Algorithms

Clustering

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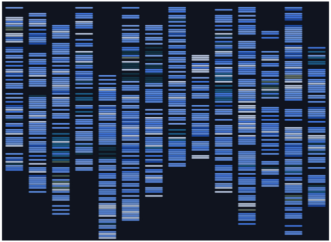
Motivation

Example: Discover groups of genes with similar functions, regardless of their particular role.



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This is a common problem in biology and other data sciences.

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What is a "good cluster"?
What does it mean to be "similar"?

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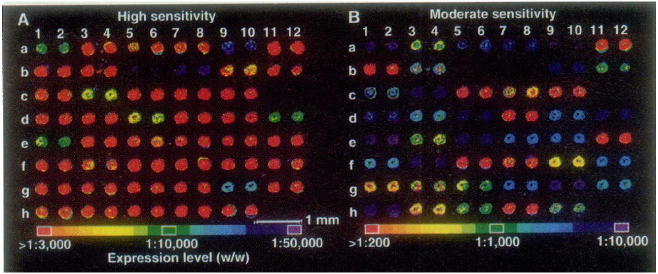

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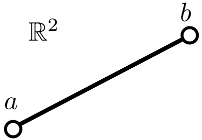

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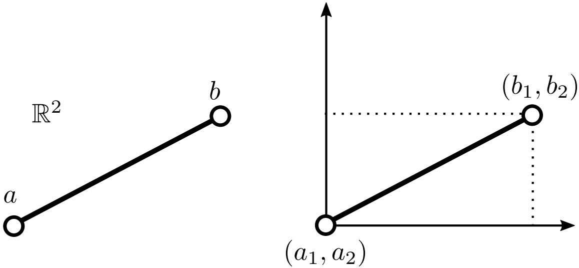

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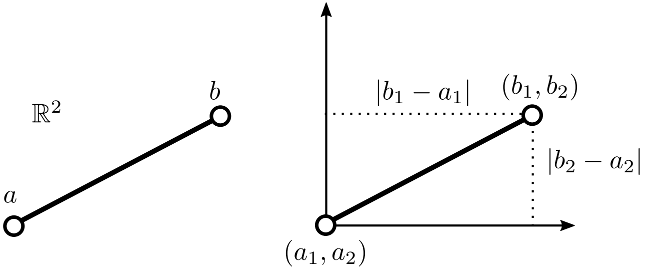

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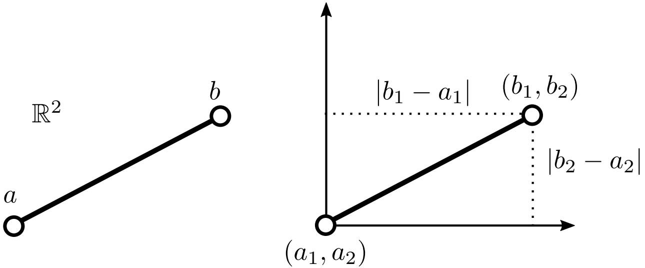

Pythagoras' theorem: $d(a,b) = (|b_1 - a_1|^2 + |b_2 - a_2|^2)^{\frac{1}{2}}$

L_p distance

One can generalize to different power coefficients $p \geq 1$:

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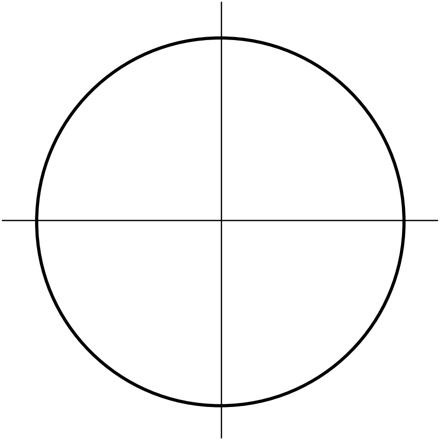
This definition gives us the L_p distance between points in $\mathbb{R}^k$.

L_p unit balls in $\mathbb{R}^2$

For $p = 2$, we get the usual intuitive idea of a circle:



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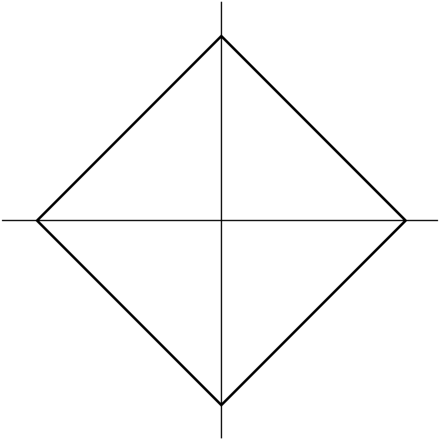
For $p = 1$, we get a diamond-shaped boundary:



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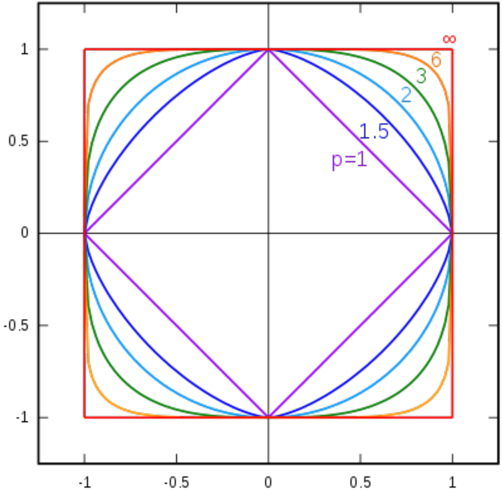
For general $p \geq 1$, we get a general notion of "ball":



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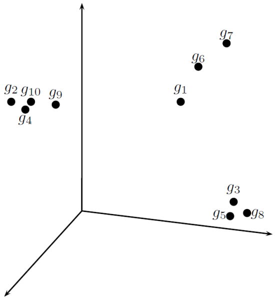

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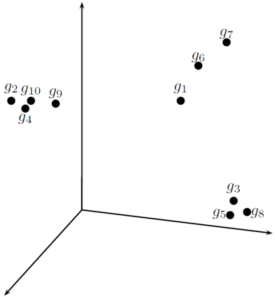
Let us look at the L_2 distances between each pair of genes:



	g_1	g_2	g_3	g_4	g_5	g_6	g_7	g_8	g_9	g_{10}
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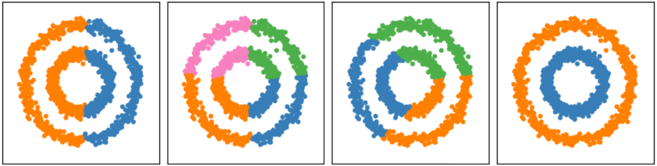
distance matrix

Good clusters

Data points can be clustered in many possible ways:



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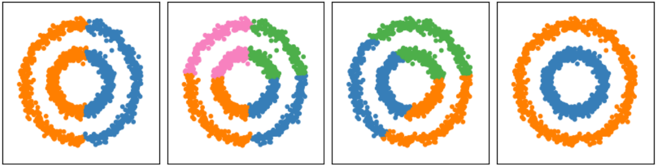

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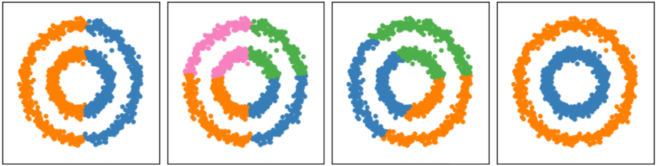

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Also: how many clusters do we want to find?

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Termination criterion: For example, when the centroids stop changing.

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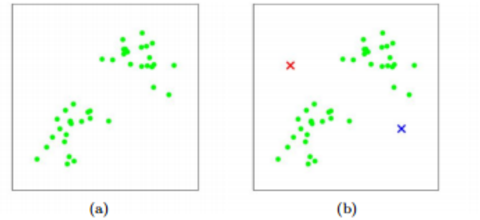

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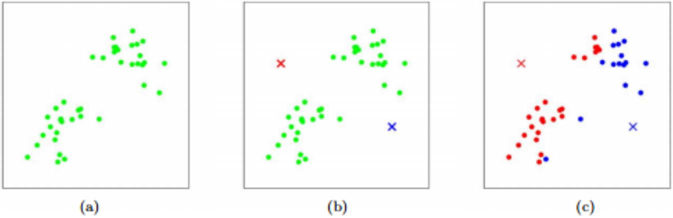

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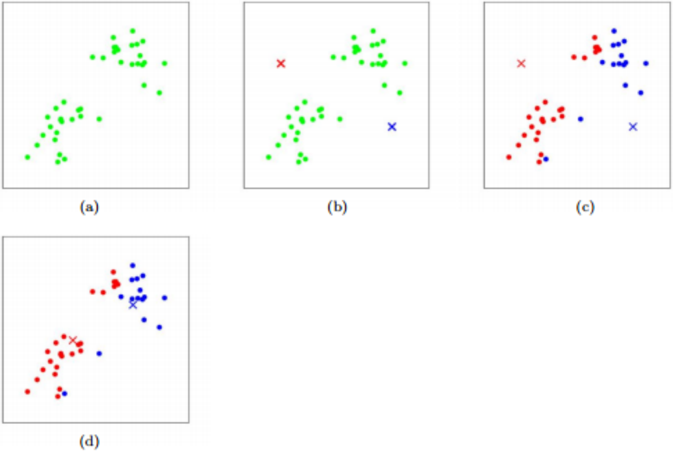

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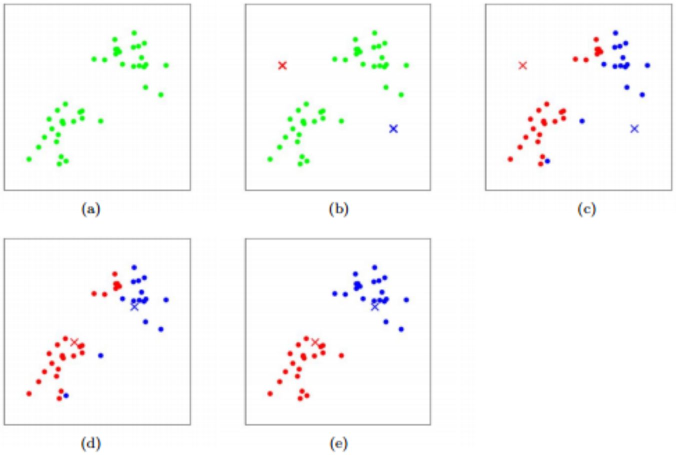

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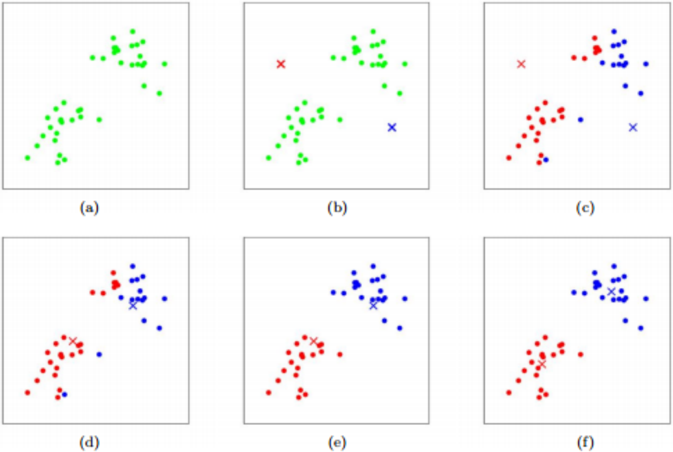

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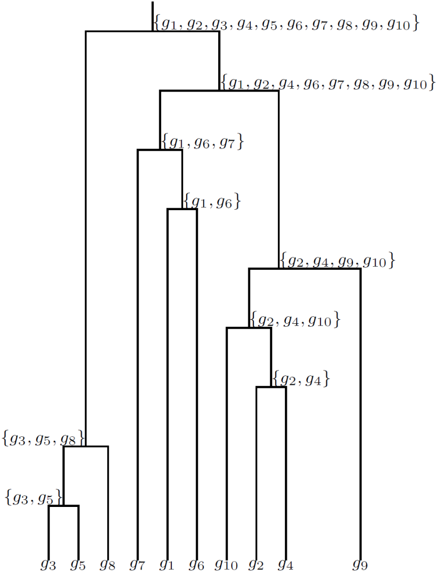
Termination: Check if the cluster assignment does not change anymore, or if centroids stop moving significantly.

Hierarchical clustering



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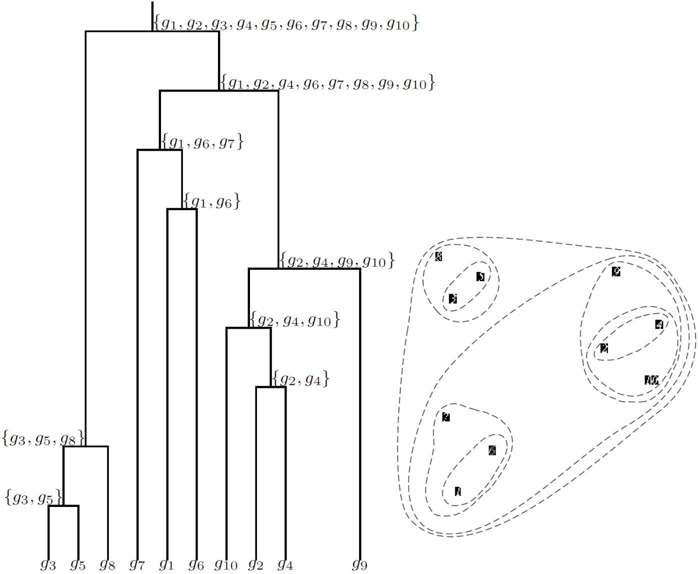

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- In general, the i-th cluster combines the two closest clusters from the $(i-1)$-th cluster.

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At the end, we have one large cluster that contains all the others.

Exercises

Implement the k-means clustering algorithm.

Test for different values of k with the given data (see course webpage).

Send me your code + some screenshots of your results.

Suggested reading

Chapters 10.1, 10.2 and 10.3 of:

“An Introduction to Bioinformatics Algorithms”, Jones and Pevzner