A Hierarchical Algorithm for Extreme Clustering

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College of Information and Computer Science
University of Massachusetts Amherst

Clustering

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Partition dataset X into clusters $C_1 \ldots C_K$

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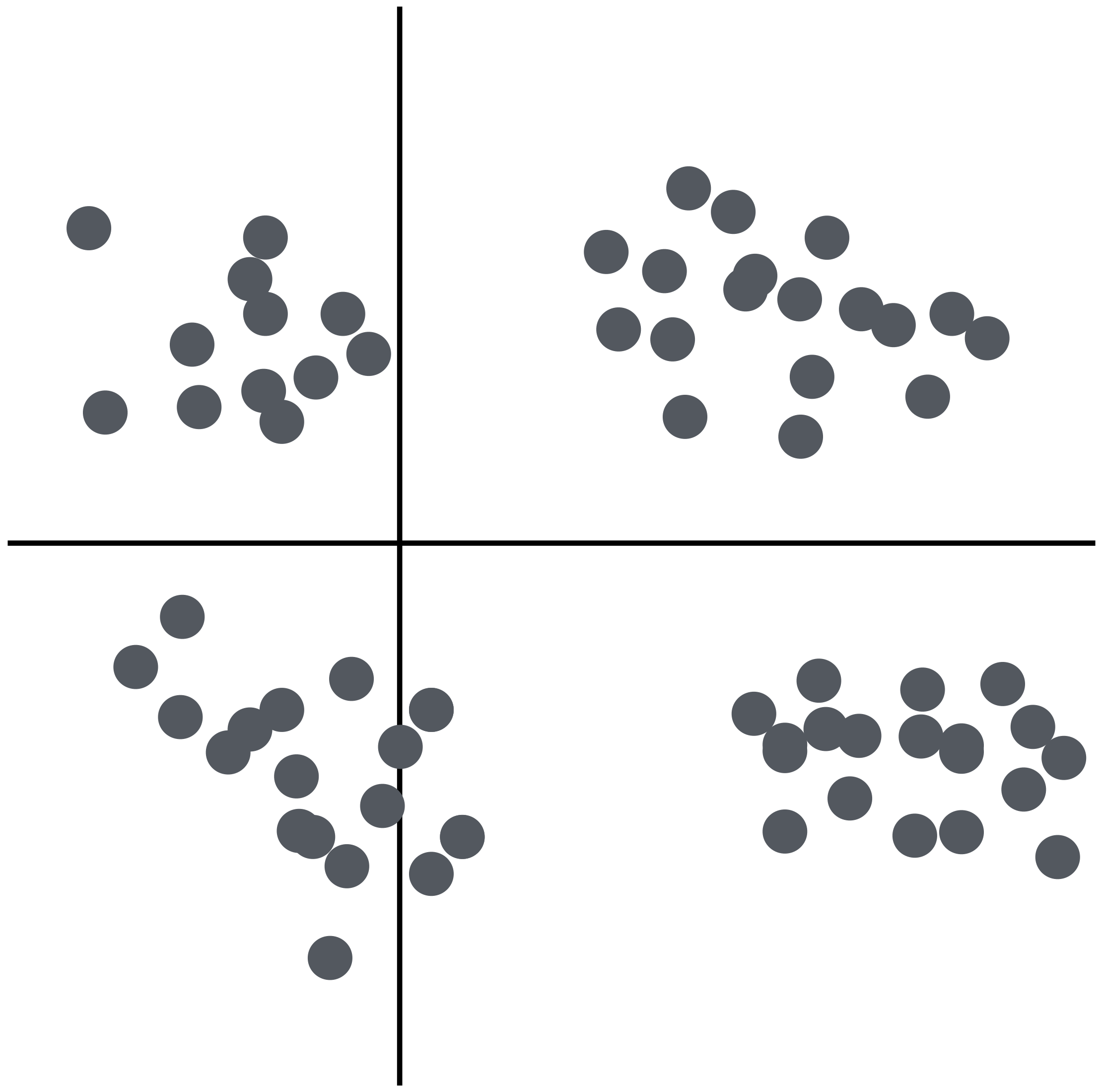

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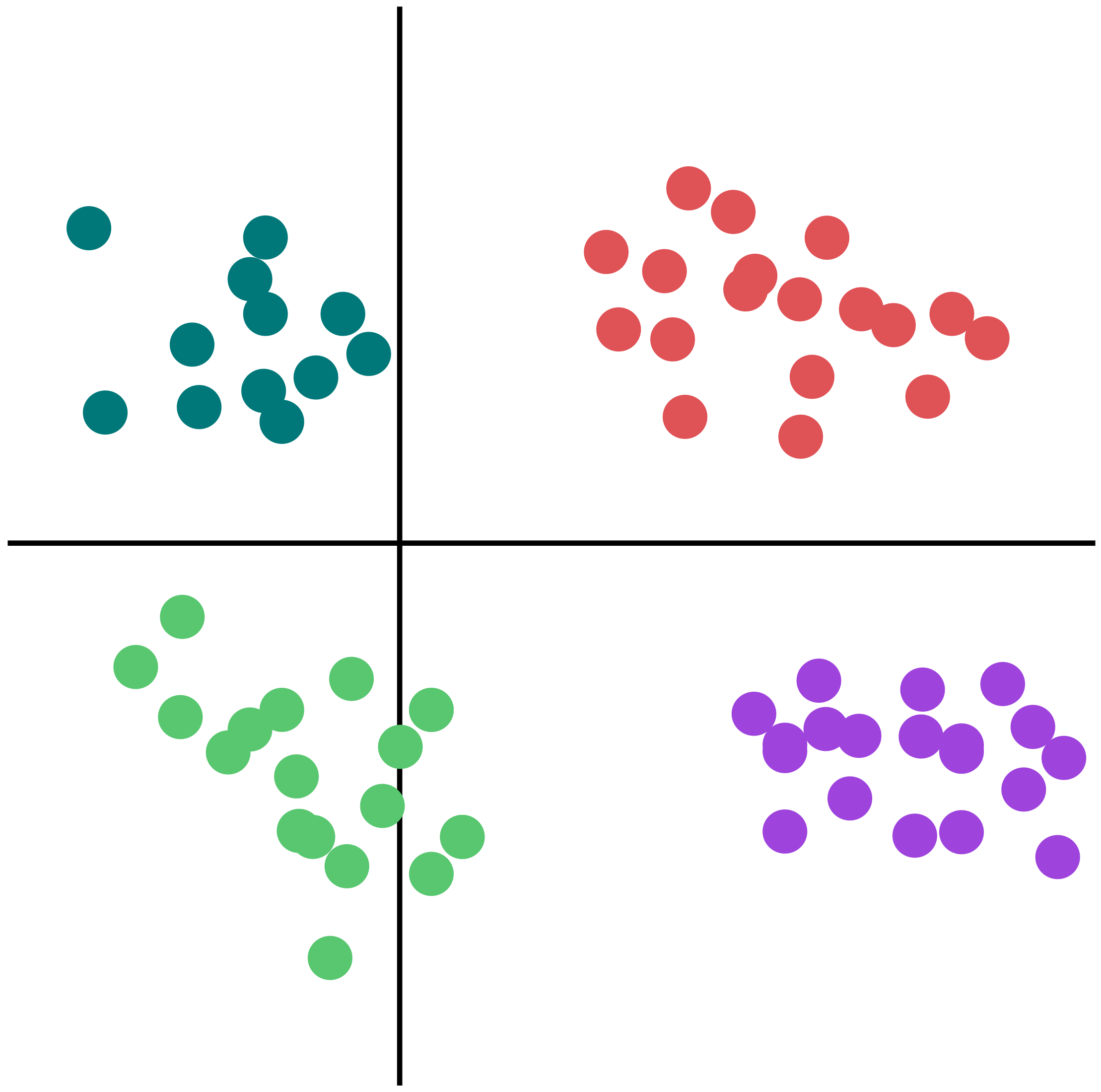

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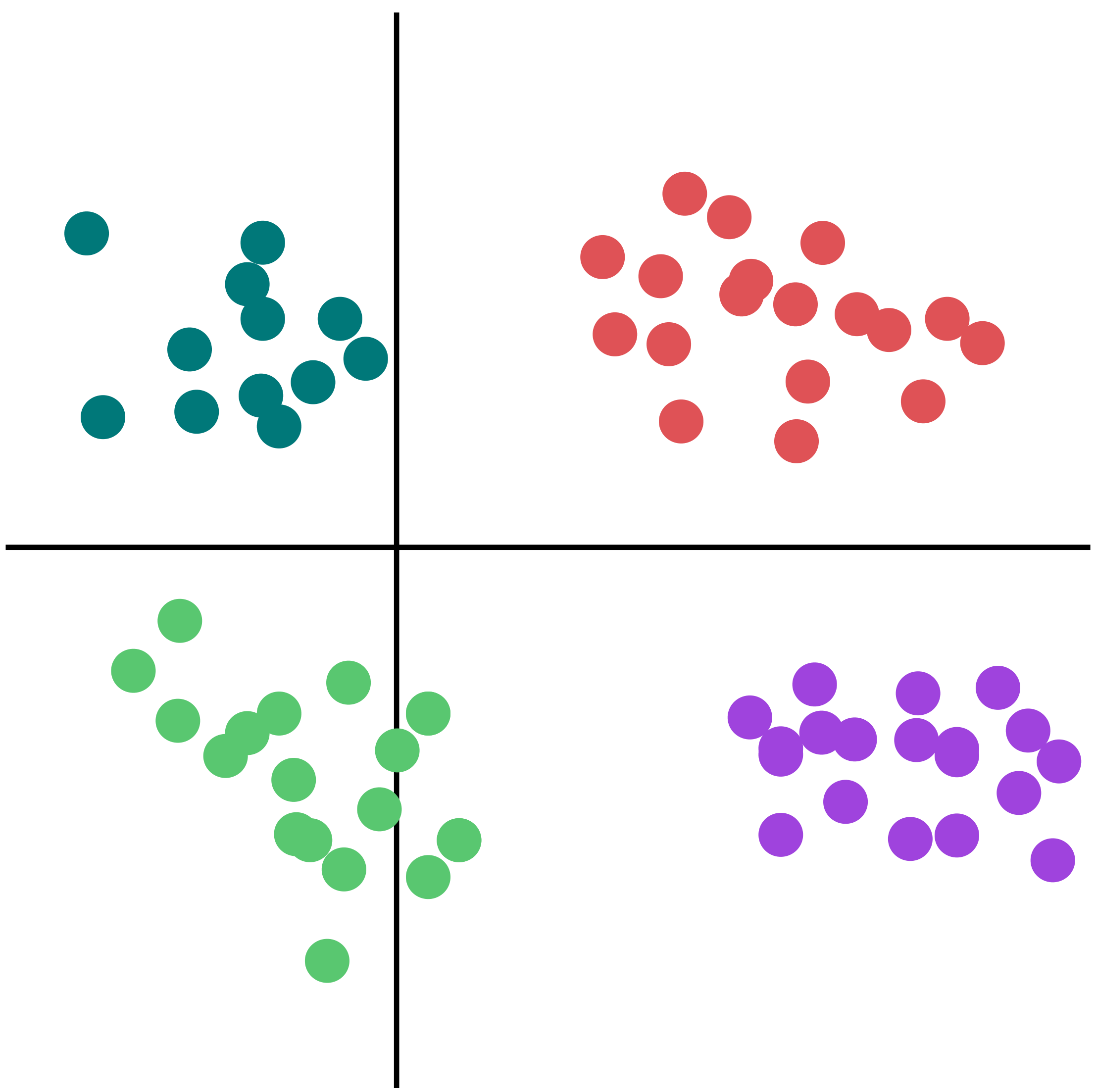
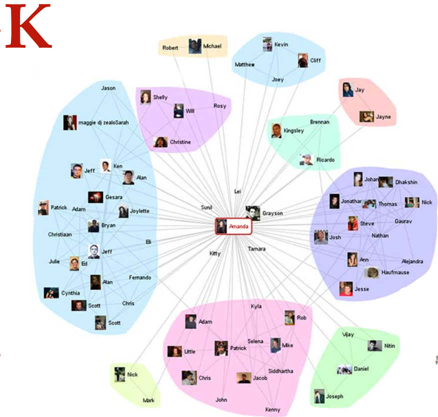
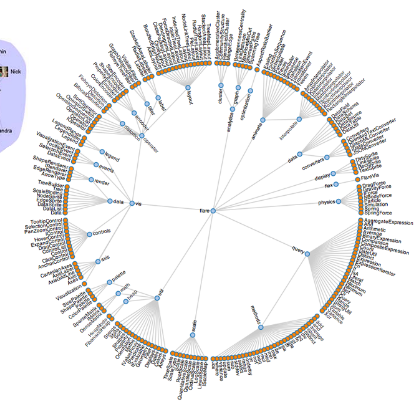


Analysis & Visualization



[Few, 2014]



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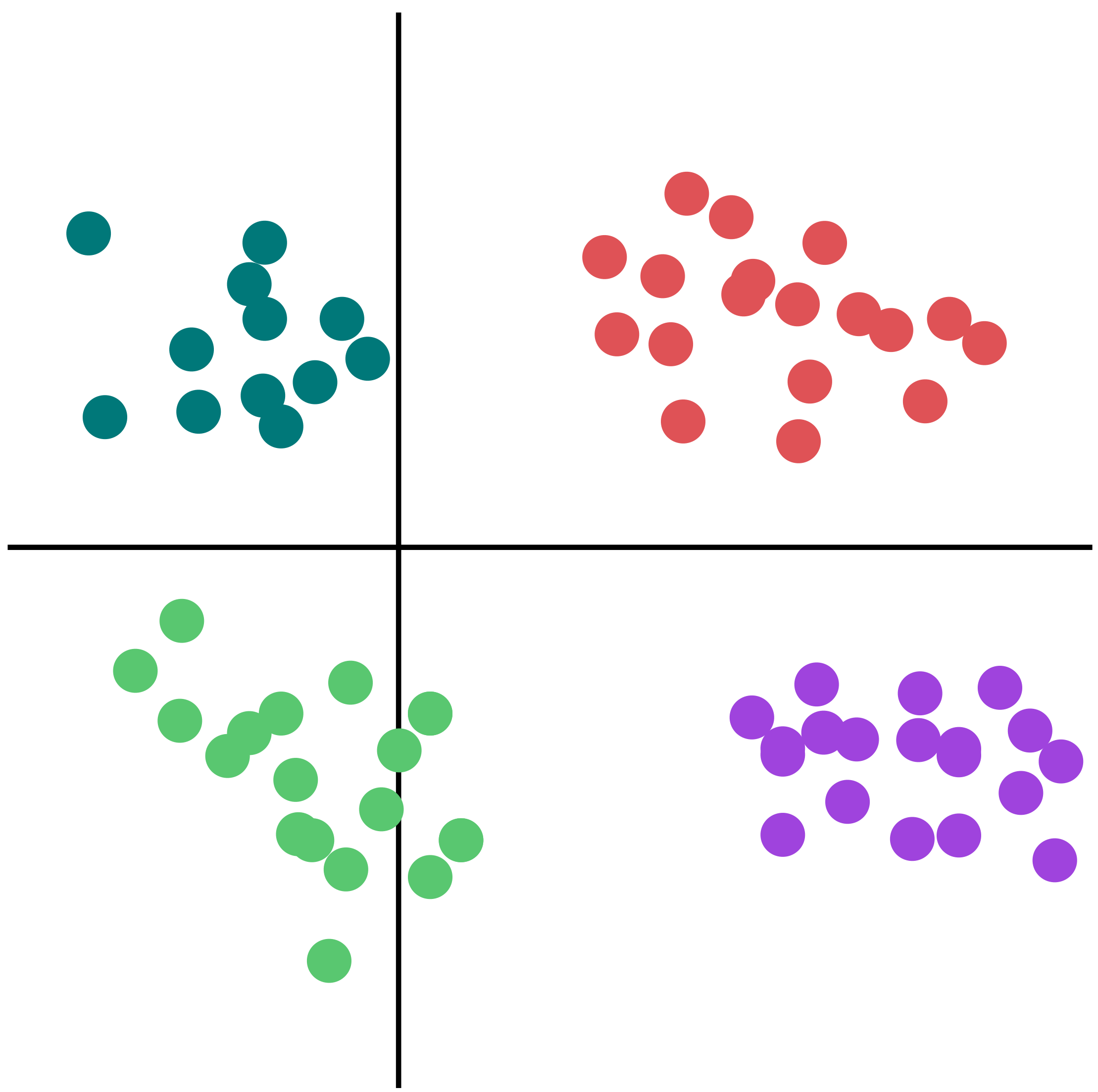

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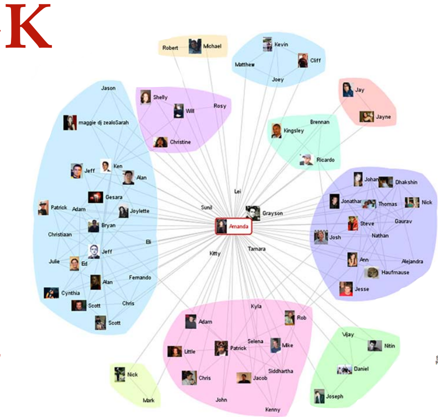

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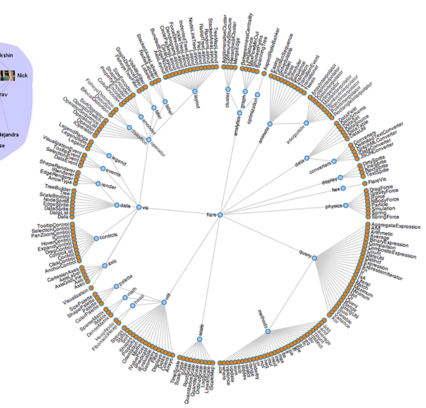

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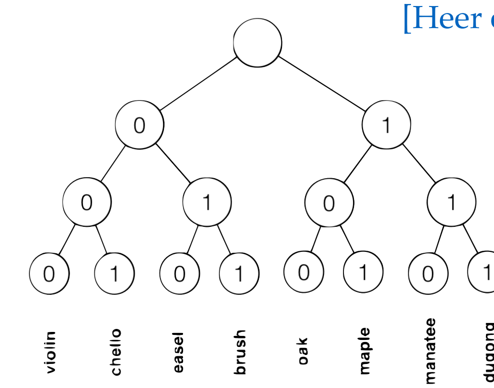
Feature Engineering

[Brown et al, 1993]



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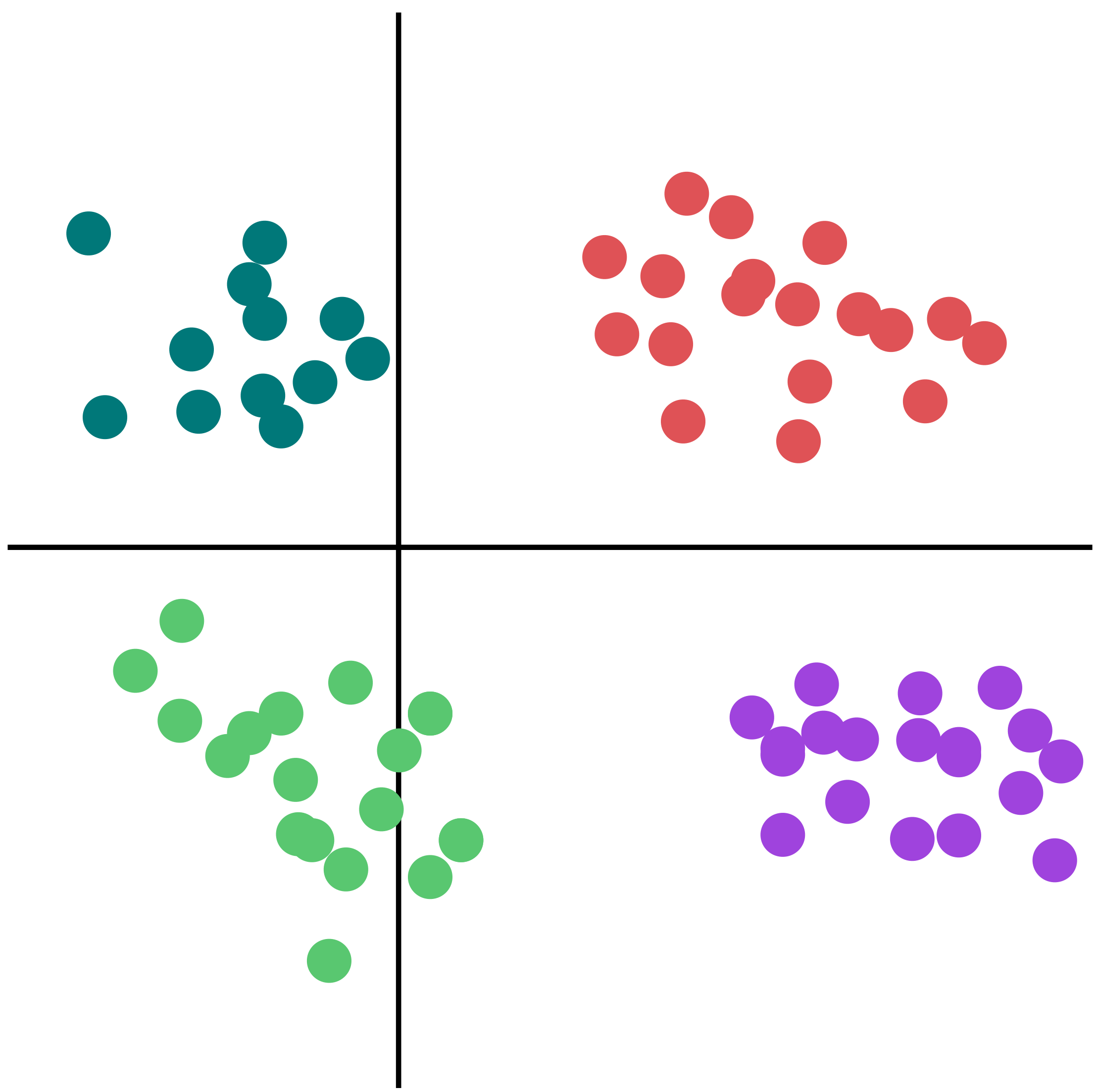

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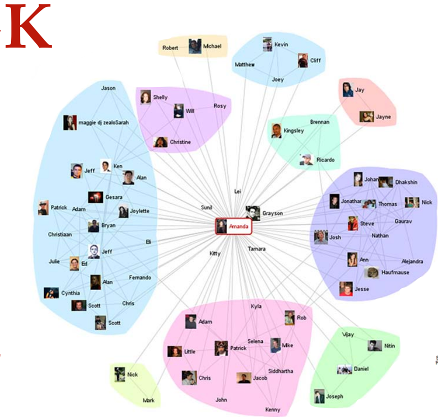

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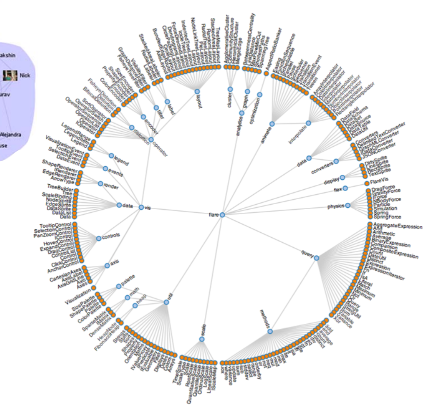

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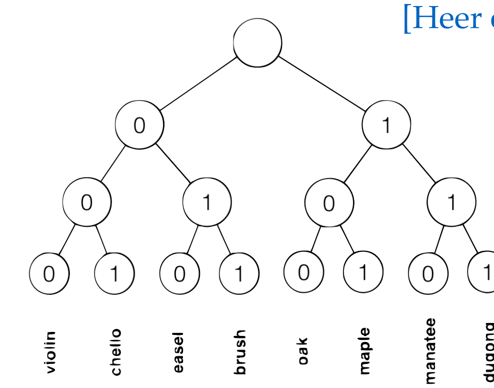

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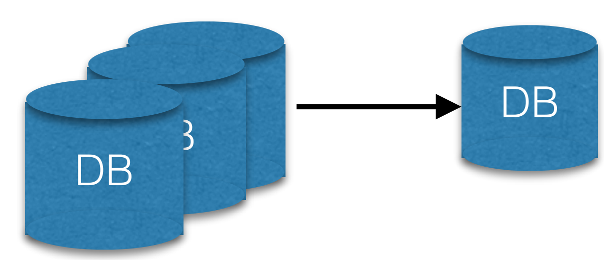

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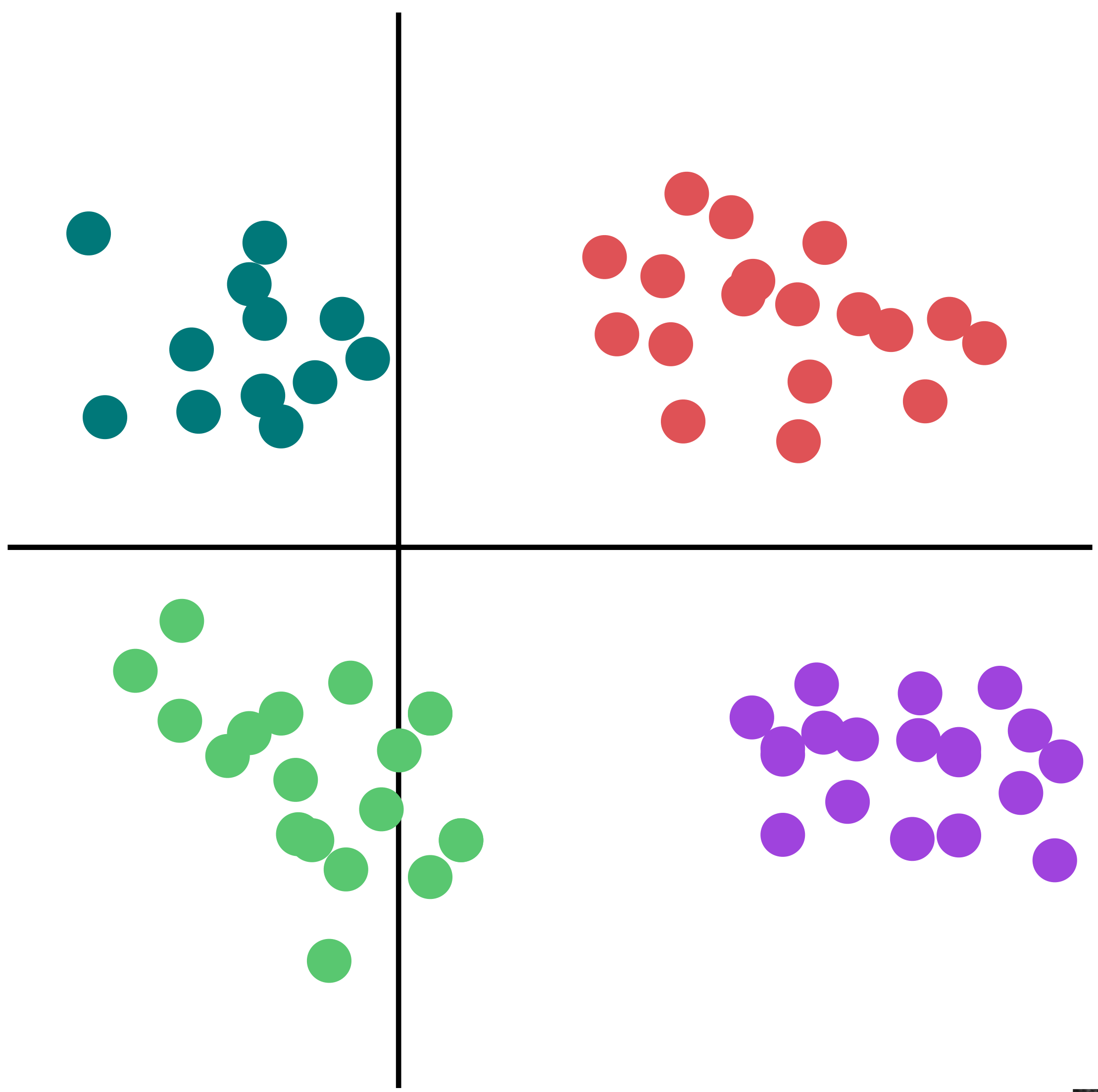

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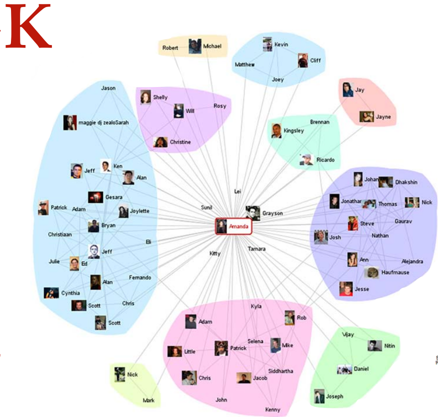

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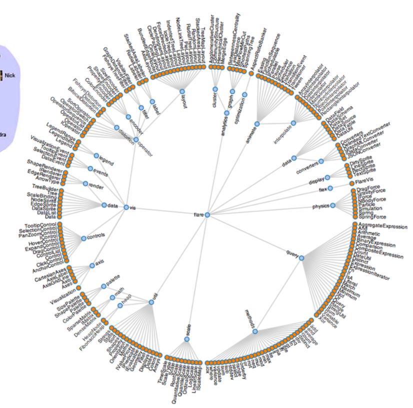

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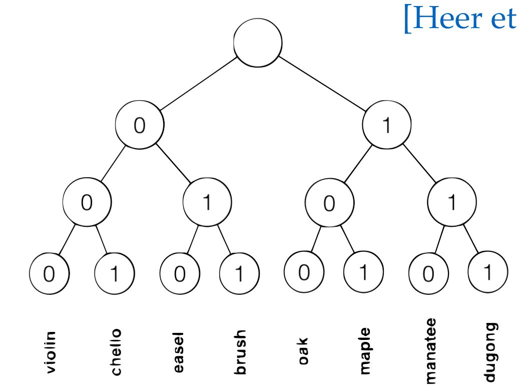

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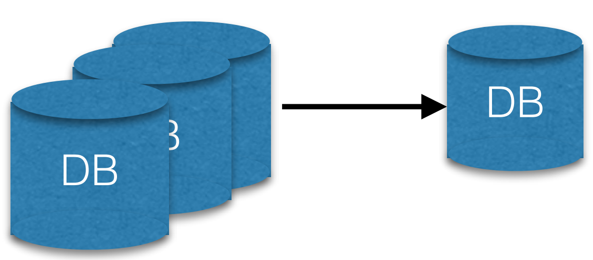
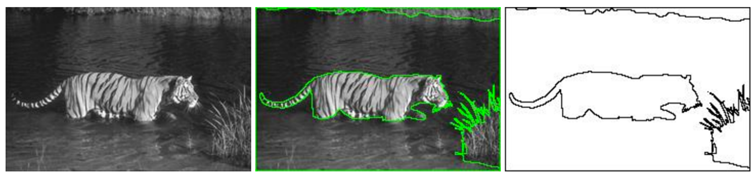


Image Segmentation



[Martin et al, 2001]

Extreme Clustering

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Large Number of Clusters *K*
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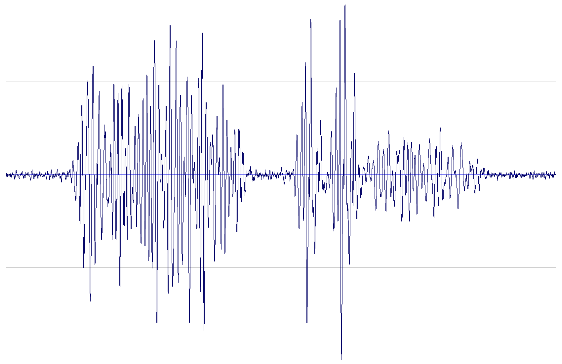
Speaker Recognition



NIST I-VECTOR Challenge

N = 36,572 Samples
K = 4,958 Speakers

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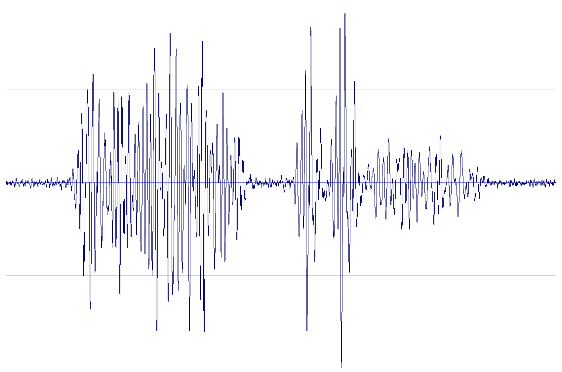

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N =14 Million Images

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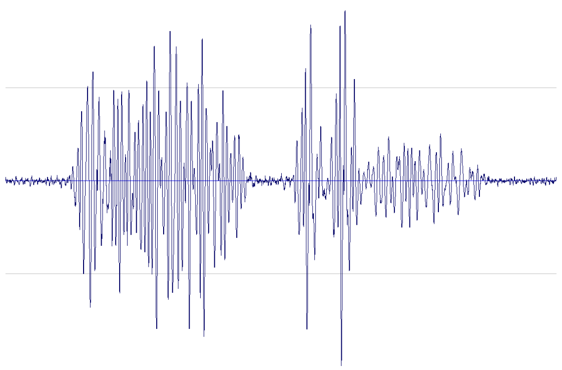

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Author Coreference. N=10M Records, K=1M Authors

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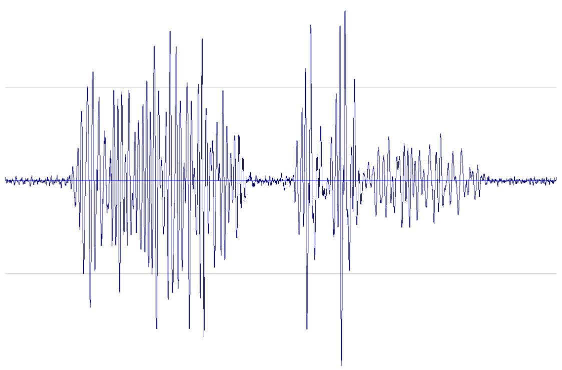

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def kmeans(x1...xN,K):
 until convergence
  for x in x1...xN:
   for c in clusters:
    if ||c - x|| < min_c:
     min_dist = ||c - x||
     min_c = x
   assign(x,min_c)
  update(clusters)
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Linear in K, O(NK)

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For large K, we'd like to be sublinear.

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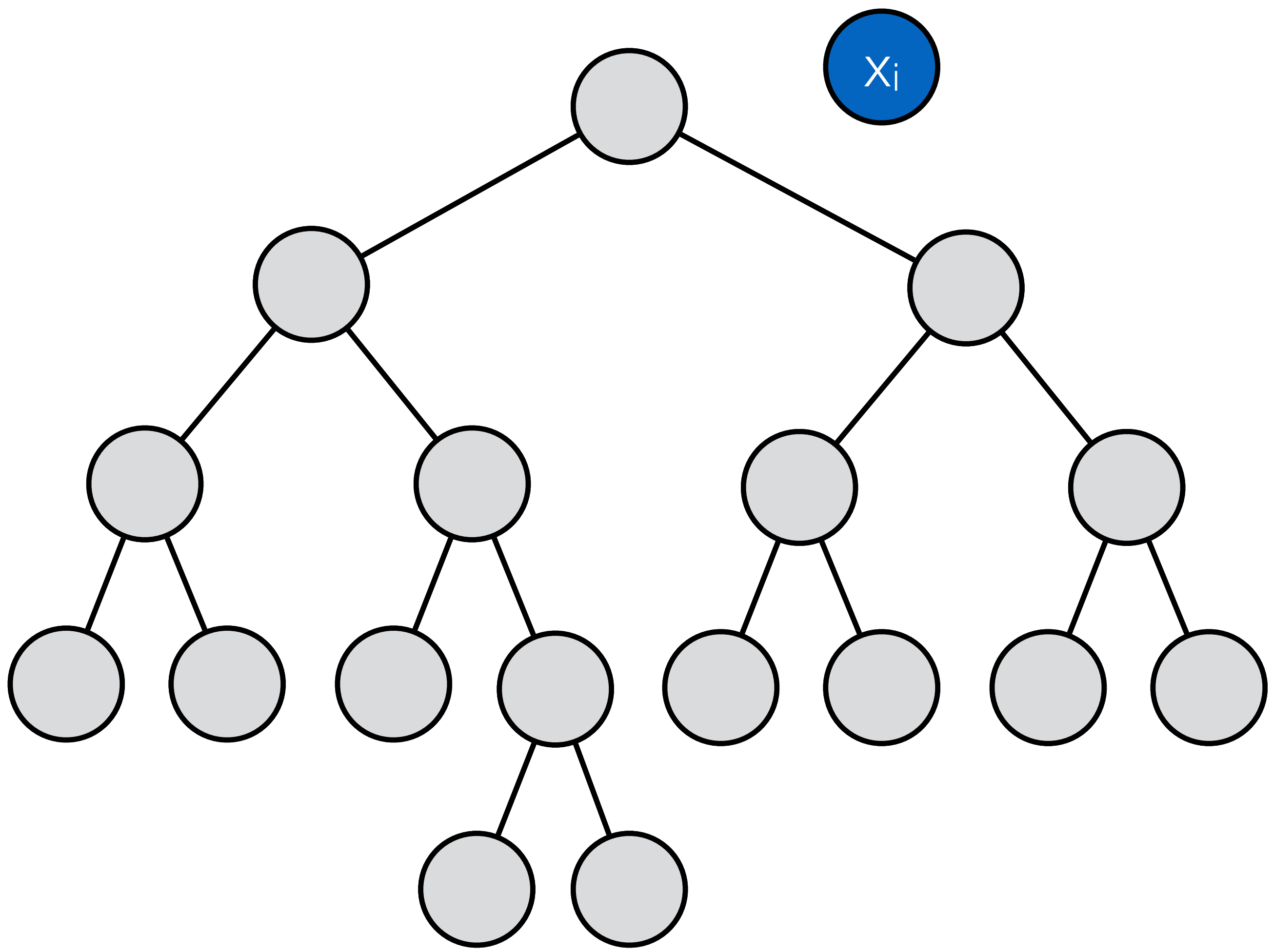
StreamKM++ BICO [Ackermann et al, 2012] [Fichtenberger, et al, 2013]	✓	✗	—	Number of coresets does not scale with K

Hierarchical Clustering

Advantages for Online Extreme Clustering

Efficiency



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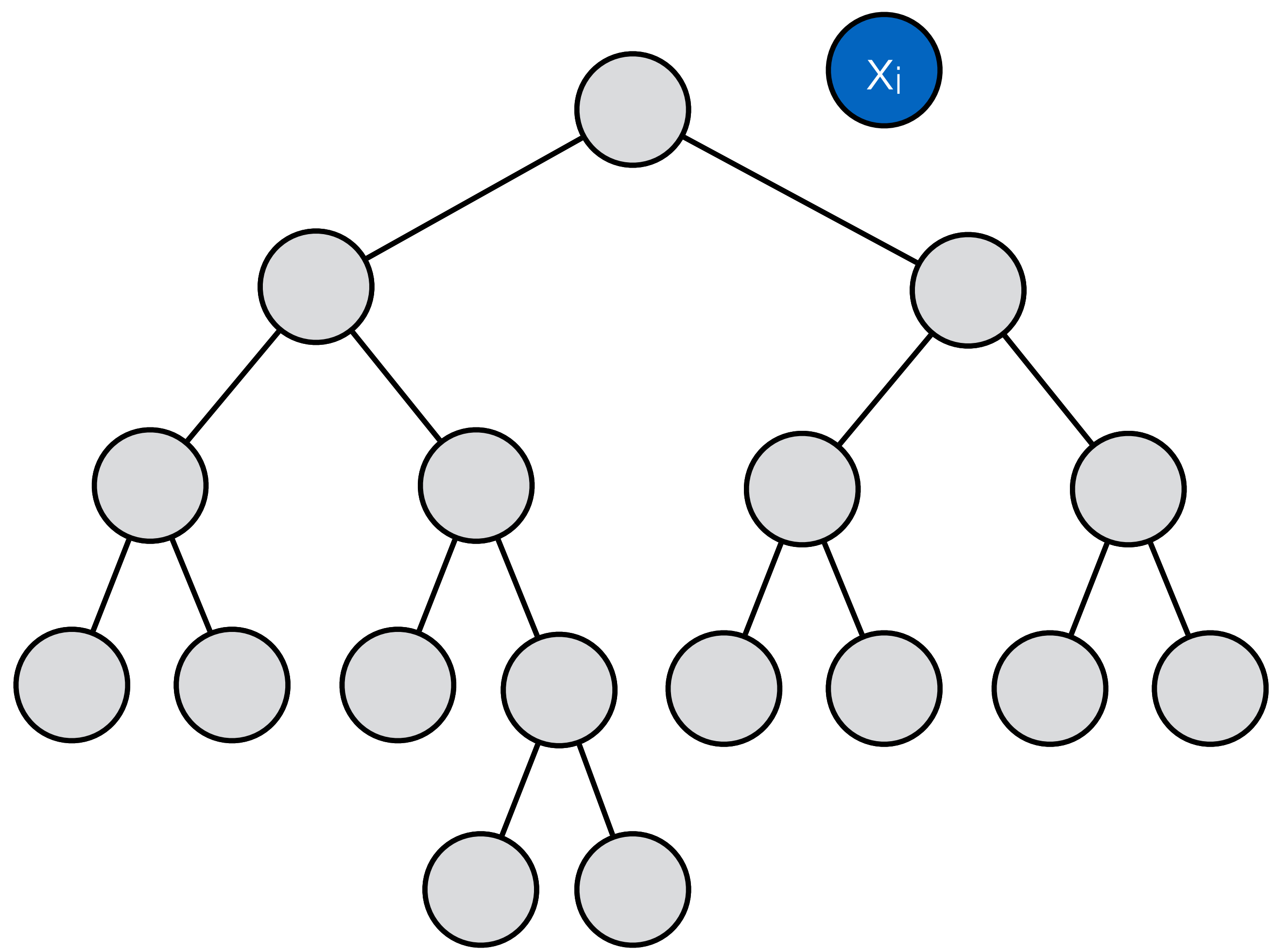

Top-Down Log-Time Search

Extreme Multiclass Classification:

[Choromanska et al, 2015]
[Daumé III et al, 2016]

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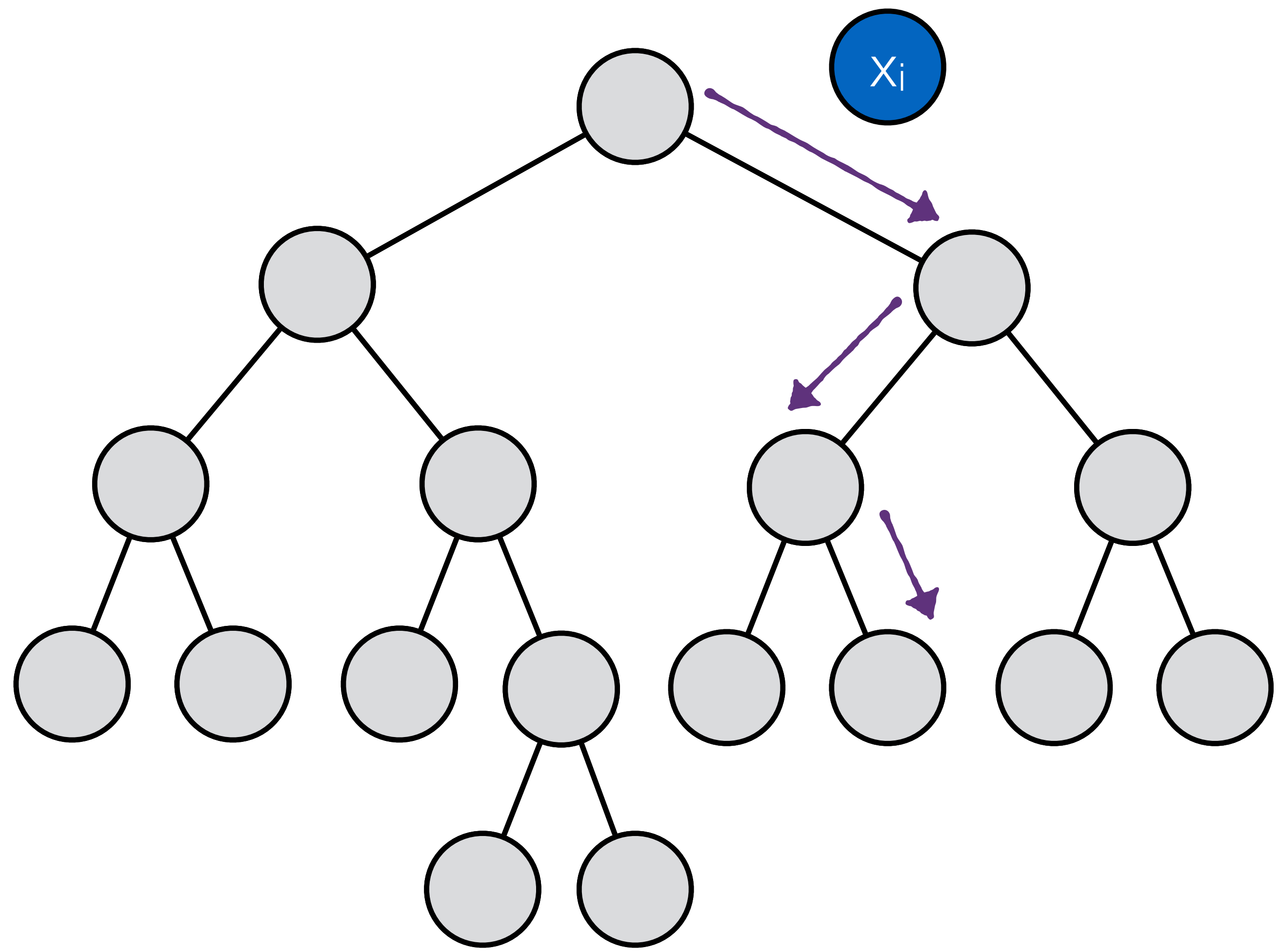

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Hierarchical Clustering

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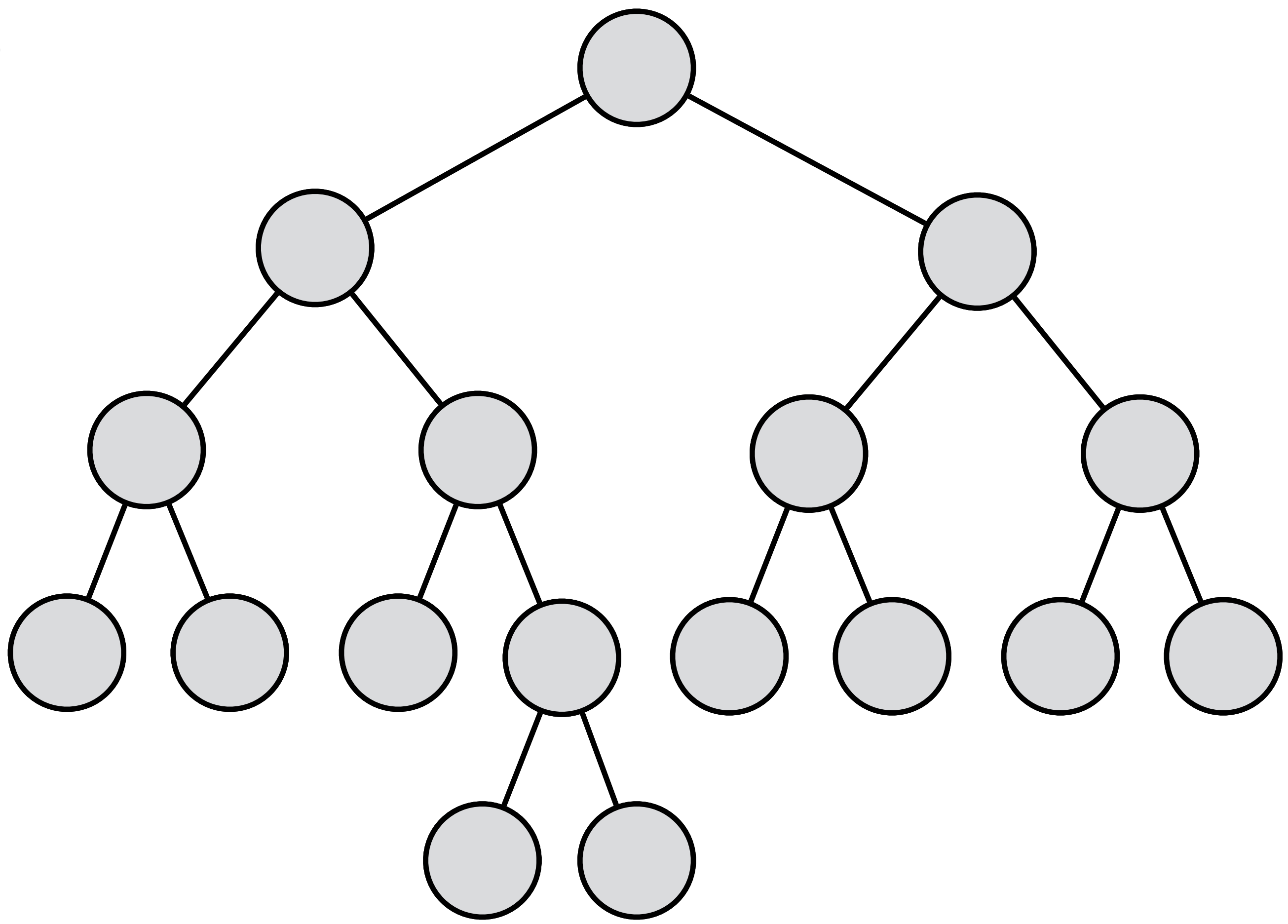

Hierarchical Clustering

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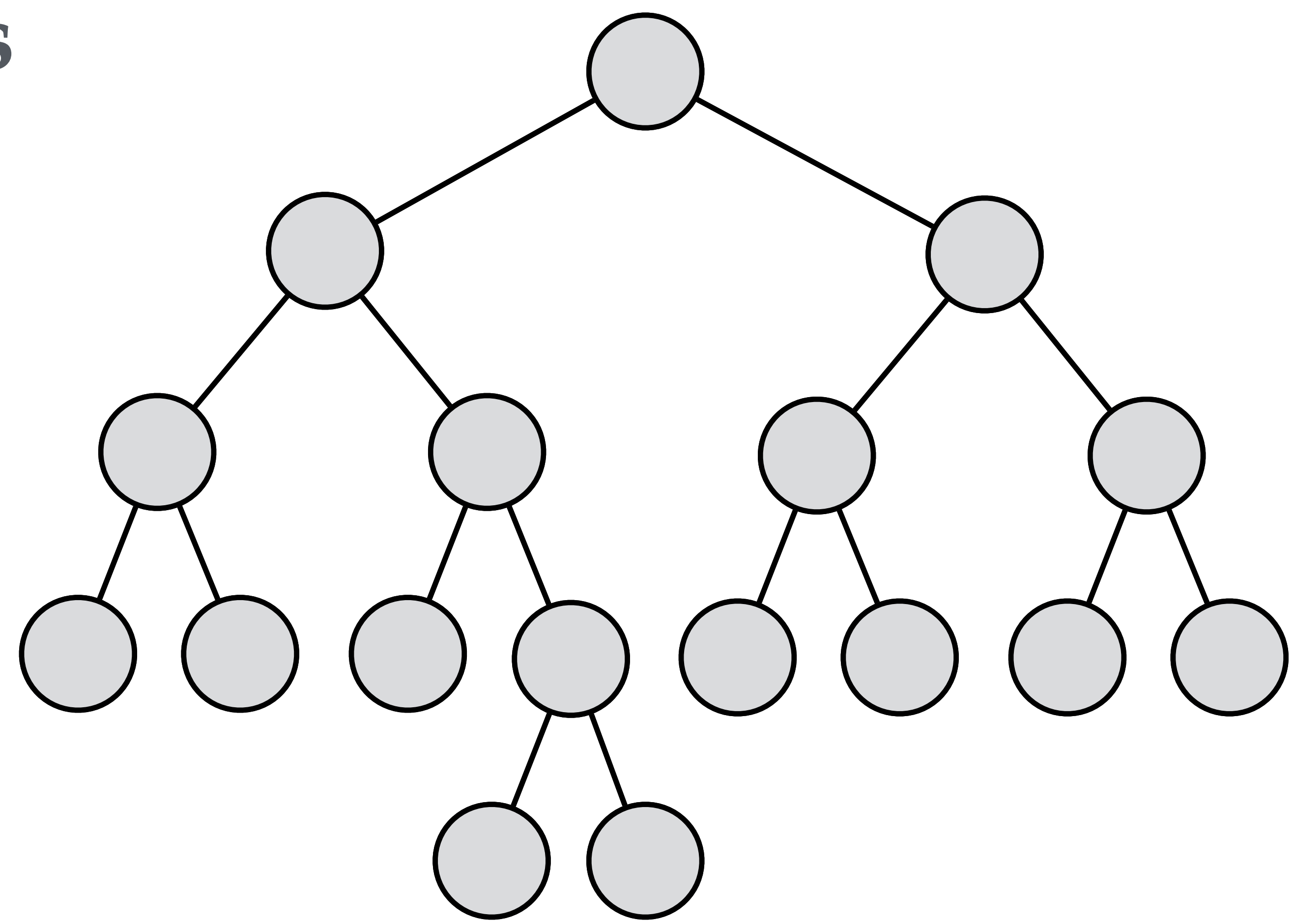

Simultaneously Represent
Multiple Alternative Clusterings

Hierarchical Clustering

Advantages for Online Extreme Clustering

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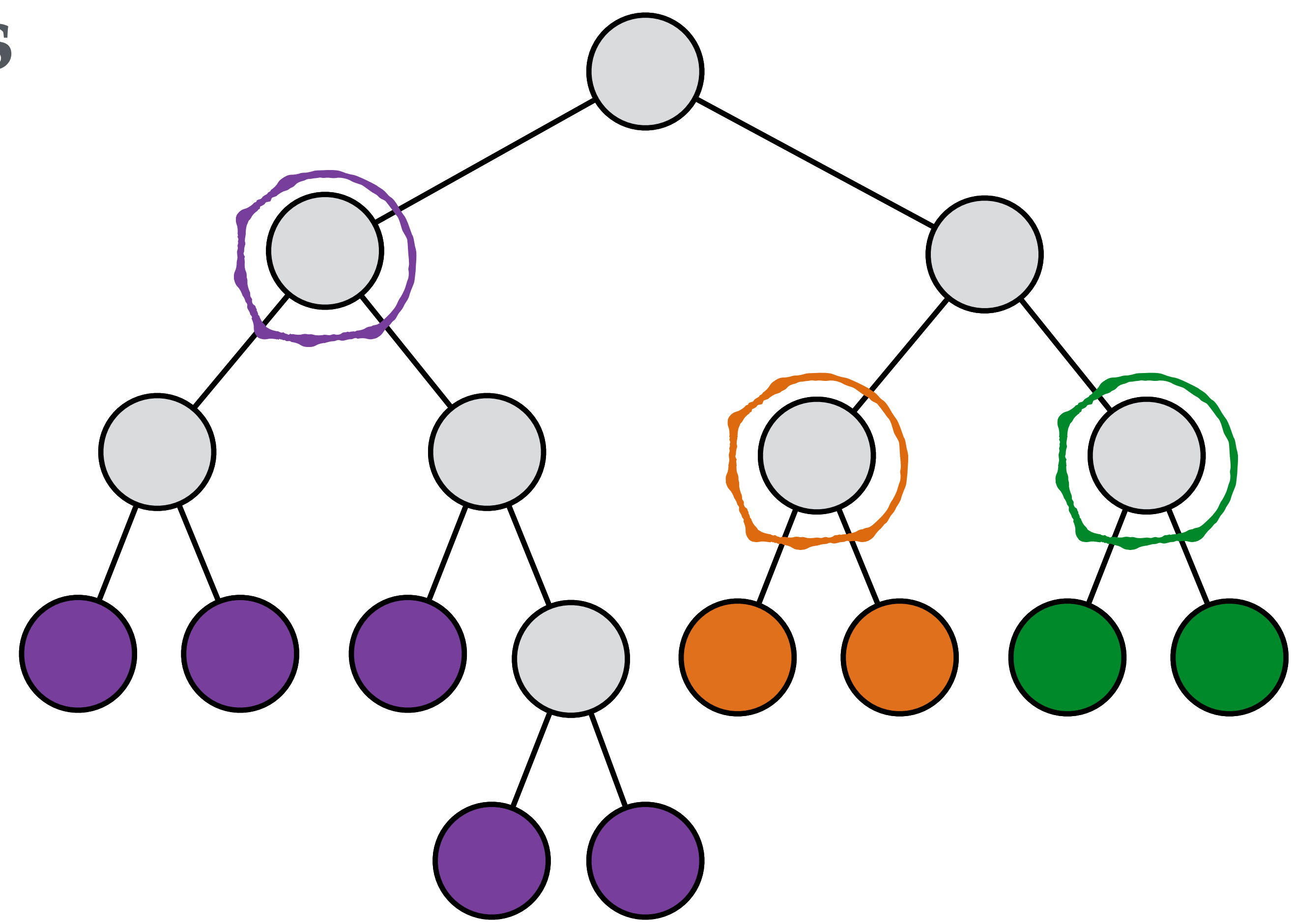

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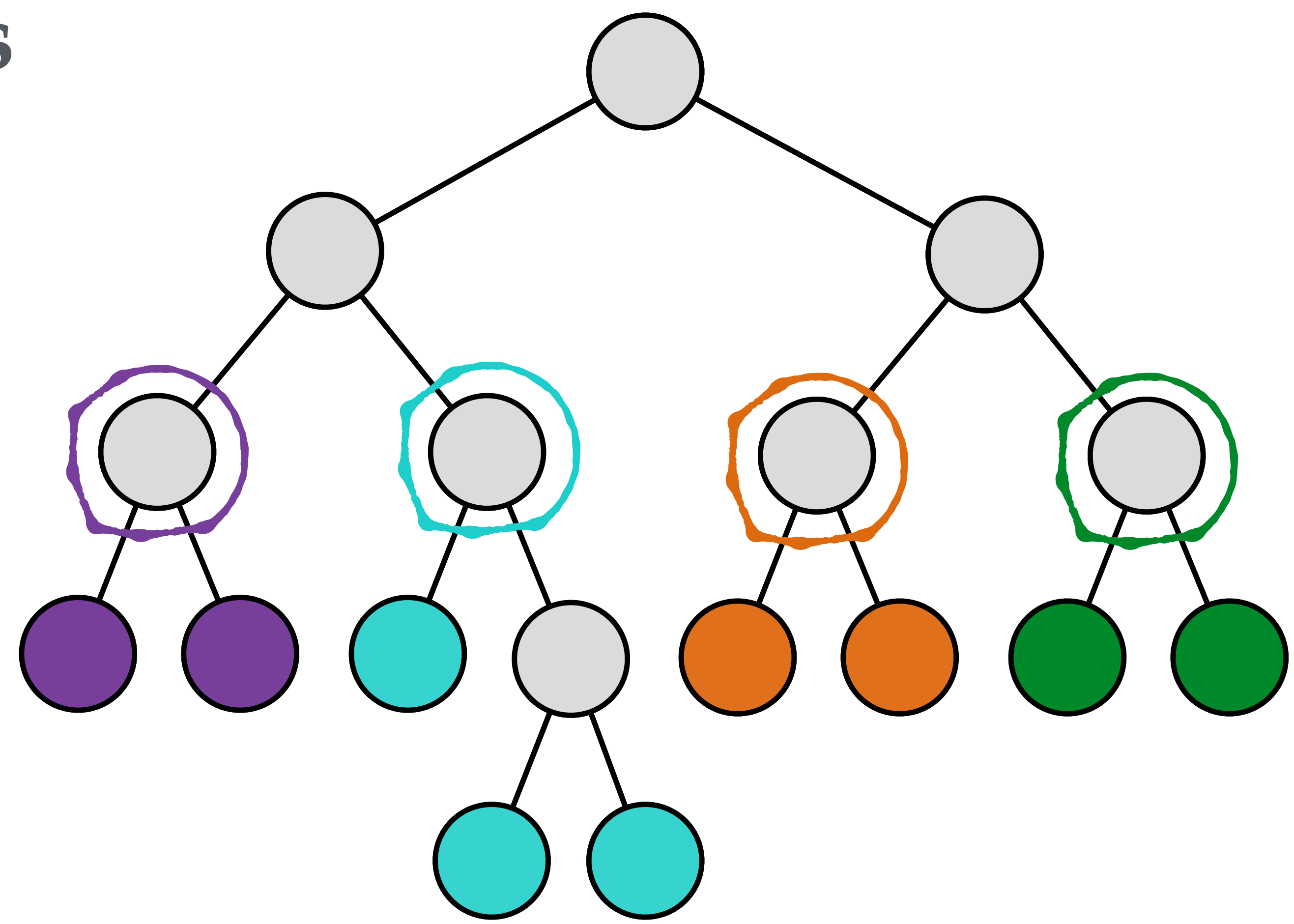

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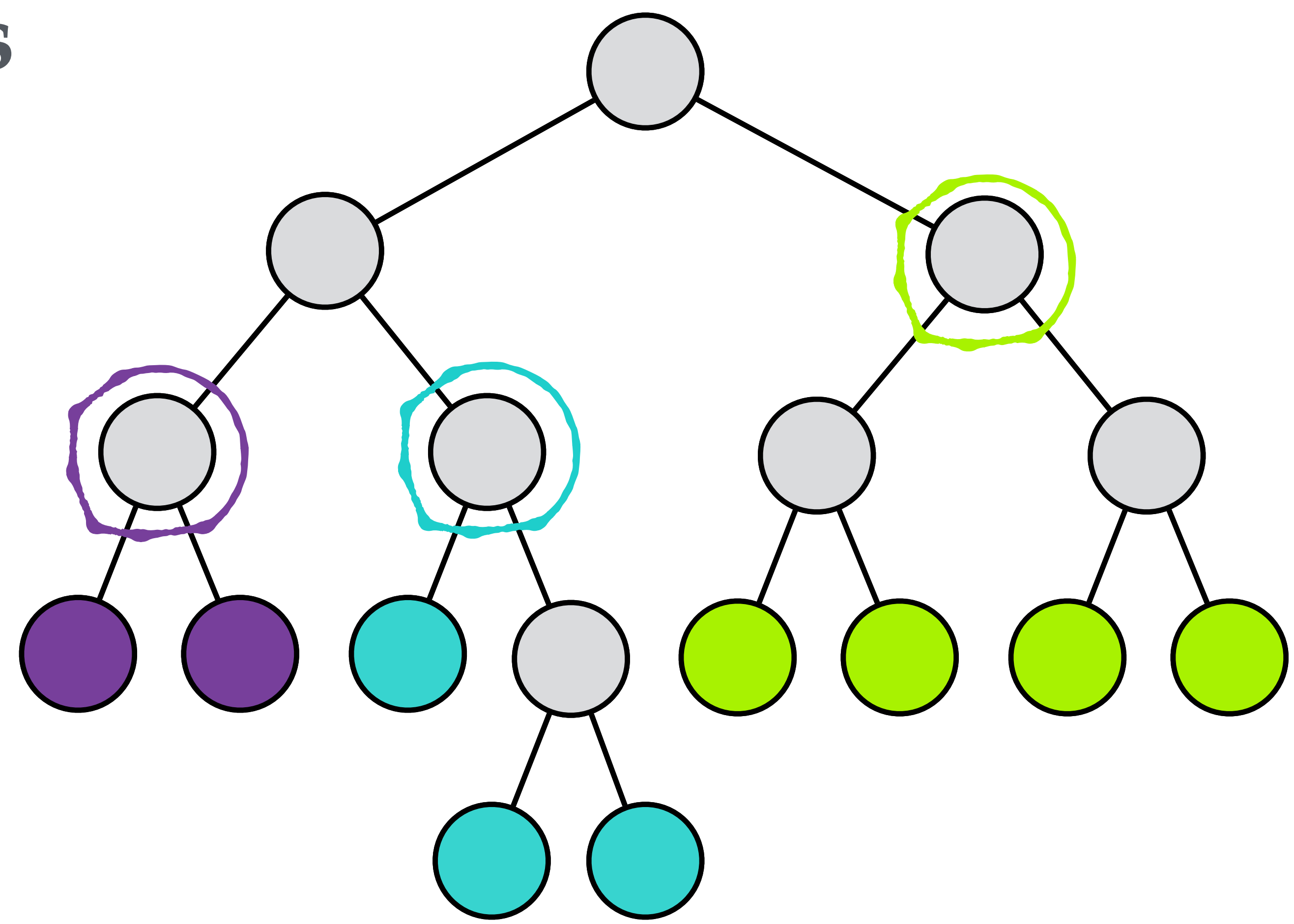

Simultaneously Represent
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PERCH

Purity Enhancing Rotations for Cluster Hierarchies

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Incrementally build hierarchical clustering

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Incrementally build hierarchical clustering

Route point to nearest neighbor

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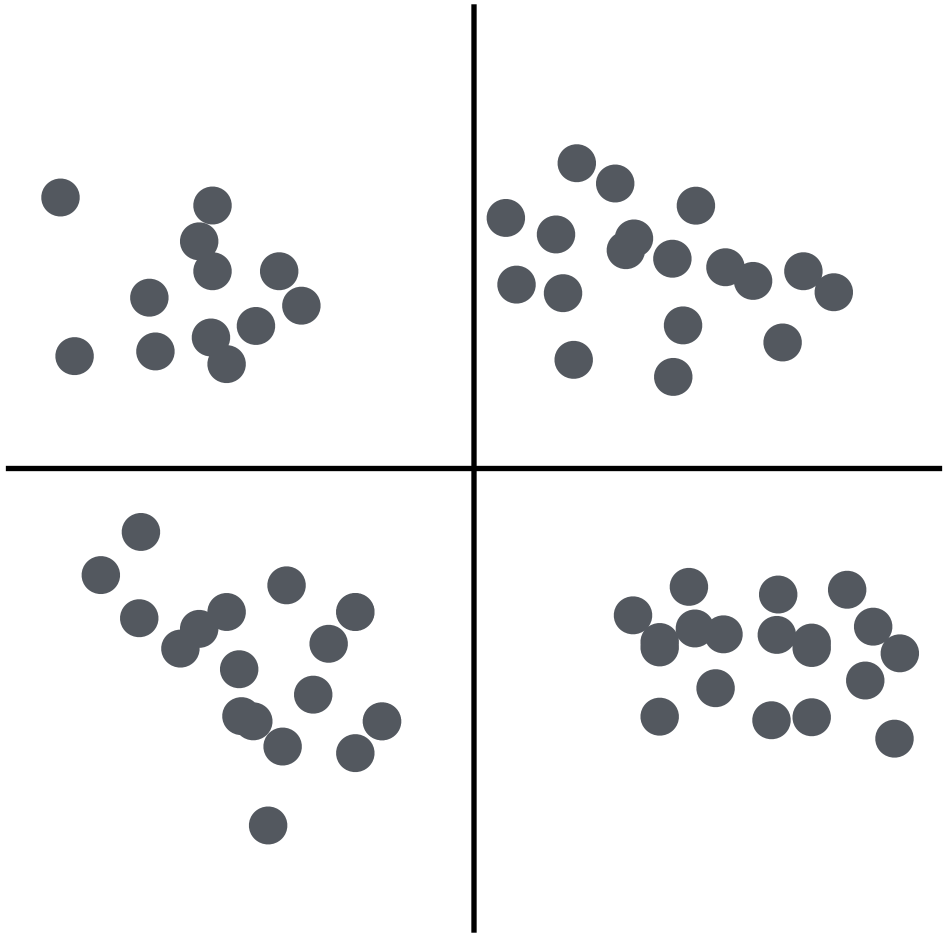
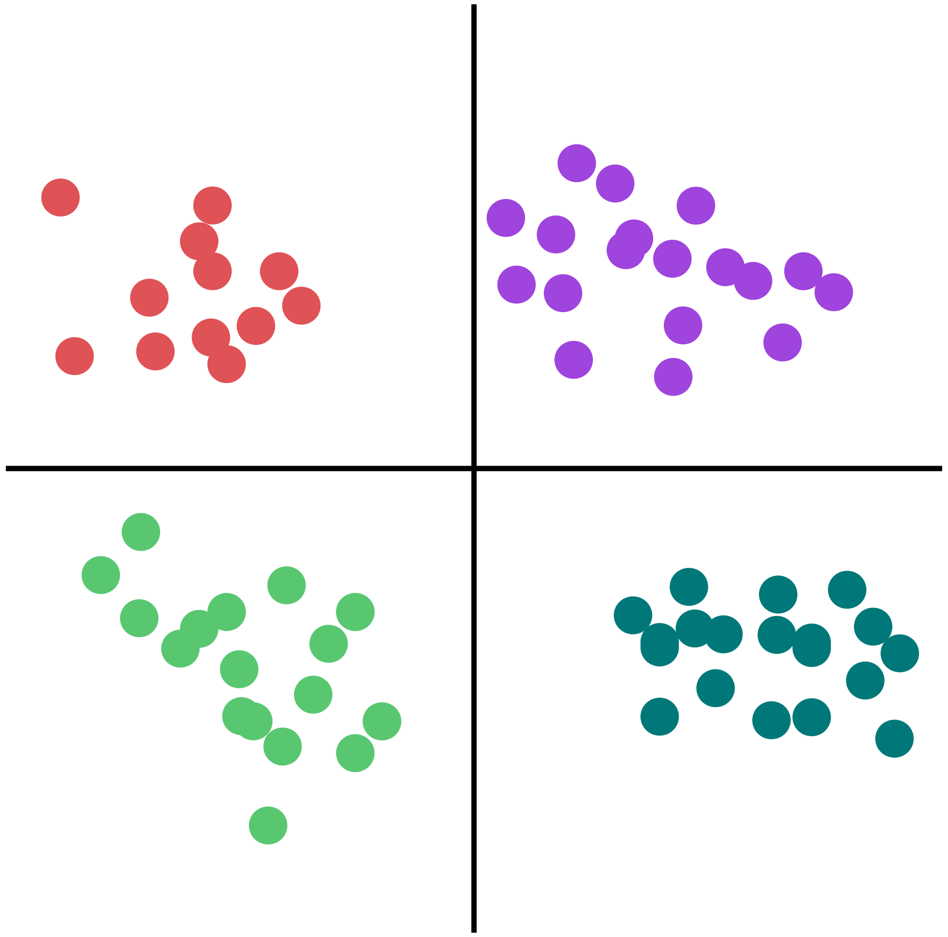
Route point to nearest neighbor

Tree maintenance using rotation operations



Dataset



True Clustering

(labels withheld from clustering algorithm)

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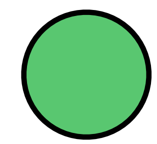

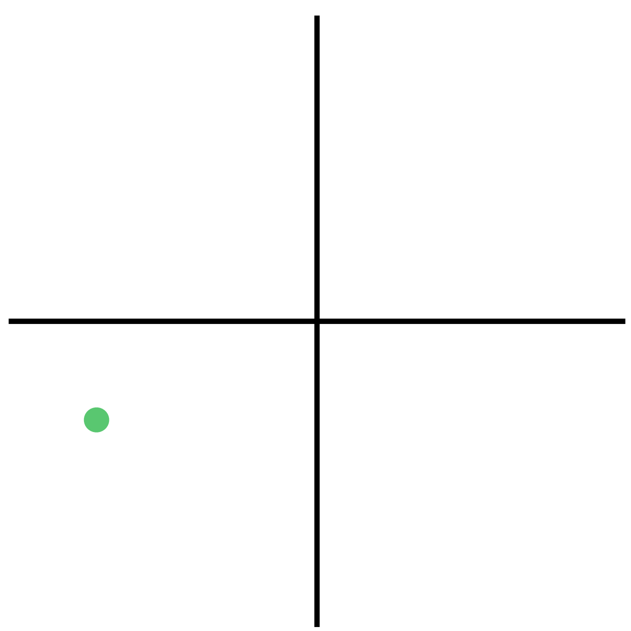

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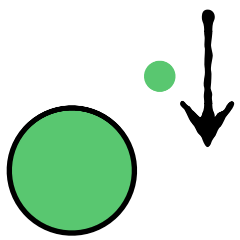

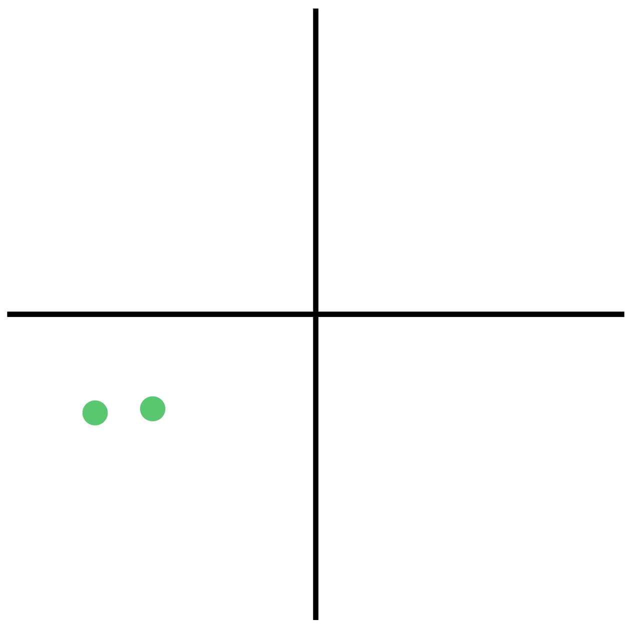

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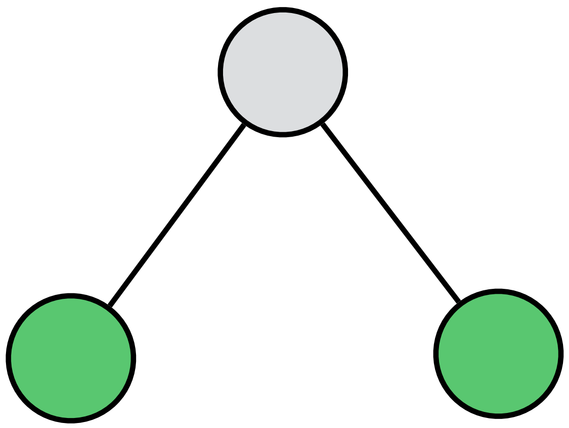

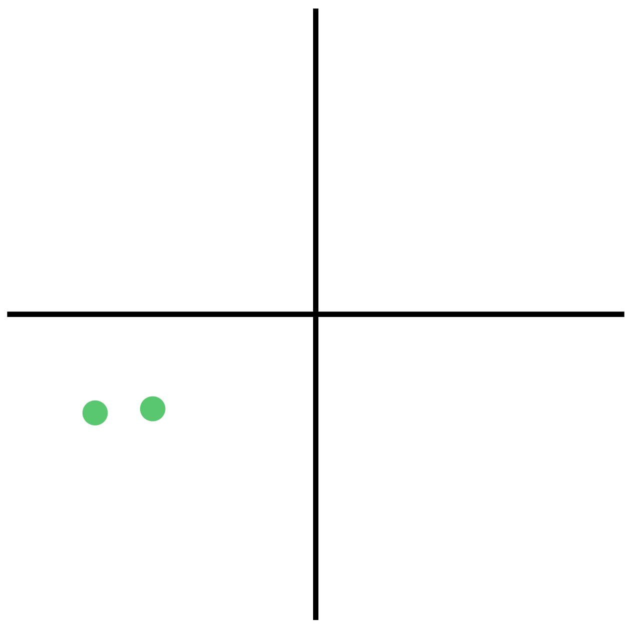

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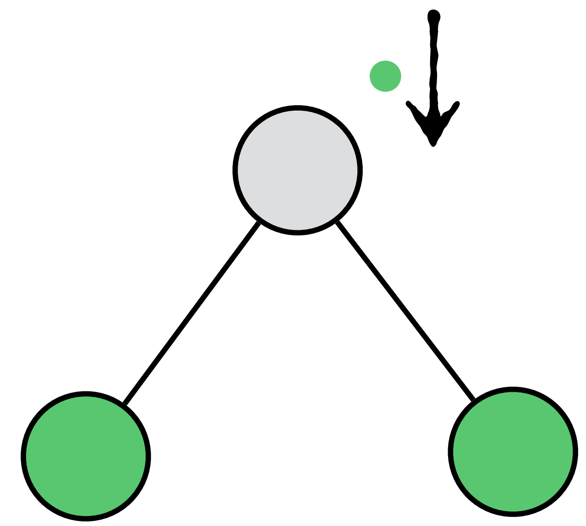

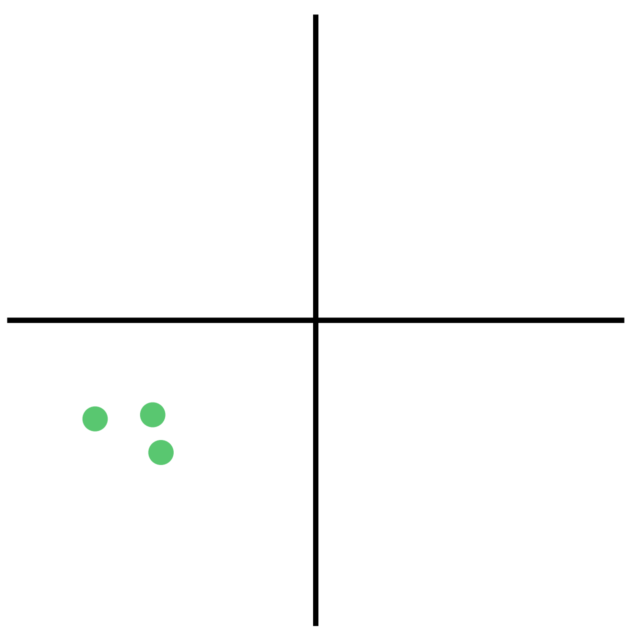

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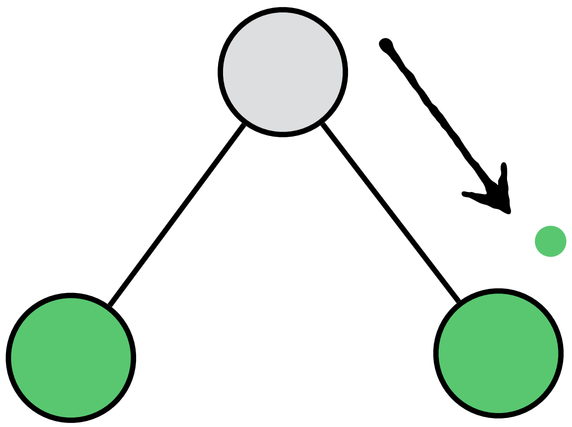

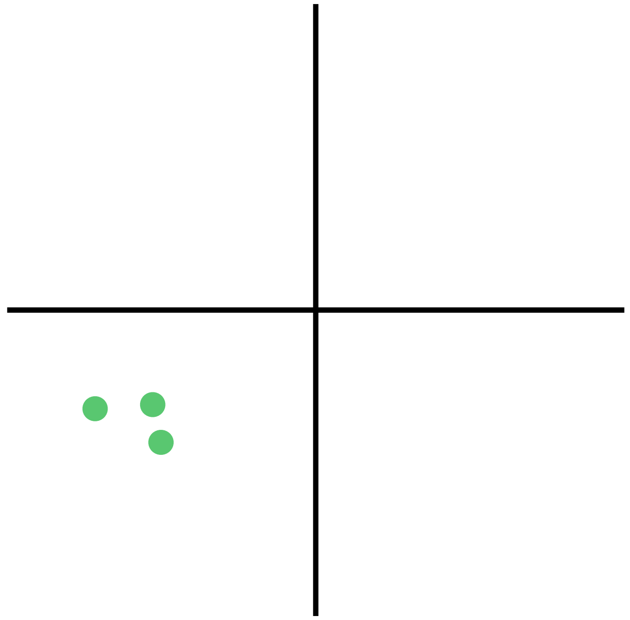

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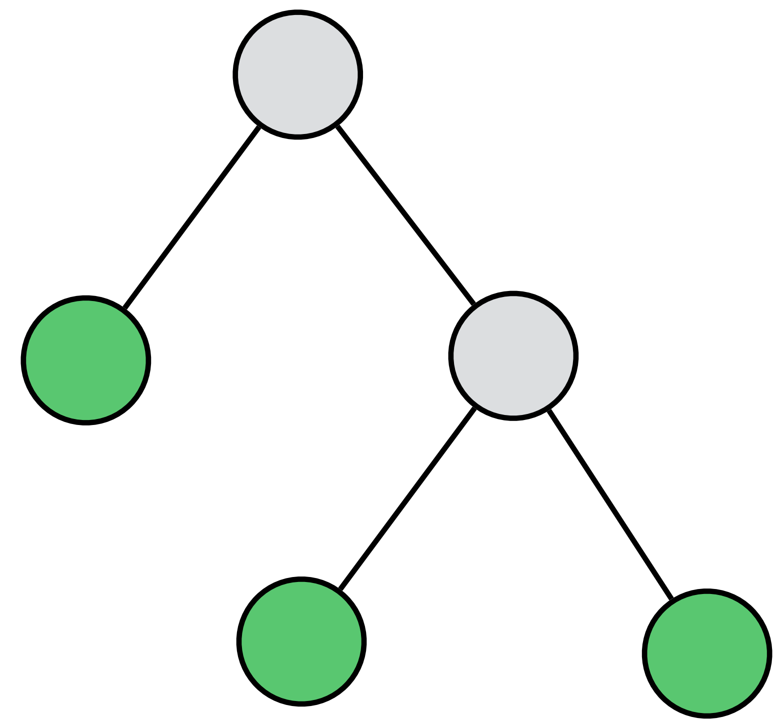

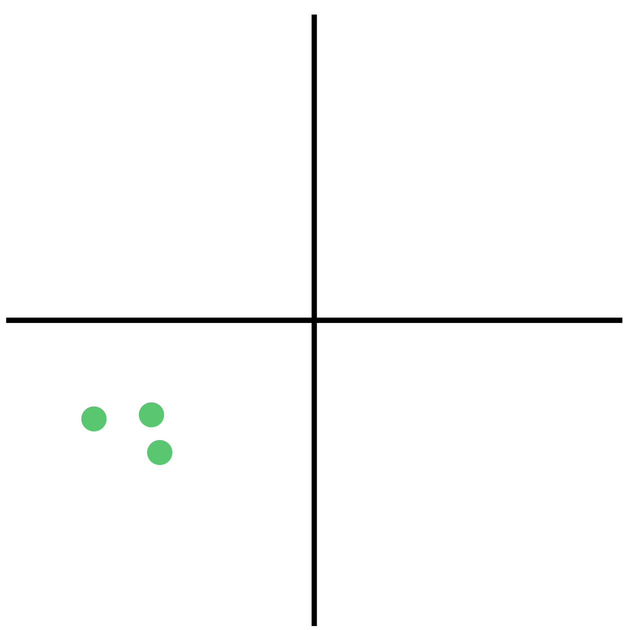

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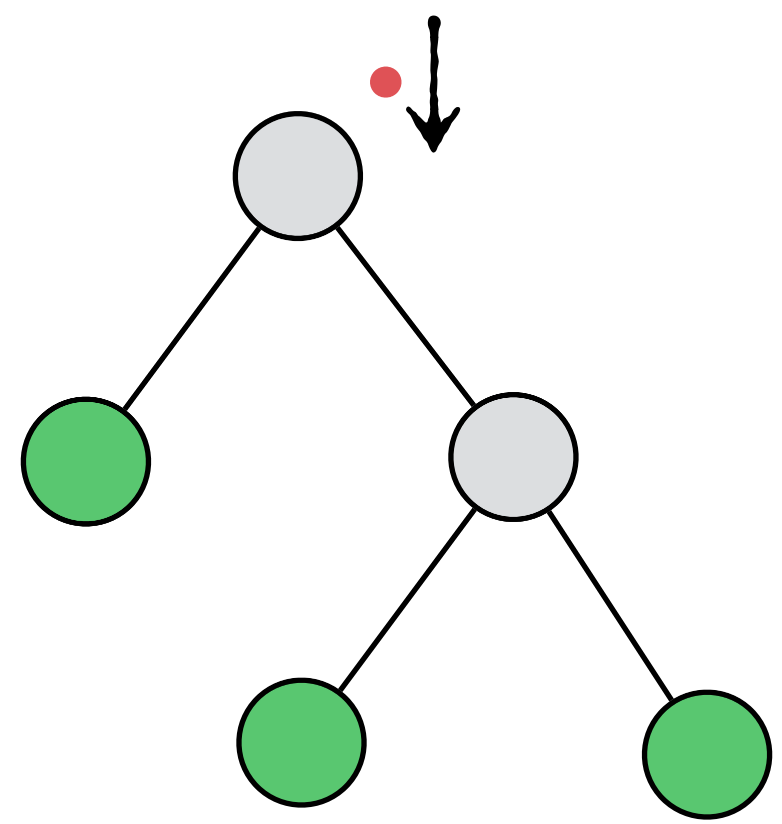

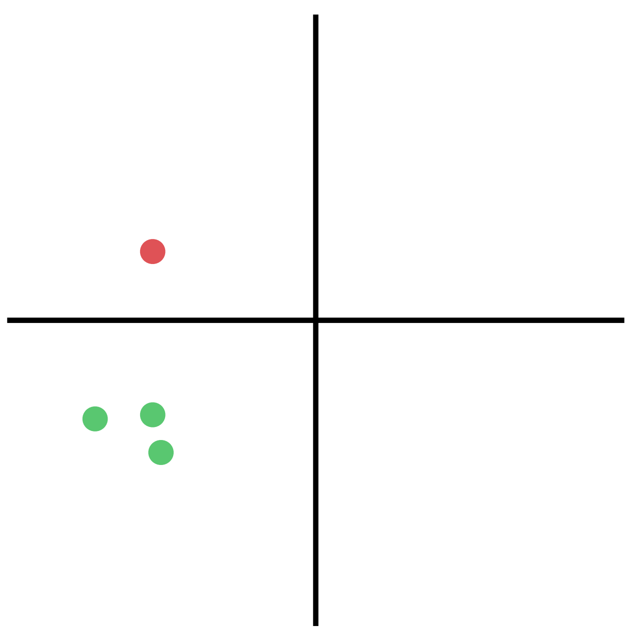

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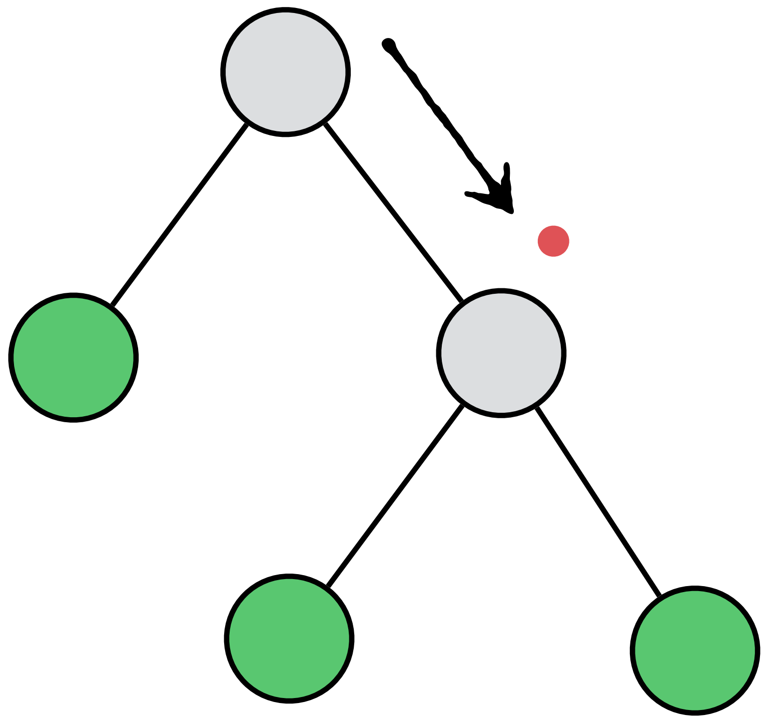

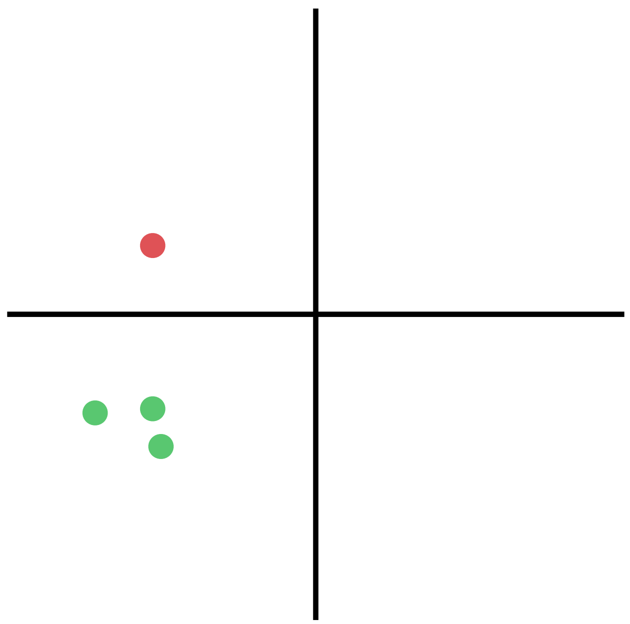

PERCH

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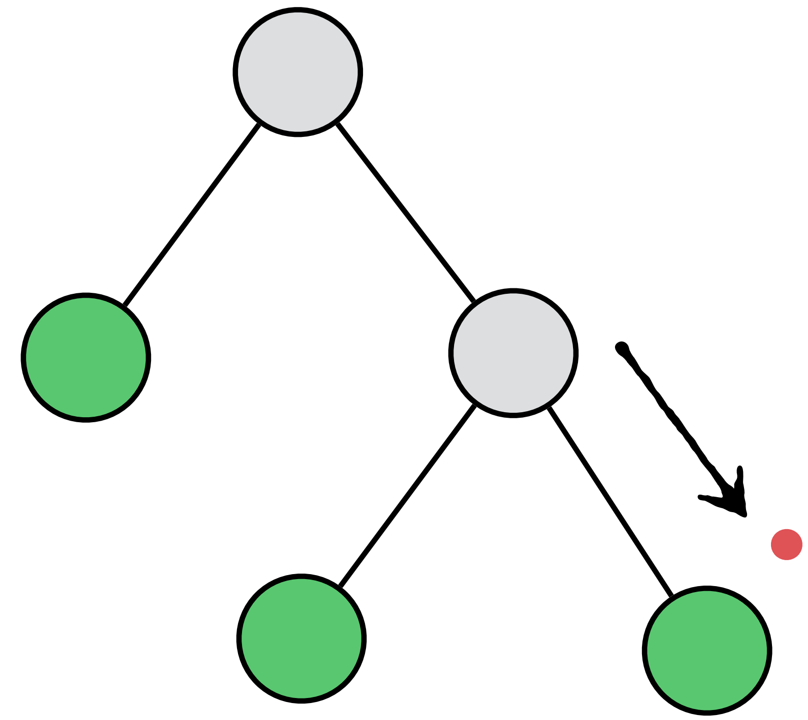

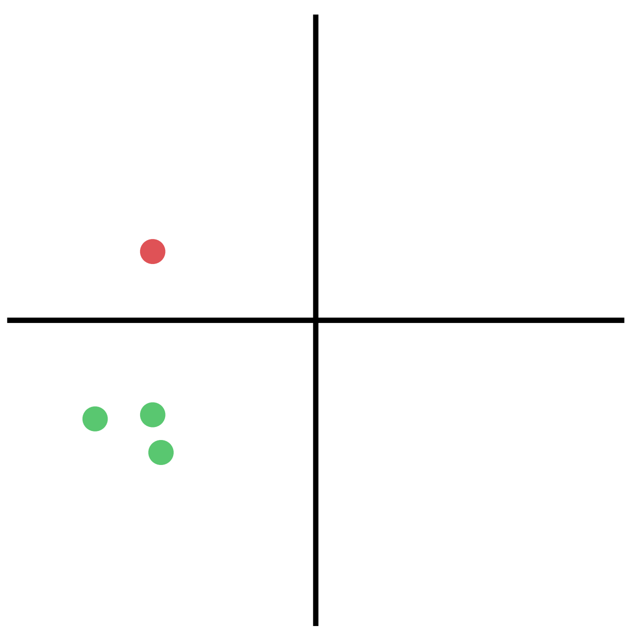

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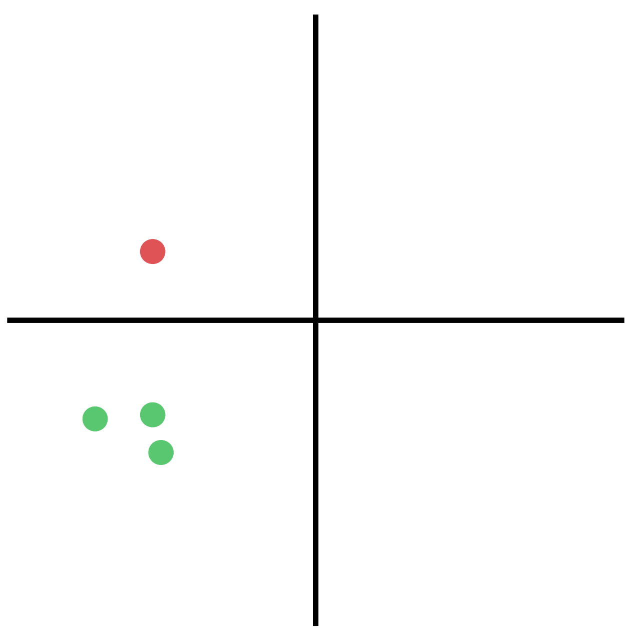

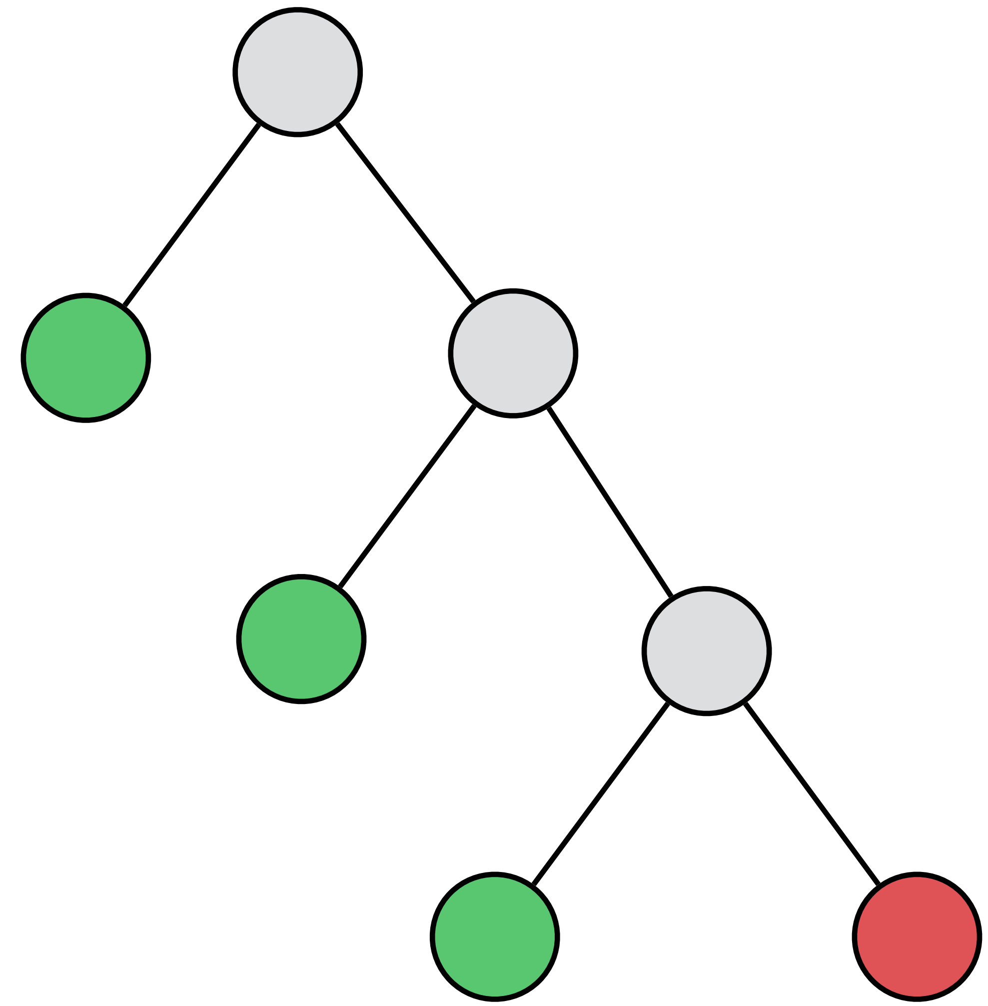

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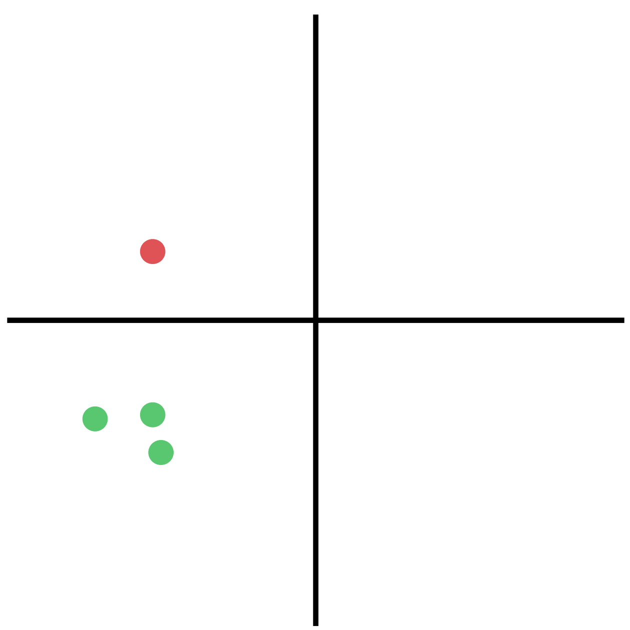

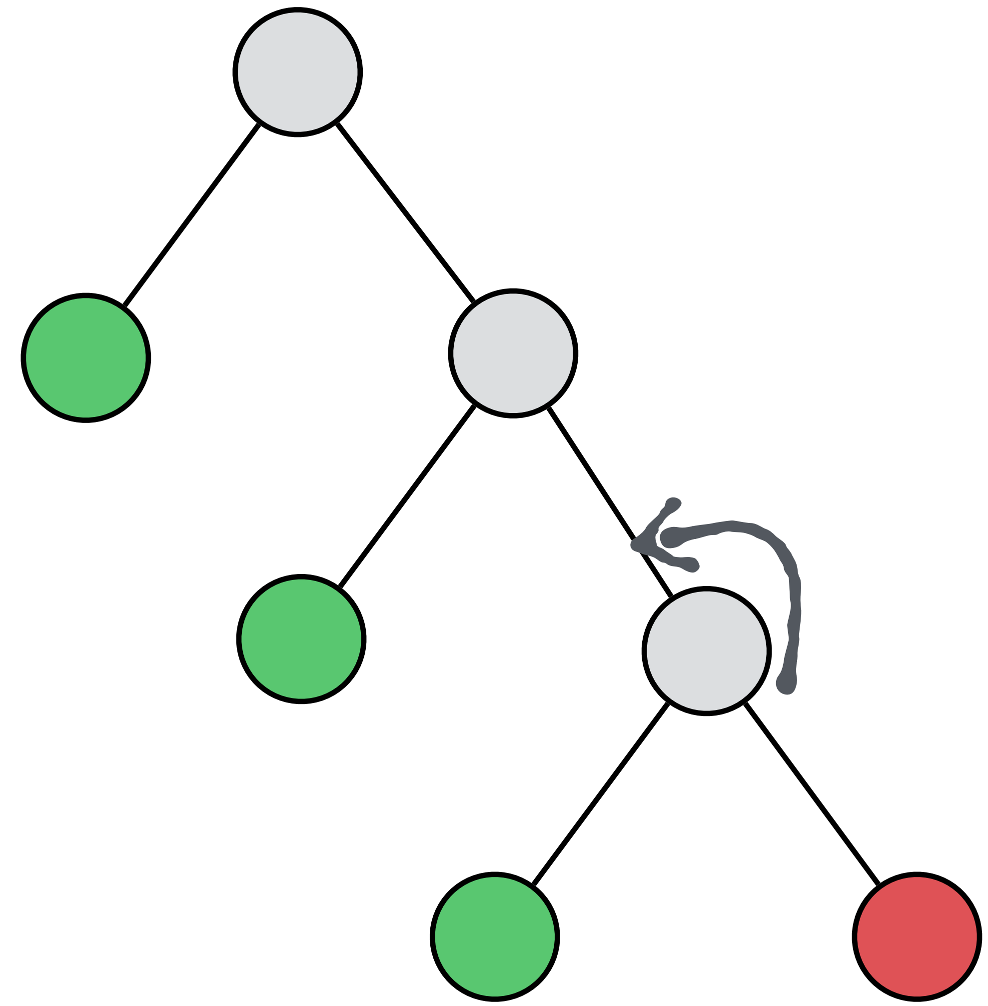

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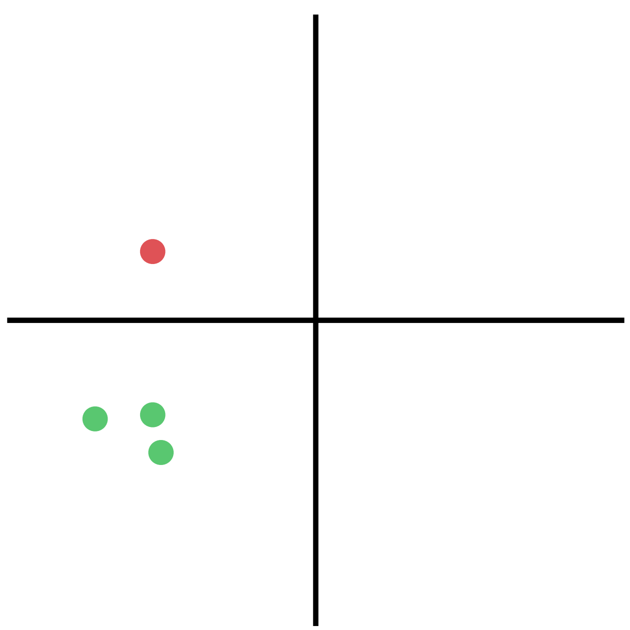

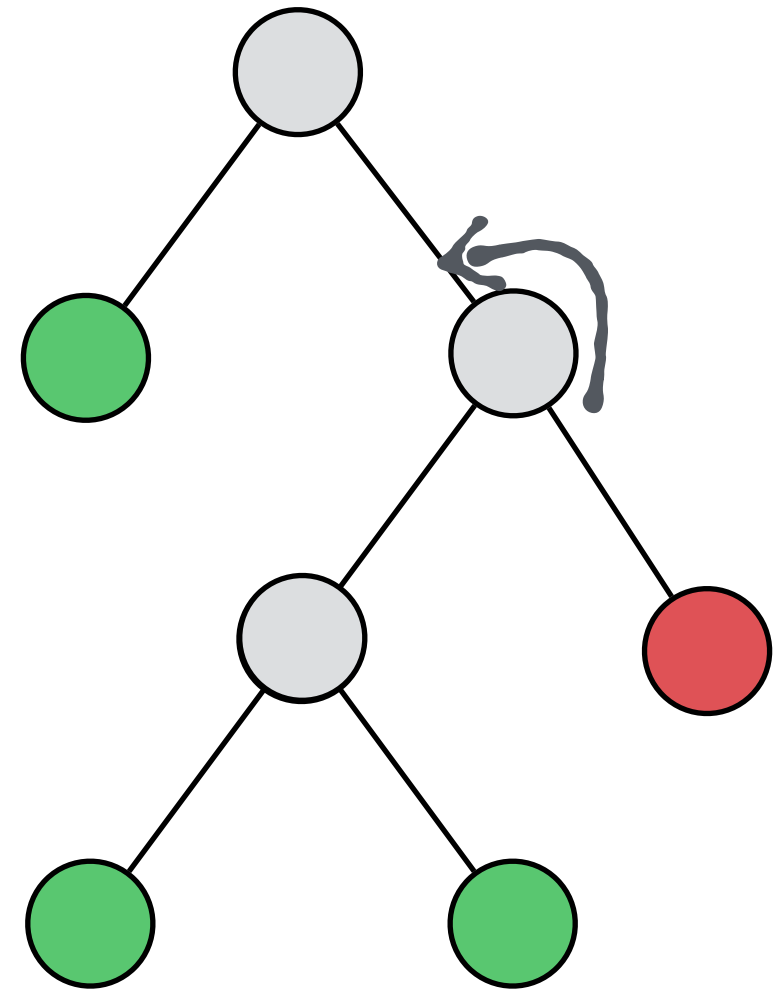

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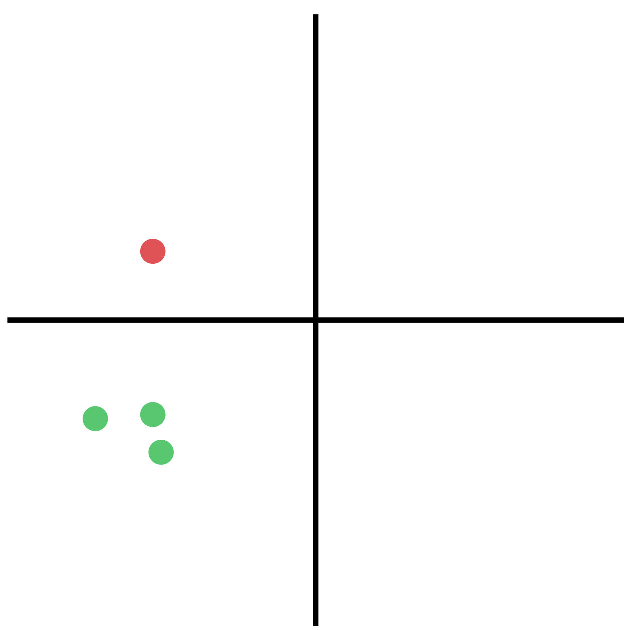

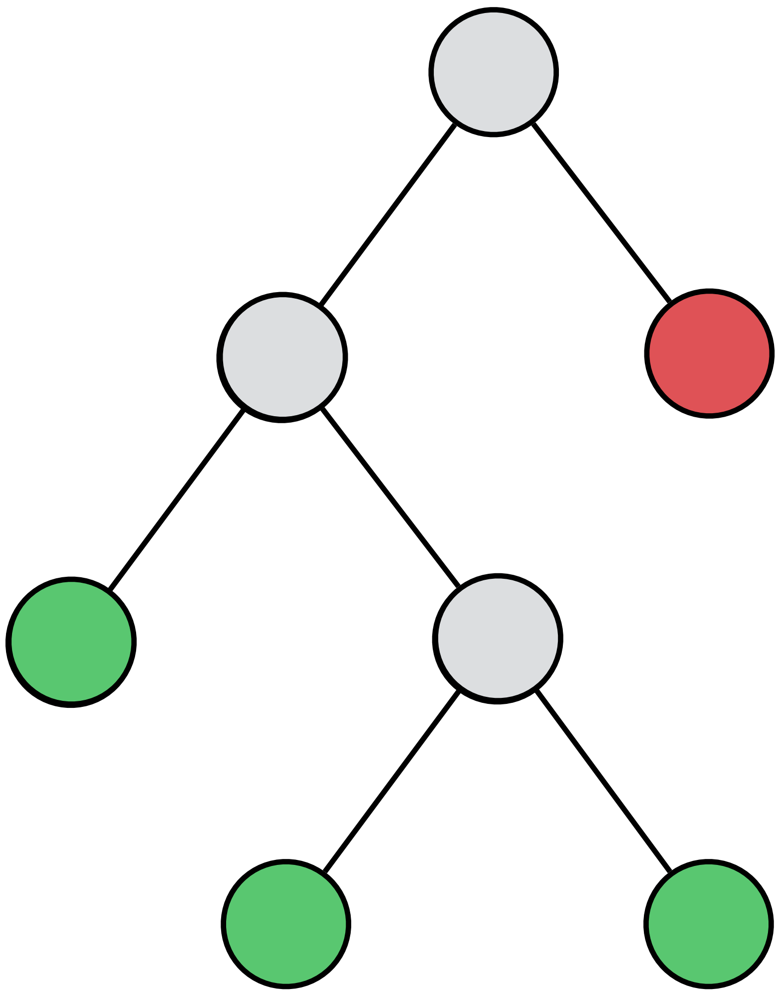

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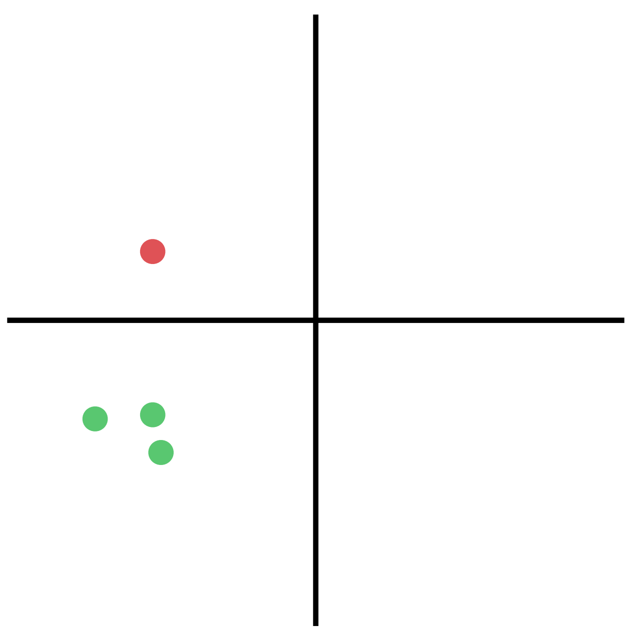
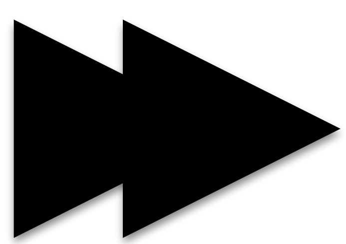
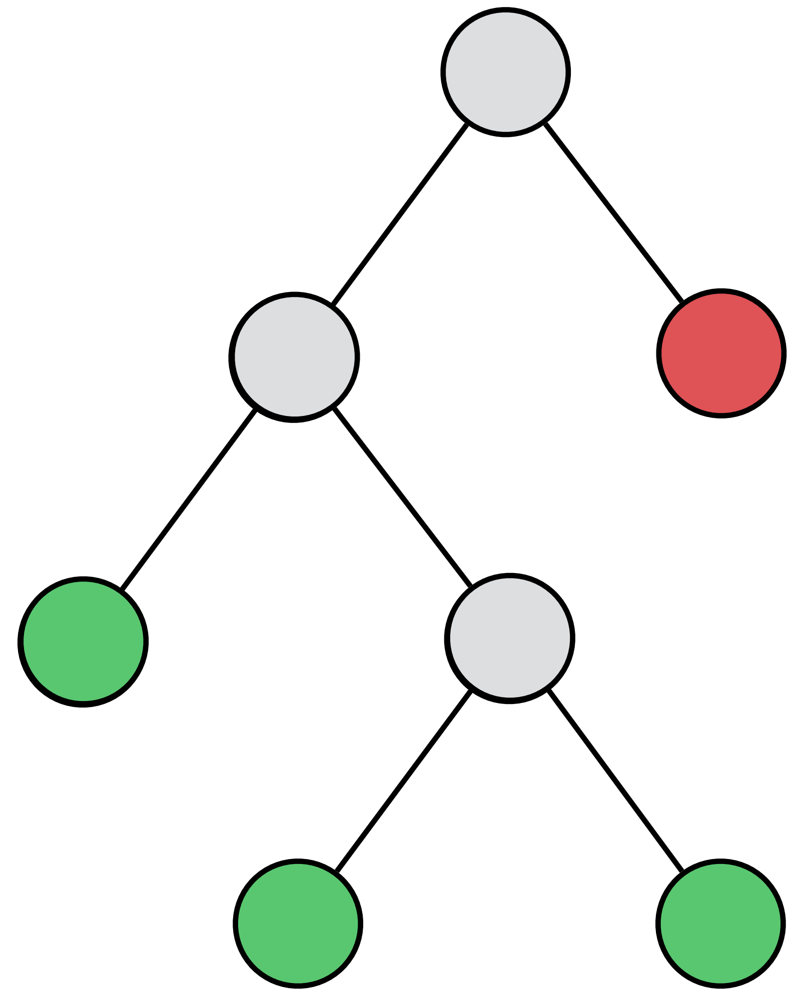




Fast Forward



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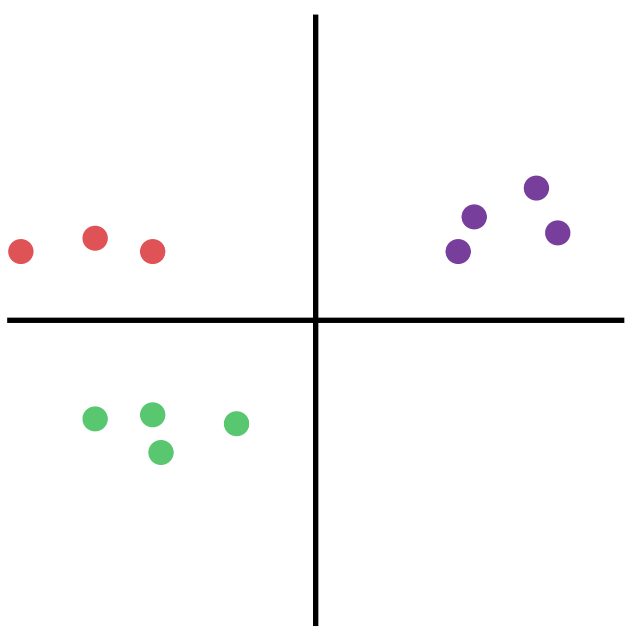

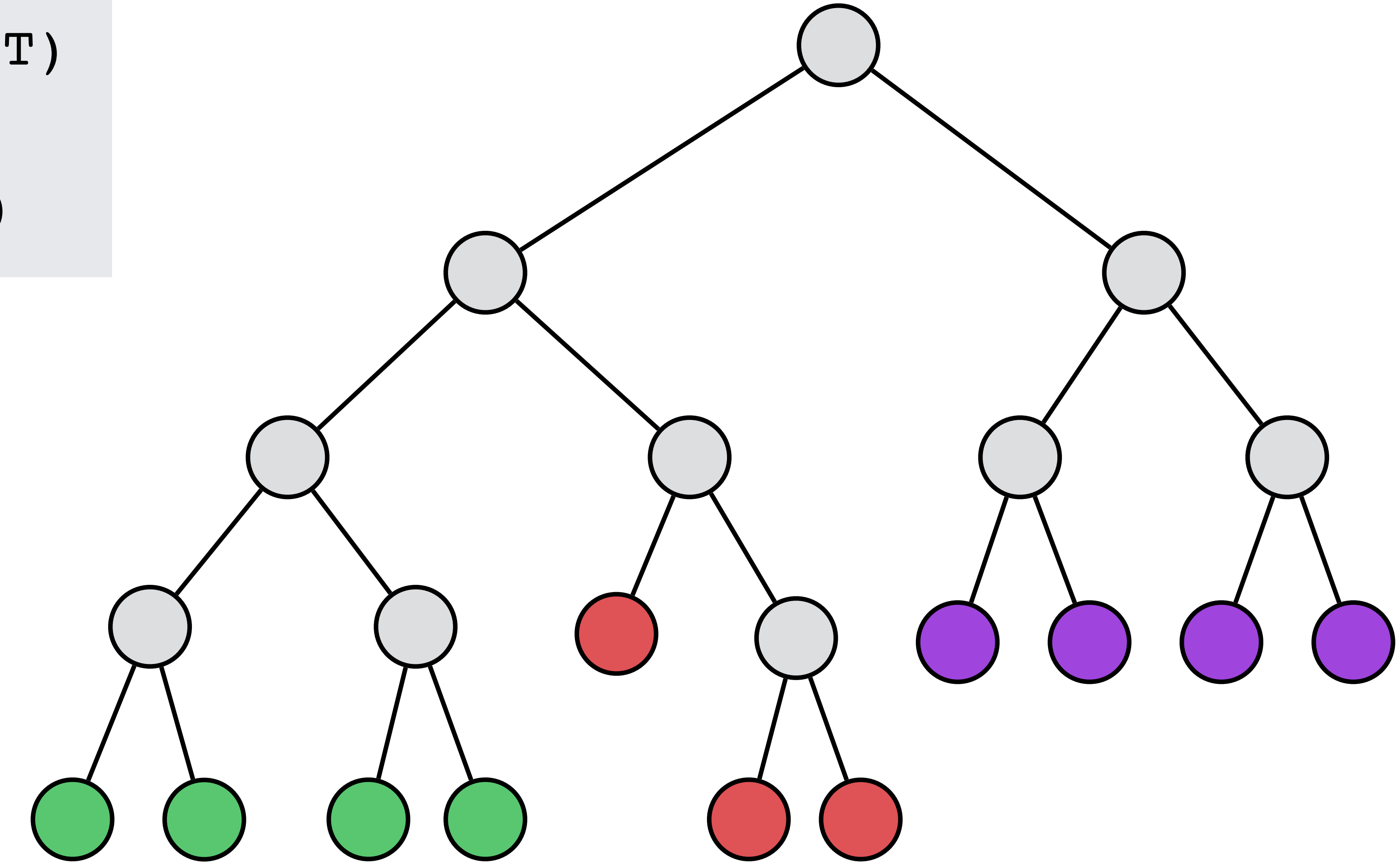

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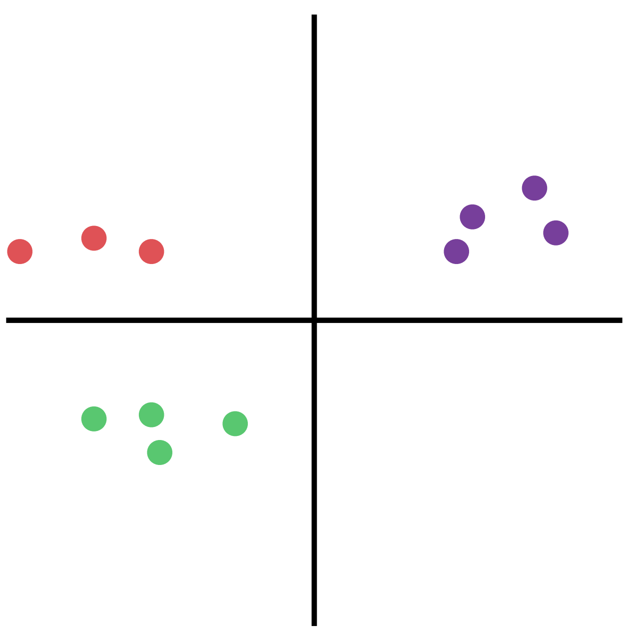

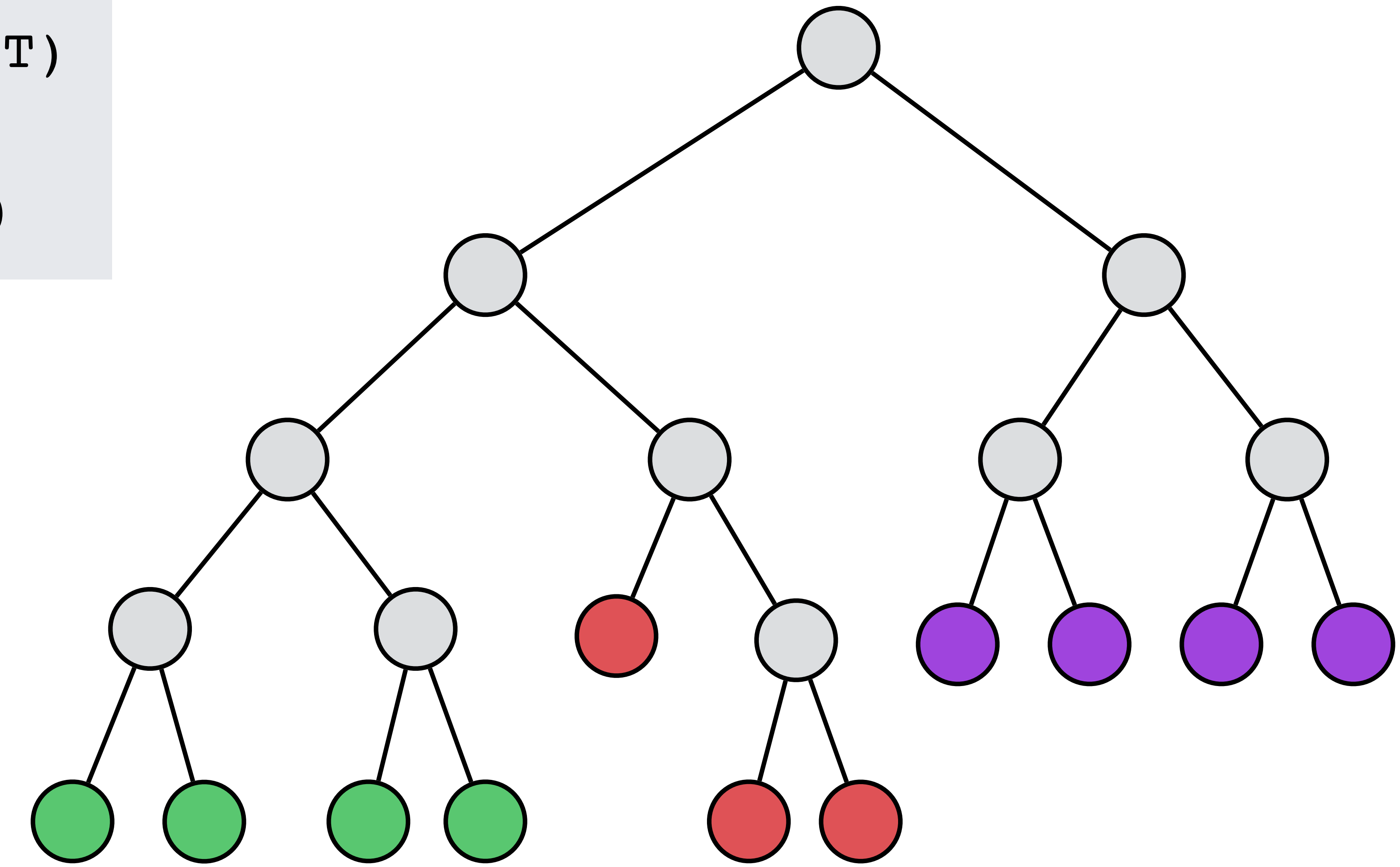

Data structures used for efficiency?

PERCH

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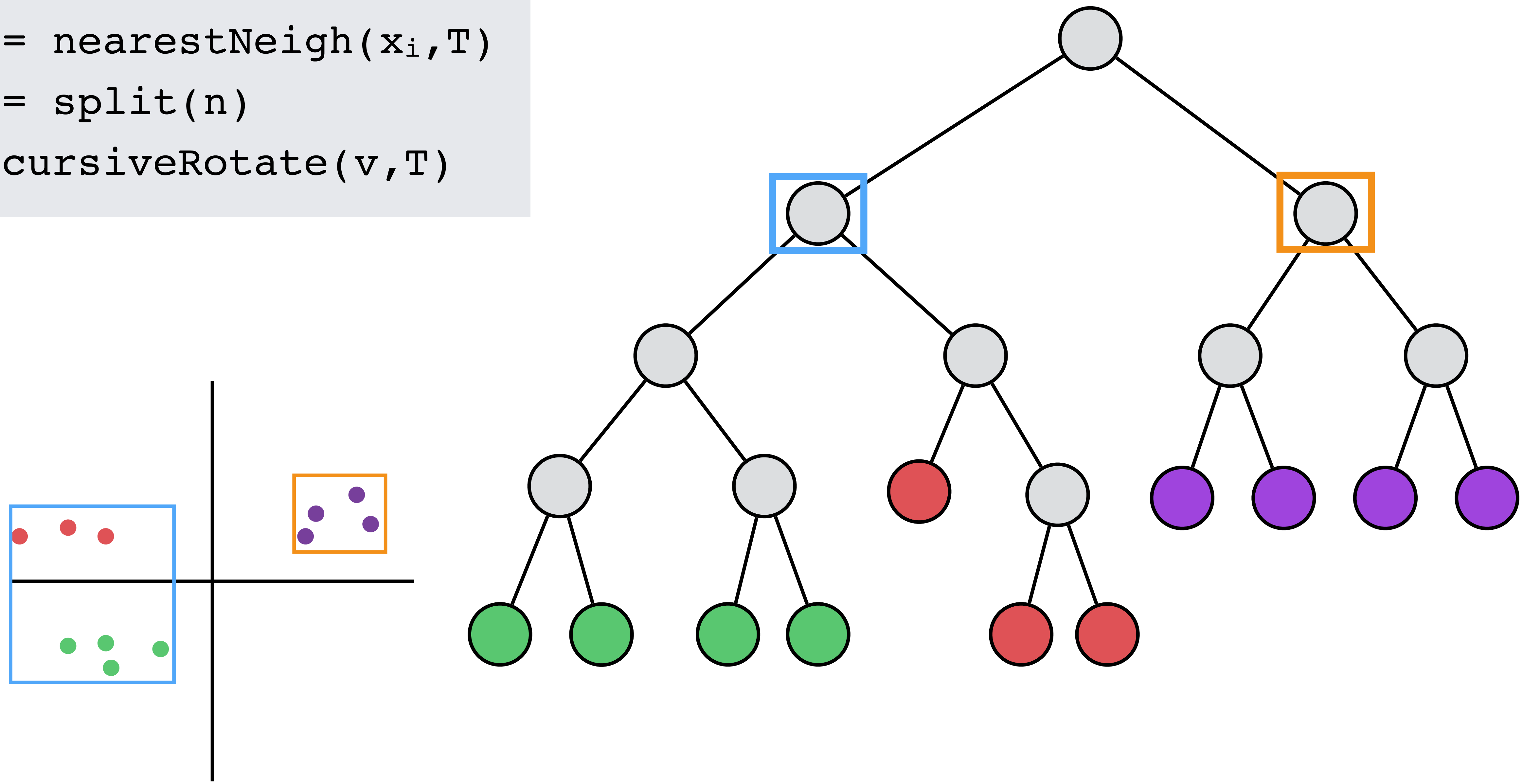

Bounding Boxes

PERCH

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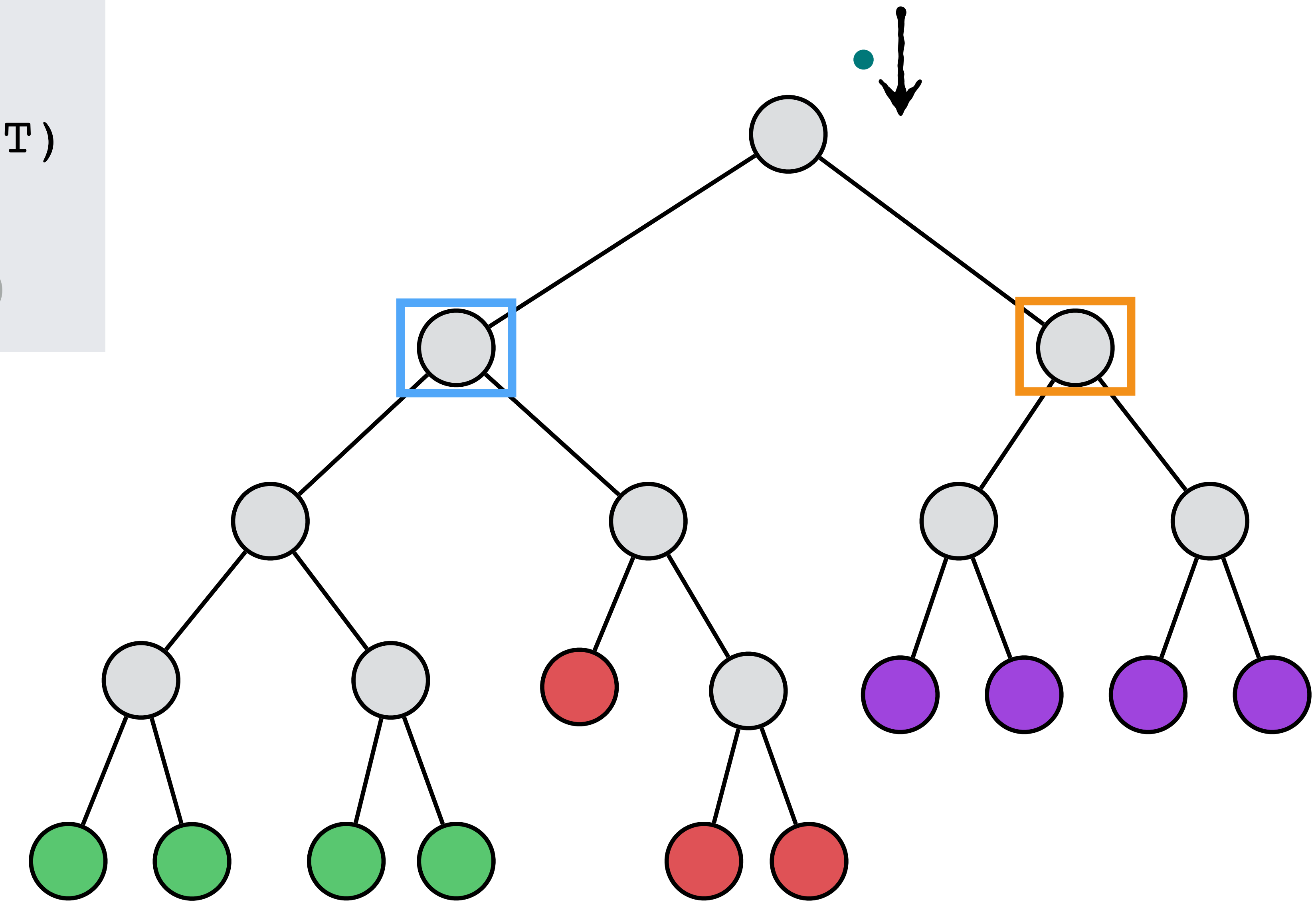

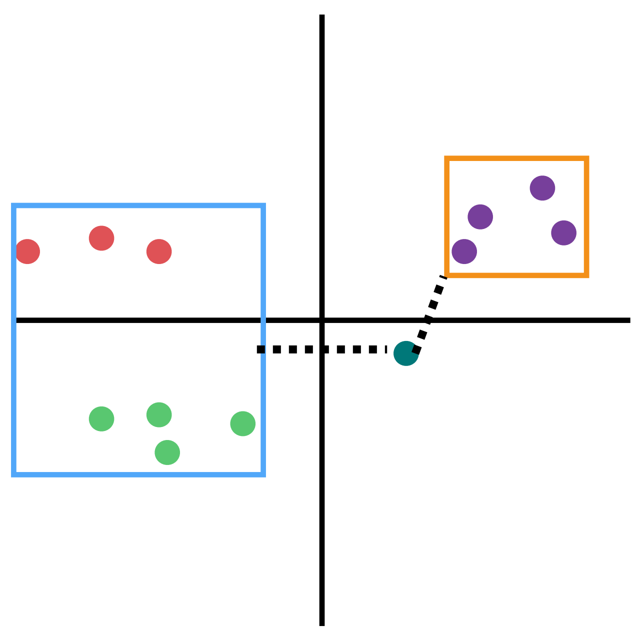

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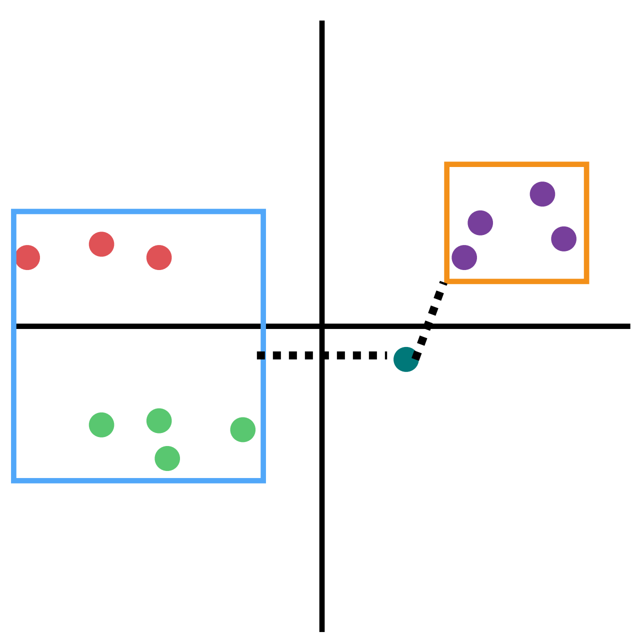

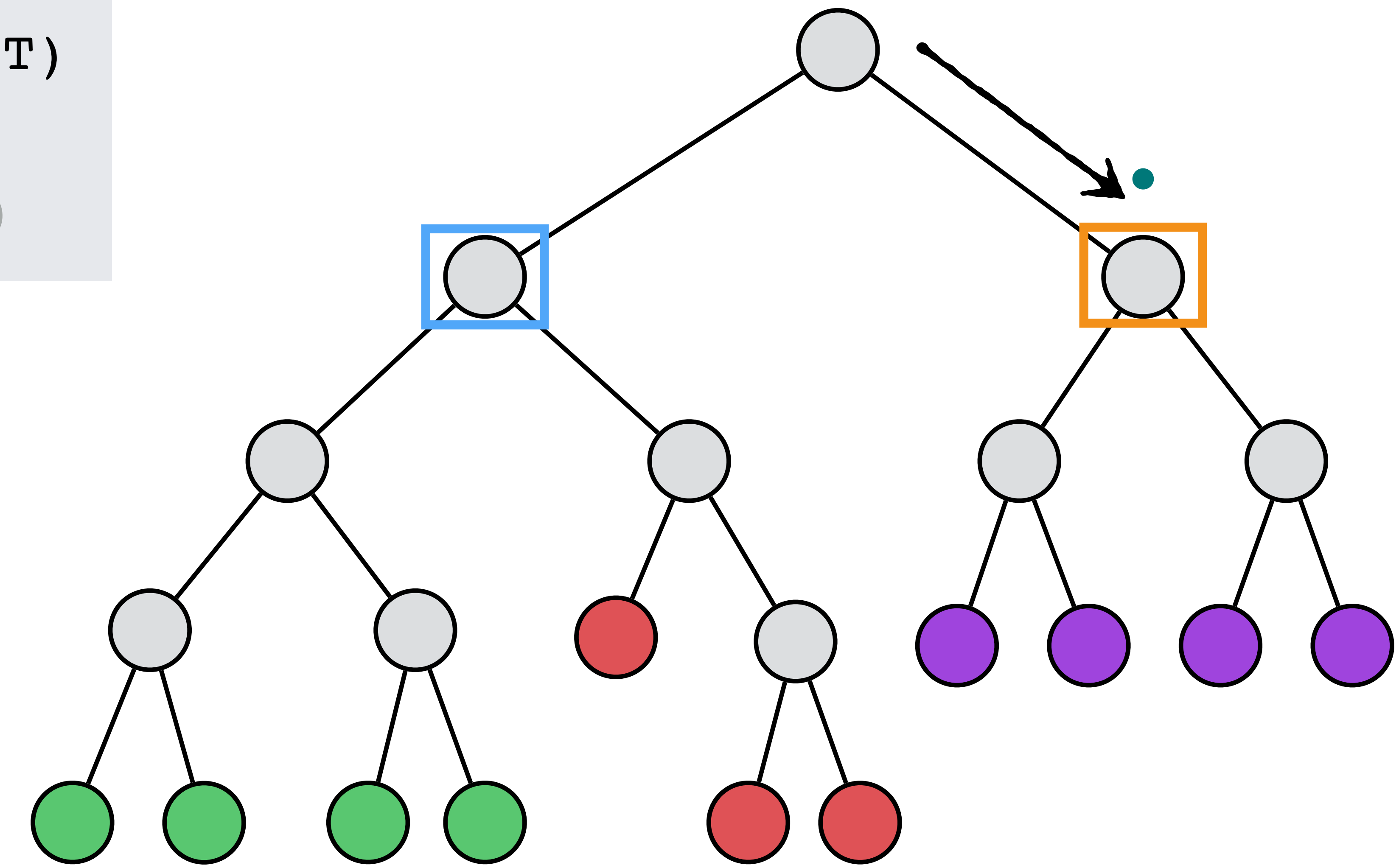

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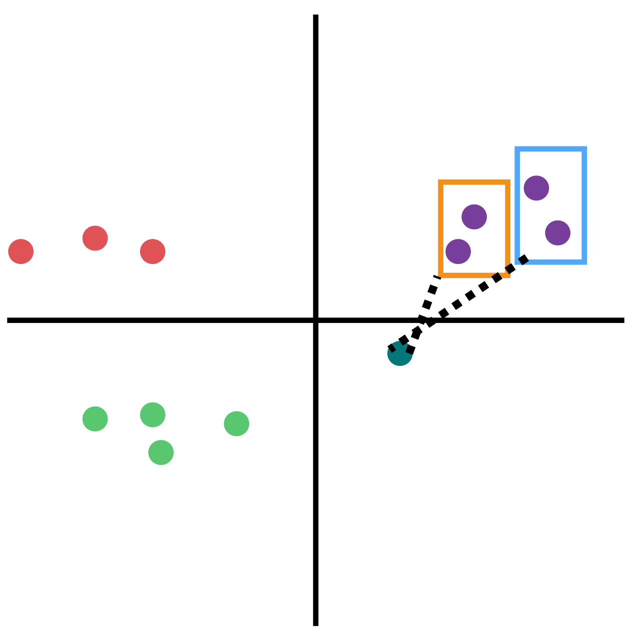

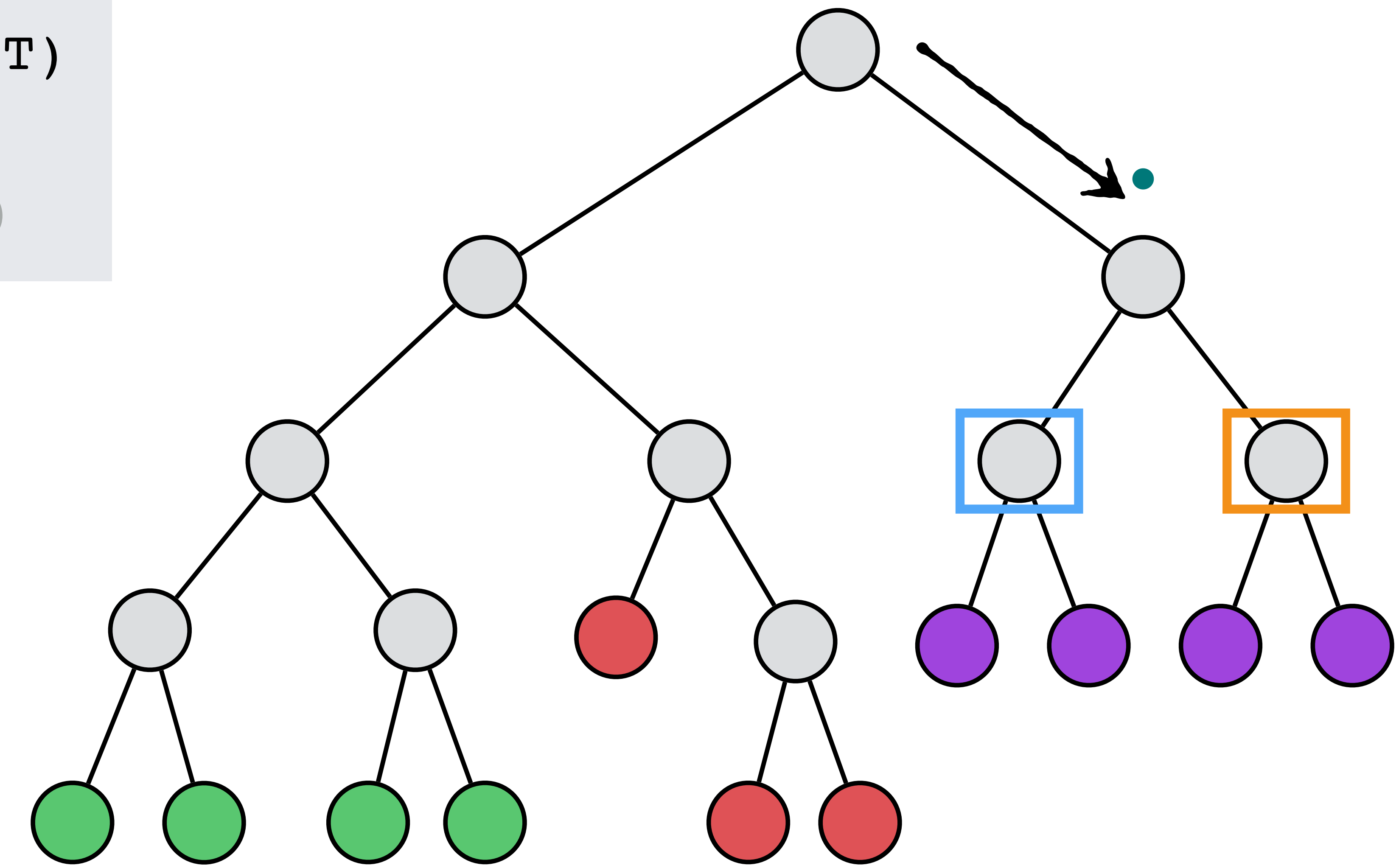

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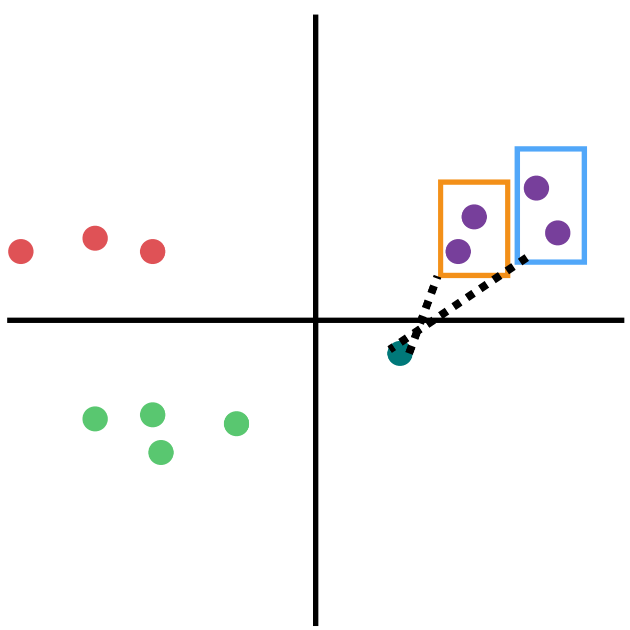

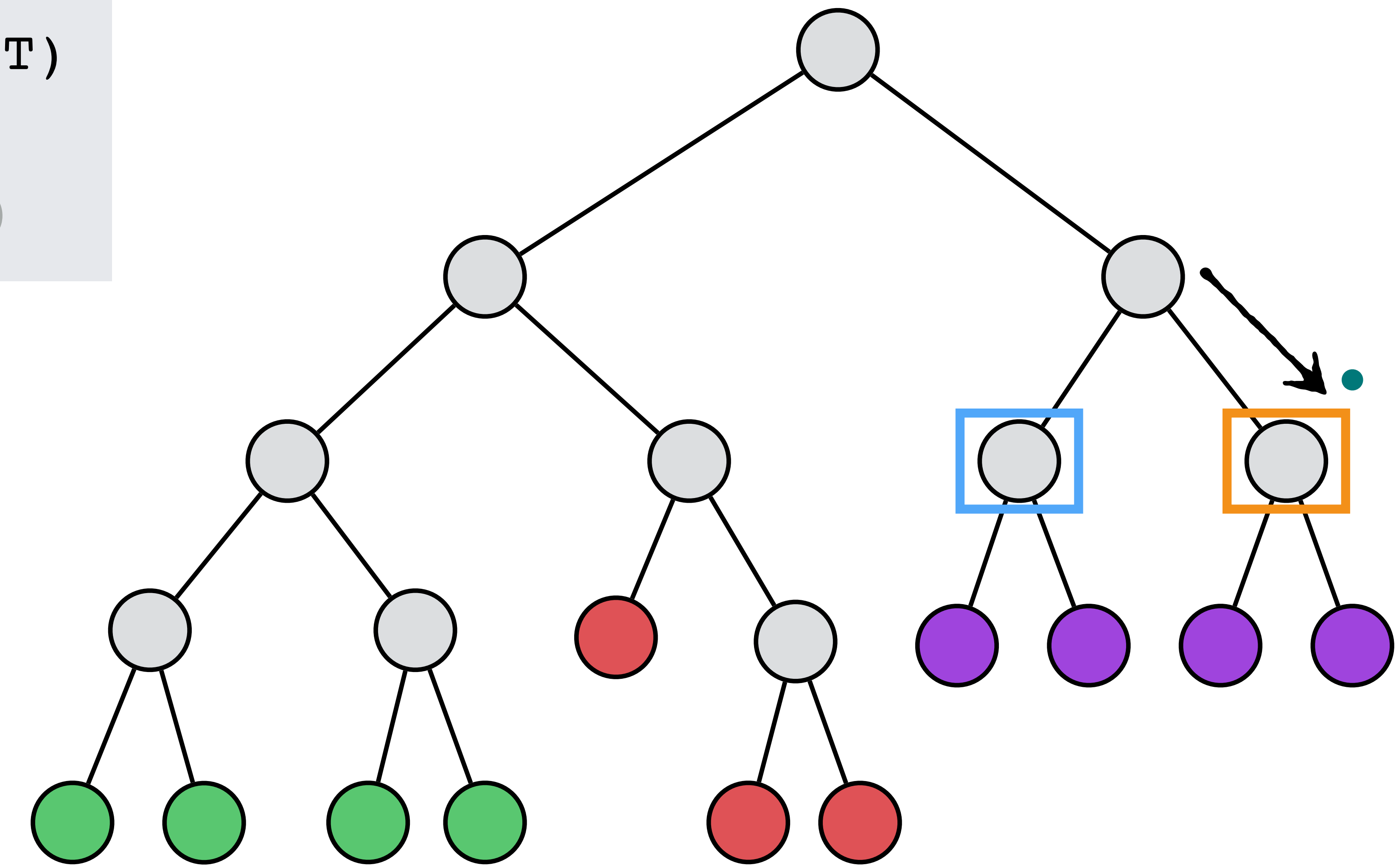

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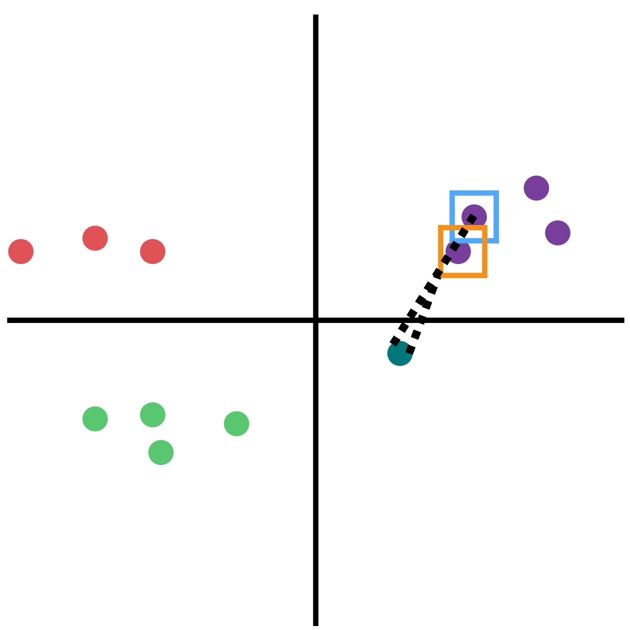

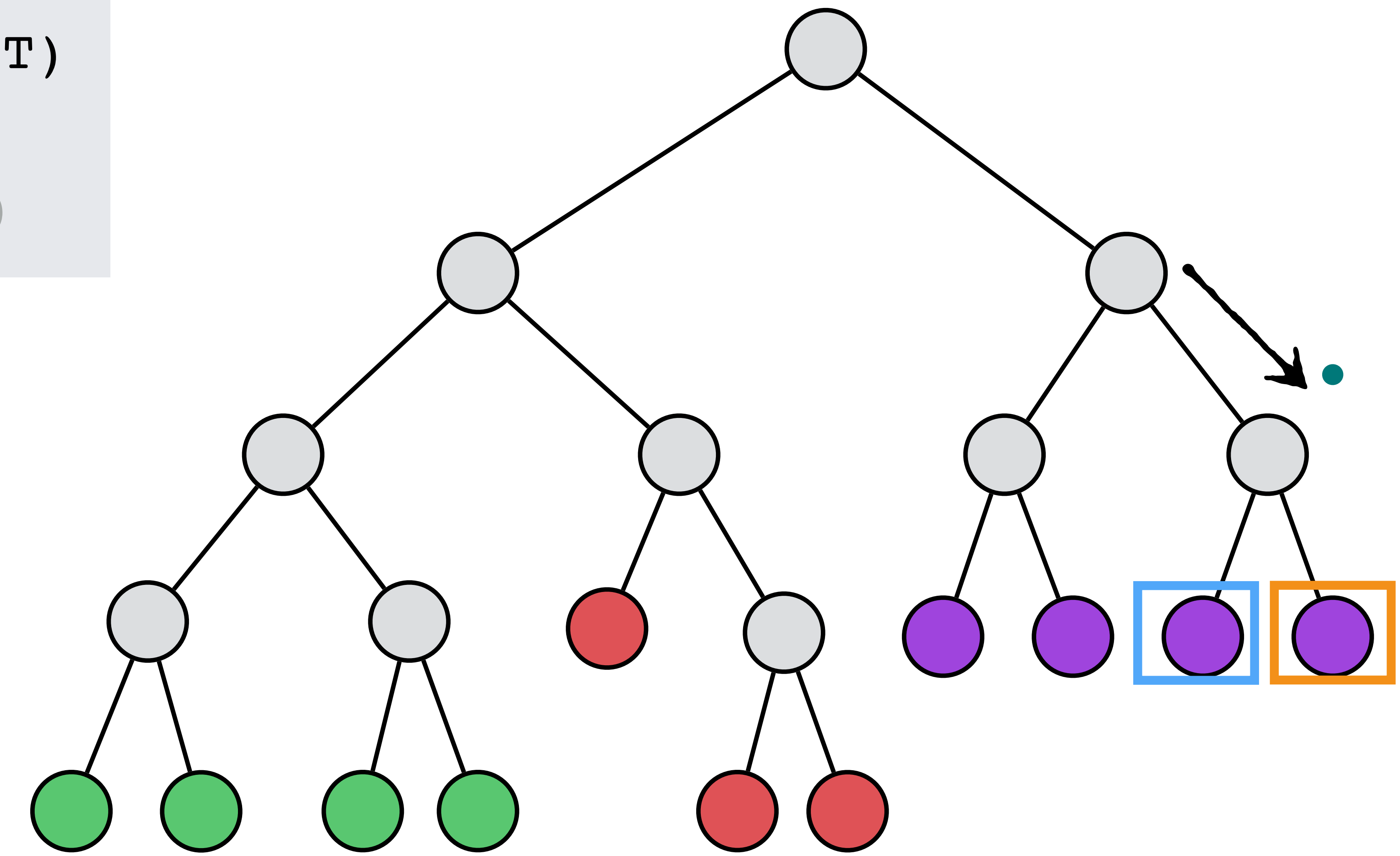

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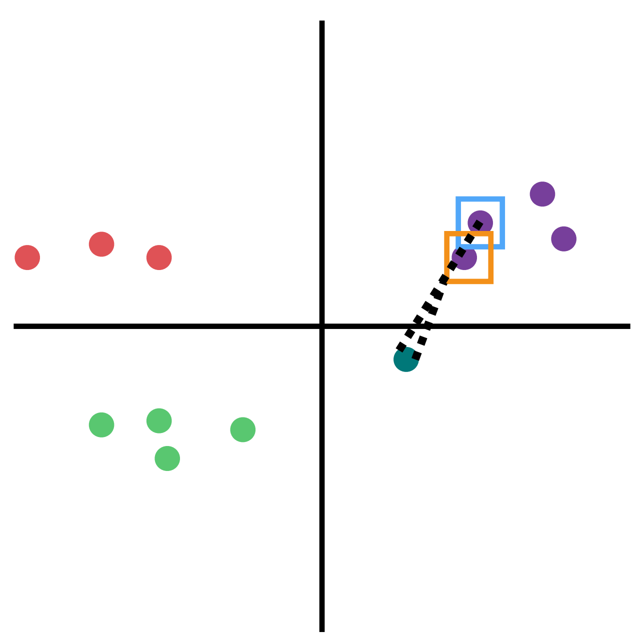

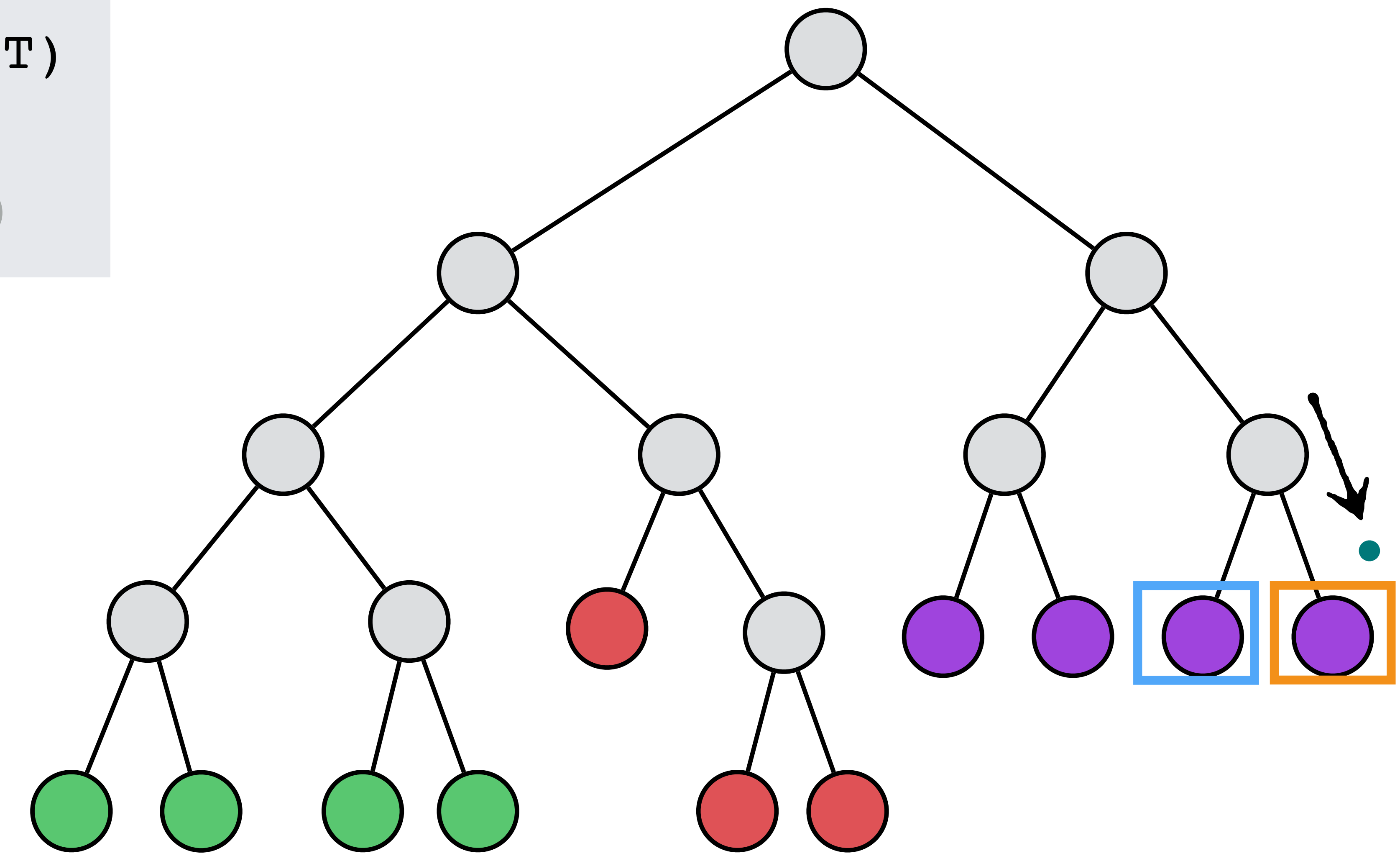

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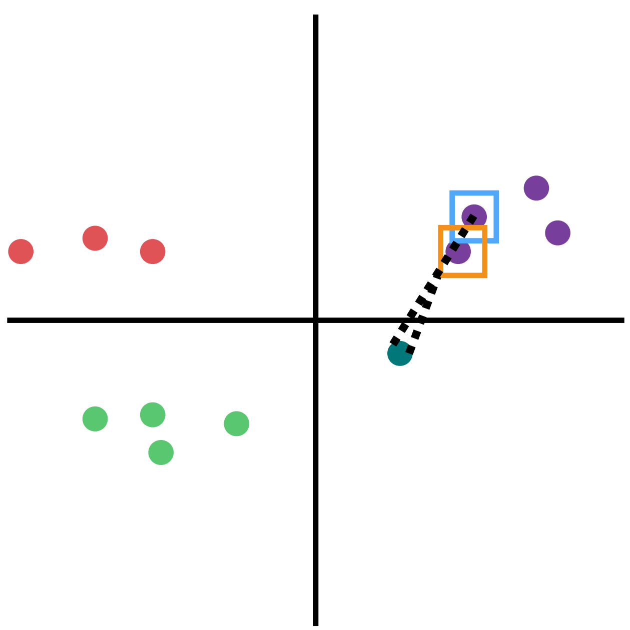

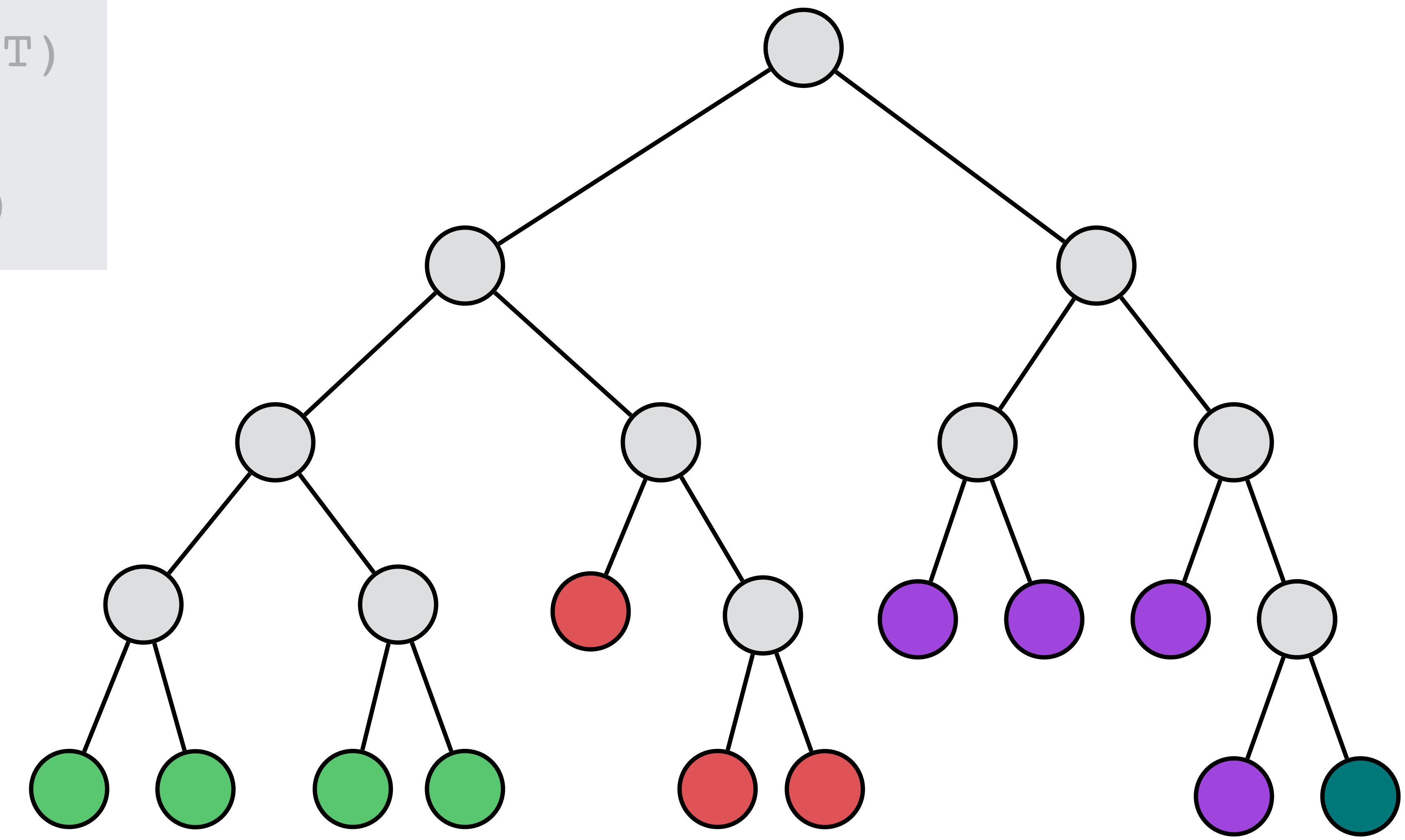

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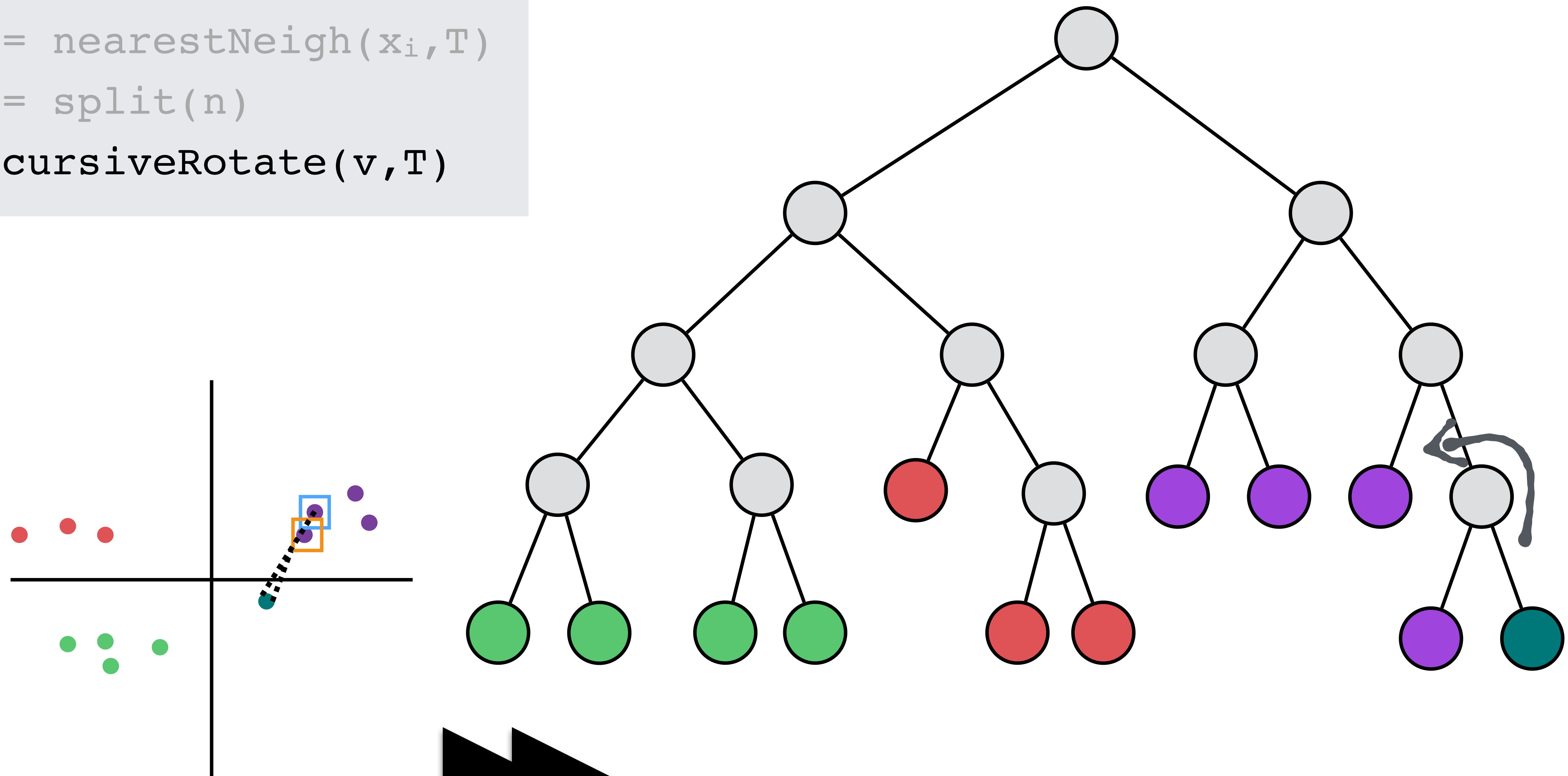

Fast Forward

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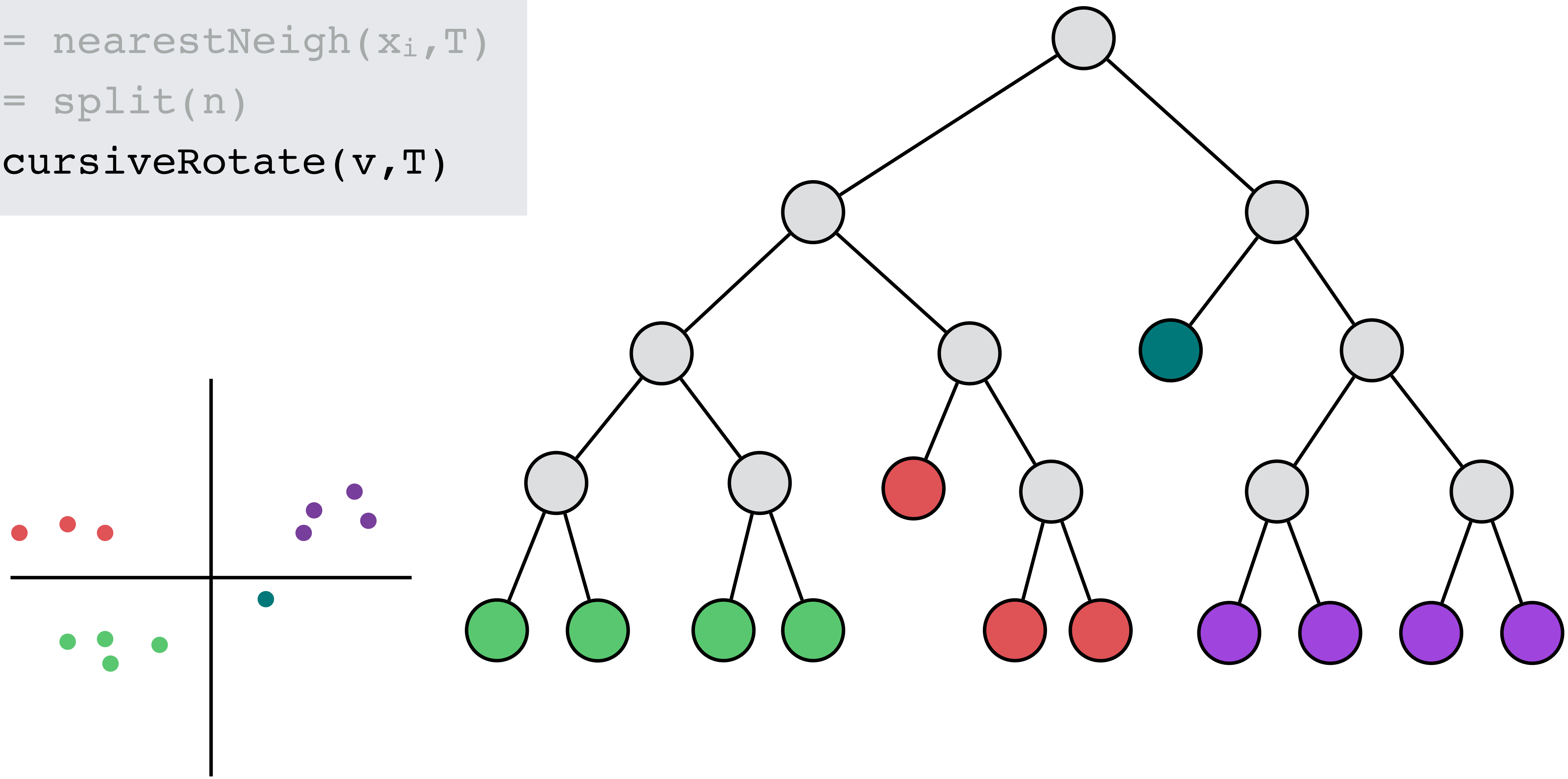

Perch

PERCH

Additional Efficiency Components:

PERCH

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Balance Rotations

- Improve tree balance without sacrificing purity
- Speed up nearest neighbor search

PERCH

Additional Efficiency Components:

Balance Rotations

- Improve tree balance without sacrificing purity
- Speed up nearest neighbor search

Collapsed Mode

- Restrict the number of nodes in the tree
- Allows for clustering data that doesn’t fit in memory

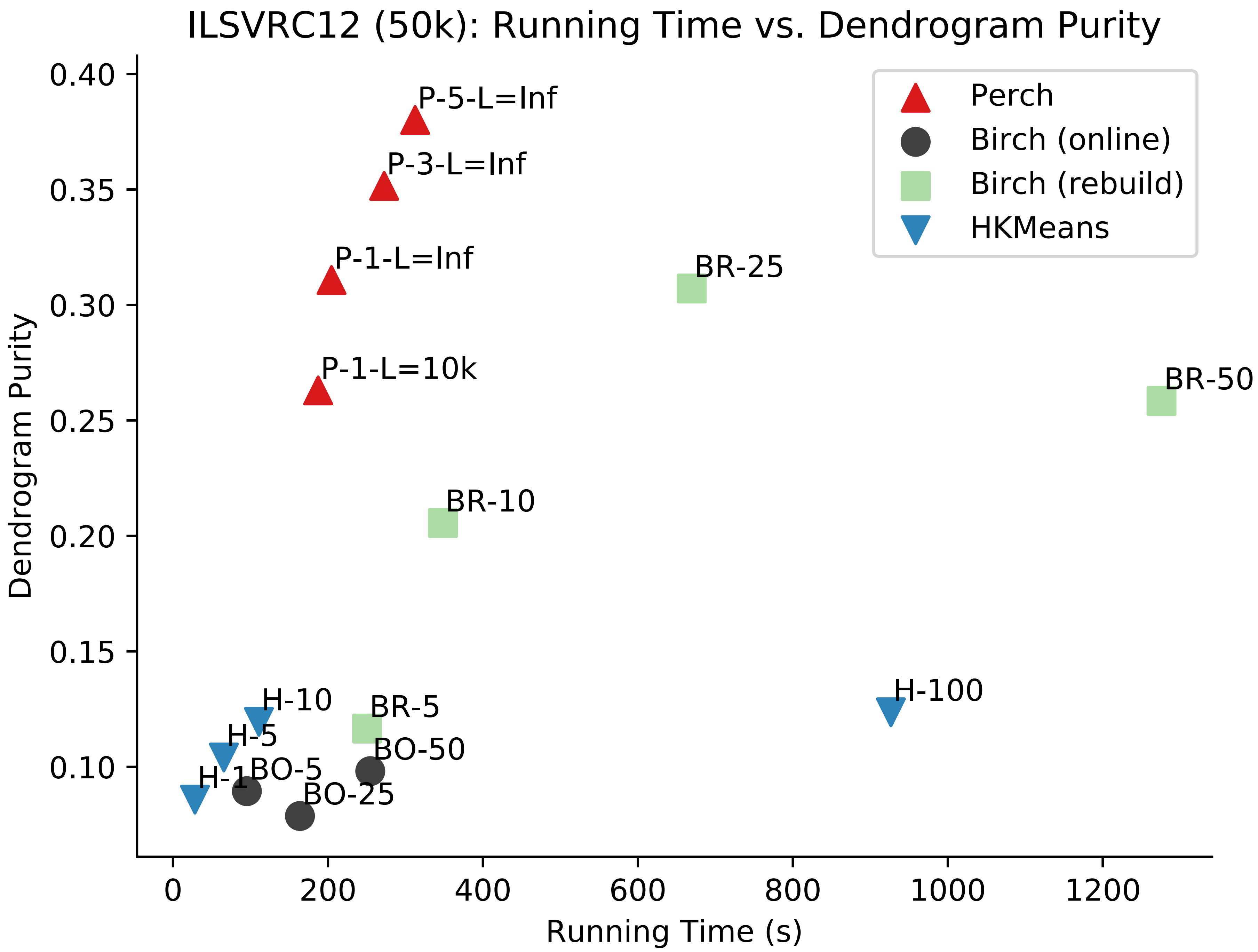
PERCH

Theoretical Guarantees:

On *separated* data, PERCH constructs trees with dendrogram purity 1.0, even when using balance rotations and collapsing.

Results

Results


ILSVRC12 (50k): Running Time vs. Dendrogram Purity
Dendrogram Purity
Running Time (s)
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0
200
400
600
800
1000
1200
Perch
Birch (online)
Birch (rebuild)
HKMeans
P-5-L=Inf
P-3-L=Inf
P-1-L=Inf
P-1-L=10k
BR-25
BR-50
BR-10
BR-5
H-10
H-5
H-1
H-100
BO-5
BO-50
BO-25

Results

Method	CovType	ILSVRC12 (50k)	ALOI	ILSVRC 12	Speaker	ImageNet (100k)
PERCH	**0.45 ± 0.004**	**0.53 ± 0.003**	**0.44 ± 0.004**	—	**0.37 ± 0.002**	**0.07 ± 0.00**
PERCH-BC	0.45 ± 0.004	0.36 ± 0.005	0.37 ± 0.008	**0.21 ± 0.017**	0.09 ± 0.001	0.03 ± 0.00
BIRCH (online)	0.44 ± 0.002	0.09 ± 0.006	0.21 ± 0.004	0.11 ± 0.006	0.02 ± 0.002	0.02 ± 0.00
MB-HAC-Com.	—	0.43 ± 0.005	0.15 ± 0.003	—	0.01 ± 0.002	—
MB-HAC-Cent.	0.44 ± 0.005	0.02 ± 0.000	0.30 ± 0.002	—	—	—
HKMmeans	0.44 ± 0.001	0.12 ± 0.002	**0.44 ± 0.001**	0.11 ± 0.003	0.12 ± 0.002	0.02 ± 0.00
BIRCH (rebuild)	0.44 ± 0.002	0.26 ± 0.003	0.32 ± 0.002	—	0.22 ± 0.006	0.03 ± 0.00

(a) Dendrogram Purity for Hierarchical Clustering.

Method	CoverType	ILSVRC 12 (50k)	ALOI	ILSVRC 12	Speaker	ImageNet (100K)
PERCH	22.96 ± 0.7	**54.30 ± 0.3**	**44.21 ± 0.2**	—	**31.80 ± 0.1**	**6.178 ± 0.0**
PERCH-BC	22.97 ± 0.8	37.98 ± 0.5	37.48 ± 0.7	25.75 ± 1.7	1.05 ± 0.1	4.144 ± 0.04
SKM++	23.80 ± 0.4	28.46 ± 2.2	37.53 ± 1.0	—	—	—
BICO	**24.53 ± 0.4**	45.18 ± 1.0	32.984 ± 3.4	—	—	—
MB-KM	24.27 ± 0.6	51.73 ± 1.8	40.84 ± 0.5	**56.17 ± 0.4**	1.73 ± 0.141	5.642 ± 0.00
DBSCAN	—	16.95	—	—	22.63	—

(b) Pairwise F1 for Flat Clustering.

Thanks!

Questions?

https://arxiv.org/abs/1704.01858

https://github.com/iesl/xcluster