Some thoughts on cluster benchmarking

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November 8, 2011

The IFCS cluster benchmarking task force

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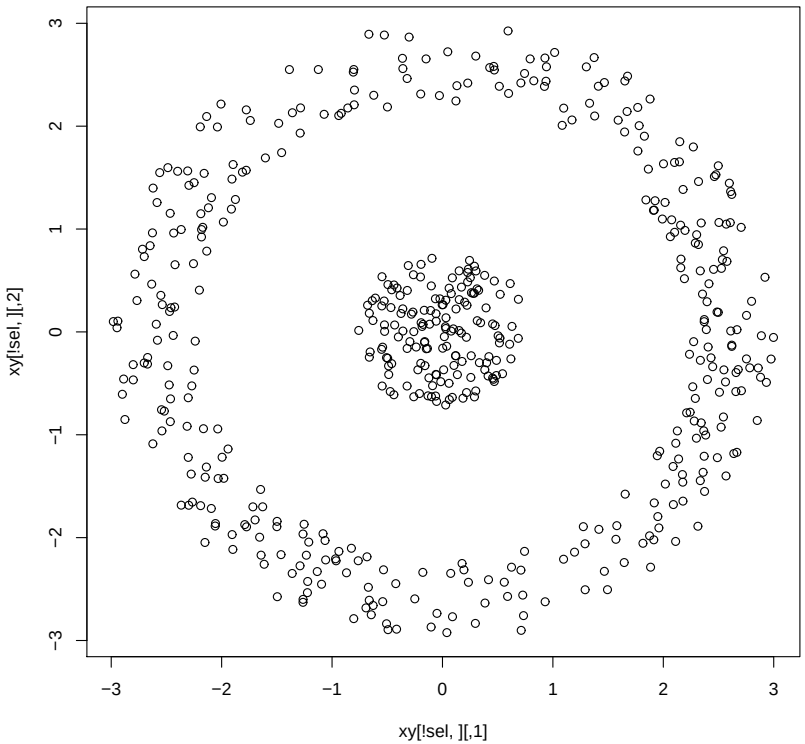
Datasets with known classes deviate *systematically* from real clustering problems.

Stupid cluster benchmarking

"*k*-means cannot do this properly!"



Benchmarking approaches

- Real datasets with known classes
- Simulated datasets (from mixture distributions?)
- Real datasets *without* known classes

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- Datasets?
- Competitors?
- Quality measurement?

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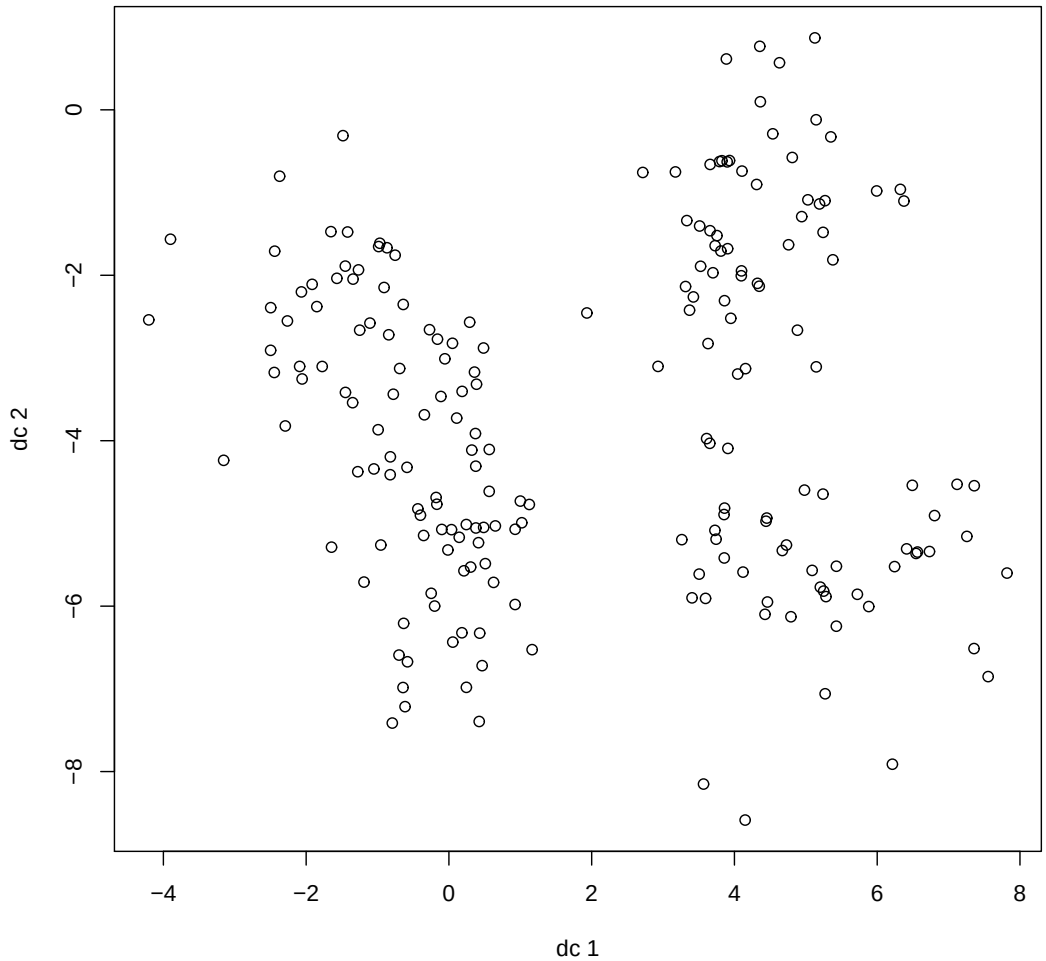
Known classes may *not* cluster in any data analytic sense.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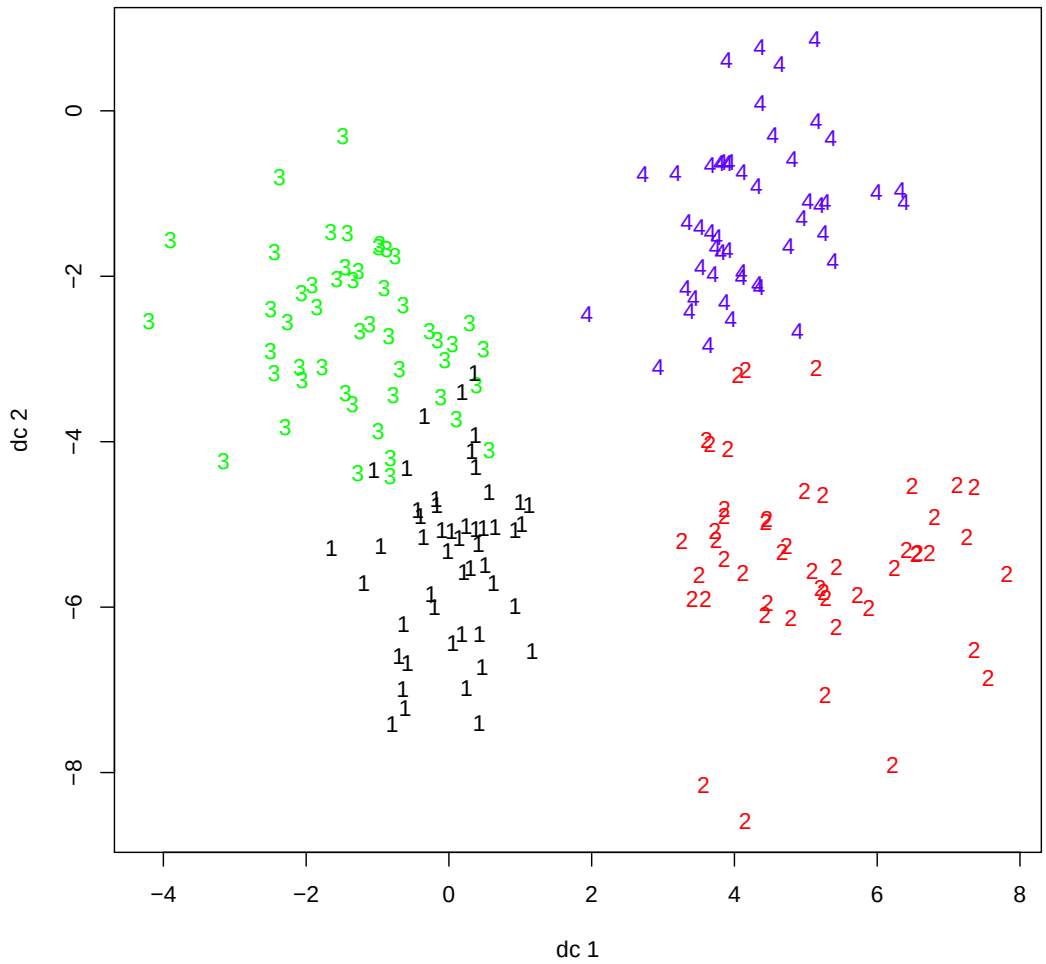
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Performance in datasets with known classes
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Therefore, for benchmarking not only datasets,
but also data analytic characteristics of classes should be presented.

Everybody who comes up with a new method
should be able to come up with an example
where one could think that the method could be applied,
and where it fails (with given reasons).

If you cannot do this, you don’t understand your own method.

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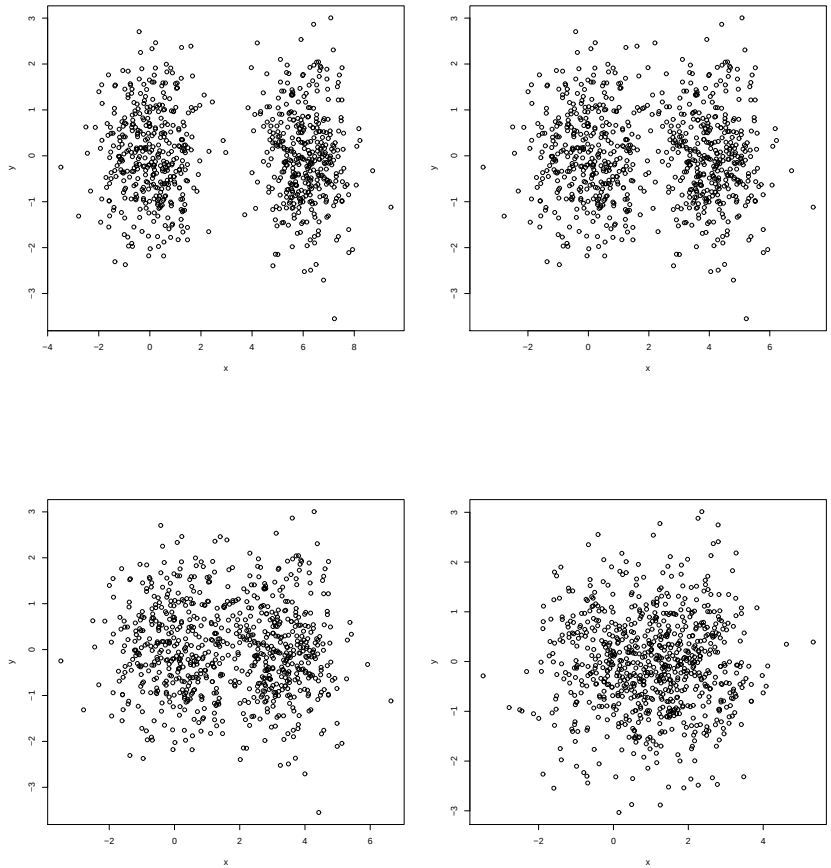
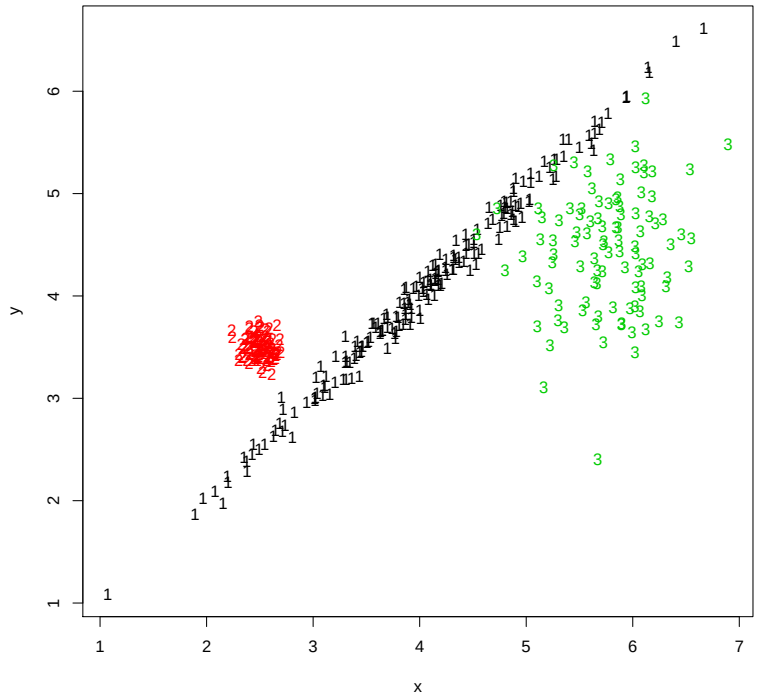
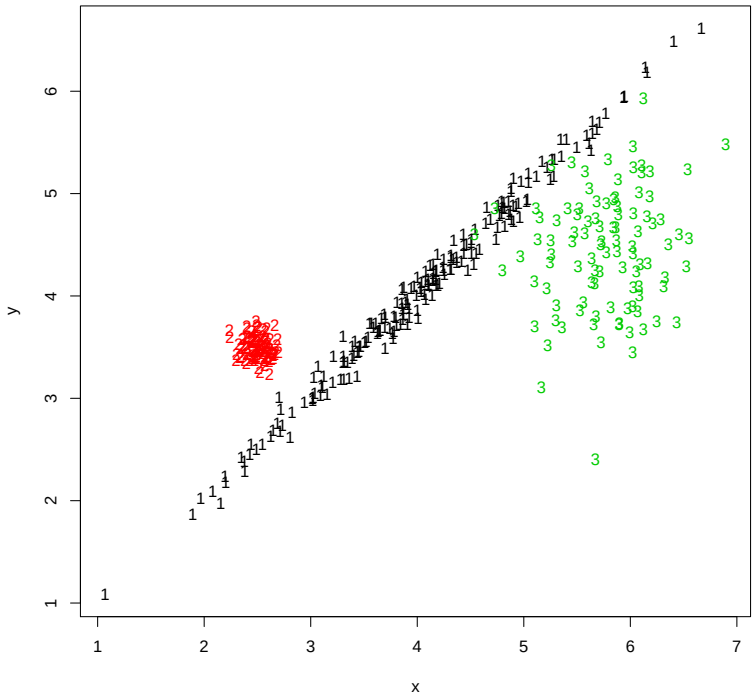
- A mixture of several Gaussians can be a single cluster (depending on what is meant by “a cluster”).
- Does a t-distribution qualify as “cluster shaped”? An exponential?

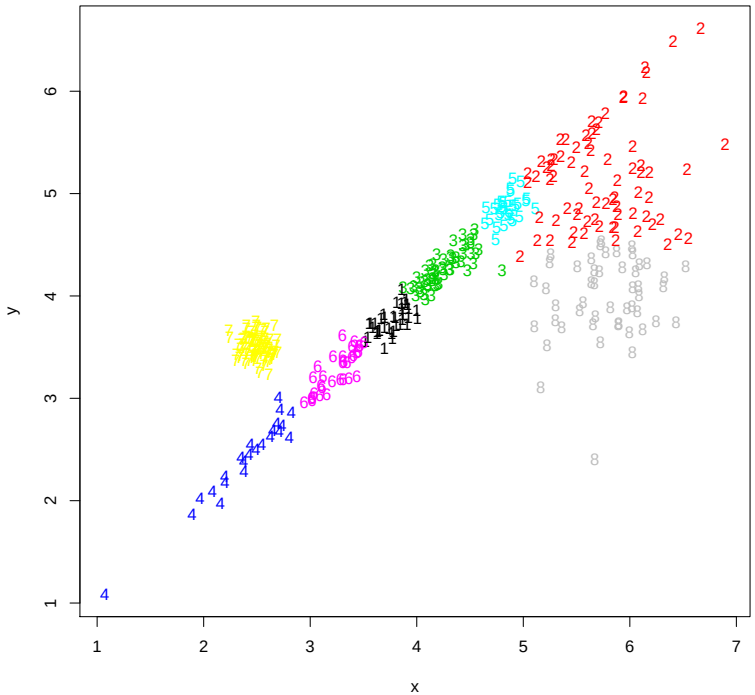

x
y

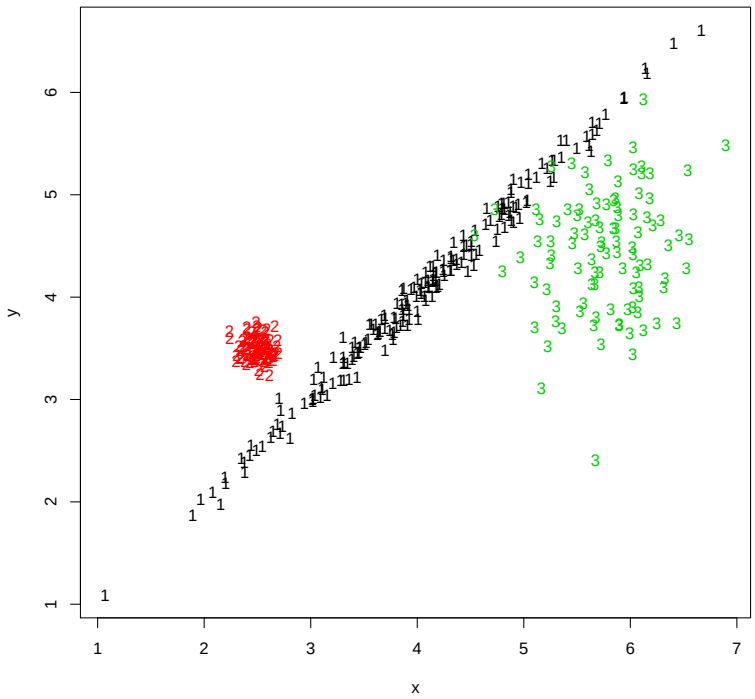
$$f(\mathbf{x}) = \sum_{i=1}^{k} \pi_i \varphi_{\mathbf{a}_i, \Sigma_i}(\mathbf{x})$$

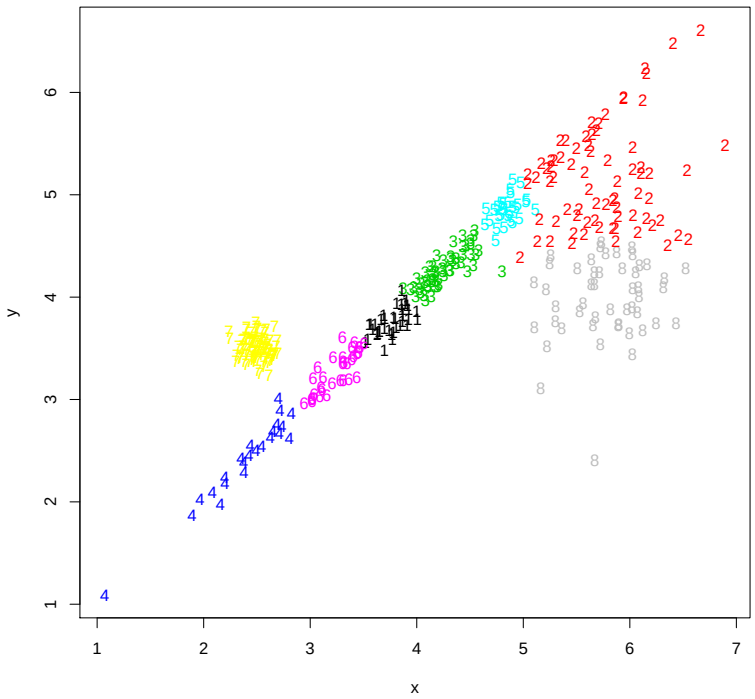


$f(\mathbf{x}) = \sum_{i=1}^{k} \pi_i \varphi_{\mathbf{a}_i, \Sigma_i}(\mathbf{x})$ - Σ_i diagonal?









Even if the true model yields visible clusters,
these are not necessarily the clusters of interest.

However, to know the performance of methods on simulated data is certainly useful for their characterisation and understanding.

Real datasets without known classes

Most clearly connected to real clustering tasks.

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Major issue: measurement of quality.
Misclassification rate won't work.

Information about clustering aim would be good,
but this is often difficult to connect to quality measurement.

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Need to be connected to clustering aims.

Benchmarking should not be ranking!

Methods need to be characterised in multidimensional ways:

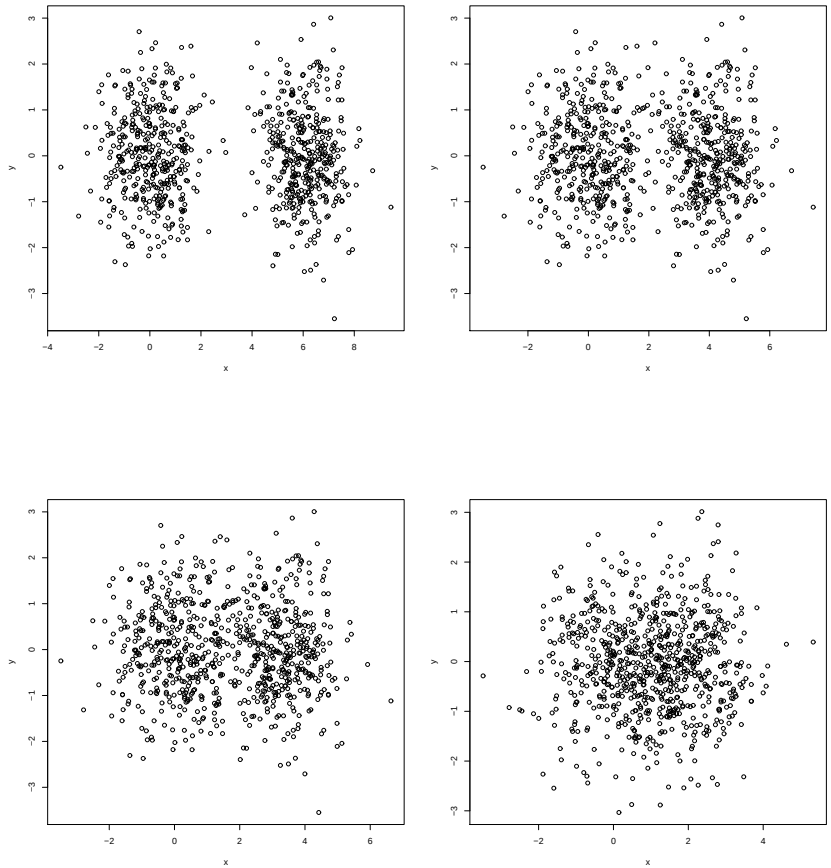
- Separation vs. homogeneity
- Cluster shapes (spherical/elliptical/skew/nonlinear)
- Small subgroups/outliers
- Stability/consistency
- Implicit similarity concept

New methods should come with specific (nontrivial) claims, and should be tested against these.

Competitors should be chosen suitable for the same aims.

Benchmarking datasets need to be documented so that it is clear for what specific claims they are relevant.

Results may not be interpreted on 1-d quality scale.



Find three clusters!