Finding Optimal Number of Clusters

TOP: Data Clustering 076/091

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Outline

Number of Clusters

Needed for common clustering models such as k-means/median/center

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- Elbow method
- Calinski-Harabasz index
- Silhouette method
- Gap statistics

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Psuedo-science alert!

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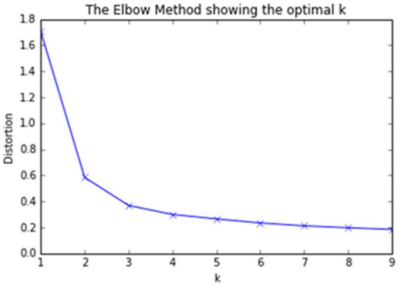
Finding Elbow of a Graph



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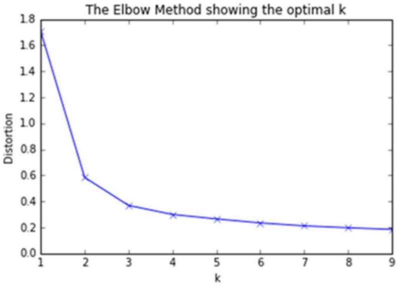

Advantages

- Simplicity of computation

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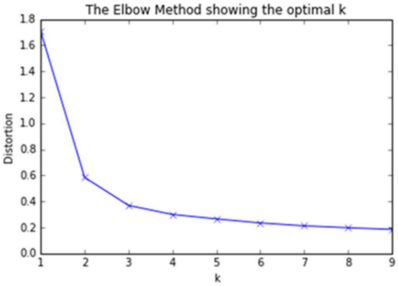
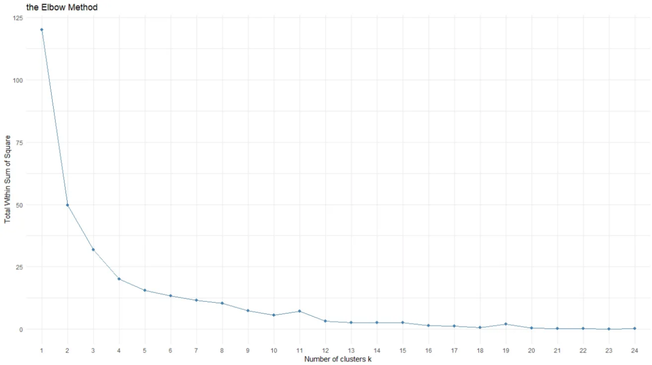


Advantages

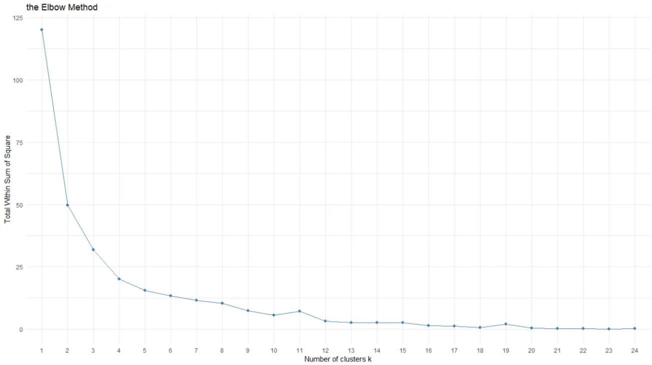
- Simplicity of computation
- Can work for any clustering model

Disadvantages



- Subjectivity in interpretation

Disadvantages



- Subjectivity in interpretation
- Can have multiple elbows: ambiguity with complex datasets

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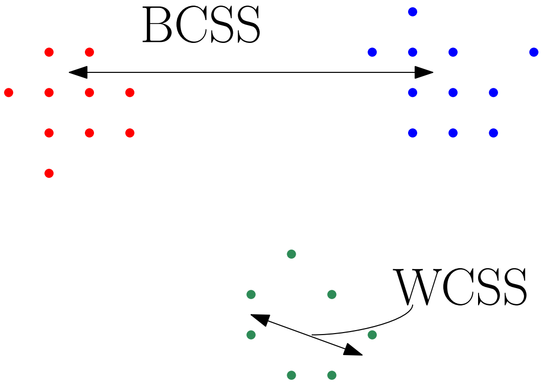
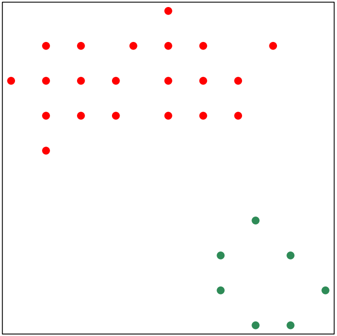
The higher is the better

Well-separated Clusters

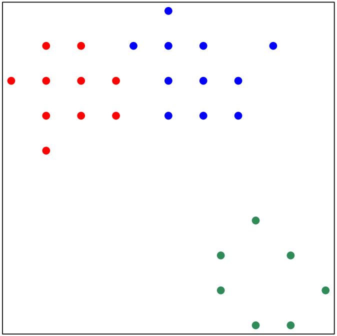


BCSS should be large and WCSS small

Why BCSS?



$k = 2$



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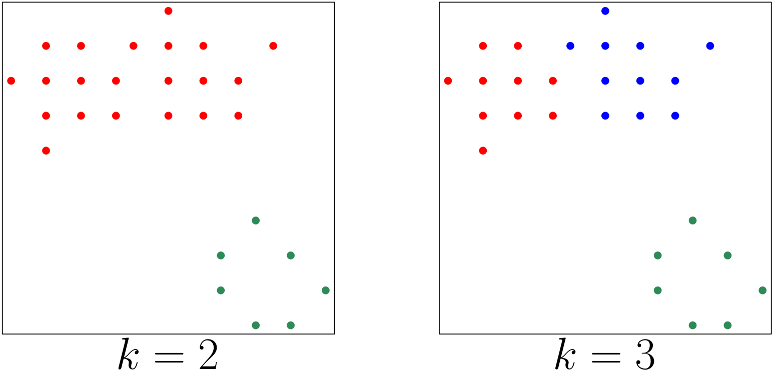

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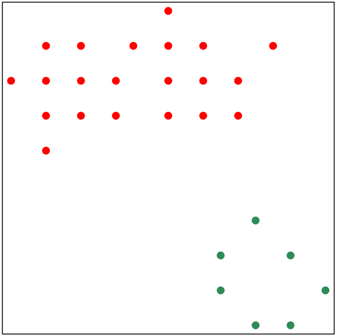

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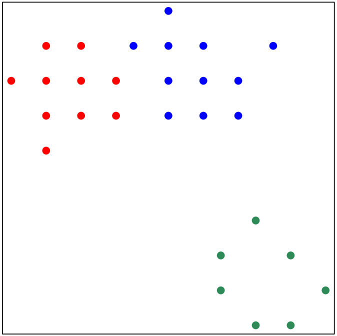

$k = 3$

CH-index might stop unnecessary splitting of clusters—>
assumes clusters are well-separated

Properties

Pros

- Objective measure
- Fast computation

Properties

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- Objective measure
- Fast computation

Cons

- Sensitivity to cluster shape
- Limited interpretability

Outline

Silhouette Coefficient

For any point x_i,

$$S(x_i) = \frac{b_i - a_i}{\max\{a_i, b_i\}}$$

a_i is proxy for WCSS; b_i is proxy for BCSS

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b_i is the smallest average distance of x_i to all points in any other cluster

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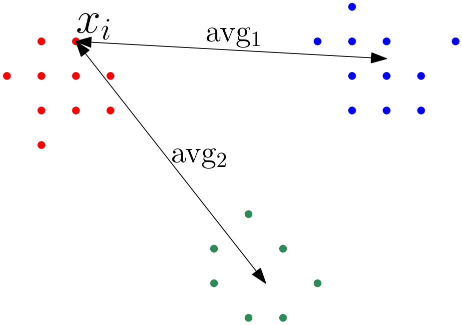

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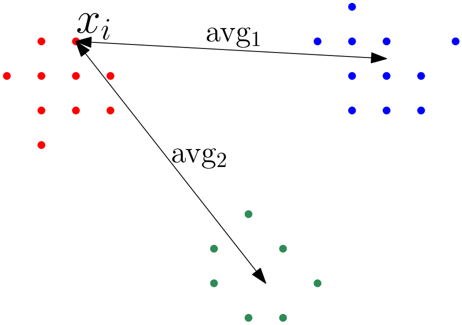

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b_i is the minimum average separation from x_i

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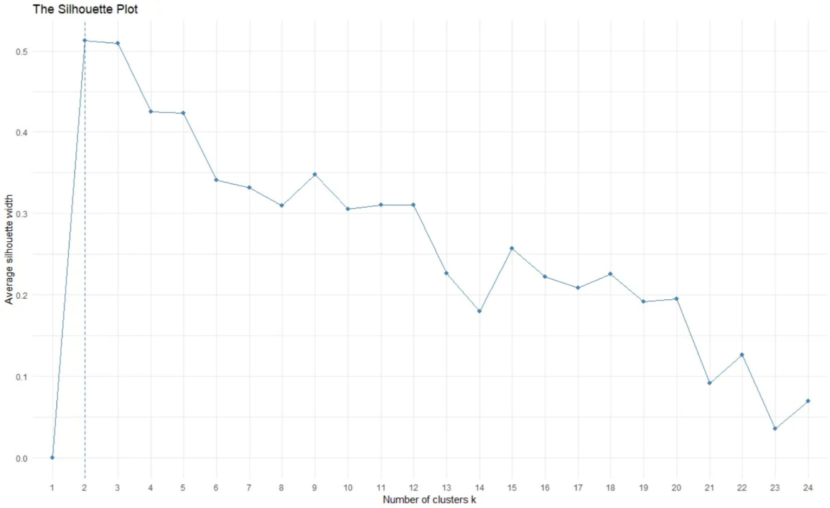
Value ranges between -1 and 1: 1 -> well-separated clusters, 0 -> overlapping or ambiguous clusters, negative -> poorly separated data points

Silhouette Plot



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- Objective measure
- Individual data point assessment
- Intuitive interpretation
- Works with different clustering models

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- Objective measure
- Individual data point assessment
- Intuitive interpretation
- Works with different clustering models

Cons

- Difficulty with overlapping clusters
- Computational complexity

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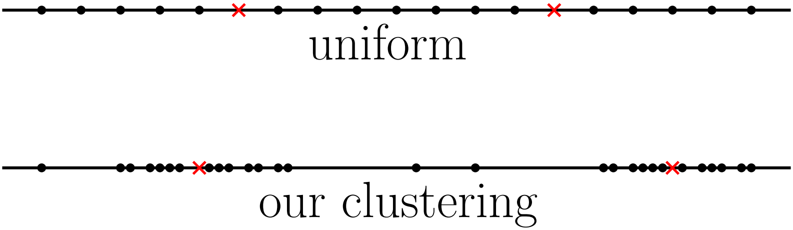
- Clustering cost of reference data is expected to be large

Uniform vs Regular Clusters



Motivation

$$Gap_n(k) = E_n^*\{WCSS(k)\} - WCSS(k)$$

- The expectation/mean is taken over B samples of size n from a reference null distribution
- Null $->$ a distribution with no obvious clustering/clusters are not well-separated
- Uniform distribution is an example $->$ for each feature, pick a value within the range of observed values
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For optimal k, the gap is expected to be maximized/falls the farthest below the reference curve

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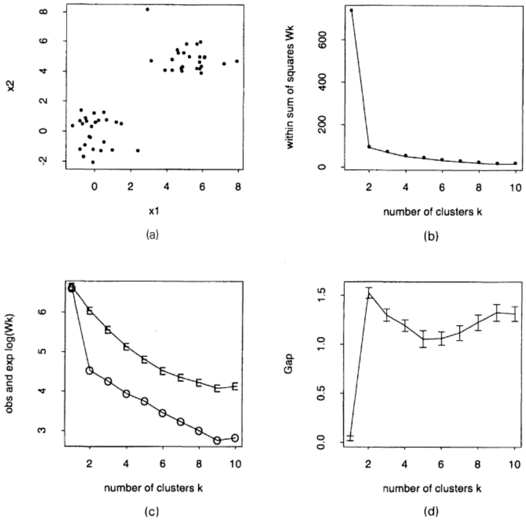
$$E_n^*\{\log WCSS(k)\} = \frac{1}{B}\sum_i \log W_i^* = \frac{1}{B}\log(\Pi_i W_i^*)$$

$$= \log(\Pi_i W_i^*)^{1/B}$$

$$Gap_n(k) = \log \frac{(\Pi_i W_i^*)^{1/B}}{WCSS(k)}$$

An Example



x2
x1
(a)
within sum of squares Wk
number of clusters k
(b)
obs and exp log(Wk)
number of clusters k
(c)
Gap
number of clusters k
(d)

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- Objective measure
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Cons

- Computationally intensive
- Limited applicability to certain datasets
- Lack of consensus on reference distribution

Take Home Message

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- Try multiple methods; compare and contrast

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- Always remember clustering is an exploratory technique

Links

[Implementation in R]

[Implementation in Python]

[Gap statistics paper]

[CH-index paper]