Naïve Bayes and Logistic Regression

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These slides are inspired based on slides from Le Song, Eric Eaton, and Chao Zhang.

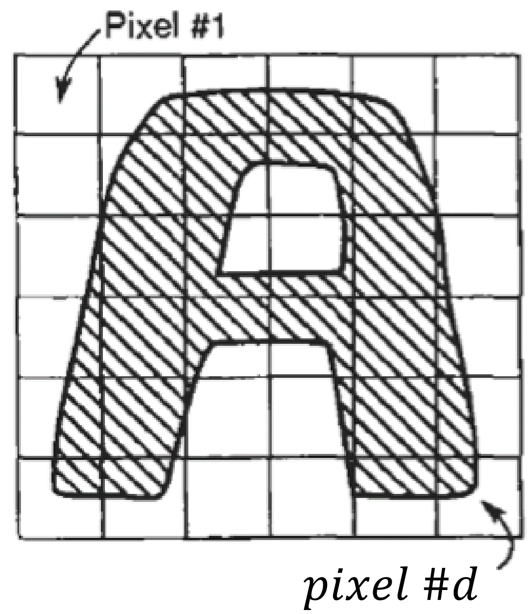

THE BEST WAY TO
EXPLAIN OVERFITTING

Outline

- Generative and Discriminative Classification
- The Logistic Regression Model
- Understanding the Objective Function
- Gradient Descent for Parameter Learning
- Multiclass Logistic Regression

Classification

- Represent the data



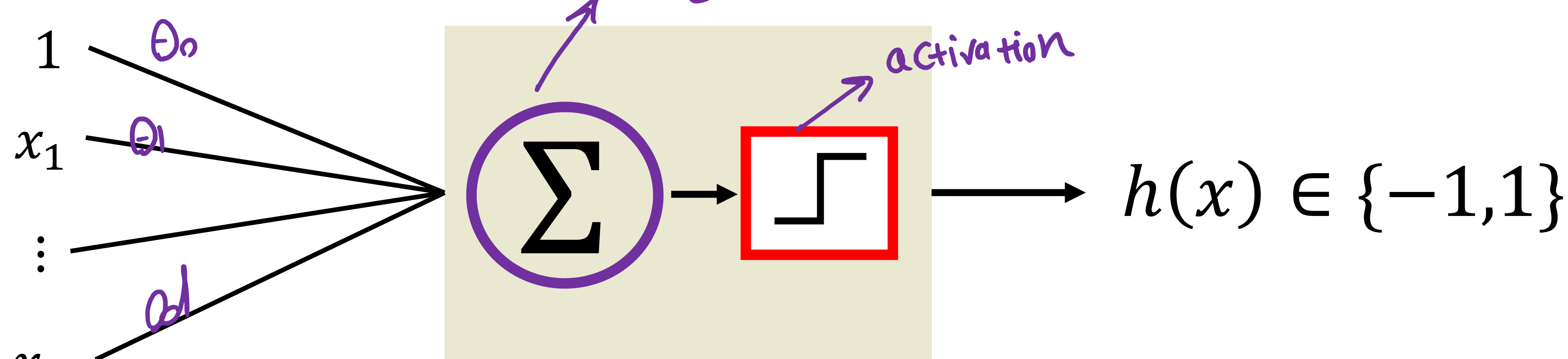
$$\Longrightarrow \quad X = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix}$$

- A label is provided for each data point, eg., $y \in \{-1, +1\}$

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

- Classifier

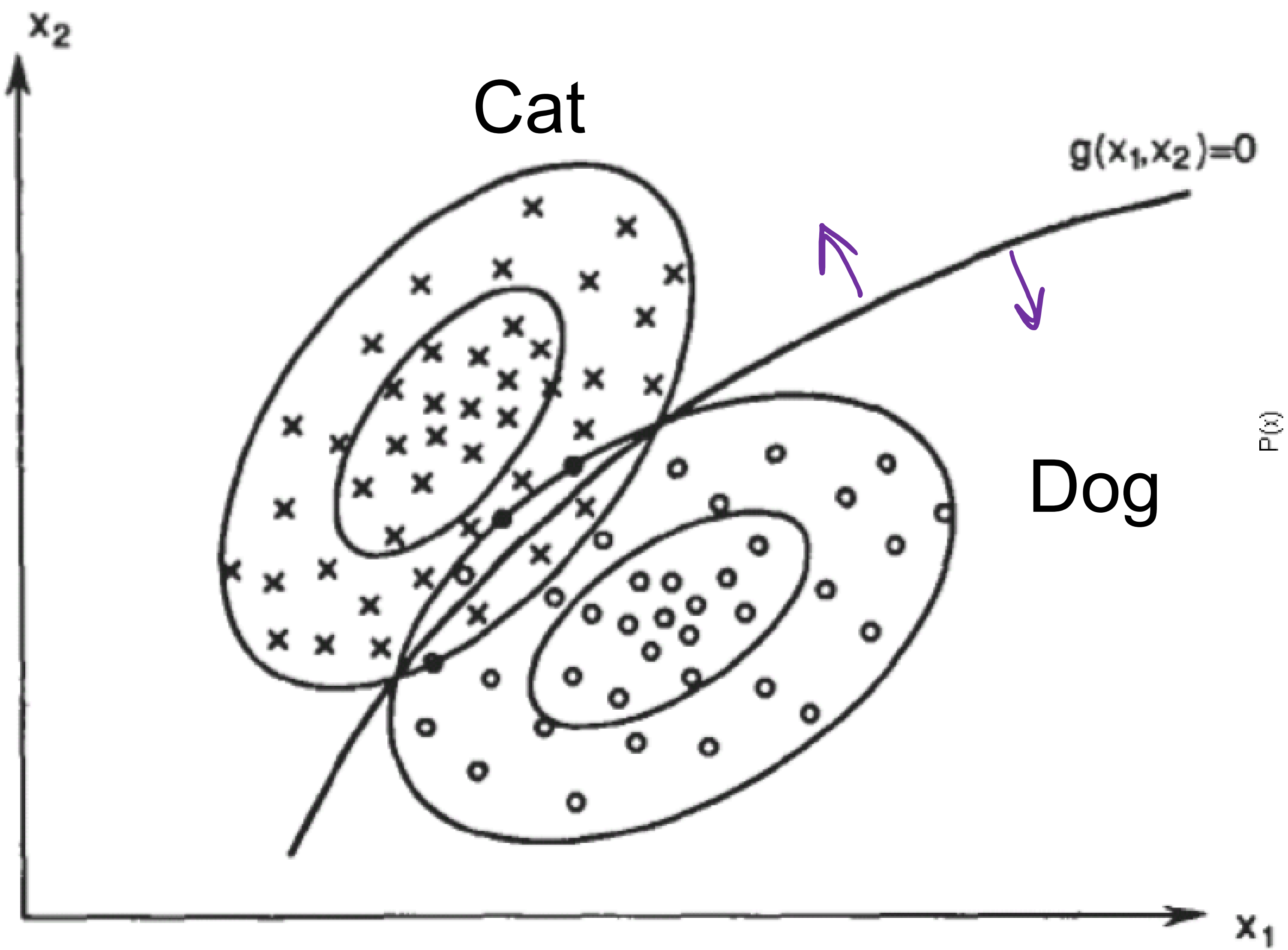
$\Sigma = 1 \times \theta_0 + x_1 \theta_1 + \dots + x_d \theta_d = x\theta \in \mathbb{R}$

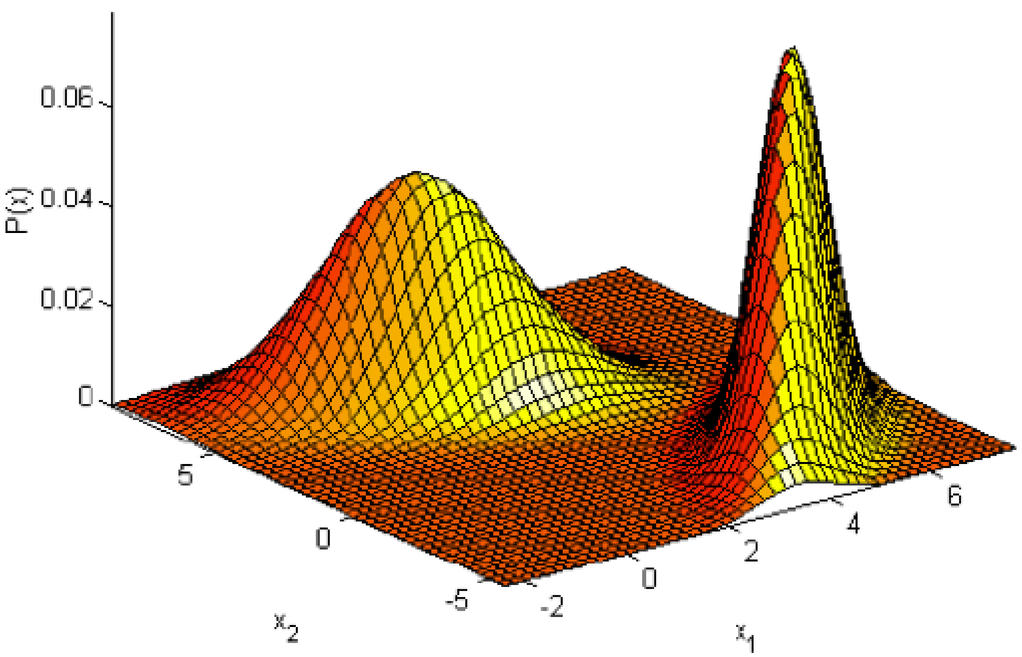


$h(x) = sign(x\theta) \rightarrow$ linear classification (Perceptron)

Decision Making: Dividing the Feature Space

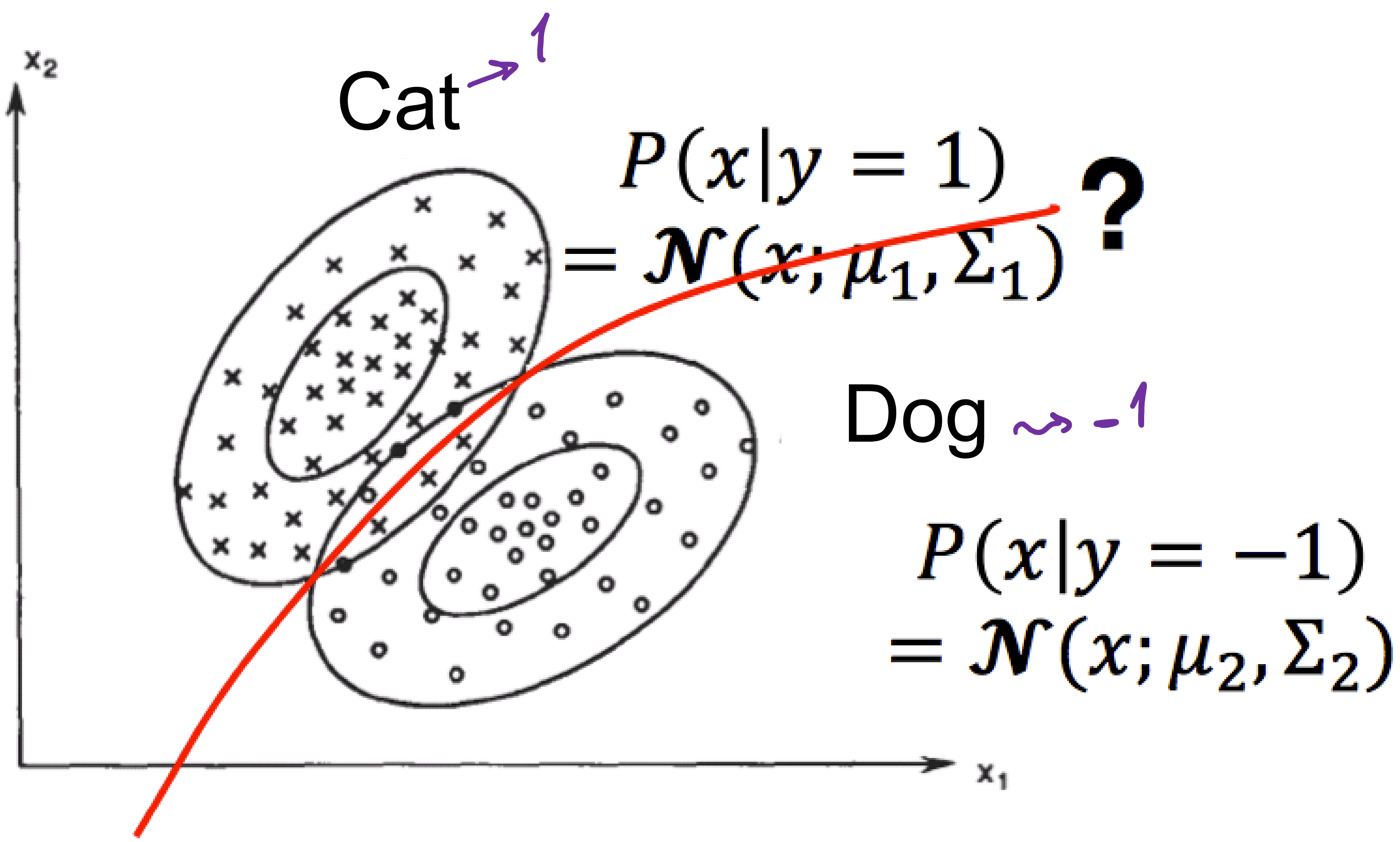
- Distributions of sample from normal (positive class) and abnormal (negative class) tissues





How to Determine the Decision Boundary?

- Given class conditional distribution: $P(x|y=1), P(x|y=-1)$, and class prior: $P(y=1), P(y=-1)$



Bayes Decision Rule

$P(x|y)$ $\to$ $+1$ cat, -1 dog

likelihood   Prior

$$P(y|x) = \frac{P(x|y)P(y)}{P(x)} = \frac{P(x,y)}{\sum_z P(x,y)}$$

posterior   normalization constant

Prior: $P(y)$

Likelihood (class conditional distribution : $p(x|y) = \mathcal{N}(x|\mu_y, \Sigma_y)$

Posterior: $P(y|x) = \frac{P(y)\mathcal{N}(x|\mu_y,\Sigma_y)}{\sum_y P(y)\mathcal{N}(x|\mu_y,\Sigma_y)}$

Bayes Decision Rule

- Learning: prior: $p(y)$,class conditional distribution : $p(x|y)$

- The poster probability of a test point

p(x,y)

$$q_i(x) := P(y = i|x) = \frac{P(x|y)P(y)}{P(x)}$$

- Bayes decision rule:
  - If $q_i(x) > q_j(x)$, then $y = i$, otherwise $y = j$

- Alternatively:
  - If ratio $l(x) = \frac{P(x|y=i)}{P(x|y=j)} > \frac{P(y=j)}{P(y=i)}$, then $y = i$, otherwise $y = j$
  - Or look at the log-likelihood ratio $\mathrm{h(x)} = -\ln \frac{q_i(x)}{q_j(x)}$

$y \in \{1, -1\} \qquad x^{\{i\}} = [h]$

$$P(y=1 \mid x^{\{i\}}) = \frac{P(x^{\{i\}} \mid y=1)\, P(y=1)}{P(x)} = \frac{\frac{1}{\sqrt{2\pi\sigma_h^2}} \exp \frac{-(x^{\{i\}} - \mu_h)^2}{2\sigma_h^2}\, P(y=1)}{P(x)}$$

for cats

$$P(y=-1 \mid x^{\{i\}}) = \frac{P(x^{\{i\}} \mid y=-1)\, P(y=-1)}{P(x)} = \frac{\frac{1}{\sqrt{2\pi\sigma_h^2}} \exp \frac{-(x^{\{i\}} - \mu_h)^2}{2\sigma_h^2}\, P(y=-1)}{}$$

for dogs

$$P(x) = \sum_y P(x, y=y) = P(x, y=1) + P(x, y=-1)$$

What do People do in Practice?

- Generative models
  - Model prior and likelihood explicitly $P(y|x) = \frac{P(x|y)\,P(y)}{P(x)}$
  - “Generative” means able to generate synthetic data points
  - Examples: Naive Bayes, Hidden Markov Models
- Discriminative models
  - Directly estimate the posterior probabilities $\rightarrow$ $P(y|x)$ directly ?
  - No need to model underlying prior and likelihood distributions
  - Examples: Logistic Regression, SVM, Neural Networks

Generative Model: Naive Bayes

- Use Bayes decision rule for classification

$P(x_1|y)\,P(x_2|y) \cdots P(x_d|y)$

$$P(y|x) = \frac{P(x|y)P(y)}{P(x)}$$

- But assume $p(x|y=1)$ is fully factorized : Dimensions are independent.

$$p(x|y=1) = \prod_{i=1}^{d} p(x_i|y=1)$$

- Or the variables corresponding to each dimension of the data are independent given the label

“Naïve” conditional independence assumption

$$P(y|x) = \frac{\boxed{P(x|y)P(y)}}{P(x)} = \frac{P(x,y)}{P(x)}$$

$P(a,b,c) = P(a|b,c)\,P(b,c)$

$P(a|b,c) = P(a)$

$a \perp b \perp c$

Joint probability model:

$$P(x, y_{label=1}) = \mathrm{P}(\mathrm{x}_1, \dots, \mathrm{x}_\mathrm{d}, \mathrm{y}_{\mathrm{label}=1}) = \mathrm{P}(\mathrm{x}_1 | \mathrm{x}_2,, \dots, \mathrm{x}_\mathrm{d}, \mathrm{y}_{\mathrm{label}=1}) P(\mathrm{x}_2, \dots, \mathrm{x}_\mathrm{d}, \mathrm{y}_{\mathrm{label}=1})$$

$$= \mathrm{P}(\mathrm{x}_1 | \mathrm{x}_2,, \dots, \mathrm{x}_\mathrm{d}, \mathrm{y}_{\mathrm{label}=1}) P(\mathrm{x}_2 | \mathrm{x}_3 \dots, \mathrm{x}_\mathrm{d}, \mathrm{y}_{\mathrm{label}=1}) P(\mathrm{x}_3, \dots, \mathrm{x}_\mathrm{d}, \mathrm{y}_{\mathrm{label}=1})$$

$$= \cdots$$

$$= \mathrm{P}(\mathrm{x}_1 | \cancel{\mathrm{x}_2,, \dots, \mathrm{x}_\mathrm{d}}, \mathrm{y}_{\mathrm{label}=1}) P(\mathrm{x}_2 | \cancel{\mathrm{x}_3 \dots, \mathrm{x}_\mathrm{d}}, \mathrm{y}_{\mathrm{label}=1}) \dots P(\mathrm{x}_{\mathrm{d}-1} | \cancel{x_d}, y_{label=1}) P(x_d | y_{label=1}) \mathrm{P}(y_{label=1})$$

Naïve Bayes assumption: let’s rewrite it as:

$$P(x, y_{label=1}) = P(x_1 | y_{label=1}) P(x_2 | y_{label=1}) \dots P(x_d | y_{label=1}) P(y_{label=1}) =$$

prior

$$P(y_{label=1}) \boxed{\prod_{i=1}^{d} P(x_i | y_{label=1})}$$

likelihood

Gaussian naïve Bayes

A typical assumption

[Example](#)

Discriminative Models

- Directly estimate decision boundary $\mathrm{h(x)} = -\ln \frac{q_i(x)}{q_j(x)}$ or posterior distribution $p(y|x)$
  - Logistic regression, Neural networks
  - Do not estimate $p(x|y)$ and $p(y)$

- Why discriminative classifier?
  - Avoid difficult density estimation problem → Generative model
  - Empirically achieve better classification results

Outline

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Gaussian Naïve Bayes

$$P(y = 1|x) = \frac{P(x|y = 1)P(y = 1)}{P(x)} = \frac{P(y = 1)\prod_{i=1}^{d} P(x_i|y = 1)}{P(x)}$$

$$\prod_{i=1}^{d} p(x_i|y = 1, \mu_{1i}, \sigma_{1i}) = \prod_{i=1}^{d} \frac{1}{\sqrt{2\pi}\sigma_{1i}} \exp\left(-\frac{1}{2\sigma_{1i}^2}(x_{1i} - \mu_{1i})^2\right)$$

Prior: $p(y = 1) = \pi_1$

Posterior: $p(y = 1 \mid x, \mu, \sigma, \pi)$

$$= \frac{\pi_1 \prod_{i=1}^{d} \frac{1}{\sqrt{2\pi}\sigma_{1i}} \exp\left(-\frac{1}{2\sigma_{1i}^2}(x_i - \mu_{1i})^2\right)}{\underbrace{\sum_{k=1}^{2}}_{\text{labels}} \pi_k \prod_{i=1}^{d} \frac{1}{\sqrt{2\pi}\sigma_{ki}} \exp\left(-\frac{1}{2\sigma_{ki}^2}(x_i - \mu_{ki})^2\right)}$$

get $\exp(\ln(u))$ of numerator and denominator

$$= \frac{\exp\left(-\sum_{i=1}^{d}\left(\frac{1}{2\sigma_{1i}^2}(x_i - \mu_{1i})^2 + \log\sigma_{1i} + C\right) + \log\pi_1\right)}{\sum_{k=1}^{2} \exp\left(-\sum_{i=1}^{d}\left(\frac{1}{2\sigma_{ki}^2}(x_i - \mu_{ki})^2 + \log\sigma_{ki} + C\right) + \log\pi_k\right)}$$

$$= \frac{\exp\left(-\sum_{i=1}^{d}\left(\frac{1}{2\sigma_i^2}(x_i - \mu_{1i})^2 + \log\sigma_i + C\right) + \log\pi_1\right)}{\sum_{k=1}^{2}\exp\left(-\sum_{i=1}^{d}\left(\frac{1}{2\sigma_i^2}(x_i - \mu_{ki})^2 + \log\sigma_i + C\right) + \log\pi_k\right)}$$

$$= \frac{1}{1 + \exp\left(-\underbrace{\sum_{i=1}^{d}\left(x_i\frac{1}{\sigma_i}(\mu_{1i} - \mu_{2i})}_{\sum_i \theta_i x_i} + \underbrace{\frac{1}{\sigma_i^2}(\mu_{1i}^2 - \mu_{2i}^2)\right) + \log\frac{\pi_2}{\pi_1}}_{\theta_0}\right)}$$

$$P(y=1|x) = \frac{1}{1+\exp\left(-\sum_{i=1}^{d}\left(x_i\frac{1}{\sigma_i}(\mu_{1i}-\mu_{2i})+\frac{1}{\sigma_i^2}(\mu_{1i}^2-\mu_{2i}^2)\right)+\log\frac{\pi_2}{\pi_1}\right)}$$

Number of parameters:

$2d+1 \rightarrow d\ mean, d\ variance, and\ 1\ for\ prior$

$$P(y=1|x) = \frac{1}{1+\exp[-(\sum_{i=1}^{d}(\theta_i x_i)+\theta_0)]} = \frac{1}{1+\exp(-s)}$$

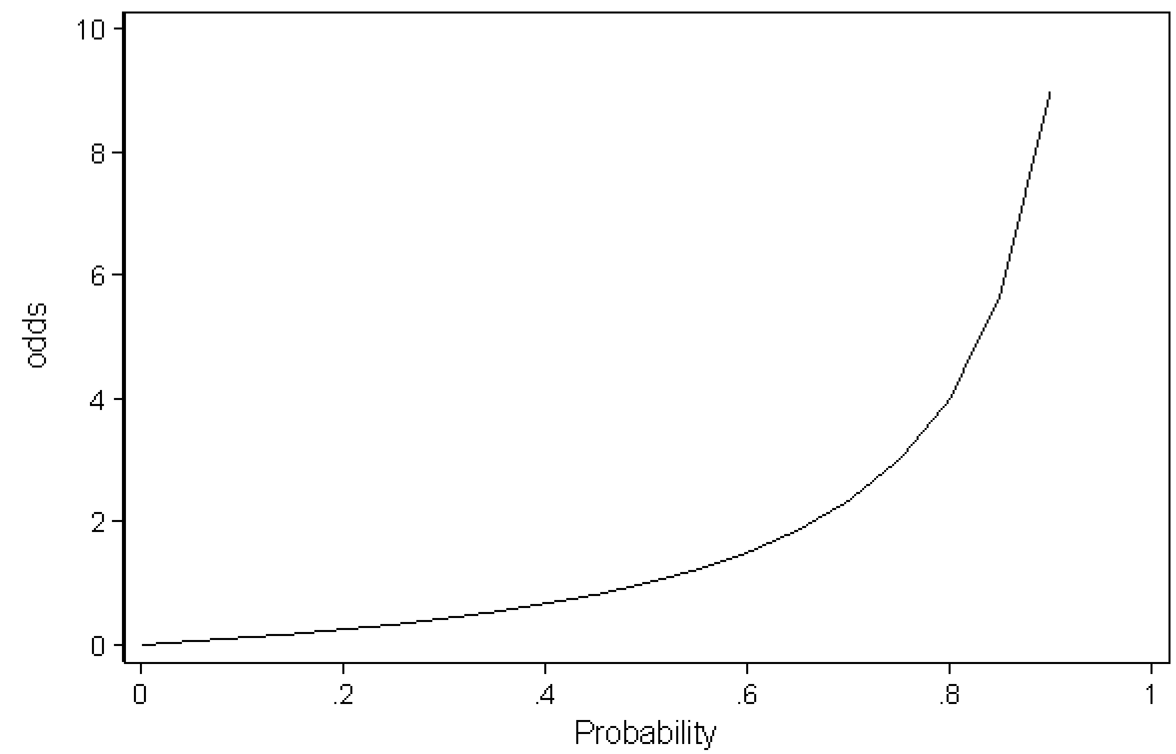
Number of parameters = $d+1 \rightarrow \theta_0, \theta_1, \theta_2, \ldots, \theta_d$

Why not directly learning $P(y=1|x)$ or θ parameters?

Gaussian Naïve Bayes is a subset of logistic regression

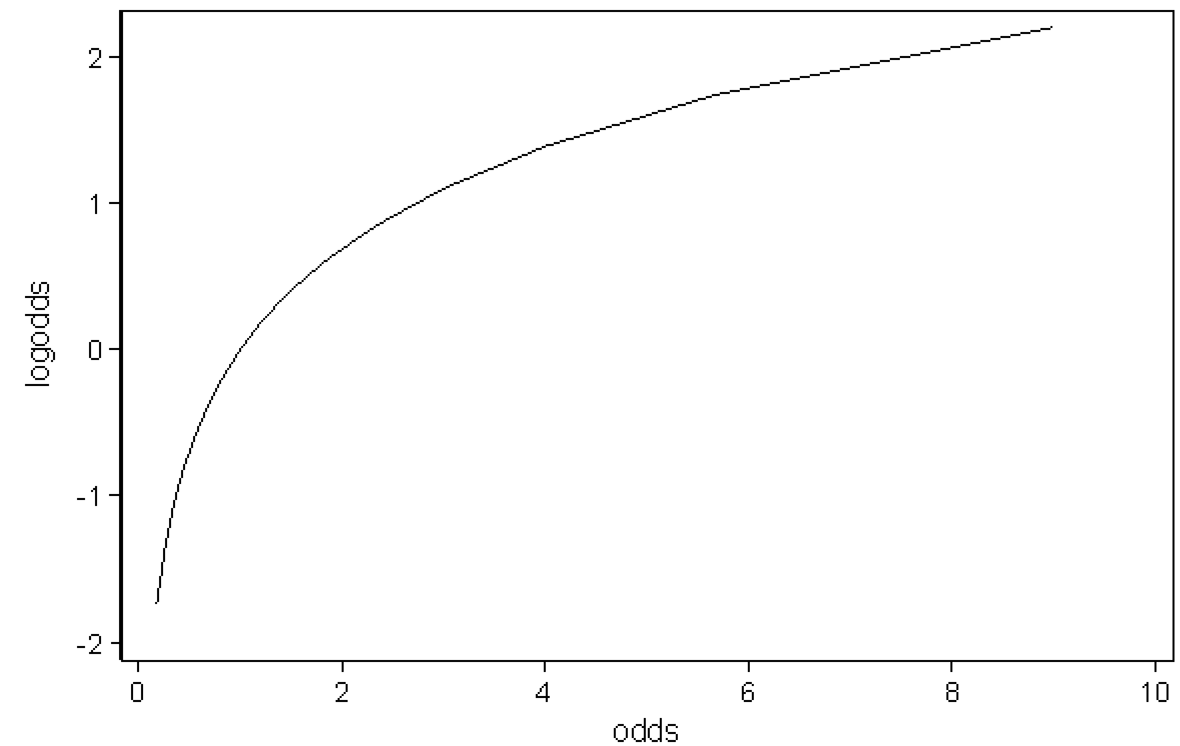
Why $\frac{1}{1+\exp(-x\theta)}$ is a probability?

$\frac{P(y=1|x)}{1-P(y=1|x)}$ is called Odds



$log(odds)\ vs\ odds$

What could be $x\theta$ domain?



What is logit function?

$$logit(p) = log(odds) = \log(\frac{p}{1-p})$$

$$\log\left(\frac{p}{1-p}\right) = \theta_0 + \theta_1 x_1 + \cdots + \theta_d x_d = \sum_{i=0}^{d} x_i \theta_i = x\theta$$

$$exp\left(log\left(\frac{p}{1-p}\right)\right) = \exp(x\theta)$$

$$p = \frac{e^{x\theta}}{1 + e^{x\theta}} = \frac{1}{1 + e^{-x\theta}}$$

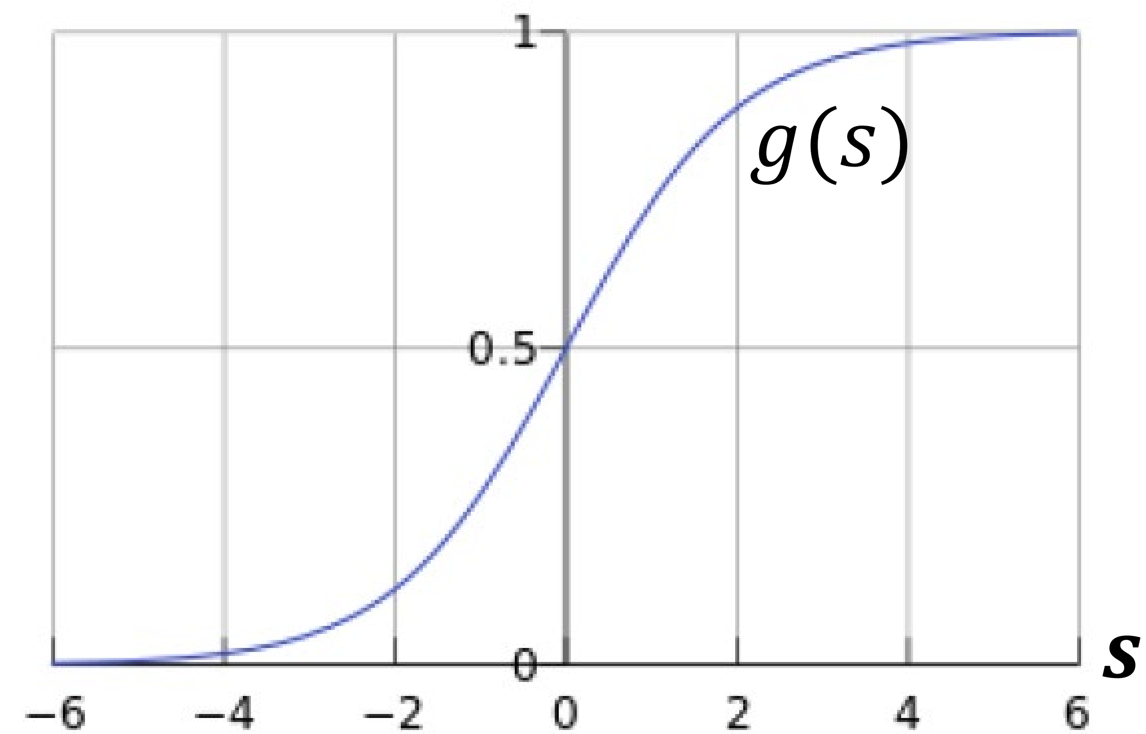
Logistic function for posterior probability

Many equations can give us this shape

Let's use the following function:

$$s = x\theta$$

$$g(s) = P(y = 1|x) = \frac{e^s}{1 + e^s} = \frac{1}{1 + e^{-s}}$$



This formula is called sigmoid function

It is easier to use this function for optimization

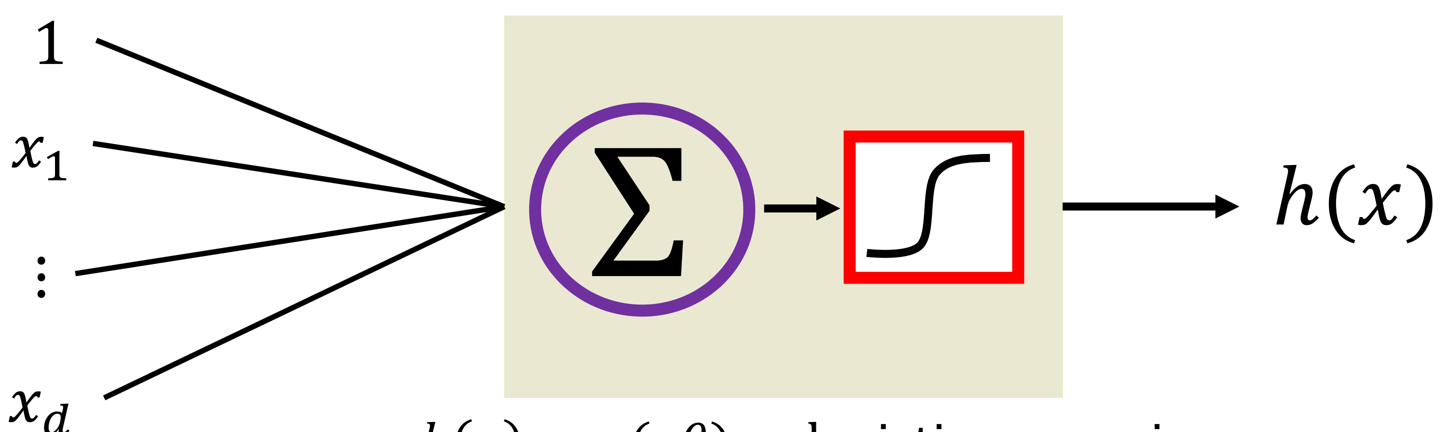
Is 0.5 threshold cut-off a good choice?

Learn about ROC and AUC (False positive rate and True positive rate) (Interactive)

Sigmoid Function

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

$$s = \sum_{i=0}^{d} x_i\theta_i = \theta_0 + \theta_1 x_1 + \cdots + \theta_d x_d$$

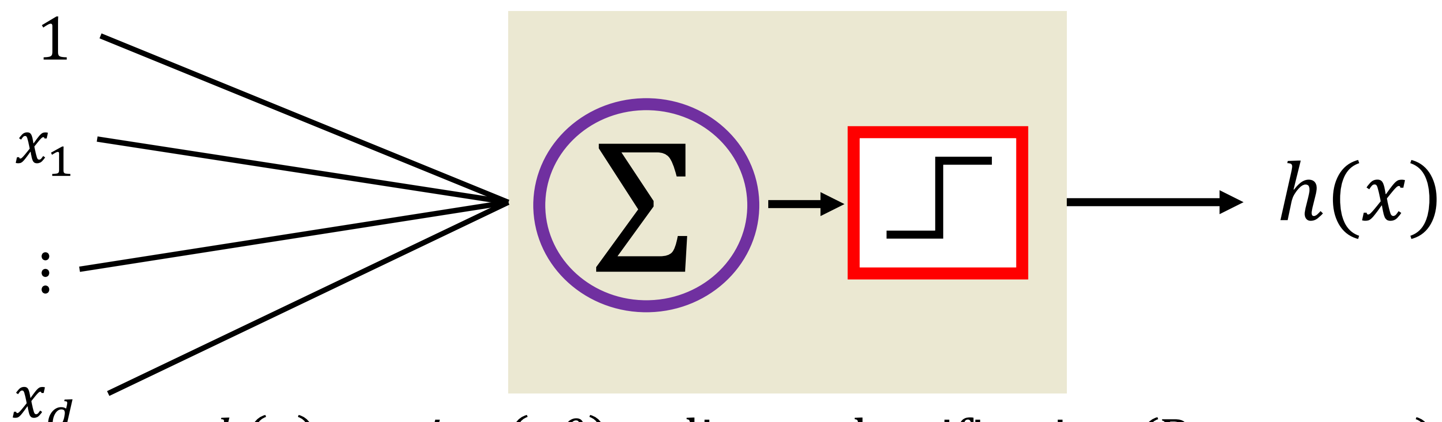


$h(x) = g(x\theta) \rightarrow$ logistic regression

Soft classification
Posterior probability

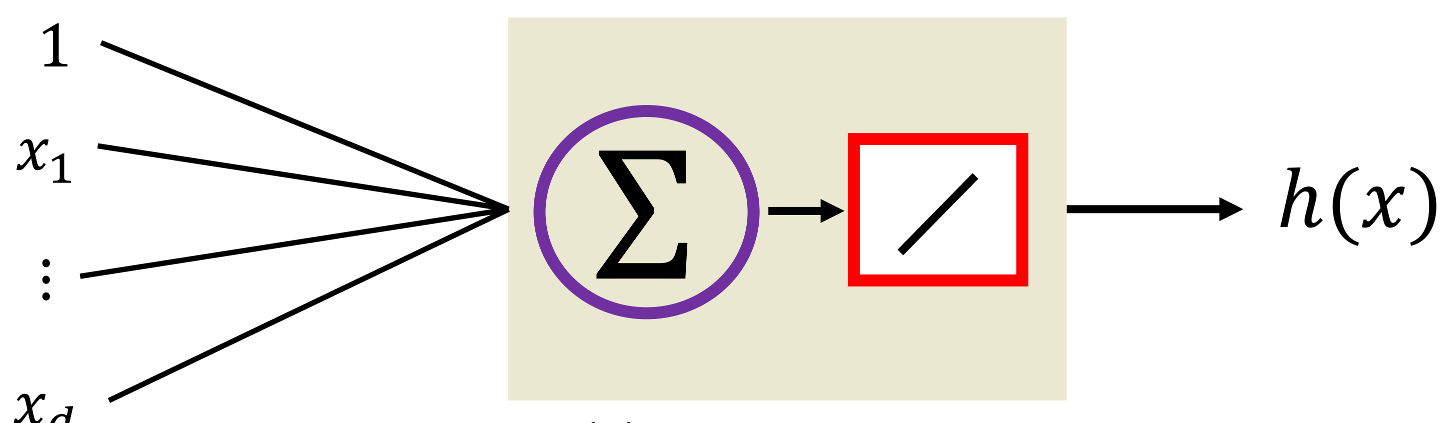
Three linear models

$$s = \sum_{i=0}^{d} x_i \theta_i = \theta_0 + \theta_1 x_1 + \cdots + \theta_d x_d$$

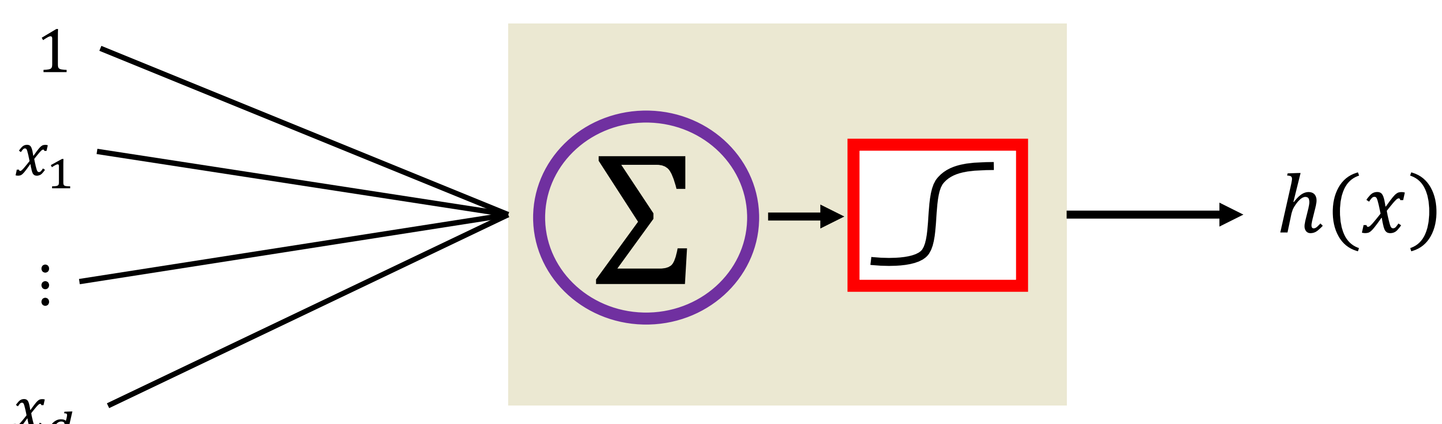


Hard classification

$h(x) = \ sign(x\theta) \rightarrow$ linear classification (Perceptron)



$h(x) \rightarrow$ linear regression



Soft classification
Posterior probability

$h(x) = g(x\theta) \rightarrow$ logistic regression

$g(s)$ is interpreted as probability

Example: Prediction of heart attacks

Input $\boldsymbol{x}$: cholesterol level, age, weight, finger size, etc.

$g(s)$: probability of heart attack within a certain time

We can't have a hard prediction here

$s = x\theta$ Let's call this risk score

$$h_\theta(x) = p(y|x) = \begin{cases} g(s), & y = 1 \\ 1 - g(s), & y = 0 \end{cases}$$

Using posterior probability directly

Logistic regression model

$$p(y|x) = \begin{cases} \dfrac{1}{1+\exp(-x\theta)} & y = 1 \\ 1 - \dfrac{1}{1+\exp(-x\theta)} = \dfrac{\exp(-x\theta)}{1+\exp(-x\theta)} & y = 0 \end{cases}$$

We need to find θ parameters, let's set up log-likelihood for **n** datapoints

$$l(\theta) \coloneqq log \prod_{i=1}^{n} p(y_i, |x_i, \theta)$$

$$= \sum_i \theta^T x_i^T (y_i - 1) - \log(1 + \exp(-x_i\theta))$$

[This form is concave, negative of this form is convex]()

The gradient of $l(\theta)$

$$l(\theta) = log \prod_{i=1}^{n} p(y_i, |x_i, \theta)$$

$$= \sum_i \theta^T x_i^T (y_i - 1) - \log(1 + \exp(-x_i \theta))$$

- Gradient

$$\frac{\partial l(\theta)}{\partial \theta} = \sum_i x_i^T (y_i - 1) + x_i^T \frac{\exp(-x_i \theta)}{1 + \exp(-x_i \theta)}$$

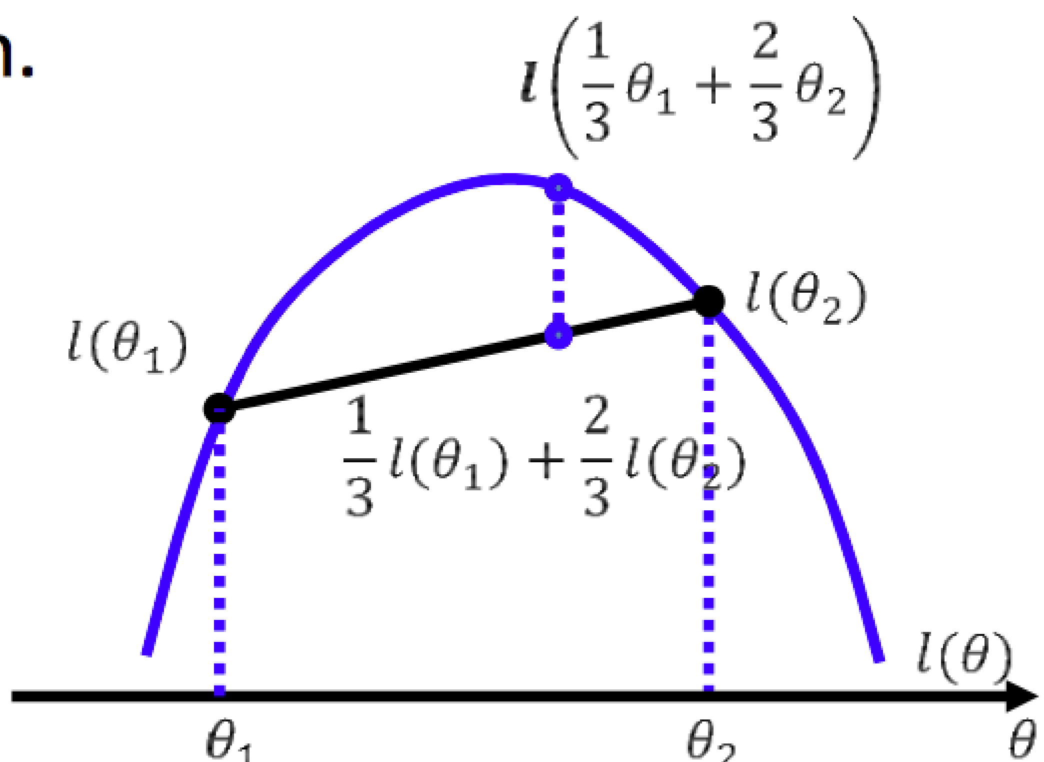
- Setting it to 0 does not lead to closed form solution

The Objective Function

- Find θ, such that the conditional likelihood of the labels is maximized

$$\max_{\theta} l(\theta) := log \prod_{i=1}^{n} p(y_i, | x_i, \theta)$$

- Good news: $l(\theta)$ is concave function of θ, and there is a single global optimum.



- Bad new: no closed form solution (resort to numerical method)

Gradient Descent

- One way to solve an *unconstrained* optimization problem is gradient descent

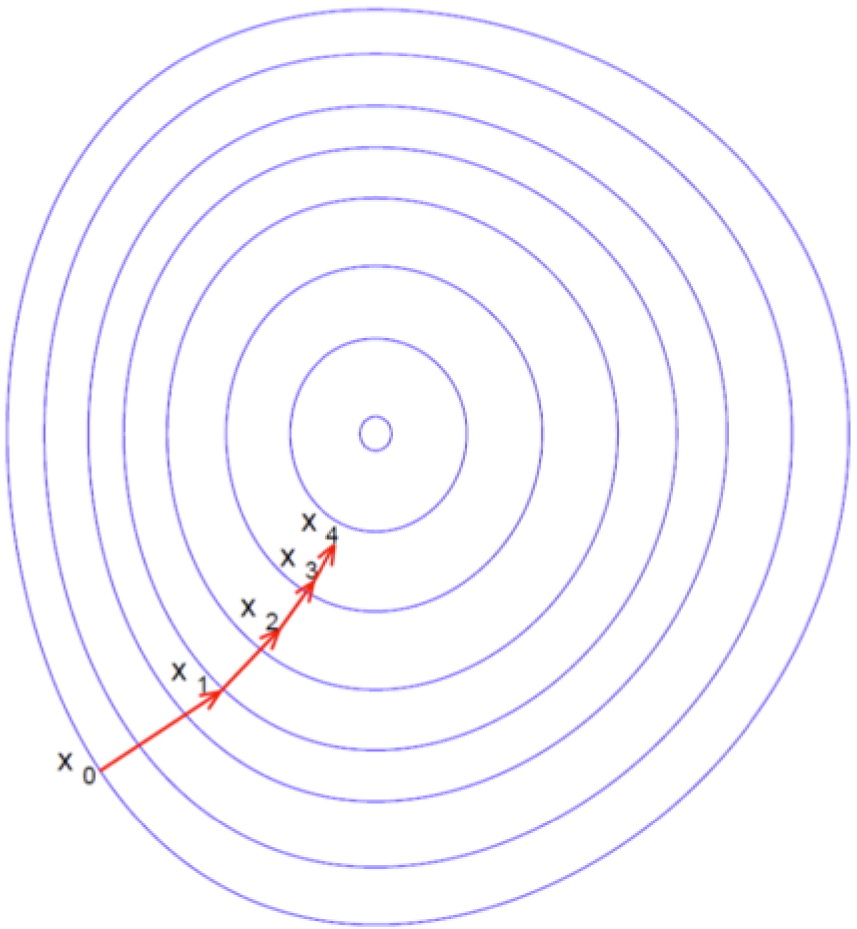
- Given an initial guess, we *iteratively* refine the guess by taking the direction of the negative gradient

- Think about going down a hill by taking the steepest direction at each step

- Update rule

$$x_{k+1} = x_k - \gamma_k \nabla f(x_k)$$

γ_k is called the step size or learning rate



Gradient Ascent(concave)/Descent(convex) algorithm

- Initialize parameter θ^0

- Do

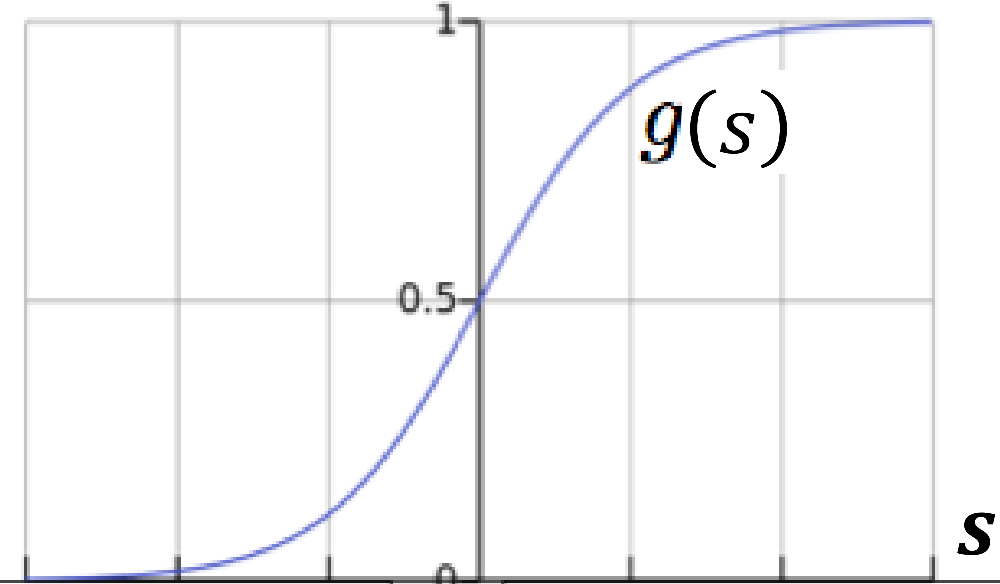
$$\theta^{t+1} \leftarrow \theta^t + \eta \sum_i x_i^T (y_i - 1) + x_i^T \frac{\exp(-x_i\theta)}{1 + \exp(-x_i\theta)}$$

- While the $||\theta^{t+1} - \theta^t|| > \epsilon$

Logistic Regression

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

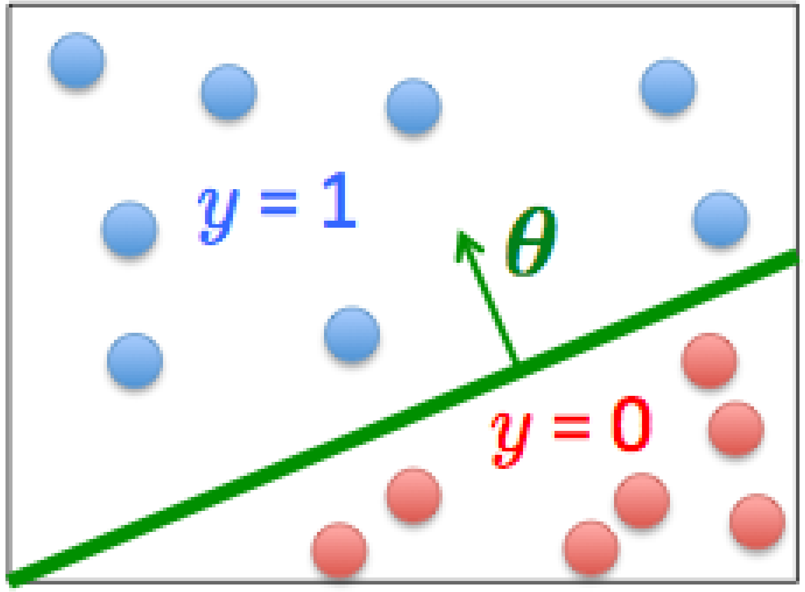
$$s = x\theta$$



$x\theta$ should be large negative values for negative instances

$x\theta$ should be large positive values for positive instances

- Assume a threshold and...
  - Predict $y = 1$ if $g(s) \geq 0.5$
  - Predict $y = 0$ if $g(s) < 0.5$



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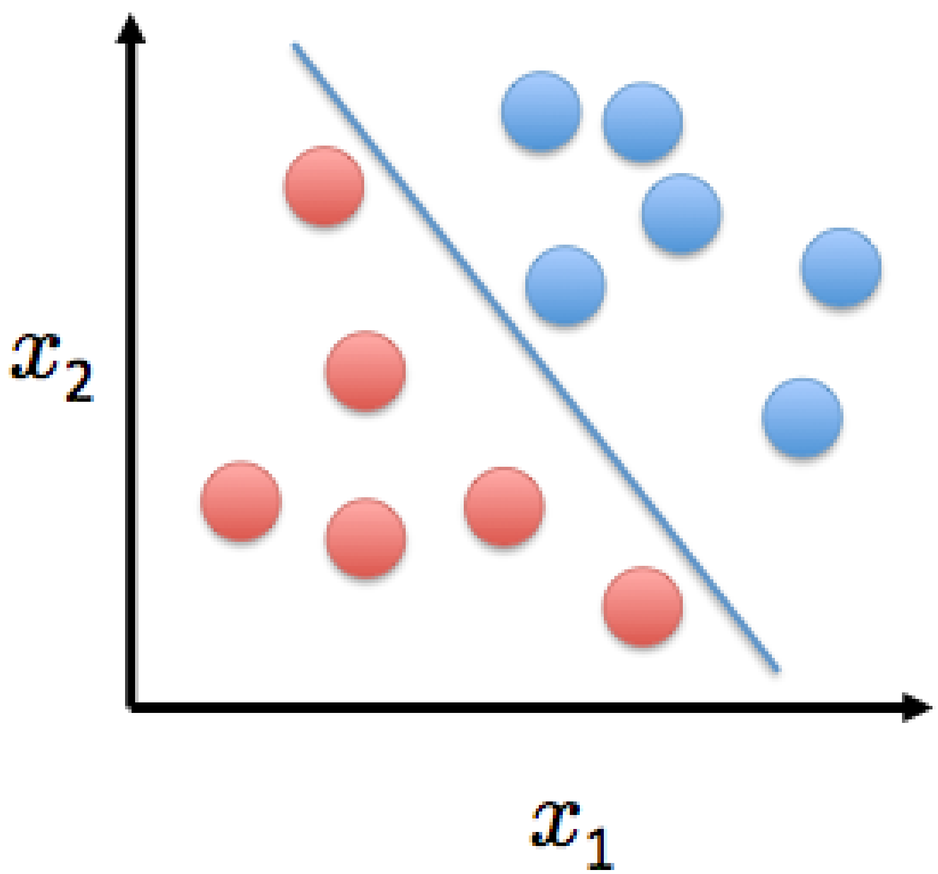
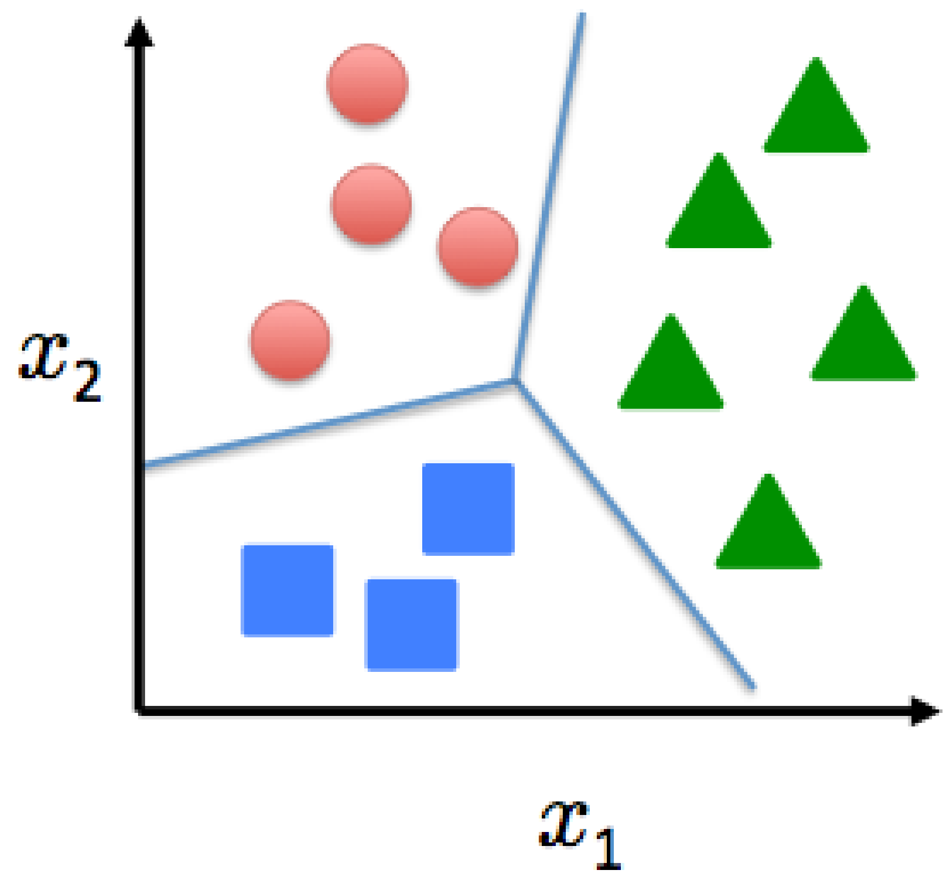
Multiclass Logistic Regression

Binary classification:



Multi-class classification:

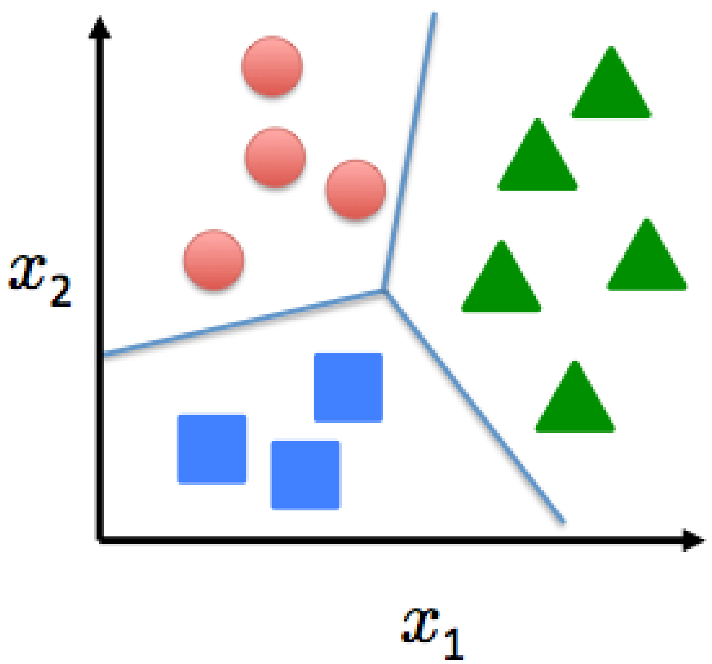


Disease diagnosis: healthy / cold / flu / pneumonia

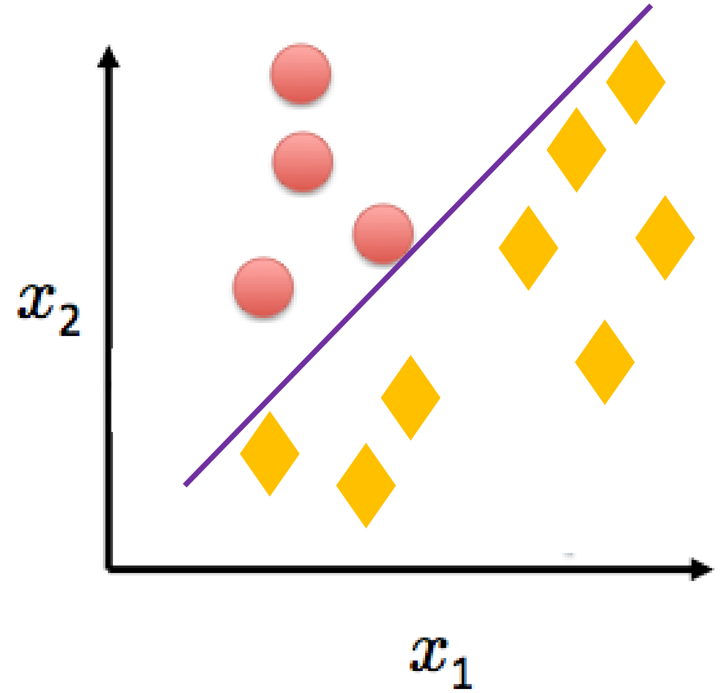
Object classification: desk / chair / monitor / bookcase

One-vs-all (one-vs-rest)

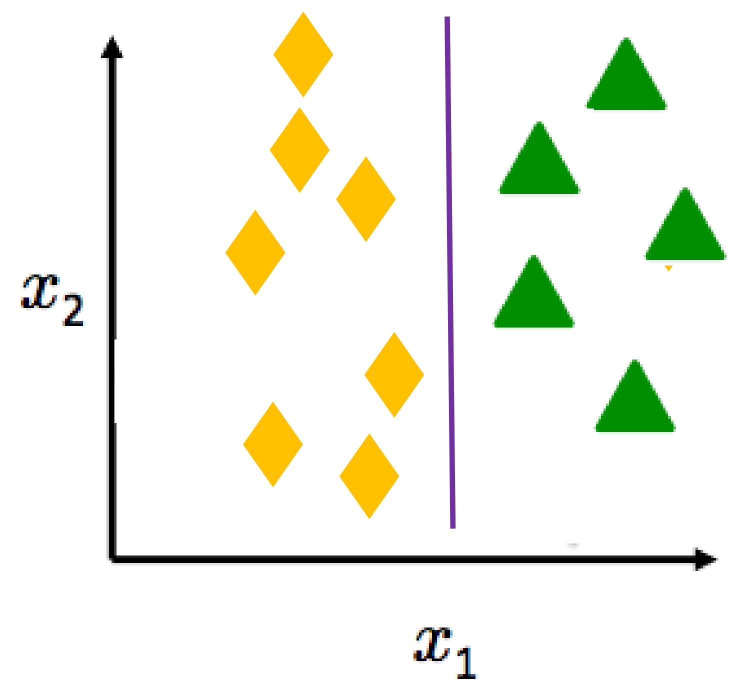
Multi-class classification:



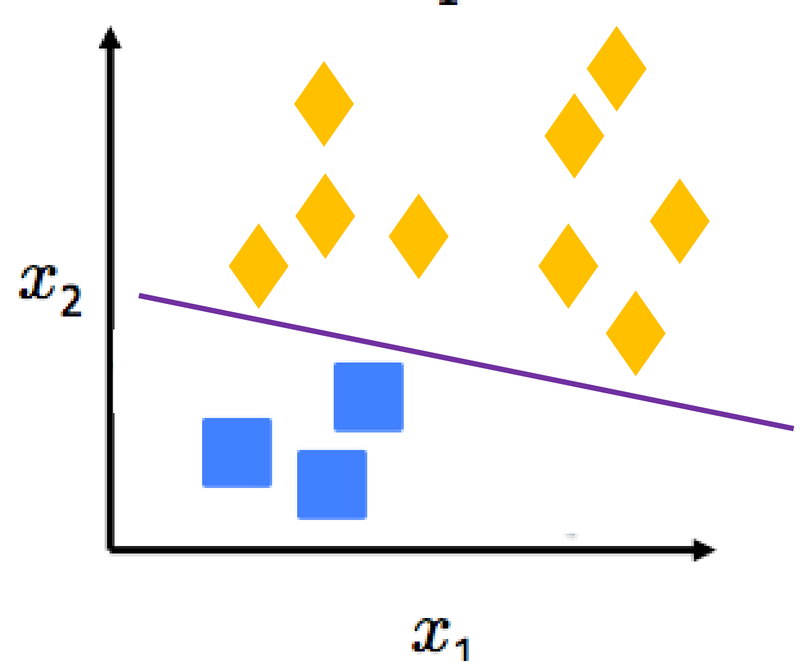
$$h_\theta^{(m)}(x) = p(y = 1|x, \theta)\ (m = 1,2,3)$$



$h_\theta^1(x)$



$h_\theta^2(x)$



$h_\theta^3(x)$

One-vs-all (one-vs-rest)

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

To predict the label of a new input x, pick class m that maximizes:

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

Using Softmax

$$L(\theta) = -\sum_{i=1}^{N} (y_a * \log(y_p)$$

$$y_a = [cat, dog, fish] = [1,0,0]$$
$$\Rightarrow there\ are\ k\ classes\ (k = 3\ in\ this\ example)$$

$$y_{p\ for\ class\ m} = softmax(x\theta) = \frac{\exp(x\theta)_m}{\sum_{j=0}^{k} \exp(x\theta)_j}$$

$$y_p = [0.6,0.3,0.1]$$

$$SGD \Rightarrow \theta^{t+1} \leftarrow \theta^t - \alpha\, \nabla L(\theta)$$

$$\theta^{t+1} \leftarrow \theta^t - \alpha\, x^T (y_p - y_a)$$

Take-Home Messages

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- Multiclass Logistic Regression