

EI5IS102 Traitement de l'Information

Lecture 3:

Introduction to Machine Learning

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Machine Learning is everywhere



NETFLIX

Series Recommenders



Music recommenders



Chatbots



Face recognition



Voice assistants



Drug discovery



AlphaGo

Games



Self-driving cars

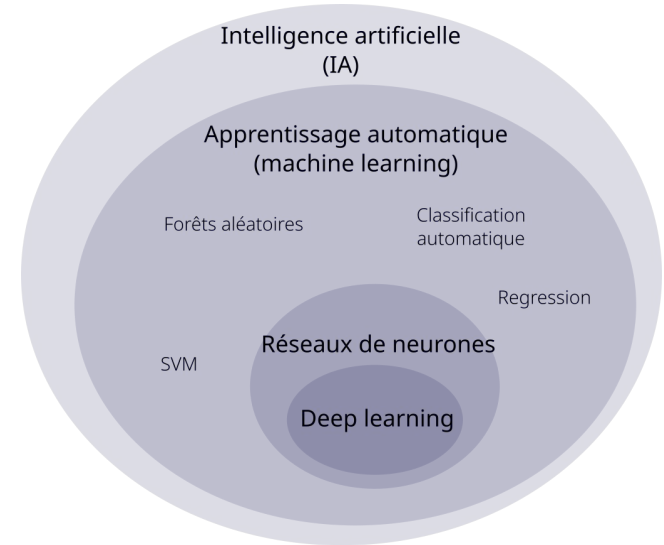


Image generators

Artificial Intelligence

Artificial intelligence?

- What is **intelligence**?
- Must have something to do with **thinking**
- What are the mechanisms of thinking?
- How to construct a model of thinking?



Wiki

Thinking

William Blake (English poet, 1757–1827) about thinking:

*“Man can only desire what he has **already perceived**”*

Noam Chomsky (American linguist, 1928–) about intelligence:

*“**Take two concepts and create a third one** without impairing the two firsts”*

Key concepts:

- Creation ex-nihilo cannot really exist
- Intelligence: the ability to assemble two ideas that seemed heterogeneous
- Thinking: finding similarity, discriminating and recognizing patterns

Learning

Past view of AI:

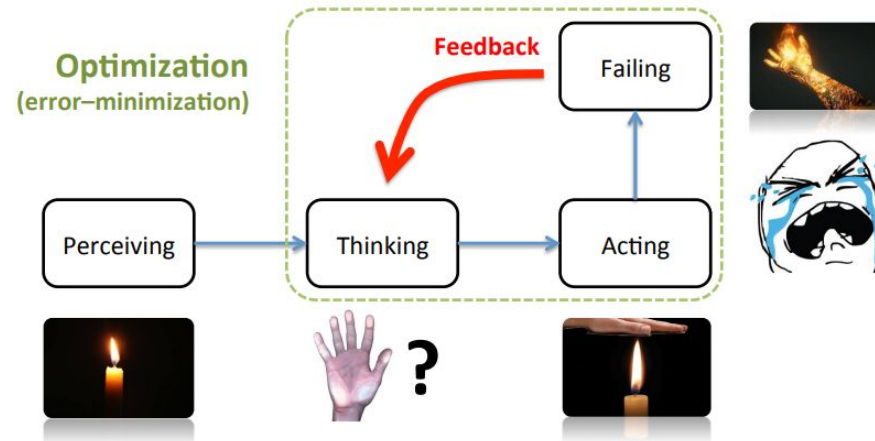
- AI was thought only about **reasoning**
- Programs with predefined rules
- Simulate intelligent decision-making

Current view of AI:

- AI is more about **learning**
- Systems that can improve through experience

Herbert Simon (American psychologist, 1916–2001) about learning:

*“Learning is any process by which a system **improves performance from experience**”*



Machine Learning



Machine Learning algorithms:

- Programs that can learn from experience to deduce new facts

Early definition of machine learning by **Arthur Samuel** (American pioneer in AI, 1901–1990):

*“Field of study that gives computer the ability **to learn without being explicitly programmed**”*

A.Samuel wrote the first self-learning program for checkers.

- Learning to improve its performance by playing against itself
- Invented alpha-beta pruning (decision tree searching)

Machine Learning



How can we have the computer learn without being explicitly programmed?

Traditional Programming

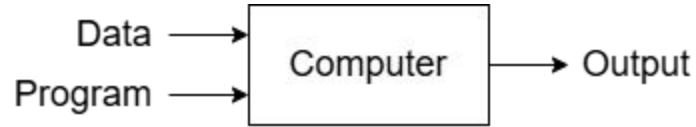


Machine Learning

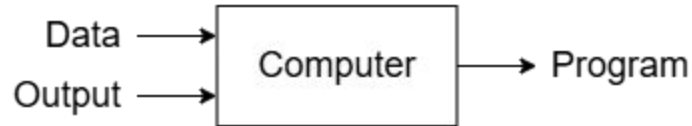


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Traditional Programming



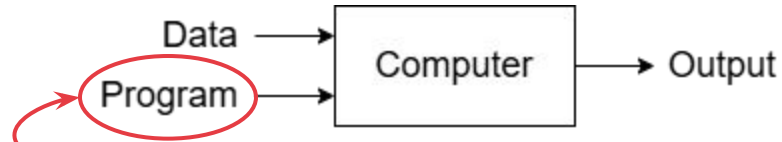
Machine Learning



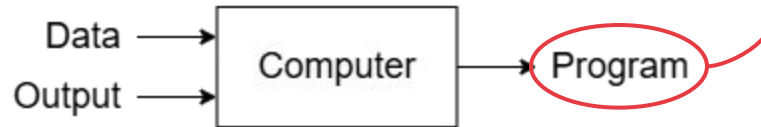
Machine Learning

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Traditional Programming



Machine Learning



Machine Learning

How to learn from data?

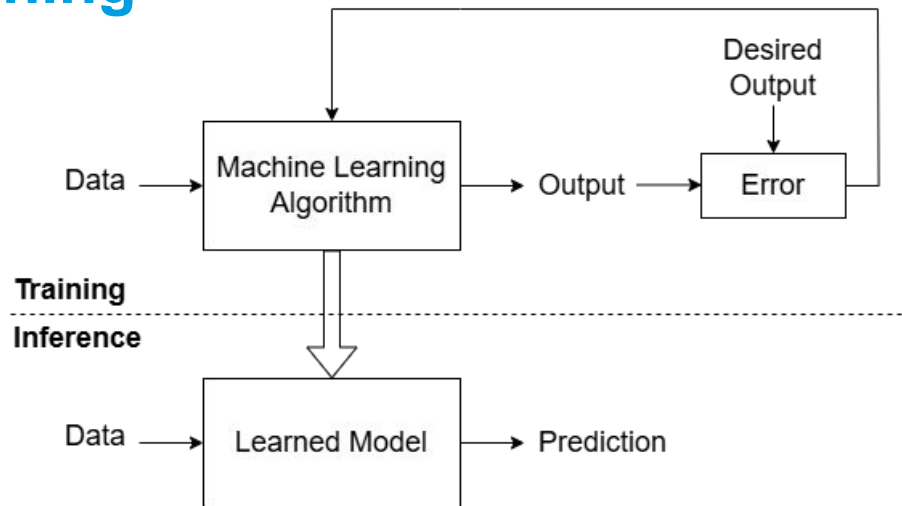
- Memorizing facts: limited by the time of observing facts, by the memory to store facts
- **Generalizing**: deduce new facts from old facts

Learning algorithm:

- A program that identifies patterns in data and uses those patterns to
- Programs that can infer useful information from implicit patterns in the data
- Need to figure out what those patterns are
- Then use those patterns to generate a program able to infer new data

Machine Learning

Pipeline:



Training phase:

- Input: a set of observations → **training data**
- Process: **learn patterns** from the training data
- Output: a **model** capable of identifying patterns in the data

Inference phase:

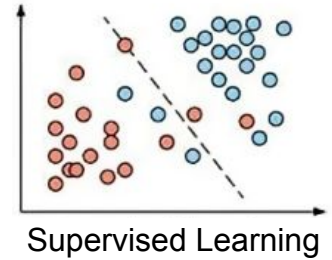
- Input: new observations → unseen data / **test data**
- Process: use the model to make new predictions

Machine Learning

3 major types of learning:

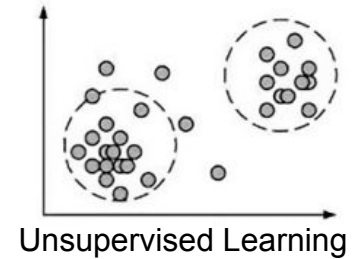
Supervised learning: labeled training data

- Training: learn a function to map inputs to their labels
- Inference: predict the label of new unseen inputs



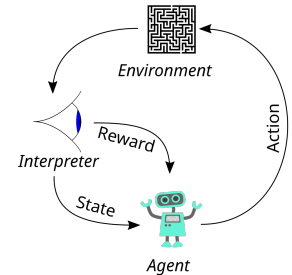
Unsupervised learning: unlabeled training data

- Training: identify hidden structures in unlabeled data
- Inference: assign new inputs to the most appropriate group



Reinforcement learning: training data with global objective (actions)

- Training: interact with an environment to maximize a cumulative reward
- Inference: make decisions to guide an agent towards an objective



Reinforcement Learning

Example: peaches vs. plums



Let's collect some data on fruits:

- weight, size
- labeled by fruit name

Plums:

- Plum 1: [147.1g, 7.8cm]
- Plum 2: [143.2g, 7.7cm]
- Plum 3: [150.2g, 7.6cm]
- Plum 4: [155.7g, 7.7cm]
- Plum 5: [145.6g, 7.5cm]
- Plum 6: [150.8g, 8.0cm]

Peaches:

- Peach 1: [151.4g, 8.2cm]
- Peach 2: [160.5g, 8.8cm]
- Peach 3: [165.3g, 9.0cm]
- Peach 4: [164.8g, 8.6cm]
- Peach 5: [158.9g, 8.6cm]

Example: peaches vs. plums

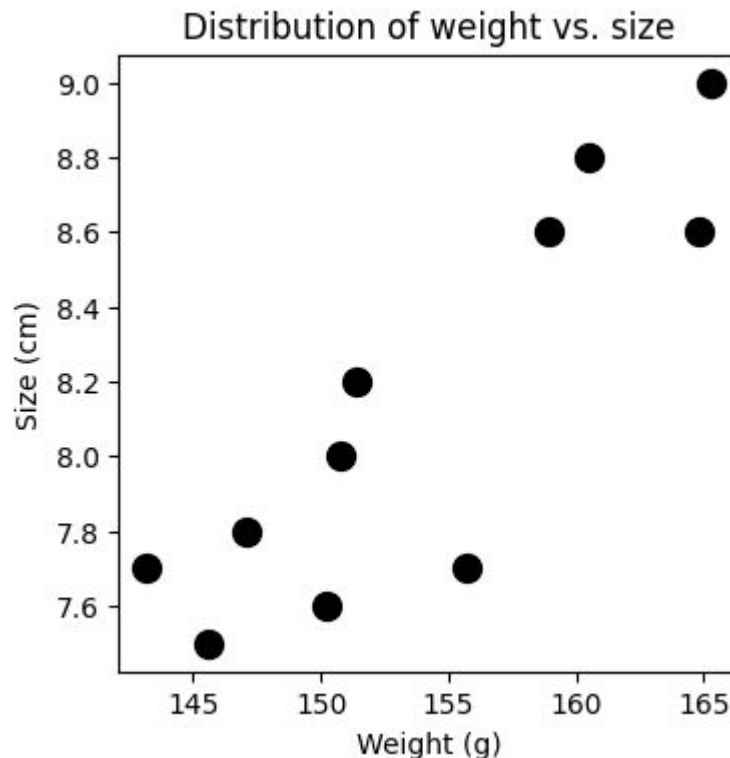
2D plot:

Can we learn patterns from data?

2 natural groups of points

How to separate them?

Clustering



Example: peaches vs. plums

2D plot:

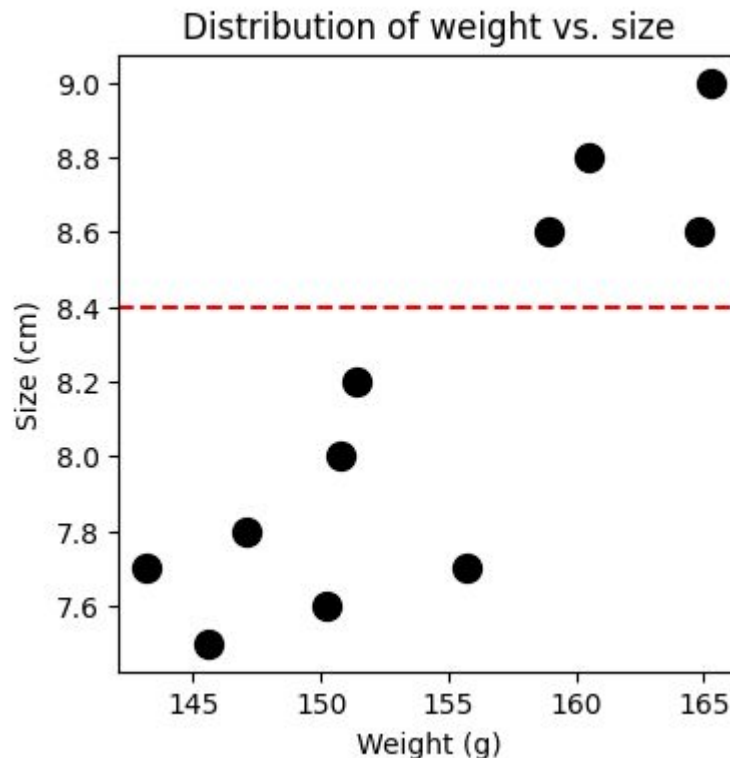
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Clustering

1) Separation on size



Example: peaches vs. plums

2D plot:

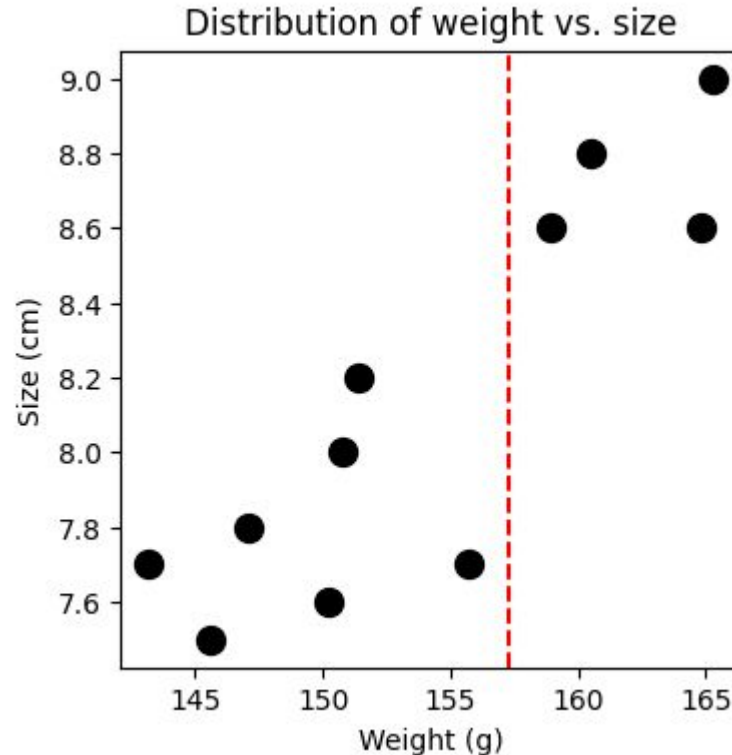
Can we learn patterns from data?

2 natural groups of points
How to separate them?

Clustering

1) Separation on size

2) Separation on weight



Example: peaches vs. plums

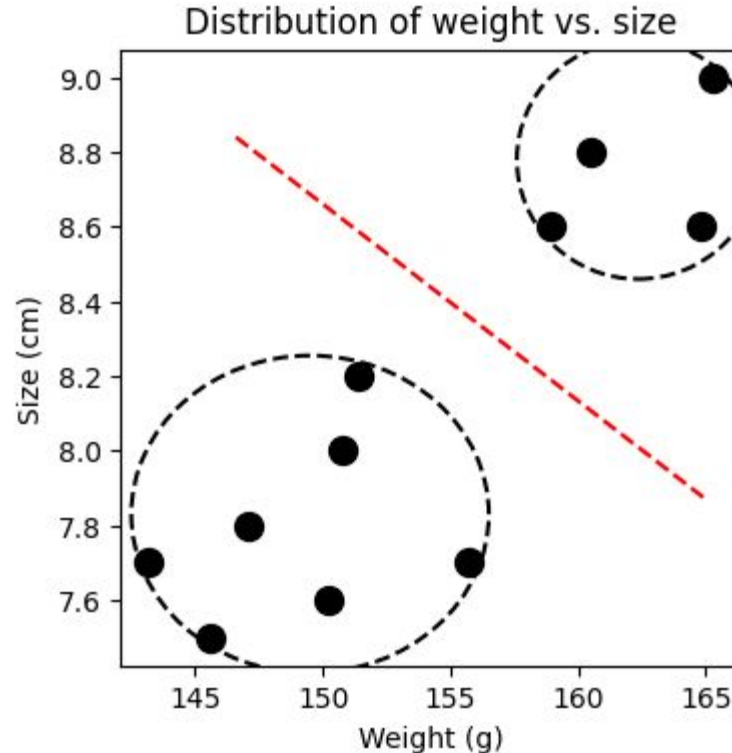
2D plot:

Can we learn patterns from data?

2 natural groups of points
How to separate them?

Clustering

- 1) Separation on size
- 2) Separation on weight
- 3) Cluster into two groups using both attributes

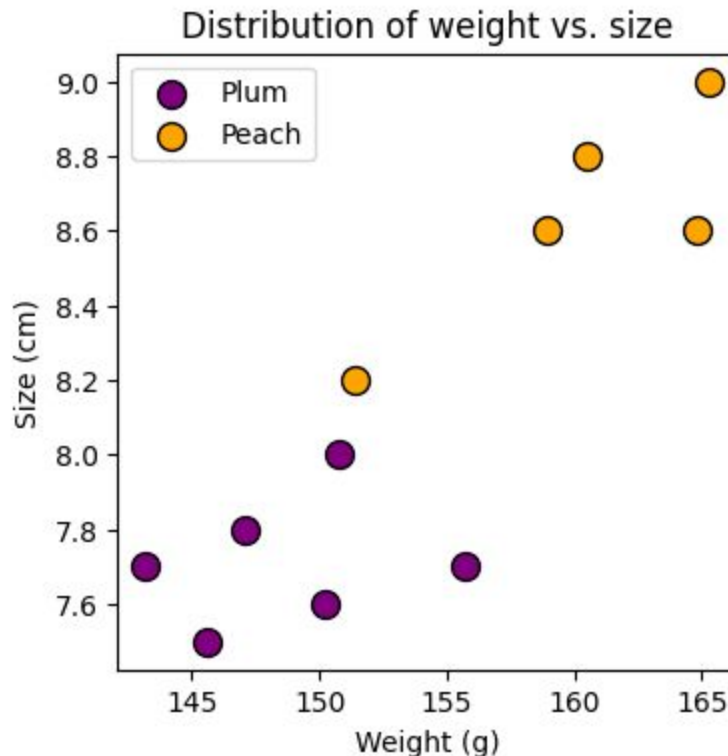


Example: peaches vs. plums

2D plot with labels:

How to take advantage of knowing the labels to divide the two groups?

Classification



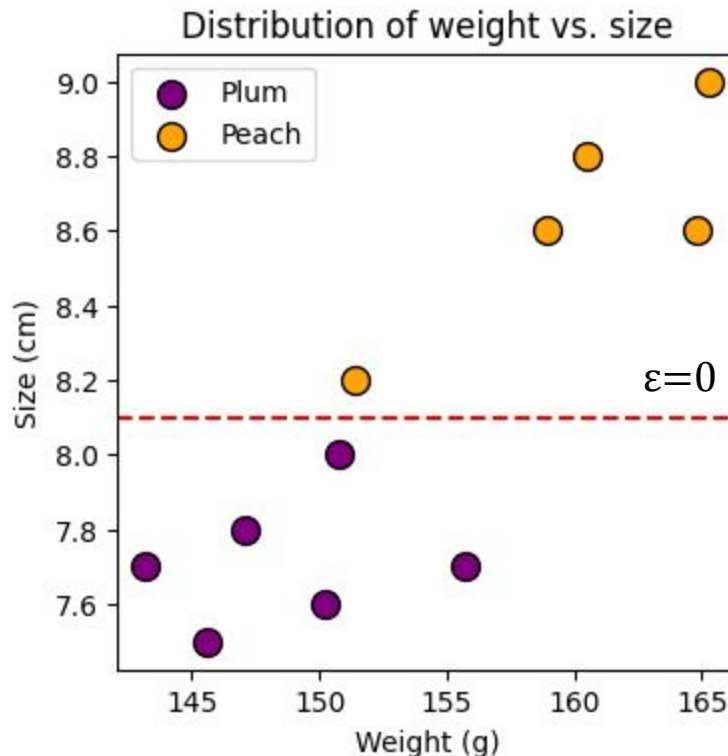
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2D plot with labels:

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Classification

1) Separation on size



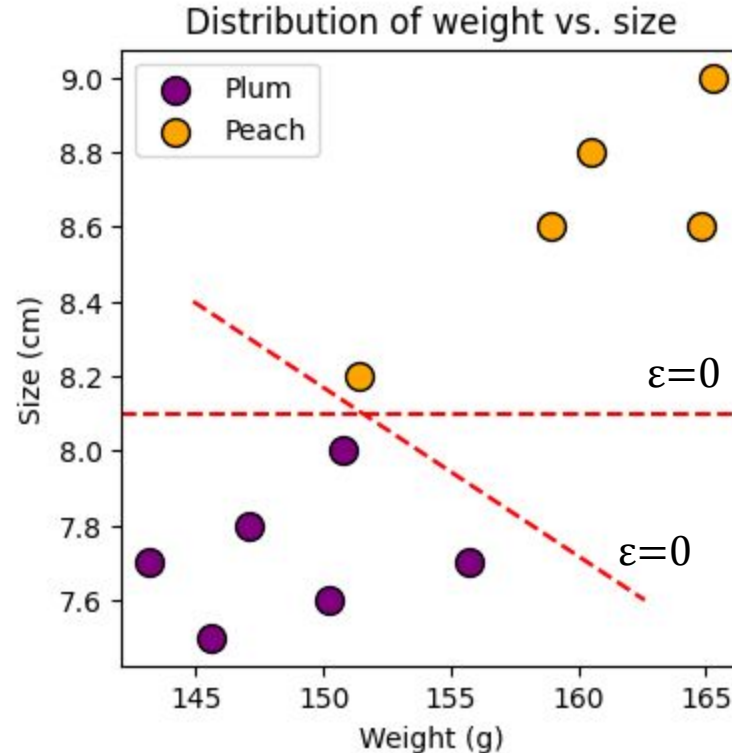
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2D plot with labels:

How to take advantage of knowing the labels to divide the two groups?

Classification

- 1) Separation on size
- 2) Separation using both attributes



Example: peaches vs. plums

2D plot with labels:

A new data point is added.

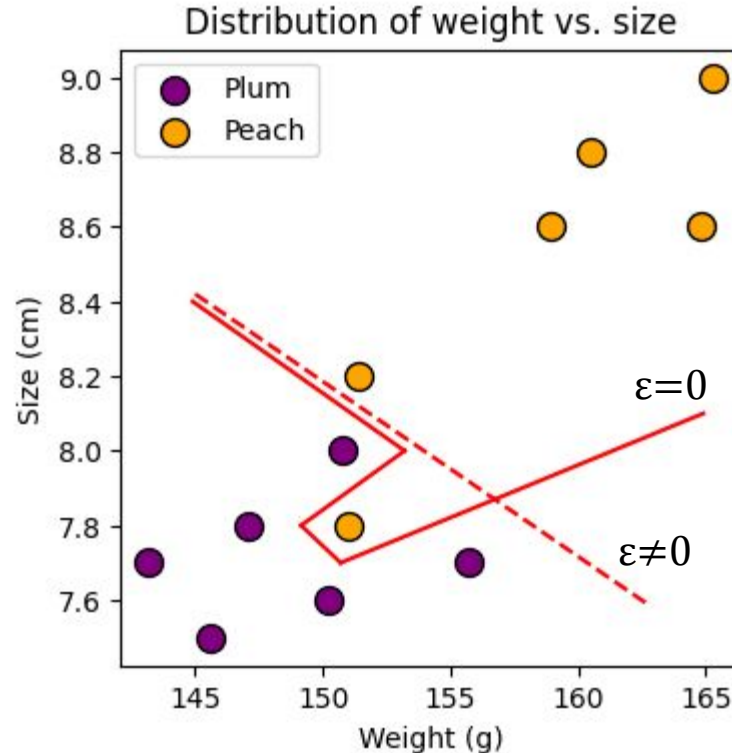
Which separator do we choose?

- 1) Dashed line: simple separator with errors
- 2) Solid line: complex separator without error

Option 2 performs well on training data
But it may fail to generalize to new data

Avoid **overfitting**:

Trade-off between **accuracy** and **simplicity**



Machine Learning: learning and generalizing

Machine Learning consists in learning from examples:

- **Training data**: a set of examples (peaches, plums, etc.) **labeled or not**
- **Features**: descriptors that describe each example (weight, size, etc.)
- **Distance** measure: quantifies “similarity” between examples
- **Objective function**: evaluates the quality of any solution

During training, we aim at optimizing the objective function (minimizing or maximizing)

Machine Learning consists in generalizing on unseen data:

- **Test data**: a set of additional examples, unknown during training

During inference, we hope to make accurate predictions on our test data

Unsupervised Learning

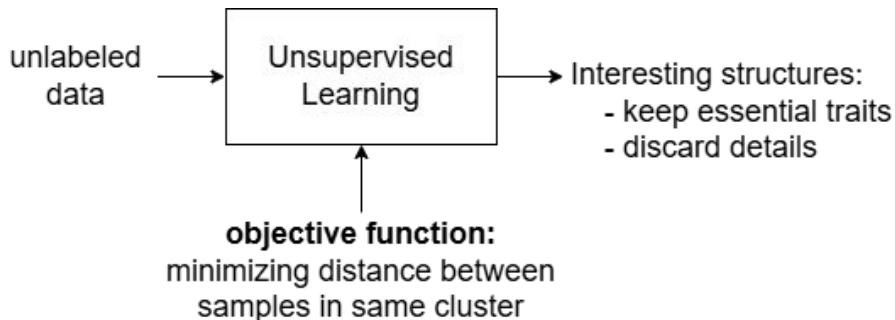
Unsupervised learning

Unsupervised learning:

- **Unlabeled** training data
- Goal: discover hidden structures in the data

Clustering:

- Group examples that are “close” together
- Assign the same label to all data points in each group
- Relies heavily on the choice of a **distance metric**
- The distance metric often matters more than the clustering algorithm itself.



Distance metric

Distances are used to measure the **similarity** or **dissimilarity** between two data points

Training data:

- n instances
- p features

$$X = \begin{pmatrix} x_1^1 & \dots & x_1^p \\ \vdots & \ddots & \vdots \\ x_n^1 & \dots & x_n^p \end{pmatrix}$$

Popular distance: **Minkowski**

- d=1: Manhattan distance
- d=2: Euclidean distance

$$d(x_i, x_j) = \sqrt[q]{|x_i^1 - x_j^1|^q + \dots + |x_i^p - x_j^p|^q}$$

Or weighted distance, ...

Clustering

K clusters $\{S_k\}$ with associated centroids $\{C_k\}$.

Goal: find the set S of clusters that minimize the **within-cluster** distance

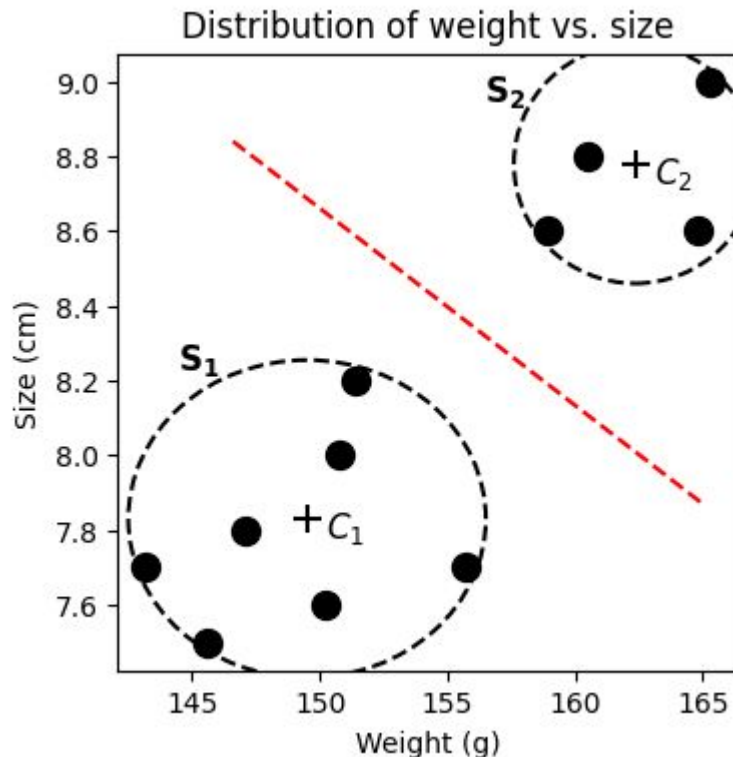
$$\arg \min_S \sum_{k=1}^K \sum_{\mathbf{x}_i \in S_k} d(\mathbf{x}_i, C_k)$$

Given centroids $\{C_k\}$, associate each data point to the closest cluster:

$$\forall i, x_i \in S_k \text{ where } k = \arg \min_j d(\mathbf{x}_i, C_j)$$

Given memberships of our data, update centroids:

$$\forall k, C_k = \frac{1}{|S_k|} \sum_{x_i \in S_k} x_i$$



K-means Clustering

K-means algorithm

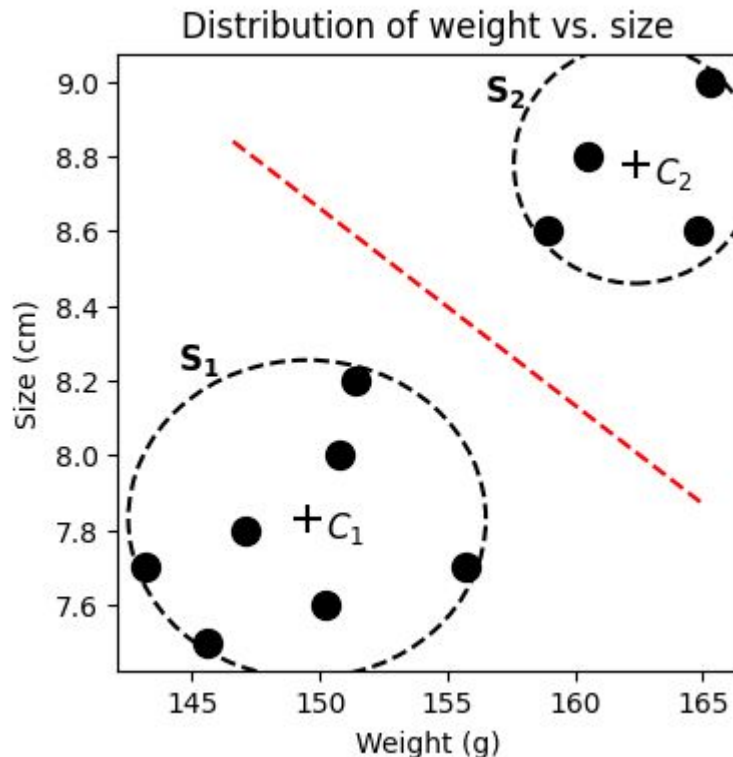
- 1) Start with a random guess of cluster centers
- 2) Determine the membership of each data point
- 3) Adjust the cluster centers



Stopping criterion:

- Number of iterations
- Clustering quality criterion $\rightarrow \sum_{k=1}^K \sum_{\mathbf{x}_i \in S_k} d(\mathbf{x}_i, C_k)$
- Evolution of the quality

In practice: we stop when $\{\mathbf{C}_j\}^{(t+1)} = \{\mathbf{C}_j\}^{(t)}$

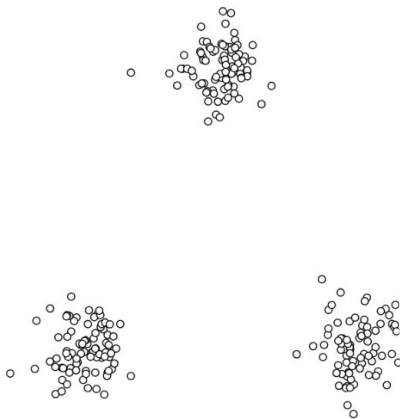


K-means Clustering



K-means algorithm

- 1) Set K the number of clusters: here $K=3$

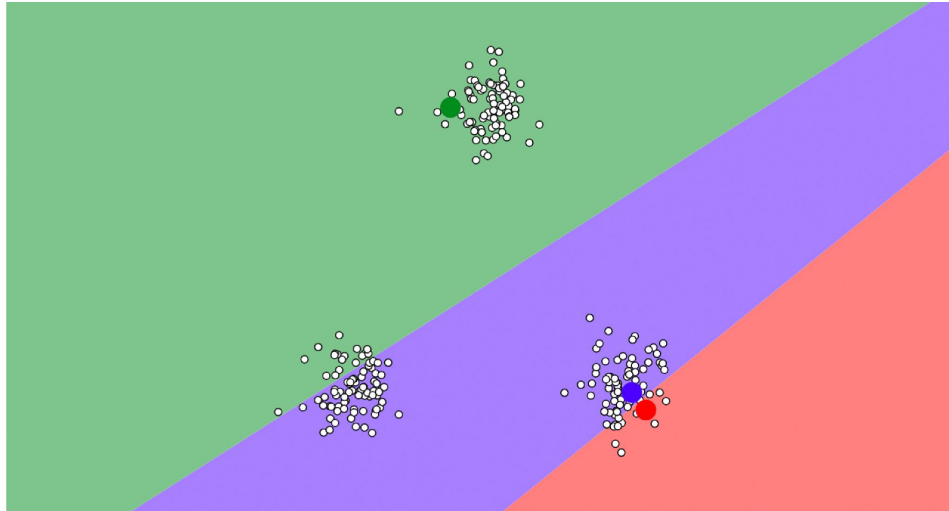


K-means Clustering



K-means algorithm

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- 2) Start with a random guess of cluster centers: select K random points

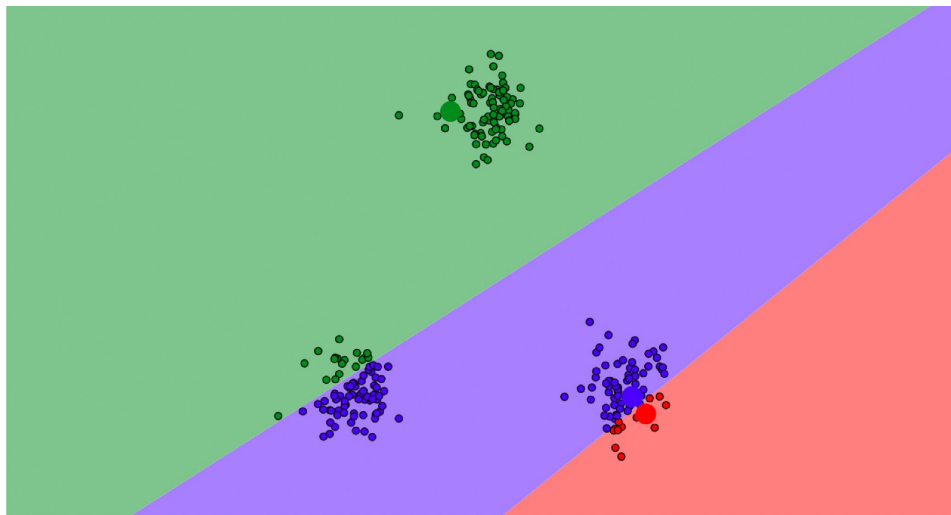


Harris, 2014

K-means Clustering

K-means algorithm

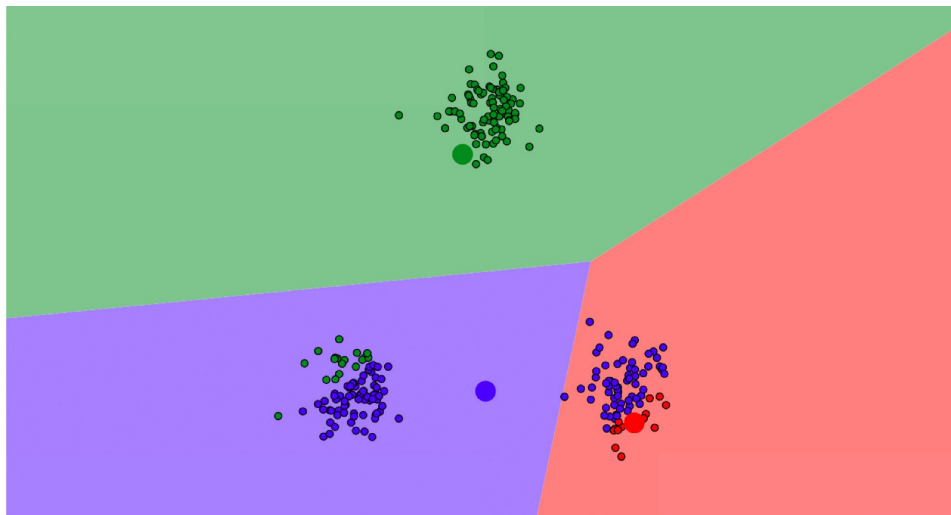
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- 3) Associate each data point to its closest cluster



K-means Clustering

K-means algorithm

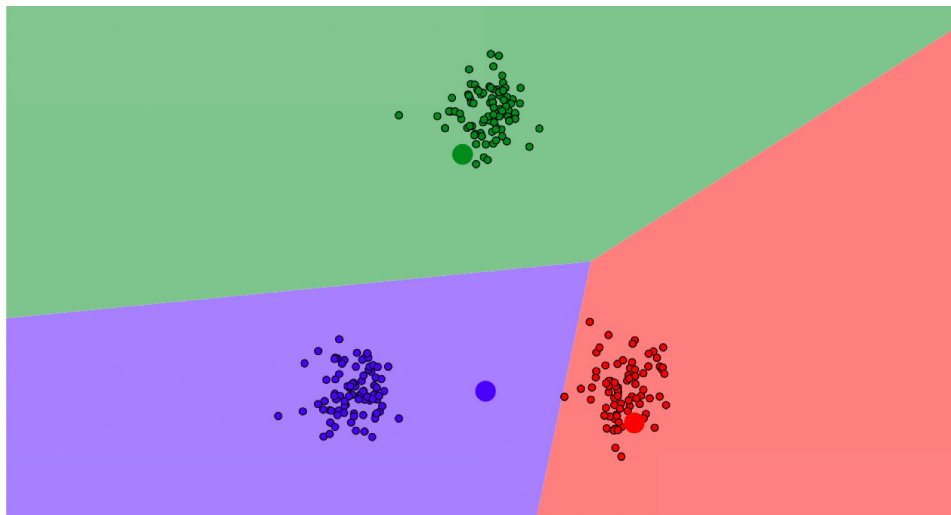
- 1) Set K the number of clusters: here $K=3$
- 2) Start with a random guess of cluster centers: select K random points
- 3) Associate each data point to its closest cluster
- 4) **Adjust centroids by computing their new mean**



K-means Clustering

K-means algorithm

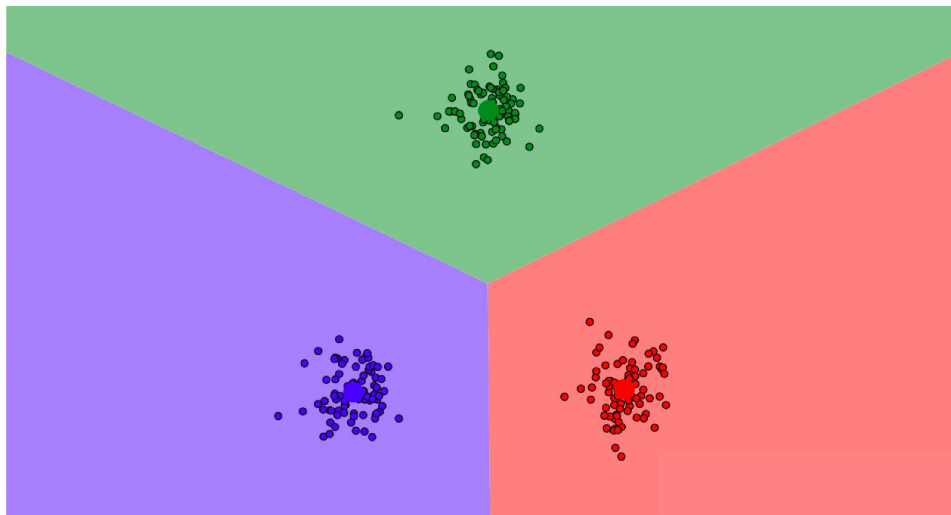
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K-means Clustering

K-means algorithm

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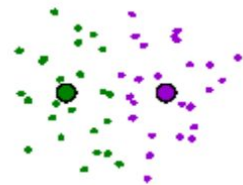
K-means Clustering

Strengths:

- Relatively efficient algorithm: $O(nkt)$ with n data points, k clusters and t iterations
- Find at least a local optimum

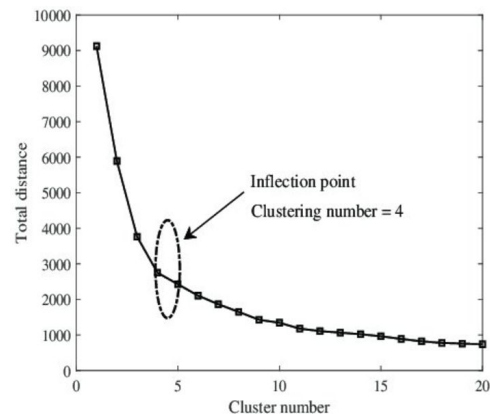
Weaknesses:

- Applicable only when the mean is defined (qualitative data?)
- Number of clusters K needs to be fixed in advance: elbow method



Variants:

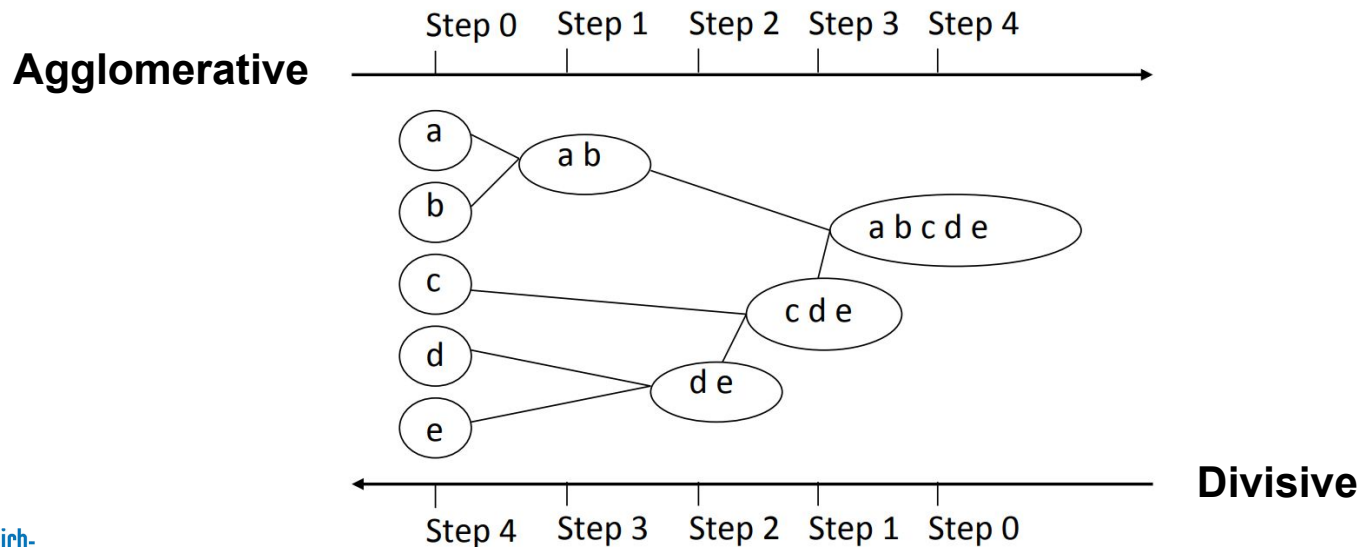
- K-medoids, K-modes, ect.



Hierarchical Clustering

Hierarchical Clustering:

- Uses distances between data points as clustering criteria
- Does not require to determine a number of clusters
- Agglomerative vs. divisive



Hierarchical Clustering



Agglomerative Clustering

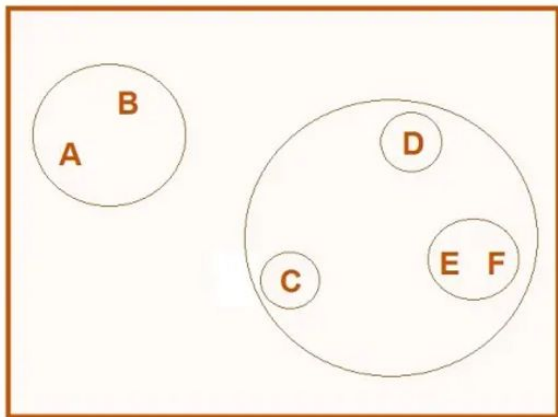
- Start with each point as individual cluster
- At each step, merge the closest pair
- Stop when only one cluster remains

Divisive Clustering

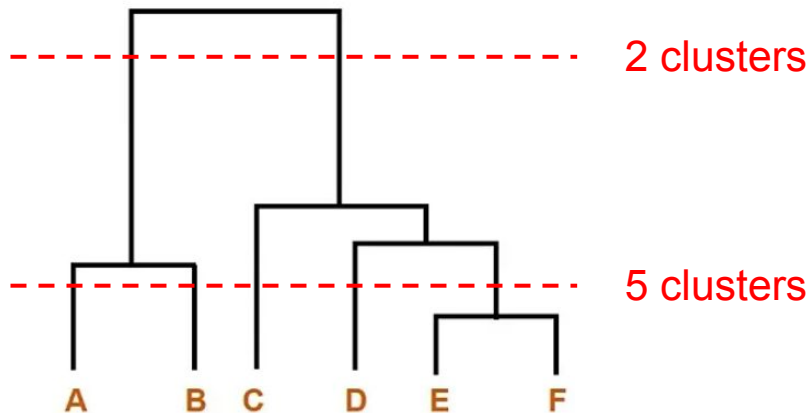
- Start with one cluster
- At each step, split a cluster
- Stop when each cluster contains a single point

Hierarchical Clustering

How many clusters do we want?



Clustering



Dendrogram

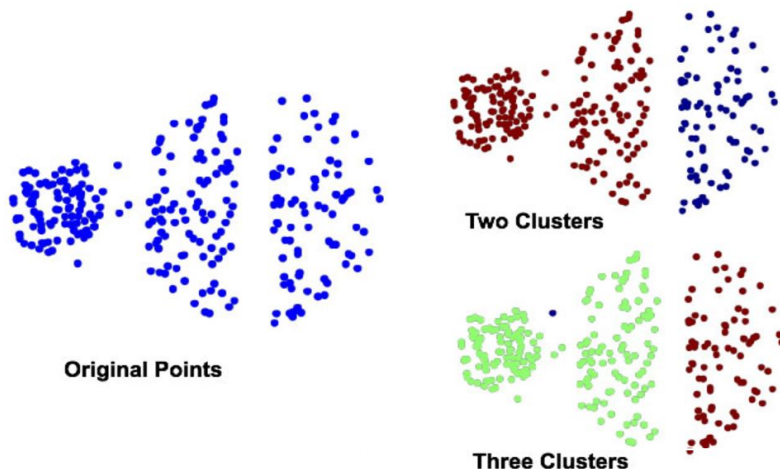
Hierarchical Clustering

Distance between two clusters?

- 1) **Single-link** distance: minimum distance between any points in S_i and S_j

$$d_{sl}(S_i, S_j) = \min_{x,y} \{d(x,y) | x \in S_i, y \in S_j\}$$

Limitations: sensitive to noise and outliers



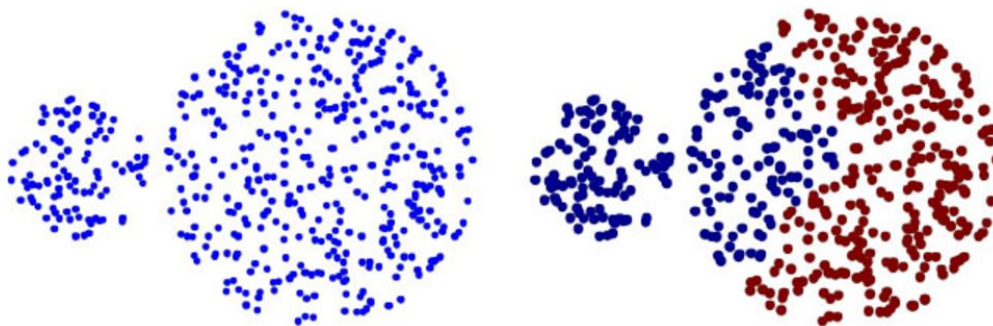
Hierarchical Clustering

Distance between two clusters?

- 2) **Complete-link** distance: maximum distance between any points in S_i and S_j

$$d_{sl}(S_i, S_j) = \max_{x,y} \{d(x, y) | x \in S_i, y \in S_j\}$$

Limitations: all clusters tend to have same diameters \rightarrow break large clusters



Original Points

Two Clusters

Hierarchical Clustering

Distance between two clusters?

- 3) **Group average** distance: average distance between any points in S_i and S_j

$$d_{ga}(S_i, S_j) = \frac{1}{|S_i| \times |S_j|} \sum_{x \in S_i, y \in S_j} d(x, y)$$

Compromise between single and complete links

- 4) **Centroid** distance

$$d_{centroids}(S_i, S_j) = d(C_i, C_j)$$

- 5) **Ward's** distance

$$d_{wards}(S_i, S_j) = \sum_{x \in S_i} (x - C_i)^2 + \sum_{x \in S_j} (x - C_j)^2 + \sum_{x \in S_{ij}} (x - C_{ij})^2$$

Hierarchical Clustering

Hierarchical Clustering

- Deterministic: always the same answer
- Greedy algorithm: local optima rather than global optimum
- Very long to compute

Complexity

- Space: $O(n^2)$ to store the distance matrix
- Time: $O(n^3)$
 - n steps
 - at each step, the distance matrix of size n^2 must be updated

Supervised Learning

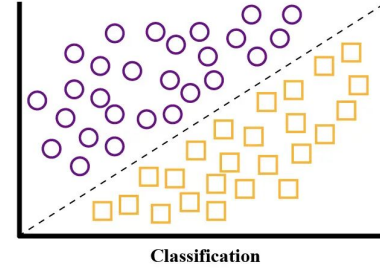
Supervised learning

Supervised learning:

- **Labeled** training data
- Goal: learn a function to map inputs to their labels

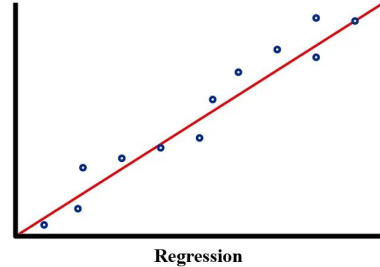
Classification:

- Labels are **discrete** classes (ex: peach/plum)
- Predict the correct class for each input

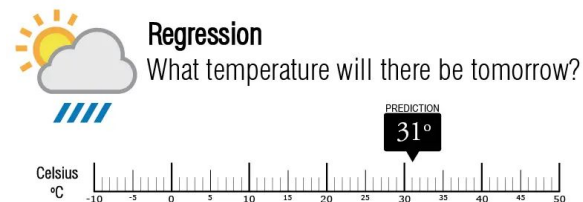
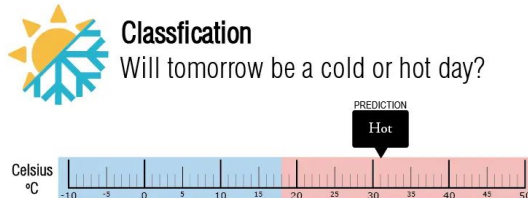


Regression:

- Labels are **continuous** values of a dependent variable (ex: ordinate)
- Make the best prediction based on a set of independent variables (ex: abscissa)



Ex:

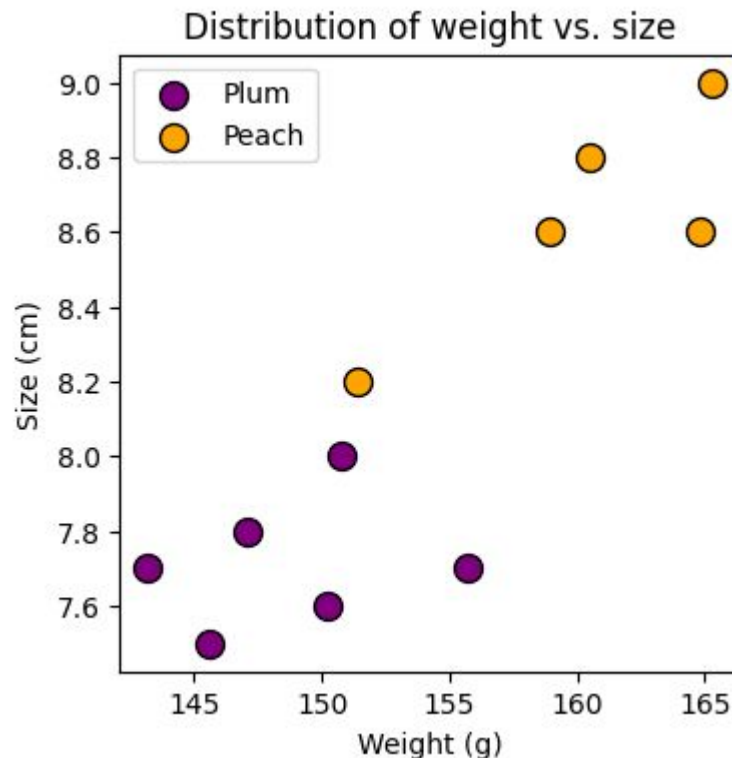


Classification

Our initial example: peaches vs. plums

- Features: weight, size
- Labels: Fruit name

How to divide the space?



Classification

Our initial example: peaches vs. plums

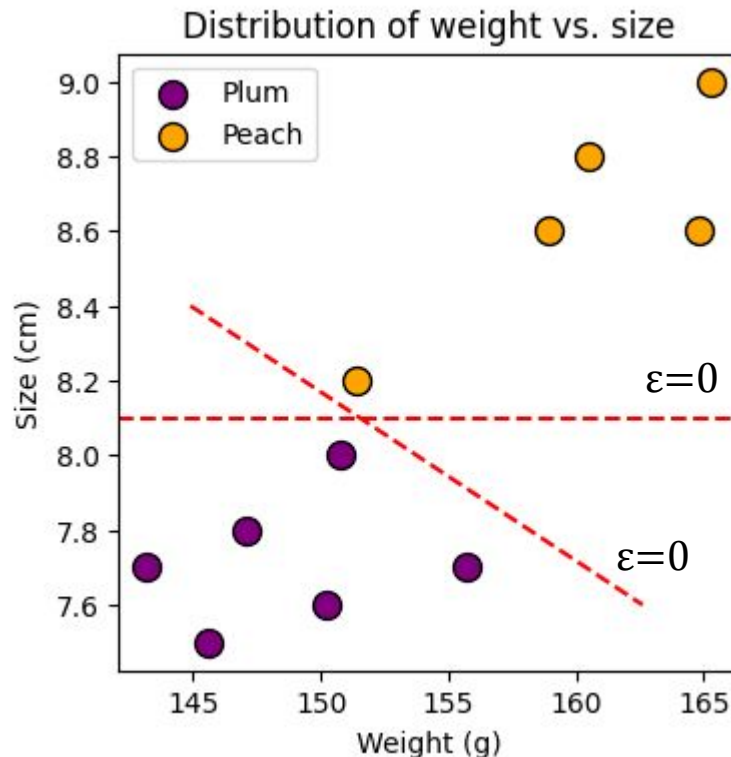
- Features: weight, size
- Labels: Fruit name

How to divide the space?

Many perfect separators exist...

How to find the best separation?

- each separator defines a “street” (margin)
- Can we find the widest street?



Classification

Our initial example: peaches vs. plums

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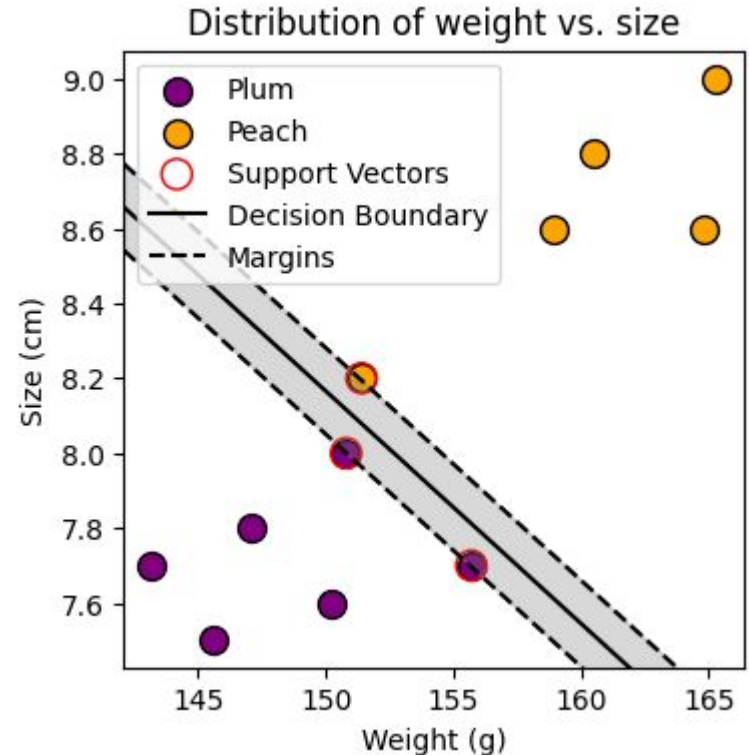
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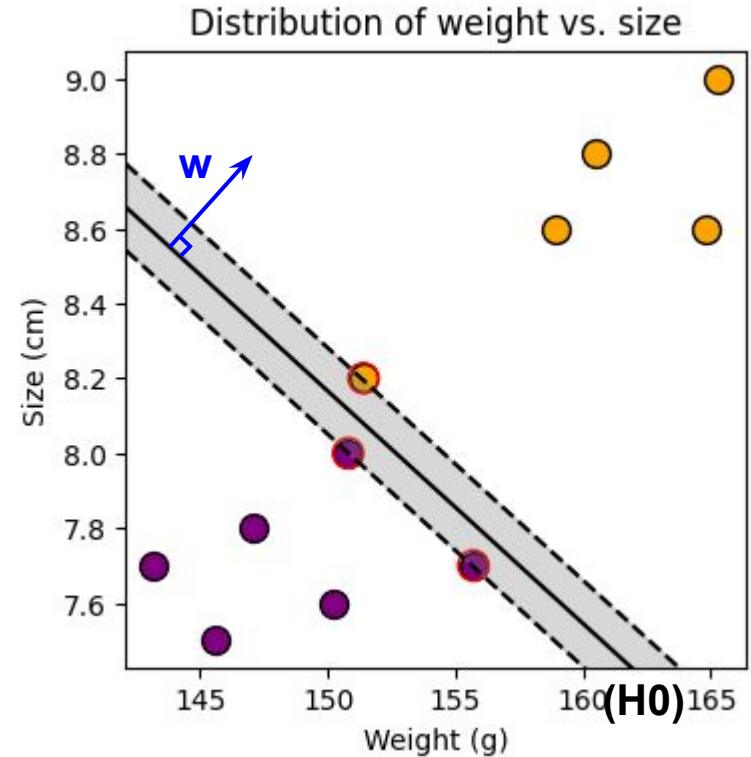
Support Vector Machines



Support Vector Machines

Let's consider $\mathbf{w} \perp (H_0)$:

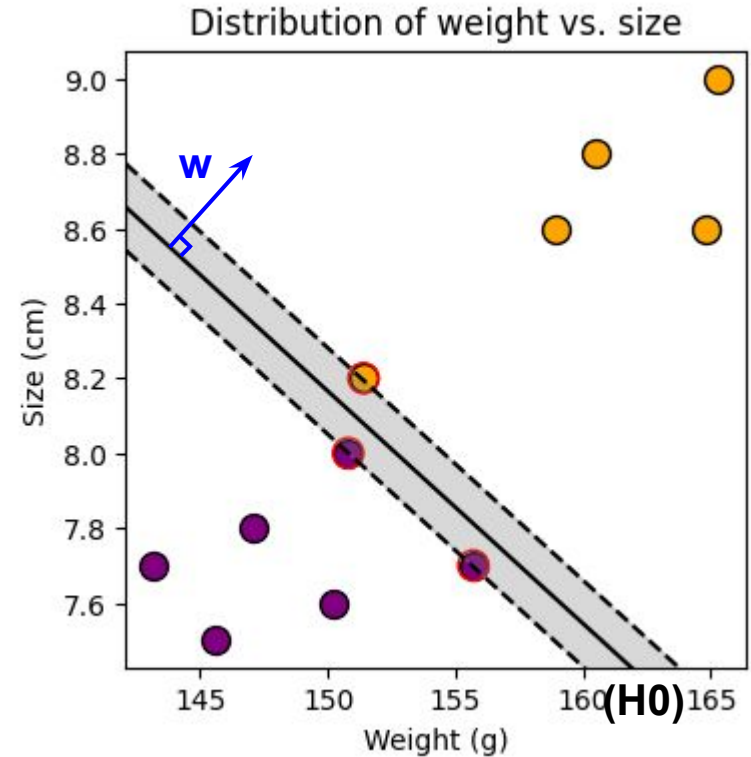
- For each point \mathbf{x} in (H_0) : $\vec{w} \cdot \vec{x} = \text{cste}$



Support Vector Machines

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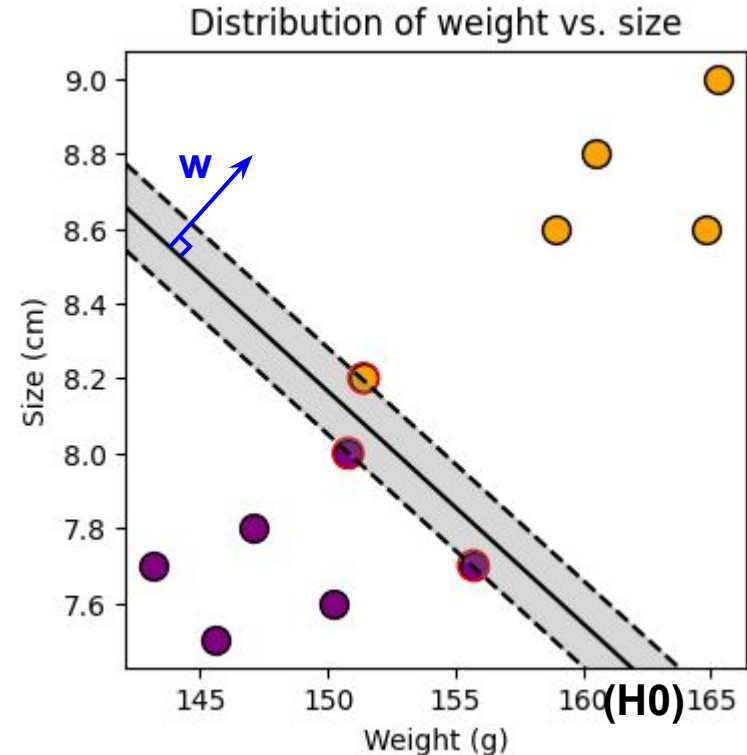
- For each point \mathbf{x} in (H_0) : $\vec{w} \cdot \vec{x} = \text{cste}$
- So we can find b such as: $\vec{w} \cdot \vec{x} + b = 0$



Support Vector Machines

Let's consider $\mathbf{w} \perp (H_0)$:

- For each point \mathbf{x} in (H_0) : $\vec{w} \cdot \vec{x} = \text{cste}$
- So we can find b such as: $\vec{w} \cdot \vec{x} + b = 0$
- Thus:
$$\begin{cases} \vec{w} \cdot \vec{x} + b \geq 0 \Rightarrow \text{peach} \\ \vec{w} \cdot \vec{x} + b < 0 \Rightarrow \text{plum} \end{cases}$$

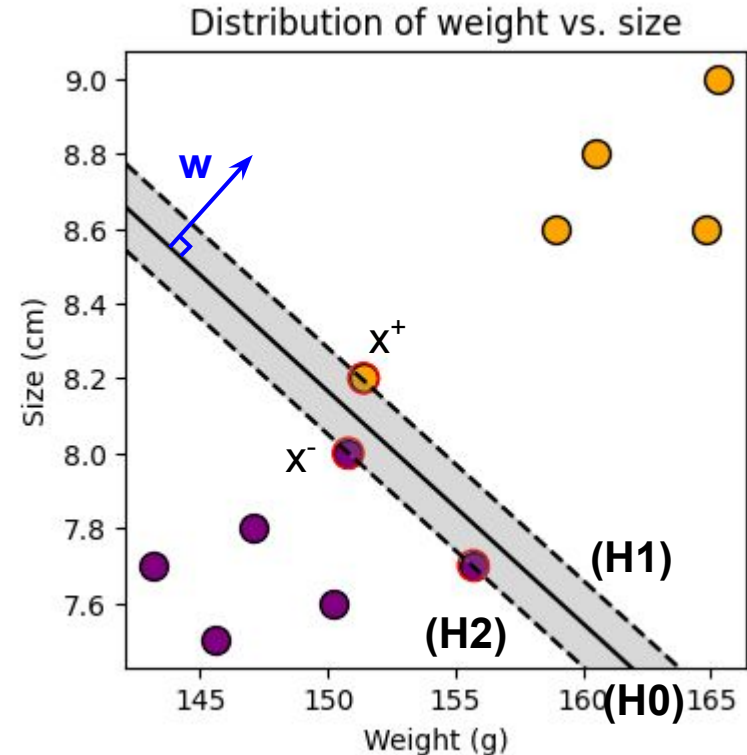


Support Vector Machines

Let's consider $\vec{w} \perp (H_0)$:

- For each point \mathbf{x} in (H_0) : $\vec{w} \cdot \vec{x} = \text{cste}$
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$$\begin{cases} \vec{w} \cdot \vec{x} + b \geq 0 \Rightarrow \text{peach} \\ \vec{w} \cdot \vec{x} + b < 0 \Rightarrow \text{plum} \end{cases}$$

Equations of (H_1) and (H_2) :
$$\begin{cases} \vec{w} \cdot \vec{x}^+ + b = +k \\ \vec{w} \cdot \vec{x}^- + b = -k \end{cases}$$



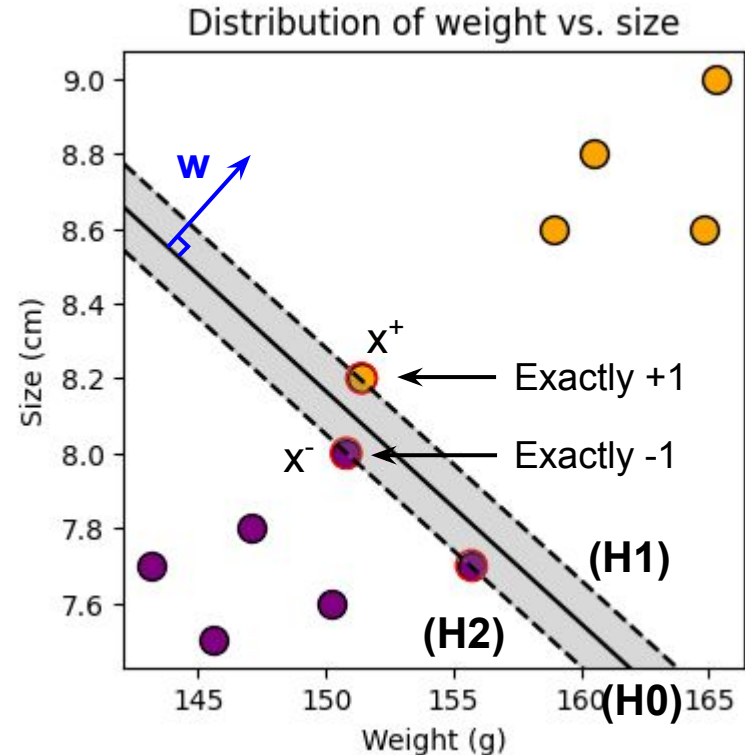
Support Vector Machines

Let's consider $\vec{w} \perp (H_0)$:

- For each point \vec{x} in (H_0) : $\vec{w} \cdot \vec{x} = \text{cste}$
- So we can find b such as: $\vec{w} \cdot \vec{x} + b = 0$
- Thus:
$$\begin{cases} \vec{w} \cdot \vec{x} + b \geq 0 \Rightarrow \text{peach} \\ \vec{w} \cdot \vec{x} + b < 0 \Rightarrow \text{plum} \end{cases}$$

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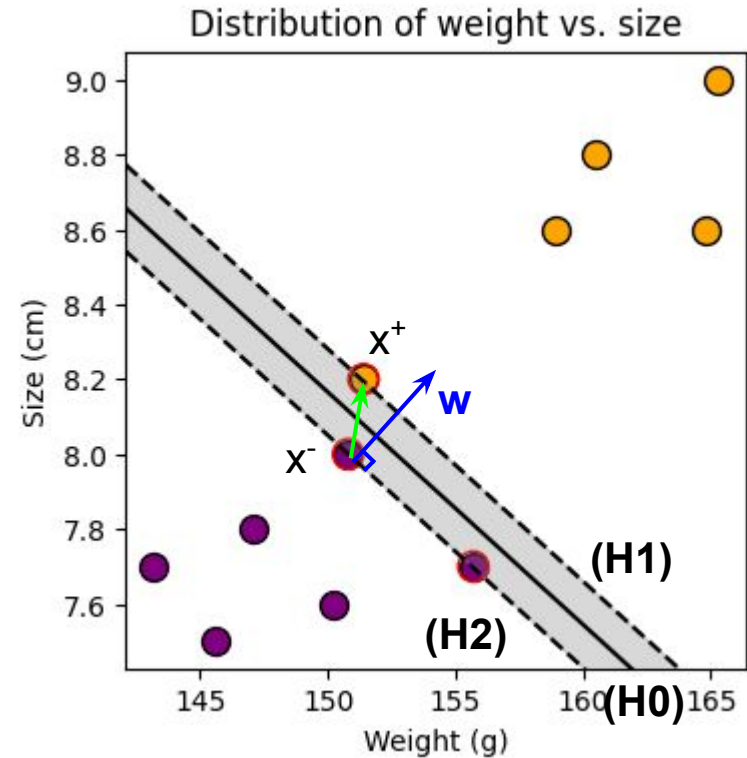
Rescaling \vec{w} and b gives:
$$\begin{cases} \vec{w} \cdot \vec{x}^+ + b = +1 \\ \vec{w} \cdot \vec{x}^- + b = -1 \end{cases}$$



Support Vector Machines

SVM maximizes the width of the margin:

$$\text{width} = \frac{\vec{w}}{\|\vec{w}\|} \cdot (\vec{x}^+ - \vec{x}^-)$$



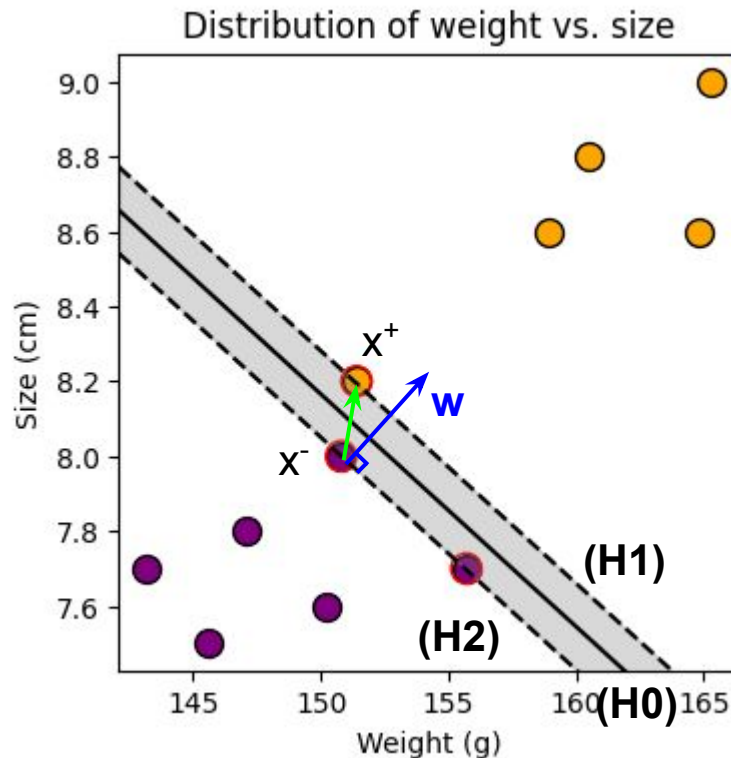
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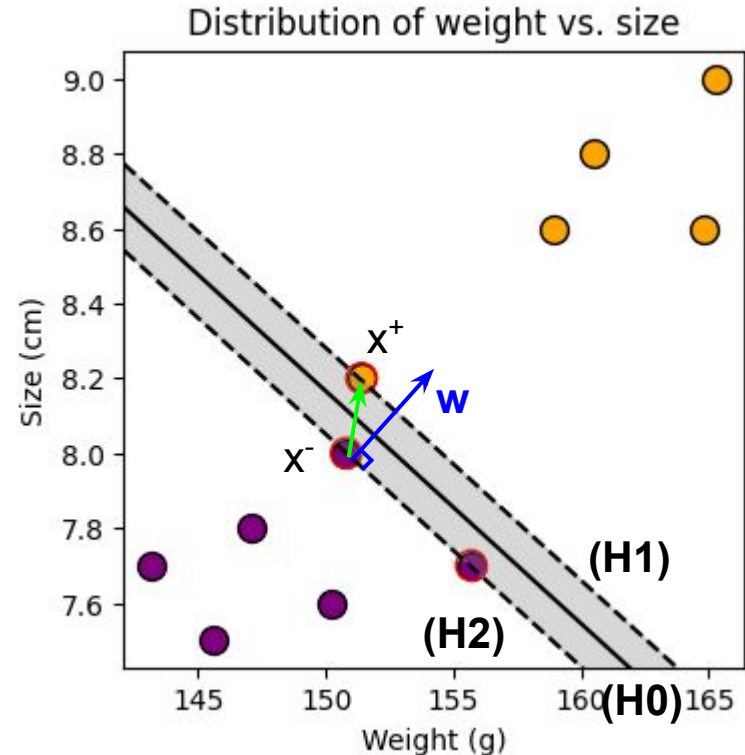
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Thus:

$$\text{maximize} \rightarrow \text{width} = \frac{2}{\|\vec{w}\|} \leftarrow \text{minimize}$$



Support Vector Machines

So the goal is to solve $\min ||\mathbf{w}||$ under $+1/-1 (y_i)$ constraints:



- Constrained optimization problem

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objective  constraints 

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Very beautiful result !!

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Support Vector Machines

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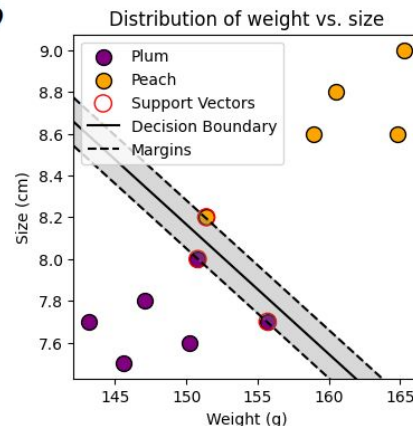
- Constrained optimization problem
- Solved via Lagrange Multiplier:

$$\mathcal{L}(\vec{w}, b) = \underbrace{\frac{\vec{w} \cdot \vec{w}}{2}}_{\text{objective}} - \sum_i \alpha_i [y_i(\vec{w} \cdot \vec{x}_i + b) - 1] \leftarrow \text{constraints}$$

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Very beautiful result !!

- \mathbf{w} linear combination of \mathbf{x}_i
- In practice, a lot of $\alpha_i = 0 \rightarrow$ so most points are useless
- Only points on the frontiers dictate the value of \mathbf{w}
 \rightarrow **Support Vectors**



Support Vector Machines

The decision rule becomes:

$$\left. \vec{w} \cdot \vec{x} + b \right\} \Rightarrow f(\vec{x}) = \sum_i \alpha_i y_i \vec{x}_i \cdot \vec{x} + b$$

All we need is:

- Optimize α_i
- Only requires the dot product

Support Vector Machines

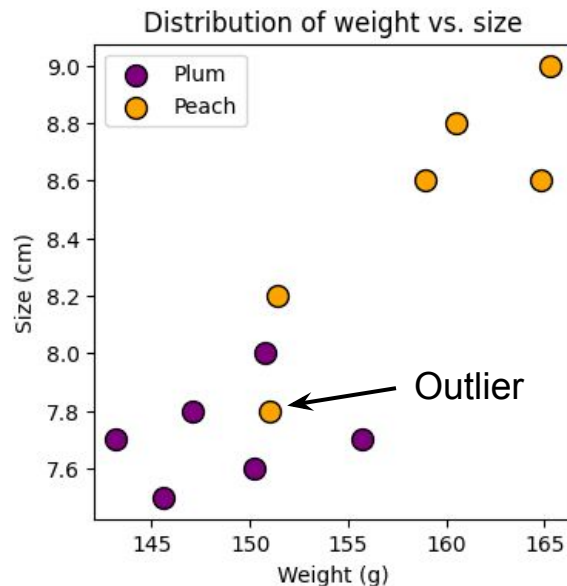
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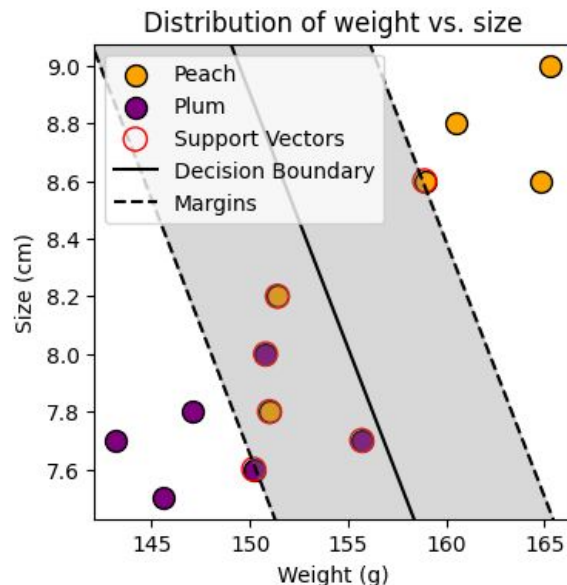
All we need is:

- Optimize α_i
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What if there are **outliers** in the data?

- Soft margin SVM
- Constrained equations: $y_i(\vec{w} \cdot \vec{x}_i + b) \geq 1 - \zeta_i$
- L1 regularization: penalizing large values of ζ_i
- Optimization function: $\frac{\vec{w} \cdot \vec{w}}{2} + C \sum_i \zeta_i$

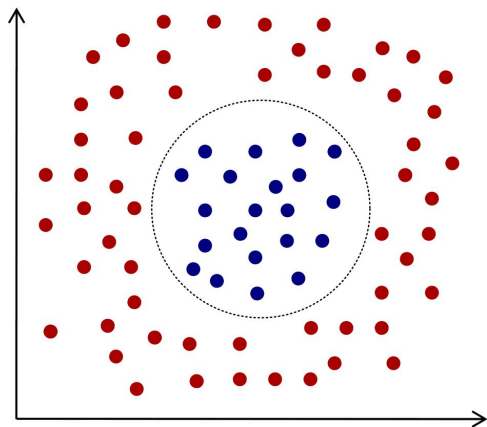
Controlling C \rightarrow controlling classification error



Support Vector Machines

SVM finds the best **straight** line

What to do when the data is **non-linearly** separable?

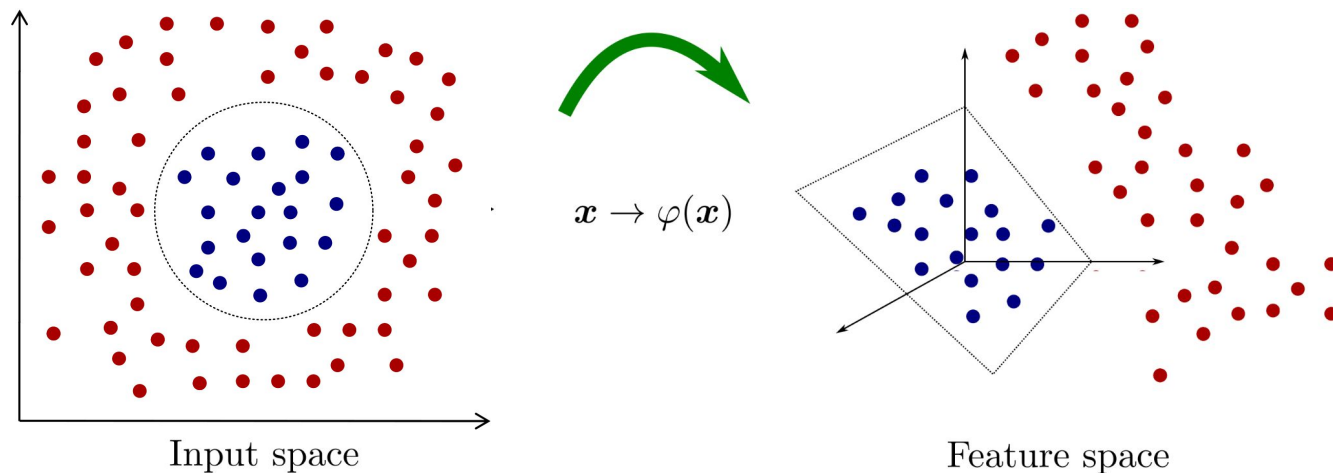


HOW?

Support Vector Machines

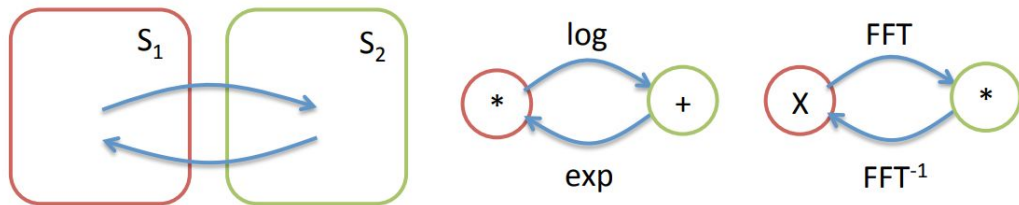
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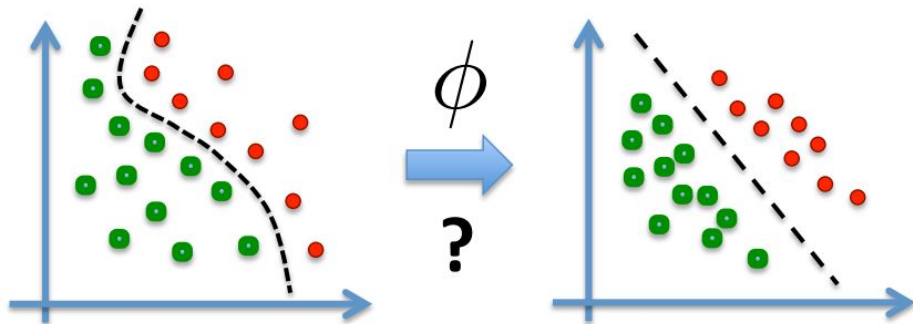


Support Vector Machines

- If the problem is hard in a given space S_1
- It is usual to go to a second space S_2 where it is easier to solve
- And then apply the inverse transformation (from S_2 to S_1)



- Same here: if we don't have a straight line in S_1 , maybe we have one in S_2



Support Vector Machines

Limitations:

- Dimensionality of Φ can be very large
- High computational costs

Solution:

- No need to compute the transform Φ
- Only need to compute its dot product!
- **Kernel trick:** $k(x, y) = \phi(x) \cdot \phi(y)$
- New problem formulation:

$$f(\vec{x}) = \sum_i \alpha_i y_i \vec{x}_i \cdot \vec{x} + b \Rightarrow f(\vec{x}) = \sum_i \alpha_i y_i \phi(\vec{x}_i) \cdot \phi(\vec{x}) + b$$

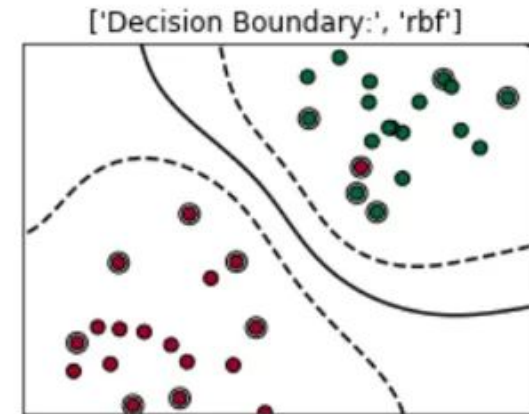
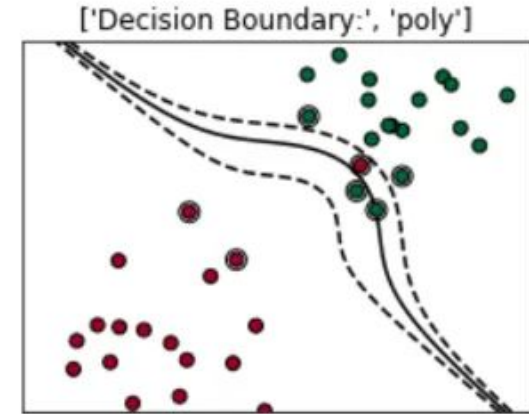
- Solved via SMO algorithm (Sequential Minimal Optimization)

Support Vector Machines



Most used kernel functions:

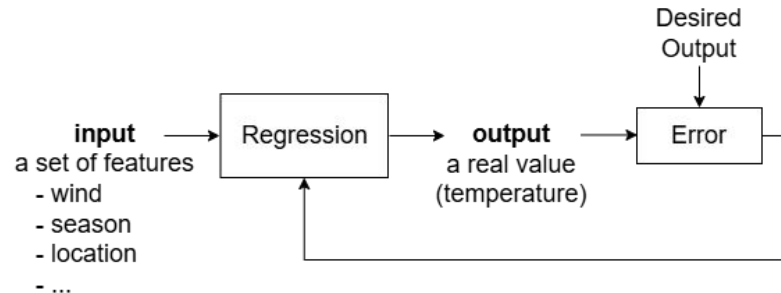
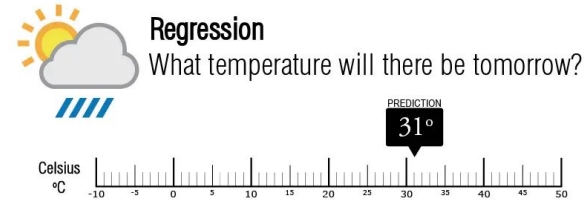
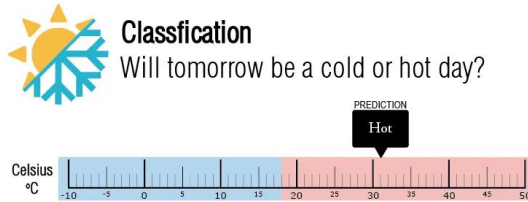
- **Polynomial:** $K(x, y) = (x^T y + 1)^d$
- **Gaussian:** $K(x, y) = \exp(-\psi(x - y)^2)$
- **Radial Basis:** $K(x, y) = \exp\left(\frac{-||x - y||^2}{2\sigma^2}\right)$
- **Sigmoid:** $K(x, y) = \tanh(kx^T y - \Theta)$



Regression

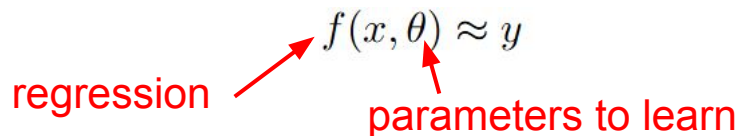
Regression:

- In classification we aim at predicting a discrete value (label)
- Here we aim at predicting a **real number** from a set of features



Regression

Objective: Learn a function f that predicts, for each input x , an output $f(x, \theta)$ that is closed to the desired value y



regression $f(x, \theta) \approx y$ parameters to learn

Let's assume a polynomial relationship between input and output:

$$f(x_i, \mathbf{w}) = w_0 + w_1 x_i + w_2 x_i^2 + \dots + w_M x_i^M = \sum_{m=0}^M w_m x_i^m$$

Objective: find parameter \mathbf{w}

Regression

Learning parameters:

- **Loss function**: quantifies the error between predicted and desired values to minimize

Example: **Mean Square Error** $\mathcal{L}(w) = \frac{1}{N} \sum_{i=1}^N (y_i - f(x_i, \theta))^2$

Regression

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Example: **Mean Square Error** $\mathcal{L}(w) = \frac{1}{N} \sum_{i=1}^N (y_i - f(x_i, \theta))^2$

- Iterative optimization: **gradient descent**
 - Compute the gradient of the loss function: $\frac{\partial \mathcal{L}}{\partial w_i}(w)$
 - Update parameters: $w_i \leftarrow w_i - \eta \frac{\partial \mathcal{L}}{\partial w_i}$

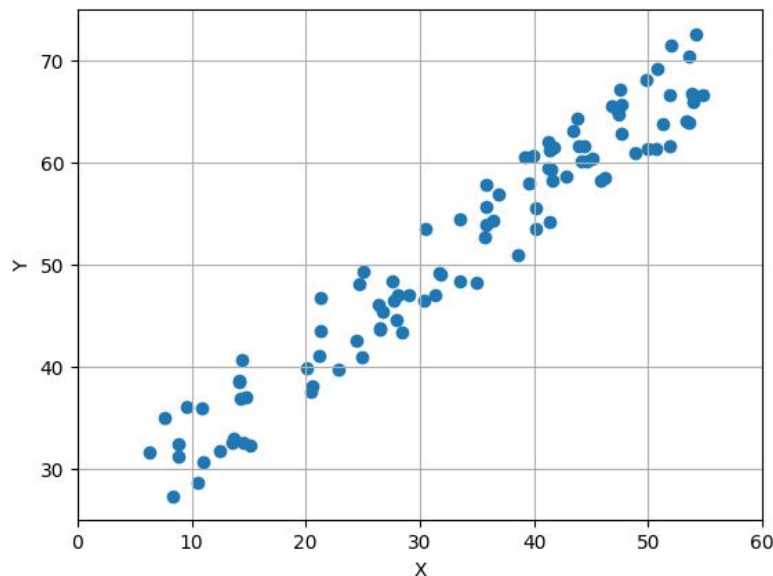
learning rate

Linear Regression



Input data: pairs of coordinates (x,y)

Model: $f(x) = ax + b$



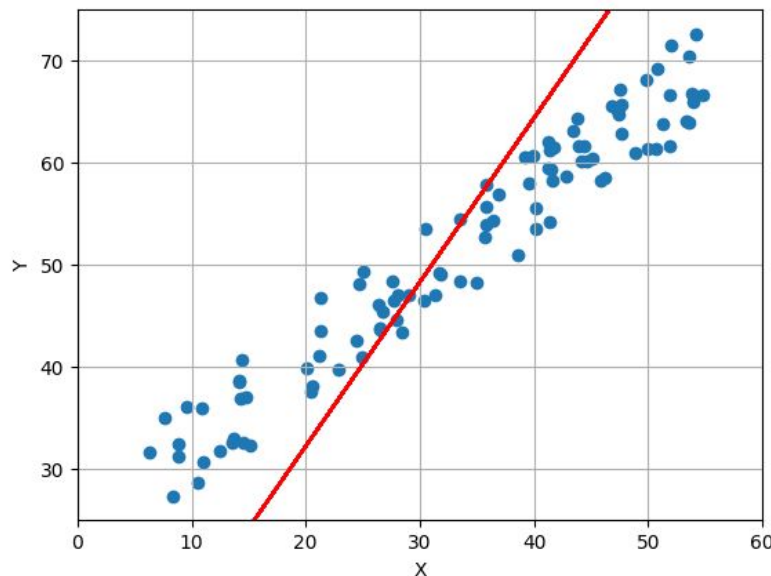
Linear Regression



Input data: pairs of coordinates (x,y)

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Learning:
epoch 1



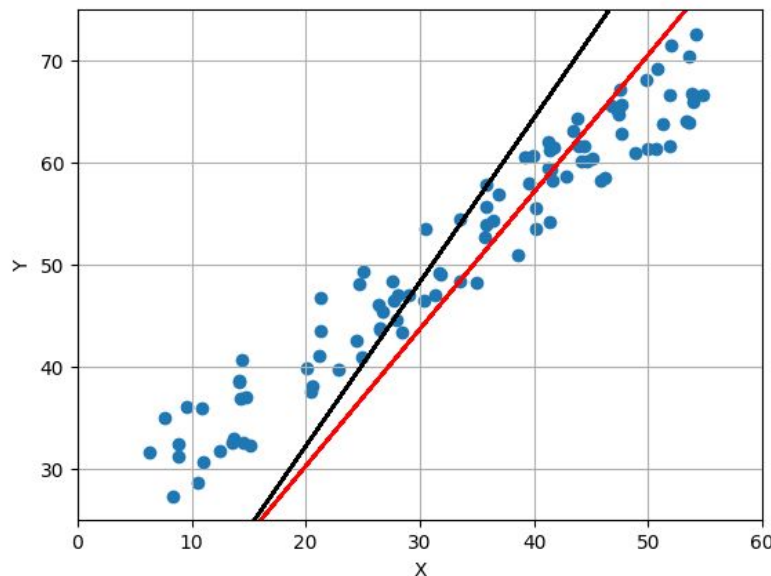
Linear Regression



Input data: pairs of coordinates (x,y)

Model: $f(x) = ax + b$

Learning:
epoch 2



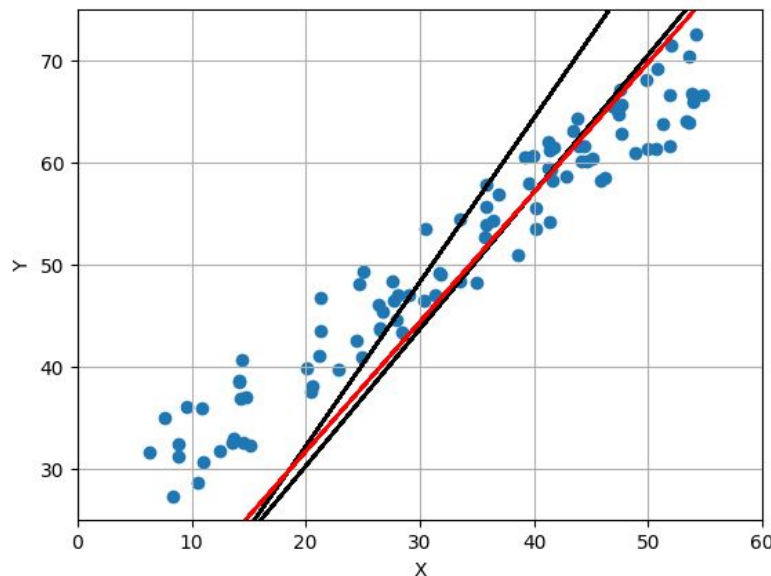
Linear Regression



Input data: pairs of coordinates (x,y)

Model: $f(x) = ax + b$

Learning:
epoch 3



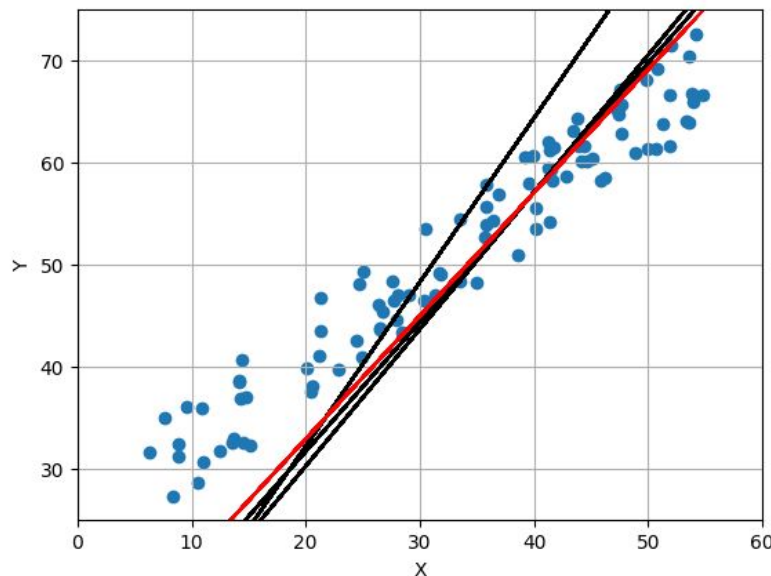
Linear Regression



Input data: pairs of coordinates (x,y)

Model: $f(x) = ax + b$

Learning:
epoch 4



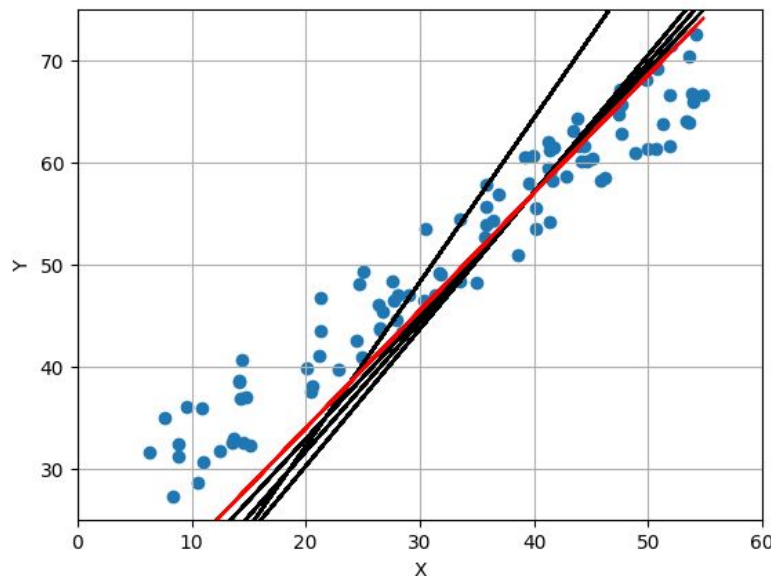
Linear Regression



Input data: pairs of coordinates (x,y)

Model: $f(x) = ax + b$

Learning:
epoch 5



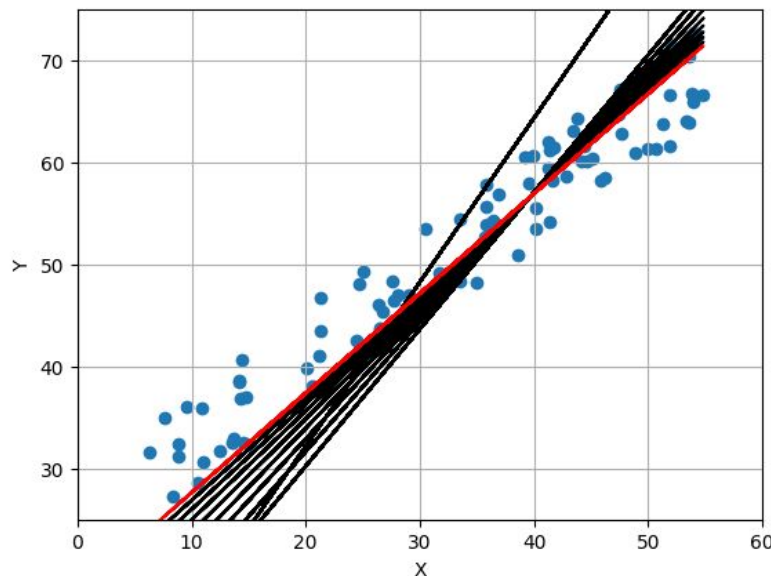
Linear Regression



Input data: pairs of coordinates (x,y)

Model: $f(x) = ax + b$

Learning:
epoch 10



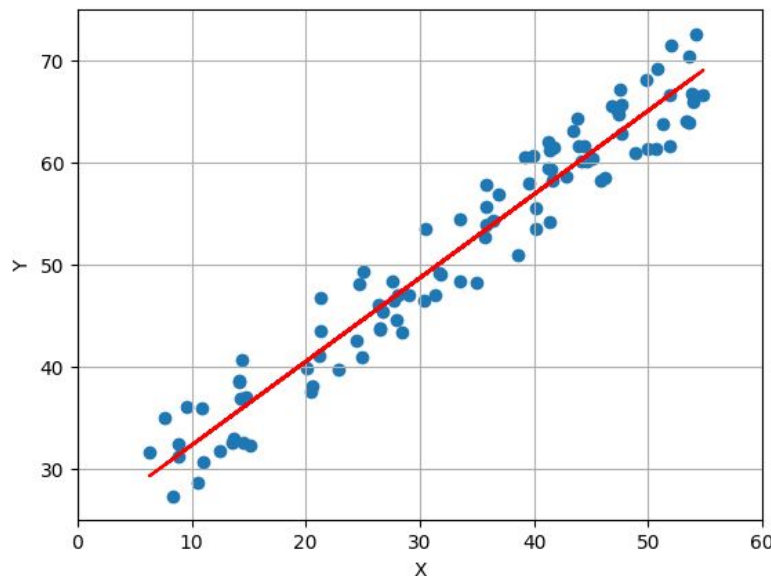
Linear Regression



Input data: pairs of coordinates (x,y)

Model: $f(x) = ax + b$

Learning:
epoch 100



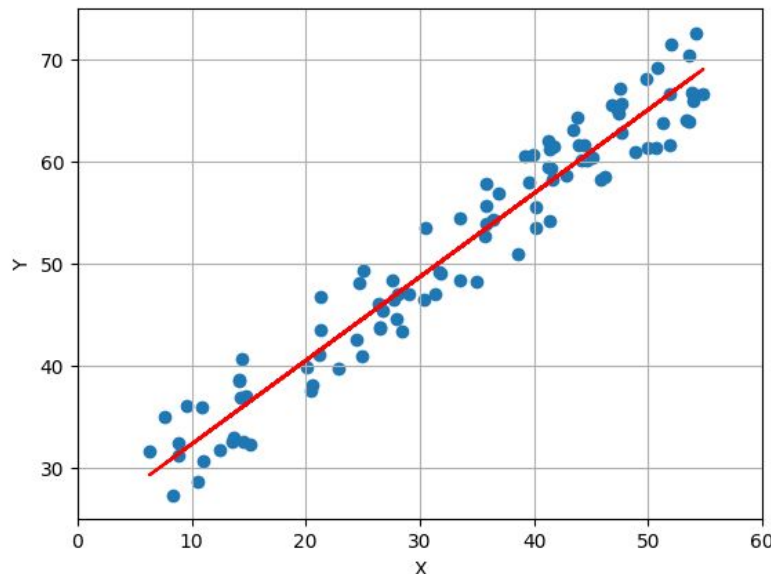
Linear Regression



Input data: pairs of coordinates (x,y)

Model: $f(x) = ax + b$

Learning:
epoch 100



Deep Learning reuse the same methodology but with extremely nonlinear models

Conclusion

Conclusion

Methods

- Unsupervised Learning: K-means clustering, hierarchical clustering
- Supervised Learning: SVM, regression

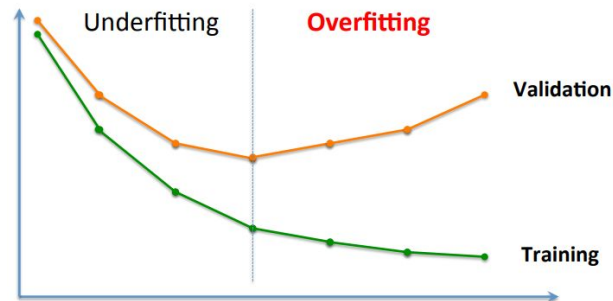
Conclusion

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- Unsupervised Learning: K-means clustering, hierarchical clustering
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Generalization and performance evaluation

- All methods are applied on a training set
- How do they perform on unseen data?
- Split dataset into train/dev/test sets to avoid **overfitting**



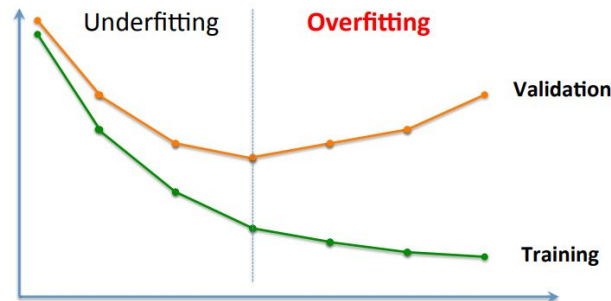
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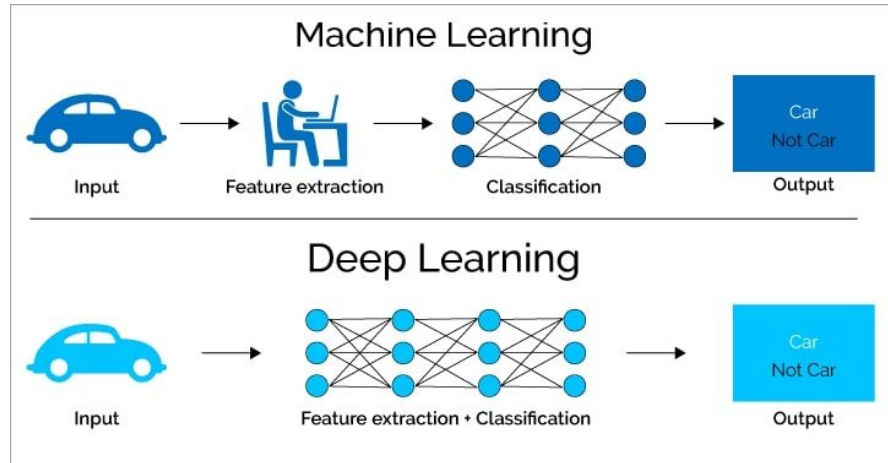


Curse of dimensionality

- We have seen that adding dimensions helps finding a separator
- Yes but overfitting!
- Growing number of features \Rightarrow amount of data to generalize grows **exponentially!**
Maybe PCA? 😊

Conclusion

From Machine Learning to Deep Learning



Going deeper:

- Apprentissage et Deep Learning (S7,S8)
- Traitement d'images (S8), Intelligence Artificielle (S8)
- Vision Artificielle (S9).

Questions?

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