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Real datasets with known classes
Simulated datasets
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Benchmarking should not be ranking

Some thoughts on cluster benchmarking

Christian Hennig

November 8, 2011
The IFCS cluster benchmarking task force
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Isn’t it what the AG DA-NK is doing anyway?
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Is there a “UCI”-approach to clustering?

Is the UCI-approach really good for *supervised* classification?

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
Benchmarks approaches

- Real datasets with known classes
- Simulated datasets (from mixture distributions?)
- Real datasets *without* known classes
- Datasets?
- Competitors?
- Quality measurement?
Real datasets with known classes

That’s not the real situation of clustering (except if the dataset had been clustered before the “true” classes became known).
Real datasets with known classes

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The existence of known “true” classes doesn’t preclude the existence of other “true” unknown classes.
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Unions and parts of known classes may qualify (i.e., there are “communities”, “species”, “subspecies” in biology).
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Known classes may not cluster in any data analytic sense.
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Just checking misclassification rates doesn’t teach us much about the characteristics of the method.
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Performance in datasets with known classes still *is* legitimate as a quality indicator, but it would be helpful to connect success or failure to the characteristics of the data and classes, so that something can be learned.
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Performance in datasets with known classes still is legitimate as a quality indicator, but it would be helpful to connect success or failure to the characteristics of the data and classes, so that something can be learned.

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.
Simulated datasets (from mixture distributions)

This is less straightforward than most people think.

- It must be “mixtures of cluster-shaped distributions” - in general, mixture/non-mixture is not a proper classification of distributions.
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- Does a \( t \)-distribution qualify as “cluster shaped”? An exponential?
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\[ f(\mathbf{x}) = \sum_{i=1}^{k} \pi_i \varphi_{a_i, \Sigma_i}(\mathbf{x}) \]
$f(x) = \sum_{i=1}^{k} \pi_i \varphi_{a_i, \Sigma_i}(x) - \Sigma_i$ 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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Validation indexes measure certain aspects of clustering, and this is relevant if somebody claims that her new method fulfills this aspect.
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Validation indexes measure certain aspects of clustering, and this is relevant if somebody claims that her new method fulfills this aspect.

Need to be connected to clustering aims.
Benchmarks 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.
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Find three clusters!