Agglomerative Hierarchical Kernel Spectral Data Clustering (AH-KSC)

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Introduction

- Clustering is widely used technique in data mining and machine learning [1].
- Core concept is to identify inherent groups present within the data.
- Real-life data exhibits hierarchical clustering organization [2].
- Spectral clustering methods [3, 4, 5] are state-of-the-art.
- Perform eigen-decomposition of a pairwise similarity matrix resulting in localized structures for the k clusters in the eigenspace.
- Computationally infeasible $O(N^3)$ and memory extensive $O(N^2)$ for large data.
- Provide flat clustering and not easy to extend it to obtain hierarchical clusters.

Background

- A kernel spectral clustering (KSC) [6] method based on weighted kernel PCA (wk-PCA) was formulated in a primal-dual setting.
- The KSC learning framework has a training, validation and test phase.
- The model parameters like k (number of clusters) and kernel parameter σ/σ_{χ^2} are obtained during validation stage.
- KSC model has a powerful out-of-sample extensions property which allows cluster affiliation for previously unseen data.

Related Work

- A hierarchical kernel spectral clustering (HKSC) was proposed in [7].
- Multiple scales of σ were used to generate KSC model for different k resulting in independent cluster memberships at various levels of hierarchy.
- Special linkage criterion [7] was designed to merge these clusters.
- One drawback is that as cluster memberships are obtained from different KSC models for different values of k, σ, the merge is usually not perfect.
- Several points are forced to merge using the majority rule [7].
- An Agglomerative Hierarchical KSC (AH-KSC) was proposed in [8, 9] for networks which overcomes the shortcomings of HKSC.

Goal

Given a dataset detect multiples levels of hierarchy with meaningful clusters at each level of hierarchy using a modified version of Agglomerative Hierarchical Kernel Spectral Clustering (AH-KSC) technique [8, 9] oriented for data and images.

Real-Image Illustration

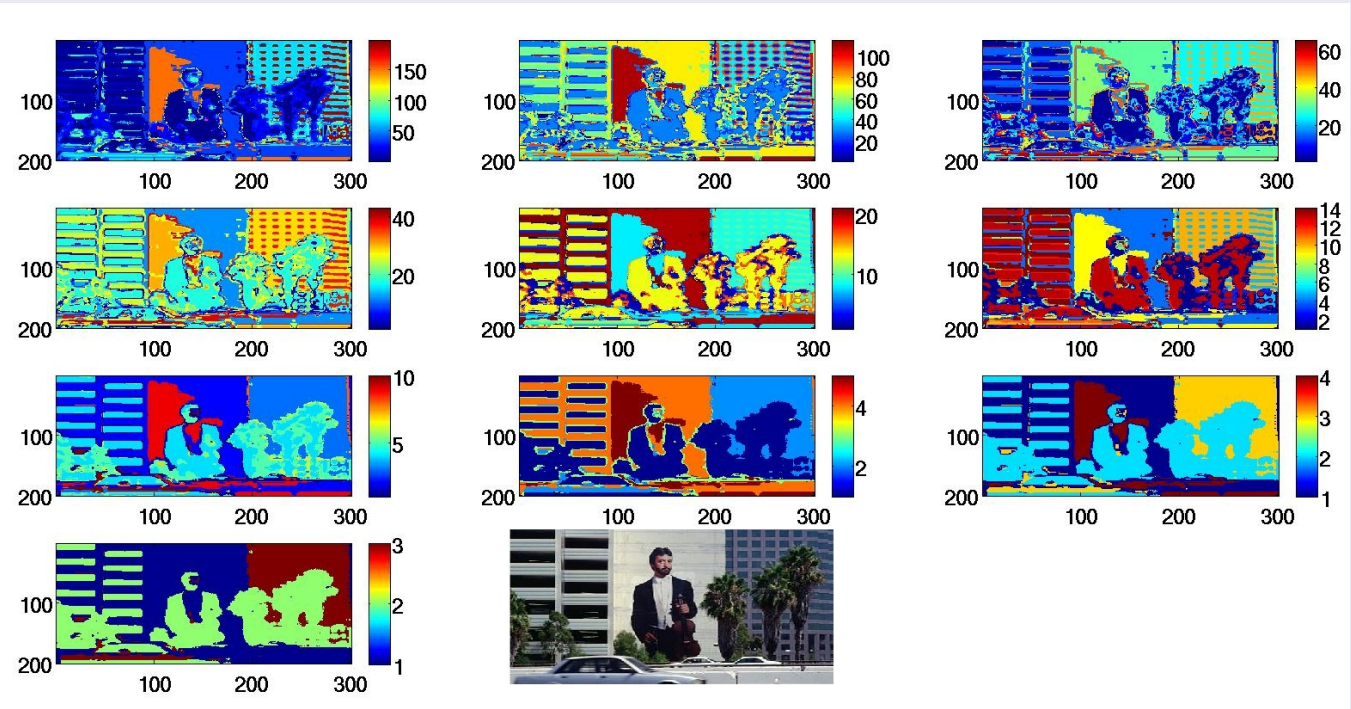


Figure: Result of AH-KSC method on a real world image dataset.

Contributions

- Extend AH-KSC technique from complex networks to datasets and images.
- Obtain optimal model parameters (σ, k) using balanced angular fitting (BAF) criterion [10] which generally corresponds to one level of hierarchy.
- BAF criterion can capture multiple peaks corresponding to different levels of hierarchy for an optimal σ.
- Exploit eigen-projections to obtain a set ($\mathcal{T}$) of distance thresholds.
- Utilize distance thresholds ($t_i \in \mathcal{T}$) to obtain multiple levels of hierarchy for datasets and images.

Building Blocks

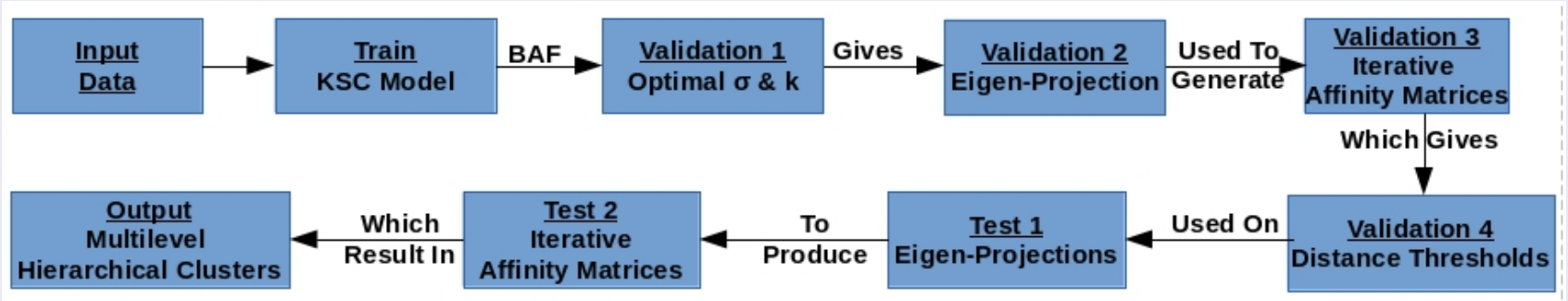


Figure: Steps of AH-KSC method [8, 9] with additional step where the optimal σ and k are estimated.

Kernel Spectral Clustering

KSC Formulation

Given $\mathcal{D} = \{x_i\}_{i=1}^{N_{tr}}$ and *maxk*, the primal formulation of the weighted kPCA is given by:

$$\min_{w^{(l)}, e^{(l)}, b_l} \quad \frac{1}{2} \sum_{l=1}^{maxk-1} w^{(l)\intercal} w^{(l)} - \frac{1}{2N_{tr}} \sum_{l=1}^{maxk-1} \gamma_l e^{(l)\intercal} D_\Omega^{-1} e^{(l)} \tag{1}$$

$$\text{such that} \quad e^{(l)} = \Phi w^{(l)} + b_l 1_{N_{tr}}, l = 1, \ldots, maxk - 1$$

KSC Primal-Dual Model

- Primal clustering model is given as: $e_i^{(l)} = w^{(l)\intercal} \phi(x_i) + b_l, i = 1, \ldots, N_{tr}$.
- Corresponding dual problem becomes: $D_\Omega^{-1} M_D \Omega \alpha^{(l)} = \lambda_l \alpha^{(l)}$.
- Dual predictive model is given as: $\hat{e}^{(l)}(x) = \sum_{i=1}^{N_{tr}} \alpha_i^{(l)} K(x, x_i) + b_l$.
- Each element of Ω, denoted as $\Omega_{ij} = K(x_i, x_j) = \phi(x_i)^\intercal \phi(x_j)$ is obtained for example using radial-basis function (RBF) kernel.

Model Selection

Balanced Angular Fitting

- The Balanced Angular Fitting (BAF) criterion [10] is defined as:

$$\begin{aligned} &\text{BAF}(k,\sigma) = \eta \sum_{p=1}^{k} \sum_{valid_{(i,\sigma)} \in Q_p} \frac{1}{k} \cdot \frac{MS(valid_{(i,\sigma)})}{|Q_p|} + (1-\eta)\frac{\min_l |Q_l|}{\max_m |Q_m|}, \\ &MS(valid_{(i,\sigma)}) = \max_j \cos(\theta_{j,valid_{(i,\sigma)}}), j = 1,\ldots,k \\ &cos(\theta_{j,valid_{(i,\sigma)}}) = \frac{\mu_j^{\mathsf{T}} e_{valid_{(i,\sigma)}}}{\|\mu_j\| \|e_{valid_{(i,\sigma)}}\|}, j = 1,\ldots,k. \end{aligned} \tag{2}$$

- Q_p represents the set of validation points belonging to cluster p.
- BAF criterion is based on angular similarity of validation points to cluster means.
- Validation points are allocated to clusters (μ_j) based on least angular distance.
- BAF criterion varies from $[-1, 1]$ and higher values are better for a given k.

Model Selection

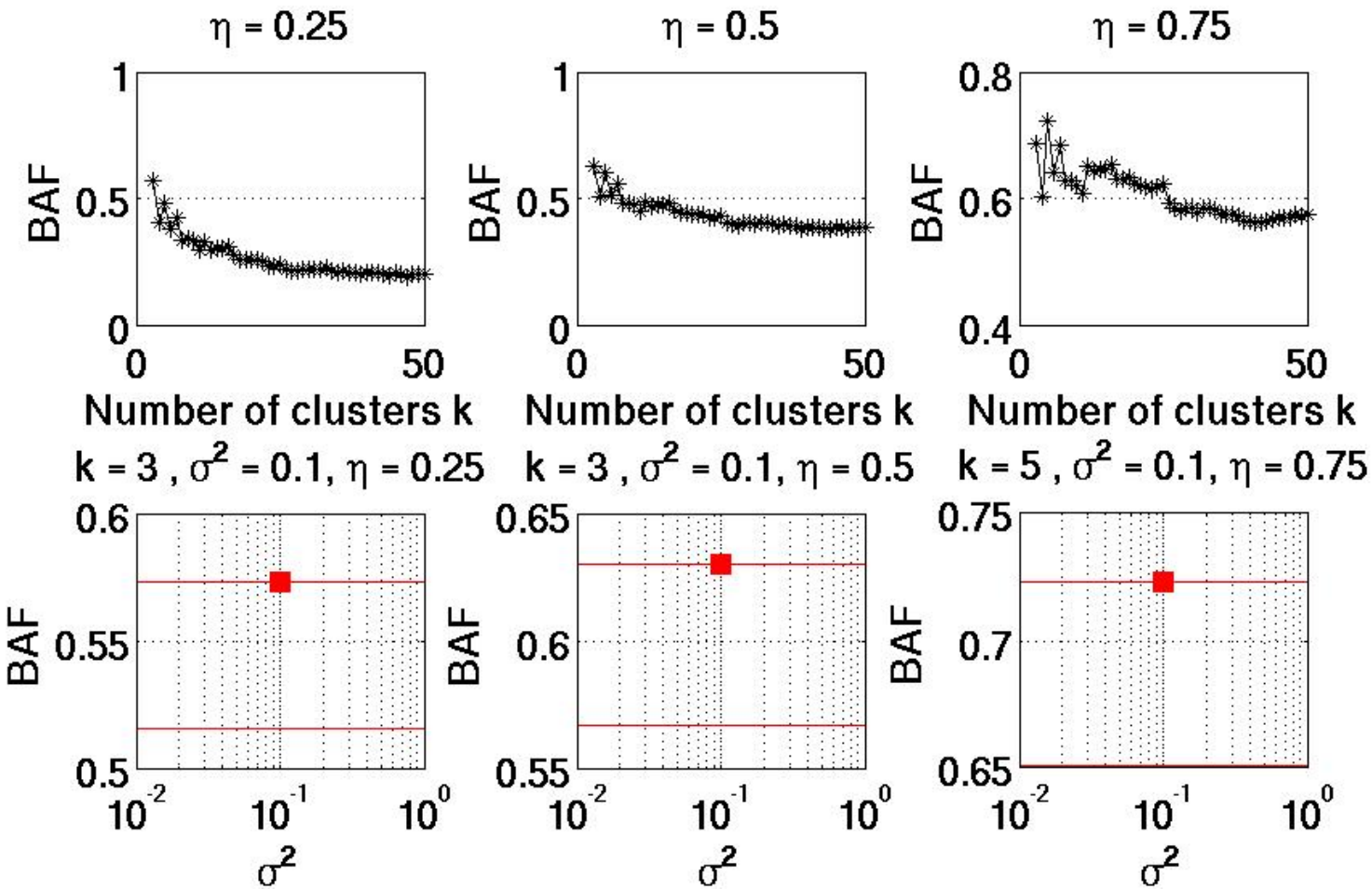


Figure: Selection of optimal σ using BAF criterion and illustration of multiple peaks in the BAF curve for different values of k for image dataset.

AH-KSC method

Determining Distance Thresholds

1. Create $S^{(0)}_{valid}$ for the validation projections (P_{valid}) as:
$$S^{(0)}_{valid}(i,j) = CosDist(e_i, e_j) = 1 - \cos(e_i, e_j) = 1 - \frac{e_i^{\mathsf{T}} e_j}{\|e_i\|\|e_j\|}.$$
2. Set initial distance threshold $t^{(0)} \in 0.15$ & $h = 0$.
3. *GreedyMaxOrder* [8, 9] gives $C^{(h)}$ and k at level h.
4. Generate affinity matrix at level h of hierarchy as:
$$S^{(h)}_{valid}(i,j) = \frac{\sum_{m \in C_i^{(h-1)}} \sum_{l \in C_j^{(h-1)}} S^{(h-1)}_{valid}(m,l)}{|C_i^{(h-1)}| \times |C_j^{(h-1)}|} \tag{3}$$
5. Threshold $t^{(h)} = \text{mean}(\min_j(S^{(h)}_{valid}(i,j))), i \neq j$ at level h.
6. Repeat Steps 4,5,6 till $k = 1$.
7. Obtain $\mathcal{T} = \{t^{(0)}, \ldots, t^{(maxh)}\}$.

AH-KSC method

Agglomerative Hierarchical KSC for Test Data

- Retrieve eigen-projections (P_{test}) for test set.
- To self-tune the approach use $t^{(i)} > t^{(0)}$, $i > 0$.
- Use *GreedyFirstOrder* [8, 9] to obtain $S_{test}^{(2)}$, $C^{(1)}$ and k.
- *For each* $t^{(h)} \in \mathcal{T}$, $h > 1$ do
  1. $[C^{(h)}, k] = GreedyMaxOrder(S_{test}^{(h)}, t^{(h)})$.
  2. Add $C^{(h)}$ to the set $\mathcal{C}$.
  3. Create $S_{test}^{(h+1)}$ using $S_{test}^{(h)}$ and $C^{(h)}$ as shown in (3).
- Results in the set $\mathcal{C}$ with cluster memberships.
- Propagate cluster memberships from lowest to coarsest level of hierarchy.

AH-KSC Illustration

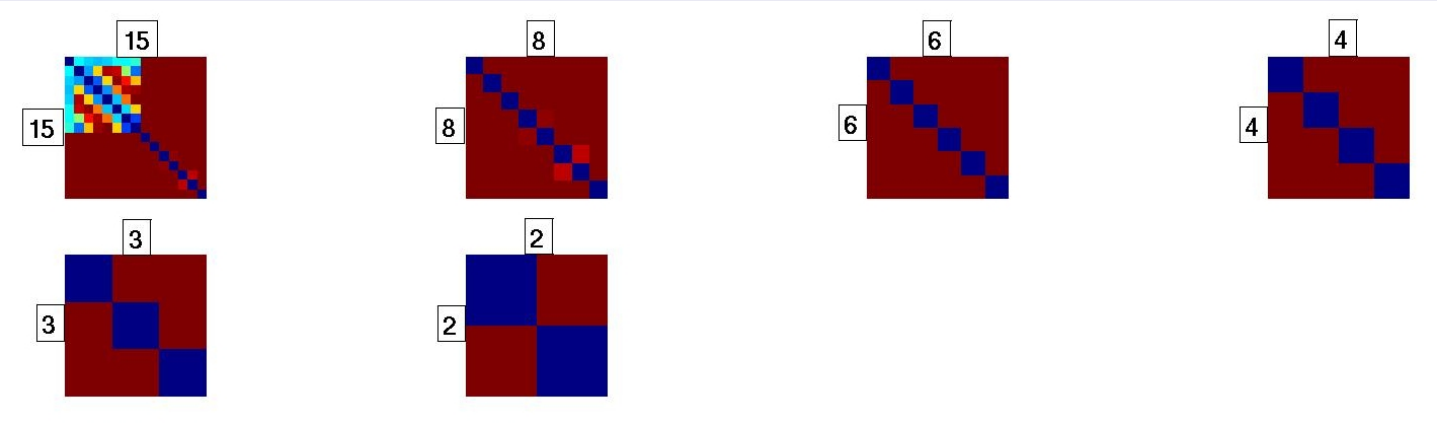


Figure: $S^{(h)}$ created at different levels of hierarchy in left to right order.

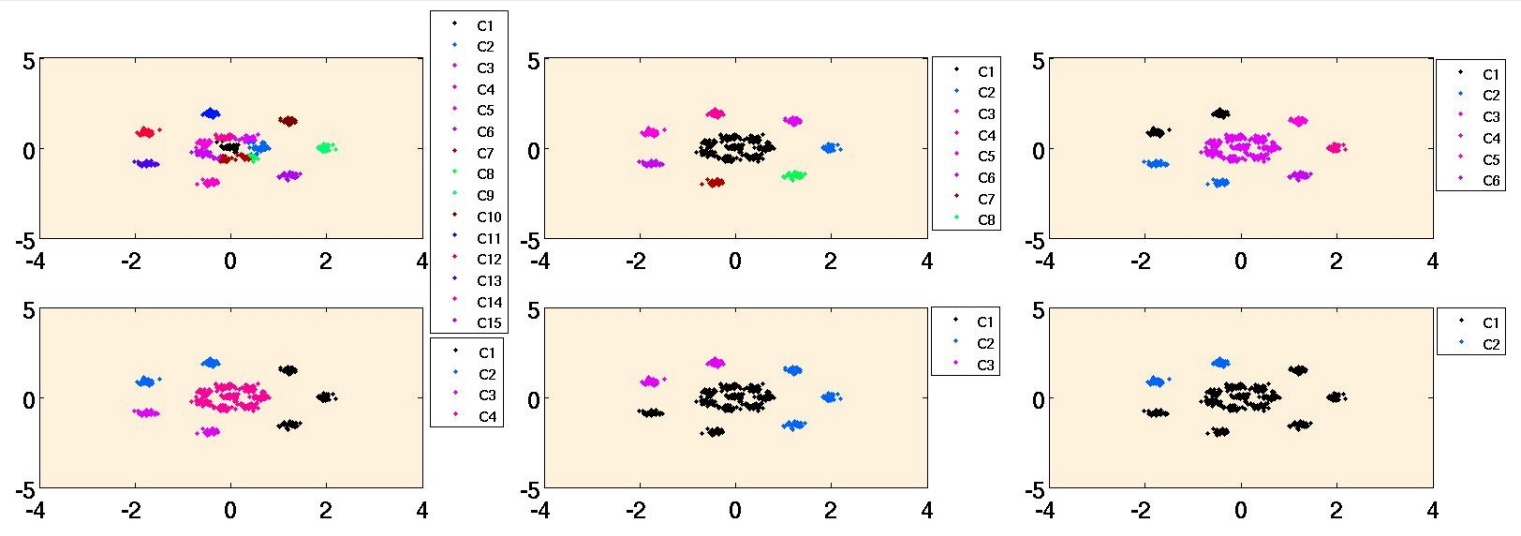


Figure: The cluster memberships at different levels of hierarchy.

Experiments

Experimental Setup

- Datasets obtained from `http://cs.joensuu.fi/sipu/datasets/` and images obtained from Berkeley image segmentation database.
- Use 30% and 40% of data as training and validation set.
- Compared on quality metrics like Silhouette (Sil), Davies-Bouldin (DB) [11] index and F-score defined as ratio between Sil and DB.
- Compared with single (SL), complete (CL), median (ML), weighted (WL) and average (AL) link hierarchical clustering techniques.

Datasets			
Name	Total Points (N)	Dimensions	Optimal k
Aggregation	788	2	7
Dim2	1351	2	9
R15	600	2	15
S1	5000	2	15
Images			
Number	Pixels		Optimal k
Id:10001	6,400		4
Id:10002	6,400		5
Id:100007	154,401		4
Id:119082	154,401		5

Table: For datasets optimal k is equal to ground truth number of clusters. For images optimal k is selected based on the maximum F-score value for SL, CL, ML, WL and AL agglomerative hierarchical clustering techniques.

Experiments

Dataset Results

Dataset	AH-KSC	SL	AL	CL	ML	WL
	F-score					
Aggregation	**1.34**	0.84	1.08	1.01	0.98	0.92
Dim2	2.27	**7.37**	5.30	4.54	5.40	5.40
R15	**4.75**	0.92	3.32	3.28	3.18	3.15
S1	**2.96**	0.0	1.81	1.55	1.58	1.76
	DB					
Aggregation	**0.466**	0.65	0.64	0.66	0.68	70
Dim2	0.37	**0.12**	0.17	0.20	0.17	0.17
R15	**0.17**	0.81	0.27	0.27	0.28	0.29
S1	**0.29**	1.7	0.45	0.51	0.50	0.46
	Sil					
Aggregation	**0.69**	0.55	**0.69**	0.67	0.66	0.65
Dim2	0.85	**0.90**	**0.90**	**0.90**	**0.90**	**0.90**
R15	0.78	0.74	**0.90**	0.90	0.90	0.90
S1	**0.88**	0.54	0.81	0.79	0.79	0.81
	ARI					
Aggregation	**0.94**	0.81	0.93	0.78	0.67	0.71
R15	0.87	0.54	**0.99**	0.98	0.98	0.99

Table: Comparison of AH-KSC method with single, average, complete, median and weight linkage techniques based on various quality measures. The highlighted result represent the best approach.

Aggregation Dataset Result

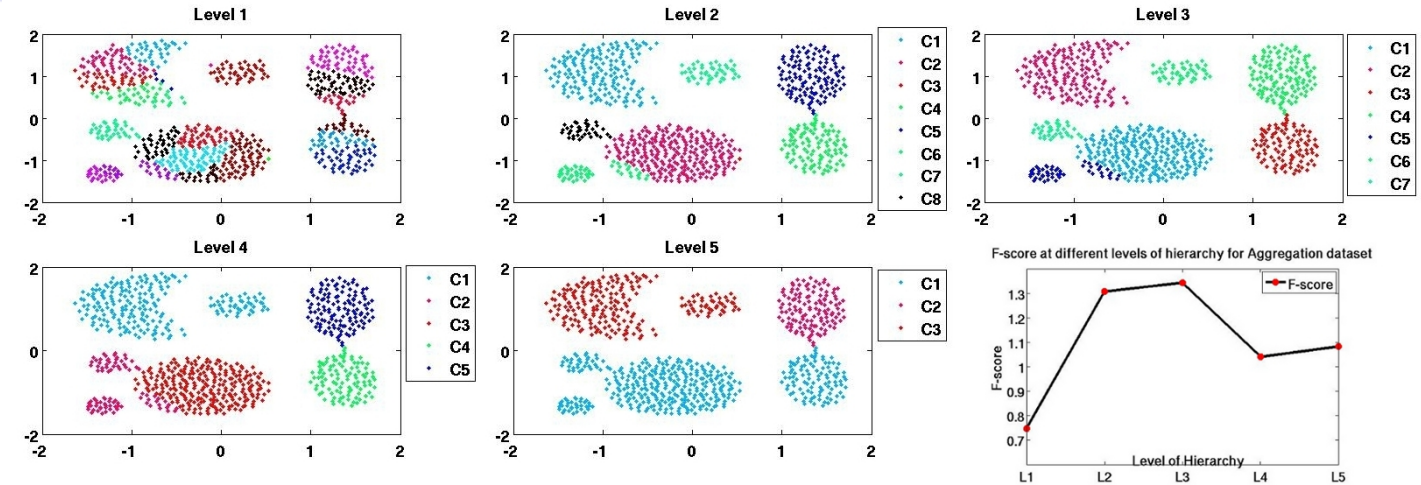


Figure: 5 levels of hierarchy produced by AH-KSC method and best F-score at $k = 7$ for Level 3.

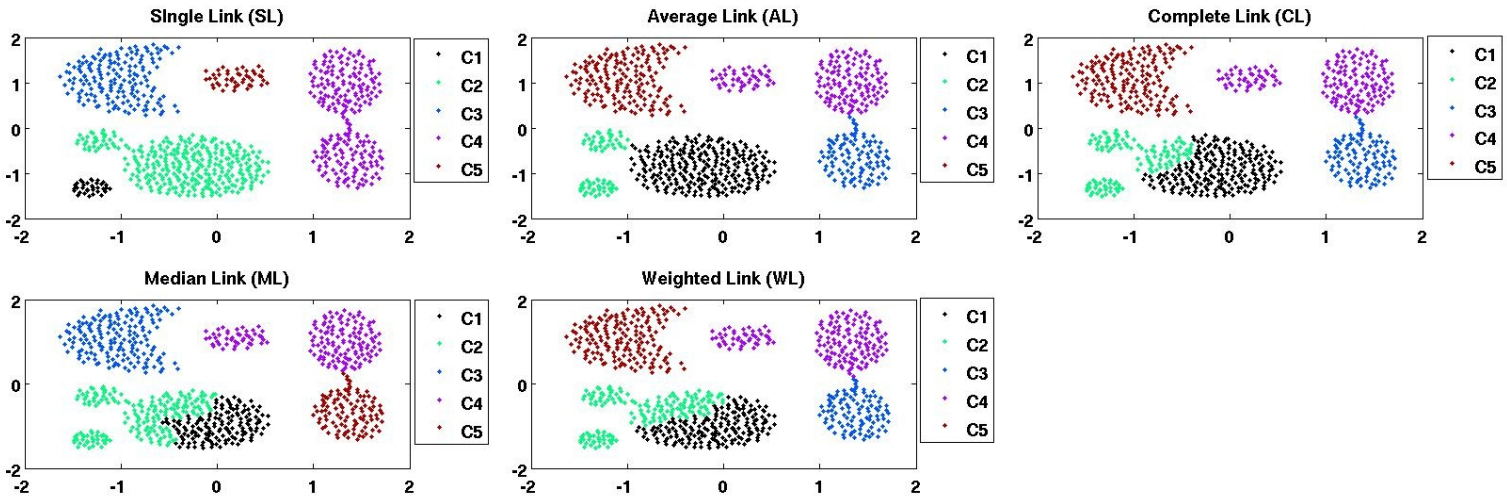


Figure: Best results for other hierarchical techniques where F-score is maximum for $k = 5$.

Image Results

Image	AH-KSC	SL	CL	ML	WL
	F-score				
Id:10001	**2.08**	0.394	1.57	1.35	1.35
Id:10002	1.02	0.70	1.37	1.2	**1.40**
Id:100007	0.73	0.38	0.41	0.68	**1.00**
Id:119082	**0.59**	0.57	0.44	0.56	0.59
	DB				
Id:10001	**0.41**	0.68	0.55	0.62	0.62
Id:10002	0.73	0.80	0.57	0.63	**0.55**
Id:100007	0.89	1.02	1.41	0.75	**0.48**
Id:119082	0.97	**0.80**	1.1	0.88	0.81
	Sil				
Id:10001	**0.85**	0.27	0.85	0.84	0.84
Id:10002	0.75	0.56	**0.77**	0.76	0.77
Id:100007	**0.65**	0.39	0.58	0.51	0.48
Id:119082	**0.57**	0.45	0.48	0.49	0.49

Table: Comparison of AH-KSC method with other agglomerative hierarchical techniques based on various quality measures for images. The highlighted result represent the best approach.

Image Segmentation Result

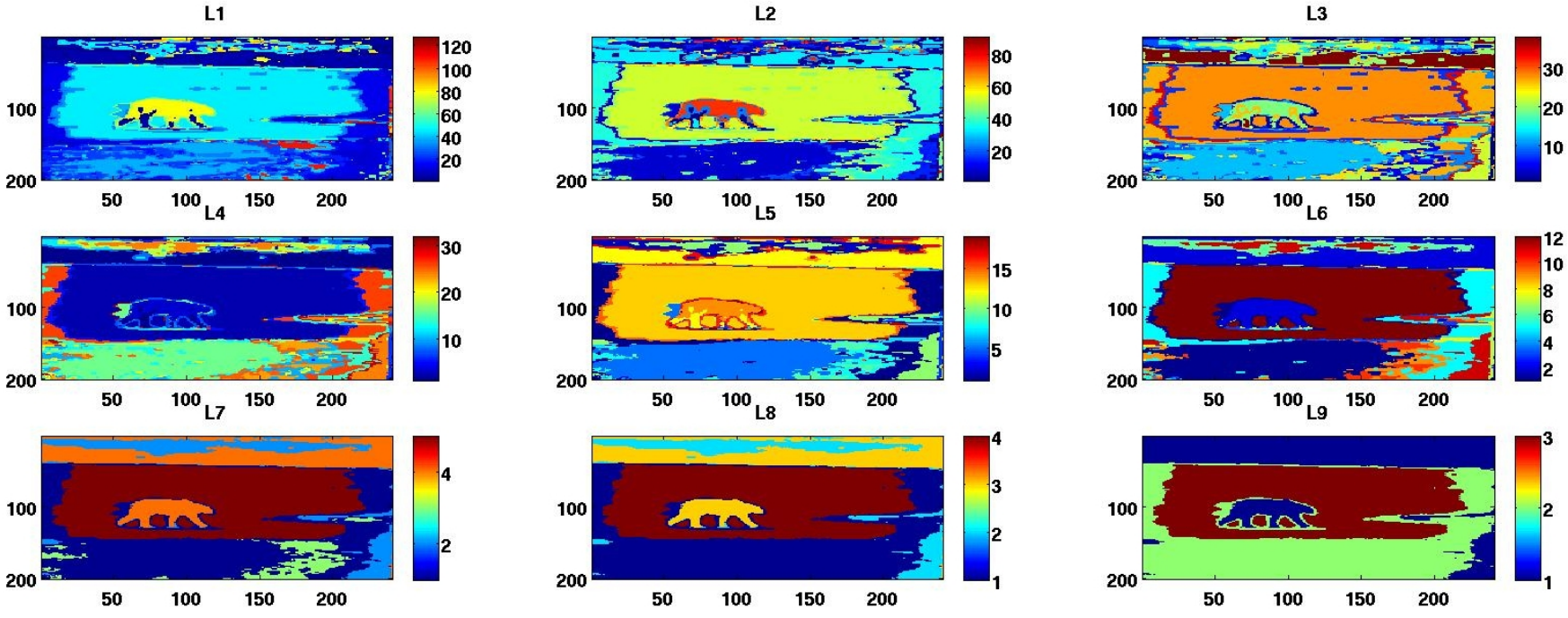
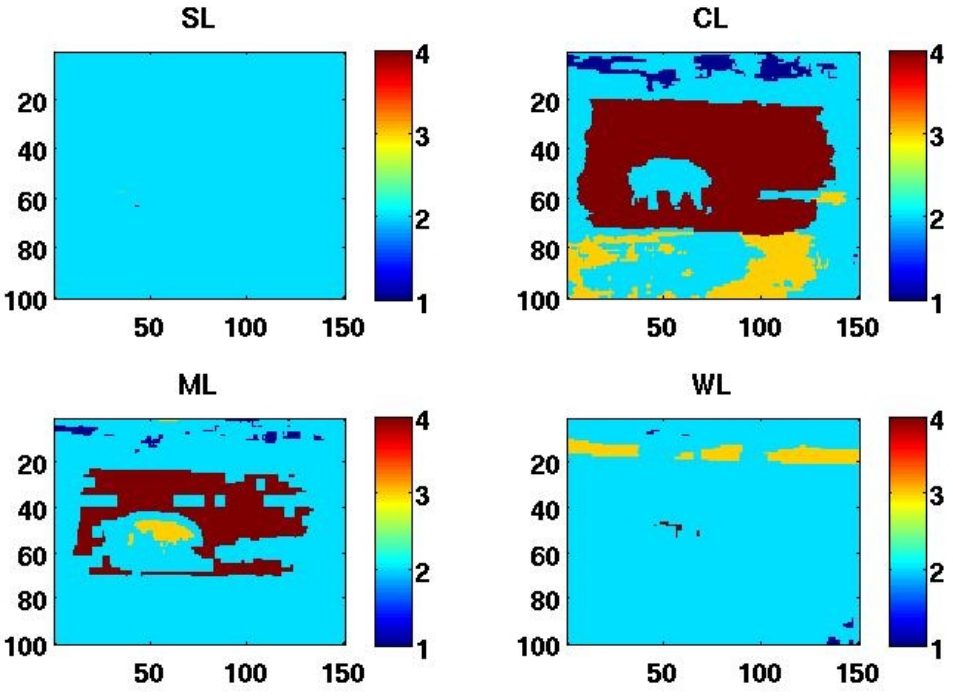
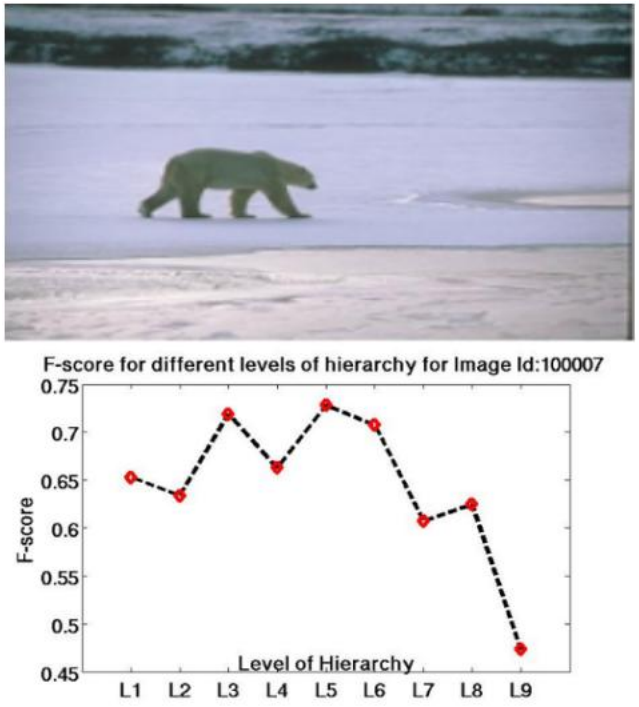


Figure: Hierarchical Segmentation by AH-KSC method from levels L1 to L9.

Image Segmentation Result



(a) Best results for other hierarchical techniques where F-score is maximum at $k = 4$.



(b) Original Image & Best F-score at L5 when $k = 19$ for AH-KSC method.

Figure: Hierarchical segmentation results by different methods on image Id:100007.

Conclusion

- Extended AH-KSC [8, 9] method from networks to datasets and images.
- Optimal kernel parameter σ selected using BAF criterion.
- Exploited the eigen-projections to obtain affinity matrices resulting in a set of increasing distance thresholds $\mathcal{T}$.
- Used these distance thresholds to perform agglomerative hierarchical clustering in bottom-up fashion.
- Compared AH-KSC method with several state-of-the-art agglomerative clustering techniques.



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