Clustering Genetic Algorithm

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Outline

Motivation

Goals

- study applicability of GAs to clustering
- design genetic operators suitable for clustering
- application to tasks with unknown number of clusters
- compare to standard techniques

Clustering

- partitioning of a data set into subsets - clusters, so that the data in each subset share some common trait
- often based on some similarity or distance measure
- the notion of similarity is always problem-dependent.
- wide range of algorithms (k-means, SOMs, etc.)

Clustering

Definition of cluster

- Basic idea: cluster groups together similar objects
- More formally: clusters are connected regions of a multi-dimensional space containing a relatively high density of points, separated from other such regions by an low density of points

Applications

- Marketing - find groups of customers with similar behaviour
- Biology - classify of plants/animals given their features
- WWW - document classification, clustering weblog data to discover groups of similar access patterns

Genetic algorithms

Genetic algorithms

- stochastic optimization technique
- applicable on a wide range of problems
- work with population of solutions - individuals
- new populations produced by genetic operators

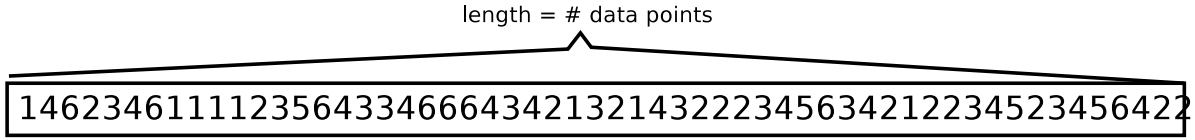
Genetic operators

- selection - the better the solution is the higher probability to be selected for reproduction
- crossover - creates new individuals by combining old ones
- mutation - random changes

Clustering Genetic Algorithm (CGA)

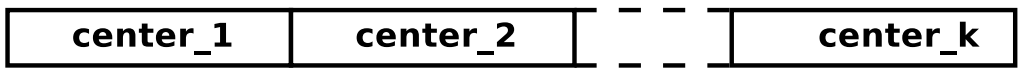
Representation of the individual

- 1. approach (Hruschka, Campelo, Castro)
  - for each data point store cluster ID



  - long individuals (high space requirements)

- 2. approach (Maulik, Bandyopadhyay)
  - store centres of the clusters



  - need to assign data points to clusters before each fitness evaluation

Fitness

Normalization

- partition the data set into clusters using the given individual
- move the centres to the actual gravity centres

Fitness evaluation

- clustering error: $fit(I) = -E_{VQ}$

$$E_{VQ} = \sum_{i=1}^{K} ||\vec{x_i} - \vec{c}_{f(x_i)}||^2, \qquad f(\vec{x_i}) = \arg\min_k ||\vec{x_i} - \vec{c}_k||^2$$

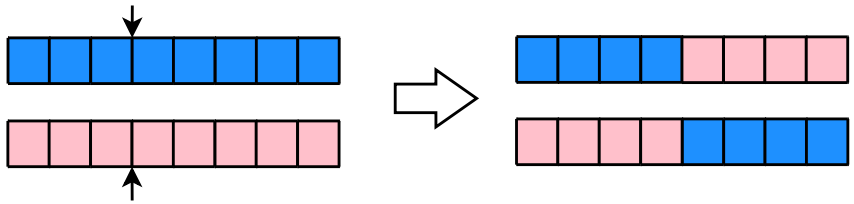
- silhouette function: $fit(i) = \sum_{i=1}^{N} s(\vec{x_i})$

$$s(\vec{x}) = \frac{b(\vec{x}) - a(\vec{x})}{max\{b(\vec{x}), a(\vec{x})\}}$$

Crossover

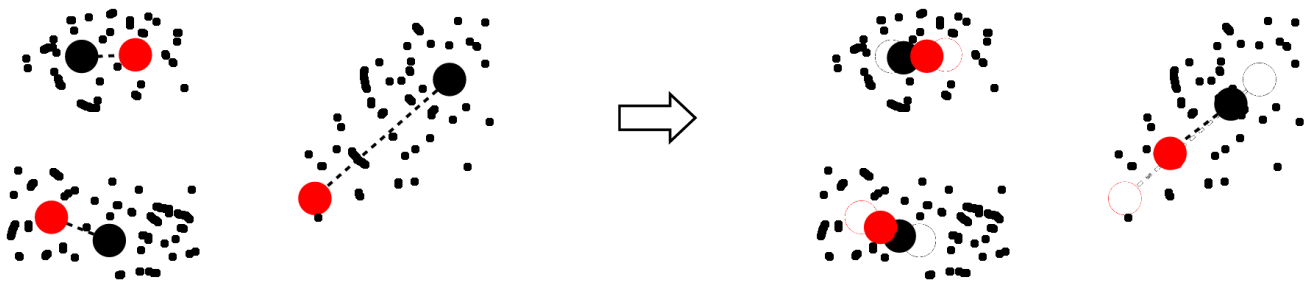
One-point Crossover

- exchange the whole blocks (i.e. centres)



Combining Crossover

- match the centres and combine them



Mutation

One-point mutation, Biased one-point mutation

- One-point Mutation:
  $\vec{c}_{new} = \vec{x}_i$, where $i \leftarrow random(1, N)$
- Bias one-point Mutation:
  $\vec{c}_{new} = \vec{c}_{old} + \vec{\Delta}$, where $\vec{\Delta}$ is a random small vector

K-means mutation

- several steps of k-means clustering

Cluster addition, Cluster removal

- *Cluster Addition* – adds one centre
- *Cluster Removal* – removes randomly selected centre

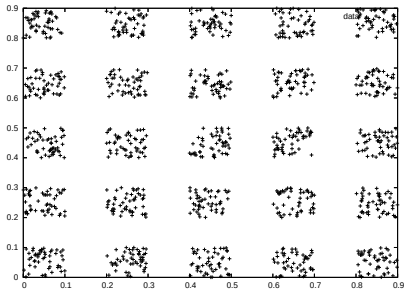
Experiments

Goals

- demonstrate the performance of CGA
- compare variants of genetic operators

Data Sets

- **25 centres**



- **vowels** (UCI machine learning repository)

  11 kinds of vowels, dimension 9
  990 examples

- **mushrooms** (UCI machine learning repository)

  23 kinds of mushrooms, dimension 125
  8124 examples

Operators Comparison

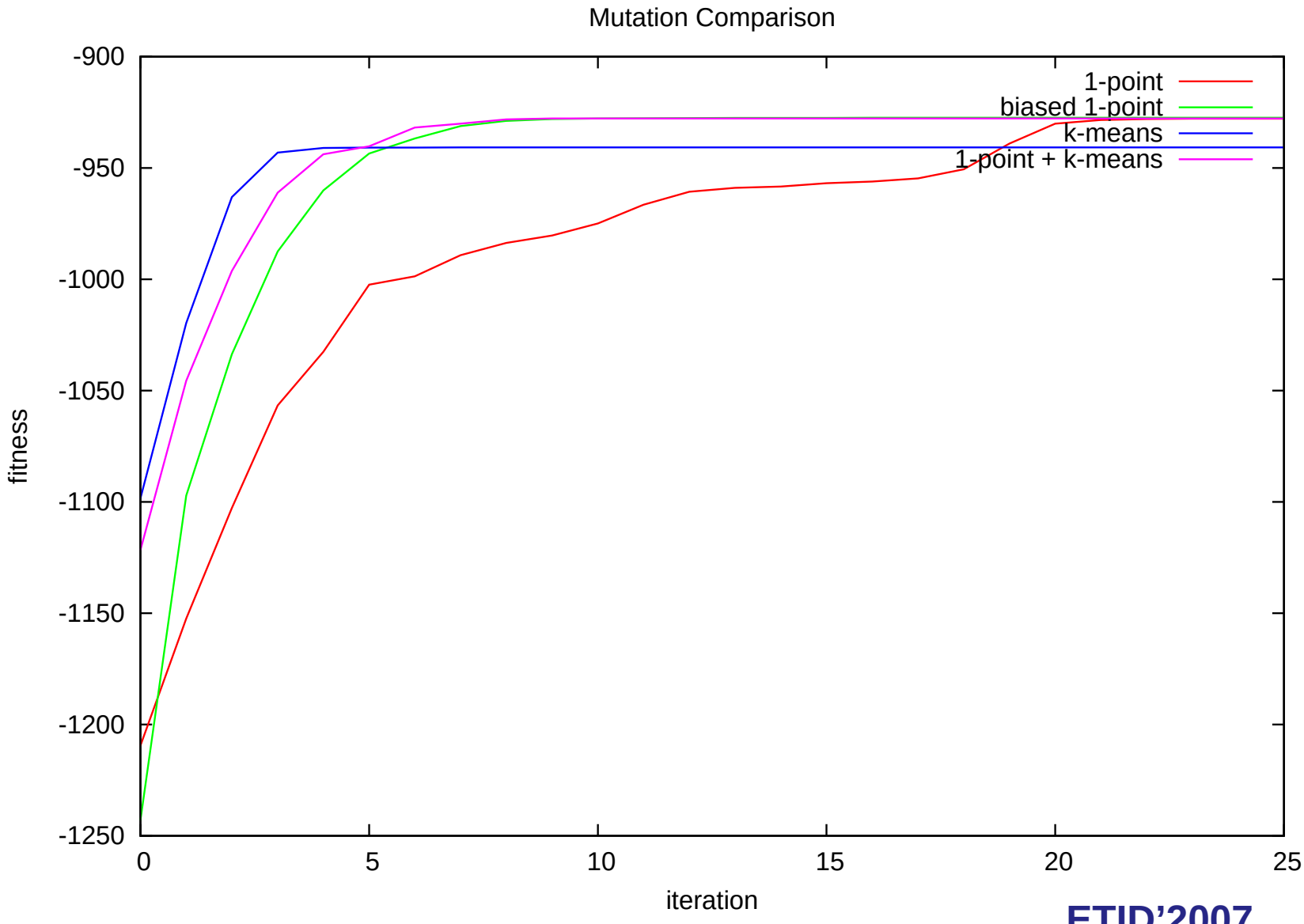
Mutation

	25clusters	Vowels
1-point	0.20	927.7
Biased 1-point	0.25	927.3
K-means	0.26	940.7
1-point + Biased 1-pt	0.21	927.3
1-point + K-means	0.21	927.6
All	0.22	927.3

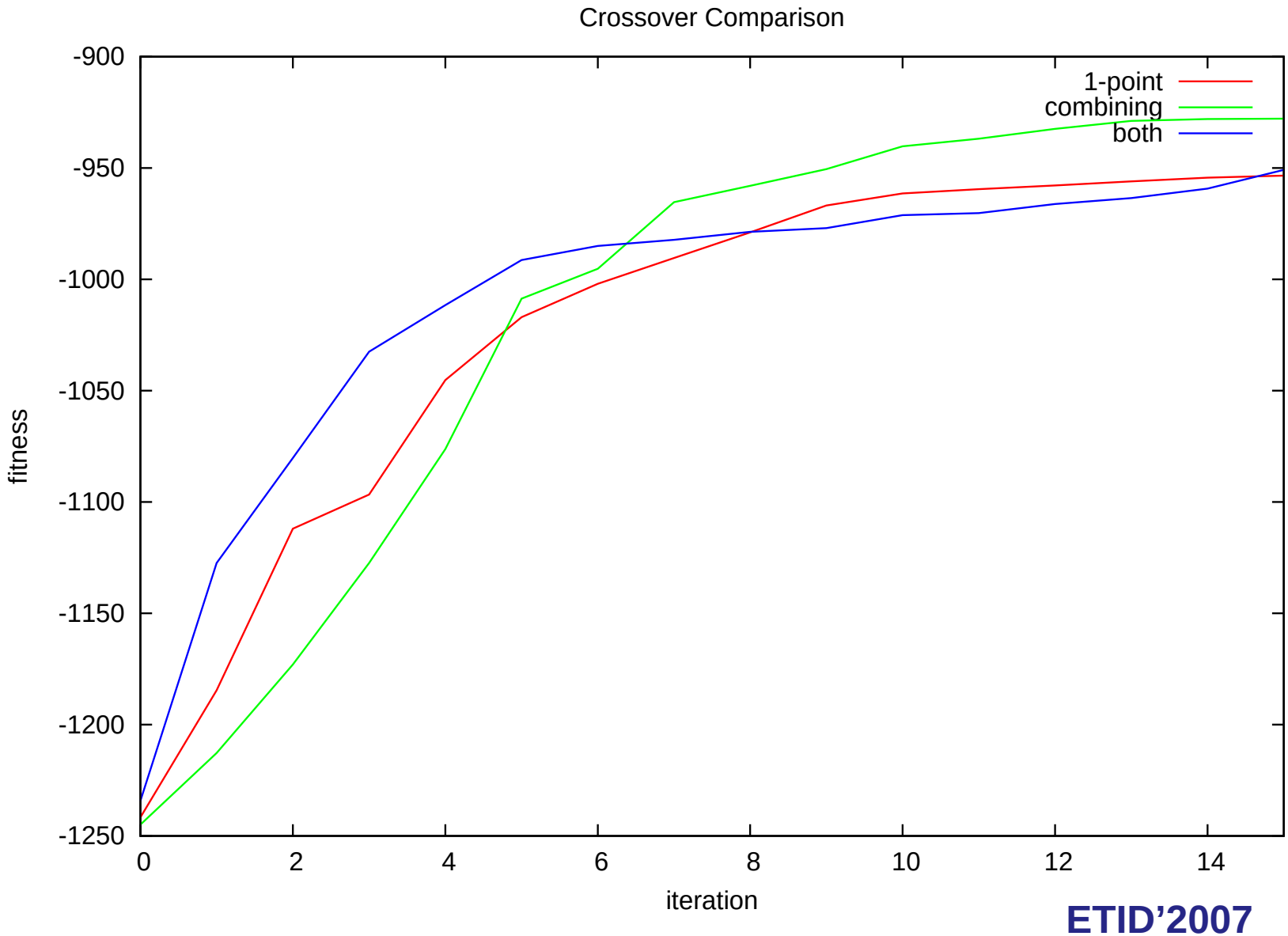
Crossover

	25clusters	Vowels
1-point	0.201	927.7
Combining	0.222	927.4
Both	0.202	927.4

Convergence Rate – Mutation



Convergence Rate – Crossover



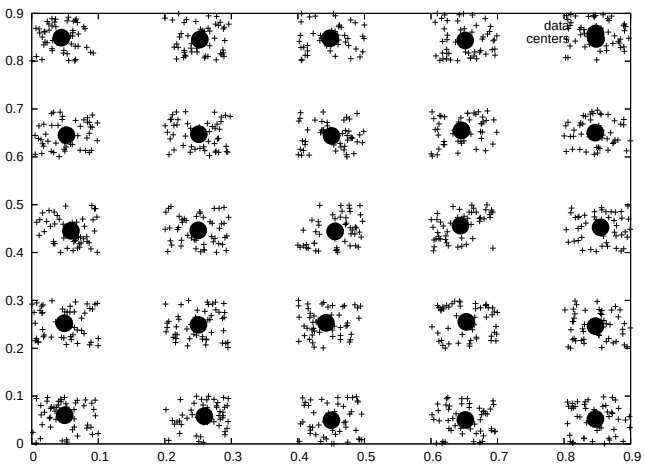
Comparison to other clustering algorithms

Mushroom data set

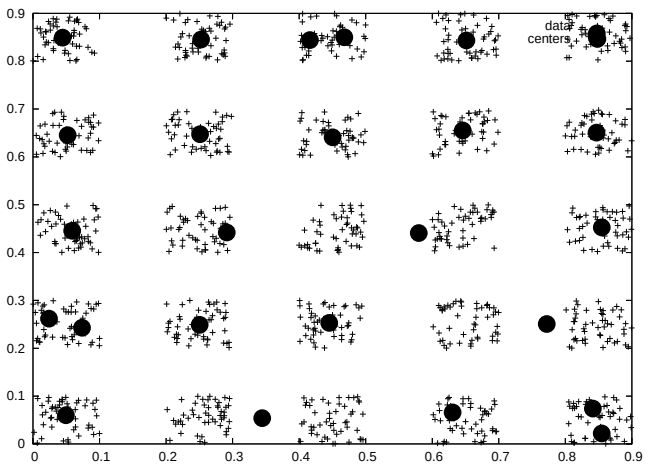
method	accuracy
k-means	95.8%
CLARA	96.8%
CGA	97.3%
HCA	99.2%

25 centers

CGA

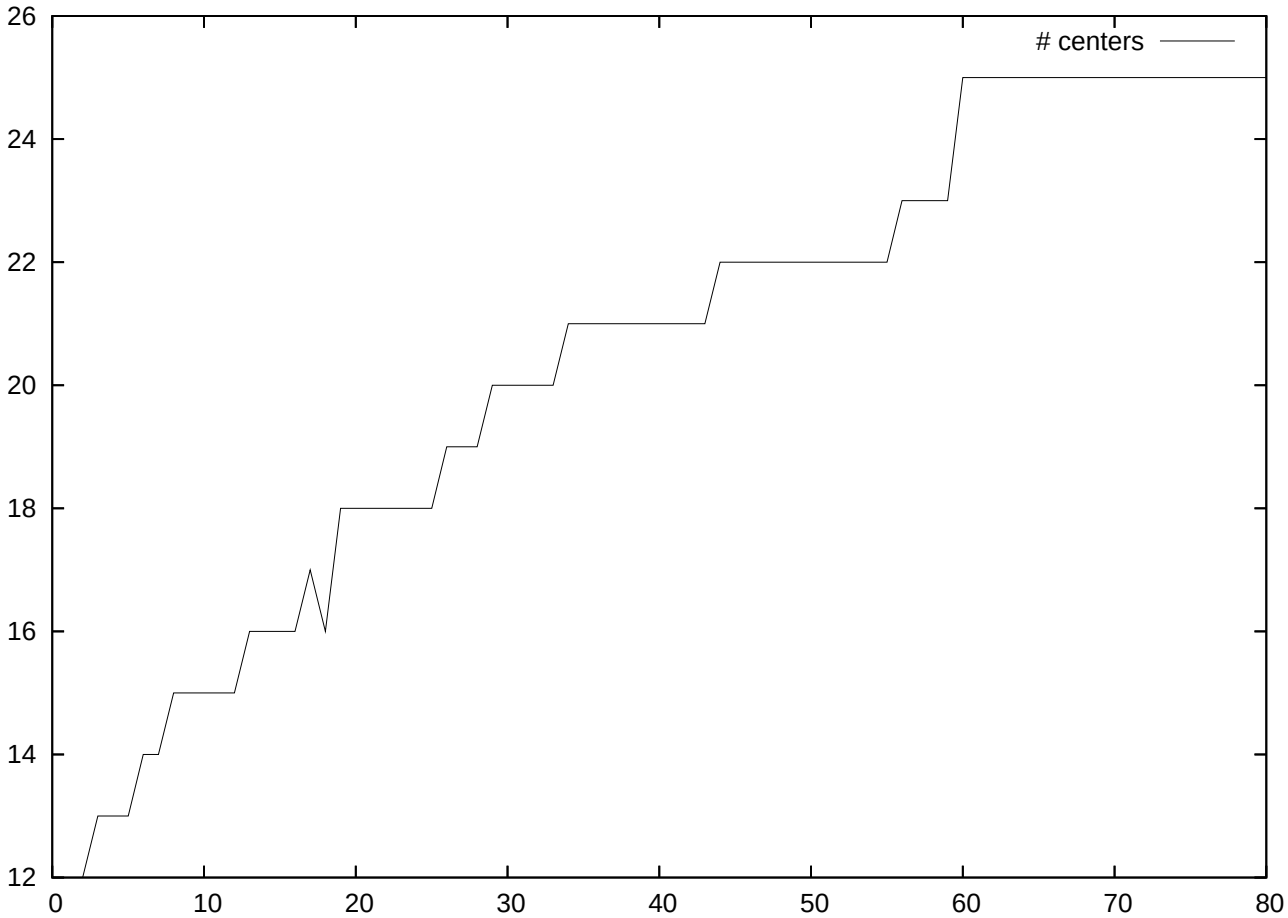


k-means



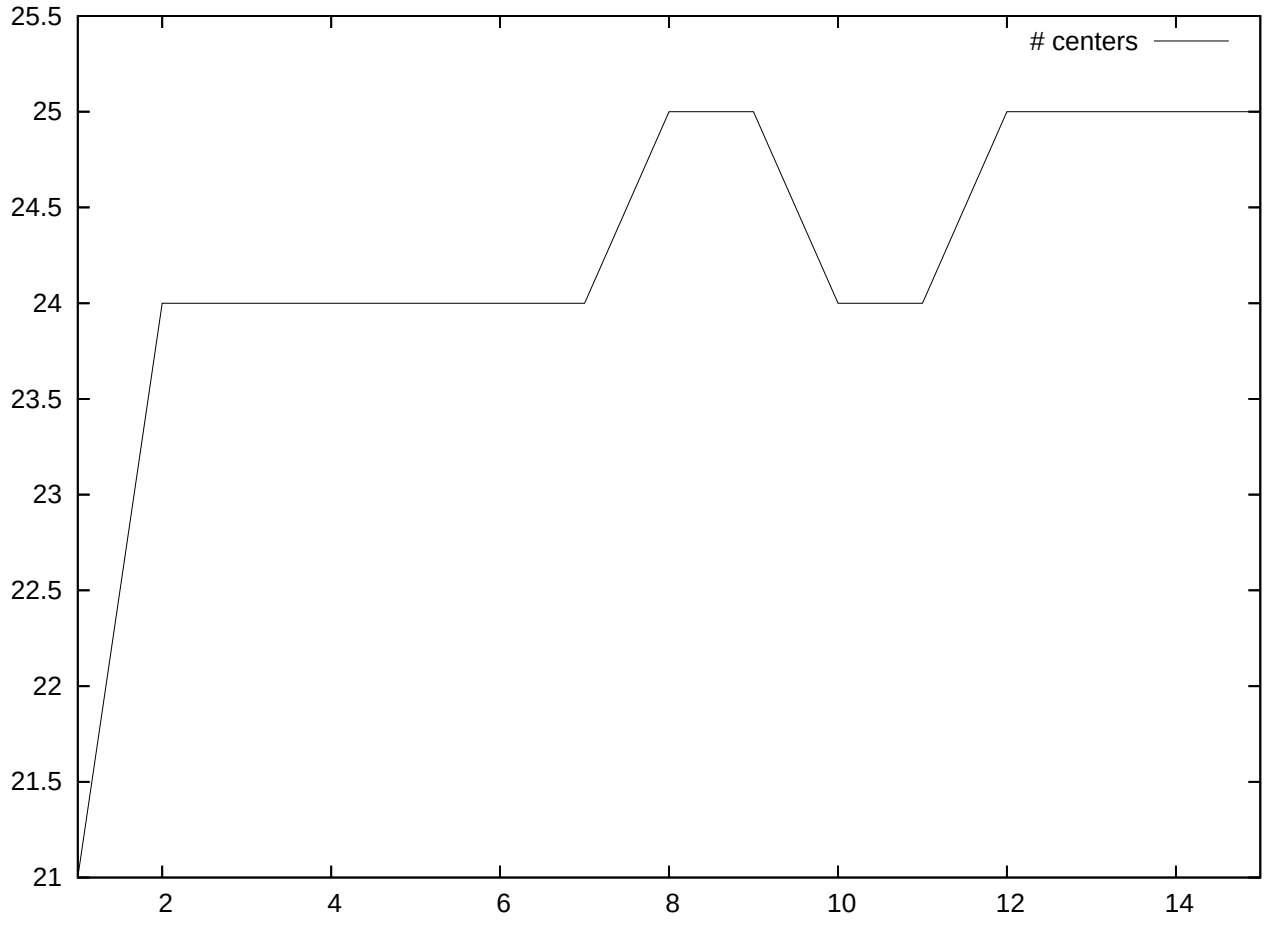
Estimating the number of clusters

Initial population: 2 to 15 centres



Estimating the number of clusters

Initial population: 10 to 30 centres



Conclusion

Summary

- *Clustering Genetic Algorithm* proposed
- several genetic operators proposed and compared
- CGA compared to available clustering algorithms
- estimating the number of clusters tested

Future work

- application of CGA to large data sets
- reducing time requirements, lazy evaluations, etc.
- applications

Thank you.
Any questions?