Approximate Hierarchical Clustering of Large Datasets

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Pedase,

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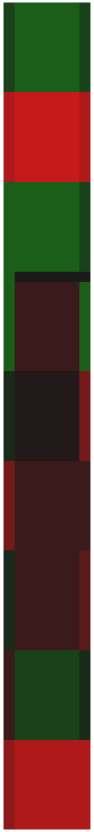
Overview

- Gene expression data
- What is clustering?
- What is hierarchical clustering?
- Why need for speedup?
- Approximate hierarchical clustering
- Finding closest pairs of data items fast
- Results
- Problems
- Future

Gene expression data (1)

Sample

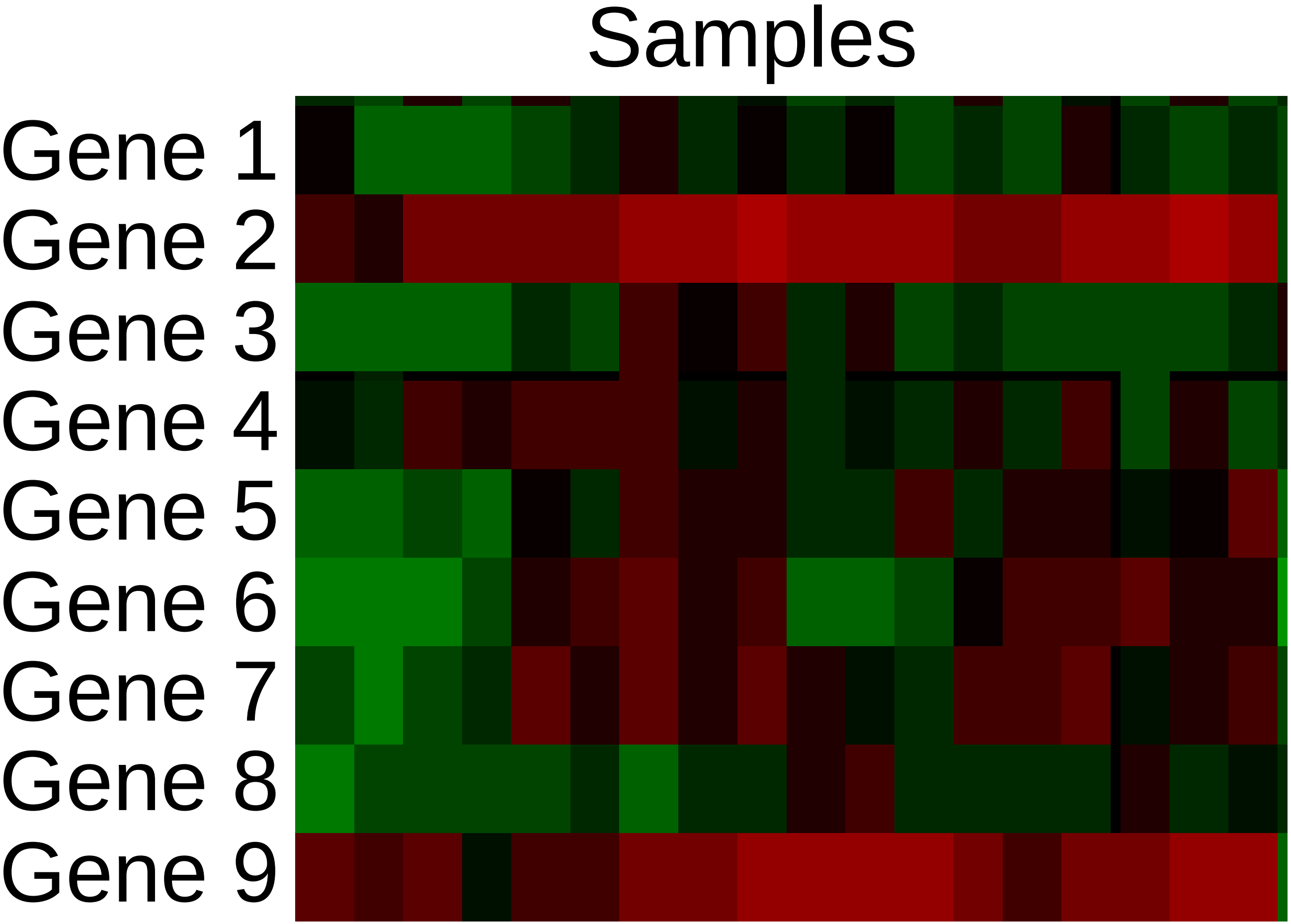


Gene 1	-2.303
Gene 2	+2.904
Gene 3	-2.235
Gene 4	+0.572
Gene 5	-1.169
Gene 6	+0.824
Gene 7	+0.343
Gene 8	-1.678
Gene 9	+2.477

🟥 Gene is highly expressed

🟩 Gene is not expressed

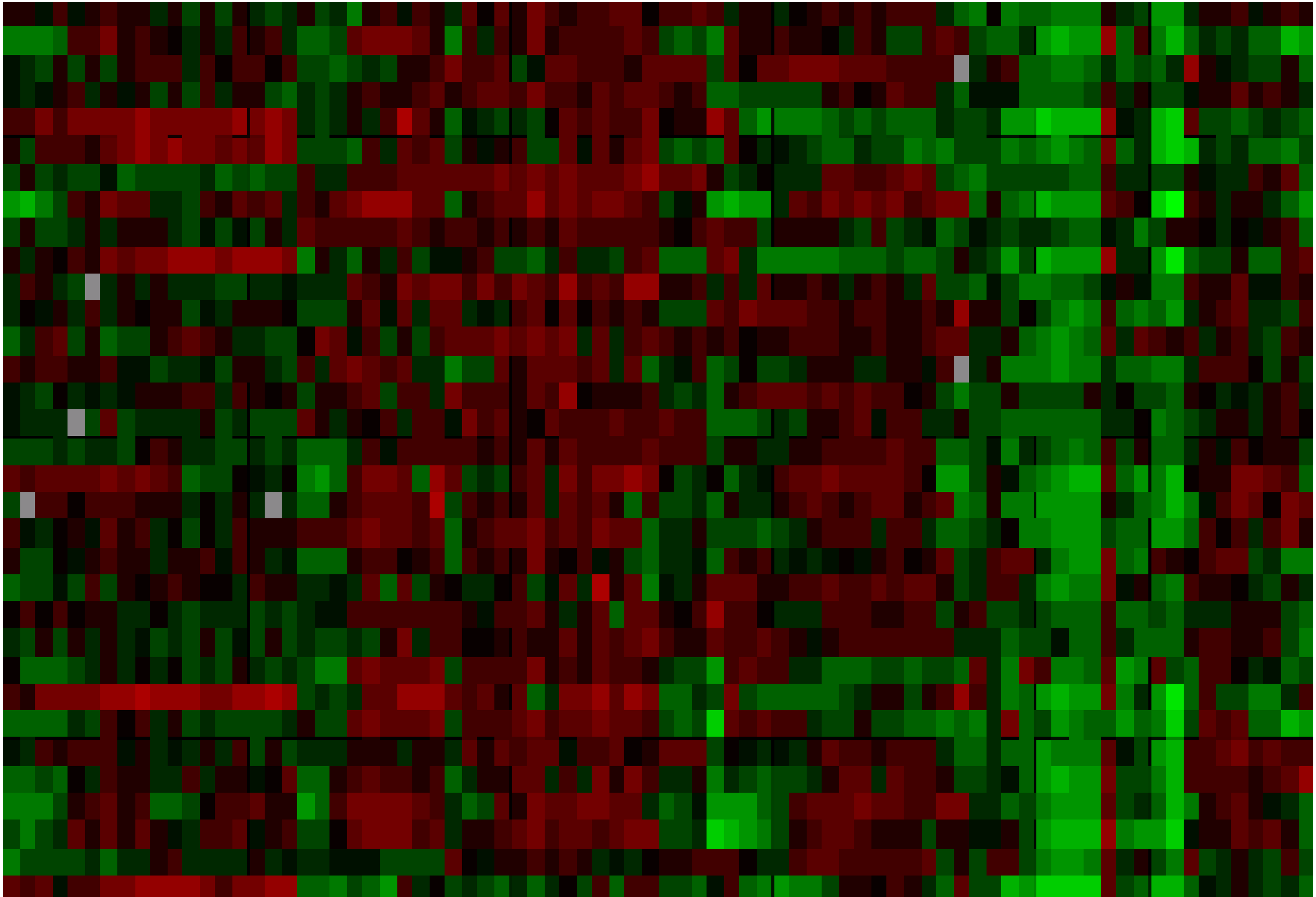
Gene expression data (1)



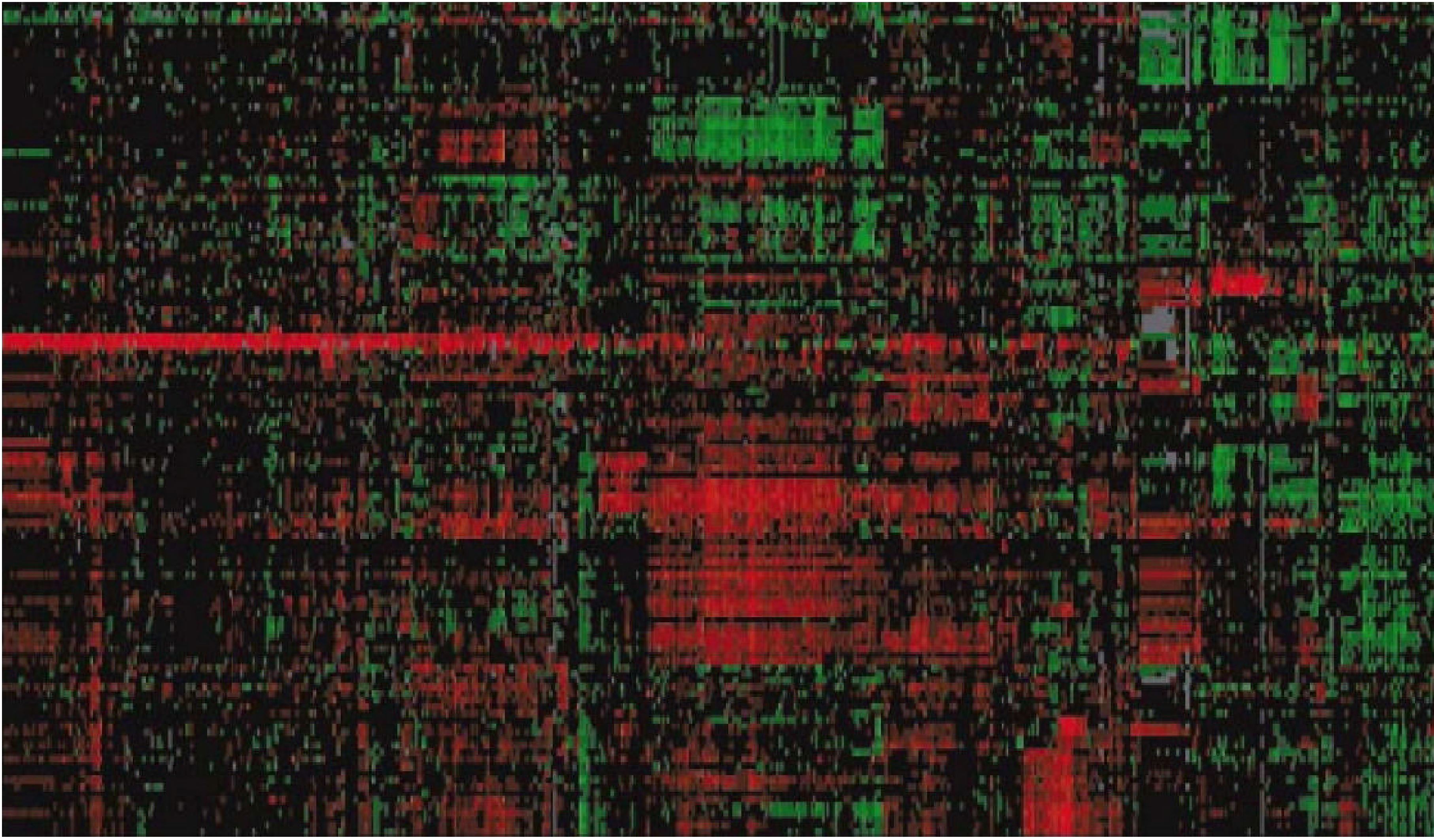
🟥 Gene is highly expressed

🟩 Gene is not expressed

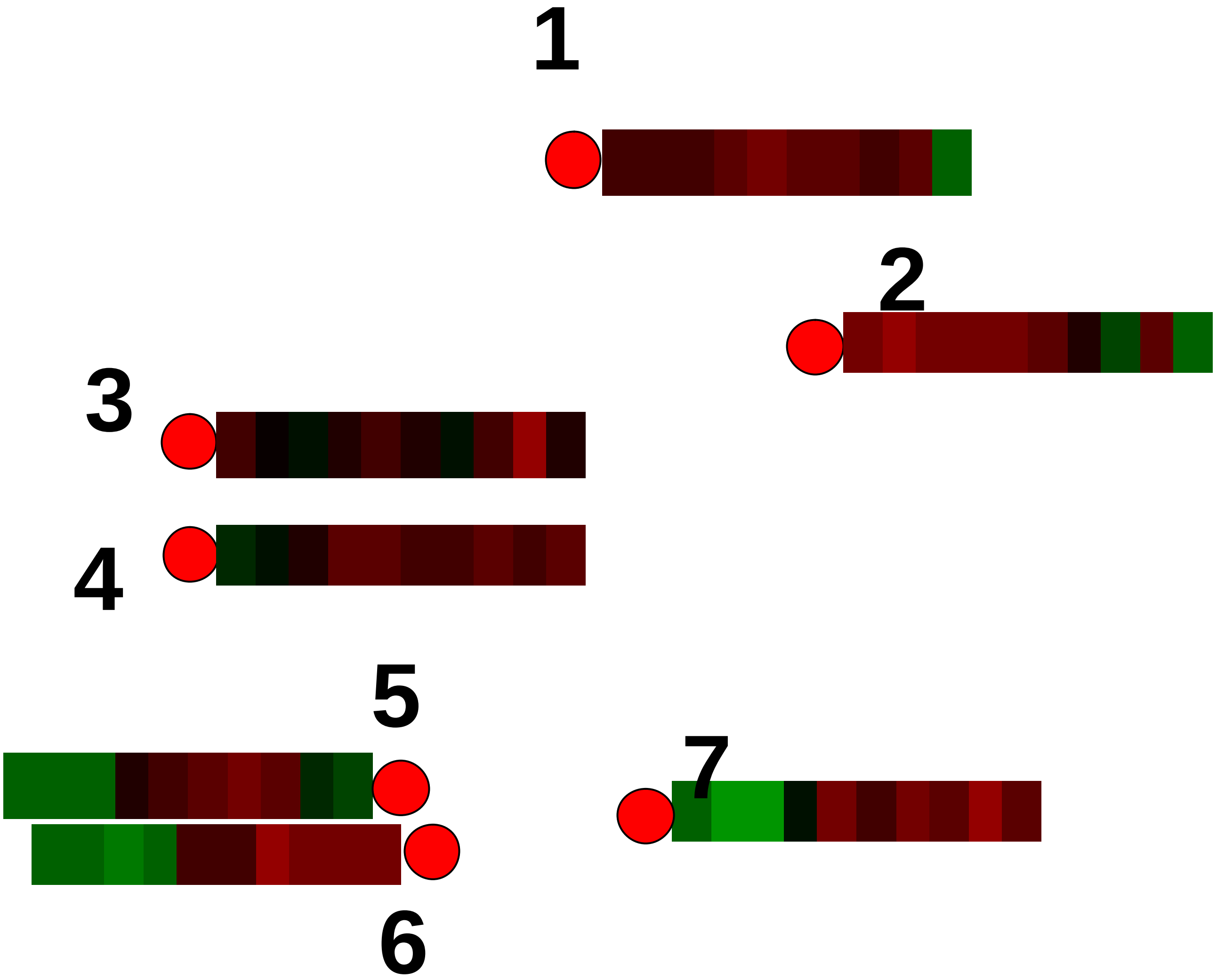
Gene expression data (2)



Gene expression data (3)



What is clustering?



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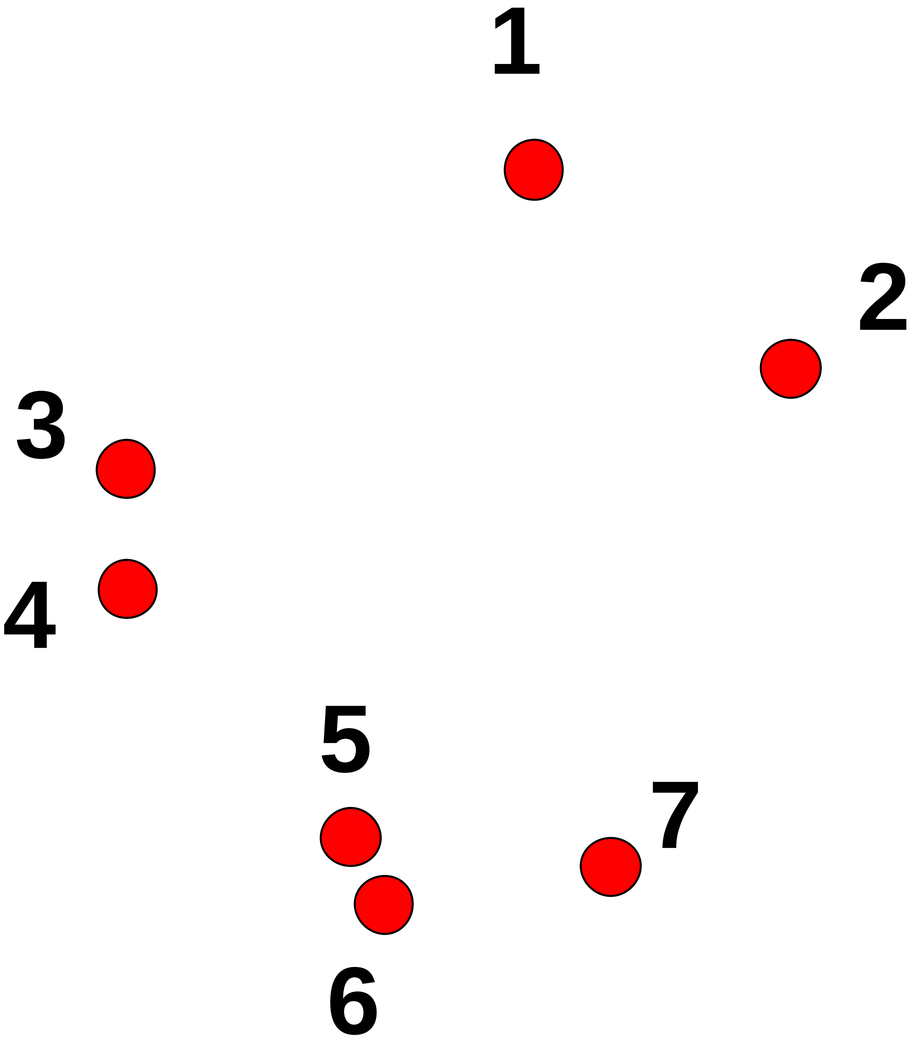

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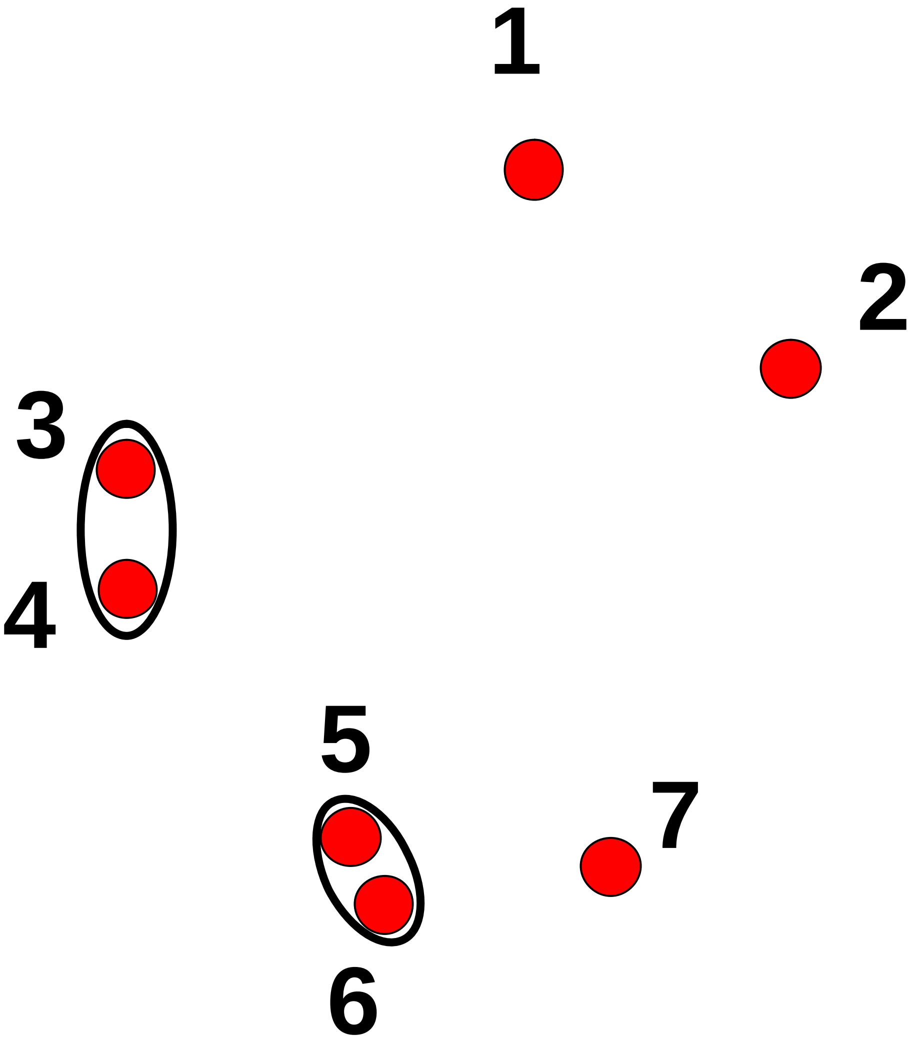

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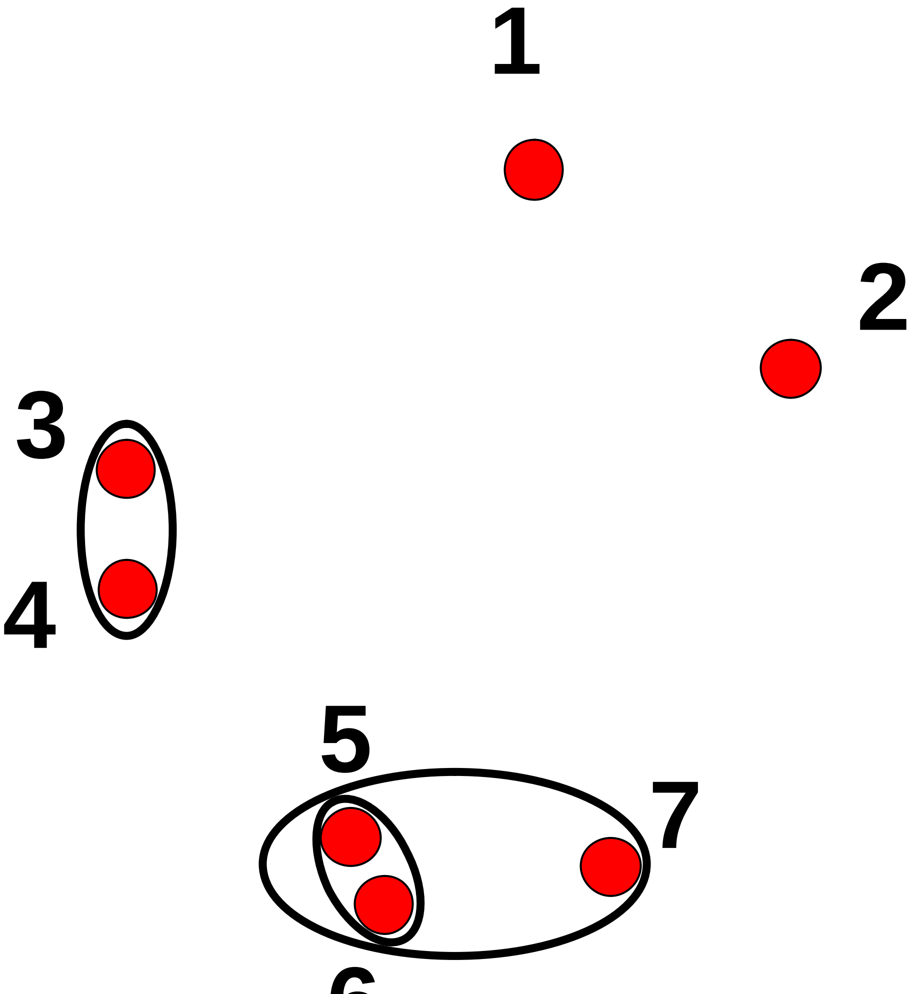

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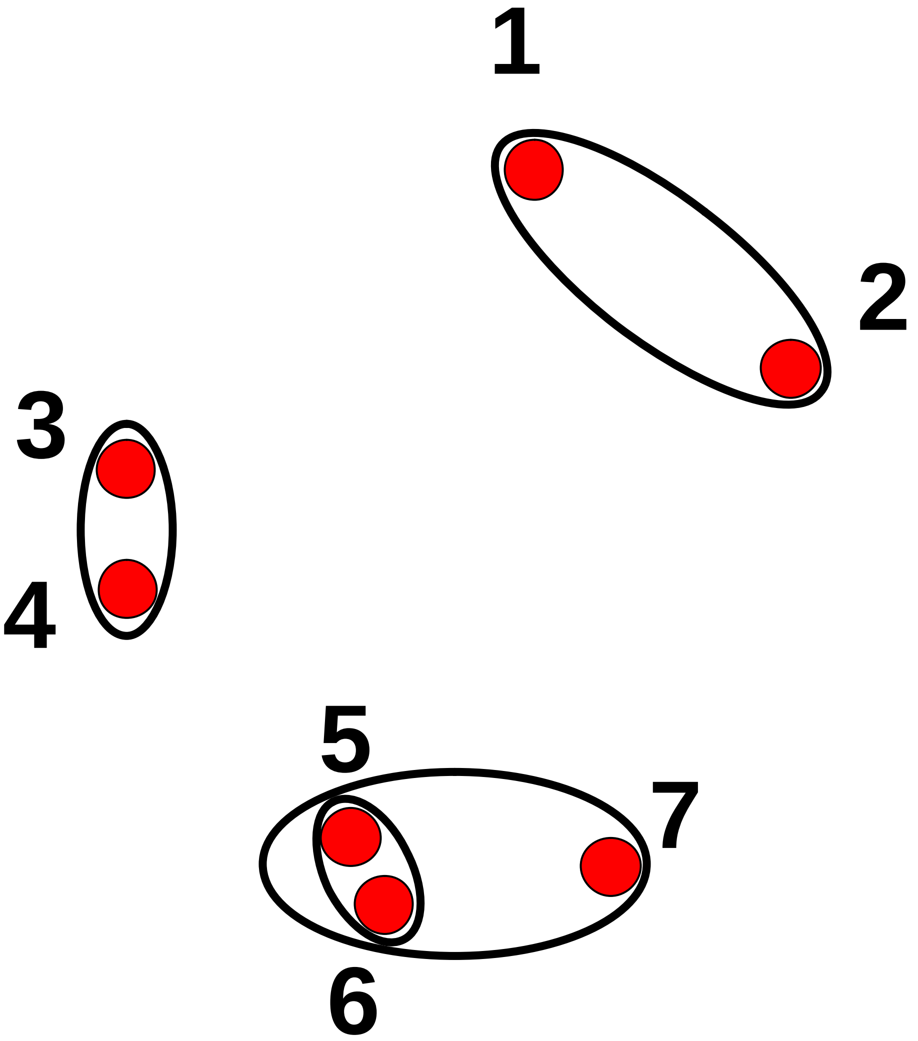

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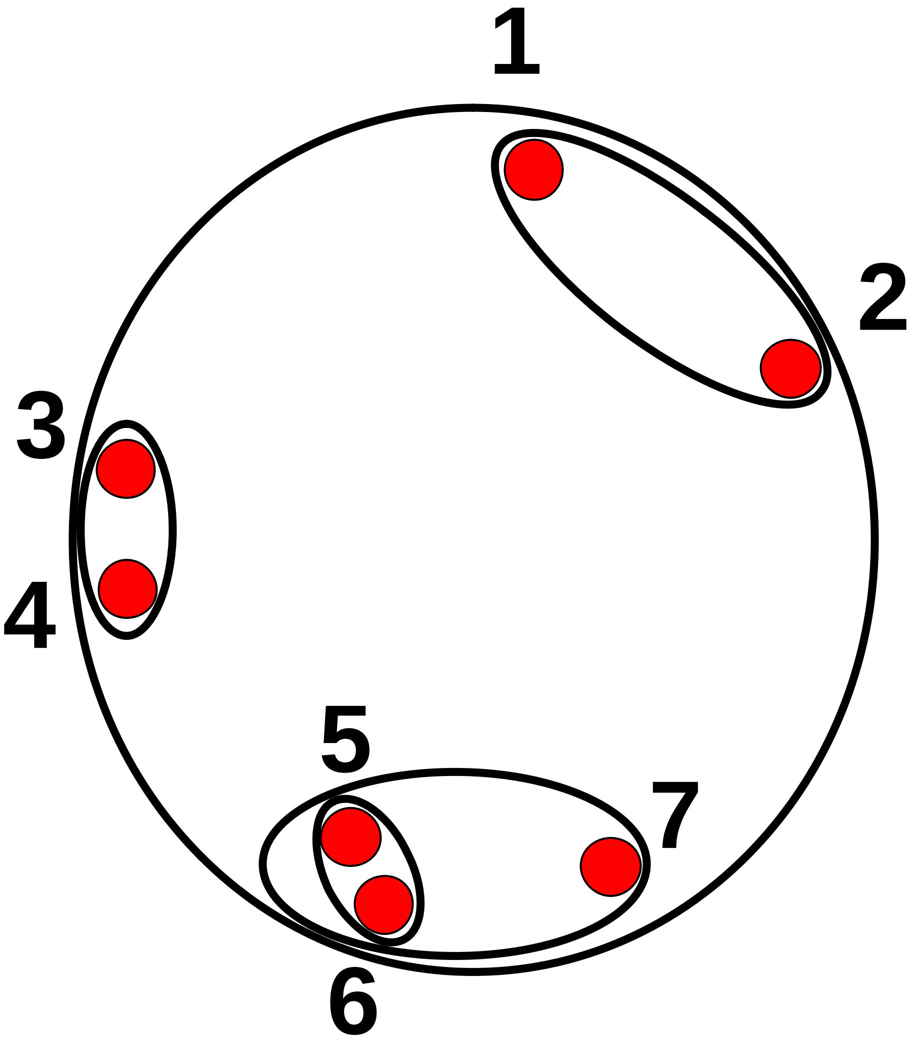
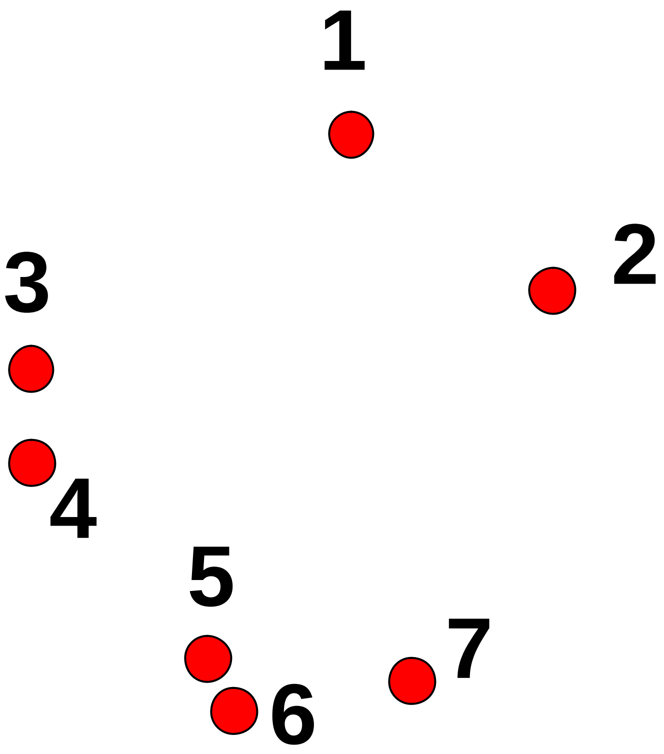


Hierarchical clustering (1)



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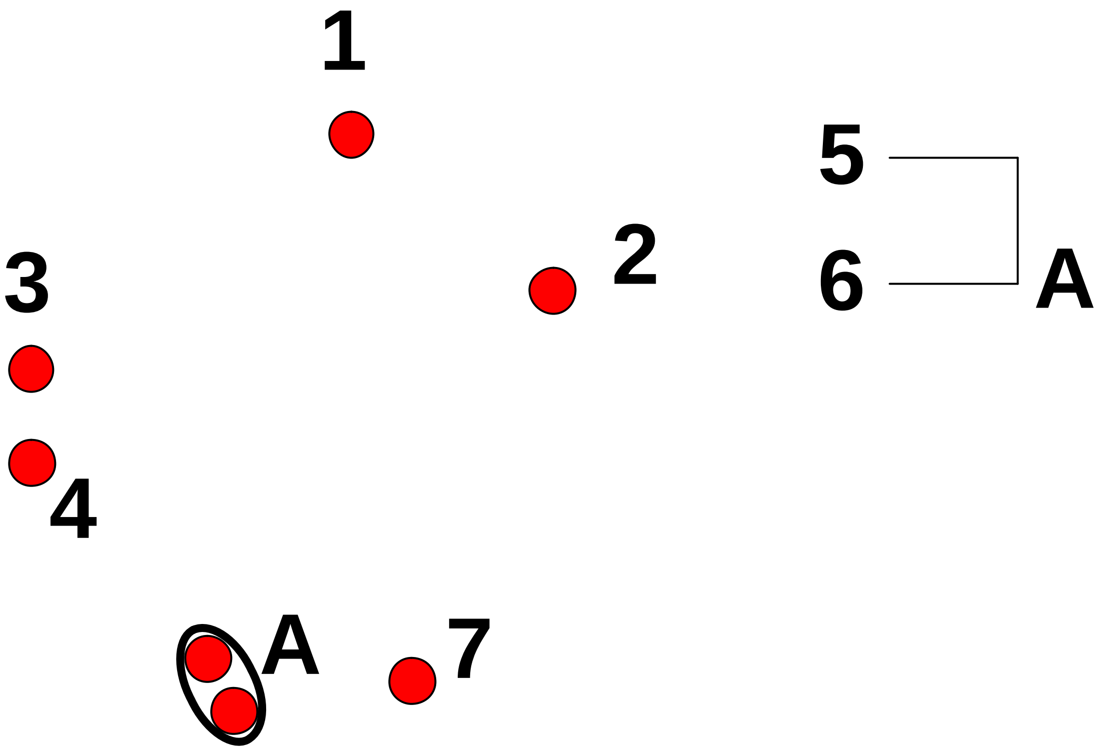

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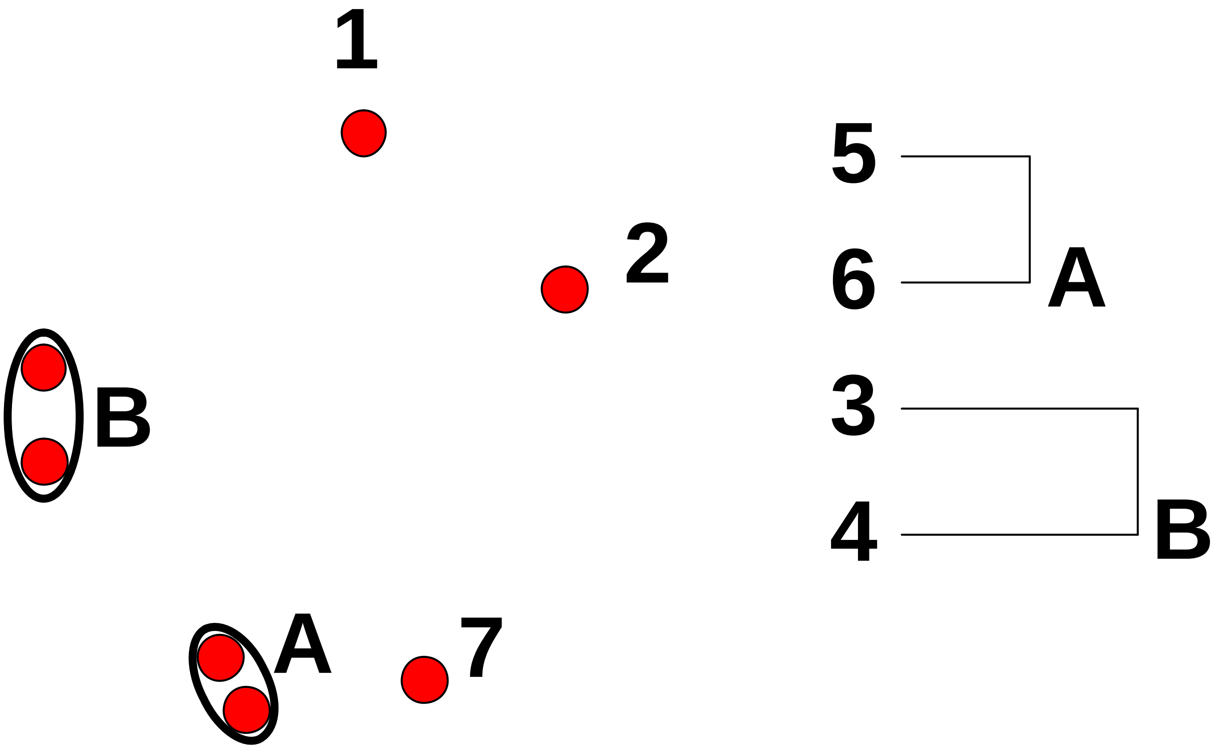

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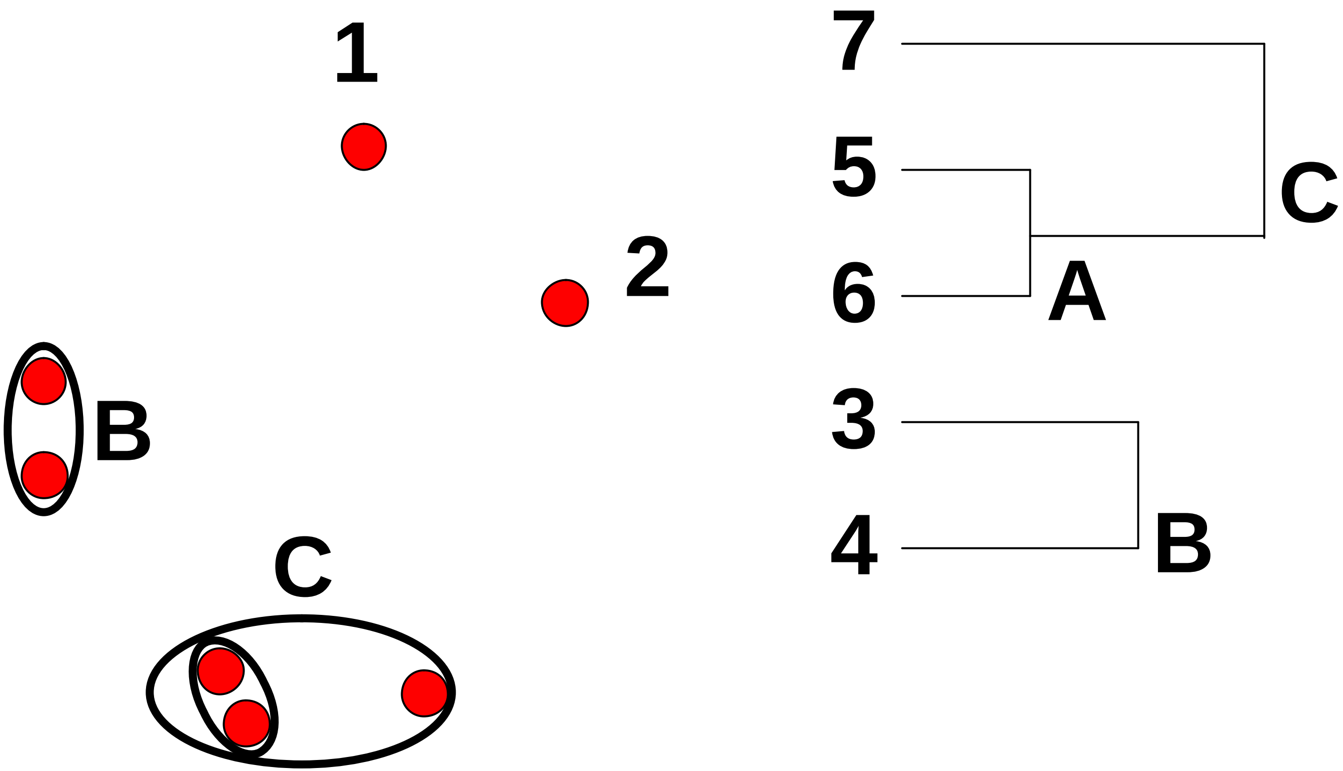

average linkage

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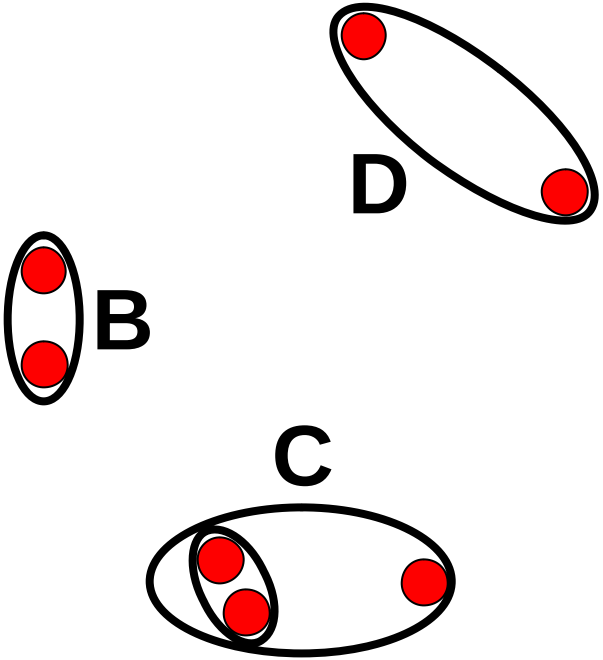

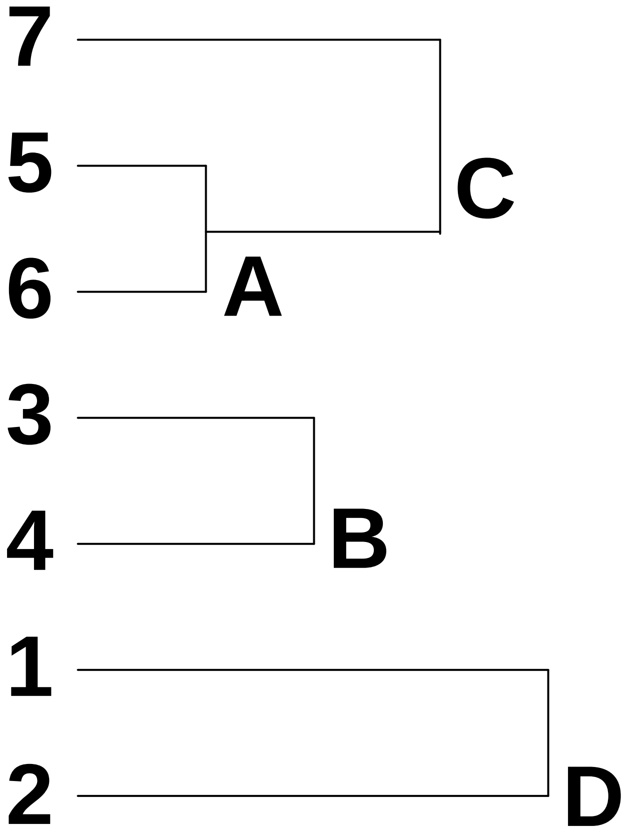

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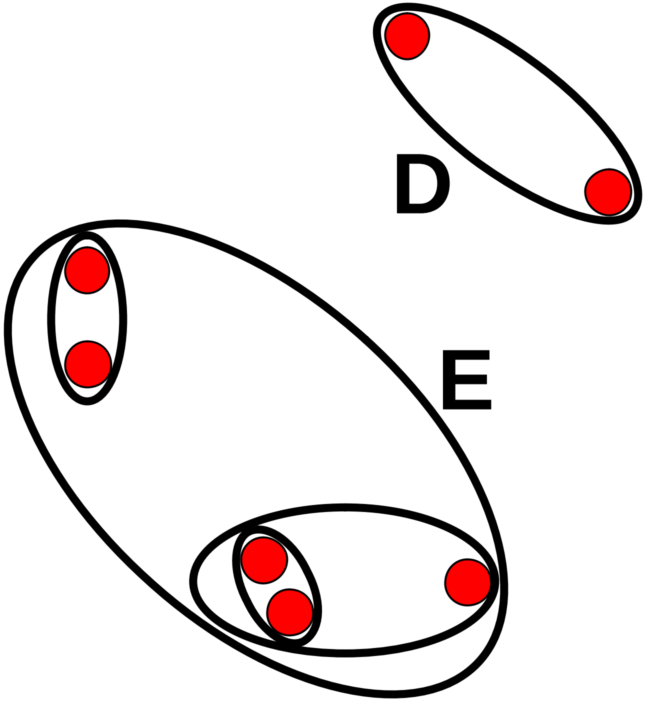

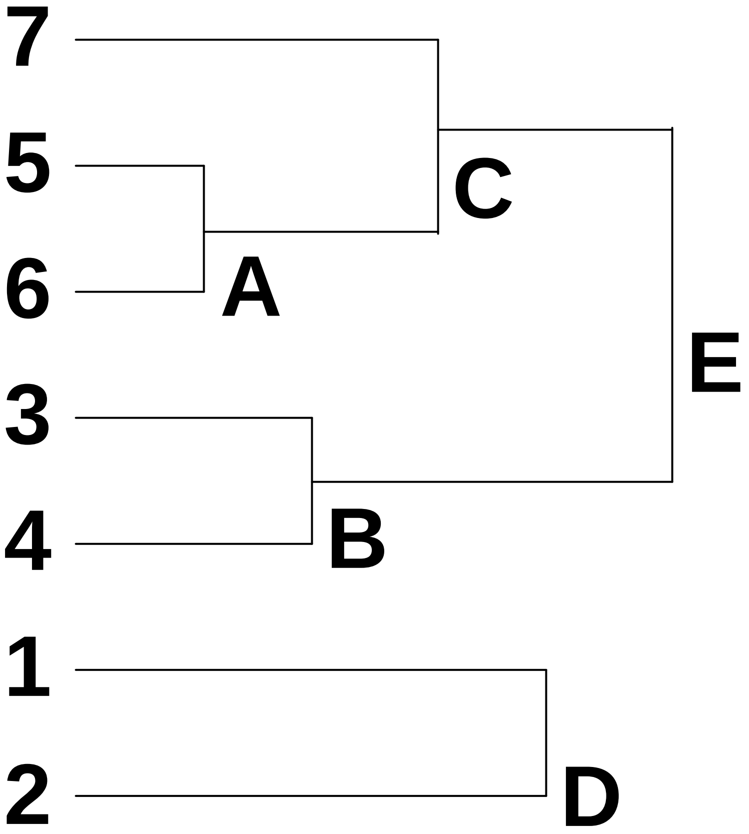

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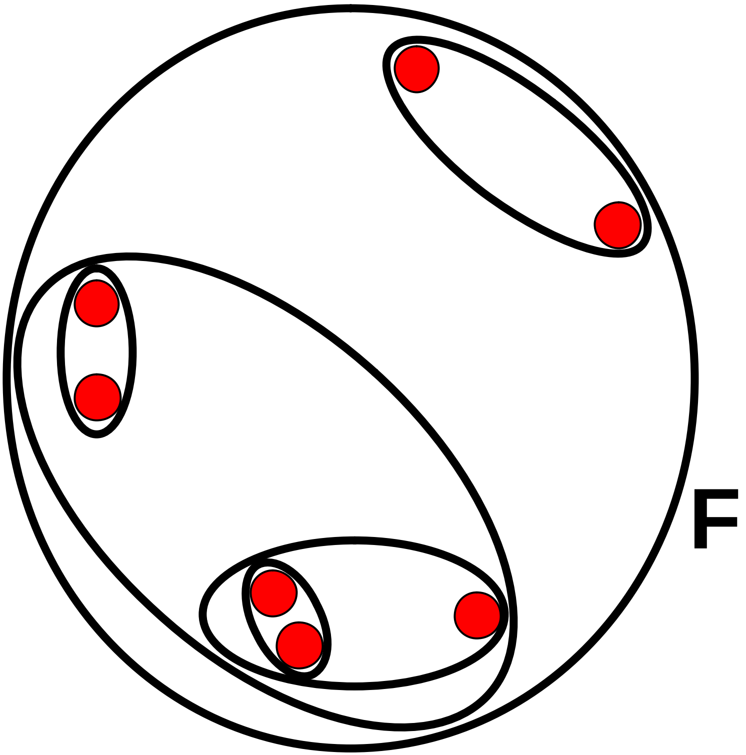

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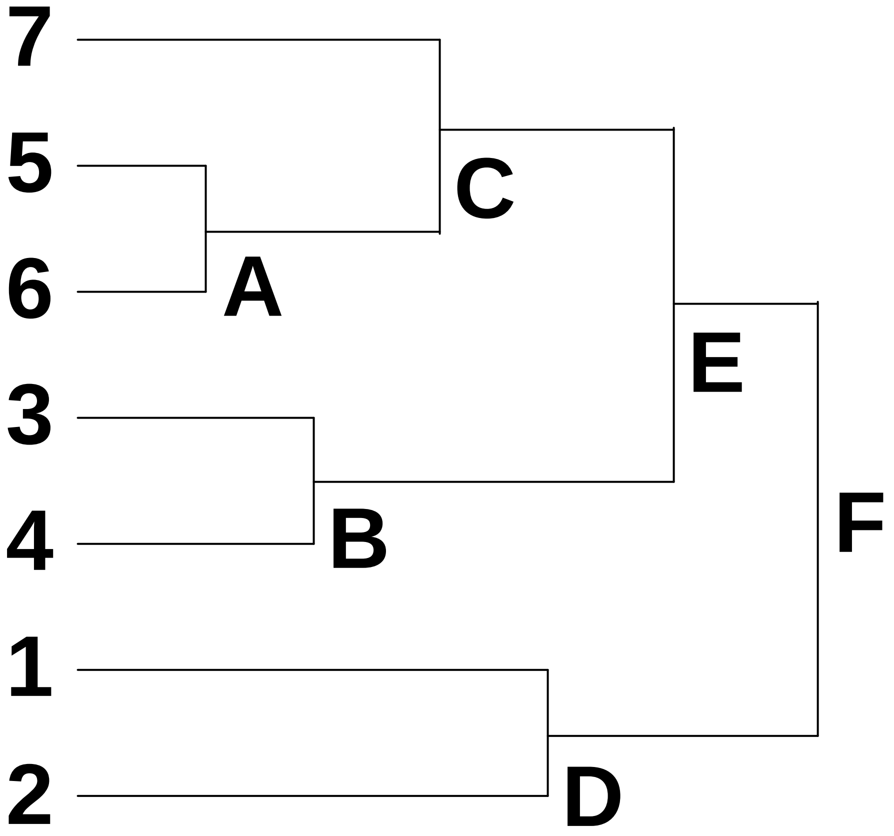

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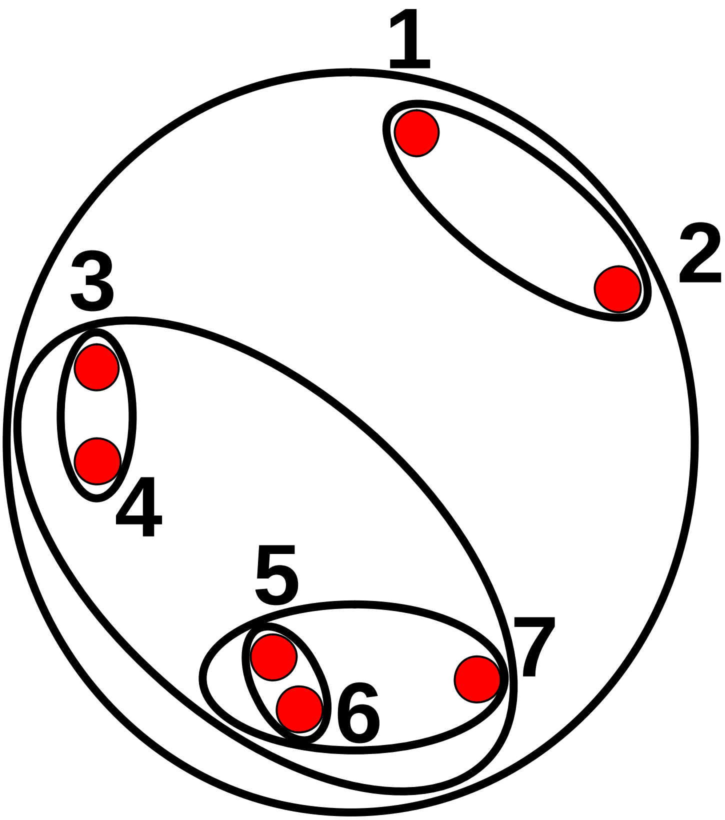

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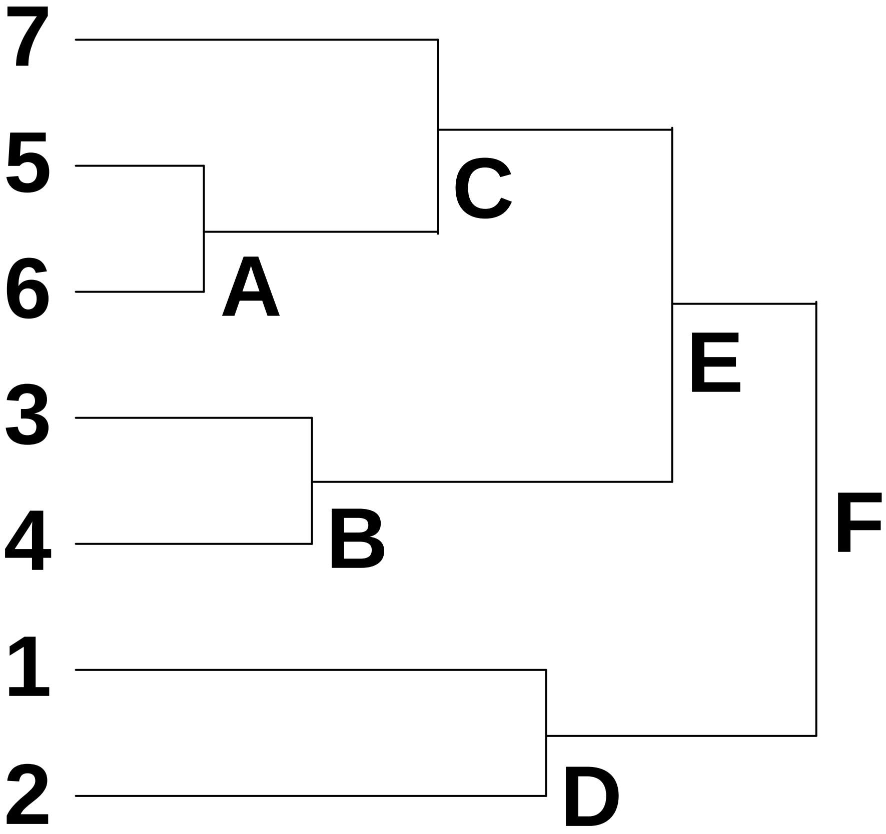
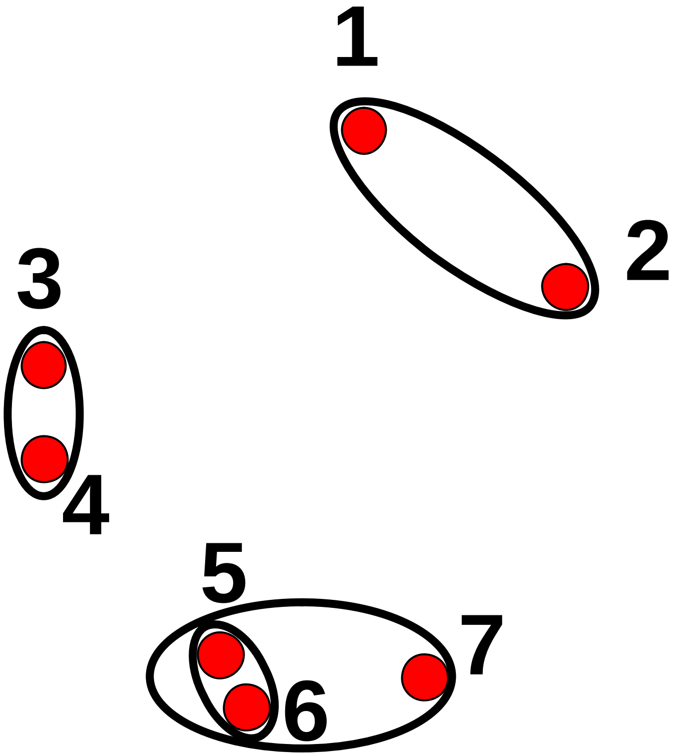


dendrogram

Hierarchical clustering (1)



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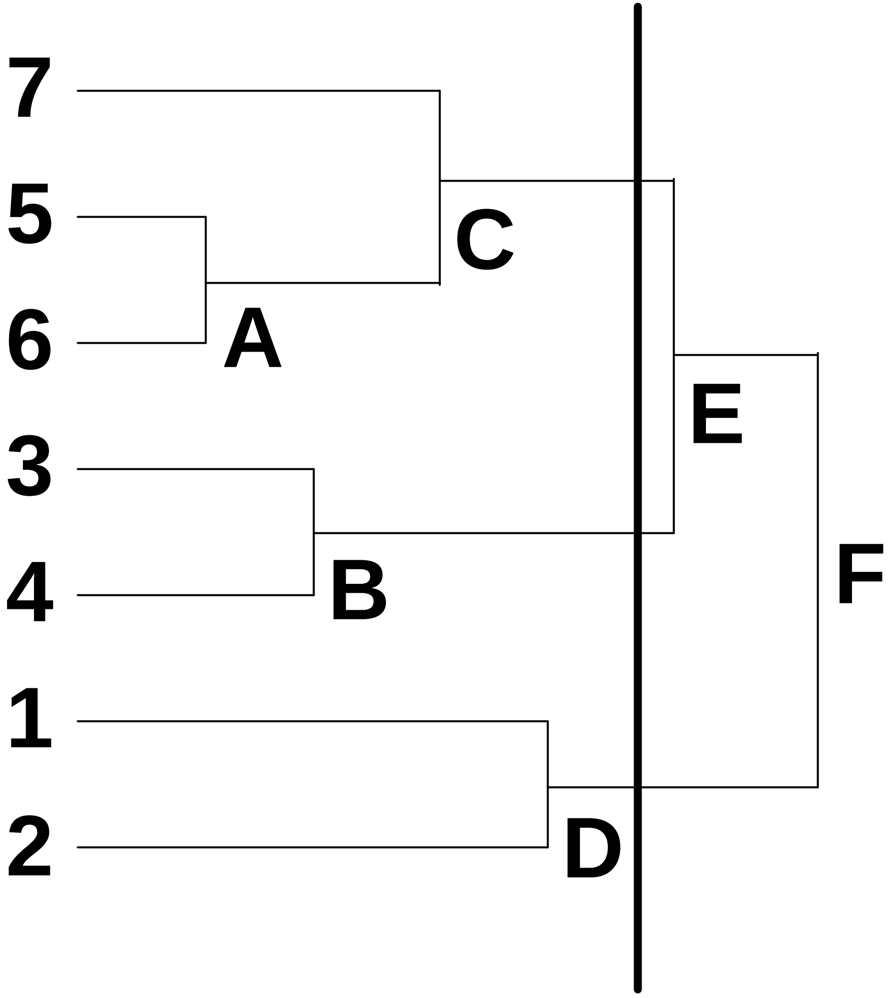
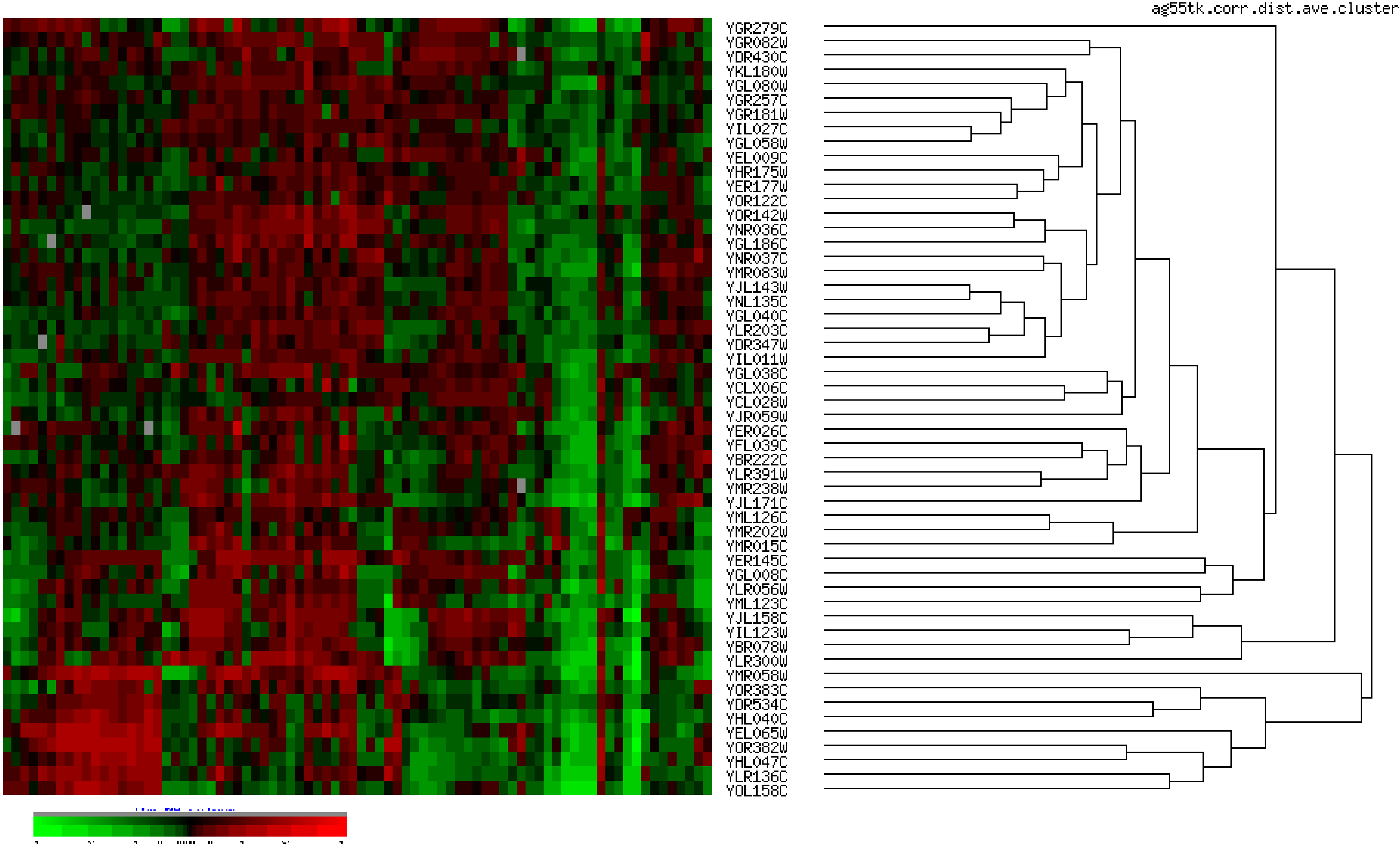
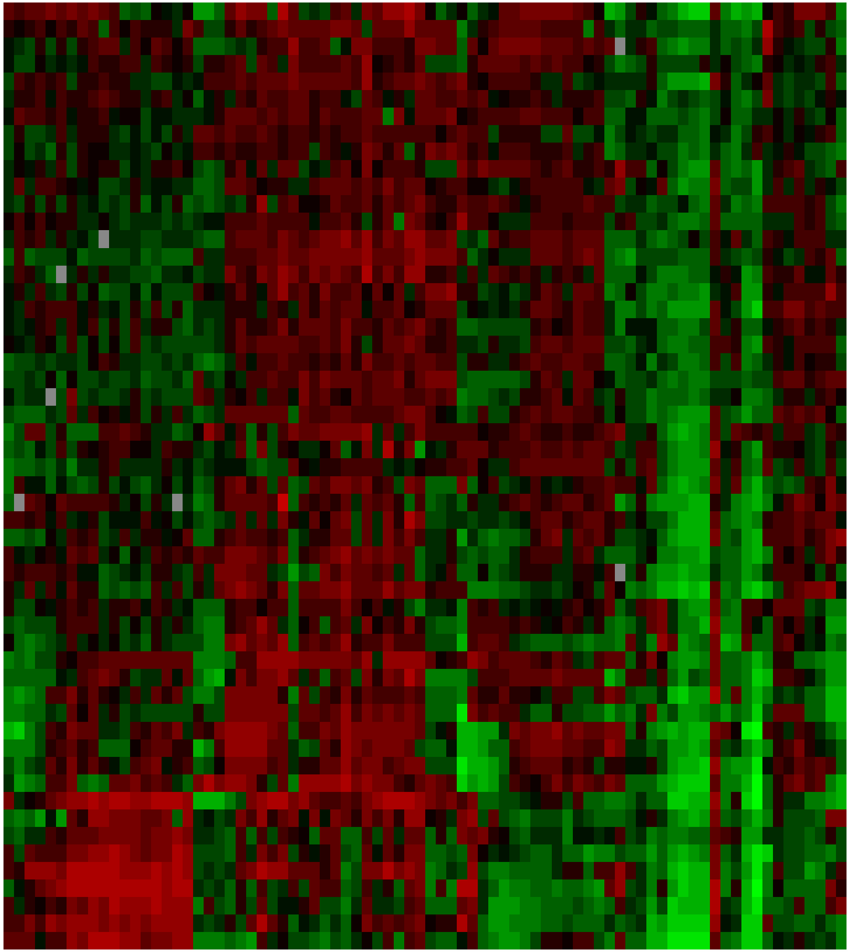


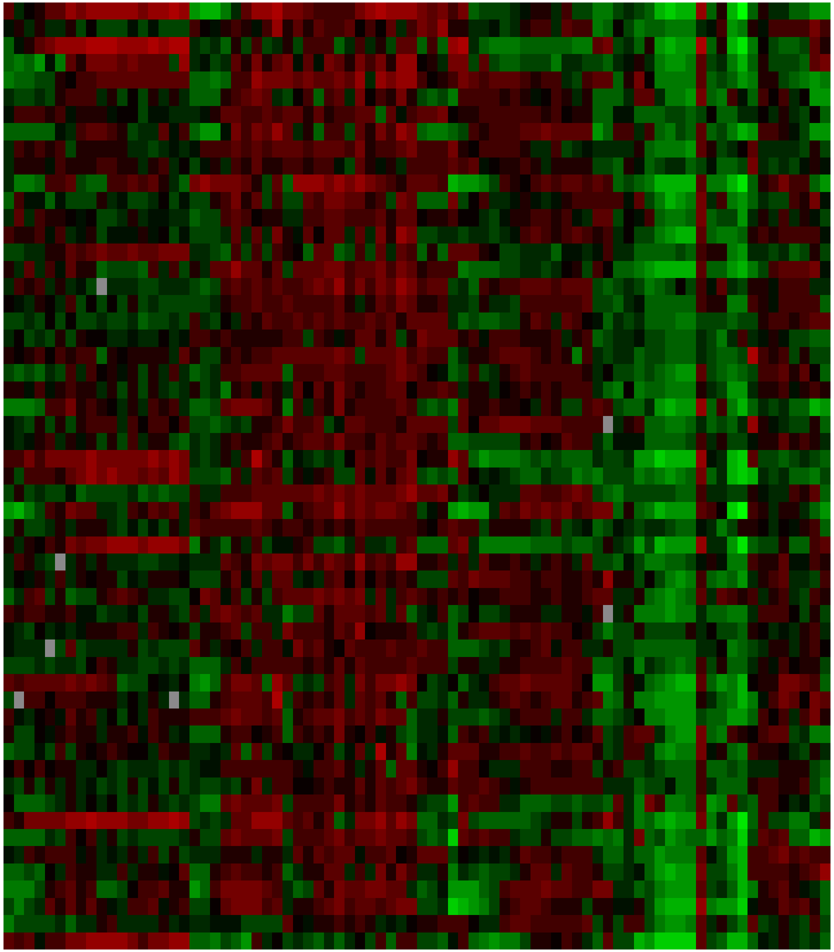
dendrogram

Hierarchical clustering (2)



Hierarchical clustering (3)





Hierarchical clustering (4)

Usually two steps:

- Calculation of all distances: $O(N^2)$ distances
- Agglomerating procedure: $O(N^2)$

Problem:

- N can be large: N>10000

We cannot afford calculating all the distances!

Hierarchical clustering (4)

Usually two steps:

- Calculation of all distances: $O(N^2)$ distances
- Agglomerating procedure: $O(N^2)$

Problem:

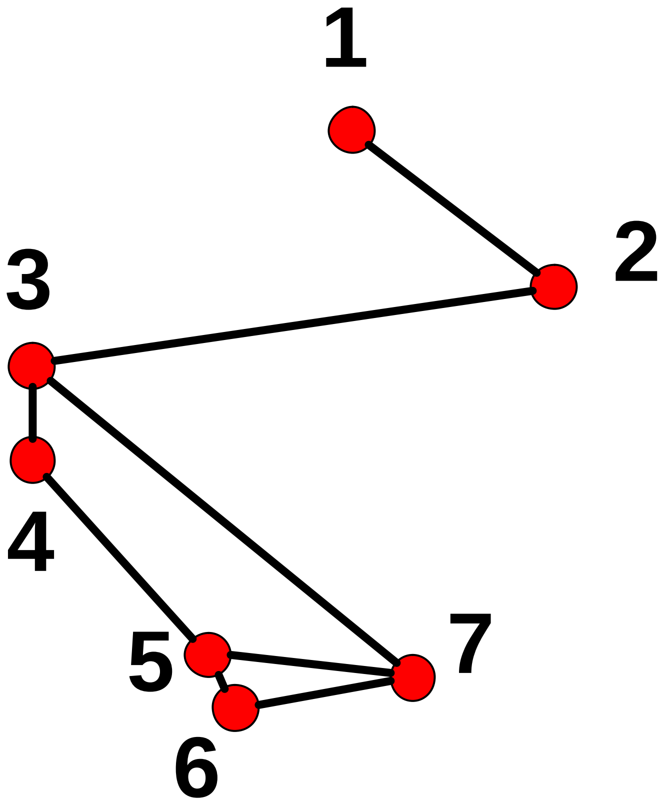
- N can be large: N>10000

We cannot afford calculating all the distances!

What if we calculate only some?

Approximate hierarchical clustering

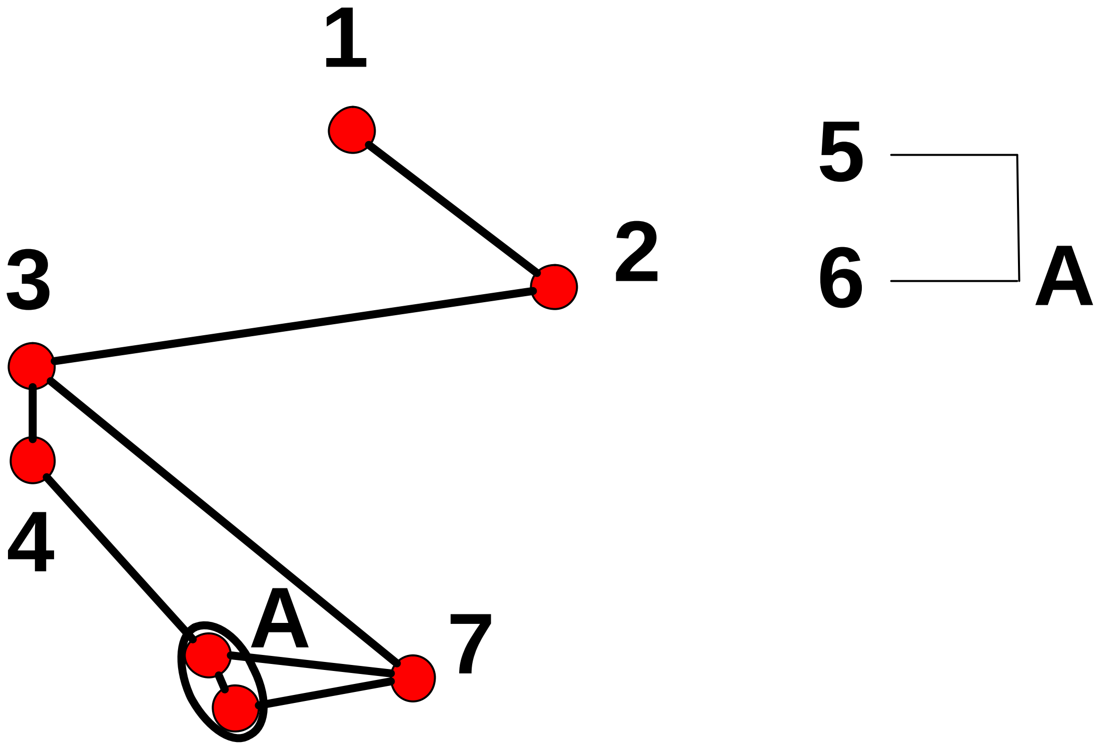
- Calculation of a subset of distances
- Approximate agglomerating procedure



1/3 of distances calculated

Approximate hierarchical clustering

- Calculation of a subset of distances
- Approximate agglomerating procedure



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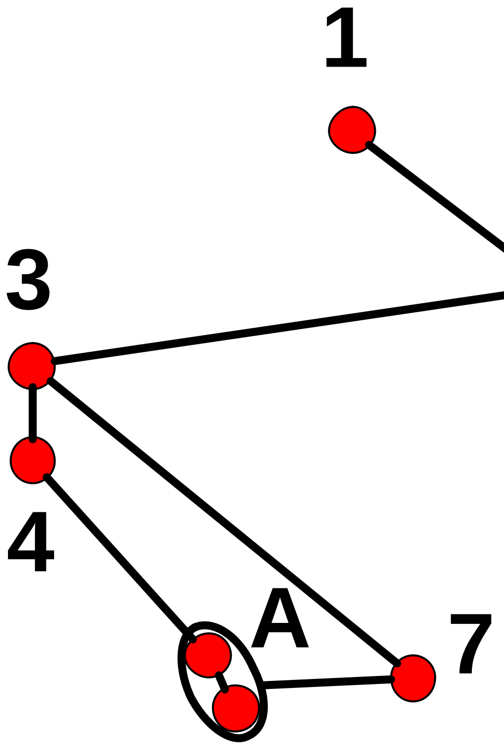

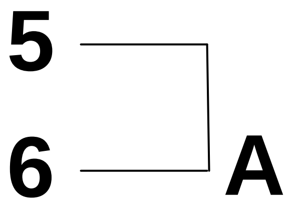

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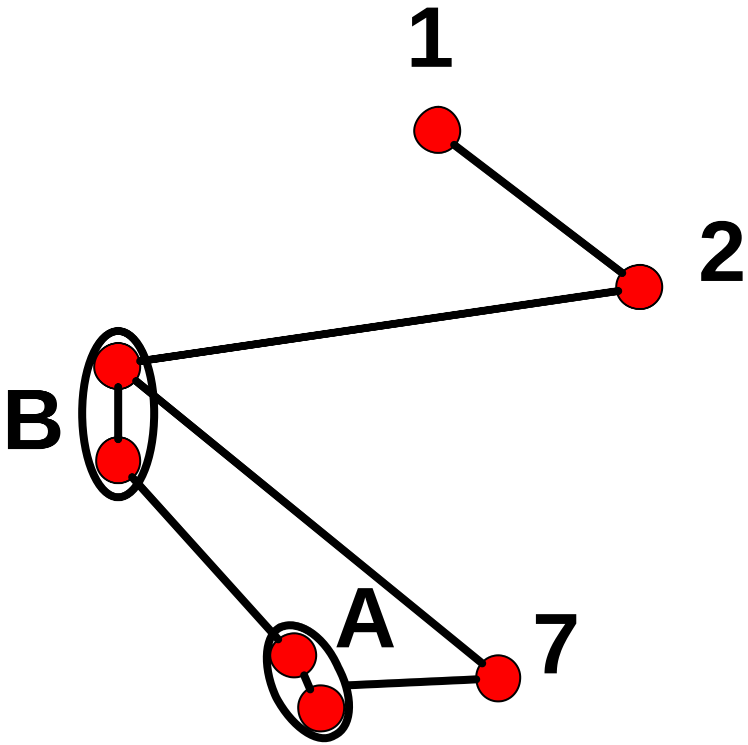

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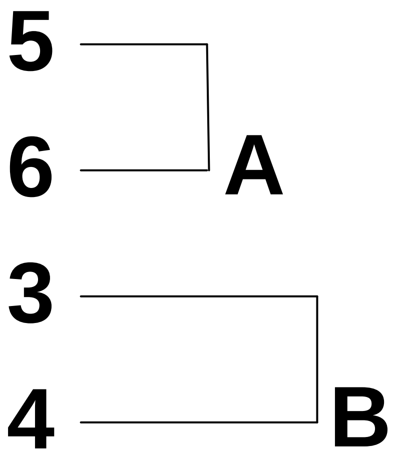

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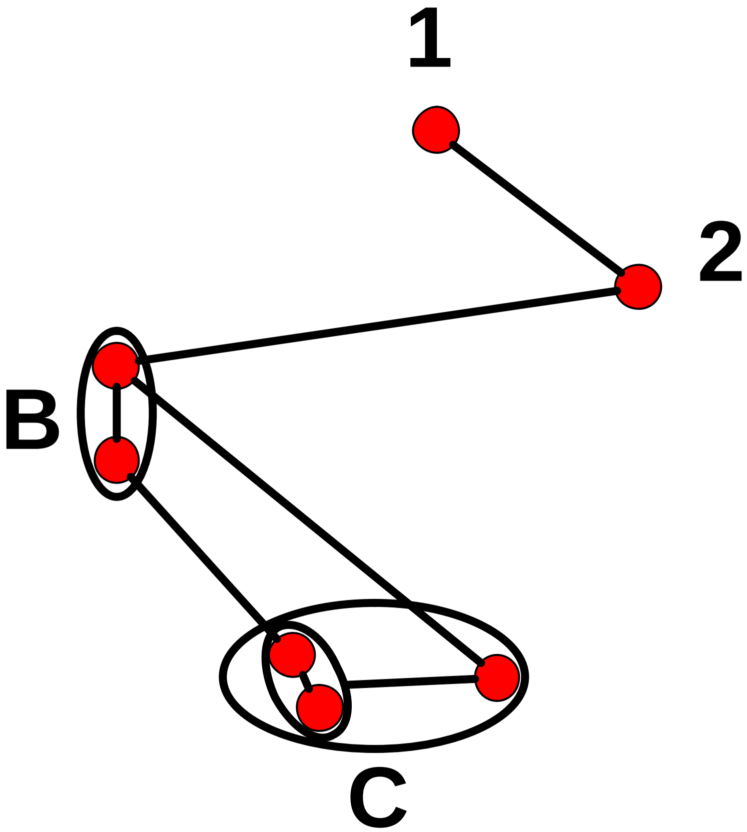

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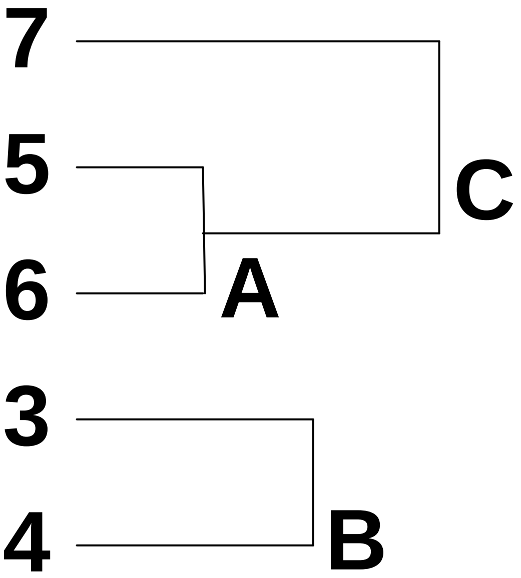

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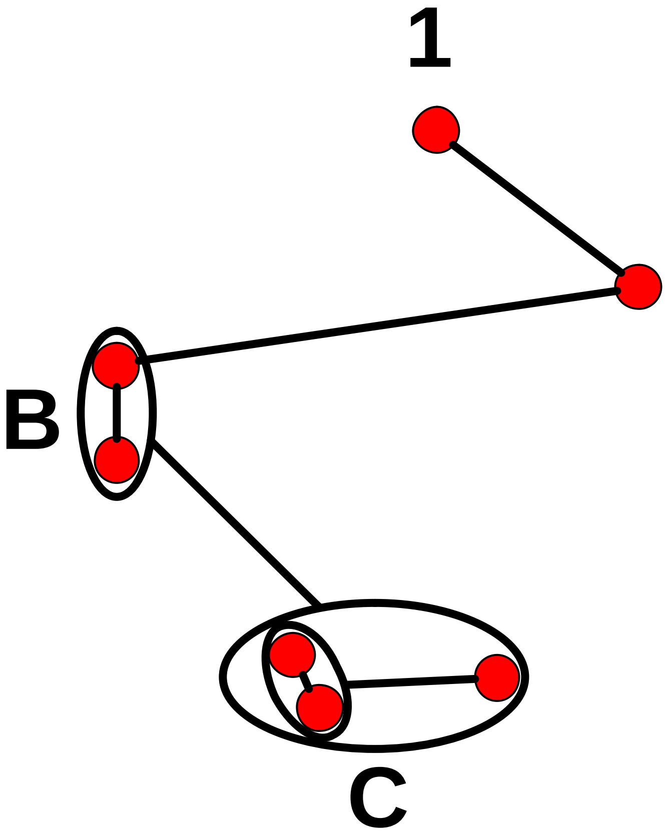

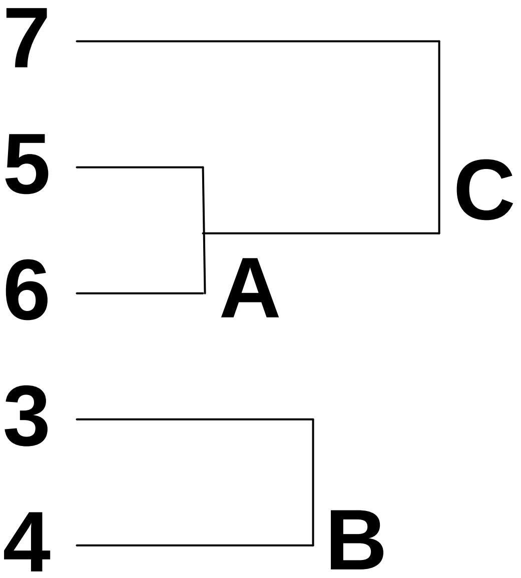

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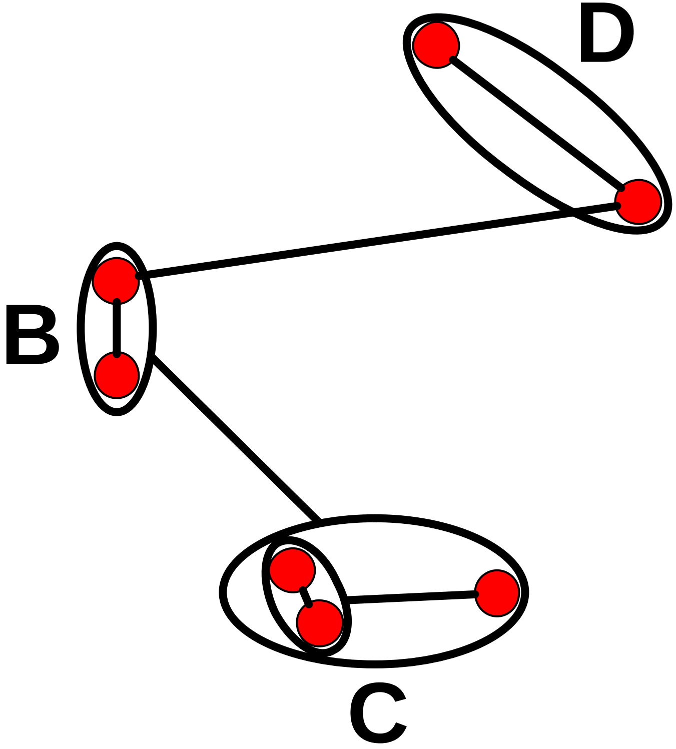

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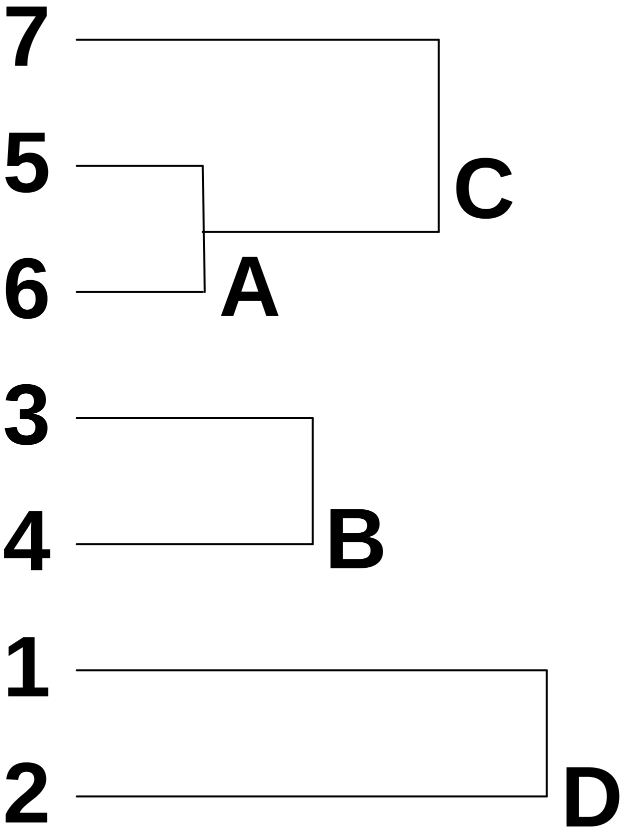

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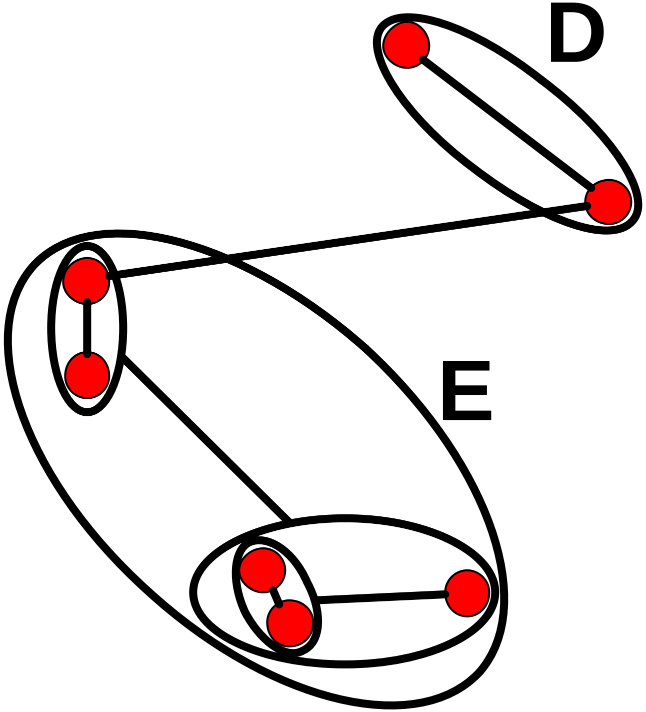

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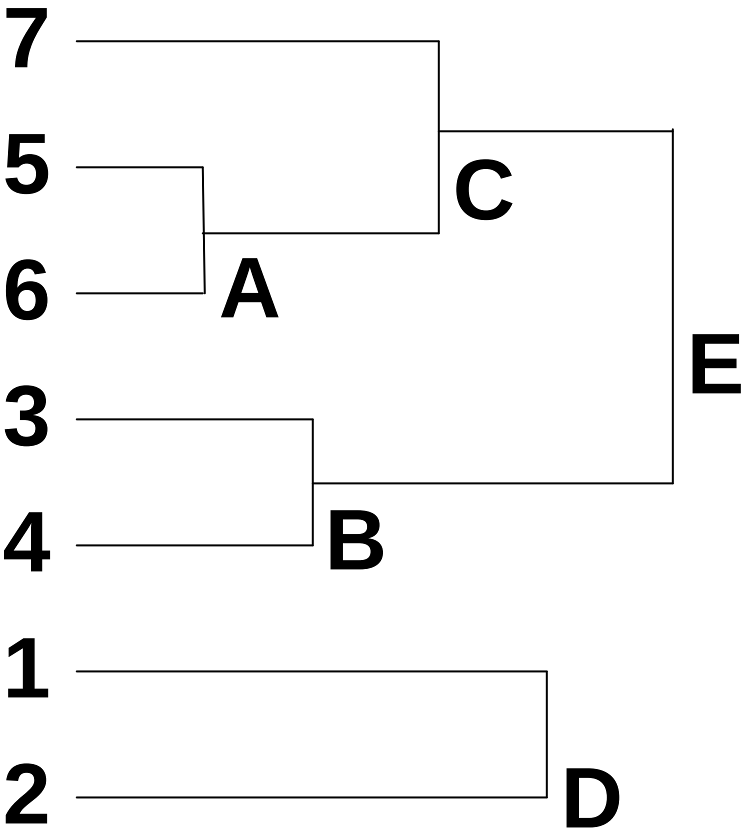

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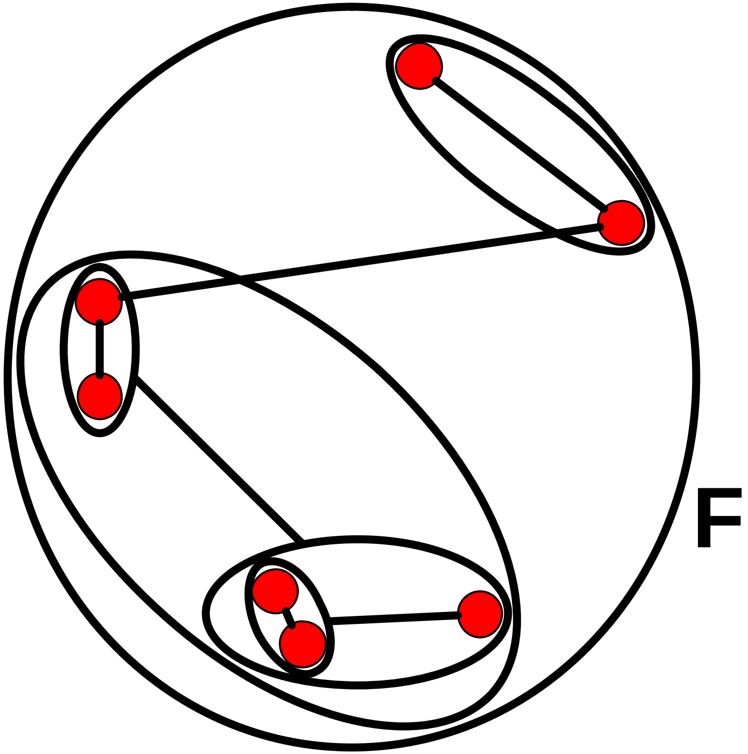

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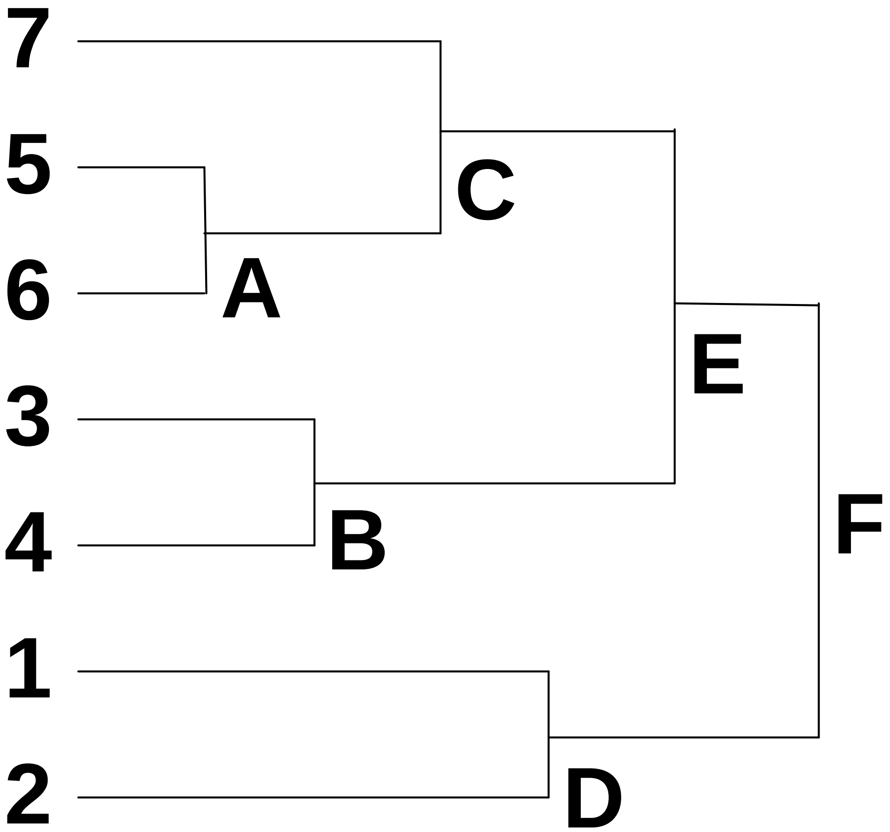

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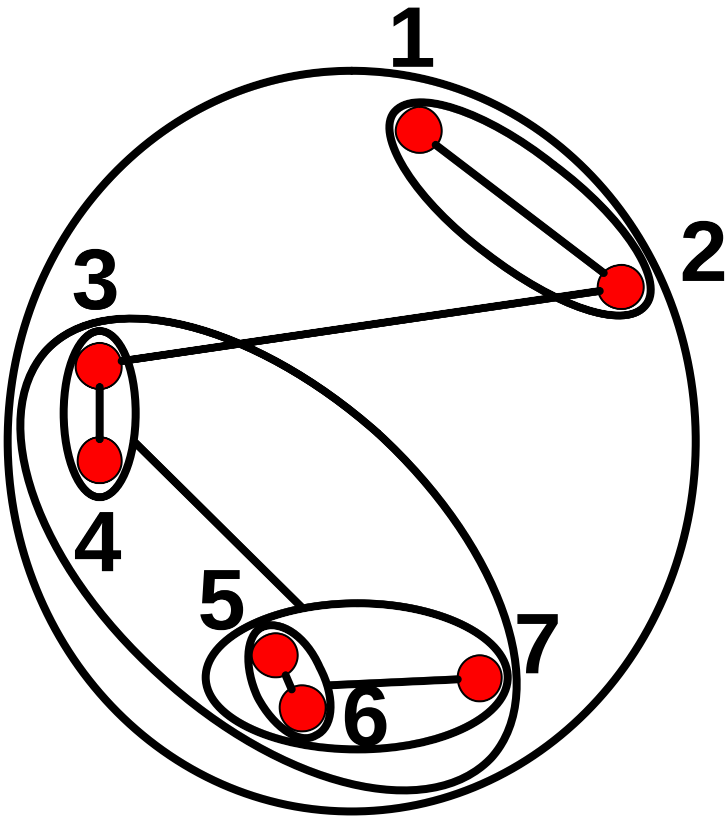

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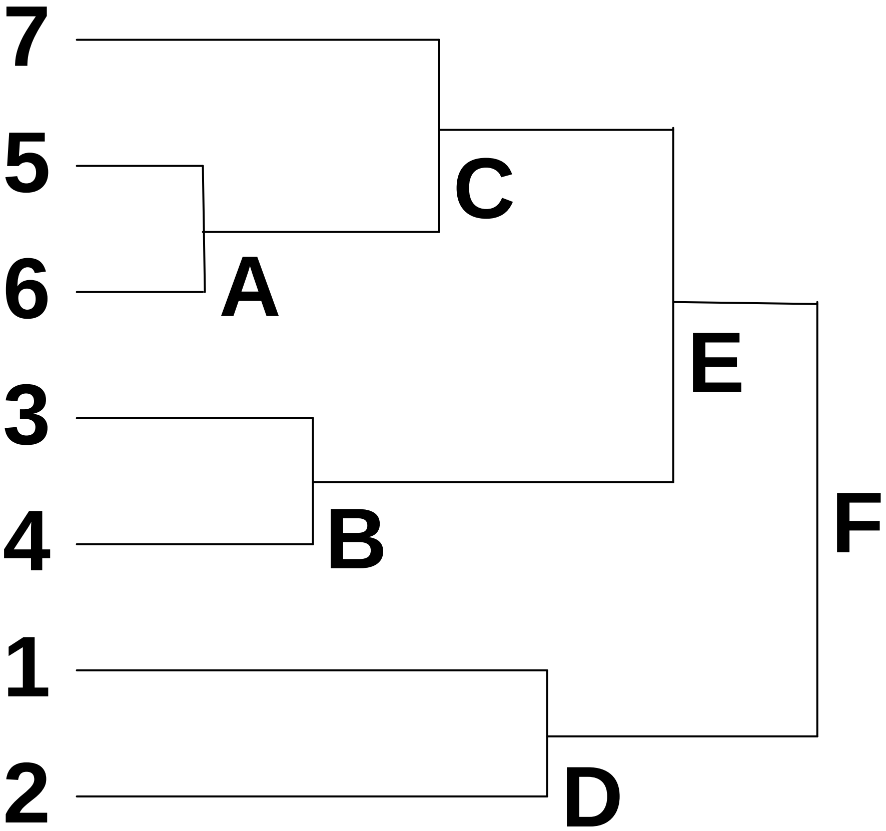
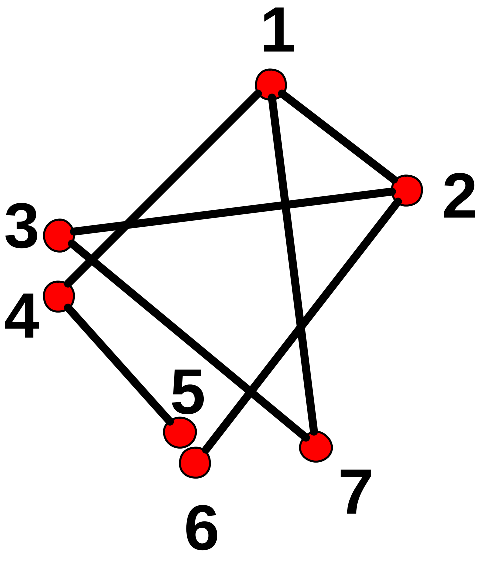


Small distances are important

Results of approximate hierarchical clustering are better when more **distances between similar data items** are used!

Otherwise:



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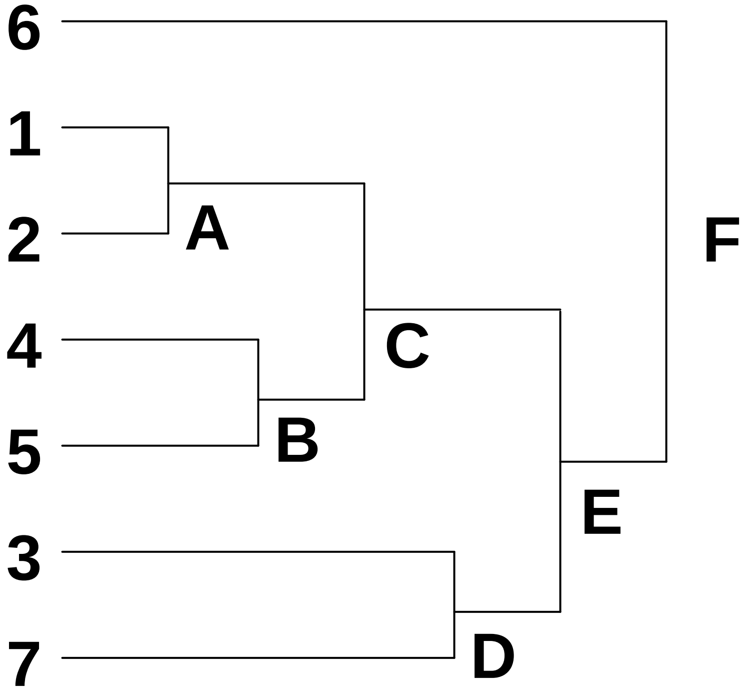
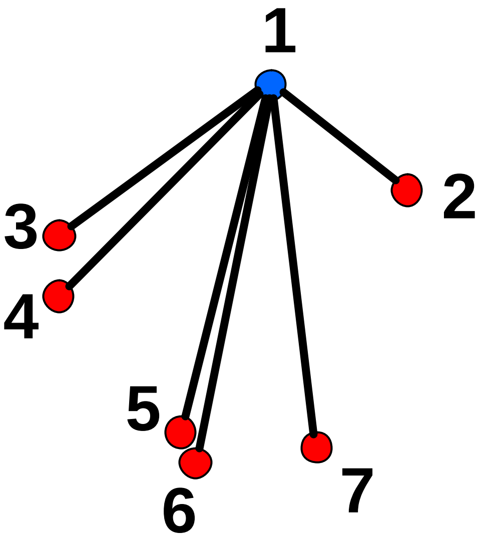


How to find all similar pairs without calculating all the distances?



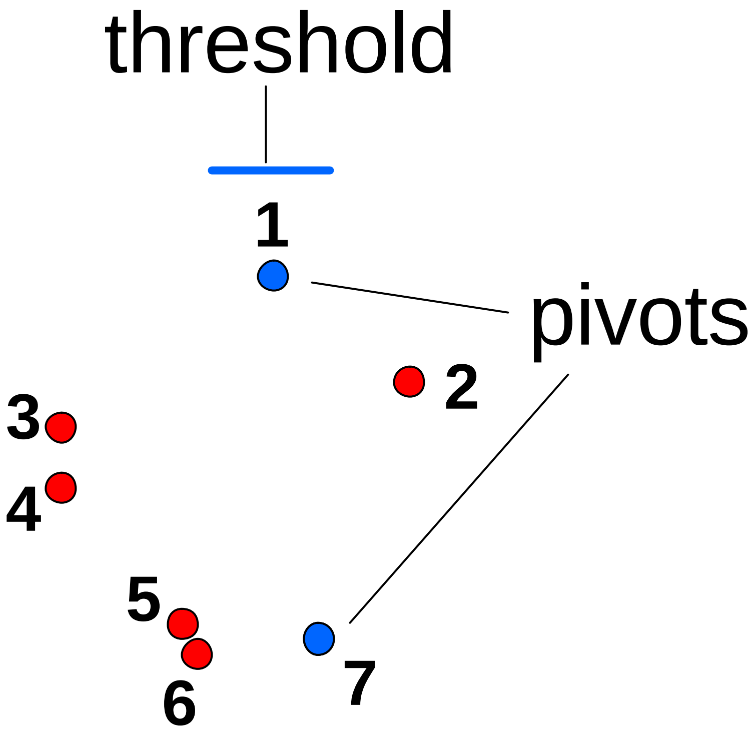
Triangle inequality: d(x,y) <= d(x,z)+d(z,y)

Corollary: d(x,y) >= |d(x,z)-d(y,z)|

d(**5**,**2**) >= |d(**1**,**5**)-d(**1**,**2**)|

d(**5**,**6**) >= |d(**1**,**5**)-d(**1**,**6**)|

Closest pairs algorithm



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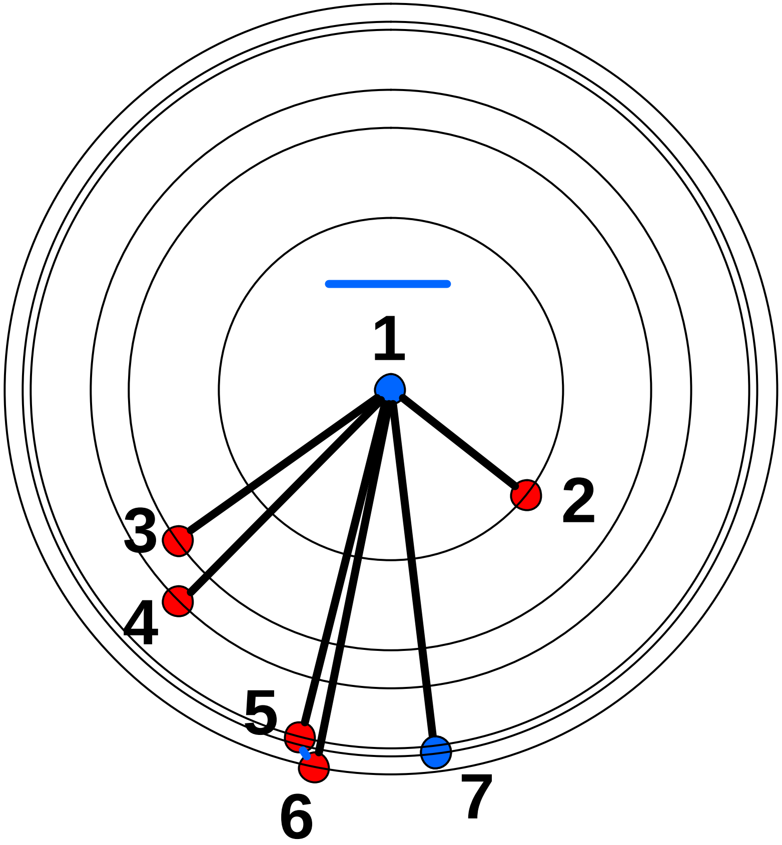

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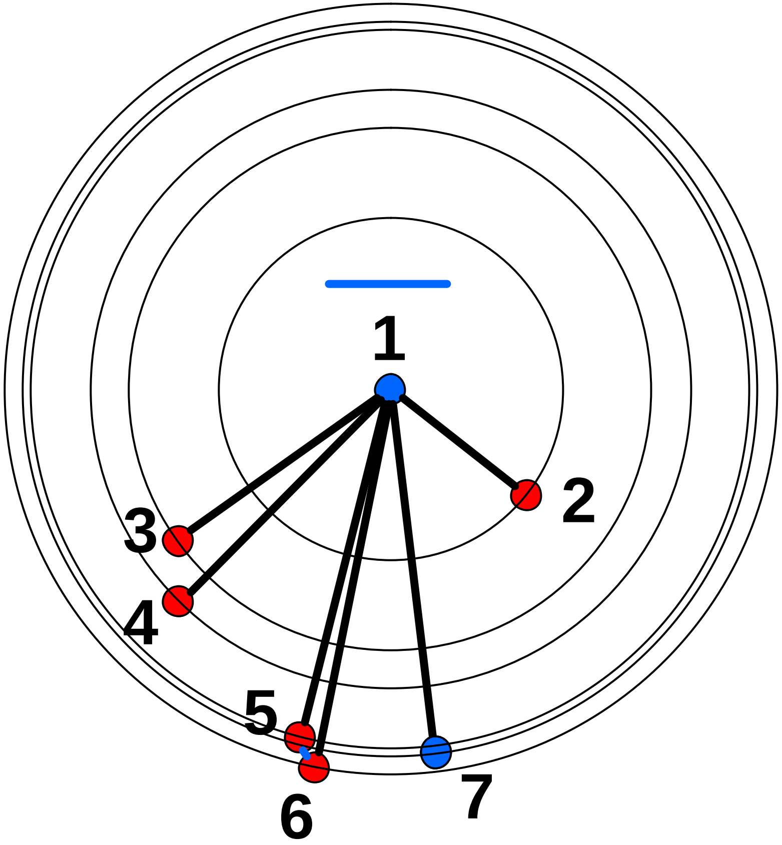
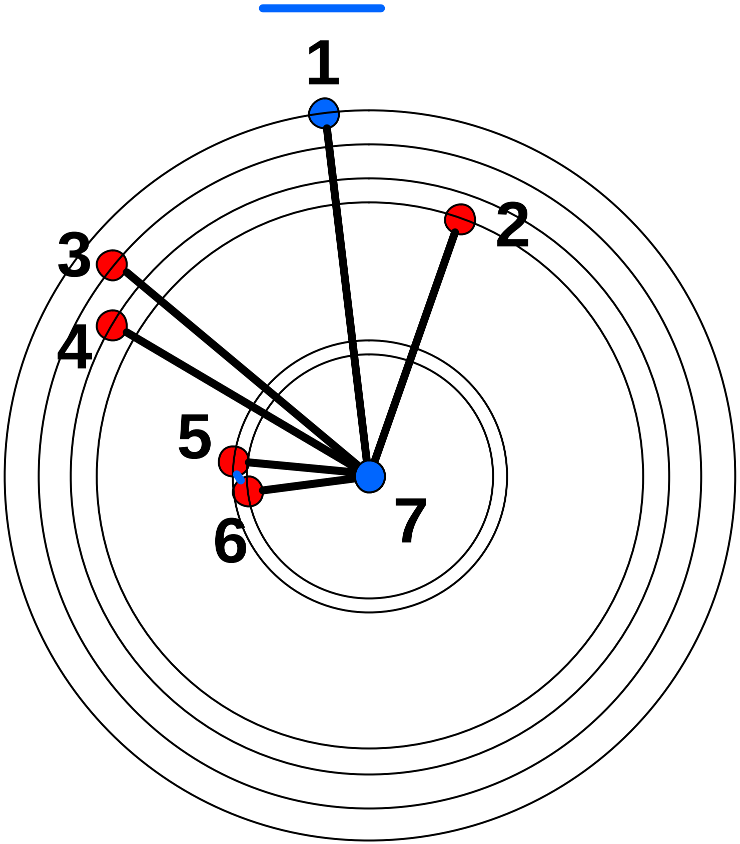


Candidates from 1:

- 2-3
- 3-4
- 3-5
- 4-5
- 4-6
- 4-7
- 5-6
- 5-7
- 6-7

Closest pairs algorithm



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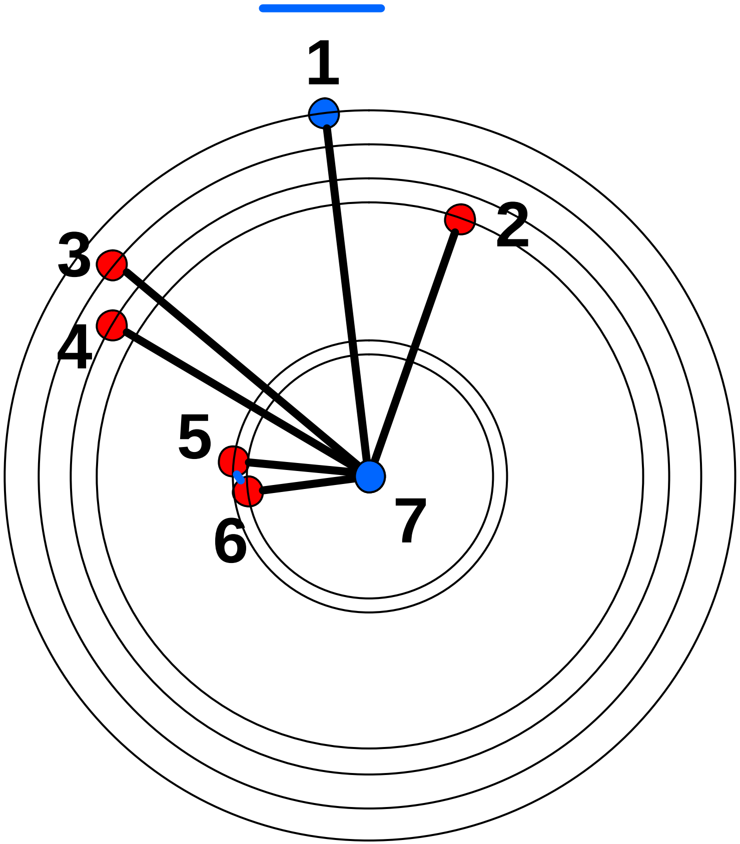


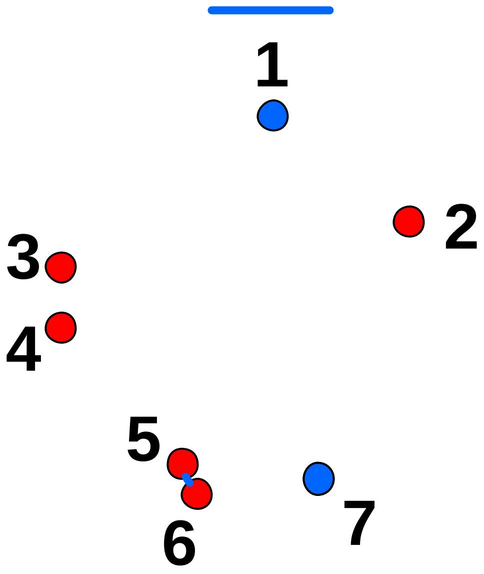
Candidates from 1:

- 2-3
- 3-4
- 3-5
- 4-5
- 4-6
- 4-7
- 5-6
- 5-7
- 6-7

Candidates from 7:

- 1-2
- 1-3
- 1-4
- 2-3
- 2-4
- 3-4
- 5-6
- 5-7
- 6-7

Closest pairs algorithm



Candidates from 1:

- 2-3
- 3-4
- 3-5
- 4-5
- 4-6
- 4-7
- 5-6
- 5-7
- 6-7

Candidates from 7:

- 1-2
- 1-3
- 1-4
- 2-3
- 2-4
- 3-4
- 5-6
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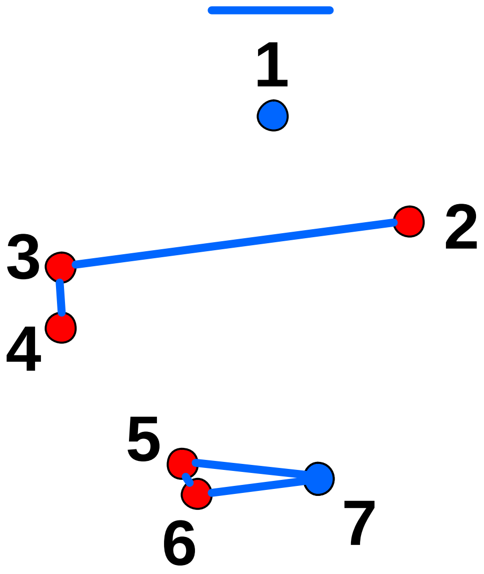
Closest pairs algorithm



Candidates from 1:

- 2-3
- 3-4
- 3-5
- 4-5
- 4-6
- 4-7
- 5-6
- 5-7
- 6-7

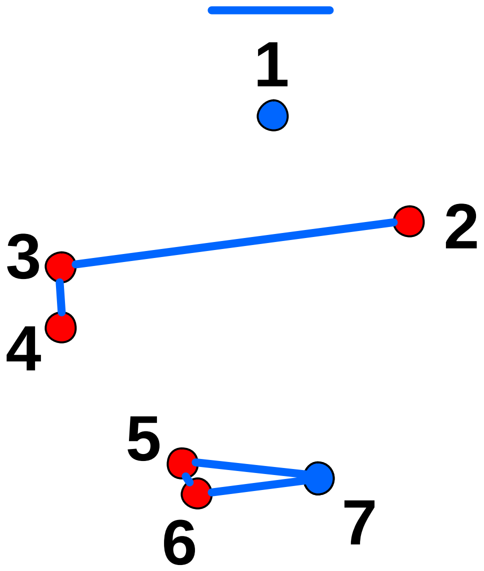
Candidates from 7:

- 1-2
- 1-3
- 1-4
- 2-3
- 2-4
- 3-4
- 5-6
- 5-7
- 6-7

Final candidates:

- 2-3
- 3-4
- 5-6
- 5-7
- 6-7

Closest pairs algorithm



Candidates from 1:

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- 4-7
- 5-6
- 5-7
- 6-7

Candidates from 7:

- 1-2
- 1-3
- 1-4
- 2-3
- 2-4
- 3-4
- 5-6
- 5-7
- 6-7

Final candidates:

- 2-3
- 3-4 +
- 5-6 +
- 5-7
- 6-7

Example continued

Dataset:

- N = **7** datapoints;
- N*(N-1)/2 = **21** pairs of datapoints.

Closest pairs algorithm

- calculated **15** distances, it means ~**70%**;
- found the **4** closest pairs (**2** of them closer than threshold).

15 randomly chosen distances contain on

the average **3** of these 4 similar pairs.

Large example

Dataset:

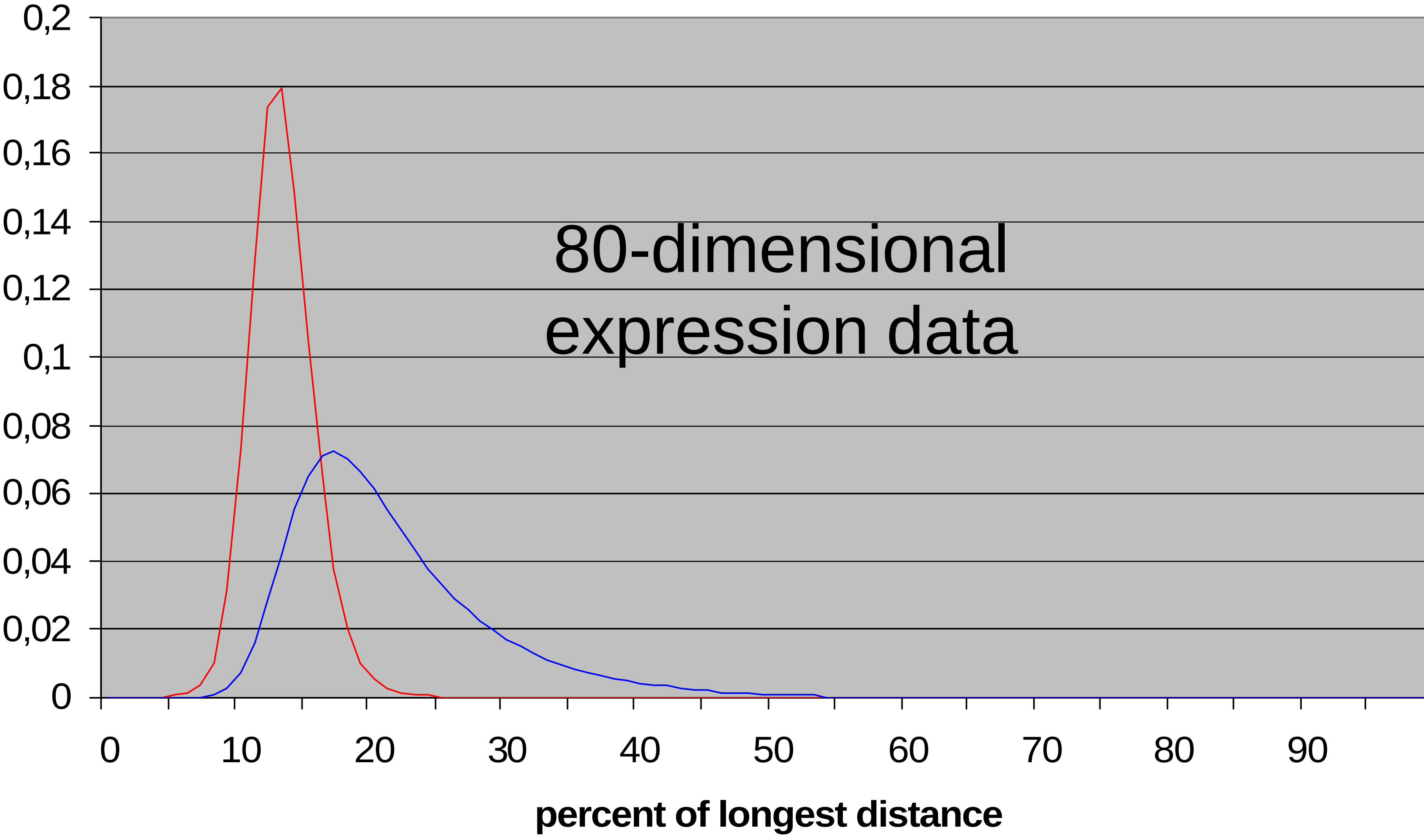
- N = **6000** datapoints;
- N*(N-1)/2 ~ **18 million** pairs of datapoints.

Closest pairs algorithm

- calculated **1.4 million** distances, i.e. ~**7%**;
- found the **10000** closest pairs (**1000** of them closer than threshold).

1.4 million randomly chosen distances contain on the average only **700** of these 10000 pairs.

Probability distributions of all distances vs distances from the closest pairs algorithm



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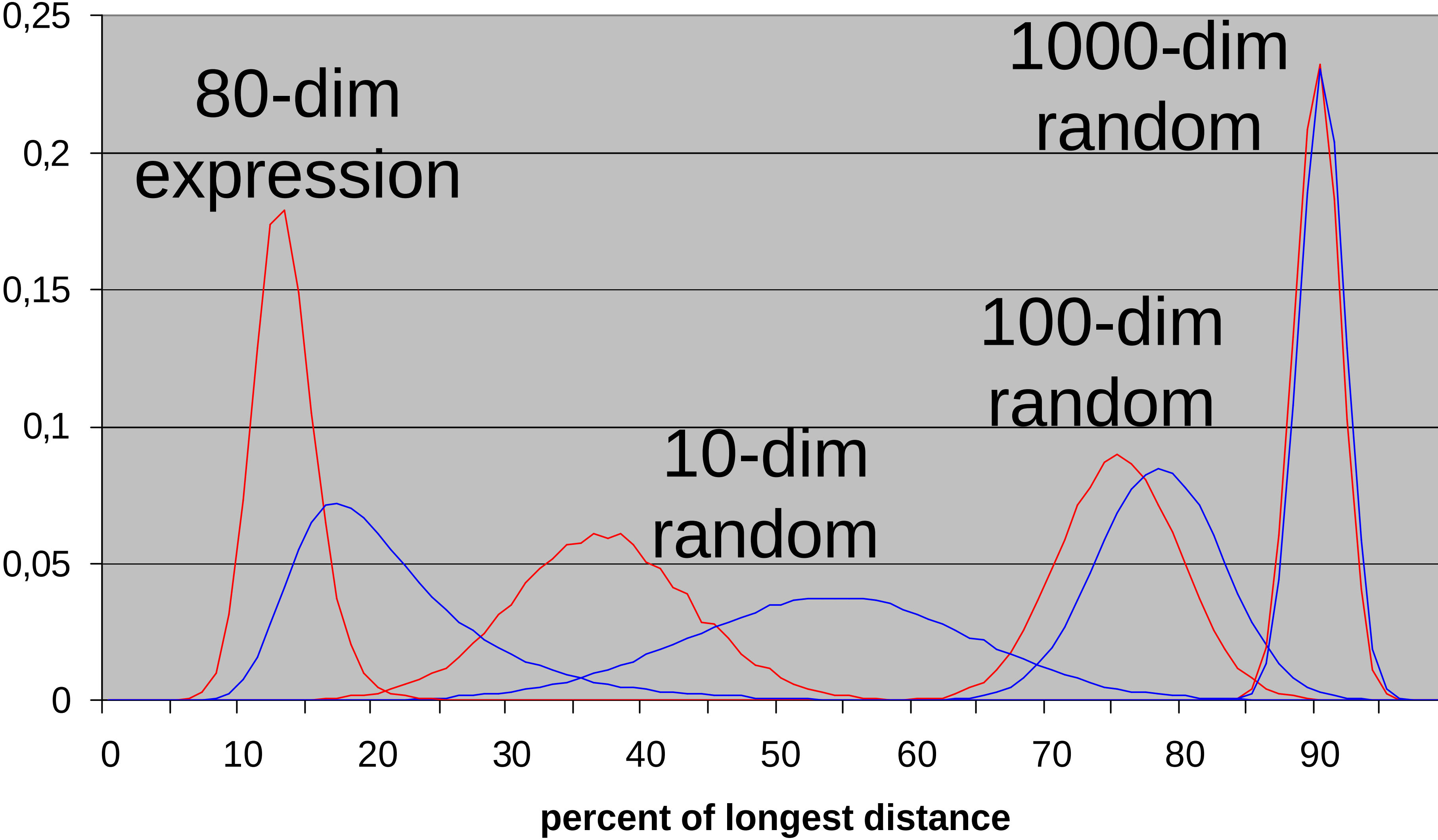

Results

- Random subset of distances
- Approximate hierarchical clustering

7% of distances measured

- Final candidates of closest pairs algorithm
- Approximate hierarchical clustering

1% of distances measured

6000 datapoints, 80-dimensional

SAME QUALITY!

Problems

- The algorithm for finding the candidates for similarity is not very efficient – if the dimensionality is small then it may be faster to calculate all the distances.
- The algorithm needs $2N^2$ bytes of memory – 1.5 GB for about 25000 human genes.

Future

- Better approximation algorithm

Future

- Better approximation algorithm
- Optimise for speed

Future

- Better approximation algorithm
- Optimise for speed
- Parallelise