

ONLINE CLUSTERING: ALGORITHMS, EVALUATION, METRICS, CHALLENGES, APPLICATIONS AND BENCHMARKING WITH RIVER

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OUTLINE

- A (very brief) introduction to River
- Online clustering algorithms:
 - Challenges and Solutions
 - Approaches
 - State-of-the-art algorithms
 - Further steps and Personal insights
- Online clustering benchmarking with River

River

<https://hoanganhngo610.github.io/river-clustering.kdd.2022/>

<https://doi.org/10.1145/3534678.3542600>

REQUIREMENTS



Process **one sample** at a time, and inspect it only **once**



Use a limited amount of **memory**



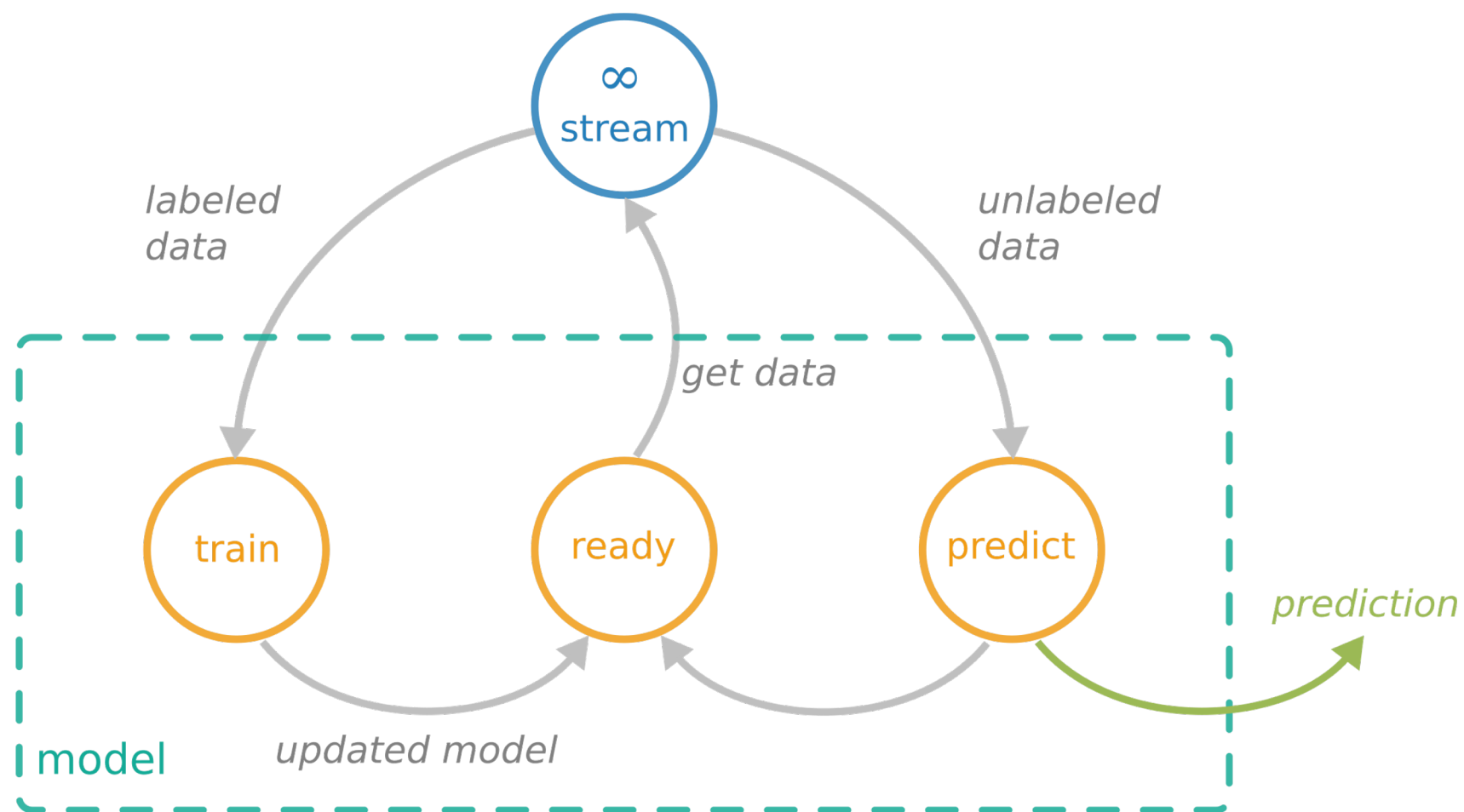
Work in a limited amount of **time**



Always ready to predict


LEARNING FROM DATA STREAMS

Supervised learning



 One sample at a time

 Limited resources

 Predict at any time

DEFINITION OF CLUSTERING

Given a set of unlabeled instances, distribute them into homogeneous groups according to some common relations or affinities

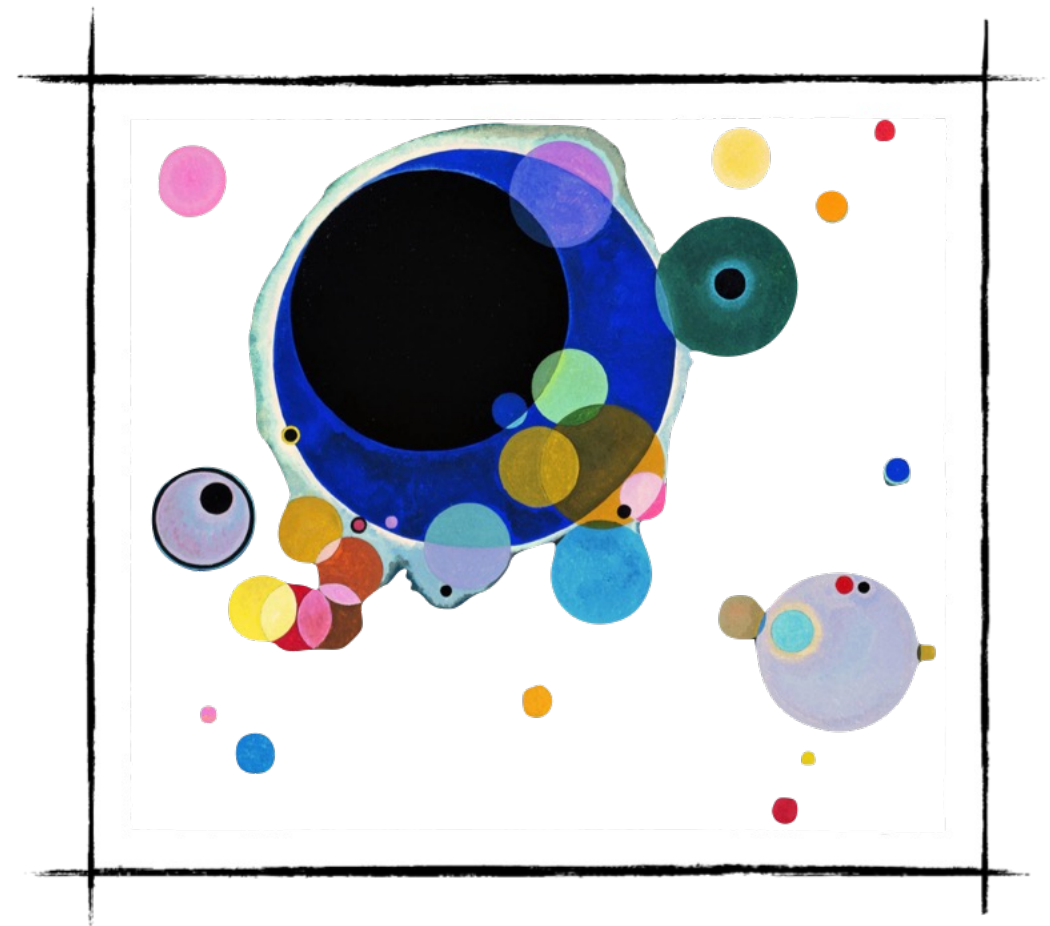


Photo source: W. Kandinsky - Several Circles (edited)

EXAMPLES

- Market segmentation
- Social network communities

AVAILABLE SOFTWARES

Very few implementations (only most prominent ones) and unified frameworks with multiple algorithms co-existing:

- **Massive Online Analysis (MOA):** Most popular framework, written by Bifet et al. (2010) in Java, including the most number (7) of clustering algorithms. However, one major **disadvantage**: only works well when information of data streams are previously known.
- **stream package:** Written in R by Hahsler et al. (2018), with newer algorithms including D-Stream, DBSTREAM and evoStream.

AVAILABLE SOFTWARES

Very few implementations (only most prominent ones) and unified frameworks with multiple algorithms co-existing:

- **Subspace MOA framework:** An extension of MOA from Java into R, written by Hassani et al. (2016), with extra algorithms including HDDStream and PreDeConStream.
- **streamDM:** Written by Huawei Noah's Ark Lab (2015) with Spark Streaming, an extension of Spark engine. Including CluStream and StreamKM++, but no plans for any further implementation

SOLUTION – RIVER

→ **River** comes into play, with a neat implementation that allows:

- Works with any arbitrary numerical data stream;
- Well-maintained, documented and includes various algorithms of different types.

Currently, River offers **6** clustering algorithms, including incremental K-Means, CluStream, DenStream, DBSTREAM, StreamKMeans (O'Callaghan et al., 2002) and evoStream (under a fully functional Pull Request) with a clear plan of further implementations.

Includes the **most** number of clustering algorithms apart from MOA.

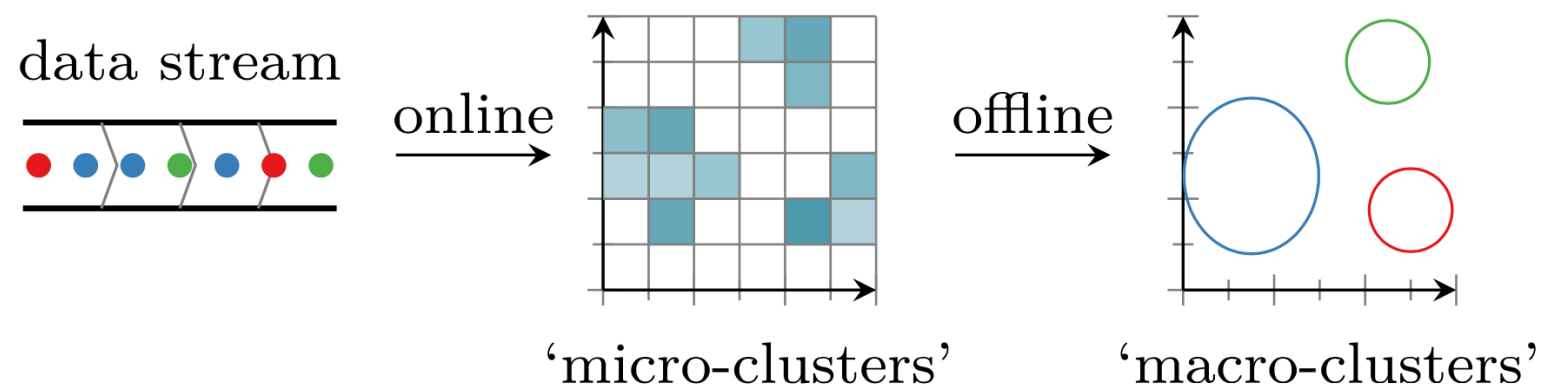
STRATEGY

Basically, finding clustering solutions is an optimization task, with the following principle strategies:

- Minimizing intra-cluster distances or radii of clusters (ensuring that objects within the same cluster are similar);
- Maximizing inter-cluster distances or heterogeneity (ensuring that objects within different clusters are well-separated);
- Maximizing likelihood estimates.

ARISING PROBLEMS

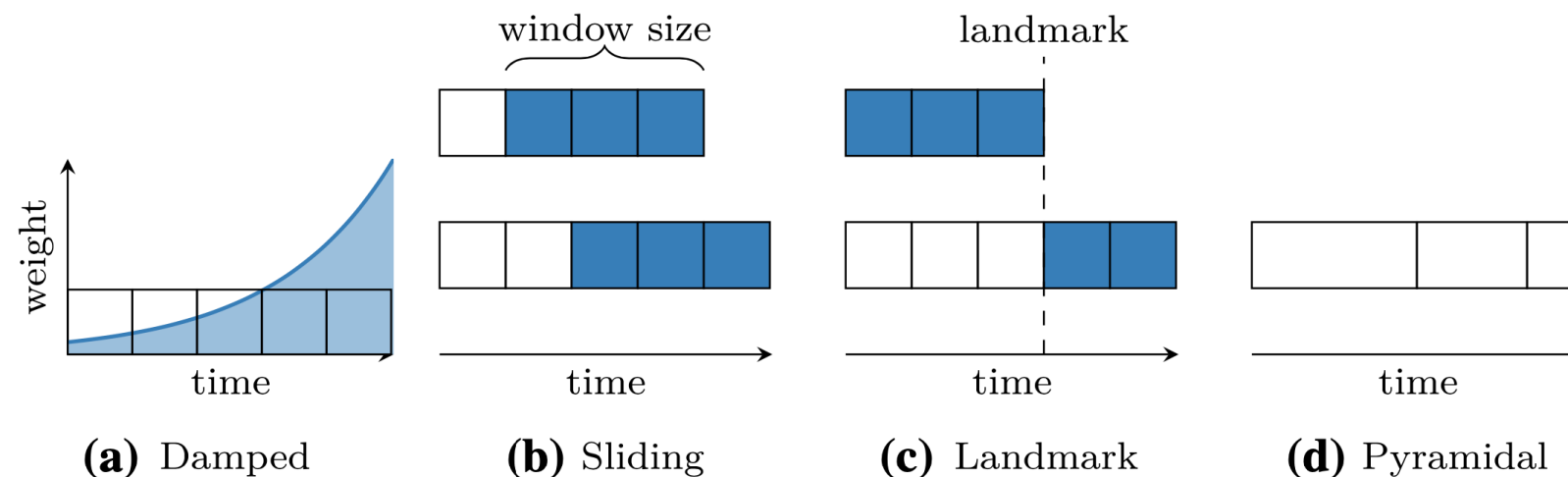
- In online clustering, historical data will be discarded and only information of formed clusters (cluster centres, number of points, linear sum, sum of squares, etc.) will be saved → Clustering algorithms are divided into **two** phases: ONLINE phase and OFFLINE phase.



Two-phase stream clustering with grid-based approach
(Source: Matthias Carnein et al. 2017. An empirical comparison of stream clustering algorithms.)

ARISING PROBLEMS

- Through time, the distribution of the stream will change. (also known as drift or concept drift) → Models can employ time-window models, which only keeps the most few recent data points to avoid bias. This approach can include damped, sliding, landmark or pyramidal models.



Two-phase stream clustering with grid-based approach
(Source: Zhu Y. and Shasha D. 2002. Statstream: statistical monitoring of thousands of data streams in real life and Silva J. A. et al. 2013. Data stream clustering: a survey.)

APPROACHES

Matthias Carnein and Heike Trautmann. 2019. Optimizing Data Stream Representation: An Extensive Survey on Stream Clustering Algorithms. *Business and Information Systems Engineering* 61, 3 (2019), 277-297. <https://doi.org/10.1007/s12599-019-00576-5>

- **Distance-based approach:** threshold the distance of the new observation to existing clusters, either to insert or initialize new clusters, including:
 - *Clustering Features (CFs), Extended CFs, Time-Fading CFs:* BIRCH, CluStream, SDStream, ClusTree;
 - *Centroids, Medoids:* StreamKM++ (coreset), STREAM, RepStream (graph of nearest neighbors);
 - *Competitive Learning:* DBSTREAM.
- **Density-based (Grid-based) approach:** capture the density of observation in a grid, by separating the data space among all dimension, including:
 - *One-time or recursive partitioning:* DUCStream, D-Stream, Stats-Grid;
 - *Hybrid Grid-Approach:* HDCStream, Mudi-Stream;

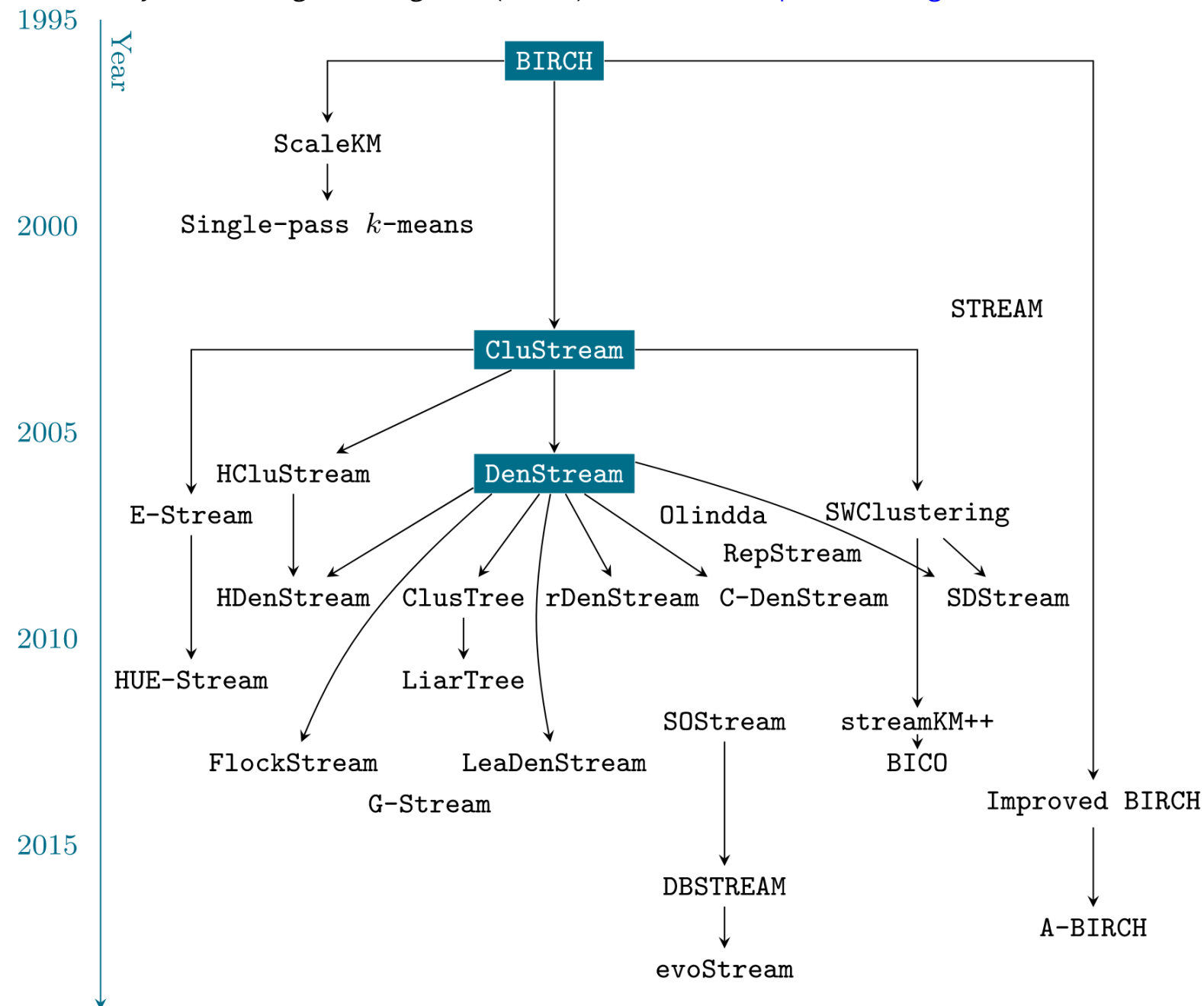
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- **Model-based approach:** Summarize the data stream as a *statistical model*, with a common area of research based on the Expectation Maximization (EM) algorithm. Others include the use of an incrementally-built classification tree or concepts from linear regression. Including CluDisStream, SWEM, COBWEB, Wstream, etc.
- **Projected approach:** This special approach deals with *high dimensional data stream*, addressing the curse of dimensionality. Including HPStream, HDDStream, and PreDeConStream along with their extensions.

EVOLUTION OF ONLINE CLUSTERING ALGORITHMS

Matthias Carnein and Heike Trautmann. 2019. *Optimizing Data Stream Representation: An Extensive Survey on Stream Clustering Algorithm*. *Business & Information Systems Engineering*, 61 (2019), 277-297. <https://doi.org/10.1007/s12599-019-00576-5>.



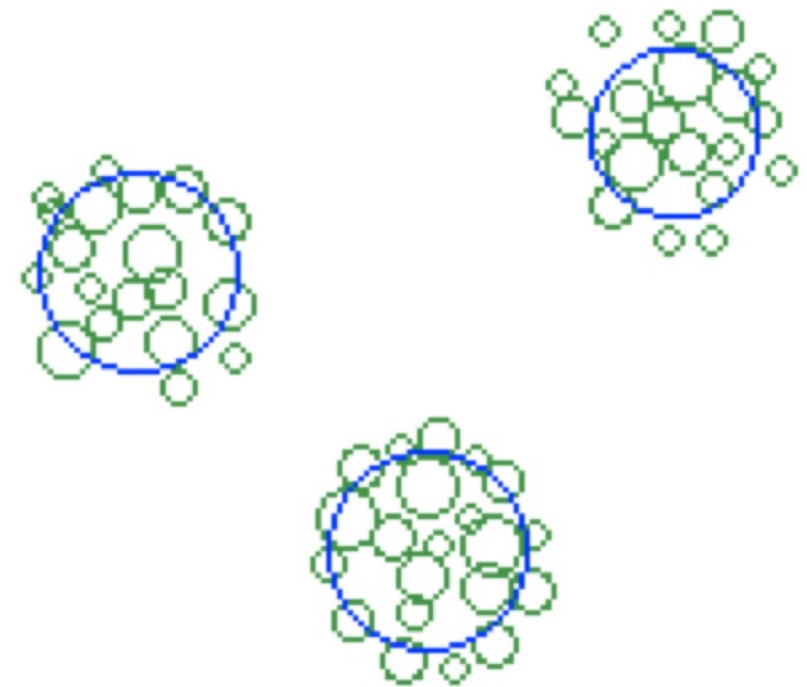
SIMPLEST IMPLEMENTED ALGORITHM: INCREMENTAL K-MEANS

- Basically the simplest, naive approach that we can think of.
- Most noticable parameter: halflife, which decides how much to move the cluster to the new point
- Obtains comparable performance compared to more complicated algorithms, while maintaining a constantly low memory usage.

MICRO-CLUSTERS

Tian Zhang, Raghu Ramakrishnan, and Miron Livny. 1996. BIRCH: An Efficient Data Clustering Method for Very Large Databases. In *SIGMOD'96: Proceedings of the 1996 ACM SIGMOD International Conference on Management of Data*. Association for Computing Machinery, New York, NY, USA. <https://doi.org/10.1145/233269.233324>

- Cluster Features \overrightarrow{CF} (statistical summary structure)
- Maintained in online phase, input for offline phase
- Data stream $\langle \overrightarrow{x_i} \rangle$, d dimensions
- Cluster Features vector includes
 - N: number of points
 - LS_j : sum of values (for dimension j)
 - SS_j : sum of squared values (for dimension j)
- Easy to update, easy to merge
- Constant space irrespective to the number of examples!



Properties:

- Centroid = LS/N
- Radius = $\sqrt{SS/N - (LS/N)^2}$
- Diameter = $\sqrt{\frac{2 \times N \times SS - 2 \times LS^2}{N \times (N-1)}}$

CLUSTREAM

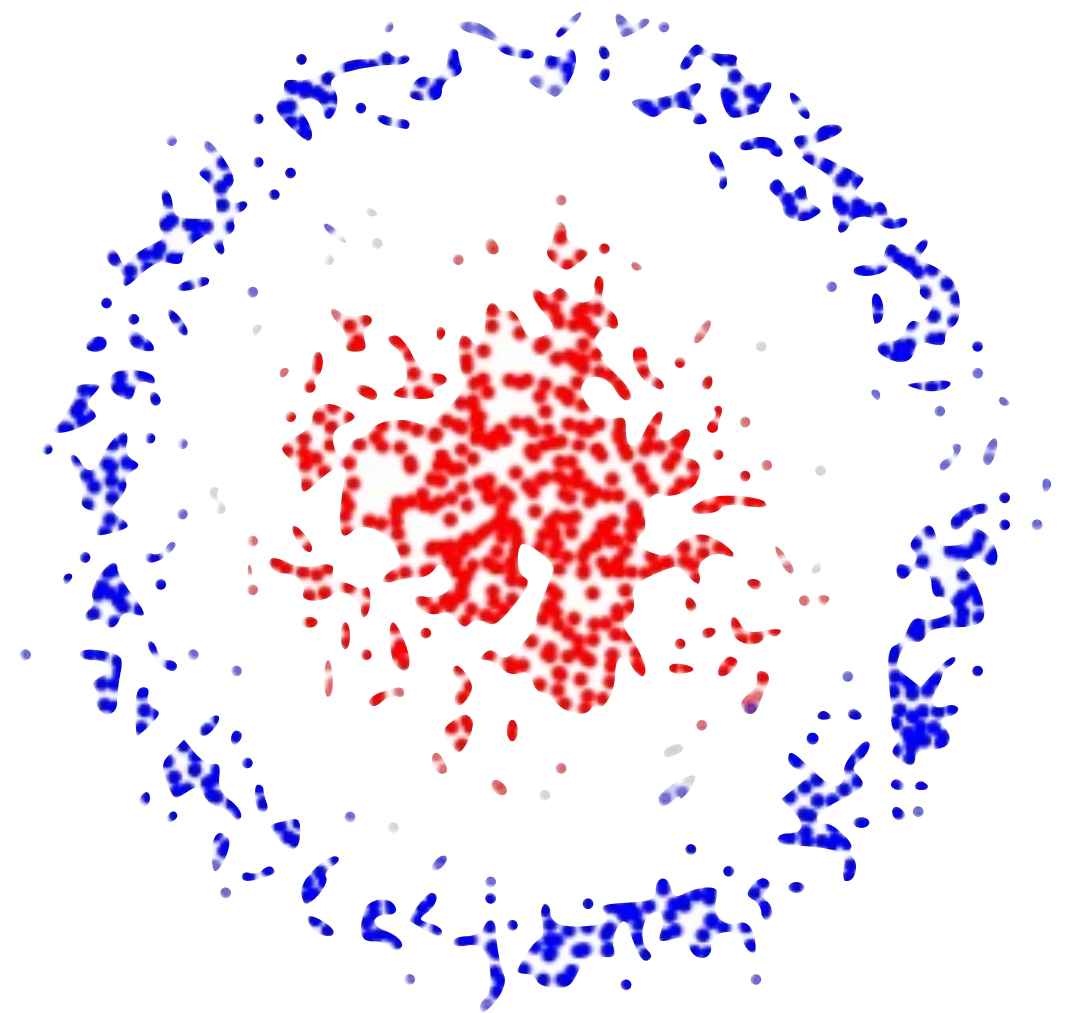
Charu C. Aggarwal, Jiawei Han, Jianyong Wang, and Phillip S. Yu. 2003. A Framework for Clustering Evolving Data Streams. In: *Proceedings of the 29th International Conference on Very Large Data Bases - Volume 29* (Berlin, Germany) (VLDB '03). VLDB Endowment, Berlin, Germany, 81–92.

- Time - stamped data stream $\langle t_i, \vec{x}_i \rangle$, represented in $d + 1$ dimensions
- Seed algorithm with q micro-clusters (K-Means on initial data)
- **ONLINE phase.** For each new point, either:
 - Update one micro-cluster (point within maximum boundary)
 - Create a new micro-cluster (delete/merge other micro-clusters)
- **OFFLINE phase.** Determine k macro-clusters on demand:
 - K-Means on micro-clusters (weighted pseudo-points)
 - Time-horizon queries via pyramidal snapshot mechanism

DBSCAN

Martin Ester and Hans-Peter Kriegel and Jörg Sander and Xiaowei Xu. 1996. A Density-Based Algorithm for Discovering Clusters in Large Spatial Databases with Noise. In *KDD'96: Proceedings of the Second International Conference on Knowledge Discovery and Data Mining*. AAAI Press, 226-231. <https://doi.org/10.5555/3001460.3001507>

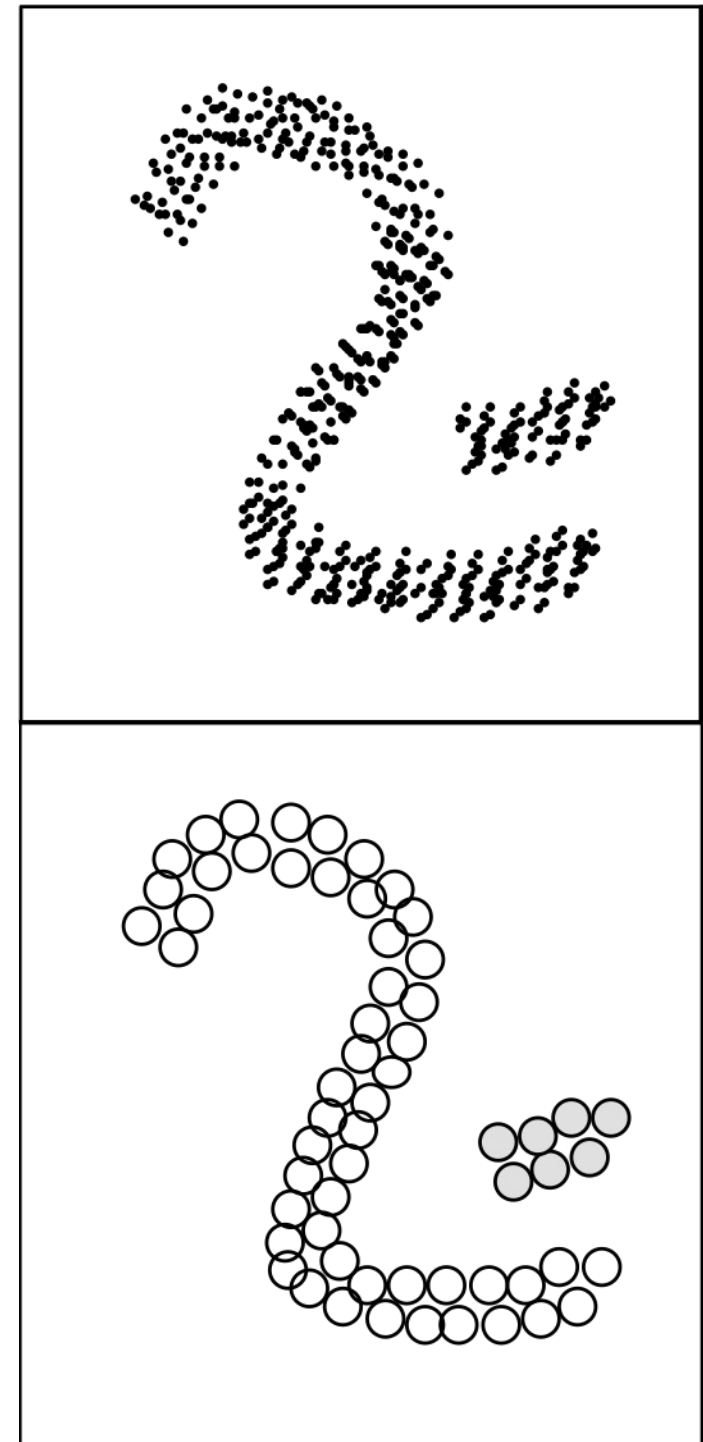
- $N_\epsilon(p)$: set of points at distance $\leq \epsilon$ from p
- Core object p iff $N_\epsilon(p)$ has weight $\geq \mu$
- p is directly density-reachable from q iff $p \in N_\epsilon(q)$ and q is a core object
- p_n is density-reachable from p_1 iff there exists chain of points p_1, \dots, p_n such that p_{i+1} is directly d – r from p_i
- **Cluster**: set of points that are mutually density-connected



DENSTREAM

Feng Cao and Martin Ester and Weining Qian and Aoying Zhou. **Density-Based Clustering over an Evolving Data Stream with Noise.** In: *Proceedings of the 2006 SIAM International Conference on Data Mining (SDM)*. Society for Industrial and Applied Mathematics (SIAM), 328-339. <https://doi.org/10.1137/1.9781611972764.29>

- Based on DBSCAN
- Core-micro-cluster: $\text{CMC}(\omega, c, r)$ with weight $\omega > \mu$, center c , radius $r < \epsilon$
- Potential/Outlier micro-clusters
- **Online phase:** merge point into p (or o) micro-cluster if new radius $r' < \epsilon$
 - Promote outlier to potential if $\omega > \beta\mu$; else, create a new o-micro-cluster
- **Offline phase:** DBSCAN



EVOSTREAM

Matthias Carnein and Heike Trautmann. 2018. **evoStream** – Evolutionary Stream Clustering Utilizing Idle Time. *Big Data Research* 14 (2018), 101-111. <https://doi.org/10.1016/j.bdr.2018.05.005>

- A fairly new online clustering algorithm.
- evoStream employs an evolutionary algorithm, first introduced by Maulik U. and Bandyopadhyay S. (2000), to utilize “idle” time efficiently to find better macro-cluster solutions.
- In the evolution algorithm, promising solutions are combined to create off-springs which can combine the best attributes of both parents.
- Include two phases: **Micro-cluster maintenance** (online learning phase) and **evolutionary step of micro-cluster generation** (offline phase)

EVOSTREAM

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Require: radius r , decay rate λ , cleanup interval t_{gap} , initialization threshold γ , Population size P , number of clusters k
Initialize: $t = 0$, $MC = \emptyset$, $\mathbf{C} = \emptyset$

<pre>1: while stream is active do 2: read \mathbf{x} from stream 3: $t \leftarrow t + 1$ 4: $new \leftarrow (\mathbf{x}, t, 1)$ 5: for $mc \in MC$ do 6: if $\text{DIST}(mc, new) < r$ then 7: $mc[\mathbf{c}] \leftarrow mc[\mathbf{c}] + h(new[\mathbf{c}], mc[\mathbf{c}]) \cdot (new[\mathbf{c}] - mc[\mathbf{c}])$ 8: $mc[t] \leftarrow t$ 9: $mc[\omega] \leftarrow mc[\omega] \cdot 2^{-\lambda(t-mc[t])} + 1$ 10: if new has not been absorbed by any $mc \in MC$ then 11: $MC \leftarrow MC \cup new$ 12: if $t \bmod t_{gap} = 0$ then 13: $\text{CLEANUP}(\cdot)$ 14: if $MC = \gamma$ and not initialized then 15: for $i \leftarrow 1, \dots, P$ do 16: $C_i \leftarrow k$ randomly chosen micro-cluster 17: while idle do 18: $\text{EVOLUTION}(\cdot)$</pre>	<div><div>▷ Temporary micro-cluster</div><div>▷ $mc := (\mathbf{c}, t, \omega)$</div><div>▷ Absorb observation</div><div>▷ h as in Equation (1)</div><div>▷ Initialize new micro-cluster</div><div>▷ Periodic adjustments</div><div>▷ see Algorithm 2</div><div>▷ Initialize macro-clusters</div><div>▷ Until new example available</div><div>▷ Repeat evolutionary step, see Algorithm 3</div></div>
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evoStream algorithm (with both online and offline phase)

EVOSTREAM

Matthias Carnein and Heike Trautmann. 2018. evoStream – Evolutionary Stream Clustering Utilizing Idle Time. *Big Data Research* 14 (2018), 101-111. <https://doi.org/10.1016/j.bdr.2018.05.005>

```
1: function CLEANUP( $\cdot$ )
2:   for each  $mc \in MC$  do
3:      $mc[\omega] \leftarrow mc[\omega] \cdot 2^{-\lambda(t-mc[t])}$                                 ▷ Update weight
4:     if  $mc[\omega] \leq 2^{-\lambda t_{gap}}$  then
5:       Remove  $mc$  from  $MC$                                                     ▷ Remove outdated
6:   Merge all  $mc_i, mc_j$  where  $DIST(mc_i, mc_j) \leq r$                         ▷ Merge colliding clusters
```

Cleanup phase (after each t_{gap} time interval)

EVOSTREAM

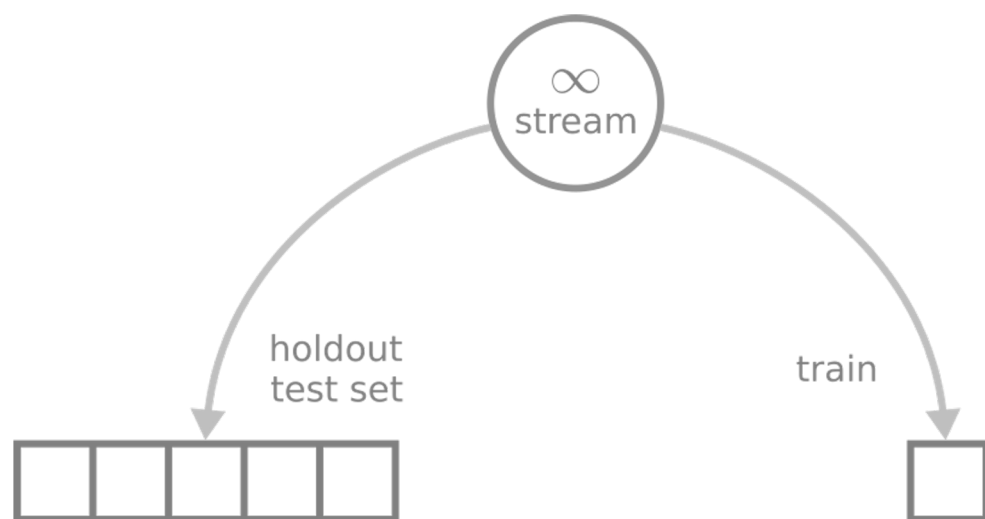
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```
1: function EVOLUTION(.)
2:    $p_1, p_2 \leftarrow$  Select two solutions proportionally to their fitness from  $\mathbf{C}$ 
3:    $o_1, o_2 \leftarrow$  Create offsprings of  $p_1, p_2$  using binary crossover
4:   for each  $g_i$  in  $o_1, o_2$  do
5:     if RANDOM(0,1) <  $P_m$  then
6:       if  $g_i = 0$  then
7:          $g_i \leftarrow 2\delta$ 
8:       else
9:          $g_i \leftarrow 2\delta \cdot g_i$ 
10:  Add  $o_1, o_2$  to  $\mathbf{C}$  and discard the two least fittest solutions
```

▷ For each child-gene
▷ Mutate with probability P_m

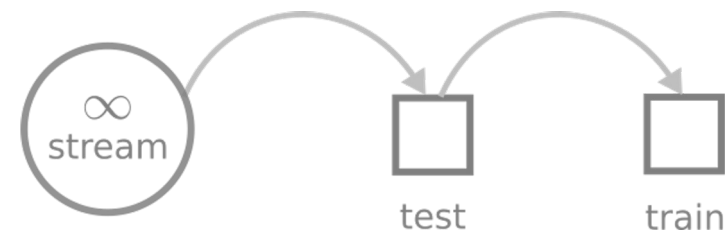
Evolution algorithm (during idle time)

EVALUATION



Holdout an independent test set

- Apply the current model to the test set, at regular time intervals
- *Unbiased* performance estimation
- Popular in *batch* and *stream* learning



Prequential

- Test *then* train each new instance
 - Order matters!
 - All data is used for training
- Performance is estimated on the sequence
- Popular in the *stream* setting

CLASSICAL STATIC EVALUATION

4 basic internal (validation) metrics include

- **Cohesion:** The average distance from a point in the dataset to its assigned cluster centroid. The smaller the better.
- **SSQ:** The sum of squared distances from data points to their assigned centroids. Closely related to cohesion. The smaller the better.
- **Separation:** Average distance from a point to the points assigned to other clusters. The larger the better.
- **Silhouette coefficient:** the ratio between cohesion and the average distances from the points to their second-closest centroid.

CLASSICAL STATIC EVALUATION

External validation metrics, requiring ground truth values, is mostly based on the following concepts

- **Accuracy:** Fraction of the points assigned to their “correct” cluster.
- **Recall:** Fraction of the points of a cluster that are in fact assigned to it.
- **Precision:** Fraction of the points assigned to a cluster that truly belong to it.
- **Purity:** In a maximally pure clustering, all points in the cluster belong to the same ground-truth class or cluster. Formally, purity is

$$\frac{1}{N} \sum_{c=1}^k (\text{number of points in cluster } c \text{ in the majority class for } c).$$

INTERNAL METRICS: ARE THEY REALLY ONLINE?

Leonardo Enzo Brito Da Silva, Niklas Max Melton and Donald C. Wunsch. 2022. Incremental Cluster Validity Indices for Online Learning of Hard Partitions: Extensions and Comparative Study. *IEEE Access*, 8 (2020), 22025-22047. <https://doi.org/10.1109/ACCESS.2020.2969849>.

- In 2020, Leonardo Enzo Brito Da Silva et al. introduced a new approach for incremental validity indices. This allows an update to a new value from a previous old value.
- However, this approach still has one huge limitation: ALL information of each previous data points still have to be available.
- As such, there is a requirement to come up with metrics that are truly incremental (facilitating the fashion of learning one sample at a time).

**Work to be submitted to IEEE Big Data 2022*

HOW TO DESIGN AN INCREMENTAL INTERNAL METRIC?

- Save the information that are needed, finite and require low computational time/resources:
 - Linear sum and/or sum of squares of distances of point x^t at time t to the nearest cluster center at the same time, i.e $\sum_t \|v_{c_t}^t - x^t\|_{1/2}$
 - Number of points passed (in total and/or within each cluster)
 - Centers and centroids of clusters (using incremental means)
 - Centers of the whole dataset
 - etc.

INCREMENTAL EVALUATION

In **River**, static evaluation metrics can be modified to continuously evaluate data streams as follows:

- **External metrics:** All external metrics implemented in River share the same **confusion matrix**, thus reducing the amount of occupied storage and computational time. This confusion matrix can easily be updated once a new predicted label and its ground truth arrive.
- **Internal metrics:** Since information on previous data points are **totally discarded** once a new data point arrives, traditional internal metrics **cannot be used incrementally**. Instead, they are slightly modified by saving the most essential information based on requirement, for example linear sum and sum of squares of data points in the same cluster, distance from data point to assigned and/or second closest cluster centre at the time of update, etc.

INCREMENTAL EVALUATION

With **20 internal metrics** and **18 external metrics**, River is currently the package with the highest number of metrics offered for data stream continuous or incremental validation.

- Internal metrics: Cohesion, SSB, SSW, Separation, Silhouette, Ball-Hall, CH, Hartigan, WB, Xie-Beni, Xu, (Root) Mean Squared Standard Deviation, R-Squared, I Index, Davies-Bouldin, Partition Separation, Dunn's indices 43 and 53, SD Validation Index, and Bayesian Information Criterion.
- External metrics: Completeness, Homogeneity, VBeta, (Adjusted, Expected, Normalized) Mutual Information, Q0 and Q2, Fowlkes-Mallows, Markedness, Informedness, Matthews Correlation Coefficient, (Adjusted) Rand Index, Purity, Prevalence Threshold, and Sorensen-Dice index.

EVALUATION

Every metric (both internal and external) in River contains the following attributes:

- **cm**: Confusion matrix;
- **update** and **revert**: Allow the metric to be updated with a new observation, or reverted to the previous state;
- **get**: Obtain the exact value of the metric;
- **bigger-is-better**: Indicate whether the metric has the property of the bigger, the better the clustering solution is;
- **work_with**: Indicate whether the metrics work with algorithms of which type (clustering, classification, regression, etc.);

FURTHER STEPS

- Benchmarking
- Implementation of more clustering algorithms and/or improvement in performance of current ones (ex. Welford's algorithm for the information of micro-clusters)
- Text-specific clustering algorithms (although this can currently be done using TFIDF + Any clustering model pipeline in River)

PERSONAL THOUGHTS

- The world of online clustering is still “chaotic”, with a lot of papers having no official implementation or implementations scattered in different frameworks/languages → Hard to evaluate.
- Are we too much dependent on the concept of online and offline phase while doing online clustering?
- Online deep clustering (ODC) with the assistance of `river-torch`? (<https://arxiv.org/abs/2006.10645>)

**Thank you for
your attention!**