PRESENTAZIONE PROGETTO MACHINE LEARNING

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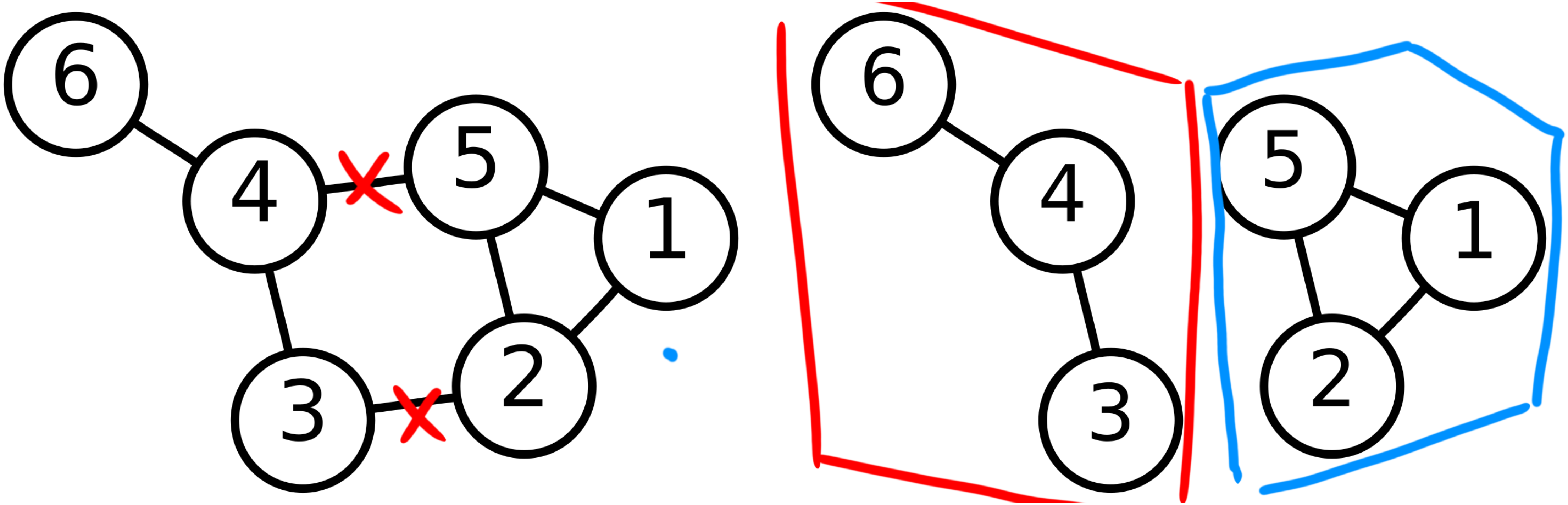
Topics:

1. Idea of Spectral Clustering, Refreshers on SVD
2. Spectral Clustering Algorithm and its SVD-based variant
3. Experiments

Spectral Clustering (Idea)

Idea: Group data by building a similarity graph, use clusters within the graph by optimal cuts



We will se how we can implement this

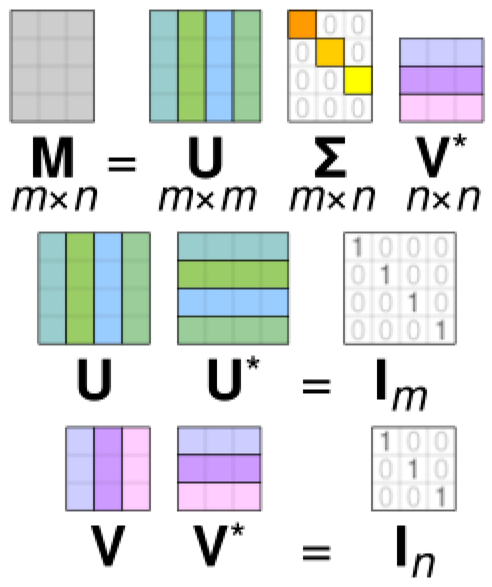
SVD (Refreshers)

The *SVD* (Singular-Value Decomposition) is a popular matrix decomposition technique based on the spectral decomposition

$$A = U\Sigma V^T$$

Applications:

- Low-Rank Reduction of Matrixes (Eckart-Young Theorem)
- Image Compression
- Dimensionality
- **We will see**: Clustering



Spectral Clustering (Non-Normalised)

Unnormalized spectral clustering

Input: Similarity matrix $S \in \mathbb{R}^{n\times n}$, number k of clusters to construct.

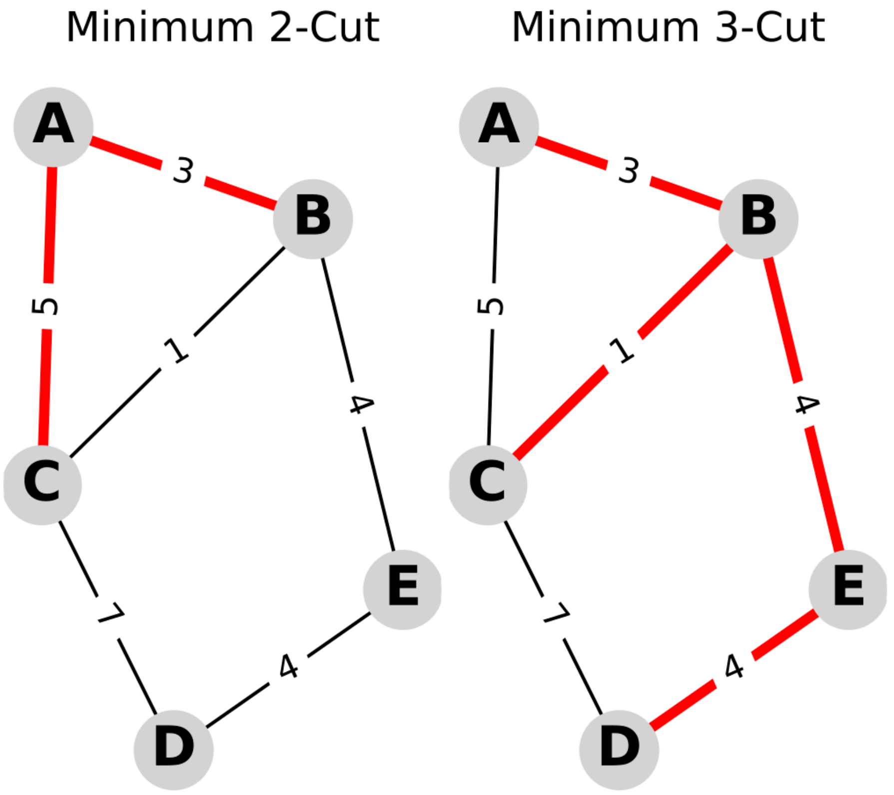
- Construct a similarity graph by one of the ways described in Sect. 2. Let W be its weighted adjacency matrix.
- Compute the unnormalized Laplacian L.
- **Compute the first k eigenvectors $u_1,\ldots,u_k$ of L.**
- Let $U \in \mathbb{R}^{n\times k}$ be the matrix containing the vectors $u_1,\ldots,u_k$ as columns.
- For $i = 1,\ldots,n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the i-th row of U.
- Cluster the points $(y_i)_{i=1,\ldots,n}$ in $\mathbb{R}^k$ with the k-means algorithm into clusters $C_1,\ldots,C_k$.

Output: Clusters $A_1,\ldots,A_k$ with $A_i = \{j \mid y_j \in C_i\}$.

> *Source: Ulrike von Luxburg, A Tutorial on Spectral Clustering*

Spectral Clustering (Remark)

> **Remark**: it can be proved that the algorithm previously described solves the relaxed version of the min. k-cuts problem of the graph G



SVD-Based Spectral Clustering (Idea)

IDEA. Instead of finding the eigenvalues of the Laplacian $L = D - A$, diagonalize the matrixes $A^T A$ and AA^T (thus determining a SVD of A)

Proposed by Zhixian Jia, in the paper "The reaserch on parameters of spectral clustering based on SVD" (2013)

SVD-Based Spectral Clustering

Parameters:

- Number of clusters k
- Amount of left-sided singular vectors to consider l (usually $l = k$)

Algorithm:

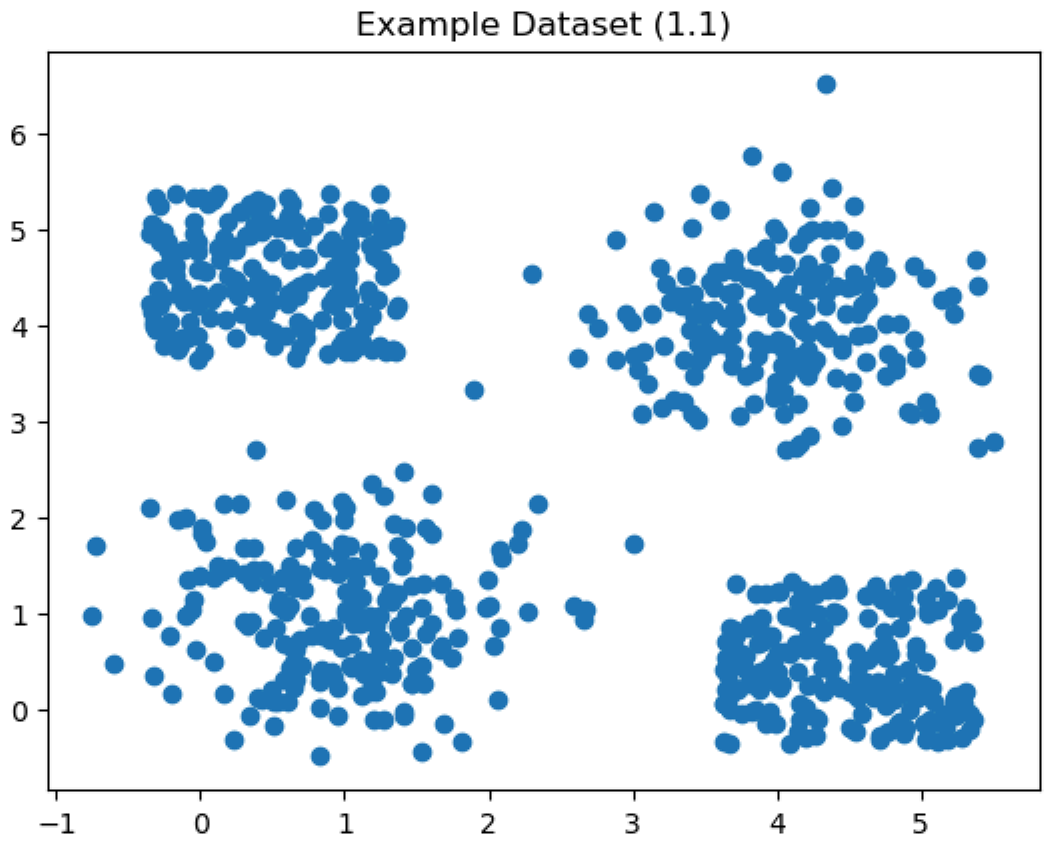
1. Create the similarity matrix A with a desired method
2. Determine a SVD of A, i.e. $A = V \Sigma U^T$
3. Take the first l columns of V, denote it as V'
4. Run *K-means* on V', the resulting clusters is the output

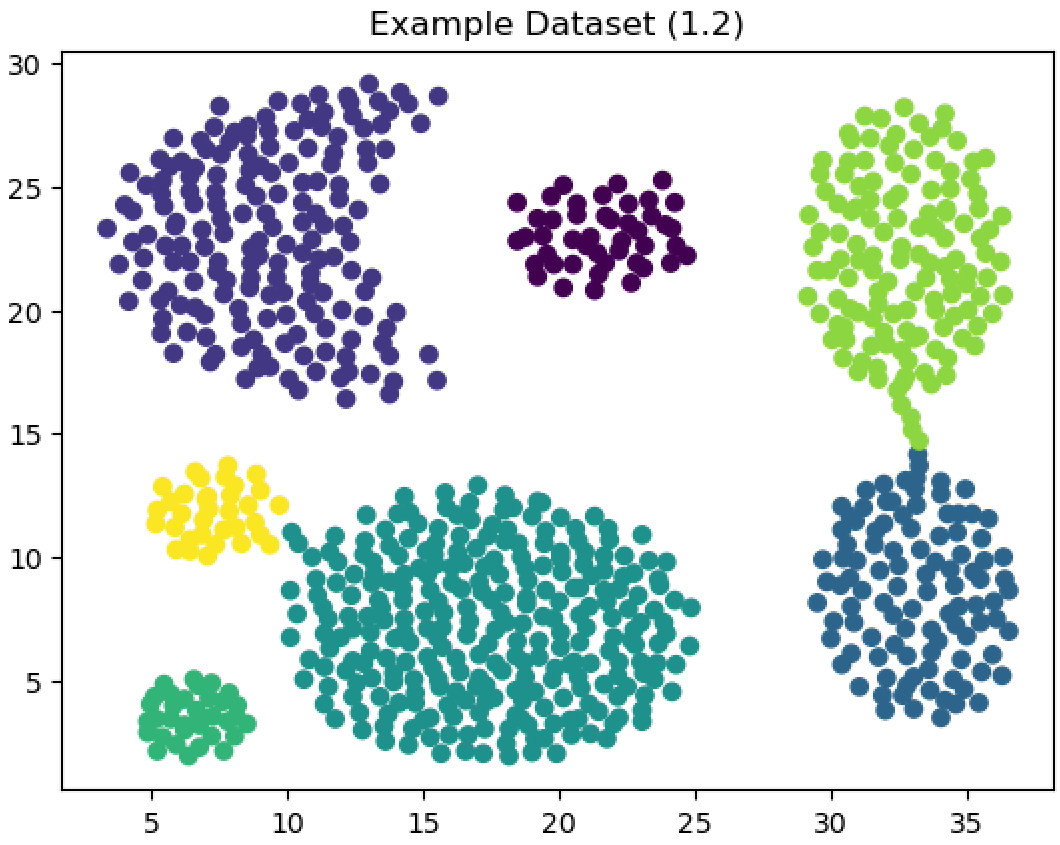
Main Results: Synthetic Datasets

Three main experiments, based on synthetically generated datasets:

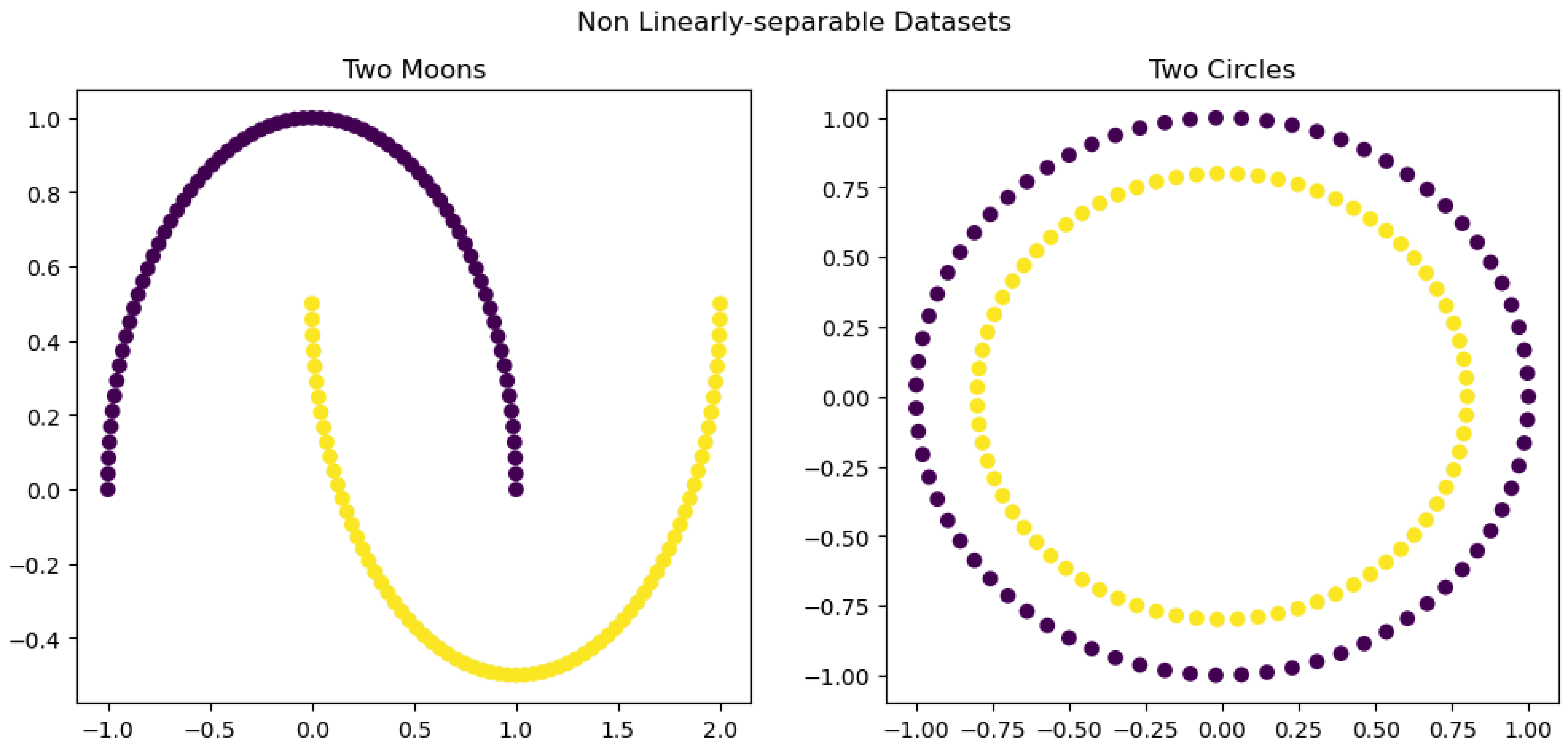
1. Compare the performances between Spectral Clustering and its SVD variant. Two similarity graph construction methods: Gaussian Kernel (fully connected graph) and KNN-graph.
2. Test the SVD-Based Clustering on non-linear datasets (with variations on the parameters)
3. Deduce the parameter k from the singular values contained in Σ

Synthetic Datasets

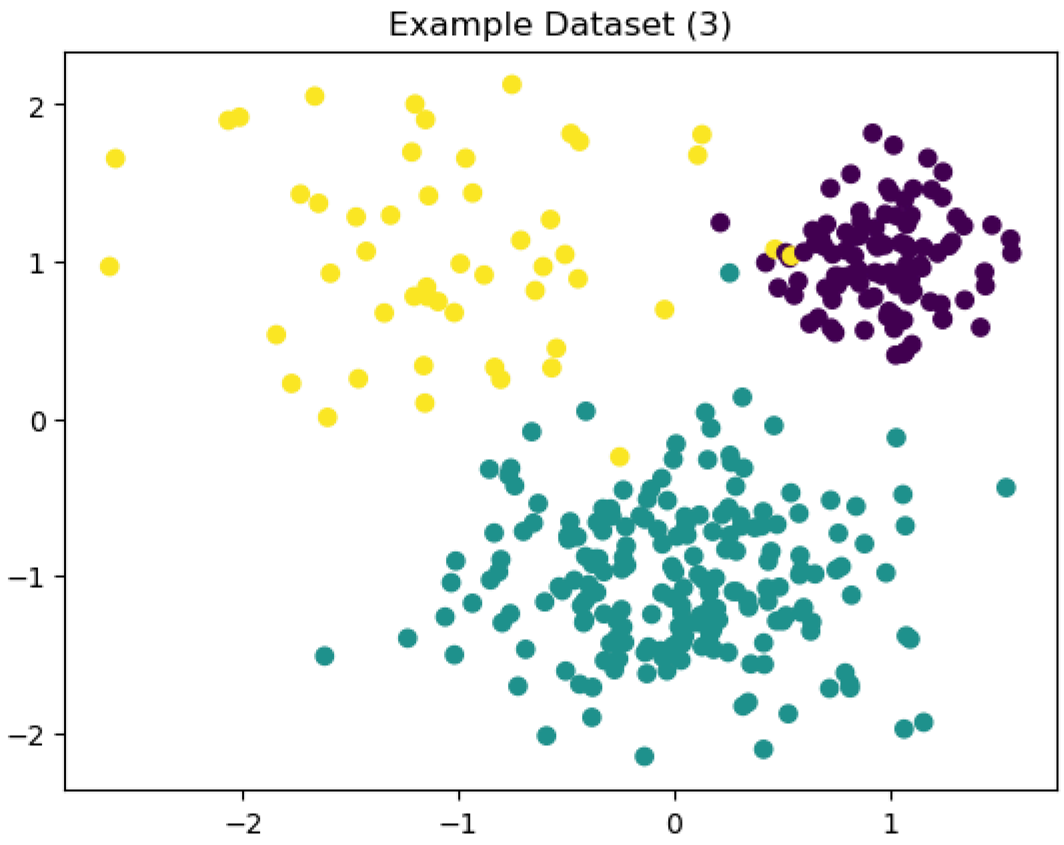




Synthetic Datasets

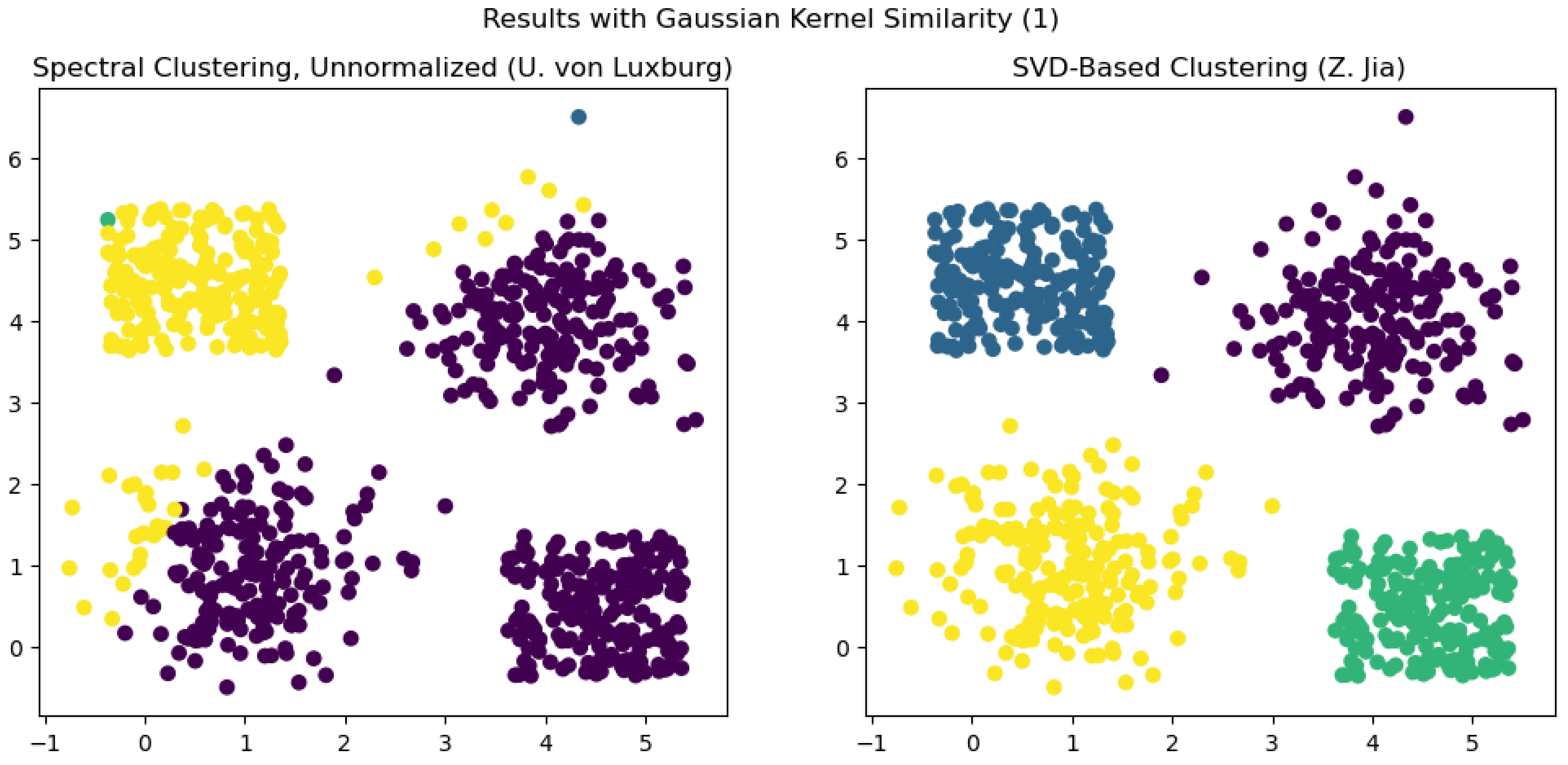


Synthetic Datasets



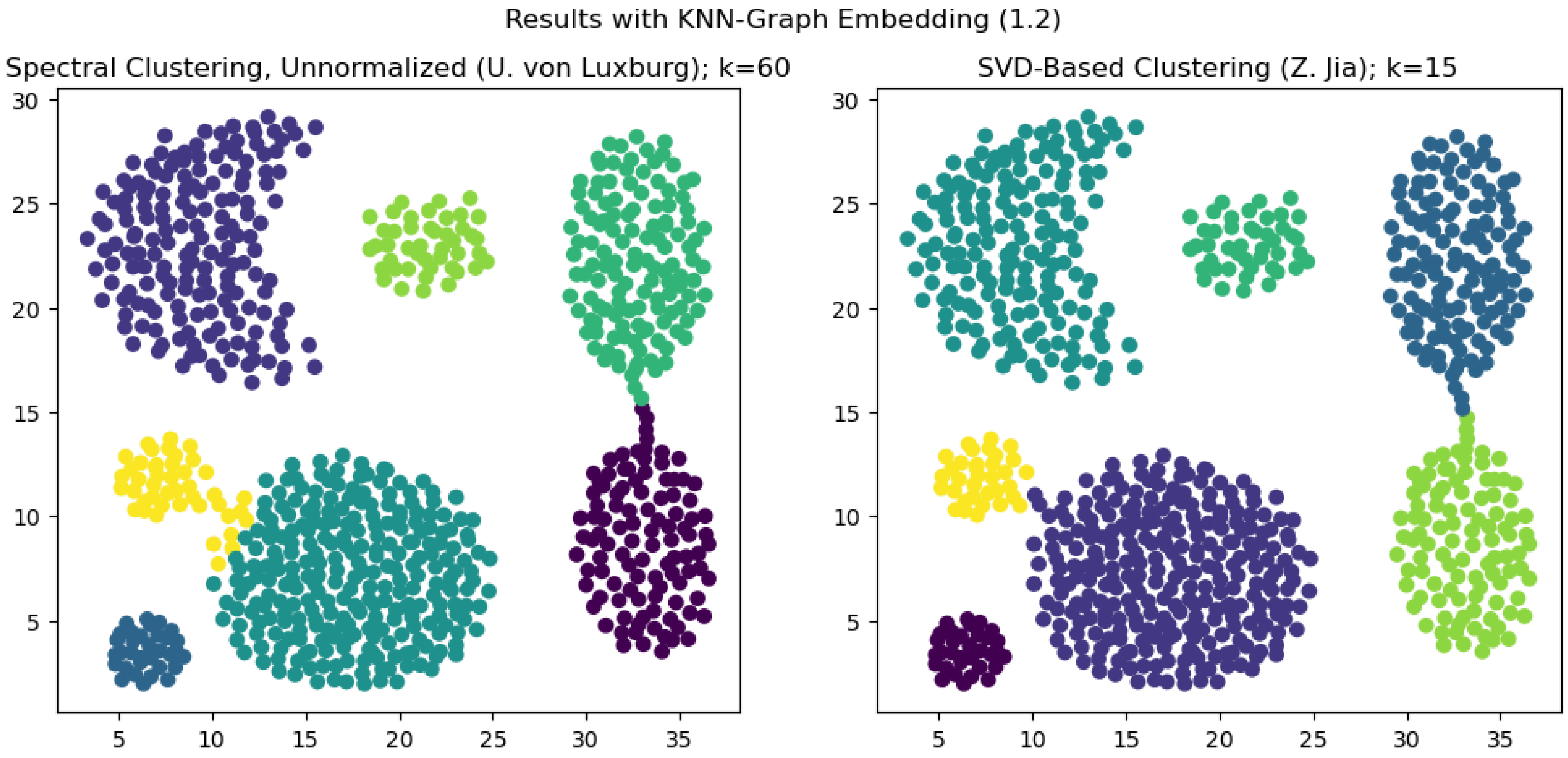
Experiment 1.1

Similarity Measure: Gaussian Kernel $s(x, y) = \exp\left(\|x - y\|_2/(2\sigma)^2\right)$ with $\sigma = 1.7$



Experiment 1.2

Similarity Measure: KNN-embedding. For classical SC, $k = 60$; for SVD-Based SC, $k = 15$.



Expriment 1 (Remarks)

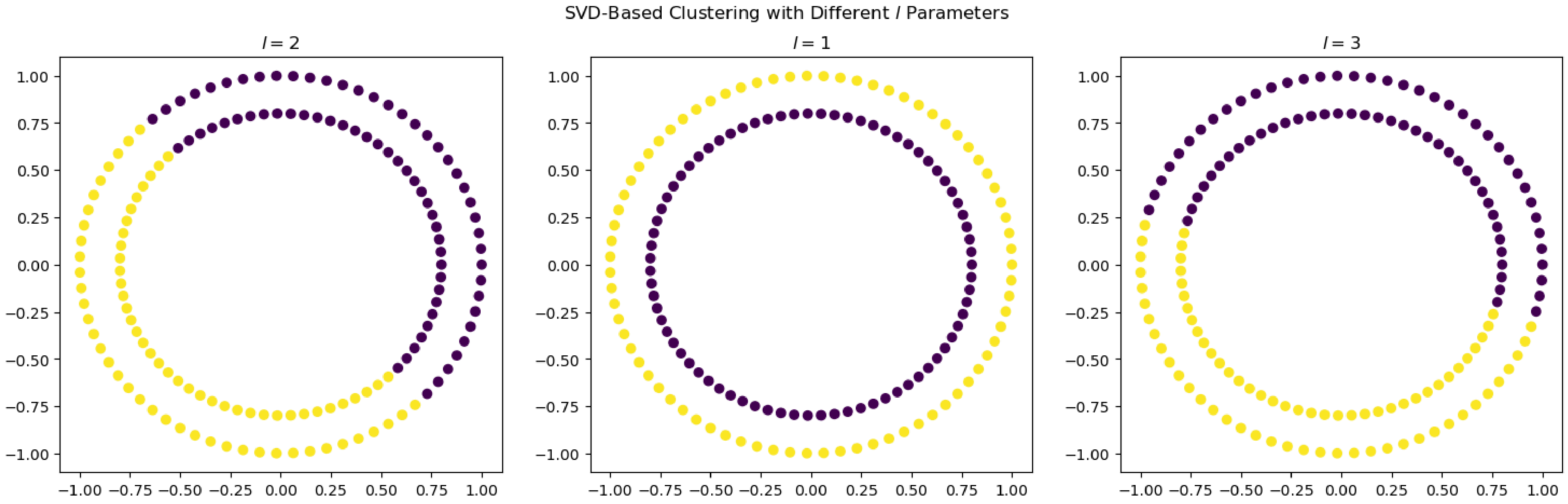
- Classical Spectral Clustering produces unsatisfying clusters
- SVD-based variant produces well-separated clusters
- To fix the issue with the classical Spectral Clustering, other approaches could have been taken:
    - Use another method to construct the similarity graph (e.g. K-nearest neighbours)
    - Use the Normalized Laplacian instead
- In fact, in experiment 1.2. both methods were able to handle the dataset with the KNN-embedding; however, the SVD-variant method requires a smaller k value

Experiment 2

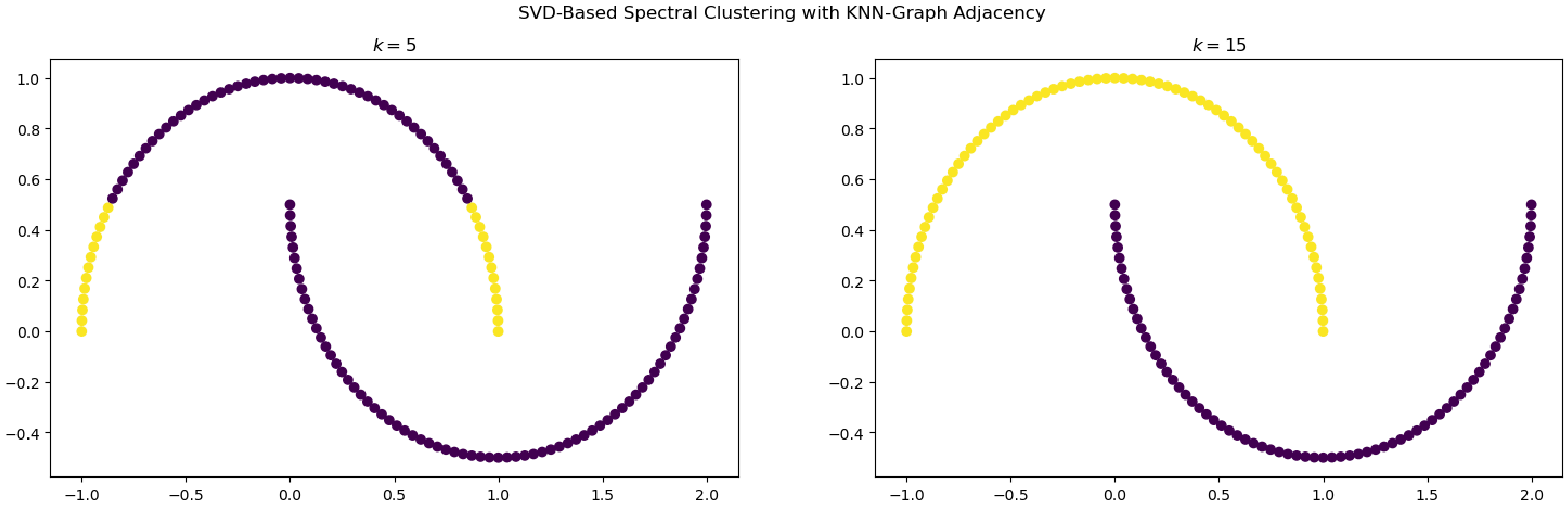
Similarity Measure: For the two circles, we used the same one in Experiment 1. For the two moons dataset, we used the K-nearest neighbours method to construct the similarity graph

Parameters: For the two circles dataset, we tweaked the hyperparameter l for $l = 1$, $l = 2$.

Experiment 2 (Results)



Experiment 2 (Results)



Experiment 2 (Remarks)

- By changing the hyperparameters, SVD-Based Spectral Clustering is able to handle non-linearly separable datasets
- In some cases, reducing the l parameter can reveal to be useful (whereas usually it is to be set $l \geq k$, usually $l = k$)

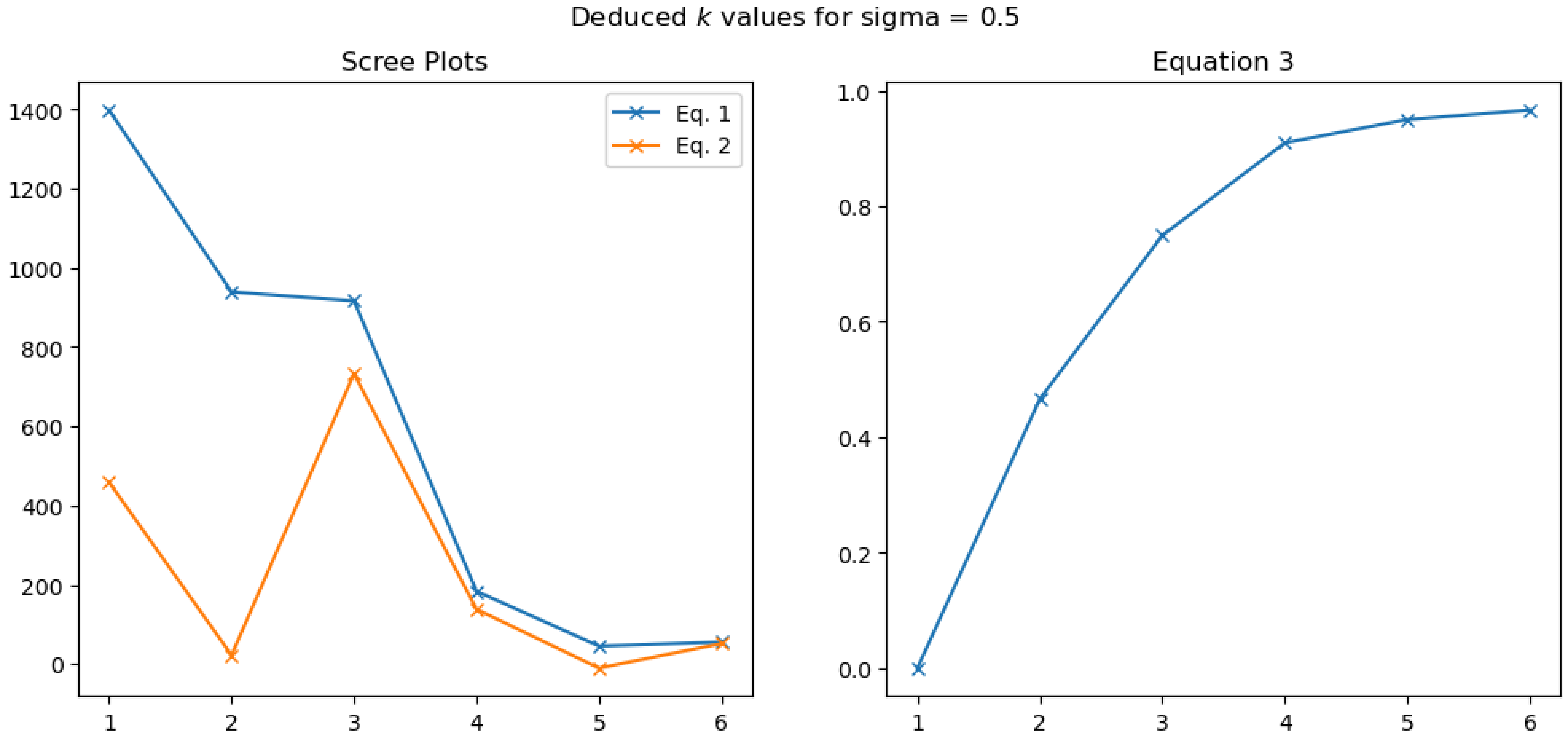
Experiment 3: Deducing Parameters

- To determine the optimal value for k, three formulas have been employed:

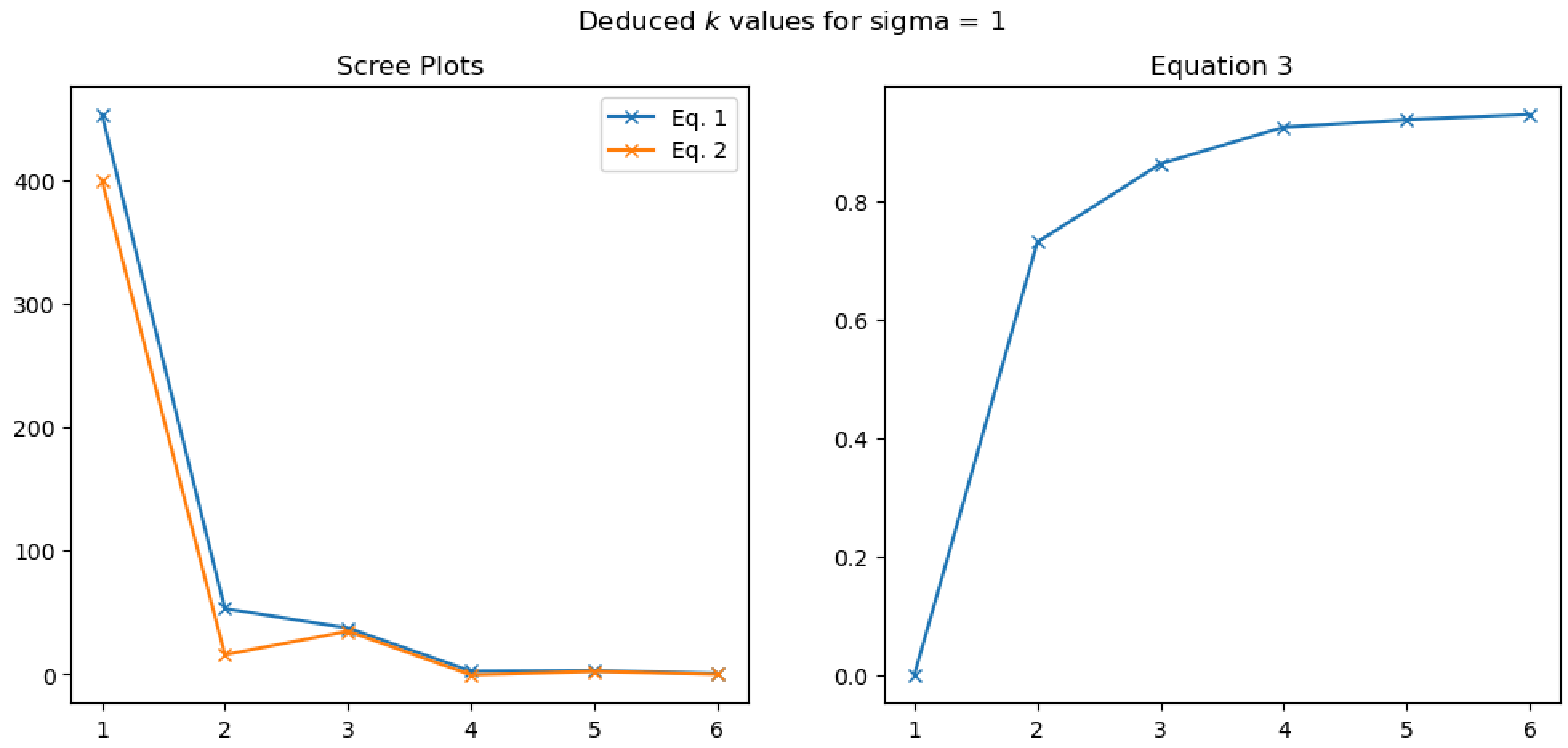
$$(1)\ \sigma_k - \sigma_{k+1}$$
$$(2)\ \sigma_k - 2\sigma_{k+1} + \sigma_{k+2}$$
$$(3)\ \frac{\sum_{i\leq k}\sigma_i}{\sum_{i\leq N}\sigma_i}$$

- Where in (1) or (2) we can find the optimal k value or use the elbow method
- In (3) we want to find the minimal k such that its value is greater than a set threshold $\theta \in (0, 1)$, which is to be derived through experimenting
- To verify the hyperparameter of the similarity measure (e.g. for the gaussian kernel it's σ), compare the k derived from (2), (3) and verify that they're consistent

Experiment 3: Analysis



Experiment 3: Analysis



Experiment 3: Results

Therefore we deduced the variables $k = 3$ and $\sigma = 1$