MACHINE LEARNING
MEI/1

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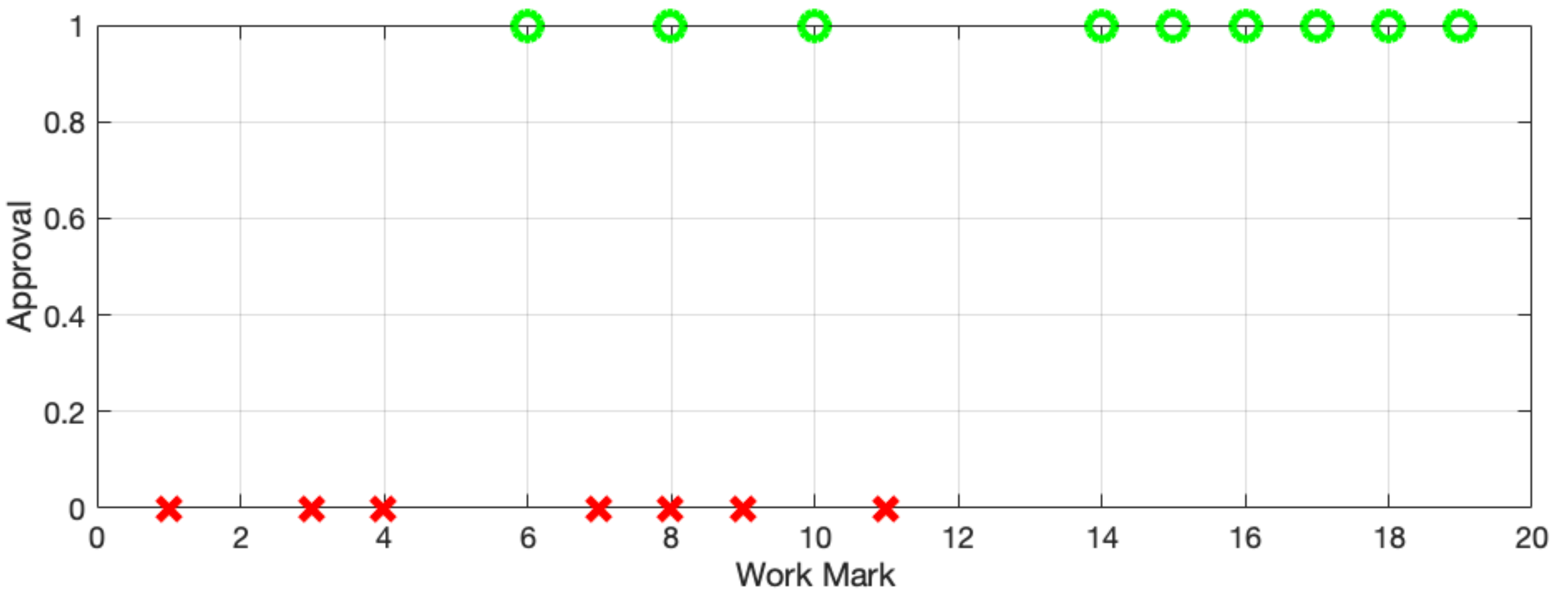
Students Performance

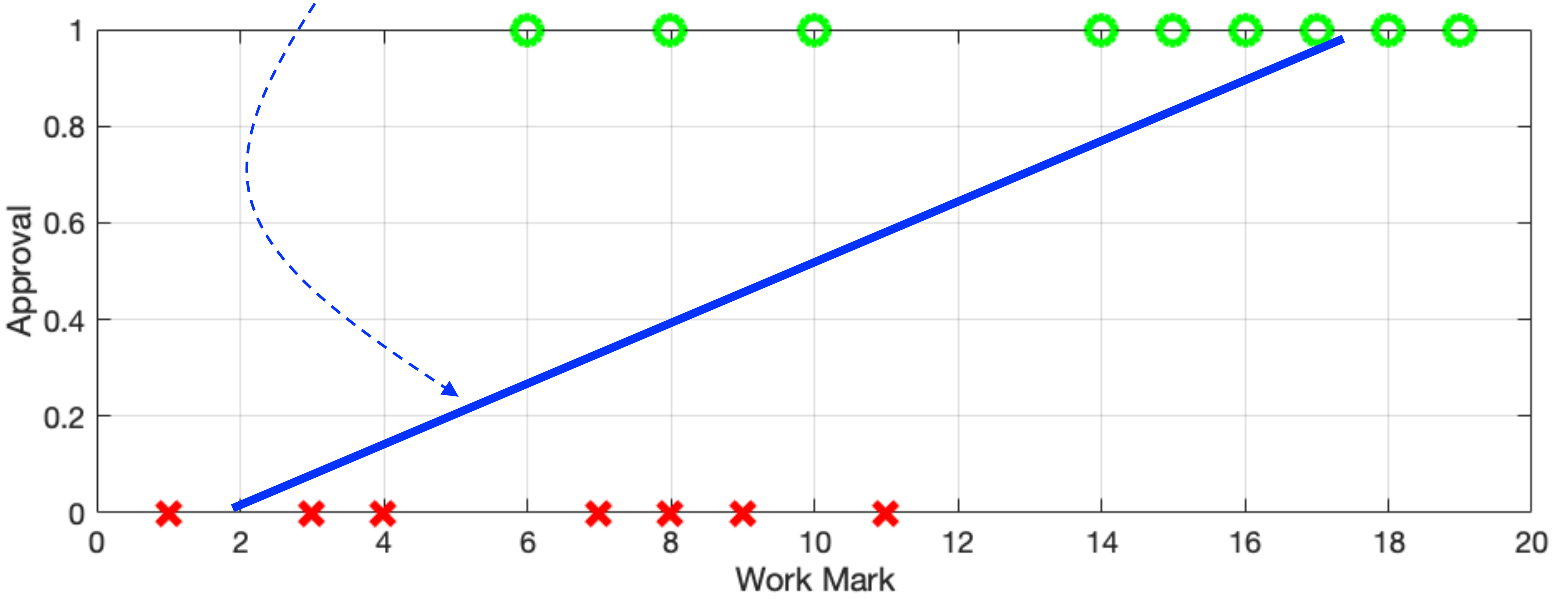
- Suppose that we are interested in predicting the **approval rate** of a class, based on the **students marks in the first practical work**.
  - Typically, students that get good marks in the first work, got approved at the course.
  - Students with very low marks at the first work tend to fail in the final examination.
- Hence, our machine learning model is expected to predict a **binary outcome** (**1: pass** vs. **0: fail**)



Students Performance

- In this kind of problems, the dependent variable assumes a reduced set of labels:
  - Emails: "is this a **spam** or **no spam** email"? $y \in \{0, 1\}$
  - Medical diagnosis: "is the patient **ill** or **healthy**" $y \in \{0, 1\}$
  - How will be the weather tomorrow?: "will it be **sunny**, **cloudy** or **rainy**"? $y \in \{0, 1, 2\}$
- In this case, a best fitting line is not enough
  - Even though this line will be the basis of our **classification model**

$$h_\theta(x) = \theta_1 . x + \theta_2$$

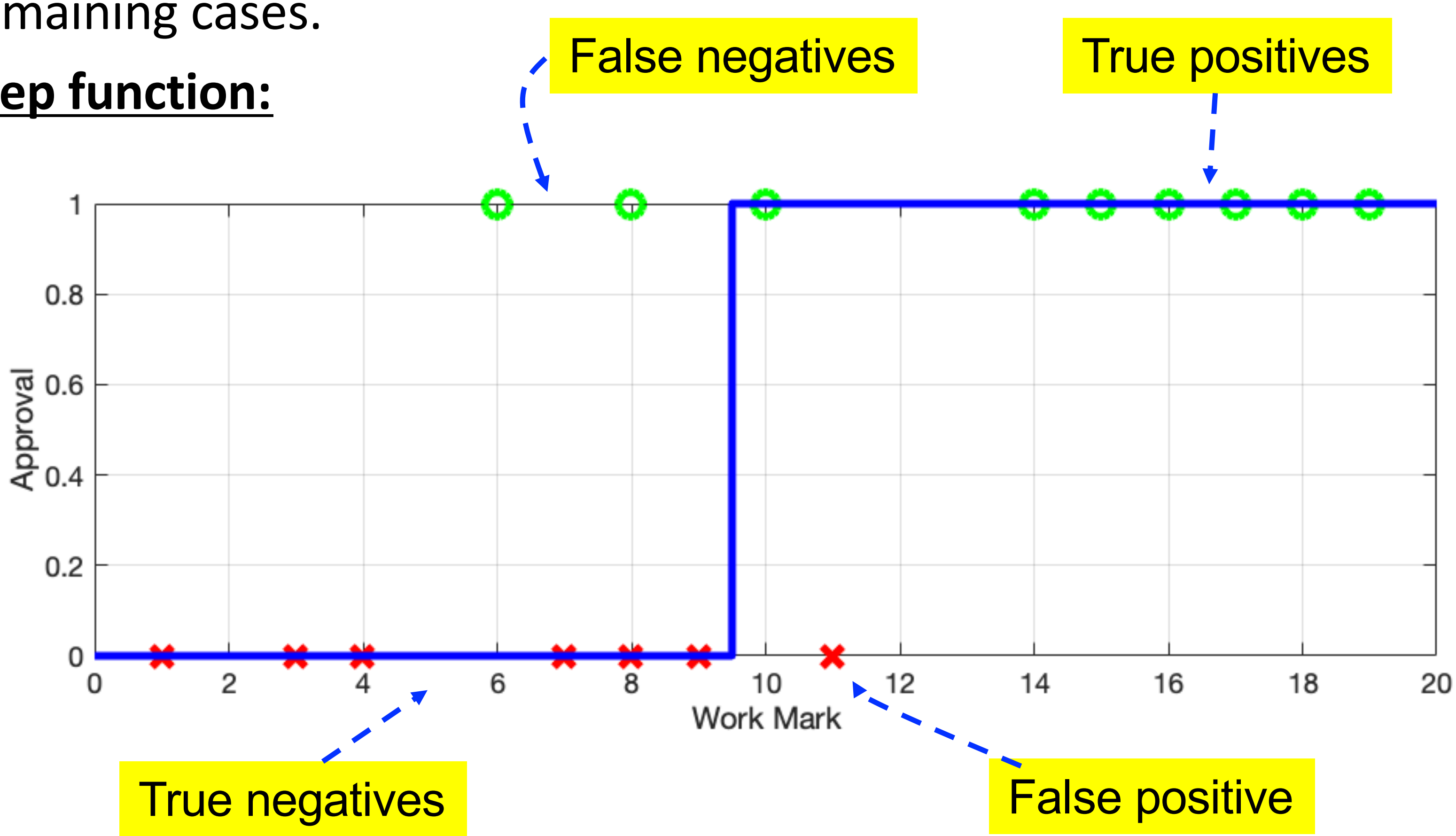


Logistic Regression: Classification

- The obvious idea will be to define a threshold at the classifier output $h_\theta(x)$, that binarizes the system response:
  - Typically, "0.5" would be the choice, for "*equal classification risks*"
    - It might be more dangerous to predict erroneously one class instead of other one.
    - For example, in a machine learning-based systems for medical diagnosis, classes have different risk.
      - Predict a "malignant cancer" on a "healthy" subject represents a unnecessary concern for the patient and would probably imply to perform additional (an unnecessary) exams.
      - However, provide a "healthy" response for a patient suffering of a "malignant cancer" might represent the patient dead sentence.
  - $f(x) = \begin{cases} 0, h_\theta(x) < 0 \\ 1, h_\theta(x) \geq 0 \end{cases}$
- Hence, the response of our classification system can be seen as a composition of two functions: $f = g\ o\ h$
  - *"f" is "g" after "h"*
- *We have seen "h" before, but what is "g"?*

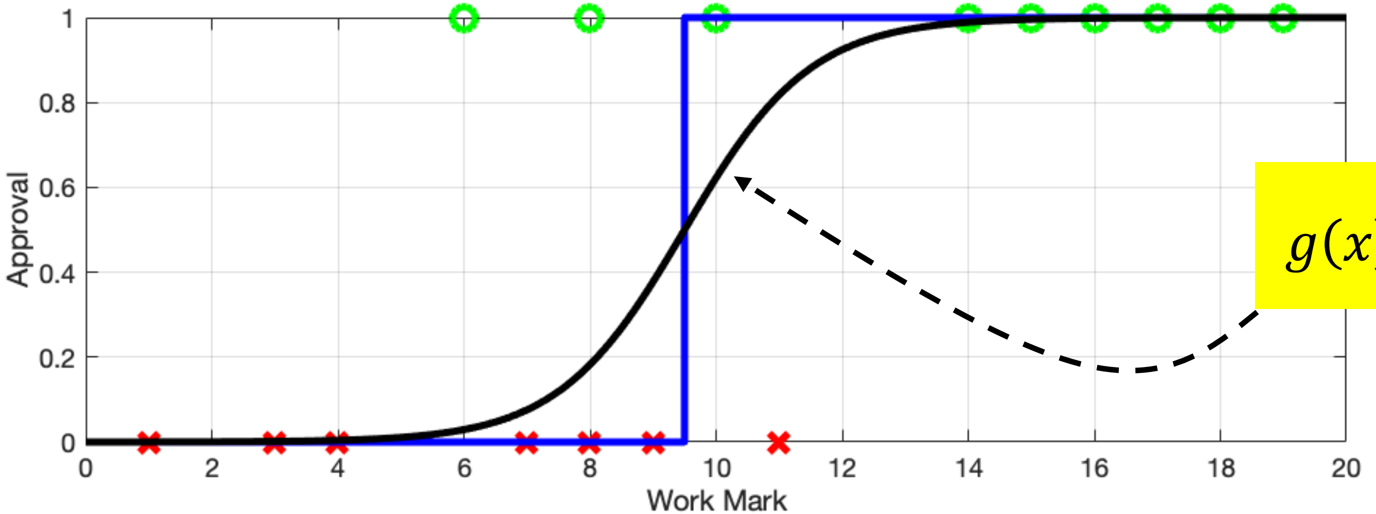
Logistic Regression: Classification

- Essentially, “g” performs a binarization of its input, and produces ”1” responses when the input is higher than some threshold, and “0” in the remaining cases.
- **Step function:**



Logistic Regression: Classification

- Assuming the step function as "g", and $f = g \ o \ h$, obtaining the automatic optimal parameterization of "f" with respect to our data (i.e., machine learning) yields two problems:
  - <u>**Problem 1**</u>: "g" is **not differentiable**
    - It has not a continuous derivative at a single point
  - **Problem 2:** in every other points **"g" has derivative 0**
- The solution is to use a function is close to the step function, without suffering of the above described problems.
  - **Sigmoid Function**



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

Logistic Regression: Classification

- Using this composition of functions, our classification system is given by:

$$f_{\boldsymbol{\theta}}(x) = \frac{1}{1 + e^{h_\theta(x)}}$$

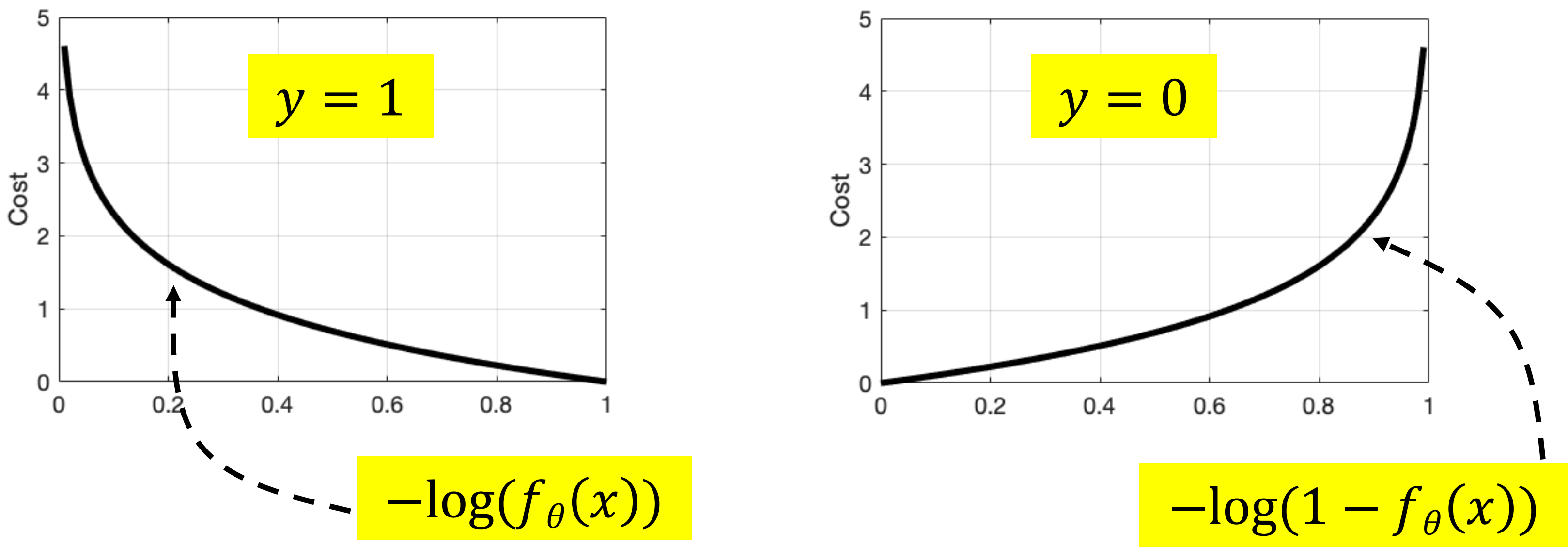
- Or:

$$f_{\boldsymbol{\theta}}(x) = \frac{1}{1+e^{\theta_1 x + \theta_2}}$$

- The remaining problema is the same as in linear regression:
  - How to find the $\boldsymbol{\theta}$ optimal parameterization?
- According to the basic principles of Machine Learning, up to now, we've only defined our model.
  - It is also required to define a "Cost Function" (Loss function) that measures how good it is na hypothesis.
  - And a systematic optimization process

Logistic Regression: Cost Function

- As previously, the cost function will measure how well the model responses ($f_{\boldsymbol{\theta}}(x)$) resemble the "ground-truth" (y)
  - Intuitively, in cases where the system is supposed to output a "1" and the model predicts a "1", the cost should be "0".
  - The same thing should hold for "0" responses.
  - However, the cost (loss) should grow in cases when the system response is far from the ground-truth.
    - The log() function is a good choice for representing the desired costs (losses)
    - It varies non-linearly with respect to the distance between the desired and actual responses
      - Attempts to avoid "**<u>ridiculously wrong responses</u>**".



Logistic Regression: Cost Function

- Hence, the cost function for one instance is given by:
  - $Cost(f_\theta(x), y) = \begin{cases} -\log(f_\theta(x)), & y = 1 \\ -\log\big(1 - f_\theta(x)\big), & y = 0 \end{cases}$
- And the cost function for the whole dataset is given by the sum of the individual costs:

$$J(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N}\Big(Cost\big(f_\theta(x^{(i)}), y^{(i)}\big)\Big)$$

- Considering that y can only assume 2 values (0 or 1), we have:

$$J(\boldsymbol{\theta}) = -\frac{1}{N}\sum_{i=1}^{N} y^{(i)} \log\big(\boldsymbol{f_\theta}(x^{(i)})\big) + (1 - y^{(i)}) \log\big(1 - \boldsymbol{f_\theta}(x^{(i)})\big)$$

Logistic Regression: Optimization

- The optimization can be done exactly as in the linear regression case.
- Using the gradient descent strategy, it is required to find the derivatives of the cost function J() with respect to the $\boldsymbol{\theta}$ parameters:

$$\frac{\int}{\int \boldsymbol{\theta}} J(\boldsymbol{\theta})$$

- In matrix form, we have:

$\boldsymbol{\theta} = [\theta_0, \theta_1]^T$

$\boldsymbol{x}^{(i)} = [x^{(i)}, 1]^T$

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

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

- $\log(1 - f_{\boldsymbol{\theta}}(\boldsymbol{x})) = -\theta\mathbf{x} - \log(\frac{1+e^{-\boldsymbol{\theta}^T \boldsymbol{x}}}{1})$

Logistic Regression: Optimization

- Plugging the two simplified expressions in the original cost function, we obtain:

$$\mathrm{J}(\boldsymbol{\theta}) = -\frac{1}{N}\sum_{i=1}^{N} - y^{(i)} \log\left(1 + \ e^{-\boldsymbol{\theta x}}\right) + (1 - y^{(i)})\,(-\boldsymbol{\theta x} \ - \ \log\left(1 + e^{-\boldsymbol{\theta x}}\right)$$

- Which can be simplified to:

$$\mathrm{J}(\boldsymbol{\theta}) = -\frac{1}{N}\sum_{i=1}^{N} y^{(i)}\,\boldsymbol{\theta x} \ - \ \log\left(1 + e^{-\boldsymbol{\theta x}}\right)$$

- Now, as

$$\frac{\int}{\int \theta j} y^{(i)}\,\boldsymbol{\theta x} \ = \ y^{(i)}\,\boldsymbol{\theta x}$$

$$\frac{\int}{\int \theta j} \log\left(1 + e^{\boldsymbol{\theta x}}\right) = \frac{\boldsymbol{x}_j e^{-\boldsymbol{\theta x}}}{1+e^{\boldsymbol{\theta x}}} = \mathrm{x}^{\mathrm{i}}_{\mathrm{j}}\, f_{\boldsymbol{\theta}}(x)$$

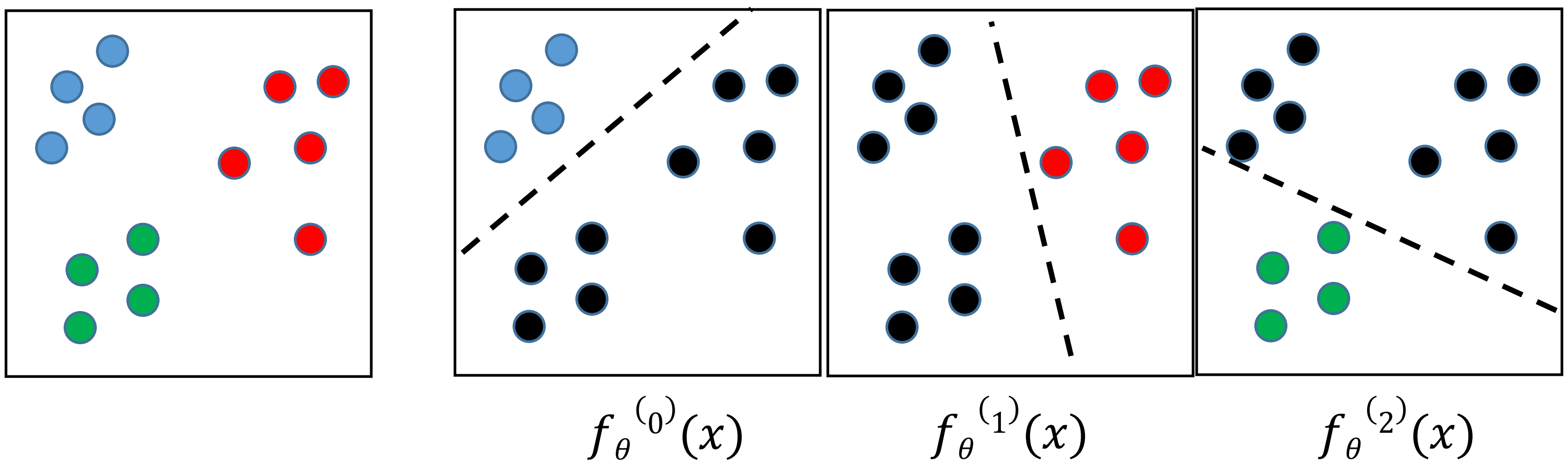
- We have:

$$\frac{\int}{\int \theta j} J(\theta) = \sum_{i=1}^{N} \ x^{i}{}_{j}\,(f_{\theta}(x^{(i)}) - y^{(i)})$$

Logistic Regression: Multi-class

- Up to now, we've only considering binary classification problems.
- When the number of classes (c) is higher than 2, the typical approach is to train "c" classifiers
  - In each classifier $f_\theta^{(i)}(x)$, instances of the ith class are considered positive examples, whereas instances of al the remaining classes are treated as negative instances.
- During classification, we pick the class that produces the maximum output response, i.e.:

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



Logistic Regression: Exercise

- Your task for today's practical class, is to adapt the "linear_regression.py" script to perform logistic regression.
  - At first, implement only the "two-classes" version
  - Generalize your script, to handle multi-class problems.
- Also, consider different feature normalization strategies:
  - Min-max
  - Z-score
- Download the data from the "**wine**" Dataset, available at the course web page.
  - In this set, the goal is to use chemical analysis to determine the origin of different wines.
  - There are 13 attributes, all numeric (either integer or real numbers):
    - *1) Alcohol*
    - *2) Malic acid*
    - *3) Ash*
    - *4) Alcalinity of ash*
    - *5) Magnesium*
    - *6) Total phenols*
    - *7) Flavanoids*
    - *8) Nonflavanoid phenols*
    - *9) Proanthocyanins*
    - *10)Color intensity*
    - *11)Hue*
    - *12)OD280/OD315 of diluted wines*
    - *13)Proline*
  - The dependent variable is provided in the first column