Turing Machine and Deep Learning
Lecture 2: Supervised Machine Learning

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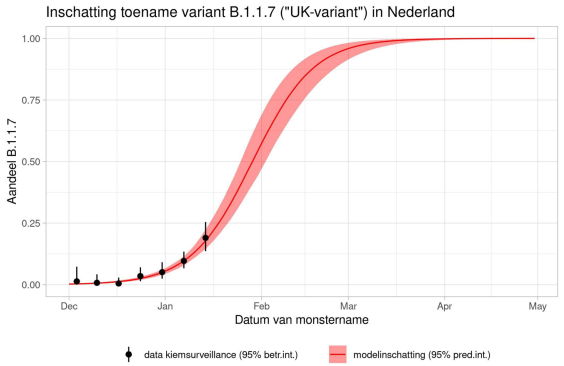
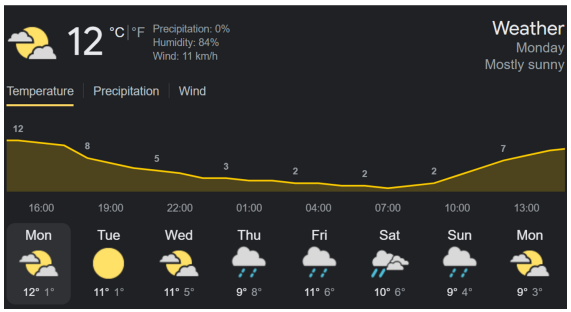
19th May 2023

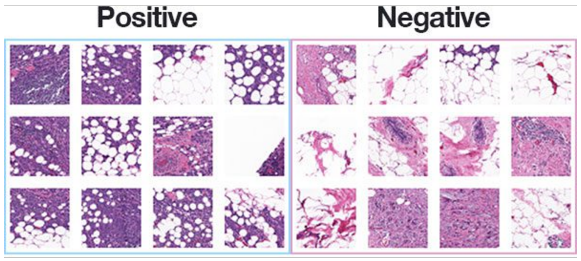
Types of Tasks

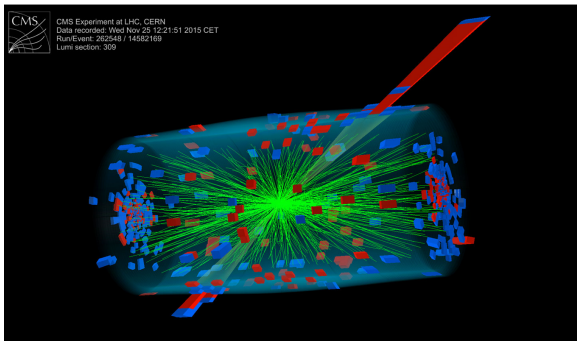
Regression





Classification





Logistic Regression

Regression $\rightarrow$ Classification

For a given 1D data point $i \in \{1, ..., N\}$, we have an estimated line:

$$\hat{y}^i = mx^i + c$$

Notation

Keep in mind here that for the next few slides, x^i means *the i^{th} data point, rather than x to the exponent i. This will be justified later.*

We can also write this as:

$$\hat{y}^i = w_0 + w_1 x^i$$

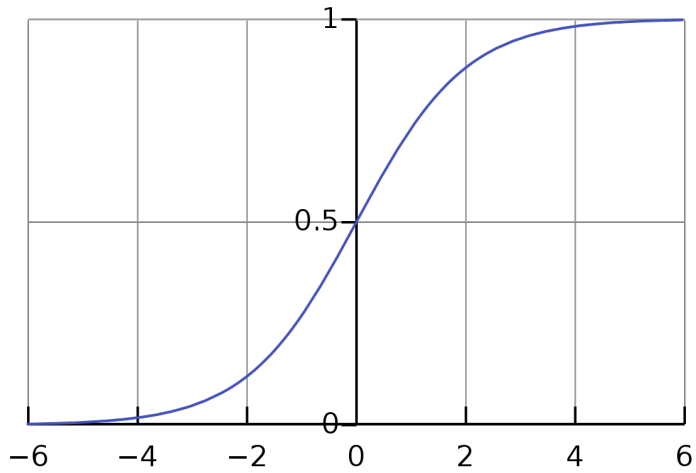
Regression $\rightarrow$ Classification

$$\hat{y}^i = \sigma(w_0 + w_1 x_1^i)$$

Regression $\rightarrow$ Classification

$$\hat{y}^i = \sigma(w_0 + w_1 x_1^i)$$

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

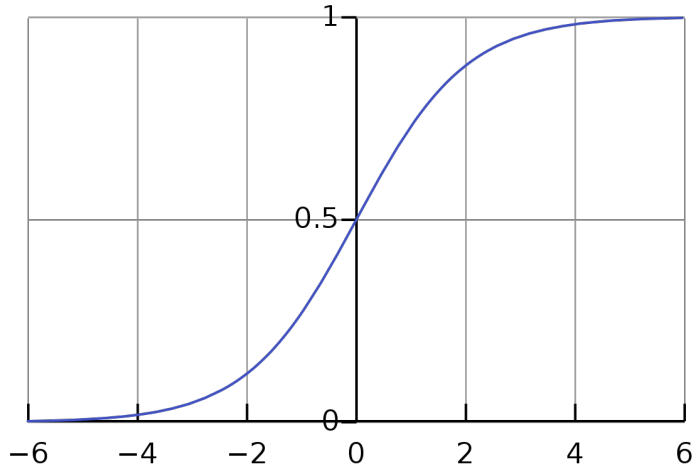


Regression $\rightarrow$ Classification

If we have k inputs,

$$\hat{y}^i = \sigma(w_0 + w_1 x_1^i + w_2 x_2^i + ... + w_k x_k^i)$$

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



Tangent: Vectorization

Machine learning is (currently) fastest when run on GPU and is vectorized, i.e. when the math is re-written as matrix/vector calculus.

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Rewritten as a vector dot product:

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Rewritten as a vector dot product:

$$\hat{y}^i = \sigma(\vec{w}^T \vec{x}^i)$$

Logistic Regression

$$\hat{y}^i = \sigma(\vec{w}^T \vec{x}^i)$$

Goal (Binary Logistic Regression)

Estimate a probability over labels parameterised by a weight vector.

To classify binary class labels, set a threshold to predict (commonly 0.5):

$$\hat{p}^i = P[y^i = 1] = \frac{1}{1 + e^{\vec{w}^T \vec{x}^i}} \in [0, 1]$$

$$\hat{y}^i = \begin{cases} 1 & \hat{p}^i \geq 0.5; \\ 0 & \hat{p}^i < 0.5. \end{cases}$$

Logistic Regression: Building blocks

Hypothesis space $\mathcal{H}$:

Logistic Regression: Building blocks

Hypothesis space $\mathcal{H}$: All functions of the form:

$$h(\vec{x}) = \sigma(\vec{w}^T \vec{x})$$

where $\vec{w}$ are weights and $\vec{x}$ are features of a data point.

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Loss function: Standard in binary classification tasks to use *binary cross-entropy* (derivable from σ):

$$\mathrm{BCE}(y, \hat{y}) = -y \log(\hat{y}) - (1 - y) \log(1 - \hat{y})$$

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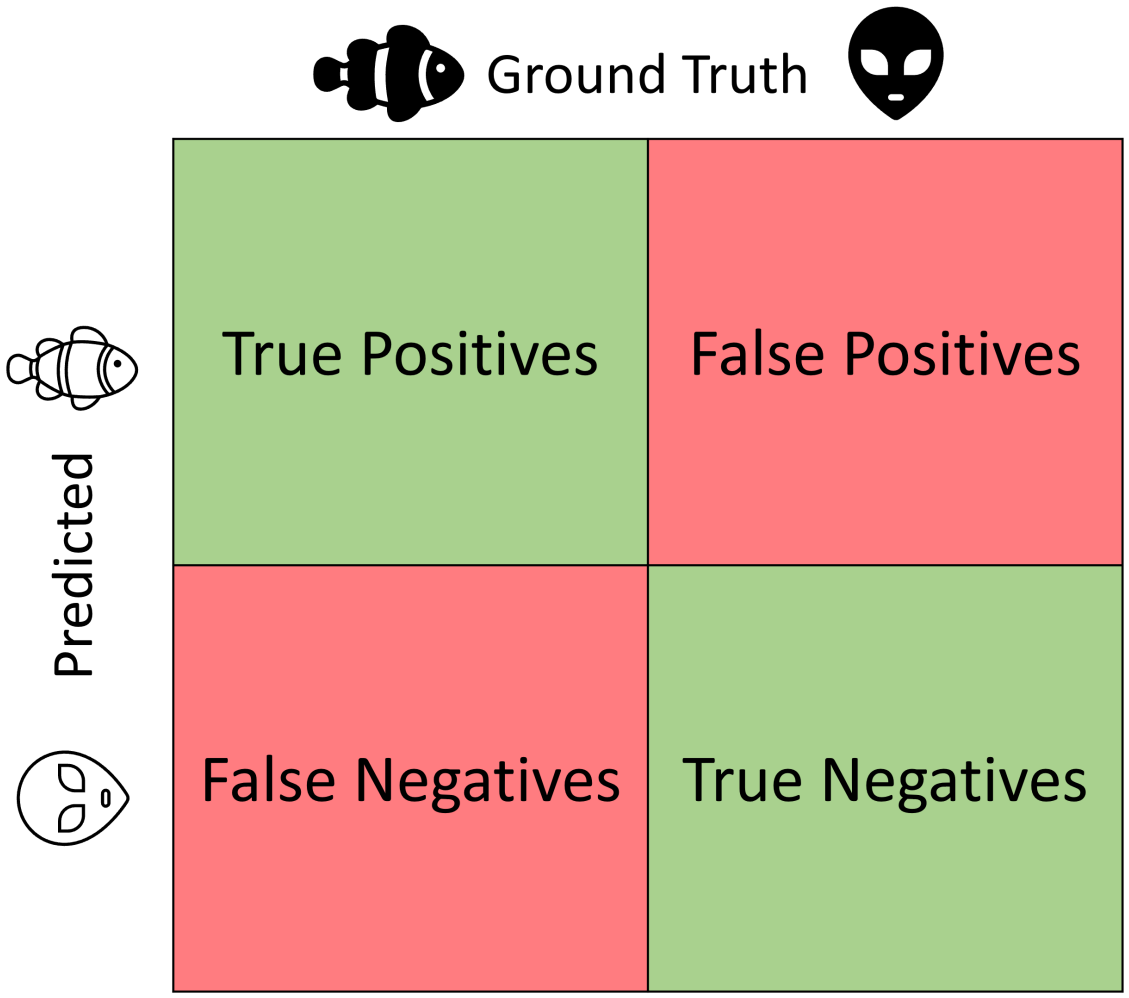
Thus, we must find h_{opt} that minimises our **empirical risk**:

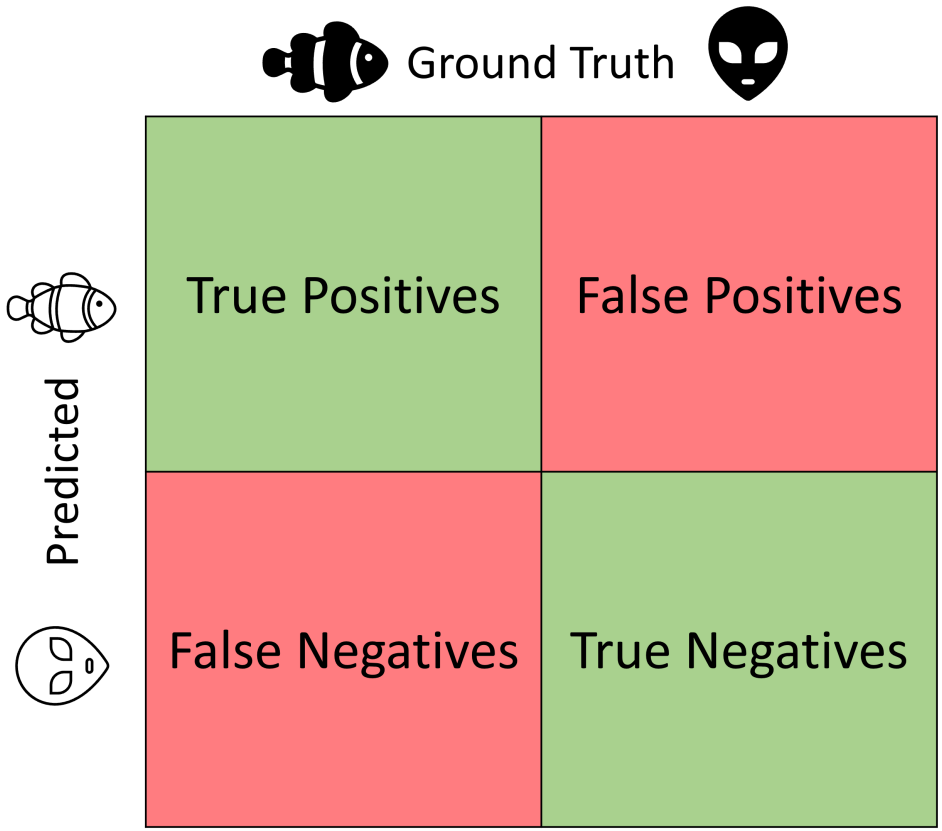
$$\hat{f} = h_{opt} = \arg\min_{h \in \mathcal{H}} \frac{1}{N} \sum_{i=1}^{N} \mathrm{BCE}(y^i, h(\vec{x}^i))$$

Classification Metrics *(a selection)*

Confusion Matrix

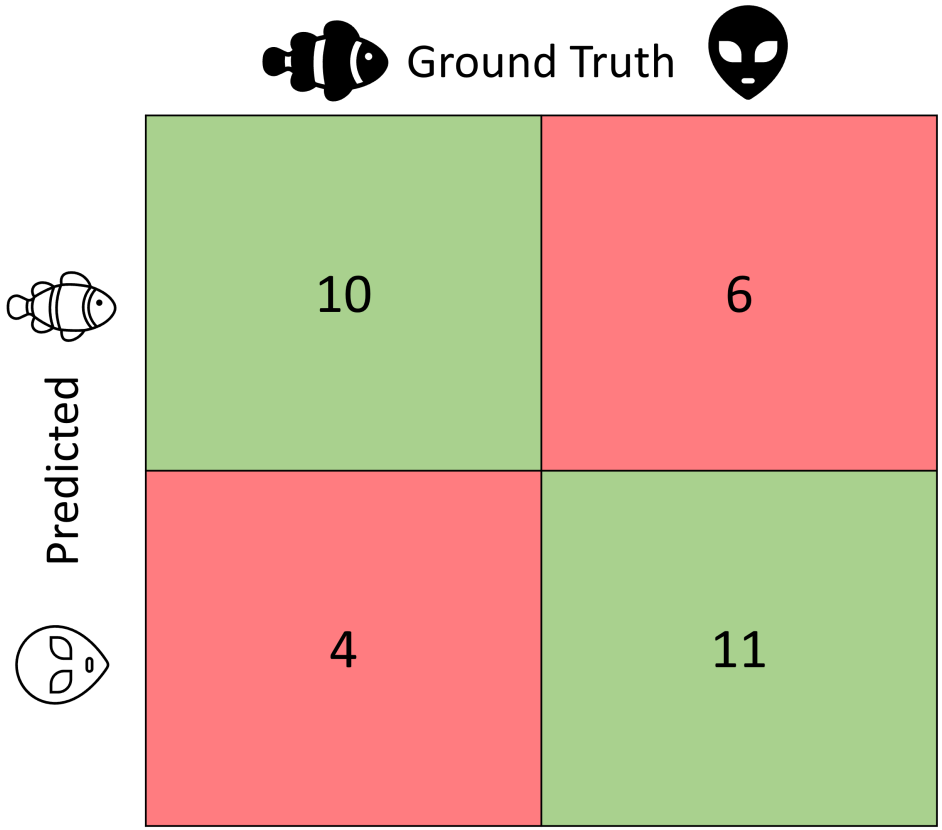


Accuracy



$$\text{Accuracy} = \frac{\text{TP}+\text{TN}}{\text{TP}+\text{TN}+\text{FP}+\text{FN}}$$

Accuracy



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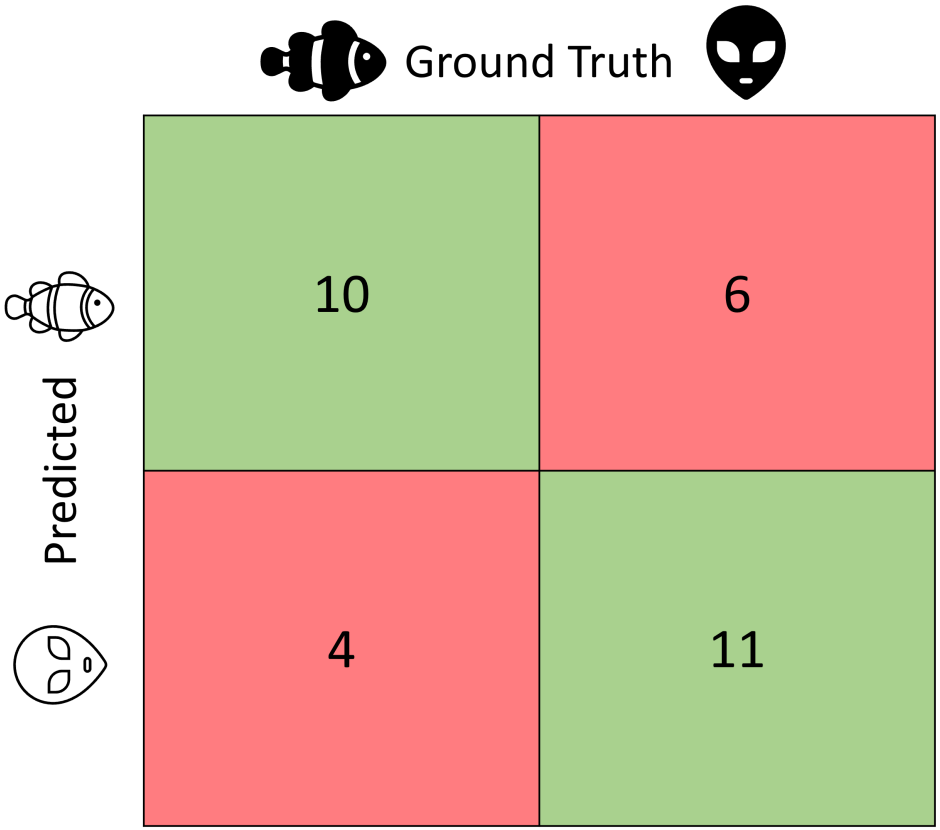
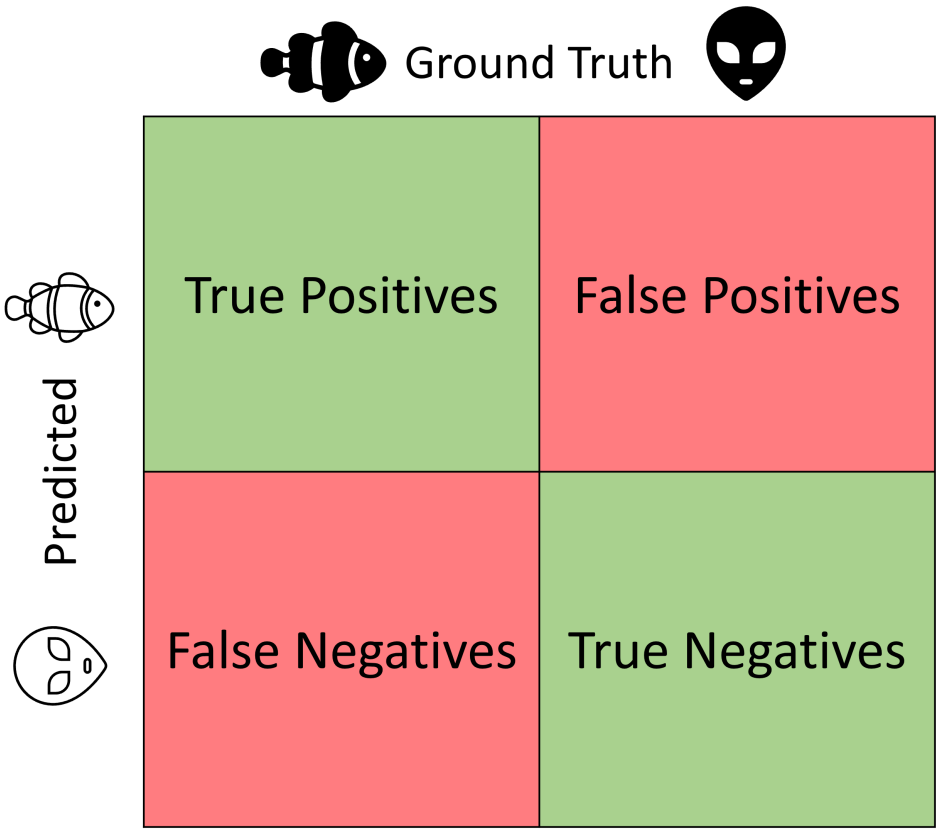


$$\text{Accuracy} = \frac{\text{TP}+\text{TN}}{\text{TP}+\text{TN}+\text{FP}+\text{FN}}$$
$$= \frac{10+11}{10+11+6+4}$$
$$= 0.677...$$

Precision



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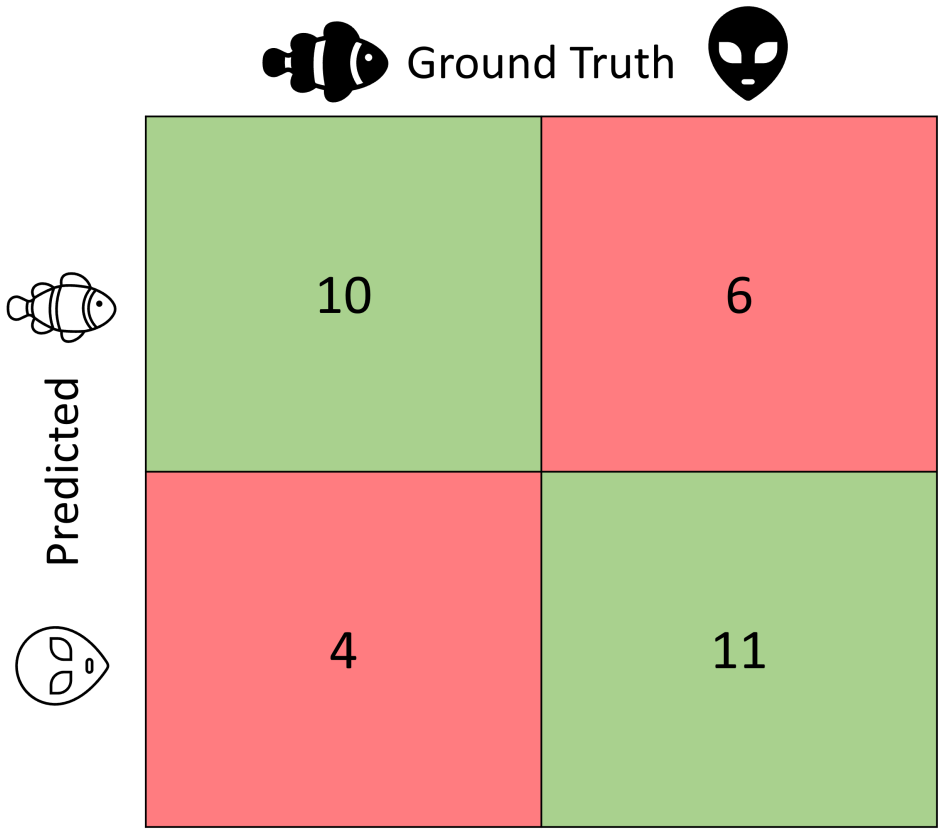
Precision



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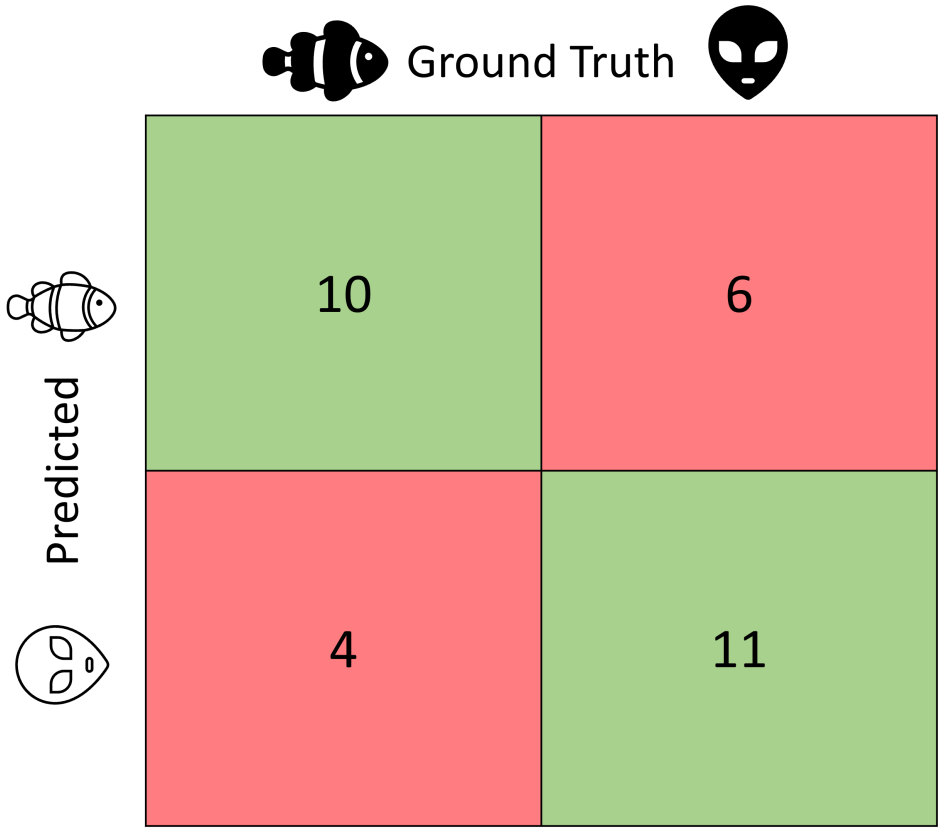
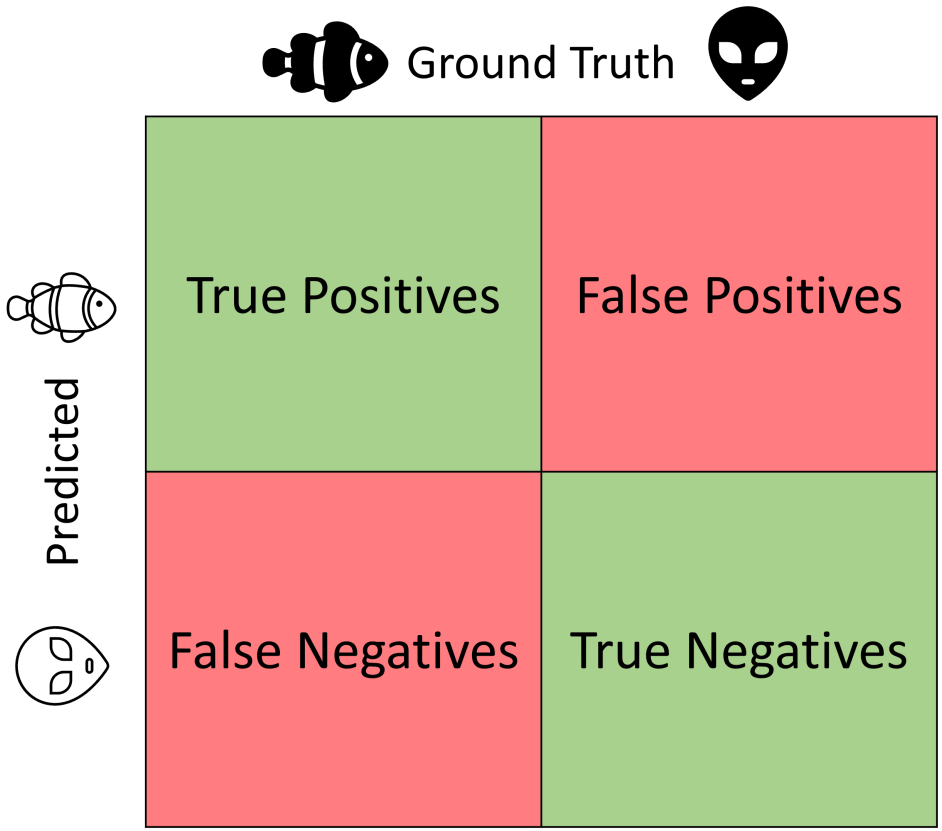
Precision



$$\text{Precision} = \frac{\text{TP}}{\text{TP}+\text{FP}} = \frac{10}{10+6} = 0.625$$

Recall



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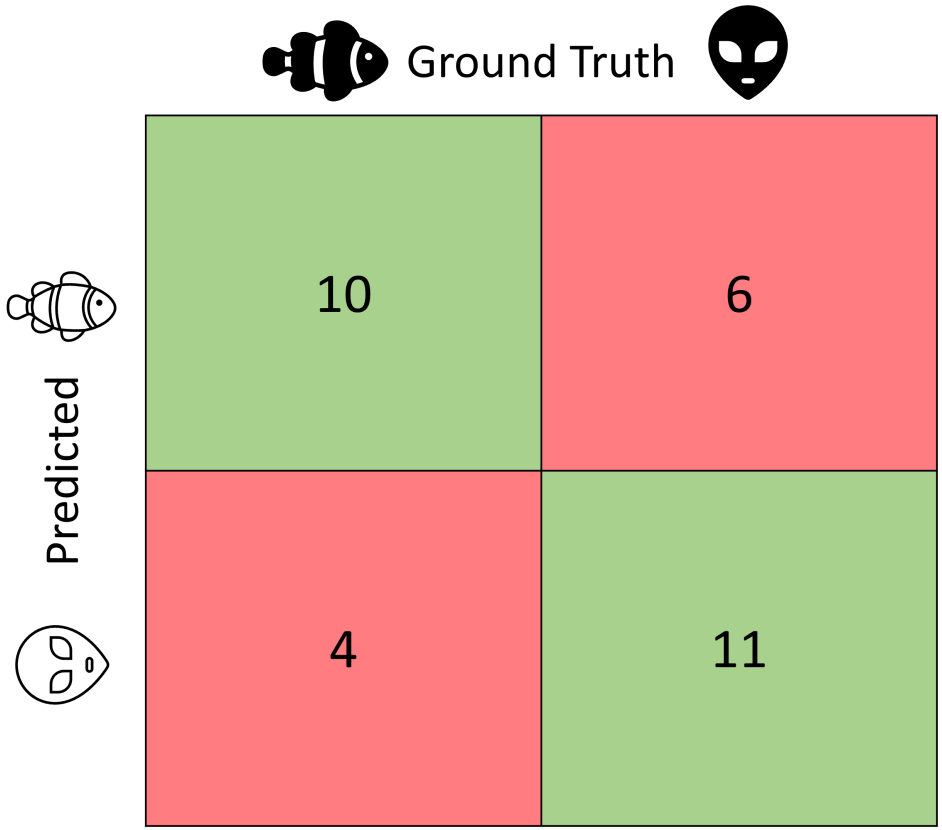
Recall



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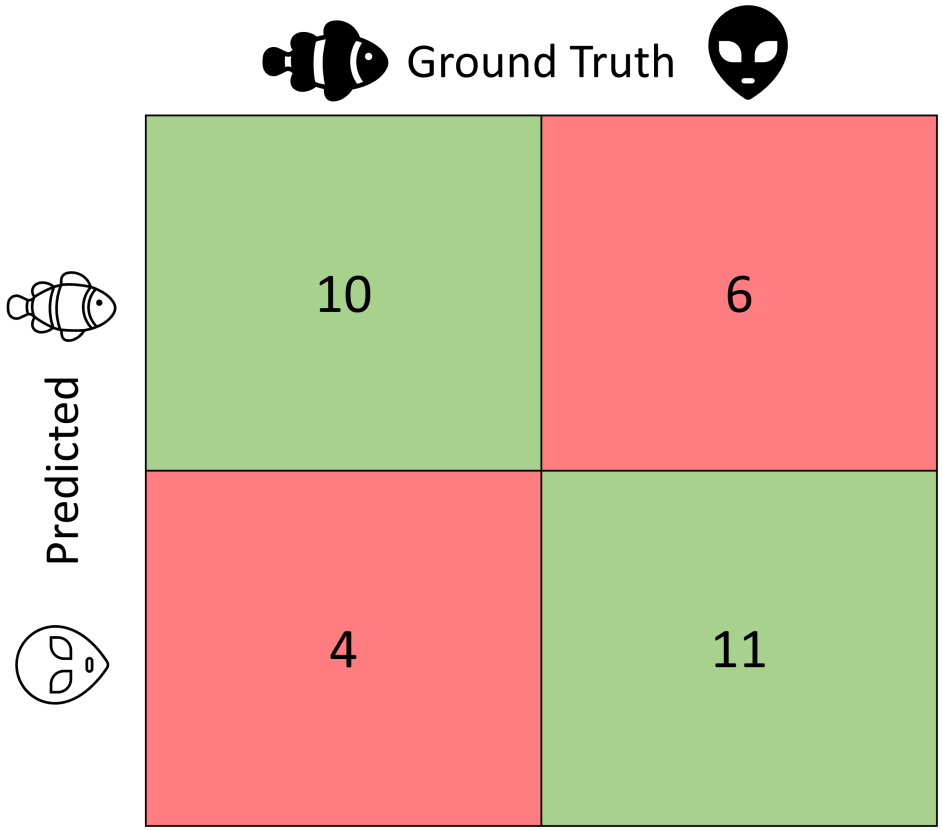
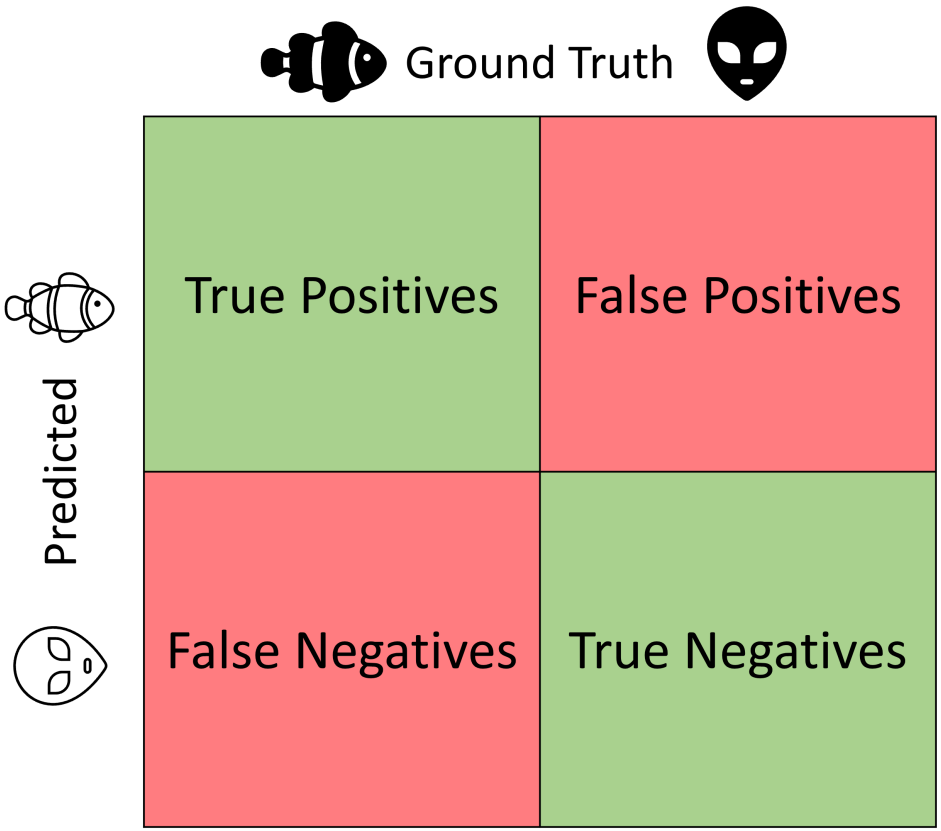
Recall



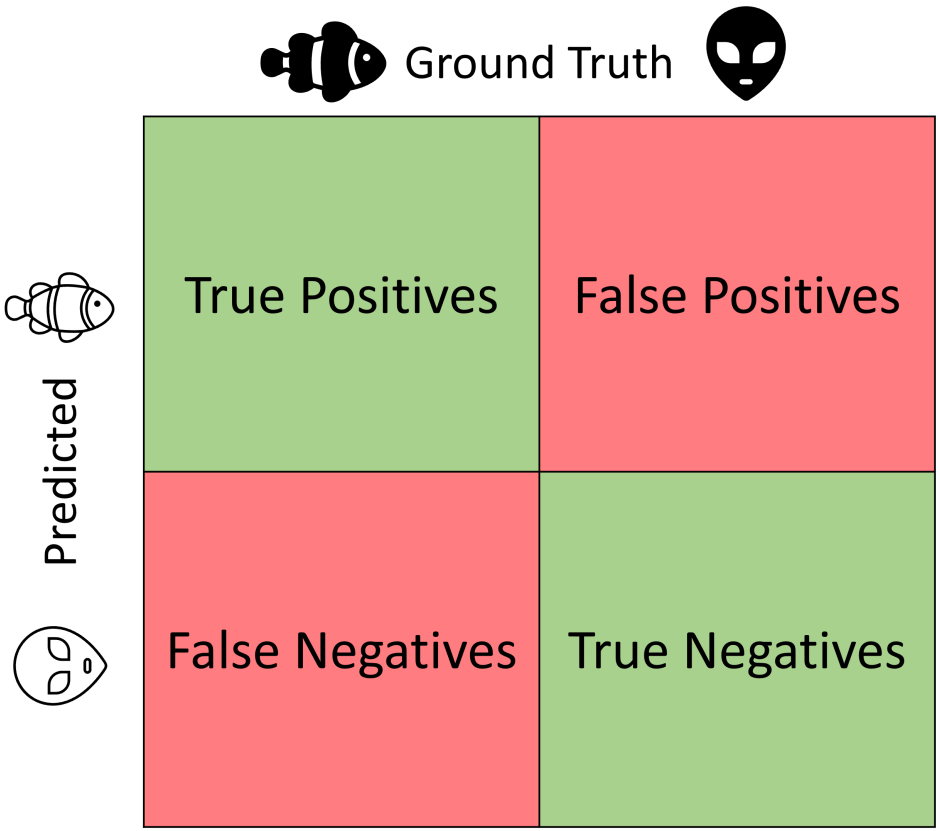
$$\text{Recall} = \frac{\text{TP}}{\text{TP}+\text{FN}}$$
$$= \frac{10}{10+4}$$
$$= 0.714...$$

F_β score



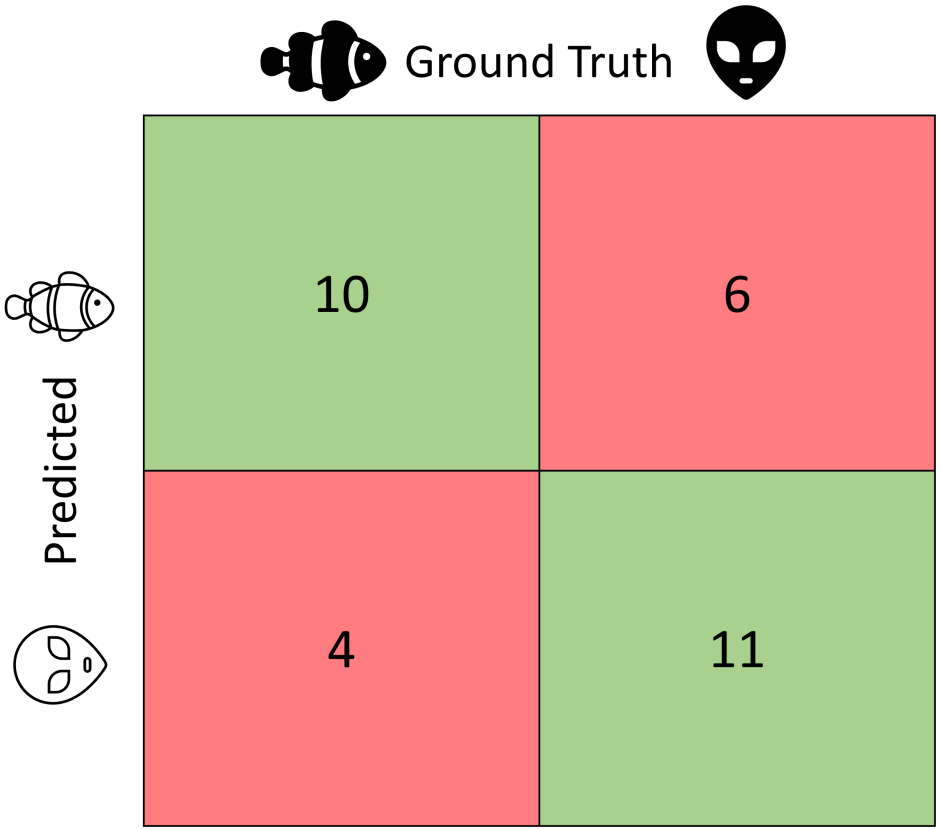
$$F_\beta = (1 + \beta^2) \cdot \frac{\text{precision} \cdot \text{recall}}{\beta^2 \cdot \text{precision} + \text{recall}}$$

F_1 score



$$F_1 = 2\frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$

F_1 score



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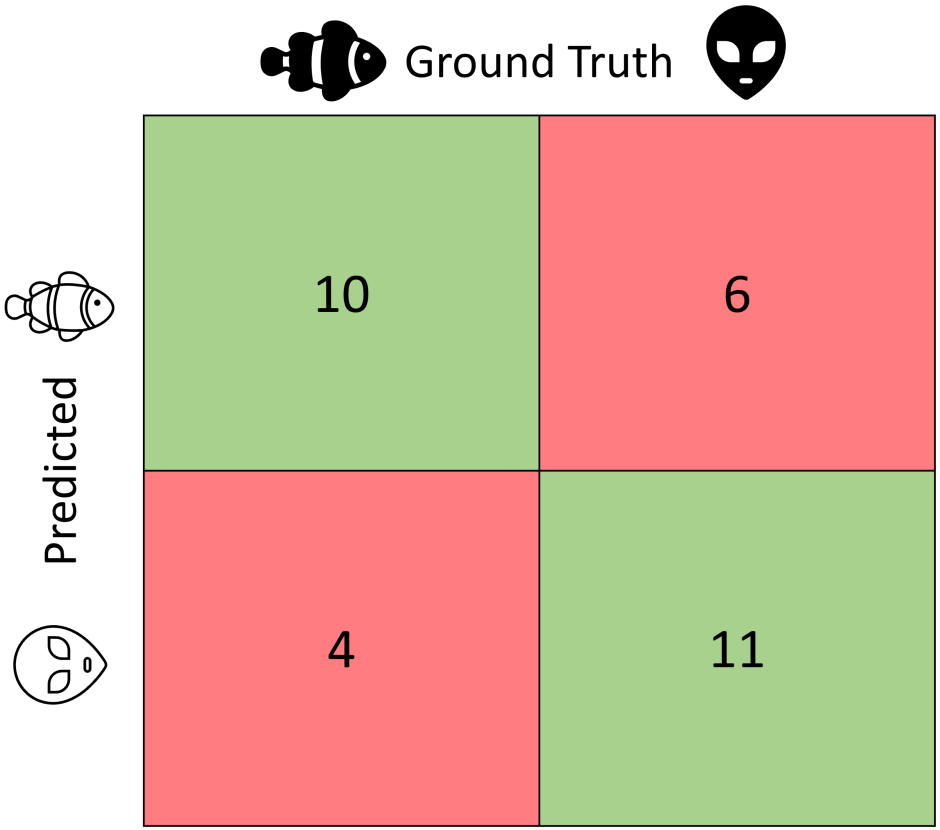


$$F_1 = 2\frac{0.625 \cdot 0.714}{0.625 + 0.714}$$
$$= 0.666...$$

Collected Measures

$$\text{Accuracy} = \frac{\text{TP}+\text{TN}}{\text{TP}+\text{TN}+\text{FP}+\text{FN}}$$

$$\text{Precision} = \frac{\text{TP}}{\text{TP}+\text{FP}}$$

$$\text{Recall} = \frac{\text{TP}}{\text{TP}+\text{FN}}$$

$$\text{F}_1 = 2\frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$

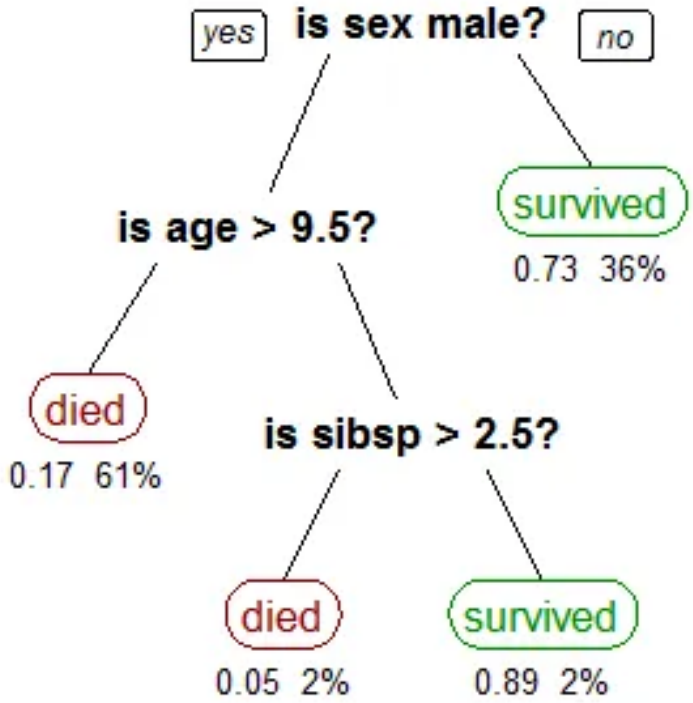
$$\text{F}_\beta = (1 + \beta^2) \cdot \frac{\text{precision} \cdot \text{recall}}{\beta^2 \cdot \text{precision} + \text{recall}}$$

Notebook time!

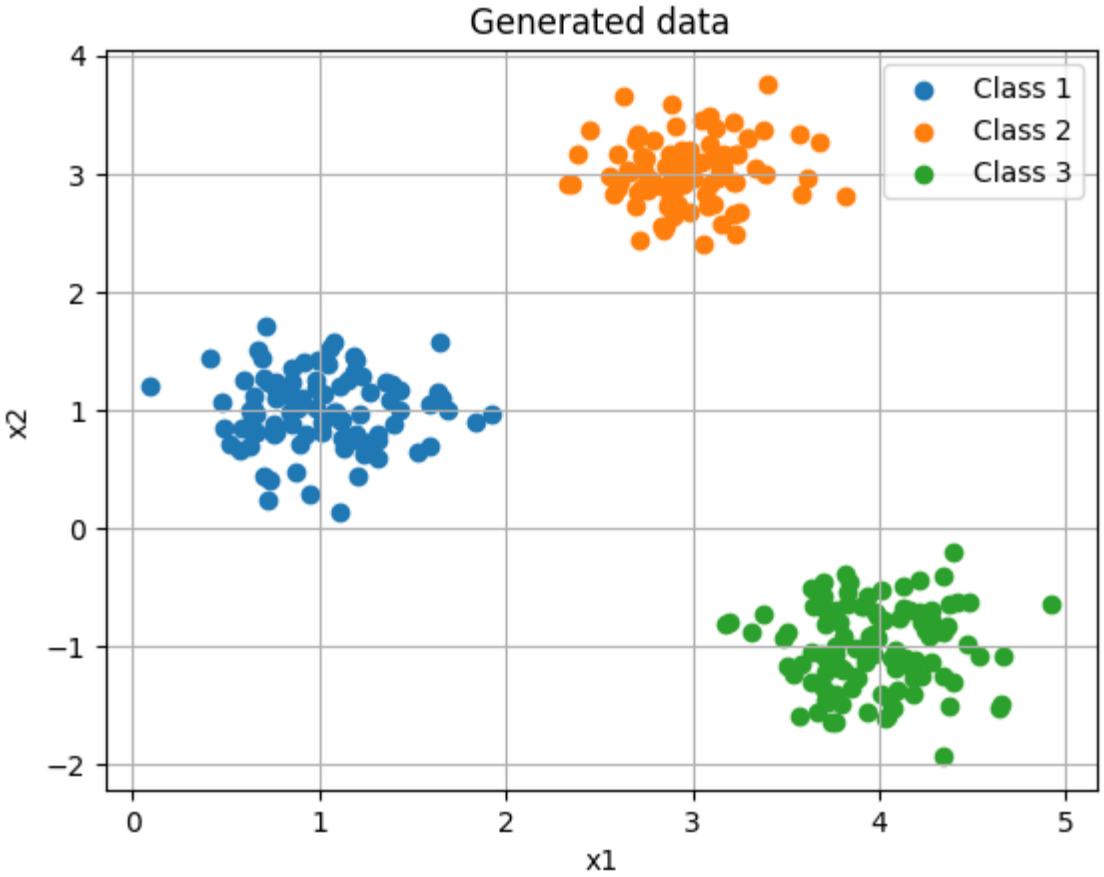
Decision Trees

Decision Trees

- Partition feature space into regions and assign labels/values to those regions.
- Each internal node represents a test on a feature, leading to different branches based on the outcome of the test.
- The leaves of the tree represent the final predicted labels or values.
- Visually appealing and (sort of) interpretable!
- Loss function for each node: *Gini index*.



Decision Trees: Example



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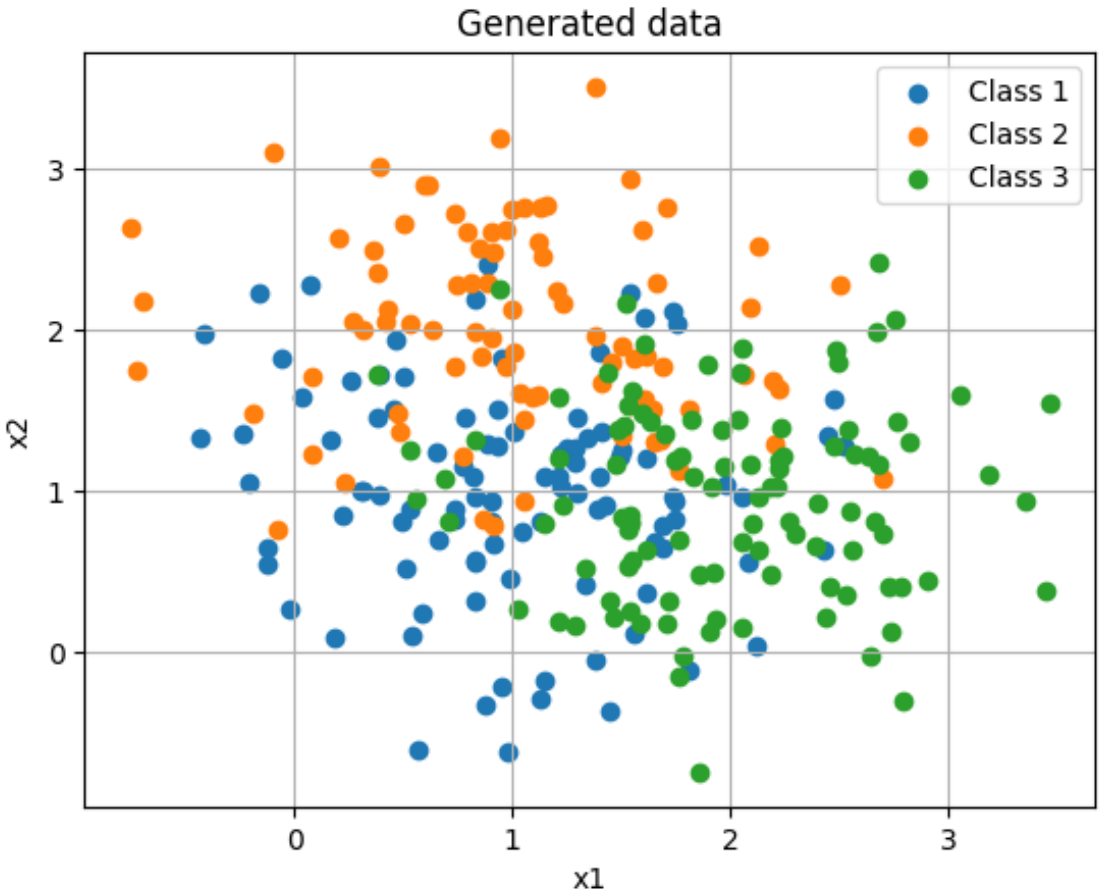
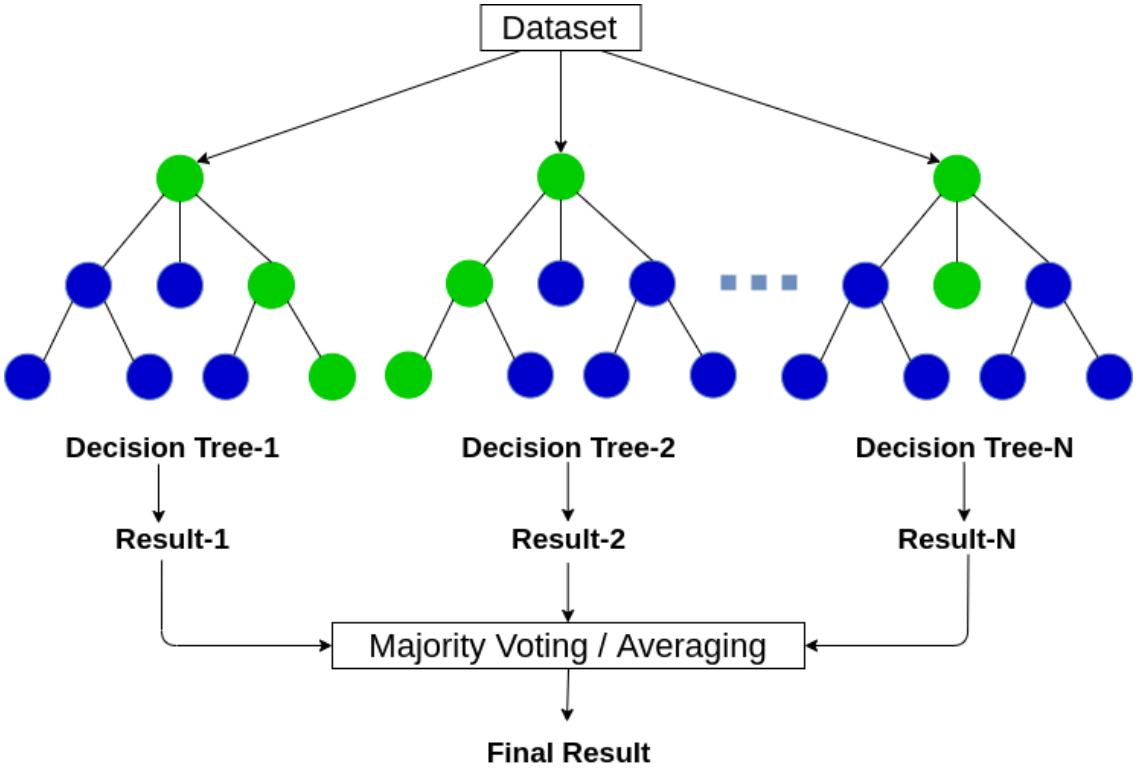


Random Forests

Random Forests

Random forest is an **ensemble learning** method that combines multiple decision trees to make predictions.



Ensemble Learning

An ML method which combines the predictions of multiple models to improve overall performance.

Random Forest: Training Process

1. Data Preparation
2. Random Sampling (Bootstrapping)
3. Decision Tree Construction + Random Feature Selection
4. Voting and Aggregation
5. Evaluation

We get better/more generalizable results (harder to overfit) *but*, we lose out on interpretability.

Support Vector Machines

SVMs: Math

SVMs: Math

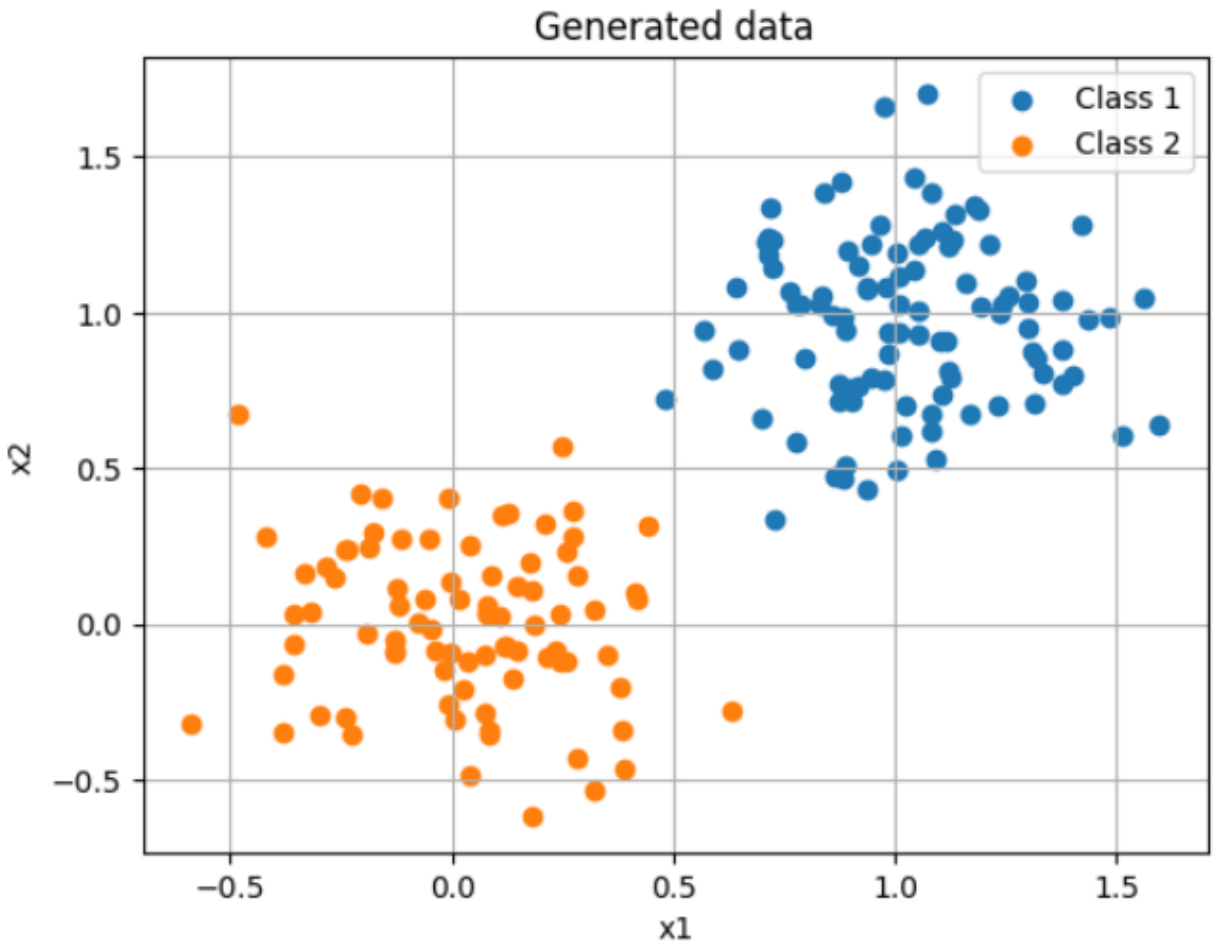
No

SVMs: Math

No

But if you're interested, look at UvA's ML1 Lecture 11: `https://youtu.be/QTzo2whcG2g`.

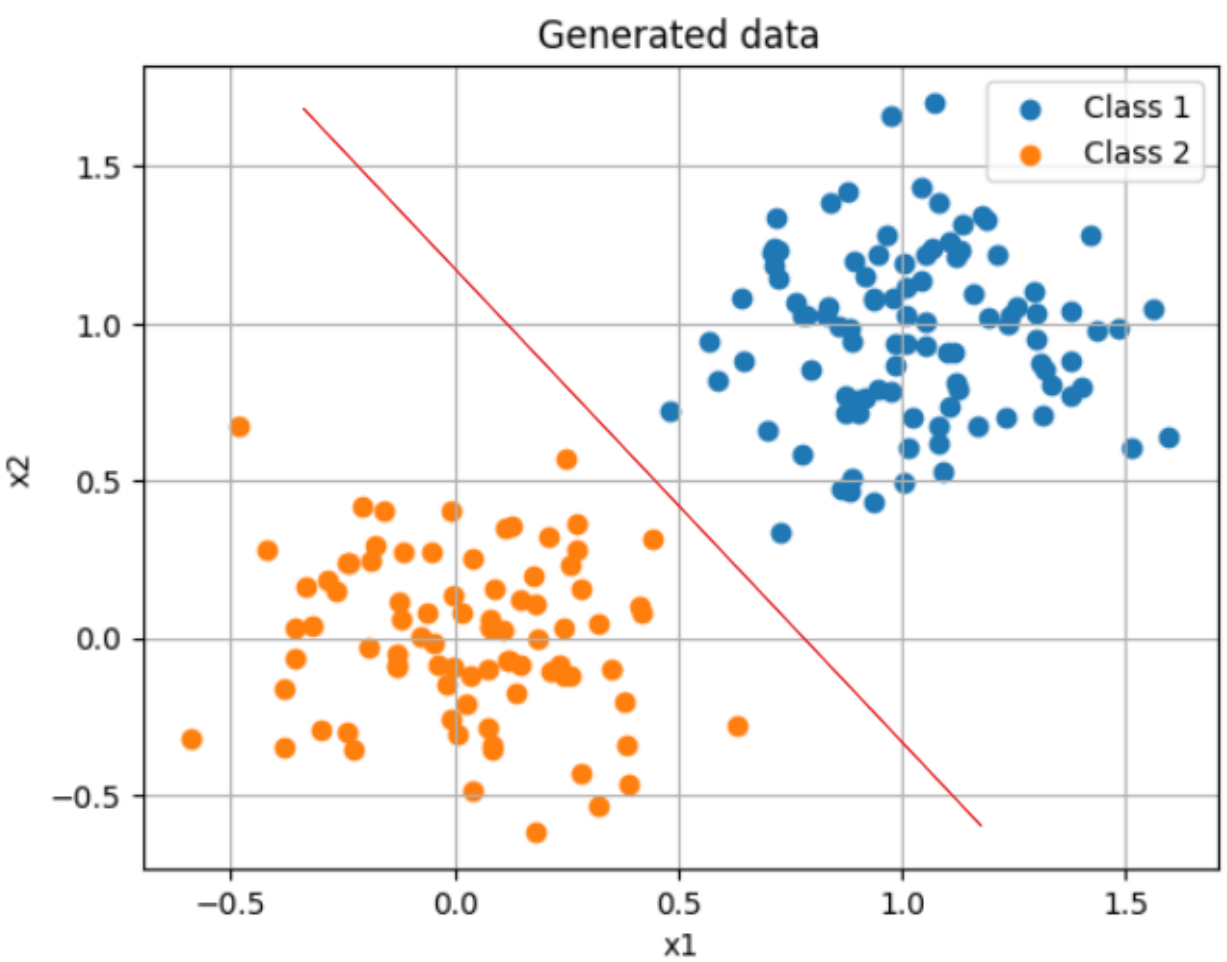
SVMs: *Intuition*



Goal

Find a *decision boundary* that maximally separates the two classes.

SVMs: *Intuition*



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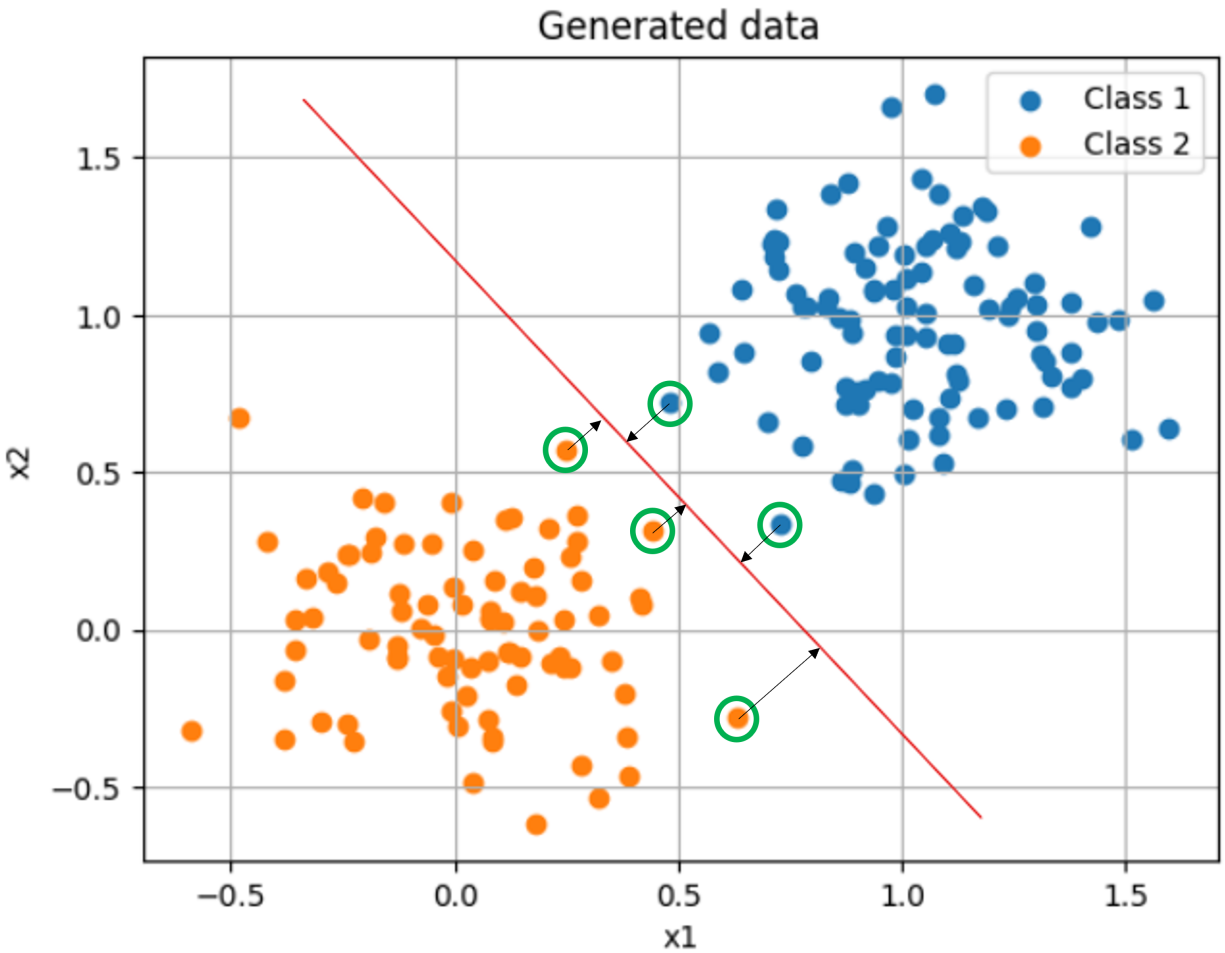

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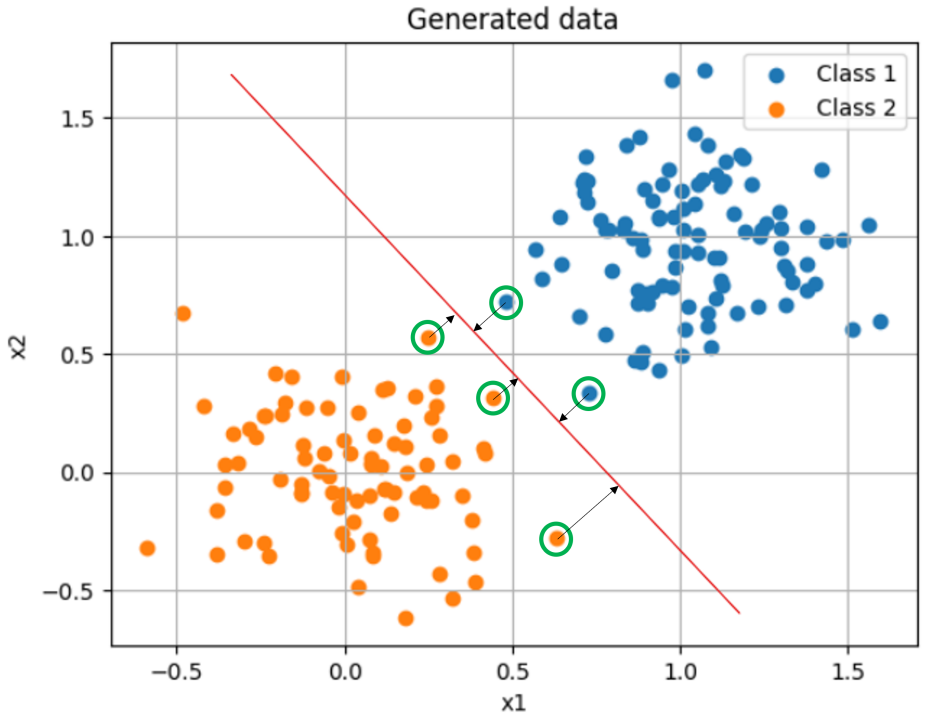
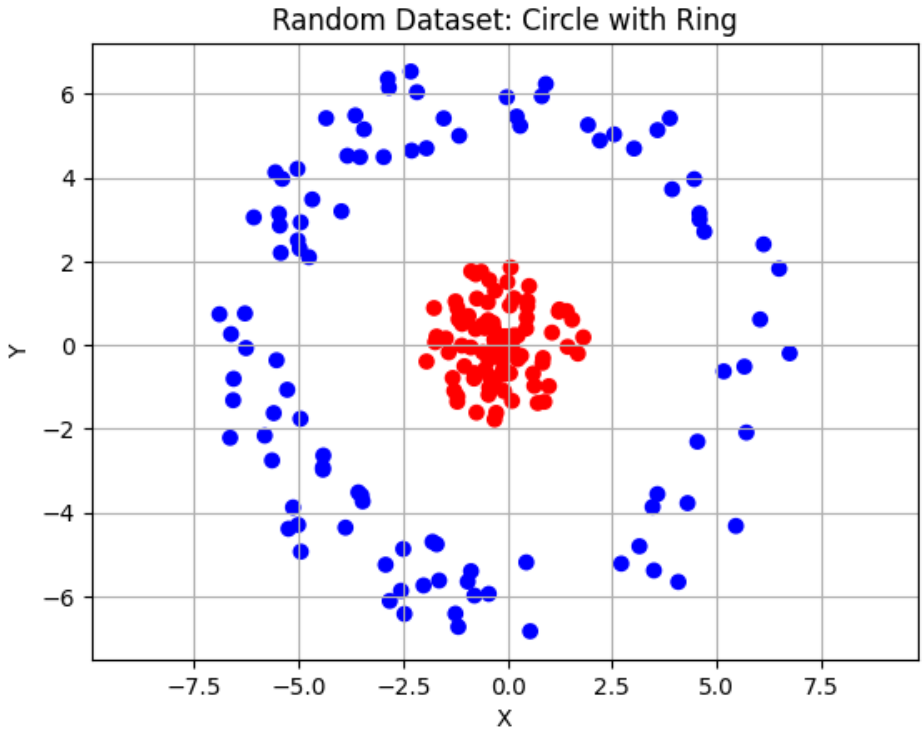


Goal

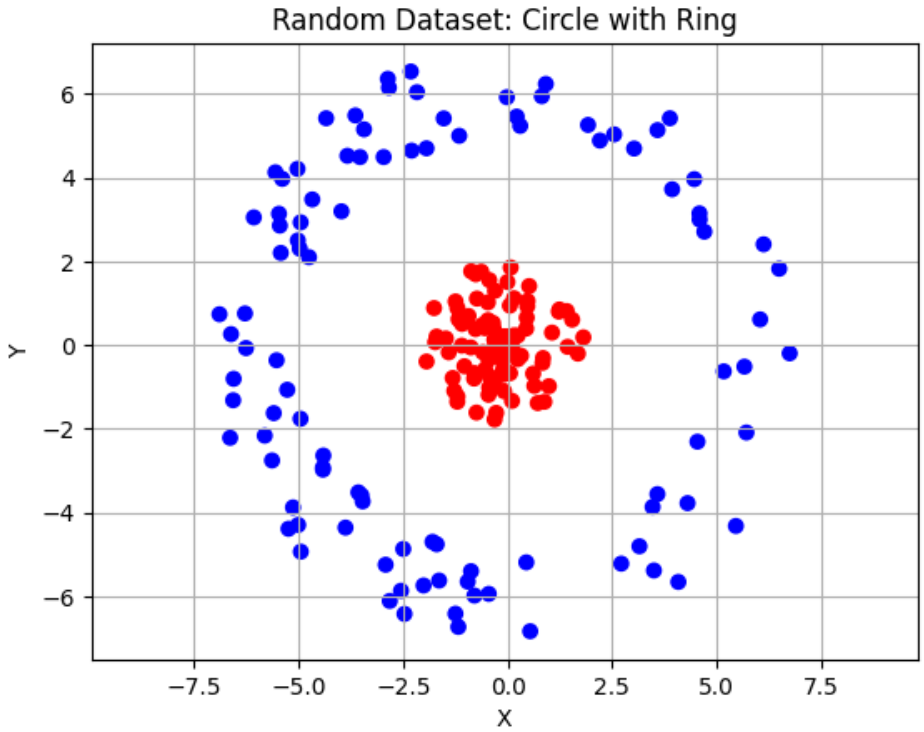
Find a *decision boundary* that maximally separates the two classes.

What about data sets that are non-linearly separable?

SVMs: Intuition II – *The Kernel Trick*

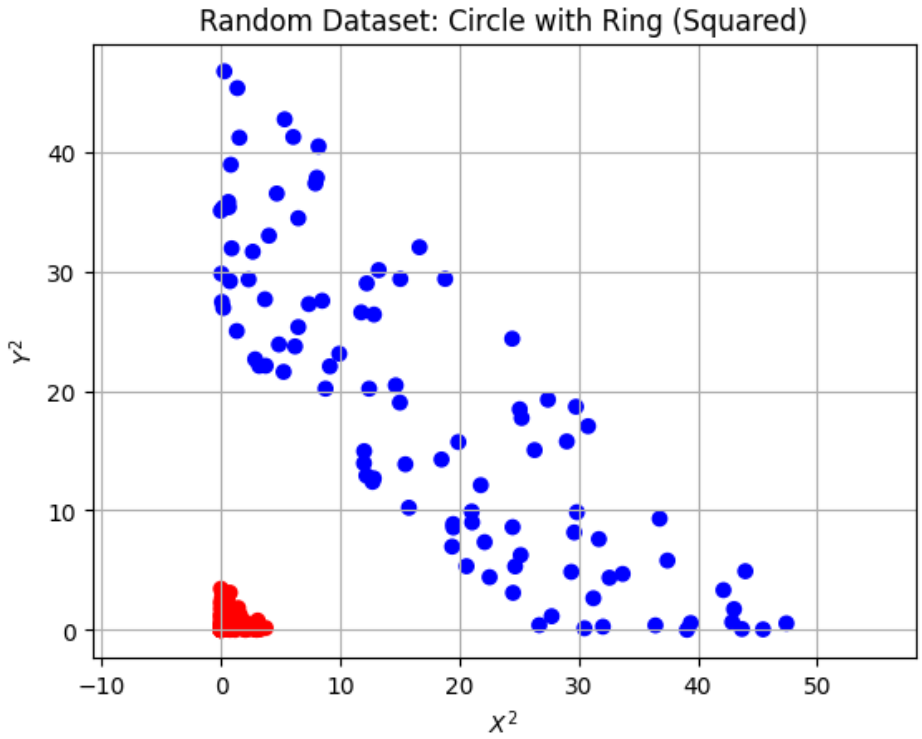


SVMs: Intuition II – *The Kernel Trick*

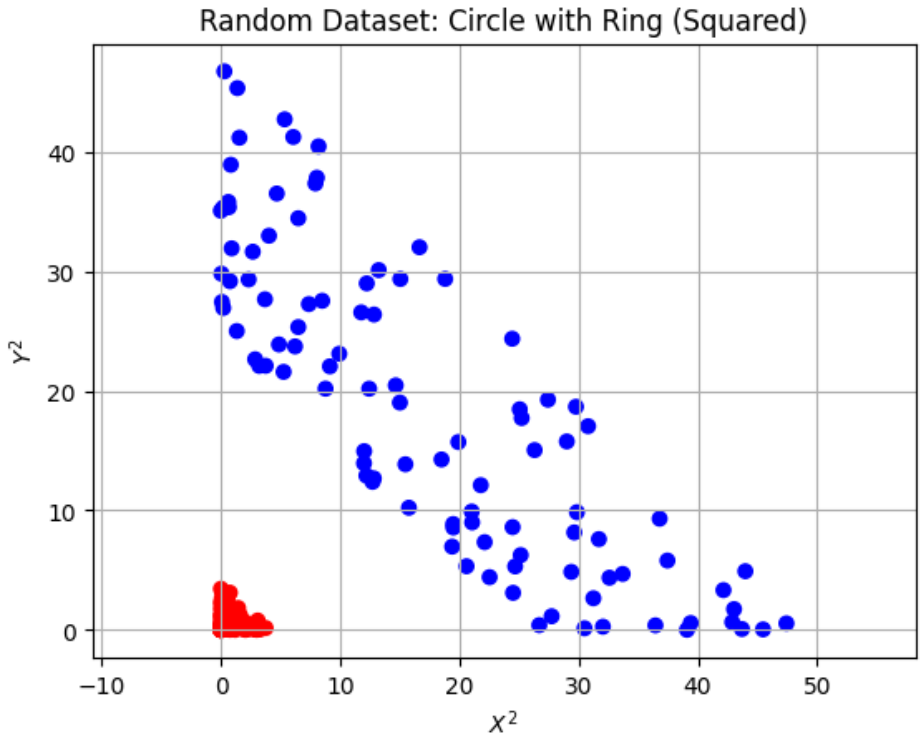


What if we could modify the data to be linearly separable?

SVMs: Intuition II – *The Kernel Trick*



SVMs: Intuition II – *The Kernel Trick*



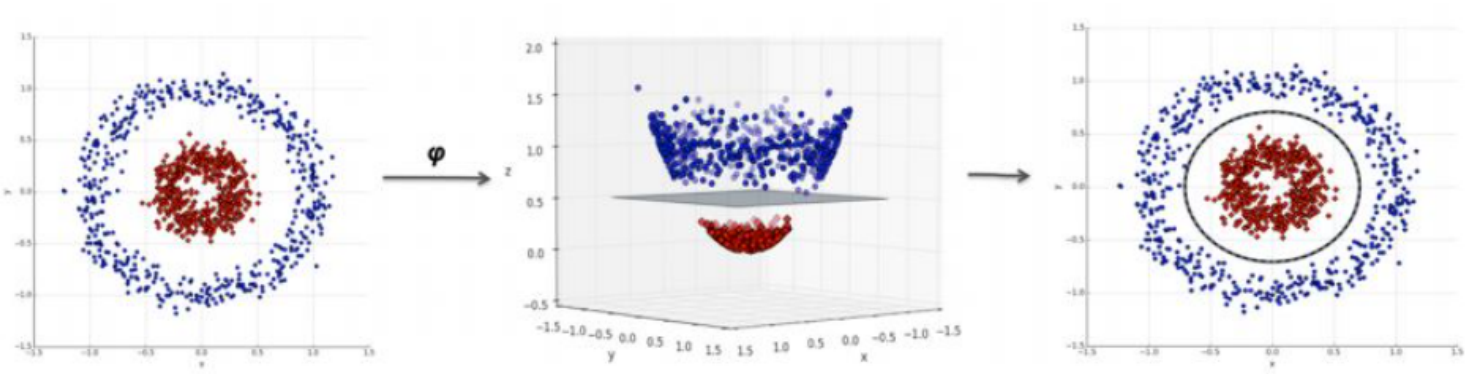
Problems

- Computationally intensive
- Hard to find a good "basis function"

SVMs: Intuition II – *The Kernel Trick*

Solution: The Kernel Trick

Learn a 'kernel' $K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j)$, representing *some* similarity measure in a higher-dimensional space between data points x_i and x_j without transforming the data itself.



Use this to learn a (hyper-)plane decision boundary.

$\Rightarrow$ SVMs are *non-parametric*.

SVMs: Types of Kernels

- Linear:
$$K(x_i, x_j) = x_i^T x_j$$
- Polynomial:
$$K(x_i, x_j) = (1 + x_i^T x_j)^d$$
- Radial Basis:
$$K(x_i, x_j) = e^{-\gamma ||x_i^T x_j||^2}, \text{ where } \gamma > 0$$

Careful!

- Different kernels have different hyperparameters.
- May not scale with data ($\approx \mathcal{O}(n^2)$ to $\approx \mathcal{O}(n^3)$ with n data points.)
- As always, beware of overfitting!

Image credits

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1. https://medium.com/analytics-vidhya/house-price-prediction-using-linear-regression-from-scratch-b2b48fd73689
2. https://weather.com
3. https://www.rivm.nl/en/coronavirus-covid-19/modelling
4. https://gsurma.medium.com/image-classifier-cats-vs-dogs-with-convolutional-neural-networks-cnns-and-google-colabs-4e9af21ae7a8
5. https://pyimagesearch.com/2019/02/18/breast-cancer-classification-with-keras-and-deep-learning/
6. https://home.cern/news/news/accelerators/lhc-collides-ions-new-record-energy

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- https://www.analyticsvidhya.com/blog/2020/05/decision-tree-vs-random-forest-algorithm/