Recent Advances in Model-Based Clustering: Image Segmentation and Variable Selection

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• Variable/feature selection for model-based clustering

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- Automatic numerical methods for finding groups in data that are
 - separated
 - internally cohesive
- Invented in the 1950s by Sokal, Sneath and others motivated by
 - biological taxonomy
 - market segmentation
- Interest now driven by new types of data:
 - Gene expression microarray data
 - finding groups and patterns in retail barcode data
 - datamining more generally
 - $\bullet\,$ analysis of Web data (finding groups of users and sites) $\longrightarrow\,$ Collaborative filtering
 - medical image segmentation, e.g. for finding tumors. Here, cluster = group of pixels
 - color image quantization (e.g. for the Internet on mobile phones)
 - automatic document clustering for technical documents and Web sites

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• Most methods heuristic or algorithmic, not statistical, for example:

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• complete link clustering

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- complete link clustering
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- single link clustering
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- Model-based clustering:
 - A framework for cluster analysis
 - Bases cluster analysis on a statistical (mixture) model: $y \sim \sum_{g=1}^{G} \tau_g f_g(y)$, where y is data and $f_g(\cdot)$ are distributions

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Cluster Analysis Methods

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- Model-based clustering:
 - A framework for cluster analysis
 - Bases cluster analysis on a statistical (mixture) model:
 - $y \sim \sum_{g=1}^{G} \tau_{g} f_{g}(y)$, where y is data and $f_{g}(\cdot)$ are distributions
 - Gives answers to questions based on standard statistical principles
 - $\bullet\,$ Here we focus on continuous data and take $f_g \sim$ multivariate normal

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• Based on a finite mixture of multivariate normal distributions:

$$y_i \sim \sum_{g=1}^{G} \tau_g \mathrm{MVN}_d(\mu_g, \Sigma_g),$$

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• where $\Sigma_g = \lambda_g D_g A_g D_g^T$

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• $\lambda_g = 1$ st eigenvalue of Σ_g : controls the *volume* of the *g*th cluster

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- λ_g = 1st eigenvalue of Σ_g: controls the *volume* of the gth cluster
 A_g = diag{1, α_{2g},..., α_{dg}}

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• $A_g = \text{diag}\{1, \alpha_{2g}, \dots, \alpha_{dg}\}$

• controls the *shape* of the *g*th cluster

• Based on a finite mixture of multivariate normal distributions:

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$$A_g = \text{diag}\{1, \alpha_{2g}, \dots, \alpha_{dg}\}$$

- controls the *shape* of the *g*th cluster
- $(1 \ge \alpha_2 \ge \ldots \ge \alpha_d > 0)$

• Based on a finite mixture of multivariate normal distributions:

$$y_i \sim \sum_{g=1}^{G} \tau_g \mathrm{MVN}_d(\mu_g, \Sigma_g),$$

- where $\Sigma_g = \lambda_g D_g A_g D_g^T$
- $\lambda_g = 1$ st eigenvalue of Σ_g : controls the *volume* of the *g*th cluster

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- D_g = Eigenvectors: Control the *orientation* of the *g*th cluster
- Different clustering models can be obtained by constraining each of *volume, shape* and *orientation* to be constant across clusters, or by allowing them to vary (Banfield & Raftery, 1993, *Biometrics*)

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 $BIC = 2 \log \max(n) \log(n)$

• This is consistent for the number of clusters (Keribin 2000), and also provides consistent density estimates (Roeder and Wasserman 1997).

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• Data: Glucose, insulin and SSPG measurements on 145 patients (Reuven and Miller 1979).

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- Data: Glucose, insulin and SSPG measurements on 145 patients (Reuven and Miller 1979).
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• Many clustering methods require that we "know" the number of clusters, but model-based clustering does not.

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Glucose



• We know the "right" model:

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- We know the "right" model:
 - The volume (Normal: small; Diabetes clusters: bigger)

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- We know the "right" model:
 - The volume (Normal: small; Diabetes clusters: bigger)
 - shape (Normal: spherical, Diabetes clusters: long and thin)

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- We know the "right" model:
 - The volume (Normal: small; Diabetes clusters: bigger)
 - shape (Normal: spherical, Diabetes clusters: long and thin)
 - and orientation (Chemical and Overt: orthogonal)



- We know the "right" model:
 - The volume (Normal: small; Diabetes clusters: bigger)
 - shape (Normal: spherical, Diabetes clusters: long and thin)
 - and orientation (Chemical and Overt: orthogonal)

• are all different



- We know the "right" model:
 - The volume (Normal: small; Diabetes clusters: bigger)
 - shape (Normal: spherical, Diabetes clusters: long and thin)
 - and orientation (Chemical and Overt: orthogonal)

are all different

• \implies Model is Σ_g all different (unconstrained)
Diabetes Data



- We know the "right" model:
 - The volume (Normal: small; Diabetes clusters: bigger)
 - shape (Normal: spherical, Diabetes clusters: long and thin)
 - and orientation (Chemical and Overt: orthogonal)
 - are all different
- \implies Model is Σ_g all different (unconstrained)
- The mclust R package is used

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BIC plot for diabetes data



Number of components

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BIC plot for diabetes data



• Model code:

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BIC plot for diabetes data

- Model code:
 - Letters refer to (Volume, Shape, Orientation):

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BIC plot for diabetes data

- Model code:
 - Letters refer to (Volume, Shape, Orientation):
 - E: Equal across clusters

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BIC plot for diabetes data

- Model code:
 - Letters refer to (Volume, Shape, Orientation):
 - E: Equal across clusters
 - V: Vary across clusters

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Number of components

BIC plot for diabetes data

- Model code:
 - Letters refer to (Volume, Shape, Orientation):
 - E: Equal across clusters
 - V: Vary across clusters

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• I: Identity (spherical) covariance matrix

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BIC plot for diabetes data

Number of components

- Model code:
 - Letters refer to (Volume, Shape, Orientation):
 - E: Equal across clusters
 - V: Vary across clusters
 - I: Identity (spherical) covariance matrix
 - Example: **EEV**: Equal volume, equal shape, varying orientations

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 BIC chooses the unconstrained (VVV) model with 3 clusters.

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- BIC chooses the unconstrained (VVV) model with 3 clusters.
- The right answer!

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Zoomed BIC plot for diabetes data

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- The right answer!

• The EII model, $\Sigma_g = \lambda I \ (\approx k \text{ means})$ not good.

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Zoomed BIC plot for diabetes data

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 - Thus *k* means would not be good for these data.

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- BIC chooses the unconstrained (VVV) model with 3 clusters.
- The right answer!



Zoomed BIC plot for diabetes data

- The EII model, $\Sigma_g = \lambda I \ (\approx k \text{ means})$ not good.
 - Thus *k* means would not be good for these data.
 - BIC allows us to assess when k means, or other methods, would work well.

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Zoomed BIC plot for diabetes data

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- The EII model, $\Sigma_g = \lambda I \ (\approx k \text{ means})$ not good.
 - Thus k means would not be good for these data.
 - BIC allows us to assess when k means, or other methods, would work well.
- Tradeoff between the clustering model and the number of clusters:

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 - Thus k means would not be good for these data.
 - BIC allows us to assess when k means, or other methods, would work well.
- Tradeoff between the clustering model and the number of clusters:
 - E.g. with the EII model (equal volume spherical), far more clusters are needed than with the VVV model (unconstrained ellipses).

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 - Thus k means would not be good for these data.
 - BIC allows us to assess when *k* means, or other methods, would work well.
- Tradeoff between the clustering model and the number of clusters:
 - E.g. with the EII model (equal volume spherical), far more clusters are needed than with the VVV model (unconstrained ellipses).
 - Thus BIC determines whether it is better to use the "peas" or the "pod."

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True Classification

Glucose



Mclust Classification: Error Rate 12%



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K means Classification: Error rate 18%





Mclust Classification: Error Rate 12%



K means Classification: Error rate 18%



Single Link Classification: Error rate 47%



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- This has good robustness properties (Hennig 2004, Ann Stat)

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• An alternative: Dynamic Magnetic Resonance Imaging (MRI):

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• Patient injected with a contrast agent, Gaudolinium

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- This has a high false positive rate, leading to
 - many unnecessary biopsies
 - unnecessary deaths
 - search for a better method
- An alternative: Dynamic Magnetic Resonance Imaging (MRI):
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 Bayesian morphology: Fast Bayesian image restoration via mathematical morphology (Forbes and Raftery 1999, JASA)

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Images at 10, 70, 150, 250 seconds



Images at 10, 70, 150, 250 seconds



Intensity curve for one voxel

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Intensity curve for one voxel

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Mclust segmentation with 4 clusters

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Mclust segmentation with 4 clusters

Bayesian morphology restoration

Breast MRI Results for 19 patients

Breast MRI Results for 19 patients

TABLE 2. Curve Type Versus Pathology Results for the 19 Patients

Curve Type	Number of Patients	Pathology Results
1 (benign)	6	5 benign, 1 unknown
2 (uncertain)	5	1 unknown, 4 cancer
3 (malignant)	8	8 cancer

Breast MRI Results for 19 patients

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Reference: Forbes et al, 2006, *J. Computer Assisted Tomography*, "Finding regions of interest in dynamic breast MRI."

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- Image segmentation with small features using incremental model-based clustering (Fraley et al, 2005, *J. Comput. Graph. Stat*)

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- Image segmentation with model-based clustering via sampling (Wehrens et al, 2004, *J. Classification*)
- Detecting features in spatial point patterns: minefields, earthquake faults (papers with Byers, Dasgupta, Walsh 1998–)

• Which variables to include in clustering?



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- General approach: Treat it as a model choice problem by vewing each combination of variables as a statistical model

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• Model for (Y_1, Y_2, Y_3) choice says that all 3 variables depend on which cluster the object is in

Variable Selection Method

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- Let Z be the matrix of (unobserved) variables that say which group each observation belongs to (as in EM and MCMC for mixtures)

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To Include or Not To Include $Y^{(?)}$? Here are the Models

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$$E(Y^{(?)} | Y^{(clust)}) = \alpha + Y^{(clust)}\beta$$

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- Thus each BIC is the sum of BICs for mixture models and possibly regression models.

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 - Inclusion and exclusion decisions are based on the approximate Bayes factors

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• We stop when two proposed changes in a row are rejected

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• First we look at an example where there are no noise variables present

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• First we look at an example where there are no noise variables present

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• Have two variables with clustering information



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- Have two variables with clustering information
- 150 observations



- First we look at an example where there are no noise variables present
- Have two variables with clustering information
- 150 observations
- The clusters are well separated with different variances

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- First we look at an example where there are no noise variables present
- Have two variables with clustering information
- 150 observations
- The clusters are well separated with different variances
- The method correctly selects both variables

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• Same 2 clustering variables as before

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• 5 noise variables added:



- Same 2 clustering variables as before
- 5 noise variables added:
 - X3, X4 and X5 are independent



- Same 2 clustering variables as before
- 5 noise variables added:
 - X3, X4 and X5 are independent
 - X6 and X7 are dependent



- Same 2 clustering variables as before
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• Compare clustering results:



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- Same 2 clustering variables as before
- 5 noise variables added:
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 - X6 and X7 are dependent
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Variables	# of	Error
	Groups	rate

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- Same 2 clustering variables as before
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Variables	# of	Error
	Groups	rate
All 7	5	44.7%

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Variables	# of	Error
	Groups	rate
All 7	5	44.7%
All 7	2 (constrained)	3.3%

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- 5 noise variables added:
 - X3, X4 and X5 are independent
 - X6 and X7 are dependent
- Compare clustering results:

Variables	# of	Error
	Groups	rate
All 7	5	44.7%
All 7	2 (constrained)	3.3%
Selected 2	2	0%

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• 4 groups: male orange, female orange, male blue and female blue

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- 4 groups: male orange, female orange, male blue and female blue
- 200 observations (50 per group)

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- 200 observations (50 per group)
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• Variables selected: 4 of the 5 variables were selected, all except length along mid-line of carapace (CL)

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- Compare clustering results:

Variables	# of	Error
	Groups	rate
All 5	7	42.5%

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- 200 observations (50 per group)
- 5 variables measuring size



- Variables selected: 4 of the 5 variables were selected, all except length along mid-line of carapace (CL)
- Compare clustering results:

Variables	# of	Error
	Groups	rate
All 5	7	42.5%
All 5	4	7.5%
	(constrained)	

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- 4 groups: male orange, female orange, male blue and female blue
- 200 observations (50 per group)
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- Variables selected: 4 of the 5 variables were selected, all except length along mid-line of carapace (CL)
- Compare clustering results:

Variables	# of	Error
	Groups	rate
All 5	7	42.5%
All 5	4	7.5%
	(constrained)	
Selected 4	4	7.5%

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• How many groups?

 Model-based clustering puts cluster analysis on a solid statistical basis and answers questions such as:

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- How many groups?
- Which clustering method to use?

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- How many groups?
- Which clustering method to use?
- How certain can we be about the clustering?

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 - Which clustering method to use?
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 - Variable selection: Raftery and Dean (2006, J. Amer. Statist. Ass.)

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• Website: www.stat.washington.edu/raftery

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