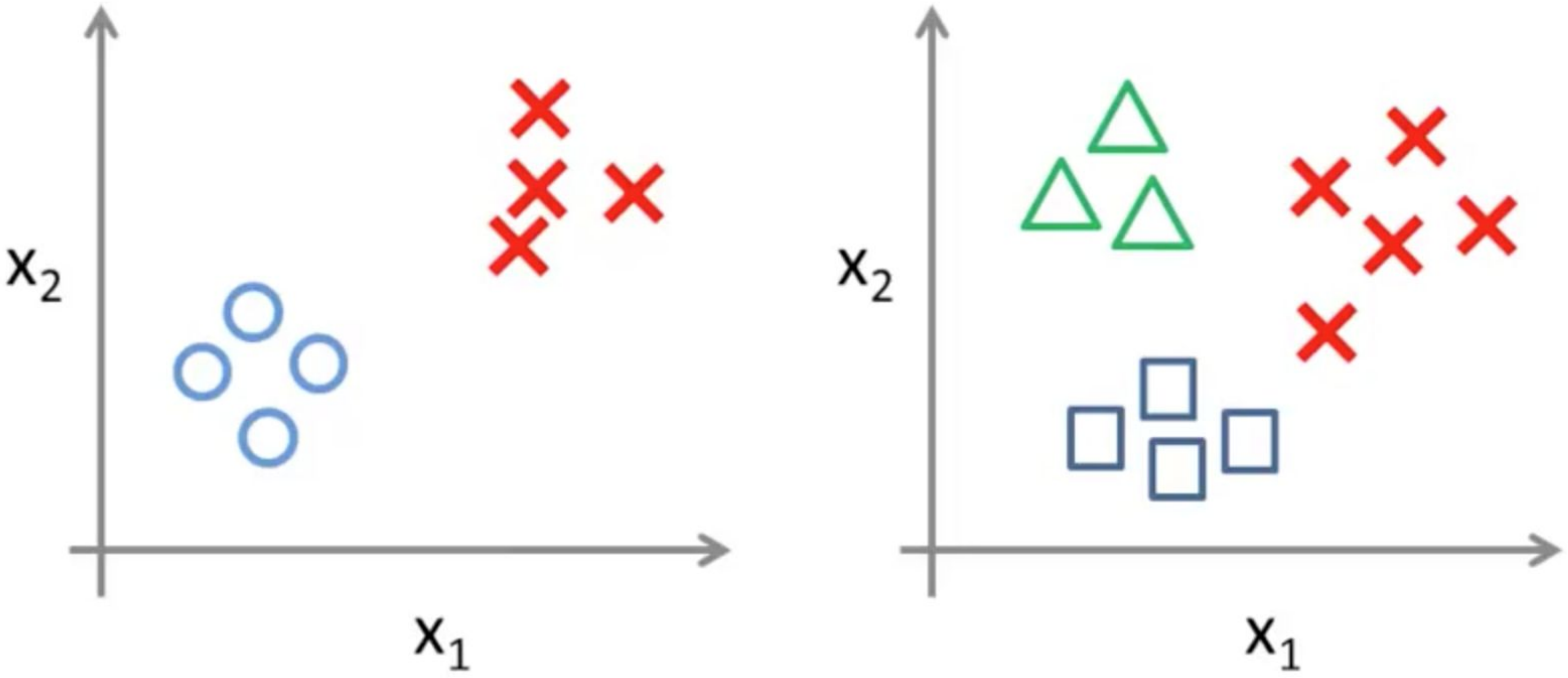
Multiclass Classification:

One vs All

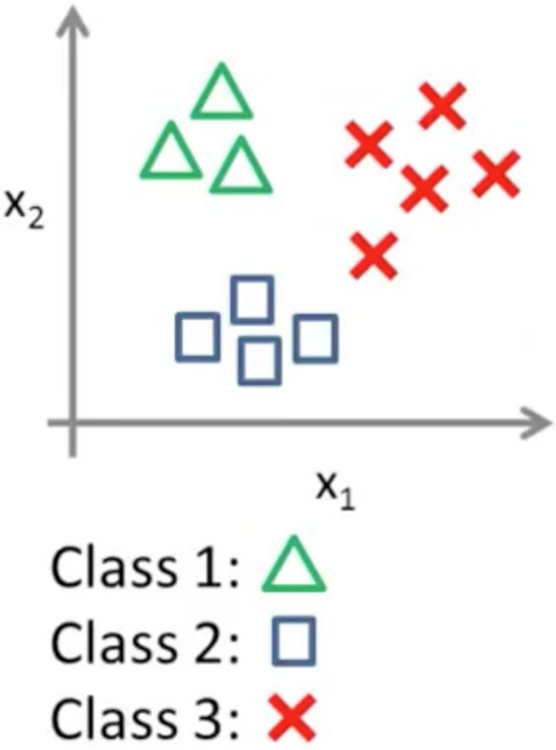
Multiclass Classification

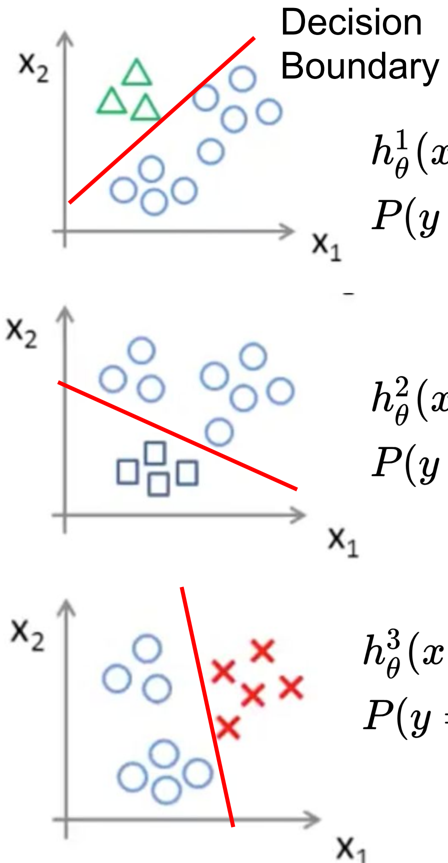
- Email foldering/tagging: work, ad, family, friends, hobby
- Medical diagrams: not ill, cold, flu
- Weather: sunny, cloudy, rain, snow

Binary vs Multiclass Classification



Multiclass Classification (One vs All)





$h_\theta^1(x)$

$P(y=1|x;\theta)$

$h_\theta^2(x)$

$P(y=2|x;\theta)$

$h_\theta^3(x)$

$P(y=3|x;\theta)$

Multiclass Classification (One vs All)

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

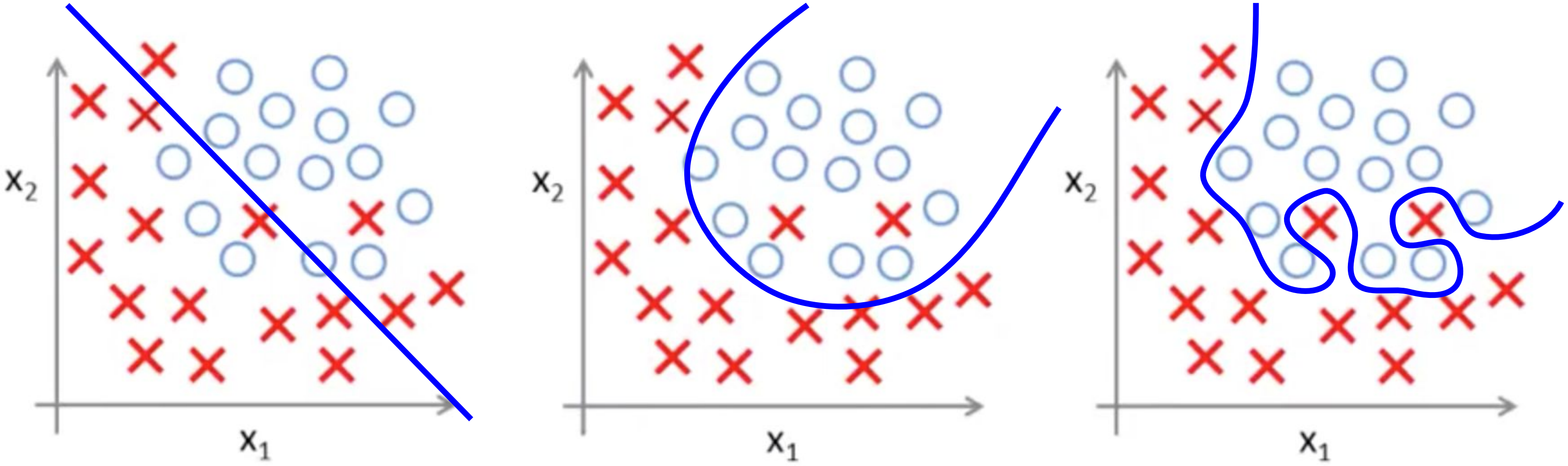
$$h_\theta^i(x) = P(y = i|x; \theta)$$

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

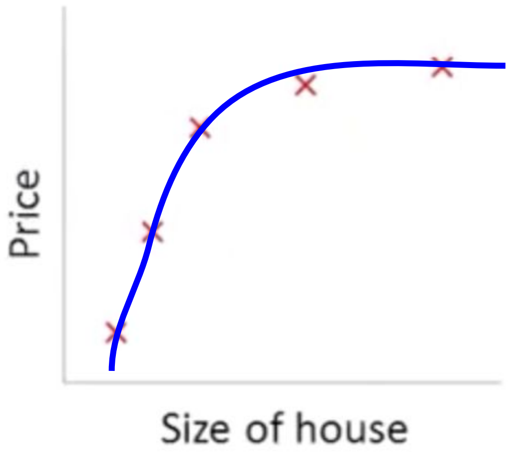
Addressing Overfitting

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.

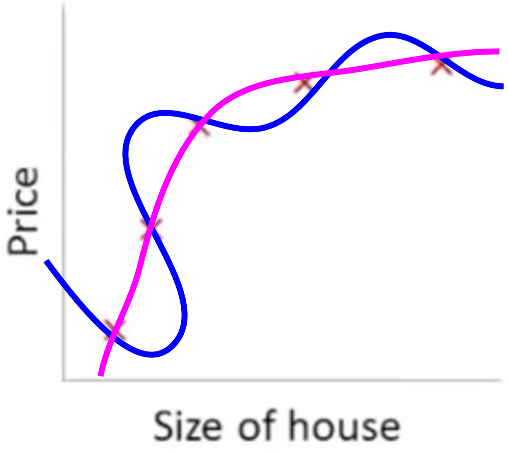
Intuition - Regularized Linear Regression

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

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

Repeat {

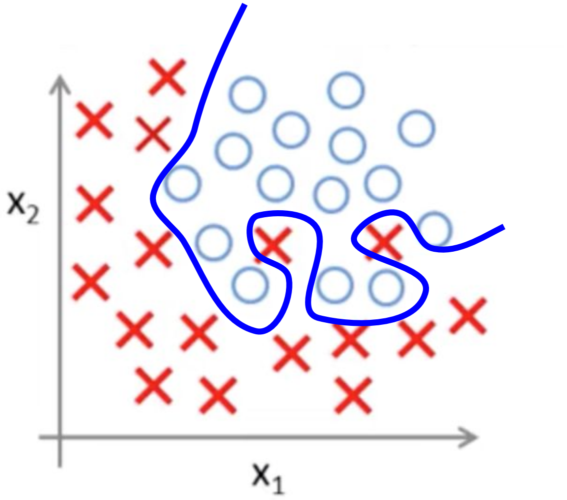
$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

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

}

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

Intuition - Regularized Logistic Regression

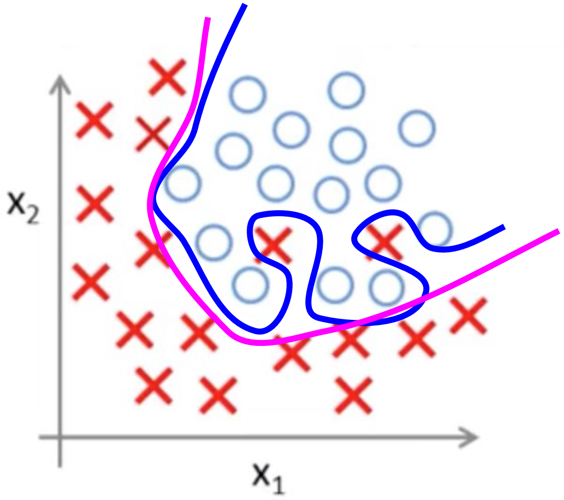


$$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 + \theta_5 x_1^2 x_2^3 + \dots)$$

Cost function:

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

Intuition - Regularized Logistic Regression



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

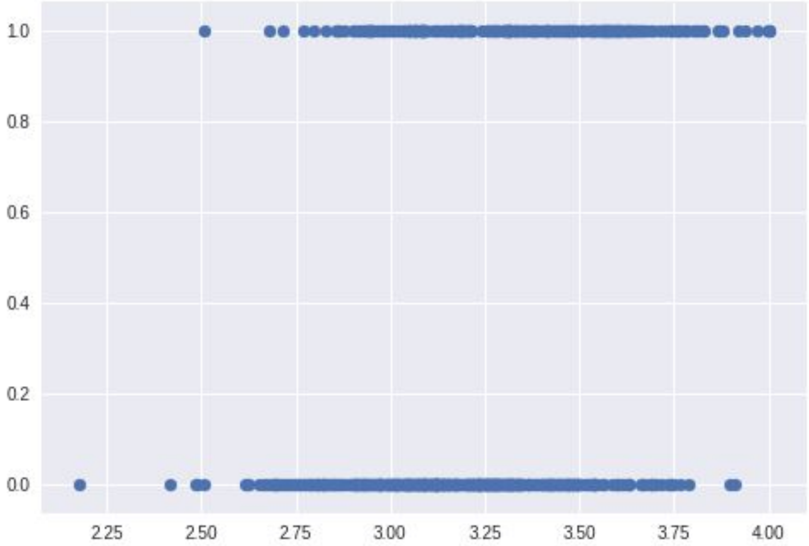
Cost function:

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

scikit
learn

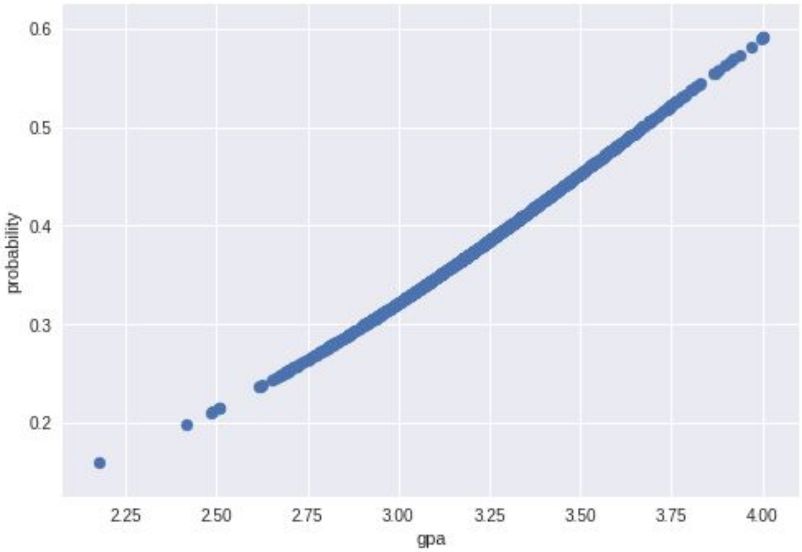
Binary Classification

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

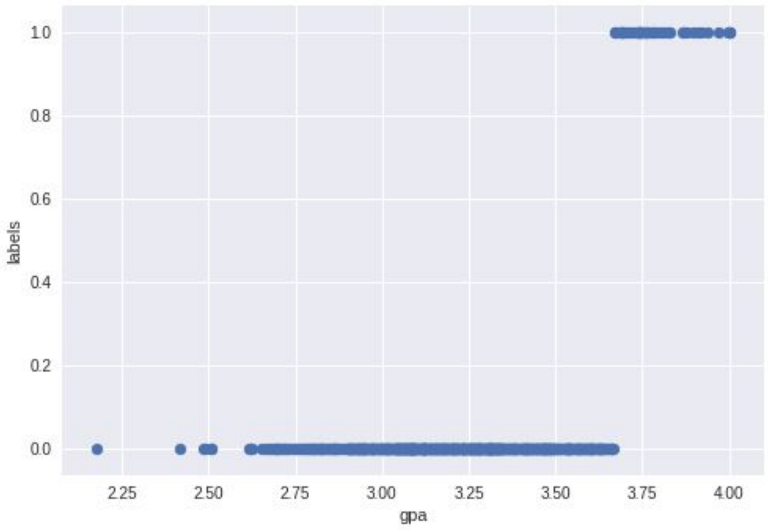


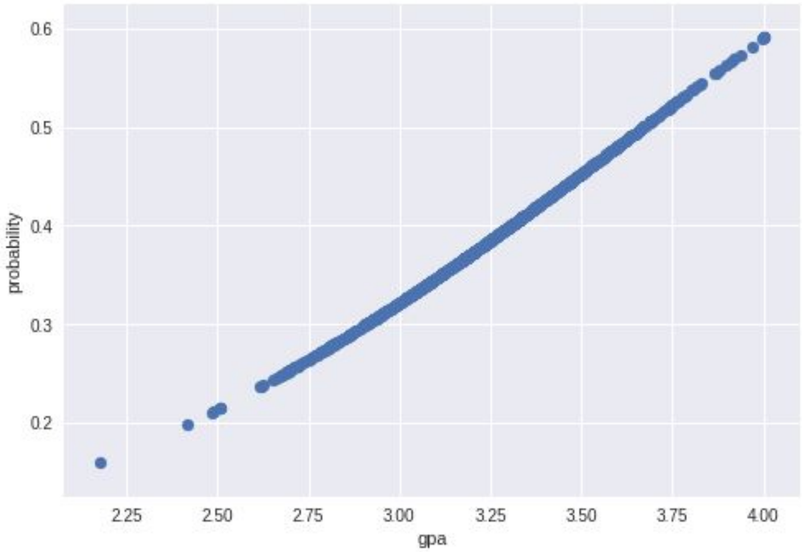
Logistic Regression Model (fit, predict prob.)

```
# create a LogisticRegression model
model = LogisticRegression()

# fit the model using gpa
model.fit(admissions[["gpa"]],
                   admissions["admit"])

# predict the probabilities for each class
pred_probs = model.predict_proba(
                    admissions[["gpa"]])
```



Logistic Regression Model (fit, predict class)





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)

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

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

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

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

```python
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