CS M146: Introduction to Machine Learning
Logistic Regression

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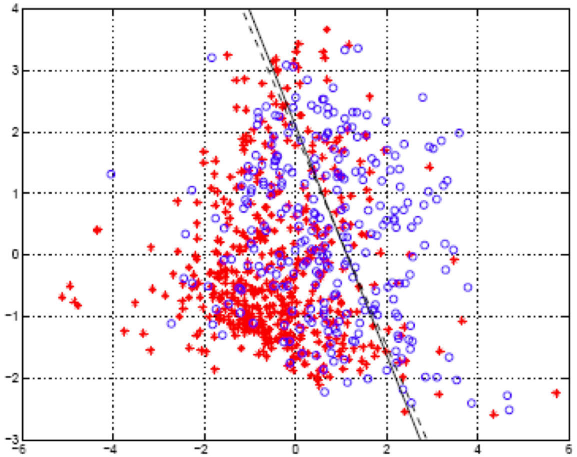
Classification Based on Probability

- Instead of just predicting the class, give the probability of the instance being that class i.e., learn $p(y|\boldsymbol{x})$
- Comparison to perceptron:
  - Perceptron doesn't produce a probability estimate
- Recall that:
  - For any event $E \in \mathcal{E}$, $0 \leq p(E) \leq 1$
  - Sum of probabilities $\sum_{E \in \mathcal{E}} p(E) = 1$
- For binary classification, we will assume $y = 1$ and $y = 0$ as the two events for an input $\boldsymbol{x}$



Logistic Regression

- Takes a probabilistic approach to learning functions (i.e., a classifier) i.e. $h_{\boldsymbol{\theta}}(\boldsymbol{x})$ outputs a probability $p_{\boldsymbol{\theta}}(y = 1 \mid \boldsymbol{x})$
  - Want $0 \leq h_{\boldsymbol{\theta}}(\boldsymbol{x}) \leq 1$ for all $\boldsymbol{x}$
- **Logistic regression model**:

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g(\boldsymbol{\theta}^T \boldsymbol{x})$$

  where g(z) is logistic function

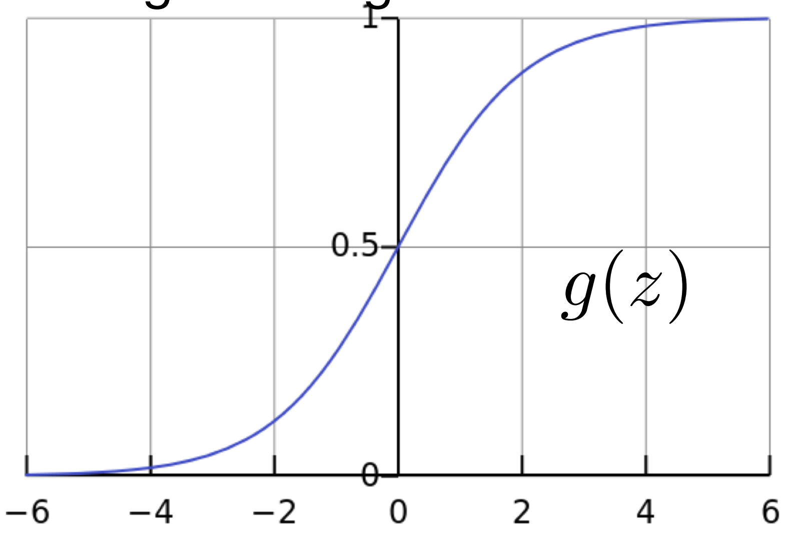
$$g(z) = \frac{1}{1+\mathrm{e}^{-z}}$$

- Hence,

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

  Not a regression model (despite the name!)

Logistic / Sigmoid Function



Interpretation of Hypothesis Output

$h_{\boldsymbol{\theta}}(\boldsymbol{x})$ should give $p_{\boldsymbol{\theta}}(y = 1 \mid \boldsymbol{x})$

Example: Cancer diagnosis from tumor size with y=1 as malignant

$$\boldsymbol{x} = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ \text{tumorSize} \end{bmatrix}$$

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = 0.7$$

Tell patient that 70% chance of tumor being malignant as per model

Note that: $p_{\boldsymbol{\theta}}(y = 1 \mid \boldsymbol{x}) + p_{\boldsymbol{\theta}}(y = 0 \mid \boldsymbol{x}) = 1$

Therefore, $p_{\boldsymbol{\theta}}(y = 0 \mid \boldsymbol{x}) = 1 - \ p_{\boldsymbol{\theta}}(y = 1 \mid \boldsymbol{x})$

Another Interpretation

Side Note: the odds in favor of an event is the quantity
p / (1 – p), where p is the probability of the event
E.g., If I toss a fair dice, what are the odds that I will have a 6?

- Equivalently, logistic regression assumes that

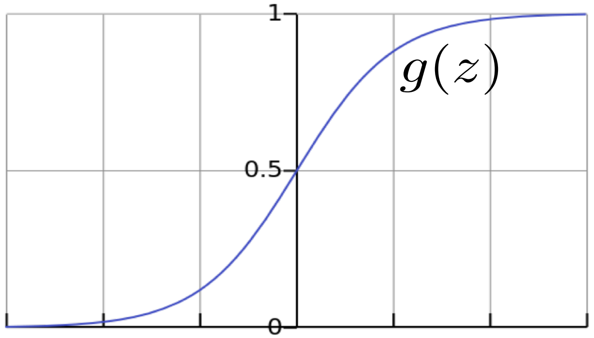
$$\log \underbrace{\boxed{\frac{p(y=1 \mid \boldsymbol{x}; \boldsymbol{\theta})}{p(y=0 \mid \boldsymbol{x}; \boldsymbol{\theta})}}}_{\text{odds of } y = 1} = \boldsymbol{\theta}^T \boldsymbol{x}$$

- In other words, logistic regression assumes that the log odds is a linear function of $\boldsymbol{x}$

Logistic Regression

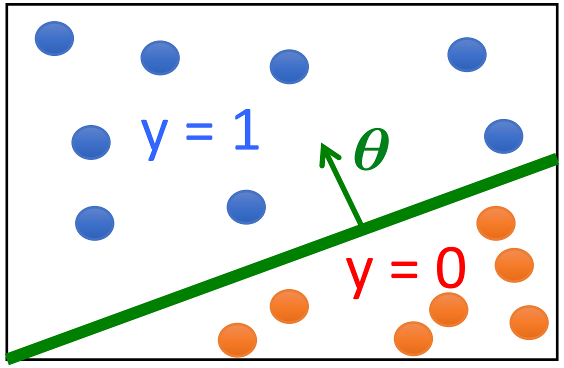
$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g(\boldsymbol{\theta}^T \boldsymbol{x})$$

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



$\boldsymbol{\theta}^T \boldsymbol{x}$ should be large <u>negative</u> values for negative instances	$\boldsymbol{\theta}^T \boldsymbol{x}$ should be large <u>positive</u> values for positive instances

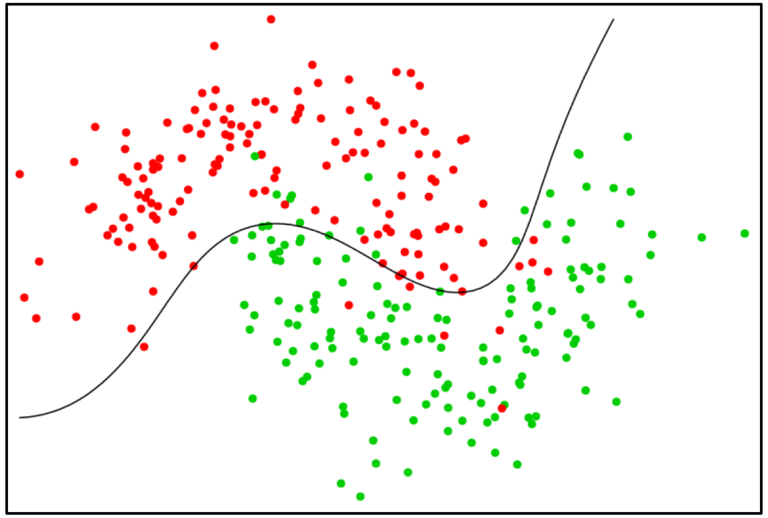
- To make hard predictions, assume a threshold t (e.g., 0.5)
  - Predict $y = 1$ if $h_{\boldsymbol{\theta}}(\boldsymbol{x}) \geq t$
  - Predict $y = 0$ if $h_{\boldsymbol{\theta}}(\boldsymbol{x}) < t$



Non-Linear Decision Boundary

- Can apply basis function expansion to features, same as with linear regression

$$\boldsymbol{x} = \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix} \rightarrow \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ x_1 x_2 \\ x_1^2 \\ x_2^2 \\ x_1^2 x_2 \\ x_1 x_2^2 \\ \vdots \end{bmatrix}$$



Loss Function

- Loss of a single instance:

$$\ell(y^{(i)}, \boldsymbol{x}^{(i)}, \boldsymbol{\theta}) = \begin{cases} -\log h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) & \text{if } y^{(i)} = 1 \\ -\log\left(1 - h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right)\right) & \text{if } y^{(i)} = 0 \end{cases}$$

- Total loss over n training instances:

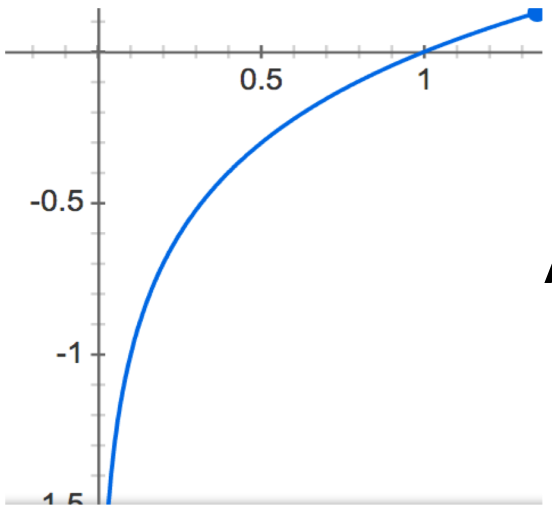
$$J(\boldsymbol{\theta}) = \sum_{i=1}^{n} \ell(y^{(i)}, \boldsymbol{x}^{(i)}, \boldsymbol{\theta})$$

Logistic regression loss:

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

Intuition Behind the Objective

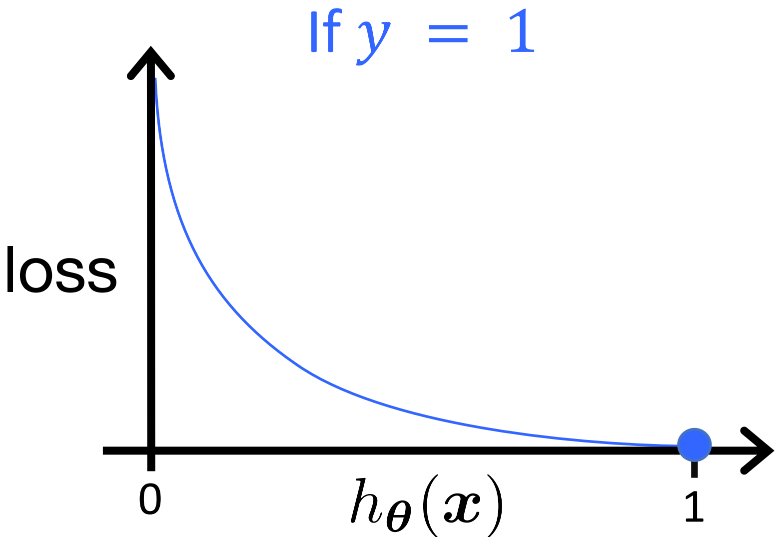
$$\ell(y^{(i)}, \boldsymbol{x}^{(i)}, \boldsymbol{\theta}) = \begin{cases} -\log h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) & \text{if } y^{(i)} = 1 \\ -\log\left(1 - h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right)\right) & \text{if } y^{(i)} = 0 \end{cases}$$



Aside: Recall the plot of log(z)

Intuition Behind the Objective

$$\ell(y^{(i)}, \boldsymbol{x}^{(i)}, \boldsymbol{\theta}) = \begin{cases} \boxed{-\log h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) \quad \text{if } y^{(i)} = 1} \\ -\log\left(1 - h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right)\right) \text{ if } y^{(i)} = 0 \end{cases}$$

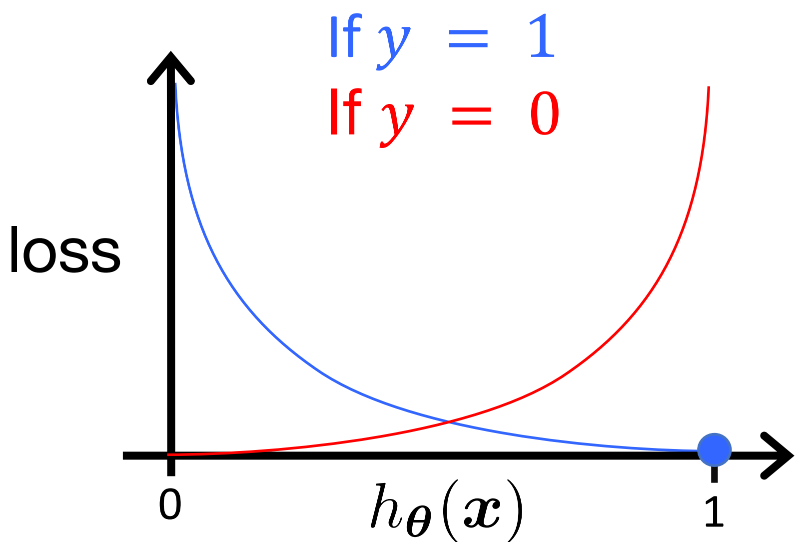


If $y^{(i)} = 1$

- As $h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) \rightarrow 1$, loss$\rightarrow 0$
- As $h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) \rightarrow 0$, loss$\rightarrow \infty$
- Captures intuition that larger mistakes should get larger penalties
  - e.g., predict $h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) = 0$, but $y^{(i)} = 1$

Intuition Behind the Objective

$$\ell(y^{(i)}, \boldsymbol{x}^{(i)}, \boldsymbol{\theta}) = \begin{cases} \boxed{-\log h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) \quad \text{if } y^{(i)} = 1} \\ \boxed{-\log\left(1 - h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right)\right) \text{ if } y^{(i)} = 0} \end{cases}$$



If $y^{(i)} = 0$

- As $h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) \rightarrow 0$, loss$\rightarrow 0$
- As $h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) \rightarrow 1$, loss$\rightarrow \infty$
- Captures intuition that larger mistakes should get larger penalties
  - e.g., predict $h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) = 1$, but $y^{(i)} = 0$

Regularized Logistic Regression

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

- We can regularize logistic regression exactly as before:

$$\begin{aligned} J_{\text{reg}}(\boldsymbol{\theta}) &= J(\boldsymbol{\theta}) + \frac{\lambda}{2}\textstyle\sum_{j=1}^{d}\theta_j^2 \\ &= J(\boldsymbol{\theta}) + \frac{\lambda}{2}\ \|\boldsymbol{\theta}_{1:d}\|_2^2 \end{aligned}$$

- $\lambda > 0$ is the regularization coefficient

Gradient Descent for Logistic Regression

$$J_{\text{reg}}(\boldsymbol{\theta}) = -\sum_{i=1}^{n}\left[y^{(i)} \log h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right)\right)\right] + \frac{\lambda}{2} \| \boldsymbol{\theta}_{1:d} \|_{\mathbf{2}}^{\mathbf{2}}$$

- Initialize $\boldsymbol{\theta}$ randomly
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

simultaneous update for j = 0 ... d

Gradient Descent for Logistic Regression

$$J_{\text{reg}}(\boldsymbol{\theta}) = -\sum_{i=1}^{n}\left[y^{(i)} \log h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) + \left(1 - y^{(i)}\right)\log\left(1 - h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right)\right)\right] + \frac{\lambda}{2}\|\,\boldsymbol{\theta}_{1:d}\|_{\mathbf{2}}^{\mathbf{2}}$$

- Initialize $\boldsymbol{\theta}$ randomly
- Repeat until convergence

[simultaneous update for j = 0 ... d]

$$\theta_0 \leftarrow \theta_0 - \alpha \sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)$$

$$\theta_j \leftarrow \theta_j - \alpha \left[\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right) x_j^{(i)} + \lambda\theta_j\right]$$

Gradient Descent for Logistic Regression

- Initialize $\boldsymbol{\theta}$ randomly
- Repeat until convergence

[simultaneous update for j = 0 ... d]

$$\theta_0 \leftarrow \theta_0 - \alpha \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right)$$

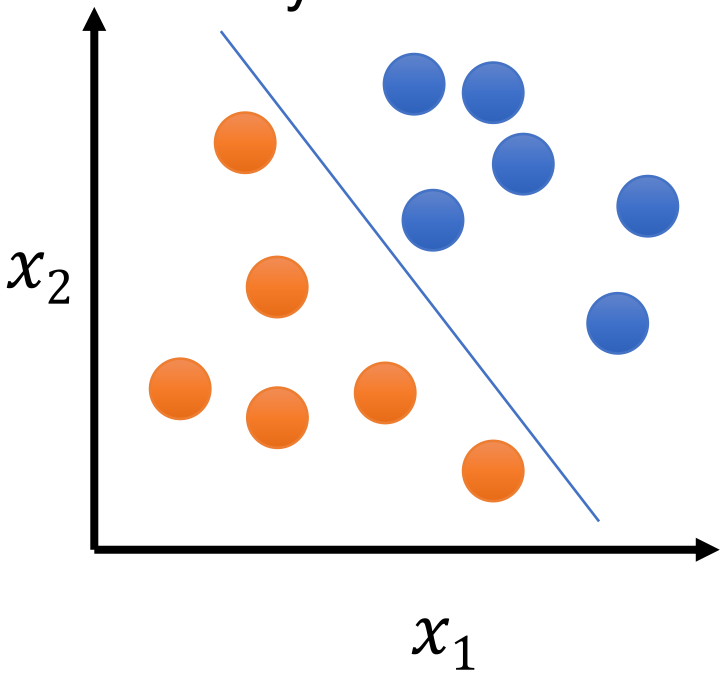
$$\theta_j \leftarrow \theta_j - \alpha \left[\sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right) x_j^{(i)} + \lambda \theta_j \right]$$

This looks IDENTICAL to linear regression!

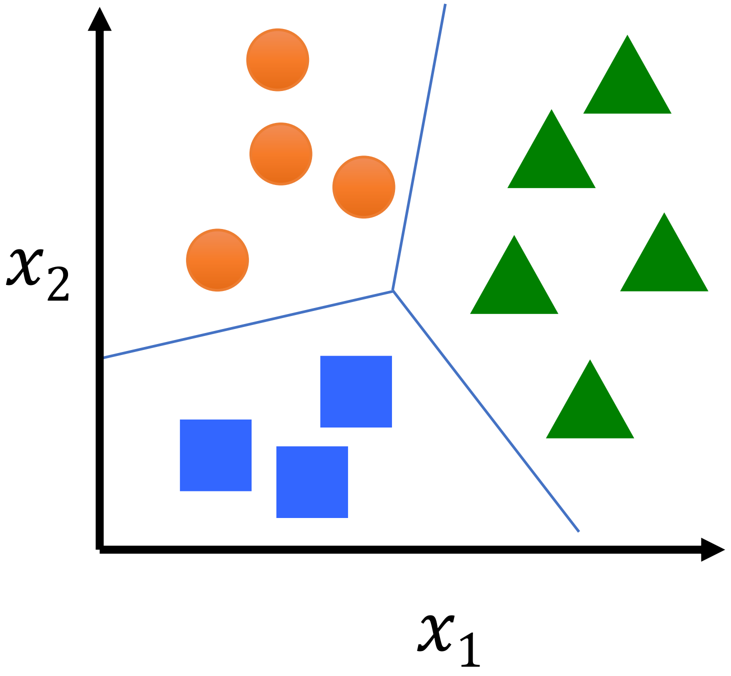
- Ignoring the 1/n constant
- However, the form of the hypothesis $h_{\boldsymbol{\theta}}(\boldsymbol{x})$ is very different

Multi-Class Classification

Binary classification



Multi-class classification



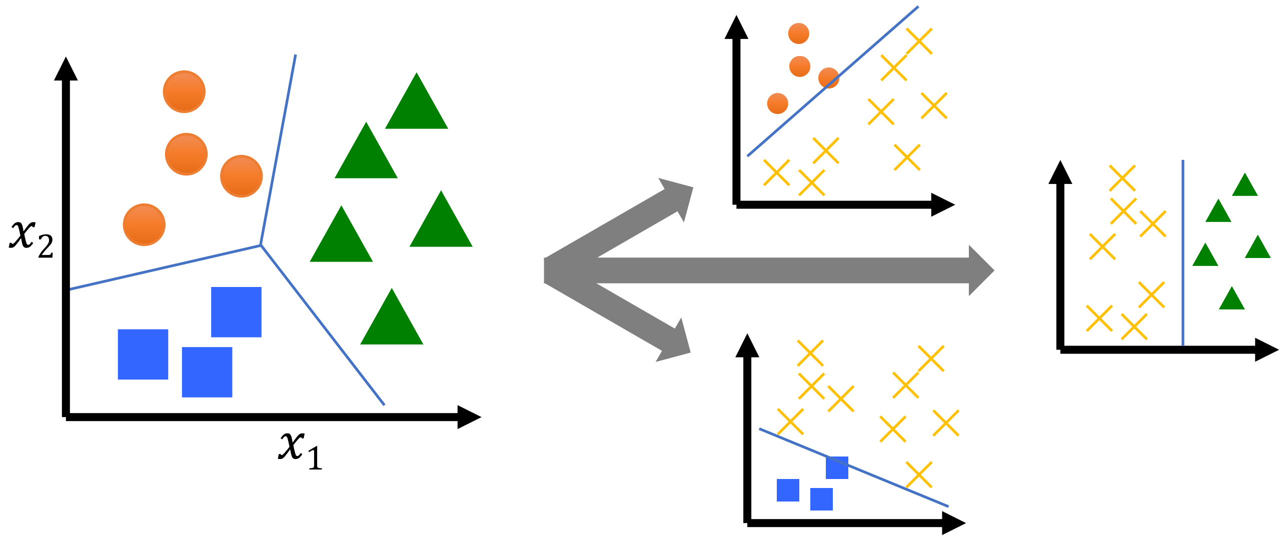
Disease diagnosis: healthy / cold / flu / pneumonia ..

Object classification: desk / chair / monitor / bookcase …

ChatGPT: next word prediction

Multi-Class Logistic Regression

Split into one v.s. rest:



- Expensive! Solving c separate classification problems

Multi-Class Logistic Regression

- For 2 classes:

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1+\exp(-\boldsymbol{\theta}^T \boldsymbol{x})} = \frac{\exp(\boldsymbol{\theta}^T \boldsymbol{x})}{\underbrace{\boxed{1}}_{\text{weight assigned to } y\,=\,0}+\underbrace{\boxed{\exp(\boldsymbol{\theta}^T \boldsymbol{x})}}_{\text{weight assigned to } y\,=\,1}}$$

- For C classes:

$$h_{\boldsymbol{\theta}_{1:C}}^{(c)}(\boldsymbol{x}) = p_{\boldsymbol{\theta}_{1:C}}(y = c \mid \boldsymbol{x}) = \frac{\exp(\boldsymbol{\theta}_c^T \boldsymbol{x})}{\sum_{k=1}^{C} \exp(\boldsymbol{\theta}_k^{\mathrm{T}} \boldsymbol{x})}$$

  - Here $\boldsymbol{\theta}_c \in \mathbb{R}^{d+1}$ is a parameter vector for class $c \in \{1, \ldots, C\}$
  - Hypothesis also called the **softmax** function
  - Note that sum of class probabilities equals 1

Multi-Class Logistic Regression

- The hypothesis for class c

$$h_{\boldsymbol{\theta}_{1:C}}^{(c)}(\boldsymbol{x}) = \frac{\exp(\boldsymbol{\theta}_c^T \boldsymbol{x})}{\sum_{k=1}^{C} \exp(\boldsymbol{\theta}_k^{\mathrm{T}} \boldsymbol{x})}$$

- Gradient descent simultaneously updates all parameters for c
  - Same derivative as before, just with the above $h_{\boldsymbol{\theta}_{1:C}}^{(c)}(\boldsymbol{x})$
- Predict class label as the most probable label

$$\hat{y} = \underset{c \in \{1,\ldots,C\}}{\arg\max}\, h_{\boldsymbol{\theta}_{1:C}}^{(c)}(\boldsymbol{x})$$

Summary

Logistic Regression

- A probabilistic linear model for classification (despite the name)

Loss function

- Binary/softmax cross-entropy loss

Basis Function, Optimization, Regularization

- Analogous to linear regression