Machine Learning

Linear and Logistic Regression

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Cours sur l'année, 2017–2018

Linear models

Problem: $\{(x_i, y_i)\}$.

Given x, predict $\hat{y}$.

Linear models

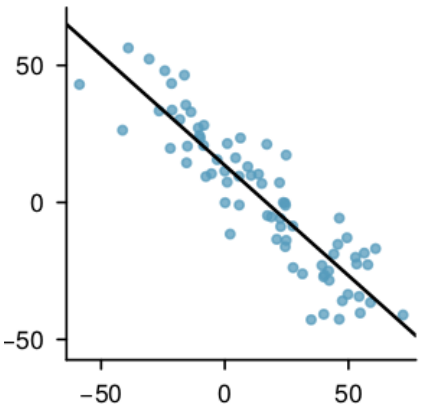
x: **explanatory** or **predictor** variable.

y: **response** variable.

For some reason, we believe a linear model is a good idea.

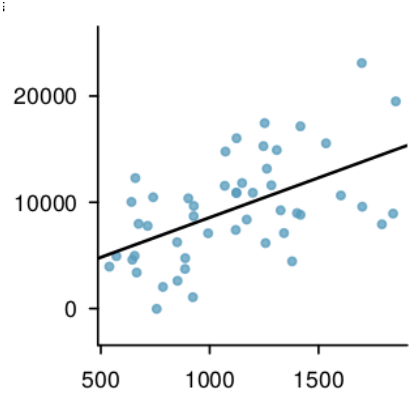
Linear models

Example:



Linear models

Example:



Linear models

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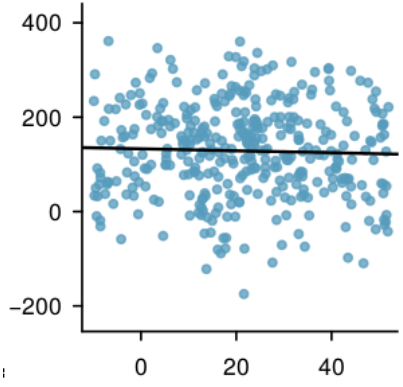
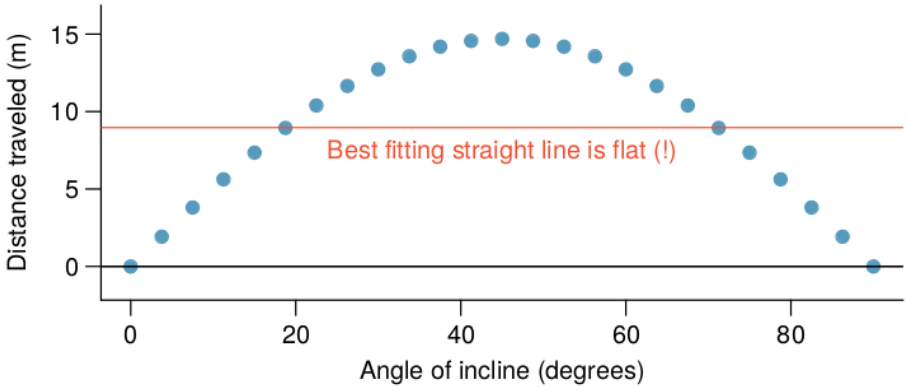


Linear models

Example:



Residuals

What's left over.

$$\text{data} = \text{fit} + \text{residual}$$

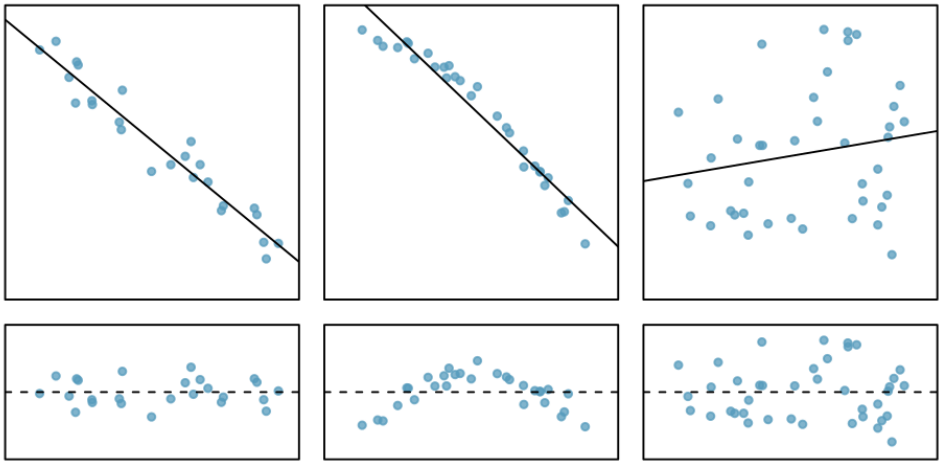
Residuals

What's left over.

$$y_i = \hat{y}_i + e_i$$

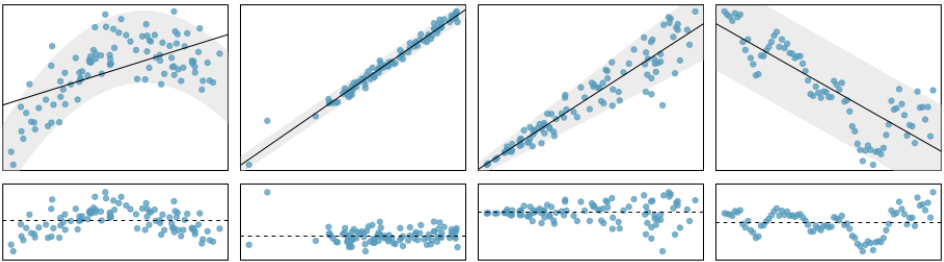
Residuals

What's left over.



Residuals

What's left over.



Residuals

What's left over.

Goal: small residuals.

$$\sum | e_i |$$

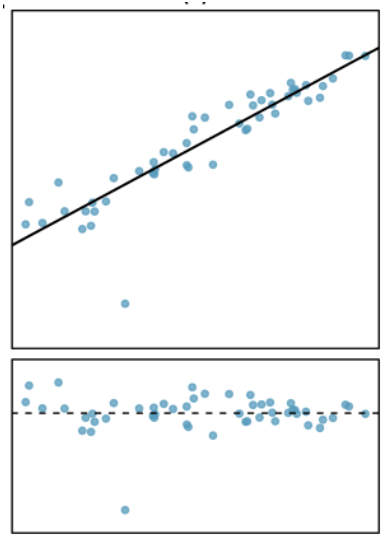
Residuals

What's left over.

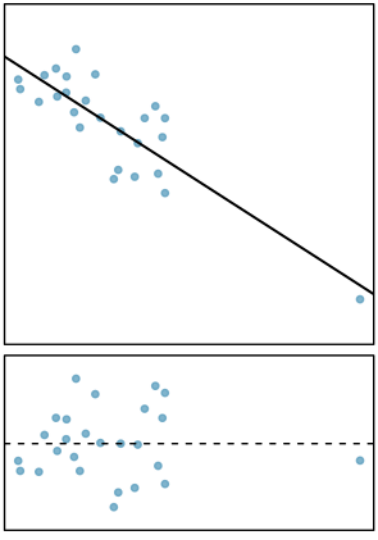
Goal: small residuals.

$$\sum e_i^2$$

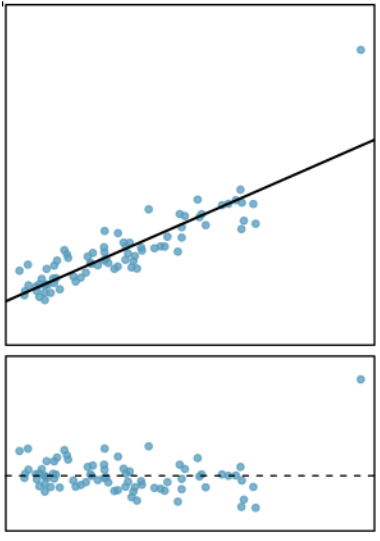
Outliers



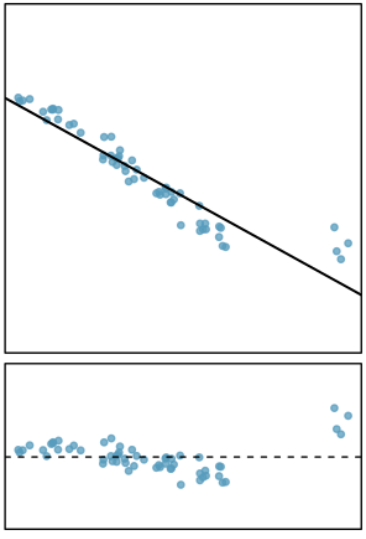
Outliers



Outliers



Outliers



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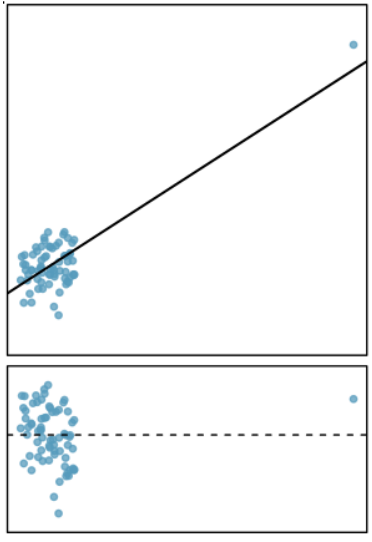
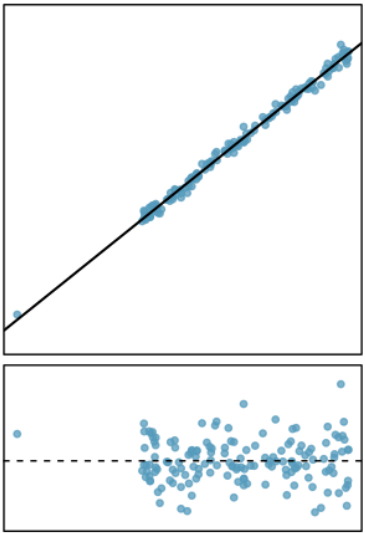


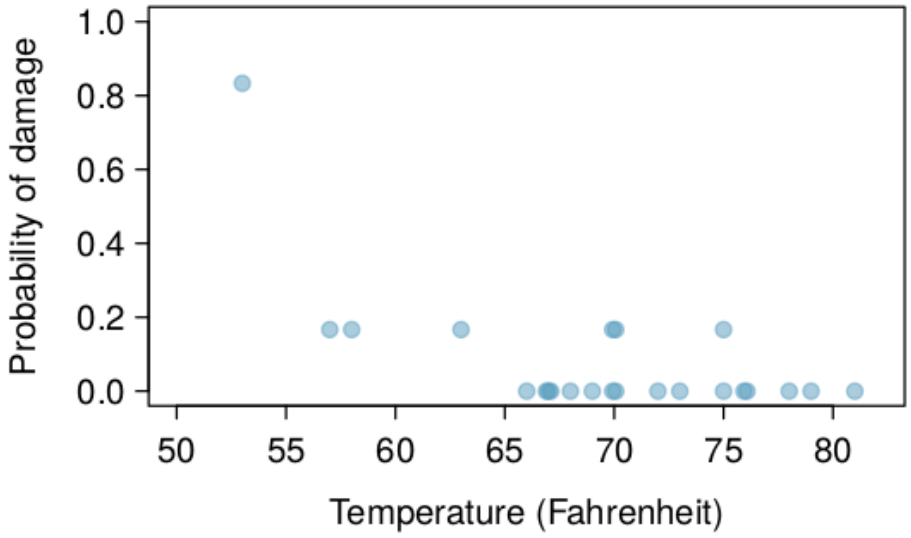
Outliers



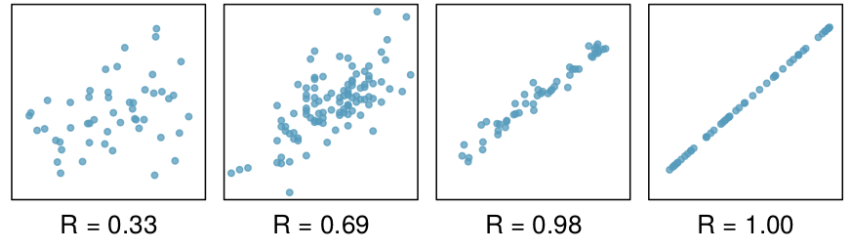
Outliers

Don’t ignore outliers.

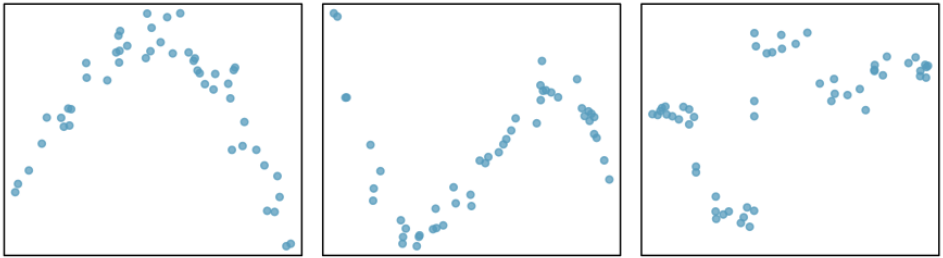
Outliers



Correlation

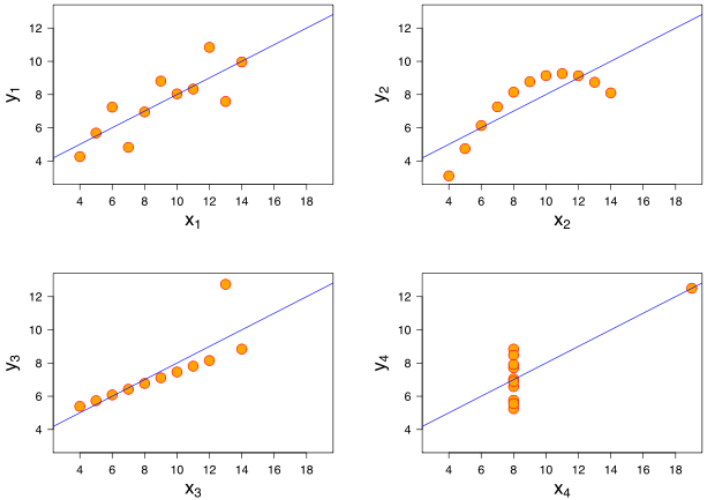


Correlation

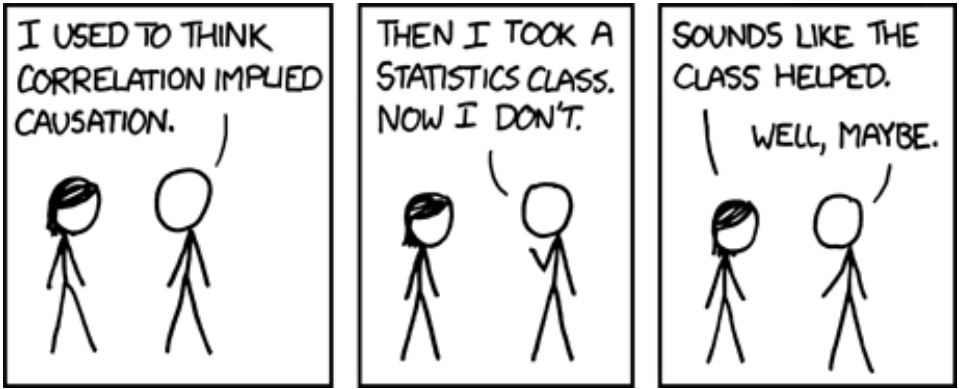


Correlation

Anscombe's Quartet



Correlation does not imply causation



https://xkcd.com/552/

Hypothesis (model)

$$h_\theta(x) = \theta_0 + \theta_1 x$$

Cost function

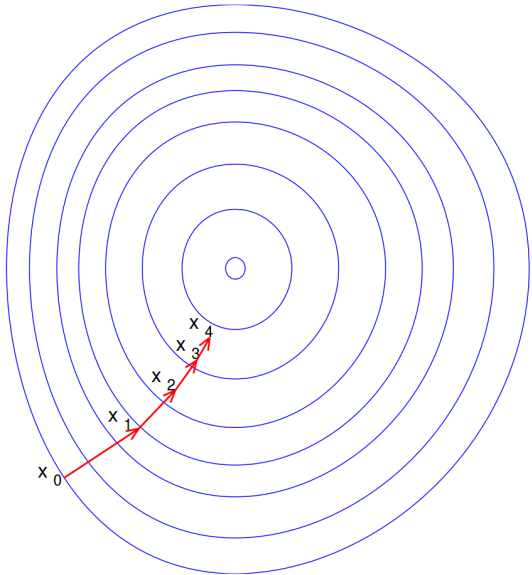
$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x_i) - y_i)^2$$

Gradient descent

$$\begin{cases} \theta_0 & \leftarrow \theta_0 - \alpha \dfrac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) \\ \theta_1 & \leftarrow \theta_1 - \alpha \dfrac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) \end{cases}$$

Gradient descent

$$\begin{cases} \theta_0 & \leftarrow \theta_0 - \dfrac{\alpha}{m} \displaystyle\sum_{i=1}^{m} (h_\theta(x_i) - y_i) \\ \theta_1 & \leftarrow \theta_1 - \dfrac{\alpha}{m} \displaystyle\sum_{i=1}^{m} (h_\theta(x_i) - y_i) \end{cases}$$



Hypothesis again

$$
\begin{aligned}
h_\theta(x) &= \theta_0 + \theta_1 x_1 \\
&= \theta_0 + \sum_{i=1}^{1} \theta_i x_i \\
&= [\theta_0, \theta_1] \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} \\
&= \theta^T x
\end{aligned}
$$

Hypothesis (multiple regression)

$$h_\theta(x) = \theta_0 + \sum_{i=1}^{n} \theta_i x_i$$

$$= [\theta_0, \cdots, \theta_n] \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$$= \theta^T x$$

Hypothesis (multiple regression)

$$h_\theta(x) = \theta^T x$$
$$= \theta^T x^{(1)}$$

Hypothesis (multiple regression)

$$X = \begin{bmatrix} | & | & \cdots & | \\ x^{(1)} & x^{(2)} & \cdots & x^{(m)} \\ | & | & \cdots & | \end{bmatrix} = \begin{bmatrix} x_0^{(1)} & x_0^{(2)} & \cdots & x_0^{(m)} \\ x_1^{(1)} & x_1^{(2)} & \cdots & x_1^{(m)} \\ \vdots & \vdots & \ddots & \vdots \\ x_n^{(1)} & x_n^{(2)} & \cdots & x_n^{(m)} \end{bmatrix}$$

Hypothesis (multiple regression)

$$
\begin{aligned}
h_\theta(X) &= \theta^T X \\
&= \left[h_0(x^{(1)}), h_0(x^{(2)}), \cdots, h_0(x^{(m)})\right] \\
&= \theta^T X
\end{aligned}
$$

Hypothesis (multiple regression)

or $X\theta$ if row vectors...

Cost function (multiple regression)

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2$$
$$= \frac{1}{2m} (X\theta - Y)^T (X\theta - Y)$$

Gradient descent (multiple regression)

$$\theta_j \leftarrow \theta_j - \frac{\alpha}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right) \cdot x_j^{(i)}$$

for $j = 1, \cdots, n$

Gradient descent (multiple regression)

$$\theta \leftarrow \theta - \nabla J(\theta)$$

$$\text{where } \nabla = \begin{bmatrix} \frac{\partial}{\partial \theta_0} \\ \frac{\partial}{\partial \theta_1} \\ \vdots \\ \frac{\partial}{\partial \theta_n} \end{bmatrix}$$

Linear regression

- Continuous output
- Normal residues
- Predict $\hat{y}$ for x given $\{(x_i, y_i)\}$

Logistic regression

- Binary output
- Classification

Logistic regression

- Have: continuous and discrete inputs
- Want: class (0 or 1)

Probabilistic inspiration

$h_\theta(x) = .75 \iff$ event has 75% of being true

Probabilistic inspiration

$$h_\theta(x) = \Pr(y = 1 \mid x; \theta) = 0.75$$

Probabilistic inspiration

So this must be true:

$$\Pr(y = 0 \mid x; \theta) + \Pr(y = 1 \mid x; \theta) = 1$$

Probabilistic inspiration

$$\text{Set } y = 1 \iff h_\theta(x) = \Pr(y = 1 \mid x; \theta) > \frac{1}{2}$$

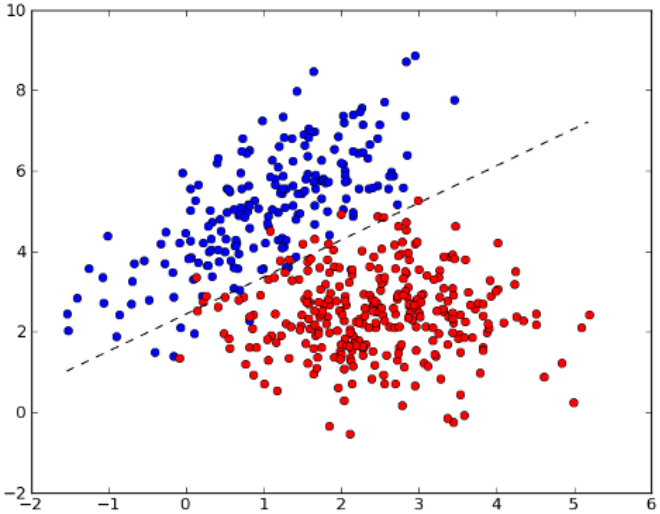
Probabilistic inspiration

Math review:

- $z = (\theta^T x)$
- $\theta^T x \geqslant 0 \iff h_\theta \geqslant 0.5$
- $\theta^T x \geqslant 0 \iff$ predict $y = 1$

Logistic Regression

Logistic Regression



Logistic (sigmoid, logit) function

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

Logistic (sigmoid, logit) function

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

Exercise: plot this

Cost function in logistic regression

In linear regression, we had

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

Cost function in logistic regression

In linear regression, we had

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

Cost function in logistic regression

In linear regression, we had

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} \text{Cost}(h_\theta(x), y)$$

Cost function in logistic regression

Here's a convex cost function:

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

Cost function in logistic regression

Here's a convex cost function:

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Exercise: Plot this (cost vs y).

Cost function in logistic regression

Here's a convex cost function:

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

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} \text{Cost}(h_\theta(x), y)$$

Cost function in logistic regression

Here's a convex cost function:

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

$$J(\theta) = y \cdot \log(h_\theta(x)) + (1 - y) \cdot \log(1 - h_\theta(x))$$

Gradient descent

$$\theta_j \leftarrow \theta_j - \frac{\alpha}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right) \cdot x_j^{(i)}$$

for $j = 1, \cdots, n$

null hypothesis

true positive, true negative

false positive, false negative

type I error
(incorrect rejection of null hypothesis)

type II error
(failure to reject null hypothesis)

sensitivity

100% sensitivity = no false negatives

specificity

100% specificity = no false positives

Precision

$$P = \frac{TP}{TP + FP}$$

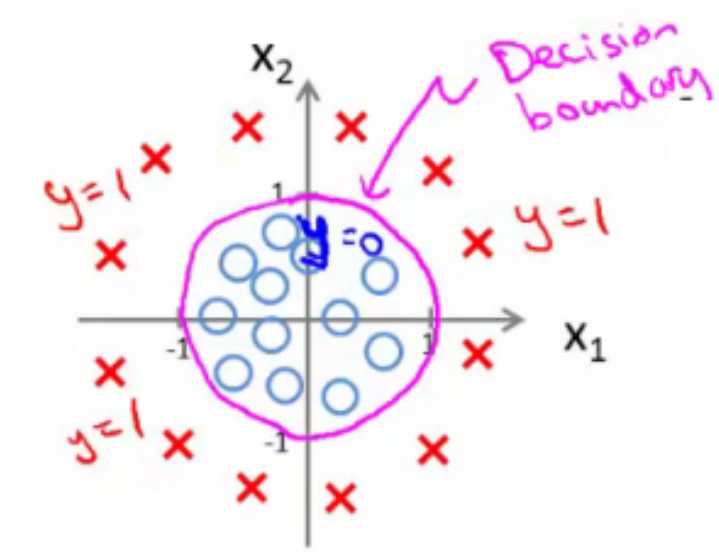
Recall

$$R = \frac{TP}{TP + FN}$$

F1 score

$$F1 = \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$

Non-linear decision boundaries



Non-linear decision boundaries

OvA = OvR

OvO

Non-linear decision boundaries

One vs All = One vs Rest

One vs One