Logistic Regression

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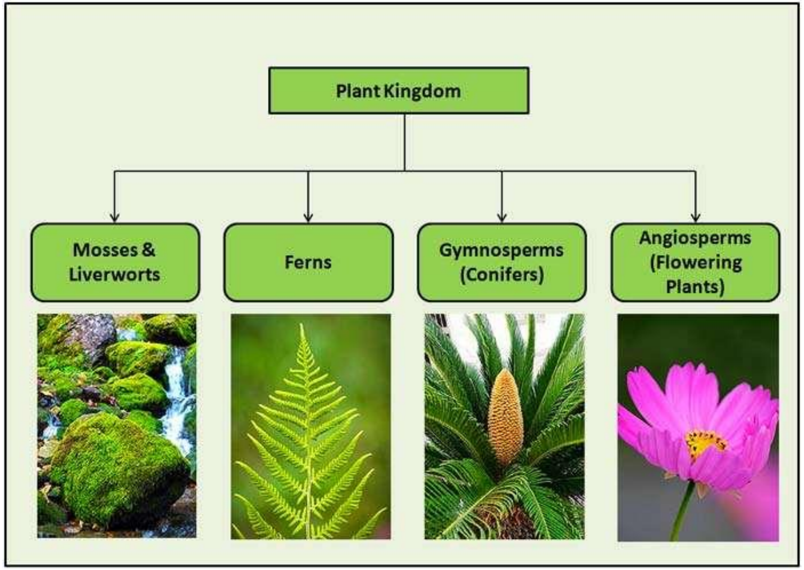
Introduction



Classification: identifying to which of a set of categories a new observation belongs, based on a training set of data.

Introduction

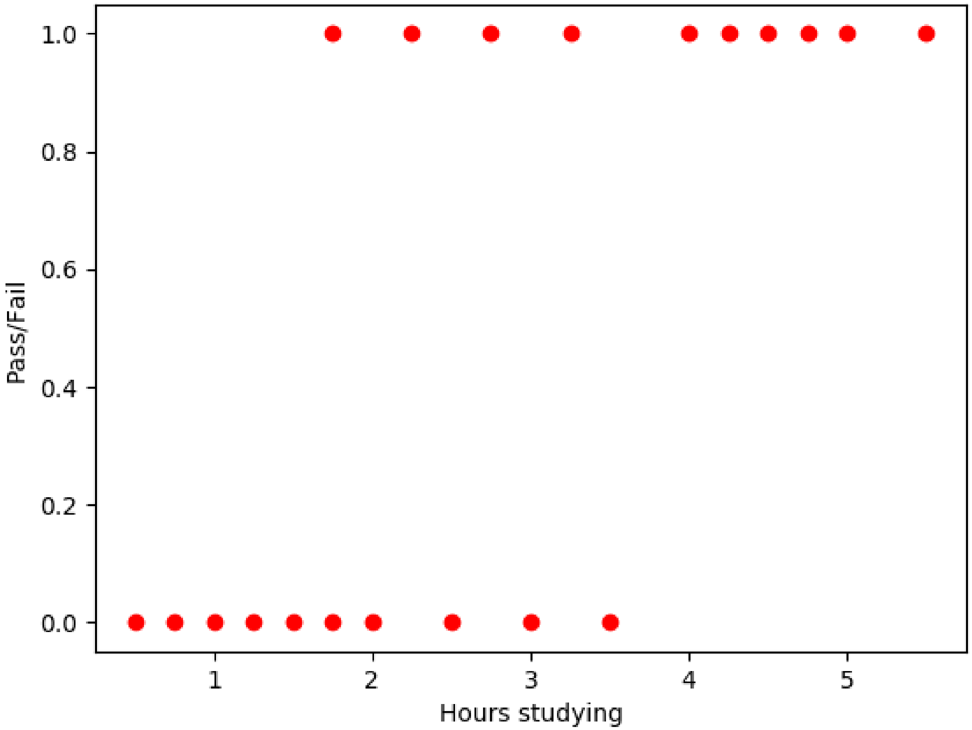
- Classification
- Examples:
  - Matter: Toxic / Not Toxic ?
  - Students: Pass / Fail ?
  - Van Gogh Painting: Real / Fake?
- Labels $y \in \{0,1\}$. 0: Negative class (Fail), 1: Positive class (Pass)
- We can have more than two labels $y \in \{0,1,2,3\}$ for DNA (cytosine [C], guanine [G], adenine [A] and thymine [T])

Example

- Performance of group of 20 students spend between 0 and 6 hours studying for an exam

Hours	Pass/Fail
0.5	Fail
0.75	Fail
1.75	Pass
2.25	Pass
…	…

Example



Original data

Fail = 0, Pass = 1

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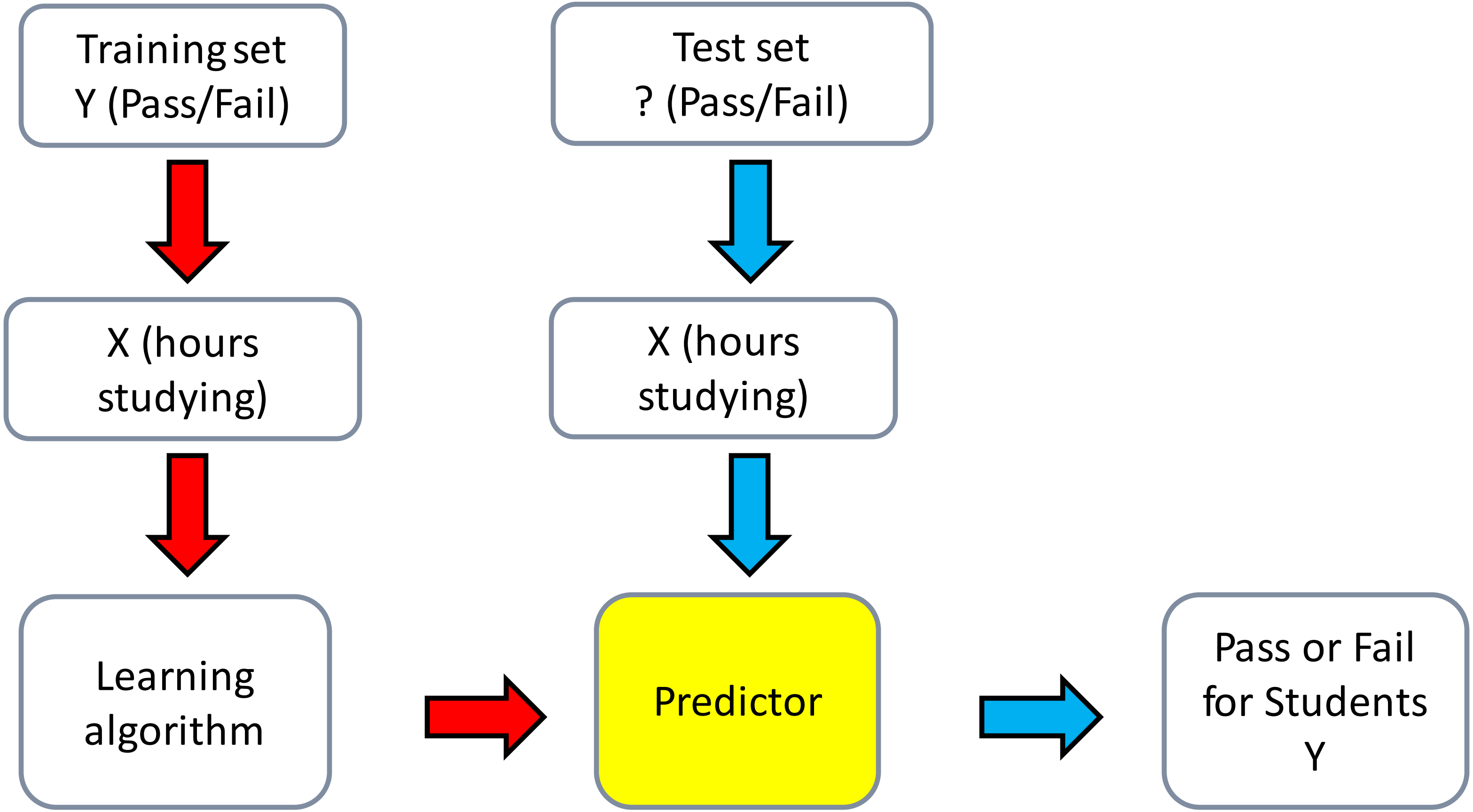
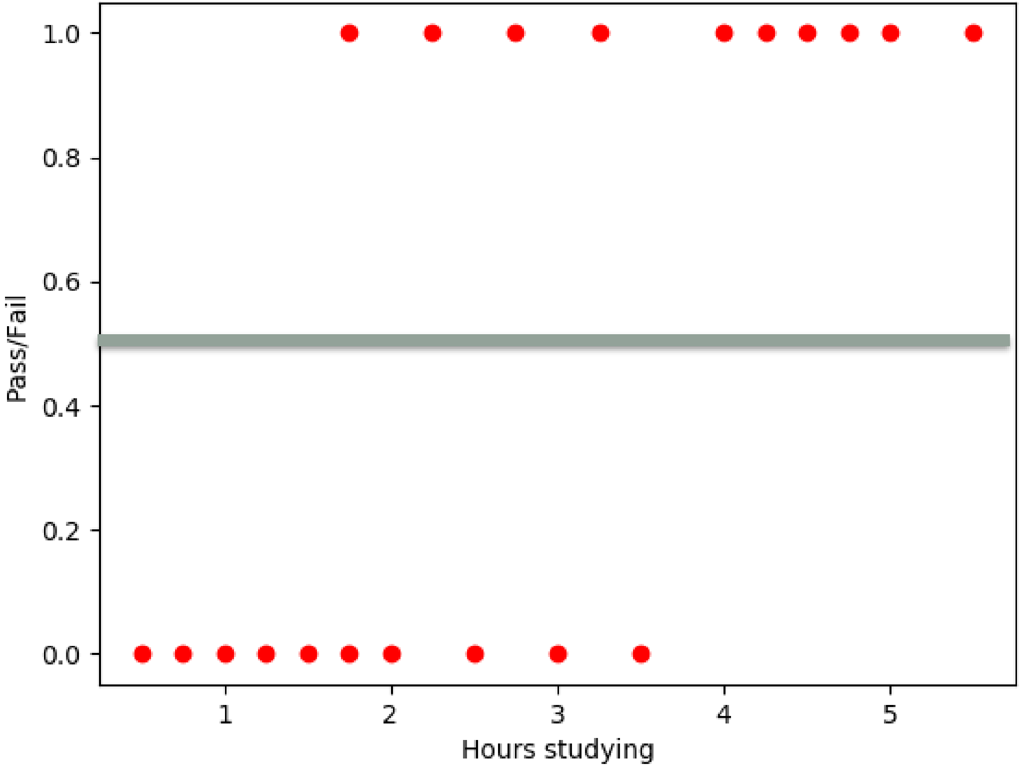
Model Representation



Predictor Construction

- Wish to construct a predictor:
$$p_{\mathbf{c}}(\mathbf{x}) = ?$$
- Our labels only has two values 0 and 1
- Predictor always give a real value
- $0 \leq p_{\mathbf{c}}(\mathbf{x}) \leq 1$
- To get classification, choose a threshold z:
$$p_{\mathbf{c}}(\mathbf{x}) < z \text{ then } y = 0$$
$$p_{\mathbf{c}}(\mathbf{x}) \geq z \text{ then } y = 1$$
- With two labels $\{0,1\}$, it is natural to choose $z = 0.5$

Predictor Construction



Predictor Construction

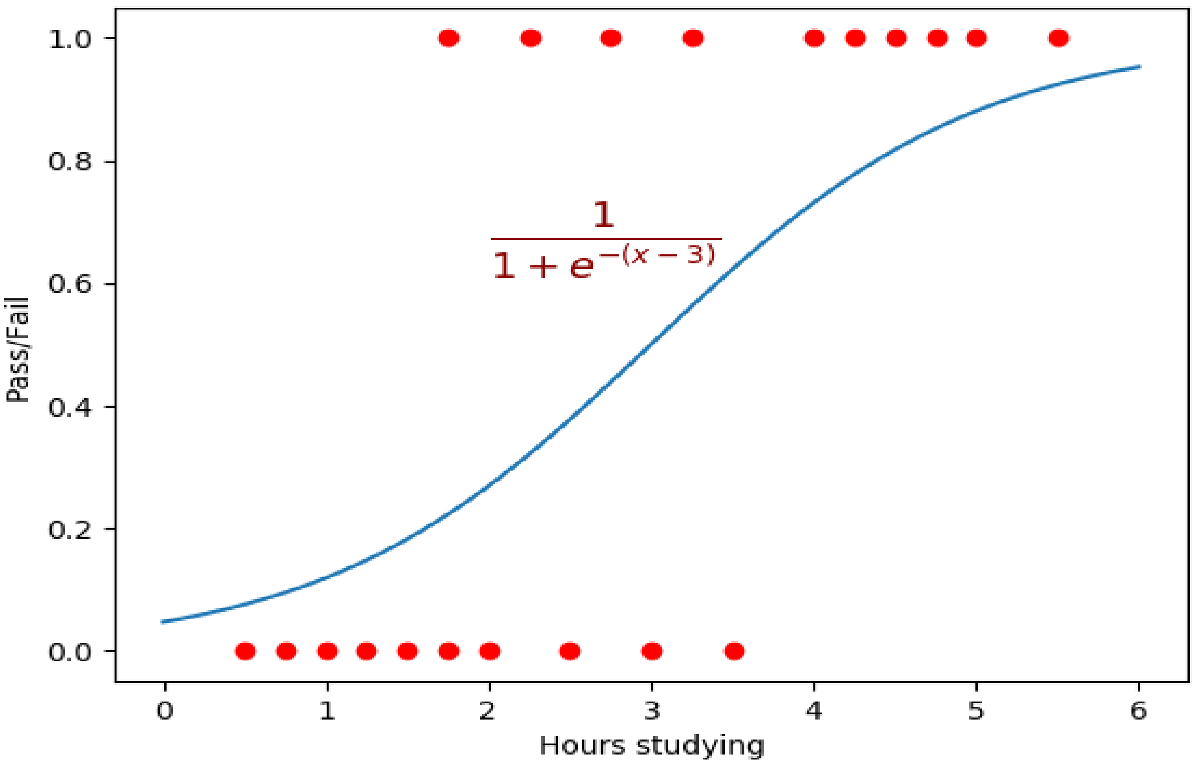
- We choose $\boxed{\text{Sigmoid / Logistic function:}}$

$$p_{\mathbf{c}}(\mathbf{x}) = \frac{1}{1 + e^{-\mathbf{c}^T\mathbf{x}}}$$

(Is this model still linear?)

- If dataset has one feature, i.e., $\mathbf{x} = (1, x_1)^T$, then $\mathbf{c} = (c_0, c_1)^T$

Predictor Construction



Predictor Construction

- If dataset has *n* features, i.e., $\mathbf{x} = (1, x_1, \ldots, x_n)^T$, then $\mathbf{c} = (c_0, c_1, \ldots, c_n)^T$
- Single-layer perceptron

$$p_{\mathbf{c}}(\mathbf{x}) = \frac{1}{1 + e^{-c_0 - c_1 x_1 - c_2 x_2 - \cdots - c_n x_n}}$$

or $$p_{\mathbf{c}}(\mathbf{x}) = \frac{1}{1+e^{-\mathbf{c}^T\mathbf{x}}}$$

is the probability that $y = 1$ on input $\mathbf{x}$

Predictor Construction

- We can also use the polynomial logistic function, e.g.,

$$p_{\mathbf{c}}(\mathbf{x}) = \frac{1}{1+e^{-c_0-c_1x_1-c_2x_1^2}}$$ or more general:

- $$p_{\mathbf{c}}(\mathbf{x}) = \frac{1}{1+e^{-c_0-c_{11}x_1-c_{12}x_1^2+,\dots,c_{n1}x_n-c_{n2}x_n^2+,\dots}}$$

- **Loss function construction:**
  - Linear regression:

$$L(\mathbf{c}) = \sum_{i=1}^{M}\left(p\left(x^{(i)}\right) - y^{(i)}\right)^2$$

  - Logistic regression (complicated by two or multiple goals):

$$L(\mathbf{c}) = ?$$

Predictor Construction

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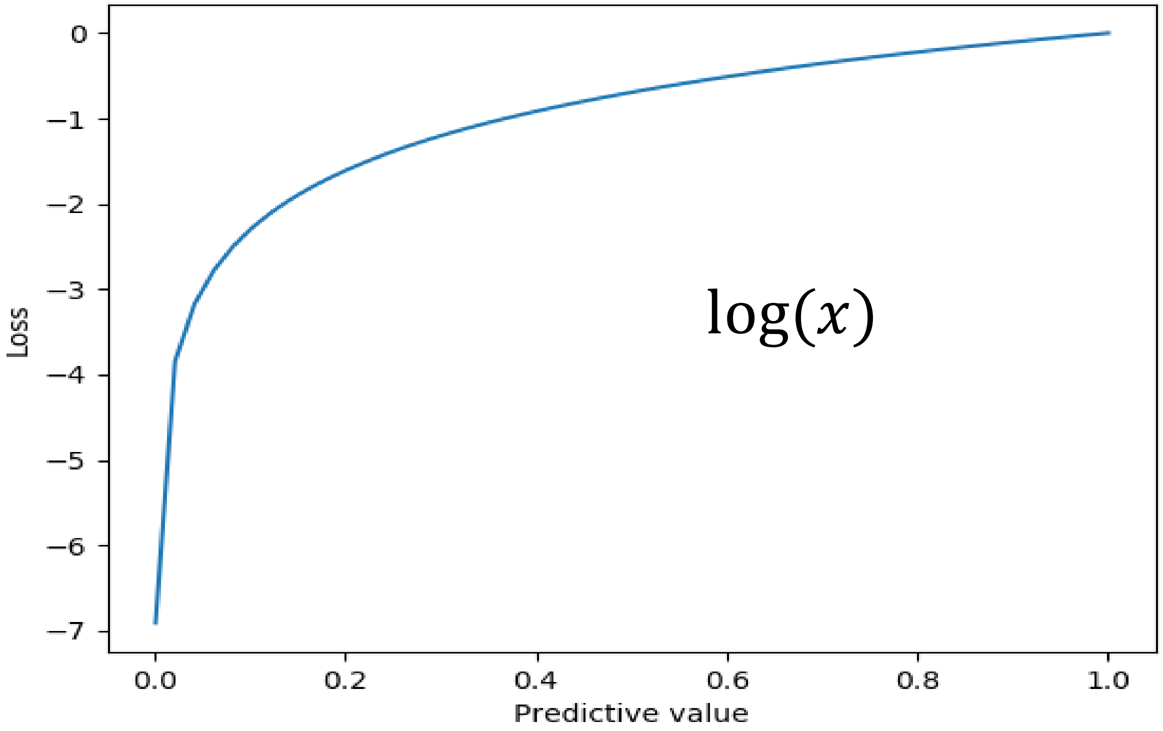
$$p_{\mathbf{c}}(\mathbf{x}) = \frac{1}{1+e^{-f(\mathbf{c},\mathbf{X})}}$$

How to determine coefficients?

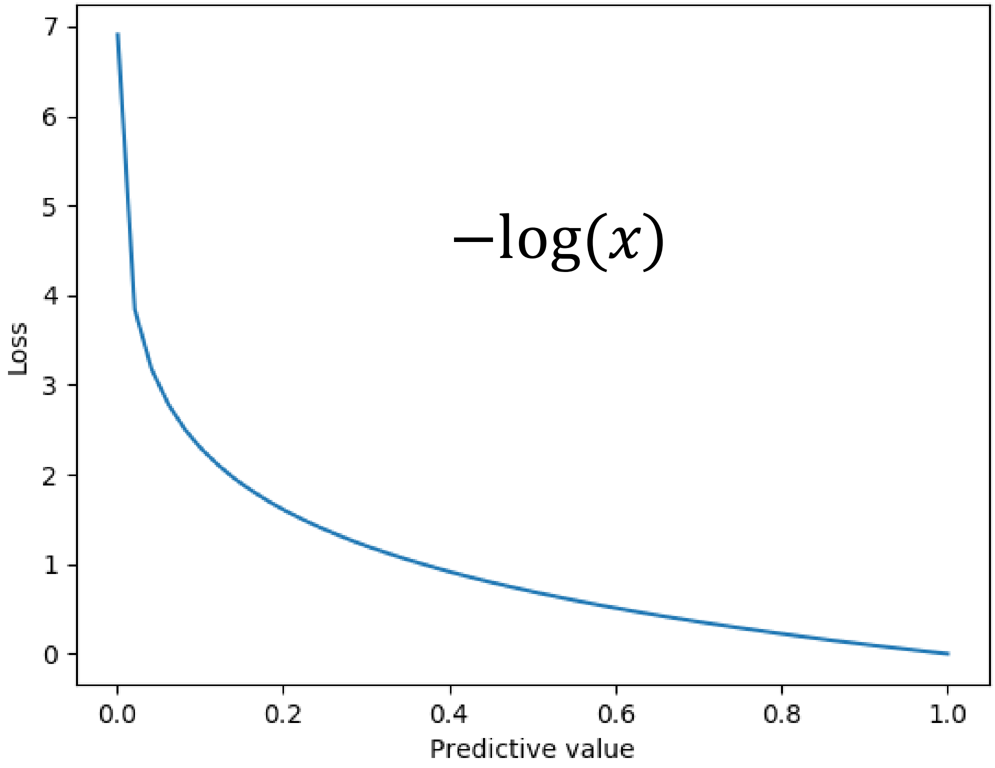
Loss Function Construction

- When $\boldsymbol{y} = \mathbf{1}$, higher $p_{\mathbf{c}}(\mathbf{x})$ is more accurate $\Rightarrow$ smaller lost
- Any function reflects that behavior?



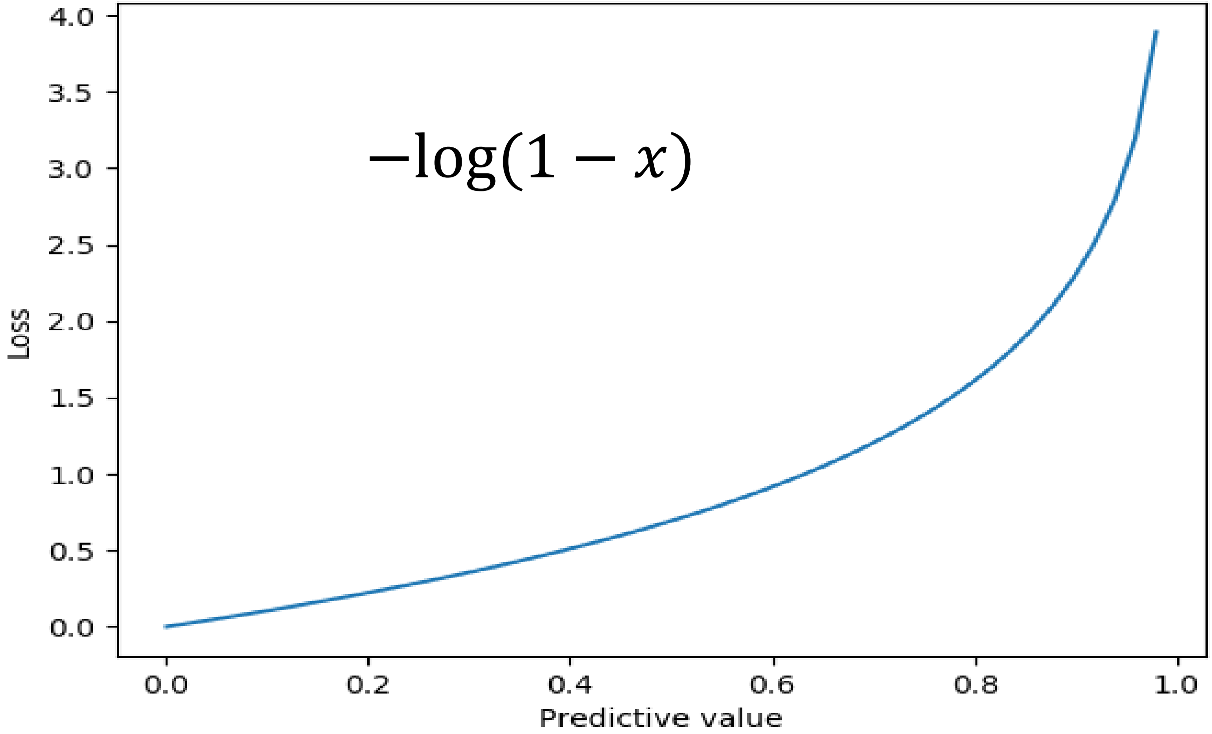
Loss Function Construction

Make it nicer!



Loss Function Construction

- When $\boldsymbol{y} = \mathbf{0}$, lower $p_{\mathbf{c}}(\mathbf{x})$ is more accurate $\Rightarrow$ smaller lost
- Any function reflects that behavior?



Loss Function Construction

- So we have

$$L(p_{\mathbf{c}}(\mathbf{x}), y) = \begin{cases} -\log\big(p_{\mathbf{c}}(\mathbf{x})\big) \text{ if } y = 1 \\ -\log\big(1 - p_{\mathbf{c}}(\mathbf{x})\big) \text{ if } y = 0 \end{cases}$$

- Combine two goals into one function:

$$L(p_{\mathbf{c}}(\mathbf{x}), y) = -y\log\big(p_{\mathbf{c}}(\mathbf{x})\big) - (1 - y)\log\big(1 - p_{\mathbf{c}}(\mathbf{x})\big)$$

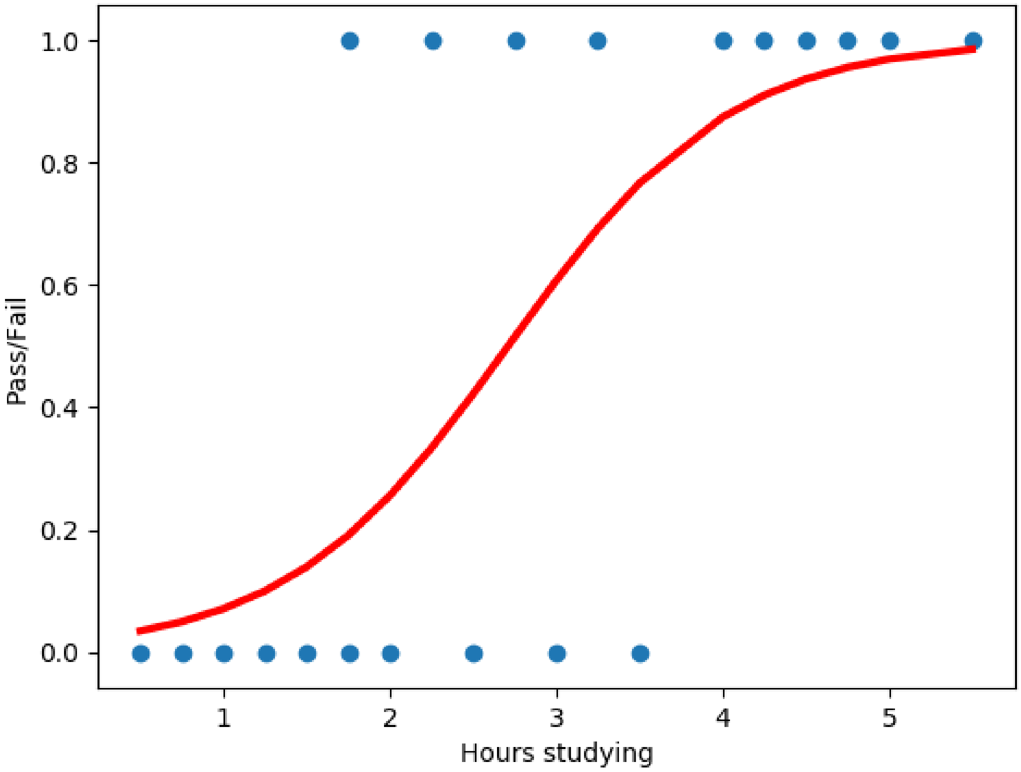
Loss Function

- Total loss for the whole dataset

$$L(\mathbf{c}) = \frac{1}{M}\sum_{i=1}^{M}\left[-y^{(i)}\log\left(p_{\mathbf{c}}\left(\mathbf{x}^{(i)}\right)\right) - \left(1-y^{(i)}\right)\log\left(1-p_{\mathbf{c}}\left(\mathbf{x}^{(i)}\right)\right)\right]$$

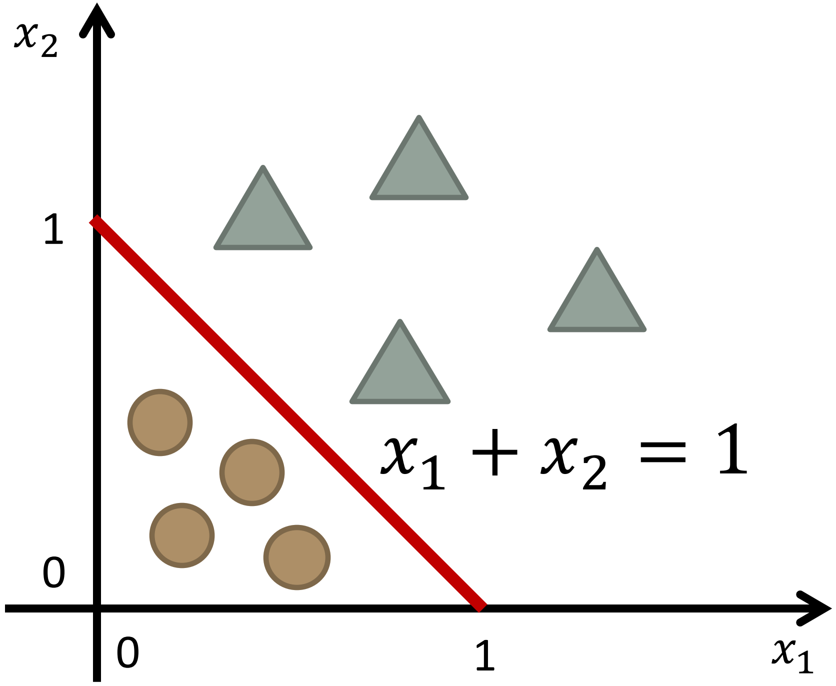
- Objective: Find parameters $\mathbf{c}$ to minimize $L(\mathbf{c})$
- How to pursue it?
- Gradient descent

Resulting Predicted Model



Decision Boundary

- Boundary that separates this class from another ones
- We can construct the **decision boundary** from optimal predictor



$$p_{\mathbf{c}}(\mathbf{x}) = \frac{1}{1 + e^{-\mathbf{c}^T\mathbf{x}}}$$

$$\mathbf{c}^T = (-1,1,1)$$

$$\mathbf{x}^T = (1, x_1, x_2)$$

$$p_{\mathbf{c}}(\mathbf{x}) = \frac{1}{1 + e^{1-x_1-x_2}}$$

When $p_{\mathbf{c}}(\mathbf{x}) = 0.5$ (threshold)

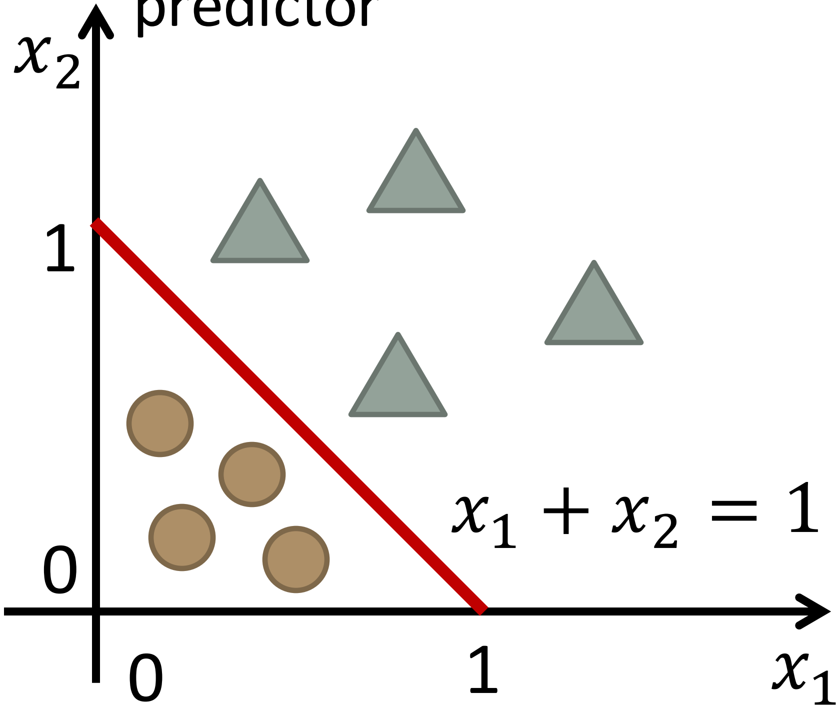
$$\frac{1}{1 + e^{1-x_1-x_2}} = \frac{1}{2}$$

$$\boxed{\Rightarrow x_1 + x_2 = 1}$$

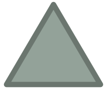
Decision boundary

Decision Boundary

- Boundary that separates this class from another ones
- We can construct the decision boundary from optimal predictor

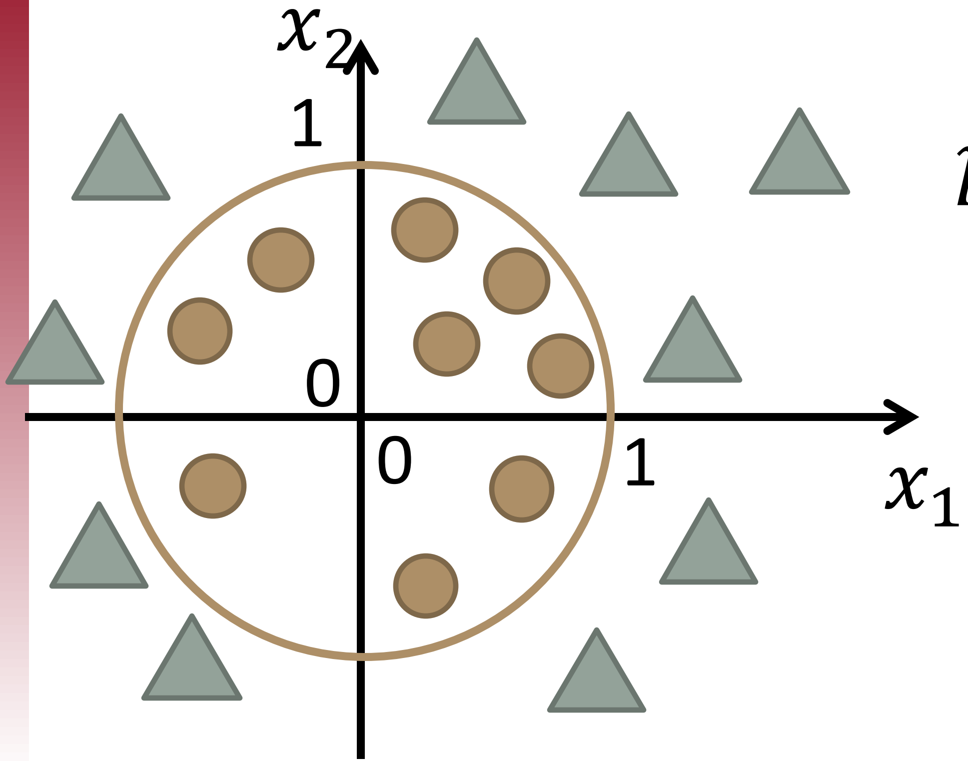


if $x_1 + x_2 \leq 1$: data point (x_1, x_2) is 

if $x_1 + x_2 > 1$: data point (x_1, x_2) is 

Decision Boundary

- Decision boundary can be a curve or manifold



$$p_{\mathbf{c}}(\mathbf{x}) = \frac{1}{1 + e^{1 - x_1^2 - x_2^2}}$$

$$p_{\mathbf{c}}(\mathbf{x}) = 0.5$$

$$\frac{1}{1 + e^{1 - x_1^2 - x_2^2}} = \frac{1}{2}$$

$$\Rightarrow x_1^2 + x_2^2 = 1$$

Multi-Class

- Loss function designs for two classes
- What if we have more than 2 classes?
- Examples:
  - Student Performance: A, B, C, D, F
  - Weather prediction: Sunny, Cloudy, Rain, Snow

Multi-Class

- One-vs-all:
  - If we have *n* classes: $l_1, l_2, \ldots, l_n$
  - For each class l_i. Consider two labels: l_i and not l_i
  - Train logistic regression classifier for this case to get the probability $p_{\mathbf{c}}^{l_i}(\mathbf{x})$ that $y = l_i$
  - Pick the class l_k that maximizes $\max_k p_{\mathbf{c}}^{l_k}(\mathbf{x})$