Streaming Hierarchical Clustering Based on Point-Set Kernel

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CONTRIBUTIONS

- Proposing the first kernel-based incremental hierarchical clustering algorithm StreaKHC for clustering massive streaming data
- Developing an efficient tree updating strategy in real-time for StreaKHC. This updating strategy does not rely on any sampling, mini-batch or approximation method.
- Verifying the effectiveness and efficiency of StreaKHC on 17 synthetic and real-world datasets.

StreaKHC

StreaKHC is a point-set kernel-based incremental hierarchical clustering algorithm. Its time and space complexity are $O(n)$ and $O(l\psi t)$, respectively.

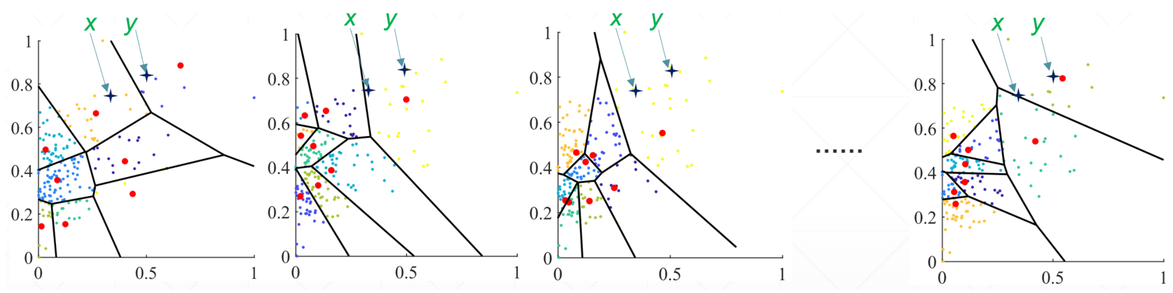
- Building an Isolation kernel and mapping points to its feature space.
- Employing a top-down search strategy to grow a tree with a new point, i.e., it recursively add the new point $\mathbf{x}$ with $\mathbf{x}$'s most similar node at each level long the path from the root to a leaf node η.
- Pruning the existing leaf to control the size of the hierarchical cluster tree, i.e., it stores the most recent l points only to reduce the over-size hierarchical tree to a pre-set size limit.

Isolation Kernel

The key idea of the Isolation kernel is using a space partitioning strategy to split the whole data space into ψ non-overlapping partitions based on a random sample of ψ points from a given dataset. The similarity between any two points is the expectation that these two points are found in the same partition.

$$K_\psi(\mathbf{x},\mathbf{y}|D) = \mathbb{E}_{\mathcal{H}_\psi(D)}[\mathbb{I}(\mathbf{x},\mathbf{y}\in\theta|\theta\in H)] \cong \frac{1}{t}\sum_{i=1}^{t}\mathbb{I}(\mathbf{x},\mathbf{y}\in\theta|\theta\in H_i),$$

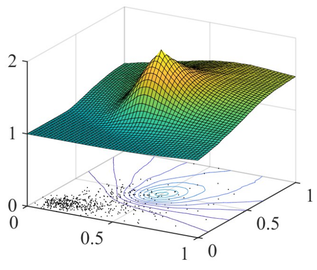
where $H \in \mathcal{H}_\psi(D)$ is one partitioning based on a subsample with size ψ, *and* $\mathbb{I}$ is an indicator function.



We can use a nearest neighbour method to split a data space into 8 non-overlapping partitions for 100 independent trials. If two points $\mathbf{x}$ and $\mathbf{y}$ are located in the same partition in 25 out of 100 trials, then the similarity between $\mathbf{x}$ and $\mathbf{y}$ is estimated as 0.25, i.e., $K_8(\mathbf{x},\mathbf{y}|D) = 0.25$.

Key Properties:

- Isolation kernel adapts to local density distribution, but the Gaussian kernel is independent of the data distribution.
- The isolation mechanism of IK produces large partitions in sparse regions and small partitions in dense regions, based on the random subsamples. The probability of two points from the dense cluster falling into the same isolating partition is lower than two points of equal inter-point distance from the sparse cluster.



Contours with reference to point (0.5, 0.5).

Two points in a sparse region are more similar than two points of equal inter-point distance in a dense region.

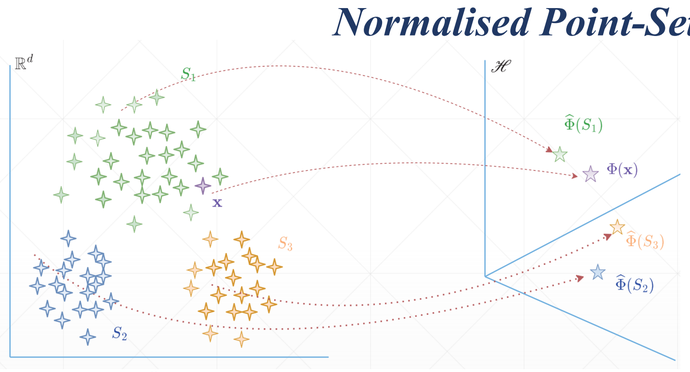
Point-Set Kernel

Given a point x and a set $A = \{\mathbf{y}_i\}_{i=1}^{p}$, and $\mathbf{x}, \mathbf{y_i} \in R^d$, the point-set similarity between $\mathbf{x}$ and A is the average pairwise similarity between $\mathbf{x}$ and every point in A, defined as follows:

$$\widehat{K}_\psi(\mathbf{x},\mathrm{A}|D) = \frac{1}{|\mathrm{A}|}\sum_{\mathbf{y}\in A} K_\psi(\mathbf{x},\mathbf{y}|D) = \frac{1}{t} < \Phi(\mathbf{x}), \widehat{\Phi}(A) >$$

Where $\widehat{\Phi}(A) = \frac{1}{|A|}\sum_{\mathbf{y}}\Phi(\mathbf{y})$ is the kernel mean map of K_ψ.

Normalised Point-Set Similarity

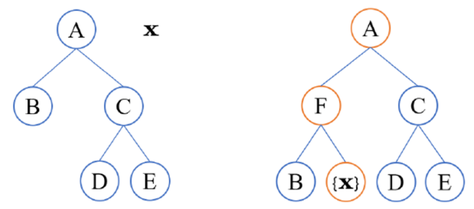


Normalise the Similarity to [0,1]:

$$\widehat{K}_\psi(\mathbf{x},A|D) = \frac{\langle\Phi(\mathbf{x}),\widehat{\Phi}(A)\rangle}{\sqrt{\langle\Phi(\mathbf{x}),\Phi(\mathbf{x})\rangle}\sqrt{\langle\widehat{\Phi}(A),\widehat{\Phi}(A)\rangle}}$$

Because $\widehat{\Phi}(A)$ can be pre-calculated, estimating the similarity between a point and a set points costs constant time $O(1)$.

Example of Growing a Tree With a New Point



(a) Original tree and new point x (b) Updated tree

1. Add $\mathbf{x}$ into the root
2. Find $\widehat{K}_\psi(\mathbf{x},S_B) \geq \widehat{K}_\psi(\mathbf{x},S_C)$
3. Replace B with a subtree having a new parent node containing $F = B \cup \{\mathbf{x}\}$

EMPIRICAL EVALUATION

- Batch Hierarchical Clustering: AHC with average-linkage (Avg.); AHC with single-linkage (Sing.); AHC with complete-linkage (Comp.); PHA - using a potential-based linkage function.
- Online Hierarchical Clustering: PERCH - adding a new point to the nearest leaf node of an existing cluster tree and then re-arrange/rotate the tree once detecting a masking situation; GRINCH -similar to PERCH with an additional grafting subroutine. 2 versions of GRINCH are used: approximate average-linkage (GRINCH-A) and cosine similarity linkage (GRINCH-C).

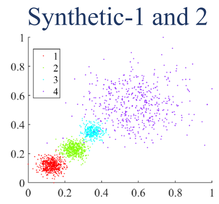
Clustering Results in Dendrogram Purity

Dataset	#Points	#Dim.	#Clus.	Avg.	Sing.	Comp.	PHA	PERCH	GRINCH-C	GRINCH-A	StreaKHC	StreaKHC-D	PERCH-IK
ALLAML	72	7,129	2	.60	.68	.67	.68	.61 ± .04	.67 ± .03	.67 ± .01	**.69 ± .03**	.68 ± .05	**.72 ± .04**
LSVT	126	310	2	.63	.58	.62	.59	**.65 ± .03**	.61 ± .01	.62 ± .01	**.65 ± .01**	.61 ± .01	**.67 ± .02**
Wine	178	13	3	.89	.68	**.92**	.73	.72 ± .09	.80 ± .06	.88 ± .04	**.91 ± .03**	.85 ± .02	.87 ± .03
Seeds	210	7	3	**.85**	.69	.75	**.84**	.69 ± .08	.68 ± .04	.79 ± .04	.83 ± .01	.81 ± .01	.79 ± .04
Musk	476	166	2	.55	.54	**.56**	.54	.55 ± .01	.55 ± .01	.55 ± .00	.55 ± .01	.54 ± .01	**.57 ± .01**
WDBC	569	30	2	**.86**	.71	.79	.73	.71 ± .05	.64 ± .02	.83 ± .05	**.89 ± .01**	.83 ± .02	.82 ± .05
LandCover	675	147	9	**.56**	.30	.52	.44	.42 ± .03	.43 ± .04	.50 ± .03	**.55 ± .03**	.45 ± .02	.48 ± .02
Hill	1,212	100	2	.50	.50	.50	.50	.50 ± .00	**.57 ± .01**	.50 ± .00	**.51 ± .00**	.50 ± .00	**.51 ± .00**
Banknote	1,372	4	2	.68	**.92**	.63	.62	.66 ± .04	.63 ± .03	.71 ± .05	**.80 ± .05**	.63 ± .01	.77 ± .07
Synthetic-1	1,800	2	4	**.95**	.77	.88	.86	.78 ± .07	.28 ± .00	.87 ± .05	**.95 ± .00**	.89 ± .03	.94 ± .02
Spam	4,601	57	2	.58	.59	.57	.55	.57 ± .01	.56 ± .02	.58 ± .01	**.68 ± .01**	.62 ± .02	**.63 ± .02**
ImageNet-10	13,000	128	10	**.87**	.77	.27	.69	.67 ± .06	.70 ± .04	.71 ± .02	**.86 ± .01**	.76 ± .03	.70 ± .01
STL-10	13,000	128	10	**.62**	.50	.22	.53	.41 ± .04	.41 ± .02	.42 ± .01	**.61 ± .01**	.54 ± .02	.42 ± .02
CIFAR-10	60,000	128	10	-	-	-	-	.42 ± .02	.43 ± .03	.45 ± .03	**.68 ± .01**	**.61 ± .03**	.45 ± .02
Mnist	70,000	128	10	-	-	-	-	.20 ± .00	.23 ± .02	.24 ± .02	**.41 ± .01**	**.36 ± .01**	.32 ± .02
CoverType	581,012	54	7	-	-	-	-	**.45 ± .00**	.43 ± .00	.43 ± .00	.43 ± .01	.41 ± .01	**.46 ± .03**
Synthetic-2	1,800,000	2	4	-	-	-	-	**.73 ± .02**	-	-	**.81 ± .03**	-	-
Average of the first 13 datasets				.70	.63	.61	.64	.61	.58	.66	.73	.67	.68

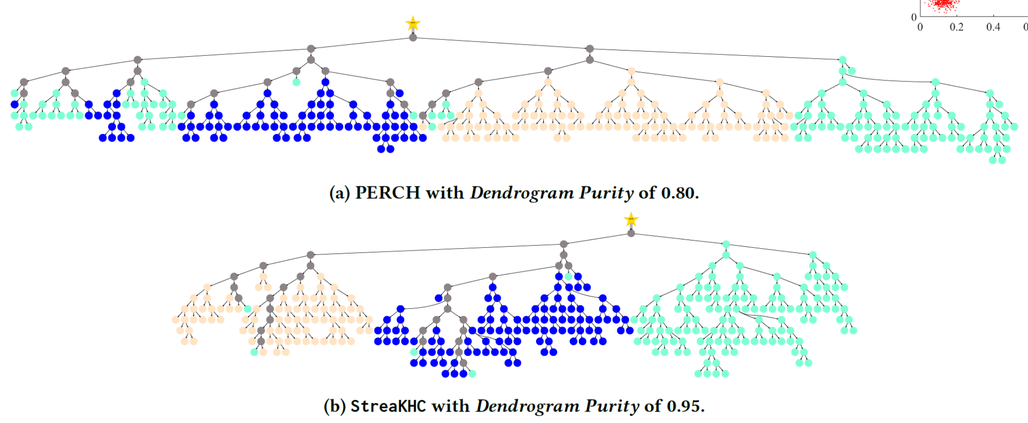
* StreaKHC-D is StreaKHC using Euclidean distance only.

* PERCH-IK: The same PERCH algorithm running on Isolation kernel space.

Synthetic-1 and 2



Visualisation on Wine Dataset

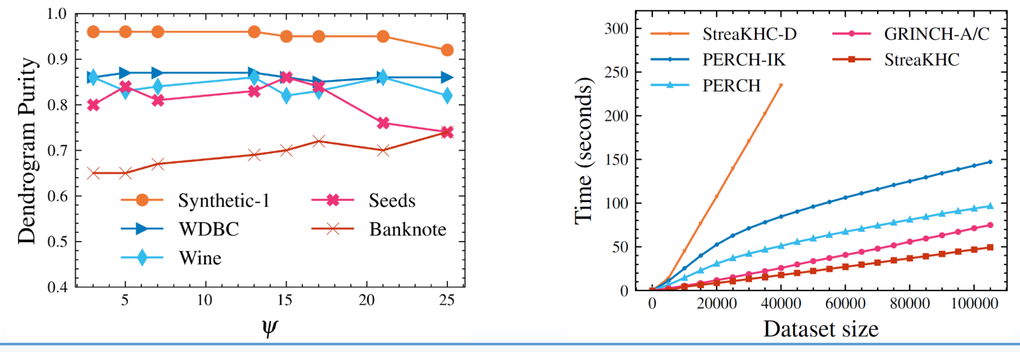


(a) PERCH with *Dendrogram Purity* of 0.80.

(b) StreaKHC with *Dendrogram Purity* of 0.95.

Figure 4: Clustering dendrograms (cluster trees) on the Wine dataset. Each leaf node contains a data point, and each colour represents a ground-truth label of a node if all the points in it belong to the same label, otherwise, the node is coloured grey.

Sensitivity and Scalability Test



StreaKHC can be obtained from https://github.com/tulip-lab/open-code/tree/master/StreaKHC