9.2 Non-linear Clustering

Machine Learning 1: Foundations

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1. Linear Clustering
2. Non-linear Clustering
3. Hierarchical Clustering

Kernel k-means clustering

The k-means clustering algorithm can be "kernelized".

```
function KMEANS(parameter k, inputs x_1, ..., x_n ∈ ℝ^d)
    initialize cluster centers c_1, ..., c_k
    repeat
        for i = 1 : n do
            label the input x_i as belonging to the nearest cluster,
                y_i := arg min_{j=1,...,k} ||x_i − c_j||^2
        end for
        for j = 1 : k do
            compute cluster center c_j as the mean of all inputs of the jth cluster,
                c_j := mean({x_i : y_i = j})
        end for
    until convergence criterion is met
    return cluster centers c_1, ..., c_k
end function
```

- Never compute mean explicitly
- Compute $\left\|\mathbf{x}_i - \mathbf{c}_j\right\|^2$ via kernel function

Kernel k-Means Clustering

- Let $\phi : \mathbb{R}^d \to \mathcal{H}$ be a kernel feature map, corresponding to a kernel $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$
- Let $I_j := \{i \in \{1, \ldots, n\} : y_i = j\}$ for all $j = 1, \ldots, k$
- Then $\mathbf{c}_j := \frac{1}{|I_j|} \sum_{i \in I_j} \phi(\mathbf{x}_i) \in \mathcal{H}$ (high dimensional!)
- However, $\left\|\phi(\mathbf{x}_i) - \mathbf{c}_j\right\|^2 = \underbrace{\|\phi(\mathbf{x}_i)\|^2}_{=k(\mathbf{x}_i,\mathbf{x}_i)} - 2\left\langle \phi(\mathbf{x}_i), \mathbf{c}_j \right\rangle + \left\|\mathbf{c}_j\right\|^2$

  can be completely expressed in terms of kernel functions:
  - $\|\mathbf{c}_j\|^2 = \frac{1}{|I_j|^2} \sum_{i,i' \in I_j} k(\mathbf{x}_i, \mathbf{x}_{i'})$ and
    $\langle \phi(\mathbf{x}_i), \mathbf{c}_j \rangle = \frac{1}{|I_j|} \sum_{i' \in I_j} k(\mathbf{x}_i, \mathbf{x}_{i'})$ □

But what if we want to cluster images?

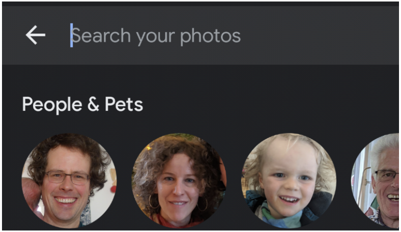
Example: Search Photo Collection For People

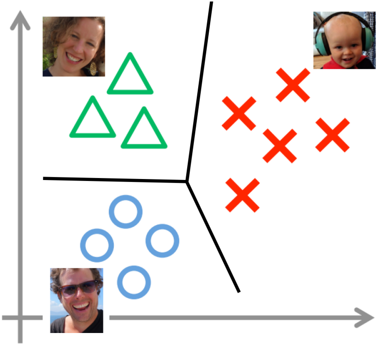
Given:

- Photo collection

Aim:

- Search for people





Solution:

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

Deep Clustering

Can we make k-means deep?

One can show:

- k-means minimizes the objective function

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

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

Deep k-means

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

But this method does not always work so well

- ongoing research topic to get this working

Another Idea: Transfer Learning

We learned this trick already in the class on overfitting:

1. Pre-training: Download an ANN with parameters W from the web that was pre-trained on huge amounts of images
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 $\phi_W(\mathbf{x}_1), \ldots, \phi_W(\mathbf{x}_n)$