Machine Learning I: Fractal 2

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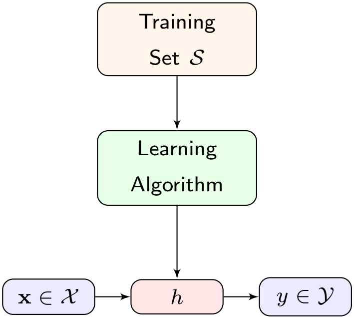
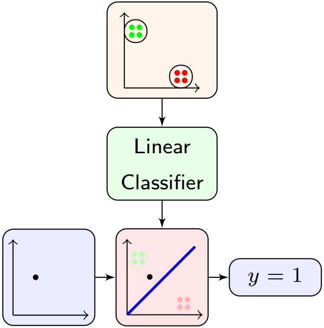
These slides are prepared from the following book:
Shalev-Shwartz, Shai, and Shai Ben-David. Understanding machine learning: From theory to algorithms. Cambridge university press, 2014.

Supervised Learning

Let $\mathcal{S} = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_m, y_m)\}$ be a training set. Here, $\mathbf{x}_i$ is the i^{th} training input, e.g. an image, and y_i is the corresponding label, e.g. "cat". Let $\mathcal{X}$ be the set of all inputs and let $\mathcal{Y}$ be the set of all possible output labels and let $h : \mathcal{X} \to \mathcal{Y}$ be a predictor. Then, our goal is to find h such that $h(\mathbf{x}_i)$ is equal to the true label of the input $\mathbf{x}_i$.

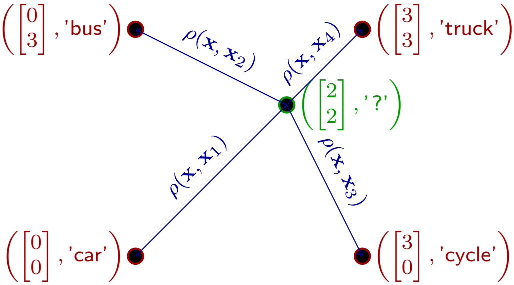




k-Nearest Neighbors Classifier

- Let $\mathcal{S} = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_m, y_m)\}$ be the training set.
- For each $\mathbf{x} \in \mathcal{X}$, let $\pi_1(\mathbf{x}), \ldots, \pi_m(\mathbf{x})$ be reordering of $\{1, 2, \ldots, m\}$ according to their distance to $\mathbf{x}$, $\rho(\mathbf{x}, \mathbf{x}')$.
- That is, for all $i < m$,

$$\rho(\mathbf{x}, \mathbf{x}_{\pi_i(\mathbf{x})}) \leq \rho(\mathbf{x}, \mathbf{x}_{\pi_{i+1}(\mathbf{x})})$$



Clustering

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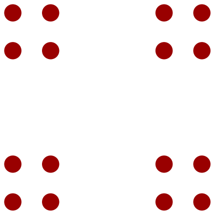

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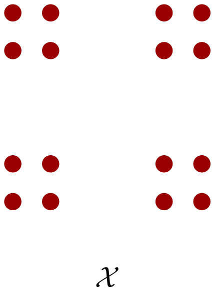

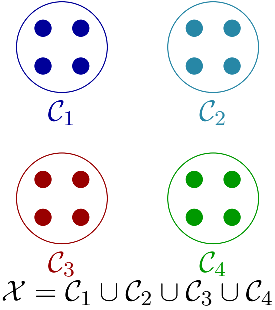

Clustering Algorithms

- Connectivity Based: Hierarchical Clustering

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- Neural models: Self-organizing map

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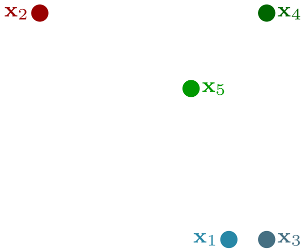

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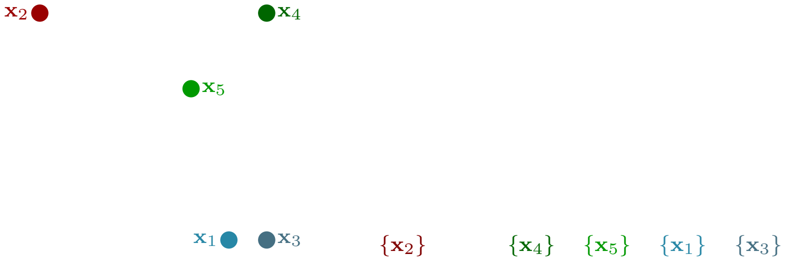

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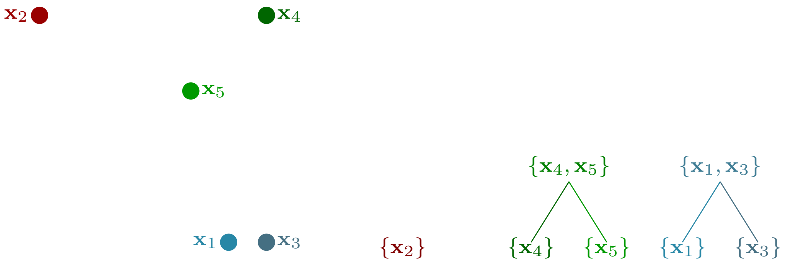

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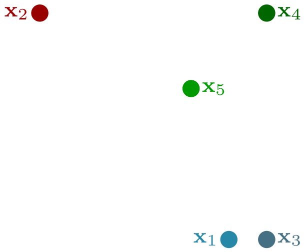

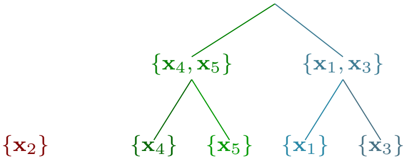

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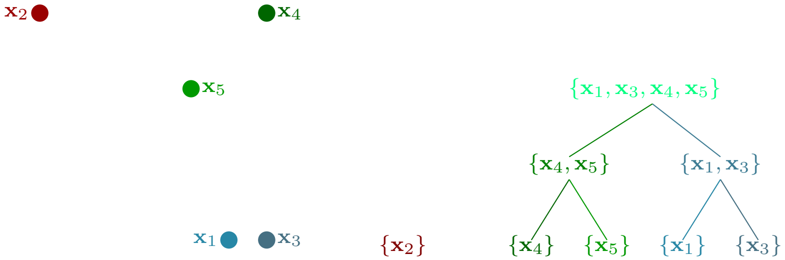

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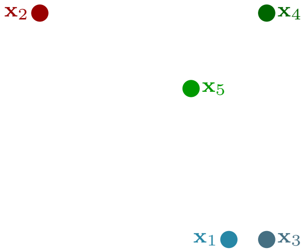

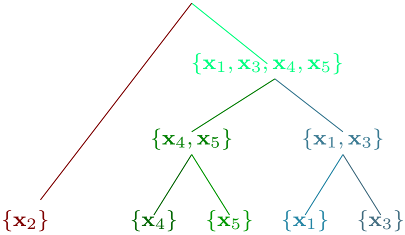

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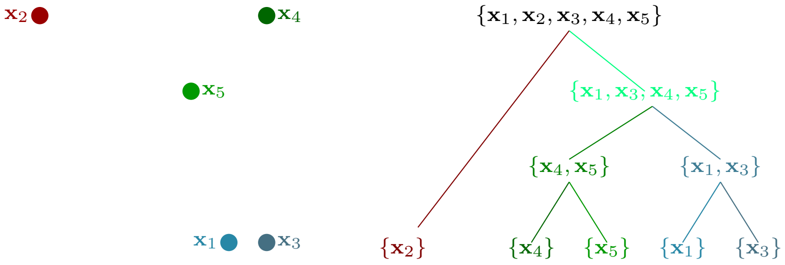

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- First, we have to decide how to measure (or define) the distance between clusters, and, second, we have to determine when to stop merging.

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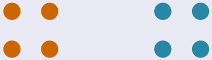

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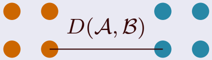

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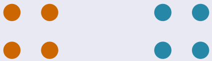

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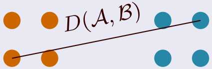

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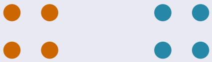

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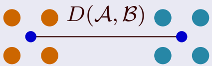

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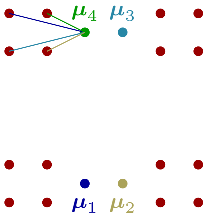

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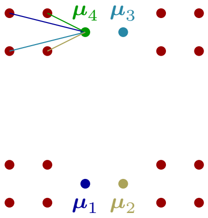

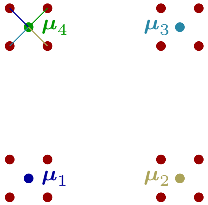

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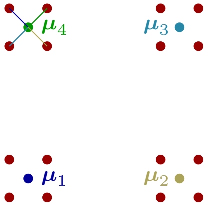

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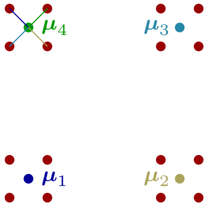

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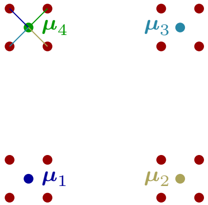

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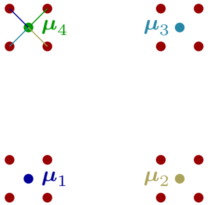
- $\underset{\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k}{\arg\min} \; f(\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k)$.

[1] MacQueen, James. "Some methods for classification and analysis of multivariate observations." Proceedings of the fifth Berkeley symposium on mathematical statistics and probability, 1967.

[2] Lloyd, Stuart P. "Least squares quantization in PCM." IEEE Transactions on Information Theory, 1982.

k-Means: Problem Formulation[3,4]

Let $\mathcal{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$ be the set data-points, where $\mathbf{x}_i \in \mathbb{R}^d$. We want to partition $\mathcal{X}$ in groups $\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_k$ containing similar objects.Let $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_k$ be their respective group representatives (centres), where $\boldsymbol{\mu}_i \in \mathbb{R}^d$.



- $f(\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k) = \sum_{i=1}^{k} \sum_{\mathbf{x} \in \mathcal{C}_i} \|\mathbf{x} - \boldsymbol{\mu}_i\|_2^2$
- $\underset{\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k}{\arg\min}\ f(\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k)$.
- $\frac{\partial f}{\partial \boldsymbol{\mu}_i} = \mathbf{0} \Rightarrow \boldsymbol{\mu}_i = \frac{\sum_{\mathbf{x} \in \mathcal{C}_i} \mathbf{x}}{|\mathcal{C}_i|}$

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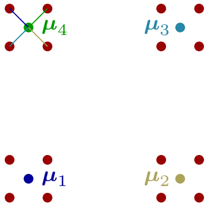

- $f(\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k) = \sum_{i=1}^{k} \sum_{\mathbf{x} \in \mathcal{C}_i} \|\mathbf{x} - \boldsymbol{\mu}_i\|_2^2$
- $\underset{\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k}{\arg\min} \; f(\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k)$.
- $\frac{\partial f}{\partial \boldsymbol{\mu}_i} = \mathbf{0} \Rightarrow \boldsymbol{\mu}_i = \frac{\sum_{\mathbf{x} \in \mathcal{C}_i} \mathbf{x}}{|\mathcal{C}_i|}$
- $\boldsymbol{\mu}_i = \text{mean}(\mathcal{C}_i) \; \forall i \in \{1, 2, \ldots, k\}$.

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Algorithm 1 k-Means Algorithm

Input: $\mathcal{X} \subset \mathbb{R}^d$, Number of clusters k

Initialize: Randomly choose initial centroids $\boldsymbol{\mu}_1^{(0)}, \ldots, \boldsymbol{\mu}_k^{(0)}$

while not converged **do**

  for $i \in [k]$ **do**

    $\mathcal{C}_i^{(t+1)} \leftarrow \left\{ \mathbf{x} : \|\mathbf{x} - \boldsymbol{\mu}_i^{(t)}\|^2 < \|\mathbf{x} - \boldsymbol{\mu}_j^{(t)}\|^2 \; \forall j \in [k] \backslash \{i\}, \mathbf{x} \in \mathcal{X} \right\}$

    $\boldsymbol{\mu}_i^{(t+1)} \leftarrow \frac{1}{|\mathcal{C}_i^{(t+1)}|} \sum_{\mathbf{x} \in \mathcal{C}_i^{(t+1)}} \mathbf{x}$

    $t \leftarrow t + 1$

  end for

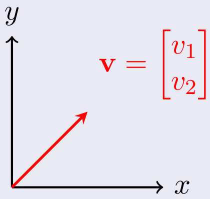
end while

Norm of a vector

Let $\mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}$ be a vector in $\mathbb{R}^n$. Then, the norm of the vector $\mathbf{v}$ is defined as

$$\|\mathbf{v}\| = \sqrt{v_1^2 + v_2^2 + \cdots + v_n^2}.$$

$$\mathbf{v}^\top \mathbf{v} = v_1^2 + v_2^2 + \cdots + v_n^2 = \|\mathbf{v}\|^2.$$



Distance Between Two Vectors

$$\|\mathbf{u} - \mathbf{v}\|_2^2 = (\mathbf{u} - \mathbf{v})^\top (\mathbf{u} - \mathbf{v}) = \mathbf{u}^\top \mathbf{u} - 2\mathbf{u}^\top \mathbf{v} + \mathbf{v}^\top \mathbf{v}.$$

$$\frac{\partial f}{\partial \boldsymbol{\mu}_i} = \mathbf{0} \Rightarrow \frac{\partial}{\partial \boldsymbol{\mu}_i} \sum_{j=1}^{k} \sum_{\mathbf{x} \in \mathcal{C}_j} \|\mathbf{x} - \boldsymbol{\mu}_j\|_2^2 = \mathbf{0},\ \forall i \in [k]$$

$$\begin{aligned}
\frac{\partial}{\partial \boldsymbol{\mu}_i} \sum_{j=1}^{k} \sum_{\mathbf{x} \in \mathcal{C}_j} \|\mathbf{x} - \boldsymbol{\mu}_j\|_2^2 &= \sum_{\mathbf{x} \in \mathcal{C}_i} \frac{\partial}{\partial \boldsymbol{\mu}_i} \|\mathbf{x} - \boldsymbol{\mu}_i\|_2^2 \\
&= \sum_{\mathbf{x} \in \mathcal{C}_i} \frac{\partial}{\partial \boldsymbol{\mu}_i} \left((\mathbf{x} - \boldsymbol{\mu}_i)^\top (\mathbf{x} - \boldsymbol{\mu}_i) \right) \\
&= \sum_{\mathbf{x} \in \mathcal{C}_i} \frac{\partial}{\partial \boldsymbol{\mu}_i} \left((\mathbf{x}^\top - \boldsymbol{\mu}_i^\top)(\mathbf{x} - \boldsymbol{\mu}_i) \right) \\
&= \sum_{\mathbf{x} \in \mathcal{C}_i} \frac{\partial}{\partial \boldsymbol{\mu}_i} \left(\mathbf{x}^\top \mathbf{x} - \boldsymbol{\mu}_i^\top \mathbf{x} - \mathbf{x}^\top \boldsymbol{\mu}_i + \boldsymbol{\mu}_i^\top \boldsymbol{\mu}_i \right) \\
&= \sum_{\mathbf{x} \in \mathcal{C}_i} \frac{\partial}{\partial \boldsymbol{\mu}_i} \left(\mathbf{x}^\top \mathbf{x} - 2\boldsymbol{\mu}_i^\top \mathbf{x} + \boldsymbol{\mu}_i^\top \boldsymbol{\mu}_i \right)
\end{aligned}$$

$$
\begin{aligned}
\frac{\partial f}{\partial \boldsymbol{\mu}_i} \sum_{j=1}^{k} \sum_{\mathbf{x} \in \mathcal{C}_j} \|\mathbf{x} - \boldsymbol{\mu}_j\|_2^2 &= \sum_{\mathbf{x} \in \mathcal{C}_i} \frac{\partial f}{\partial \boldsymbol{\mu}_i} \left(\mathbf{x}^\top \mathbf{x} - 2\boldsymbol{\mu}_i^\top \mathbf{x} + \boldsymbol{\mu}_i^\top \boldsymbol{\mu}_i \right) \\
&= \sum_{\mathbf{x} \in \mathcal{C}_i} (-2\mathbf{x} + 2\boldsymbol{\mu}_i) \\
\Rightarrow \sum_{\mathbf{x} \in \mathcal{C}_i} (-2\mathbf{x} + 2\boldsymbol{\mu}_i) &= \mathbf{0} \\
\Rightarrow \sum_{\mathbf{x} \in \mathcal{C}_i} \boldsymbol{\mu}_i &= \sum_{\mathbf{x} \in \mathcal{C}_i} \mathbf{x} \\
\Rightarrow \boldsymbol{\mu}_i \sum_{\mathbf{x} \in \mathcal{C}_i} 1 &= \sum_{\mathbf{x} \in \mathcal{C}_i} \mathbf{x} \\
\Rightarrow \boldsymbol{\mu}_i |\mathcal{C}_i| &= \sum_{\mathbf{x} \in \mathcal{C}_i} \mathbf{x} \\
\Rightarrow \boldsymbol{\mu}_i &= \frac{1}{|\mathcal{C}_i|} \sum_{\mathbf{x} \in \mathcal{C}_i} \mathbf{x}
\end{aligned}
$$