TECHNISCHE UNIVERSITÄT KAISERSLAUTERN

9.2 Non-linear Clustering

Machine Learning 1: Foundations

Marius Kloft *(TUK)*

1 Linear Clustering

2 Non-linear Clustering

3 Hierarchical Clustering

Kernel k-means clustering

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function KMEANS(parameter k, inputs $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$)
  initialize cluster centers $\mathbf{c}_1, \ldots, \mathbf{c}_k$
  repeat
    for $i = 1 : n$ **do**
      label the input $\mathbf{x}_i$ as belonging to the nearest cluster,

$$y_i := \arg\min_{j=1,\ldots,k} \left\| \mathbf{x}_i - \mathbf{c}_j \right\|^2$$

    end for
    for $j = 1 : k$ **do**
      compute cluster center $\mathbf{c}_j$ as the mean of all inputs of the jth cluster,

$$\mathbf{c}_j := \mathrm{mean}(\{\mathbf{x}_i : y_i = j\})$$

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- Compute $\left\|\mathbf{x}_i - \mathbf{c}_j\right\|^2$ via kernel function

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  can be completely expressed in terms of kernel functions:
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But what if we want to cluster images?

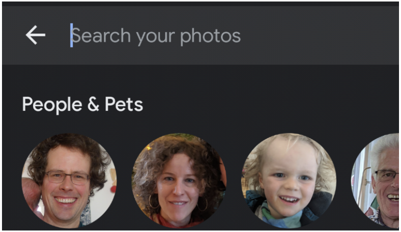
Example: Search Photo Collection For People

Given:

- Photo collection

Aim:

- Search for people



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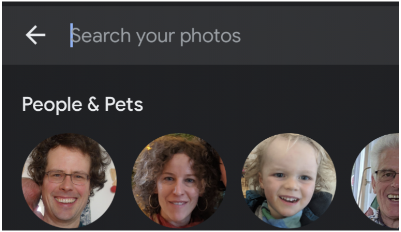
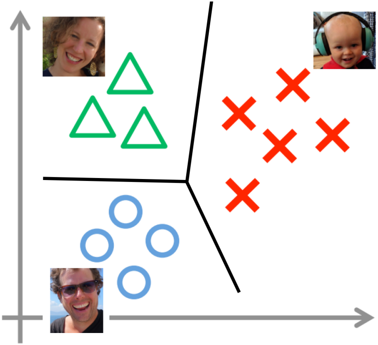


Solution:

- Automatically crop out portraits
- **Cluster the portraits**



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$$\min_{c=(\mathbf{c}_1,\ldots,\mathbf{c}_k)\in\mathbb{R}^{d\times k}} \sum_{i=1}^{n} \min_{j\in\{1,\ldots,k\}} \left\| \mathbf{x}_i - c_j \right\|^2$$

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Analog to regression and classification, we could "deepify" k-means as follows:

Deep k-means

$$\min_{W,\mathbf{c}} \; \frac{1}{2}\sum_{l=1}^{L} \left\|W^{(l)}\right\|_{\text{Fro}}^2 + \sum_{i=1}^{n} \min_{j\in\{1,\ldots,k\}} \left\|\phi_W(\mathbf{x}_i) - c_j\right\|^2$$

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But this method does not always work so well

- ongoing research topic to get this working

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2. Deep representation of data: For each input $\mathbf{x}_i$, compute its vector of activations in the last hidden layer $\phi_W(\mathbf{x}_i)$
3. Clustering: Run k-means on $\phi_W(\mathbf{x}_1), \ldots, \phi_W(\mathbf{x}_n)$