Data Wrangling and Data Analysis
Unsupervised learning:
Model-based clustering

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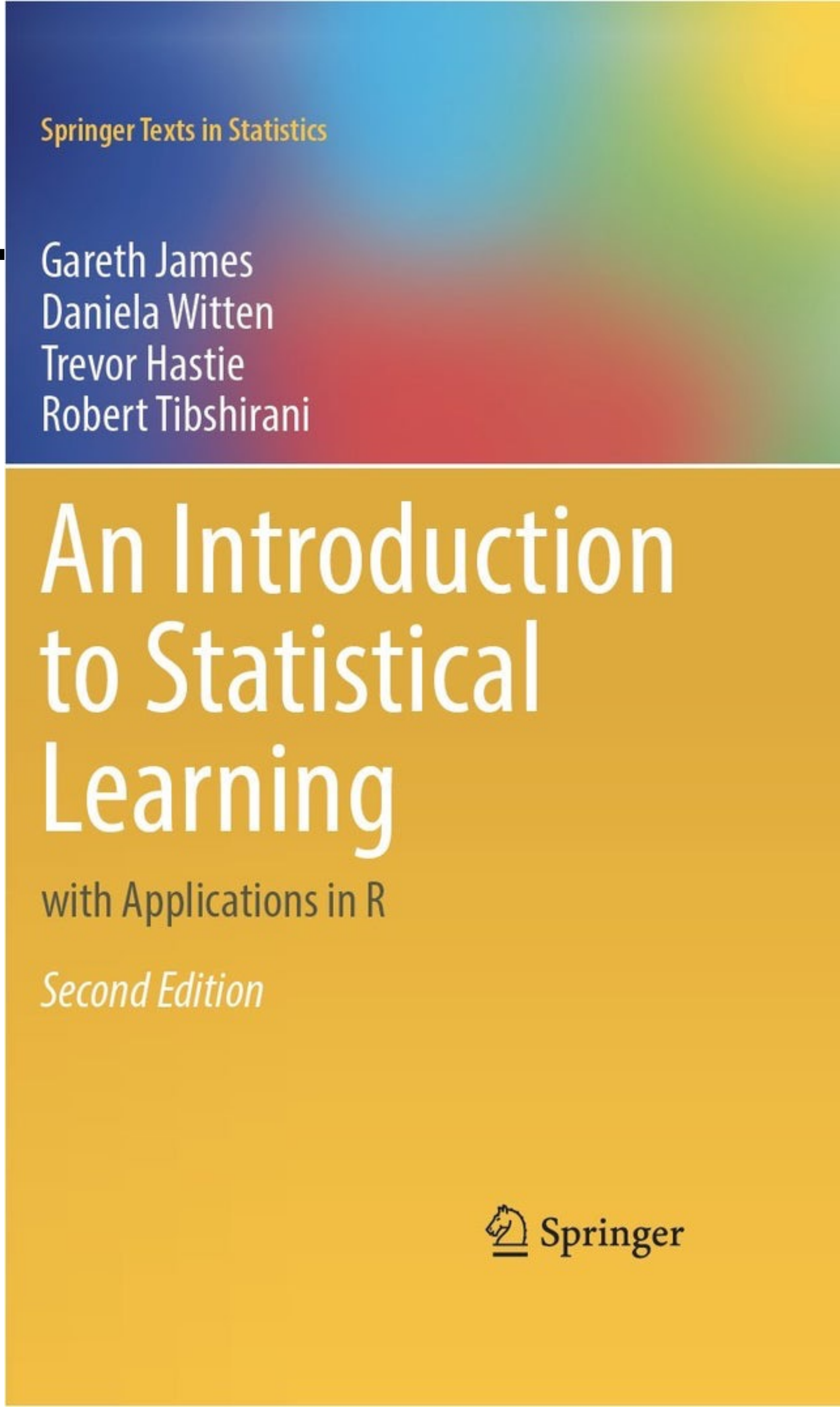
This week

- **Day 1: Clustering #2: Model-based clustering**
- Day 2: Text mining #1
- Day 3: Text mining #2

Reading materials about clustering (this week & nex

- Selected paragraphs from **Introduction to Statistical Learning (ISLR)** §12.1 and 12.4
- “Mixture models: latent profile and latent class analysis” [Oberski, 2016] §1, §2
  http://daob.nl/wp-content/papercite-data/pdf/oberski2016mixturemodels.pdf



Optional, much more in-depth material

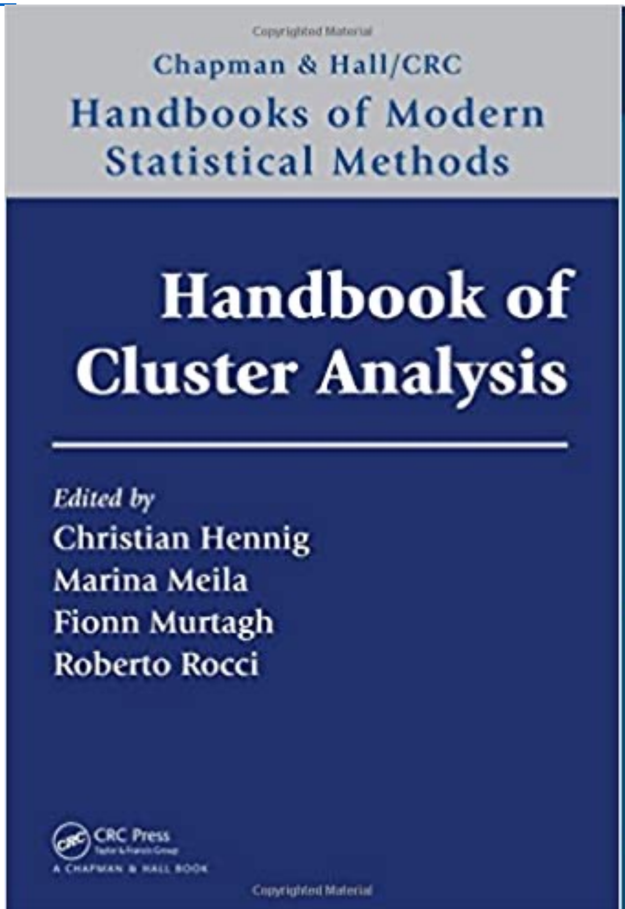
Clustering strategy and method selection (ch. 31),
[*https://arxiv.org/pdf/1503.02059.pdf*](https://arxiv.org/pdf/1503.02059.pdf)

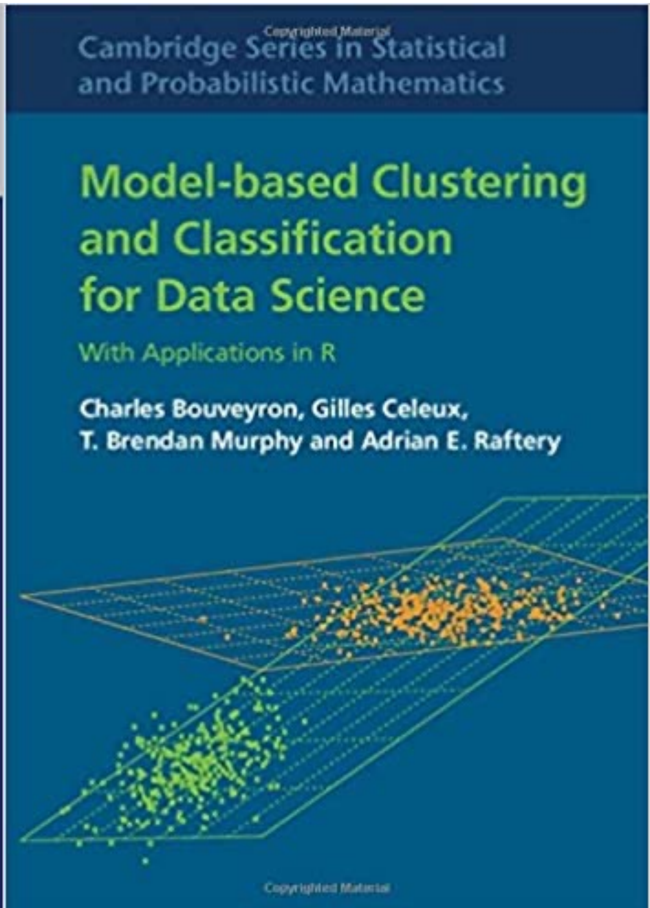
Handbook of Cluster Analysis

Hennig et al. (2016)

Model-based Clustering and Classification for Data Science

Bouveyron et al. (2018)





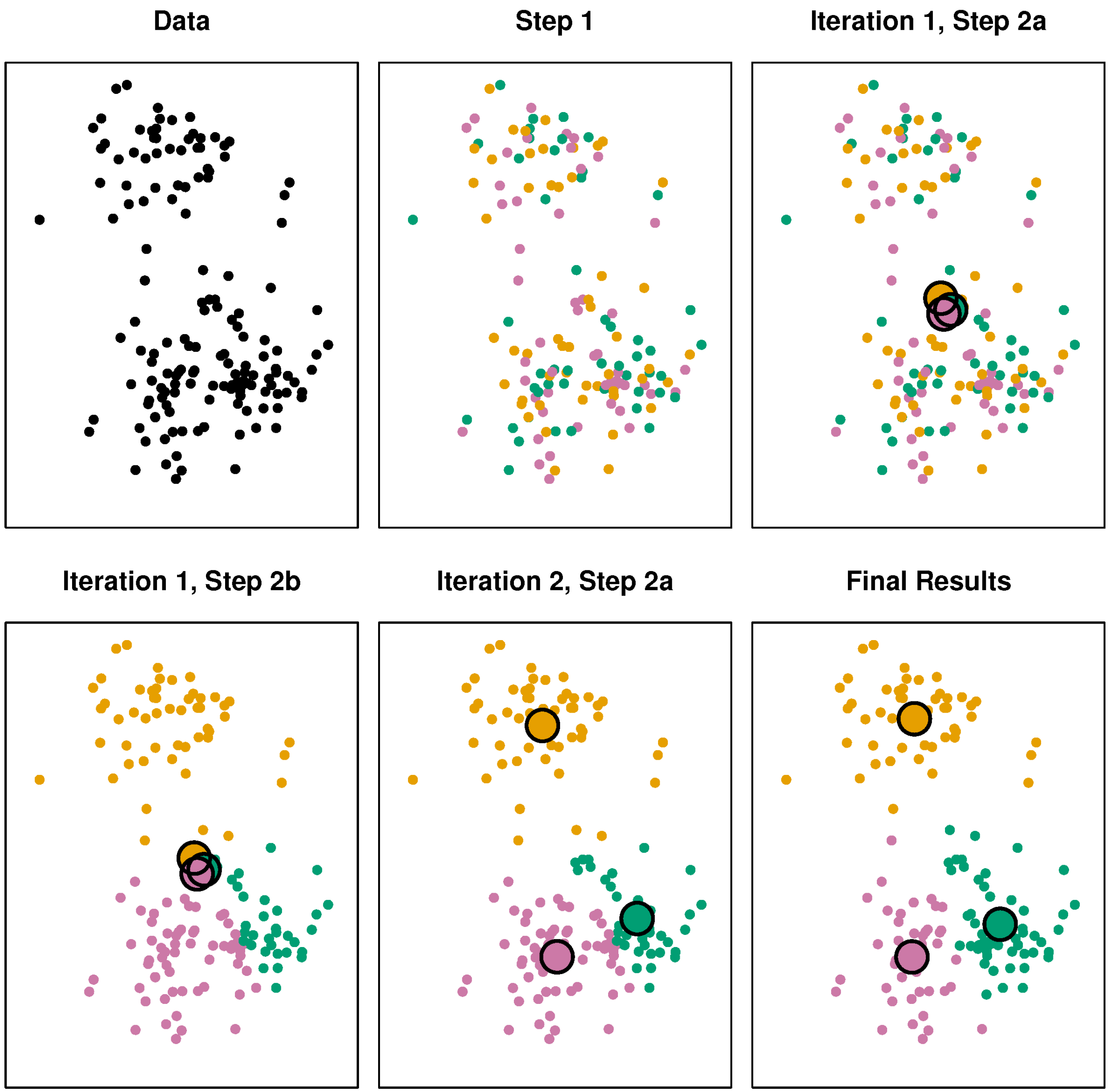
Model-based clustering

K-means again

1. Assign examples to K clusters

2.
   a. Calculate K cluster centroids;
   b. Assign examples to cluster with closest centroid;

3. If assignments changed, back to step 2a; else stop.



K-means again

- K-means is based on a **rule**
- Why this rule and not some other rule?
- What kind of data does the rule work well for?
- In what situations would the rule fail?
- What happens if we want to change the rule?

All **difficult to answer by staring at the algorithm.**

"I propose we hire some new management consultants to reverse-engineer the previous consultants' re-engineering plan."

Model-based clustering

Steps:

1. Pretend we believe in some *statistical model* that describes data as belonging to unobserved ("latent") groups;
2. Estimate ("train") this model using the data.

- **The rule follows from the model!**
- Instead of worrying about *algorithm*, we worry about *model*.
- Questions are easy to answer.

Model-based clustering

- Assumptions about the clusters are explicit, not implicit.
- We will look at the most commonly used family of models,

Gaussian mixture models (GMMs):

- Data within each cluster *(multivariate) normally distributed.*
- Parameters can be either the same or different across groups:
    - Volume (size of the clusters in data space);
    - Shape (circle or ellipse);
    - Orientation (the angle of the ellipse).

Model-based clustering

Another major advantage:

- For each observation, get a **posterior probability** of belonging to each cluster;
- Reflects that cluster membership is uncertain;
- Cluster assignment can be done based on the highest probability cluster for each observation.

Model-based clustering

Specific examples of model-based clustering:

- Gaussian mixture models
- Latent profile analysis
- Latent class analysis (categorical observations)
- Latent Dirichlet allocation

Gaussian mixture modeling

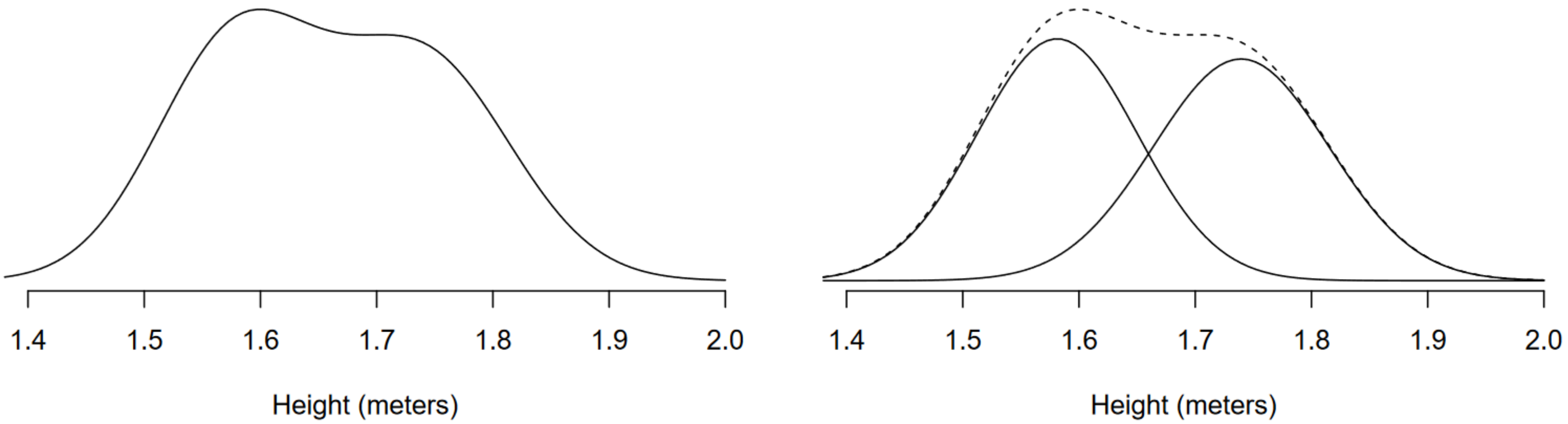


Fig. 1 Peoples' height. Left: observed distribution. Right: men and women separate, with the total shown as a dotted line.

Model-based clustering

- Statistical model + assumptions defines a likelihood

$$p(\text{data} \mid \text{parameters}) = p(y \mid \theta)$$

- Maximum likelihood estimation: find the parameters θ that make it most likely to observe the data we actually observed, y

- The above procedure automatically gives algorithm for computing clusters from data, given the model.

Model-based clustering

Likelihood (*density*) for height data:

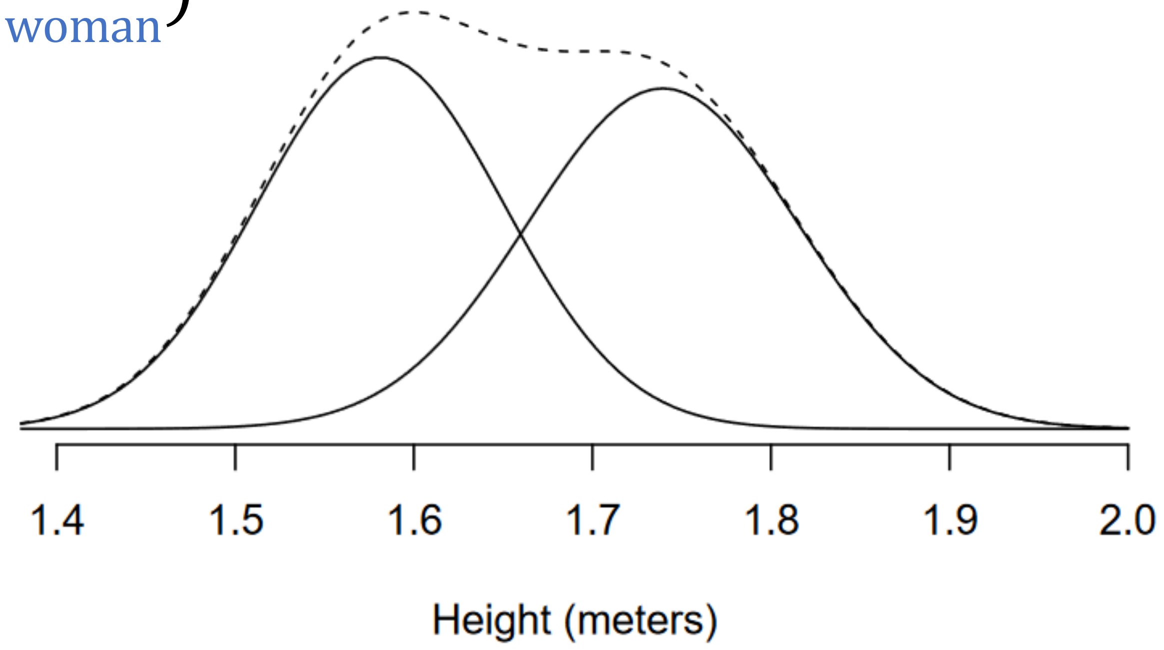
$p(\text{height} \mid \theta) =$

$$\Pr(\text{man}) \cdot \text{Normal}(\mu_{\text{man}}, \sigma_{\text{man}}) +$$
$$\Pr(\text{woman}) \cdot \text{Normal}(\mu_{\text{woman}}, \sigma_{\text{woman}})$$

Or, more concise notation:

$p(\text{height} \mid \theta) =$

$$\pi_1^X \text{Normal}(\mu_1, \sigma_1) +$$
$$(1 - \pi_1^X)\text{Normal}(\mu_2, \sigma_2)$$



Model-based clustering

Gaussian mixture model **parameters**:

- π_1^X determines the relative cluster sizes
  - Proportion of observations to be expected in each cluster
- μ_1 and μ_2 determine the locations of the clusters
  - Like centroids in K-means clustering
- σ_1 and σ_2 determine the volume of the clusters
  - how large / spread out the are clusters are in data space

Together, these 5 unknown parameters describe our model of how the data is generated.

Estimation: the EM algorithm

- If we knew in advance who is a man and who is a woman, it would have been easy to find the estimates for μ and σ:

$$\hat{\mu}_1 = \frac{\sum_{i=1}^{N_1} \mathtt{height}_i}{N_1}, \qquad \hat{\sigma}_1 = \sqrt{\frac{\sum_{i=1}^{N_1} (\mathtt{height}_i - \hat{\mu}_1)^2}{N_1}}$$

(and same for $\hat{\mu}_2$ and $\hat{\sigma}_2$.)

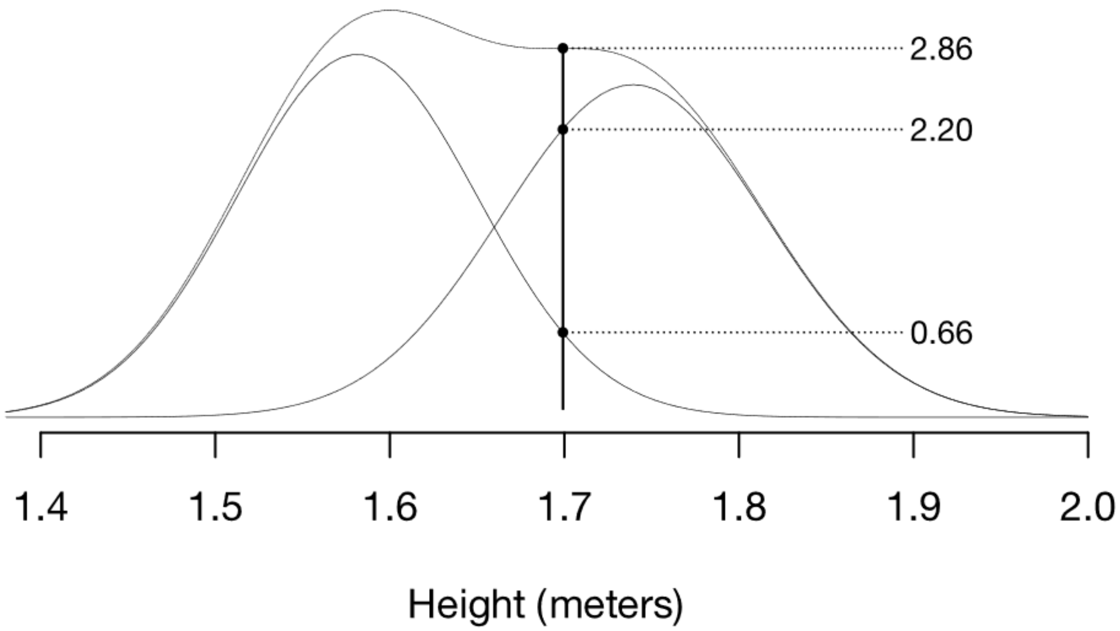
- But we don't know this!

-> Assignments need to be estimated too.

Estimation: the EM algorithm

- Solution: Figure out the posterior probability of being a man/woman, given the current estimates of the means and sds
- If we know cluster locations and shapes, how likely is it that a 1.7m person is a man or a woman?

$$\pi_{man}^{X} = \frac{2.20}{2.86} \approx 0.77$$

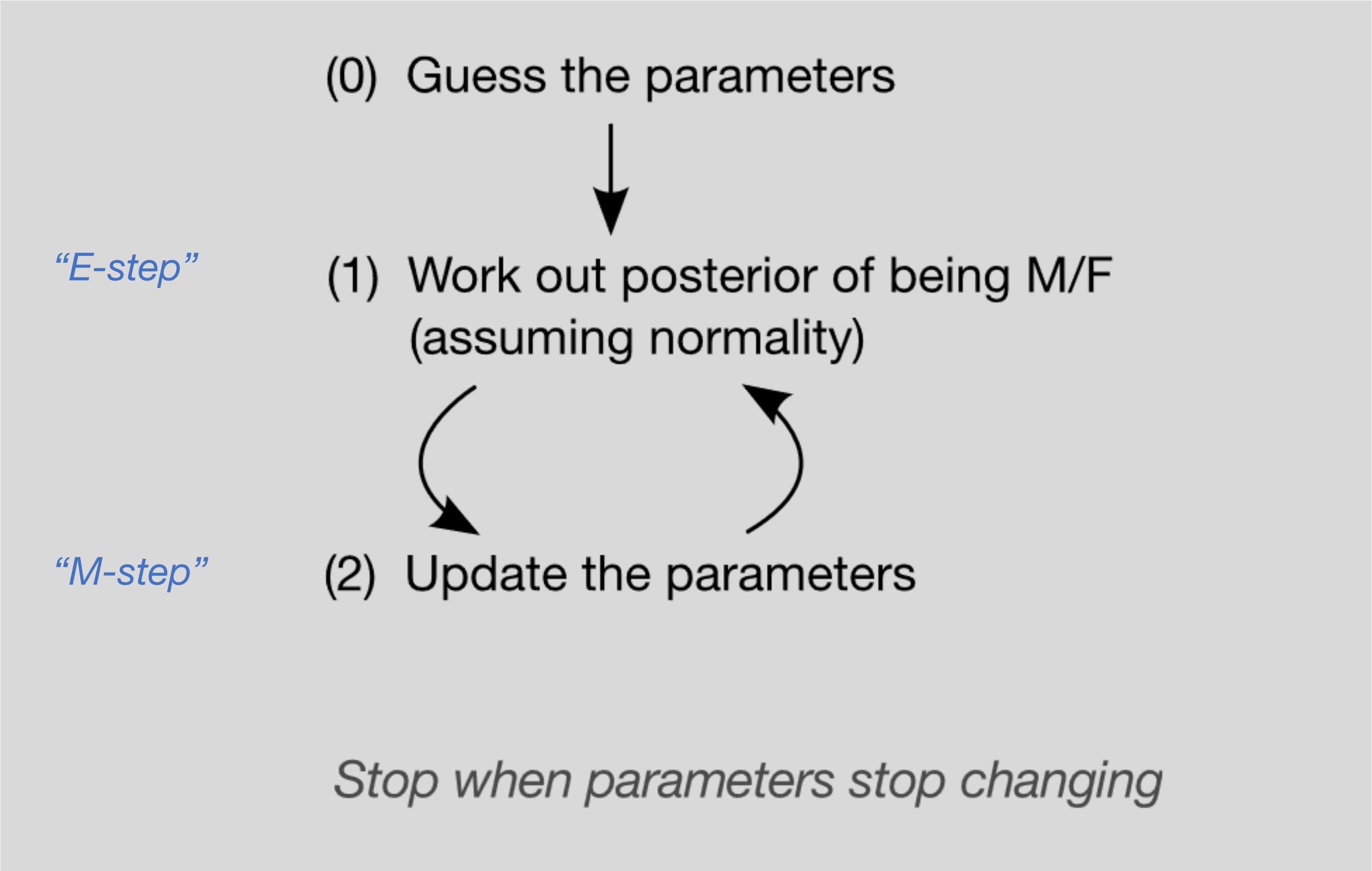


Estimation: the EM algorithm

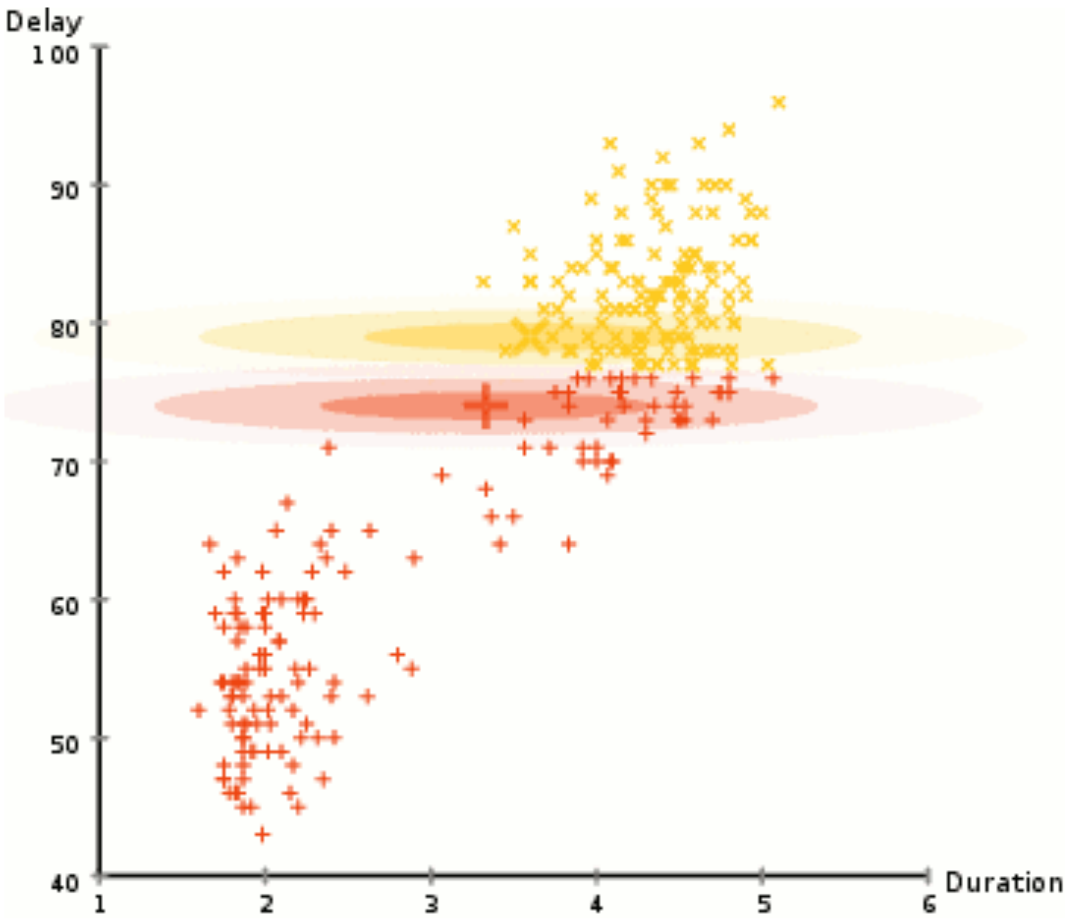
- Now we have some class *assignments* (probabilities);
- So we can go back to the parameters and update them using our easy rule (M-step)
- Then, we can compute new posterior probabilities (E-step)

Does it remind you of something…?

Estimation: the EM algorithm



Estimation: the EM algorithm

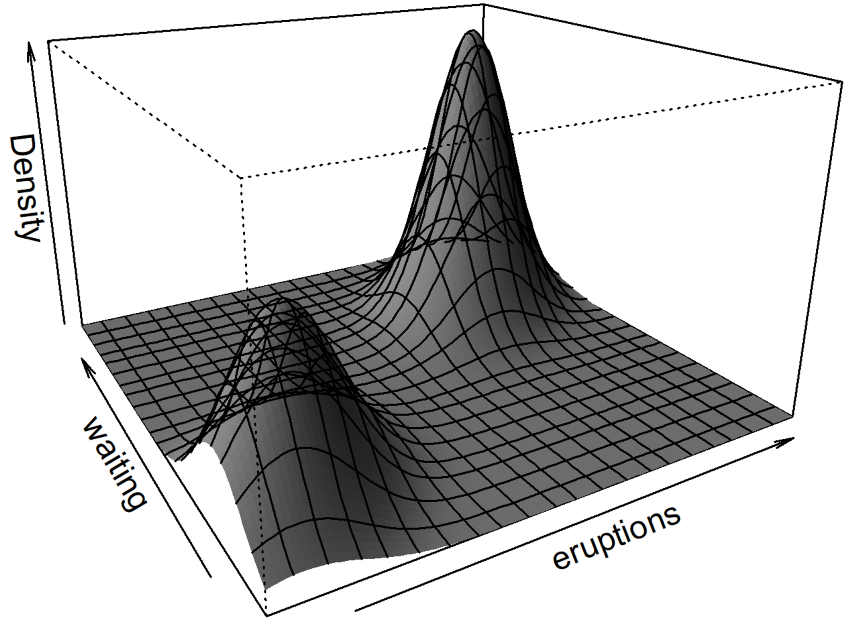


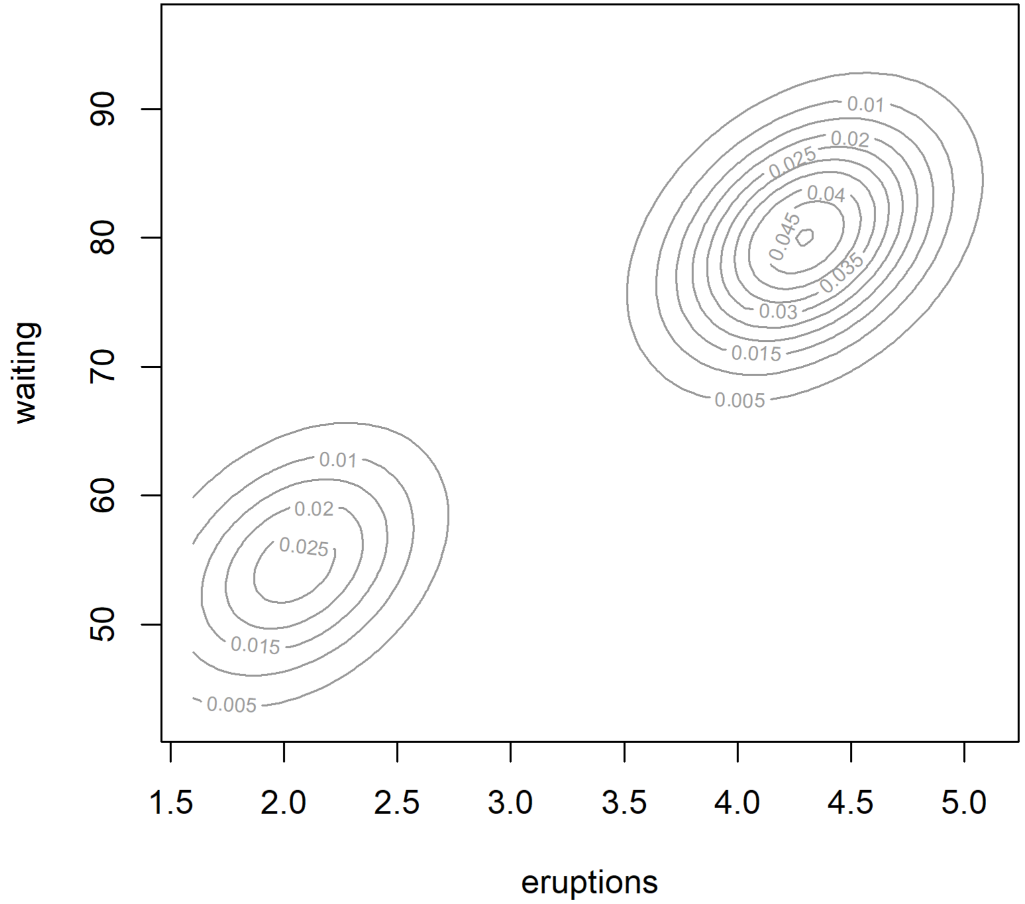
Multivariate model-based clustering

- With 2 observed features:
  - mean becomes a vector of 2 means
  - standard deviation turns into a 2x2 variance-covariance matrix determining the shape of the cluster
- So we have multiple within-cluster parameters:
  - Two means
  - Two variances, one for each observed variable
  - A single covariance among the features
- Together, the 11 parameters define the likelihood in bivariate space, which from the top looks like ellipses

Multivariate model-based clustering

$$p(\boldsymbol{y}|\,\theta) = \pi_1^X MVN(\boldsymbol{\mu_1}, \boldsymbol{\Sigma_1}) + (1\ - \pi_1^X)MVN(\boldsymbol{\mu_2}, \boldsymbol{\Sigma_2})$$





Number of parameters in a (multivariate) Gaussian mixture model

The number of parameters in a multivariate mixture model is:

- (the π_k^X) The number of components (classes), minus one, i.e. $K - 1$
- (the $\boldsymbol{\mu}_k$), i.e. $\mathrm{K} \cdot p$ (where p is the number of variables)
- (the $\boldsymbol{\Sigma}_k$), i.e.
    - $K \cdot p$ variances,
        - (or p variances when variances **equal over classes**)
    - $K \cdot p\ (p - 1)/2$ covariances
        - (or $p\ (p - 1)/2$ when covariances **equal over classes**)
        - (or 0 when variables are uncorrelated, spherical clusters)

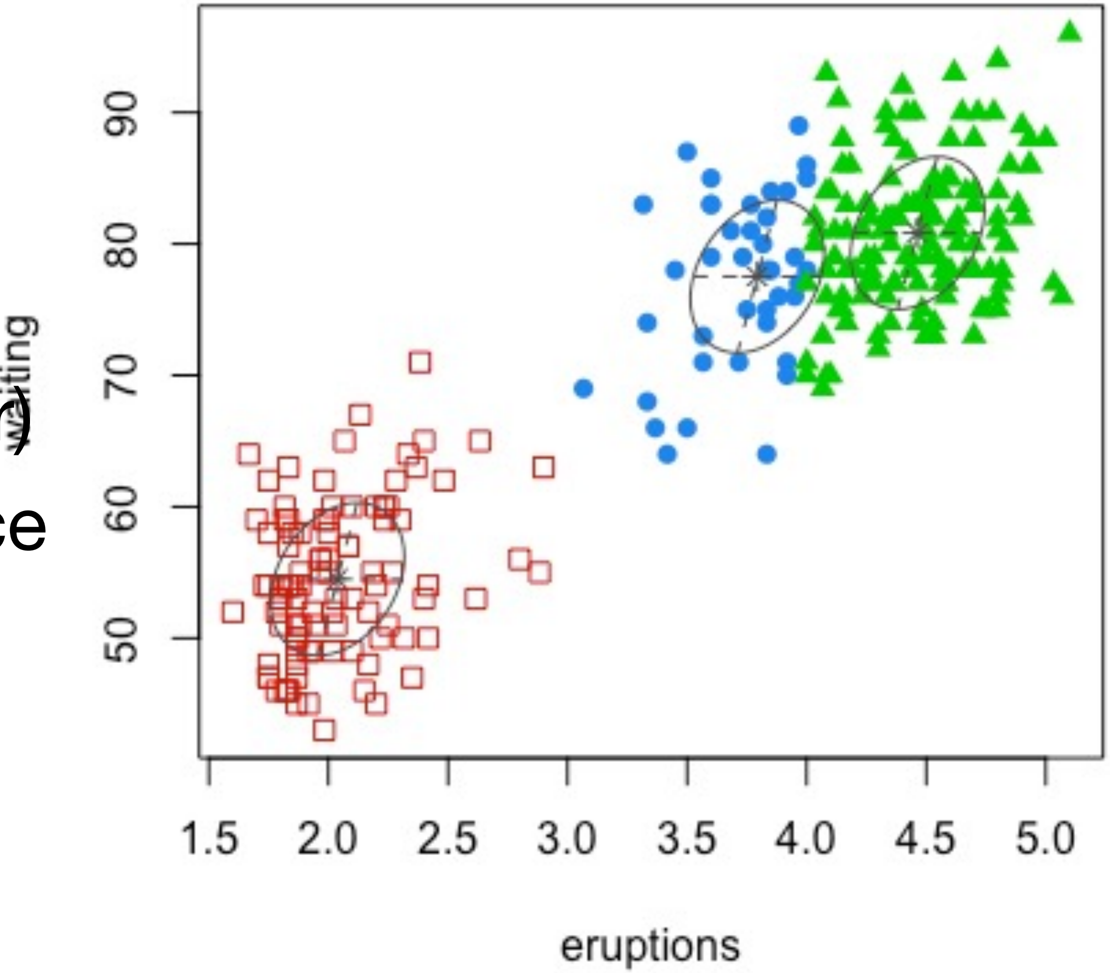
Number of parameters

$$m = (K-1) + Kp + Kp + K\frac{p(p-1)}{2}$$

For example:

- $K = 3$
- $p = 2$
- Ellipsoidal (correlated within cluster)
- But: equal variances and covariance

$$m = (K-1) + Kp + p + \frac{p(p-1)}{2}$$
$$= 2 + 3\times 2 + 2 + 1$$
$$= 11$$



Multivariate model-based clustering

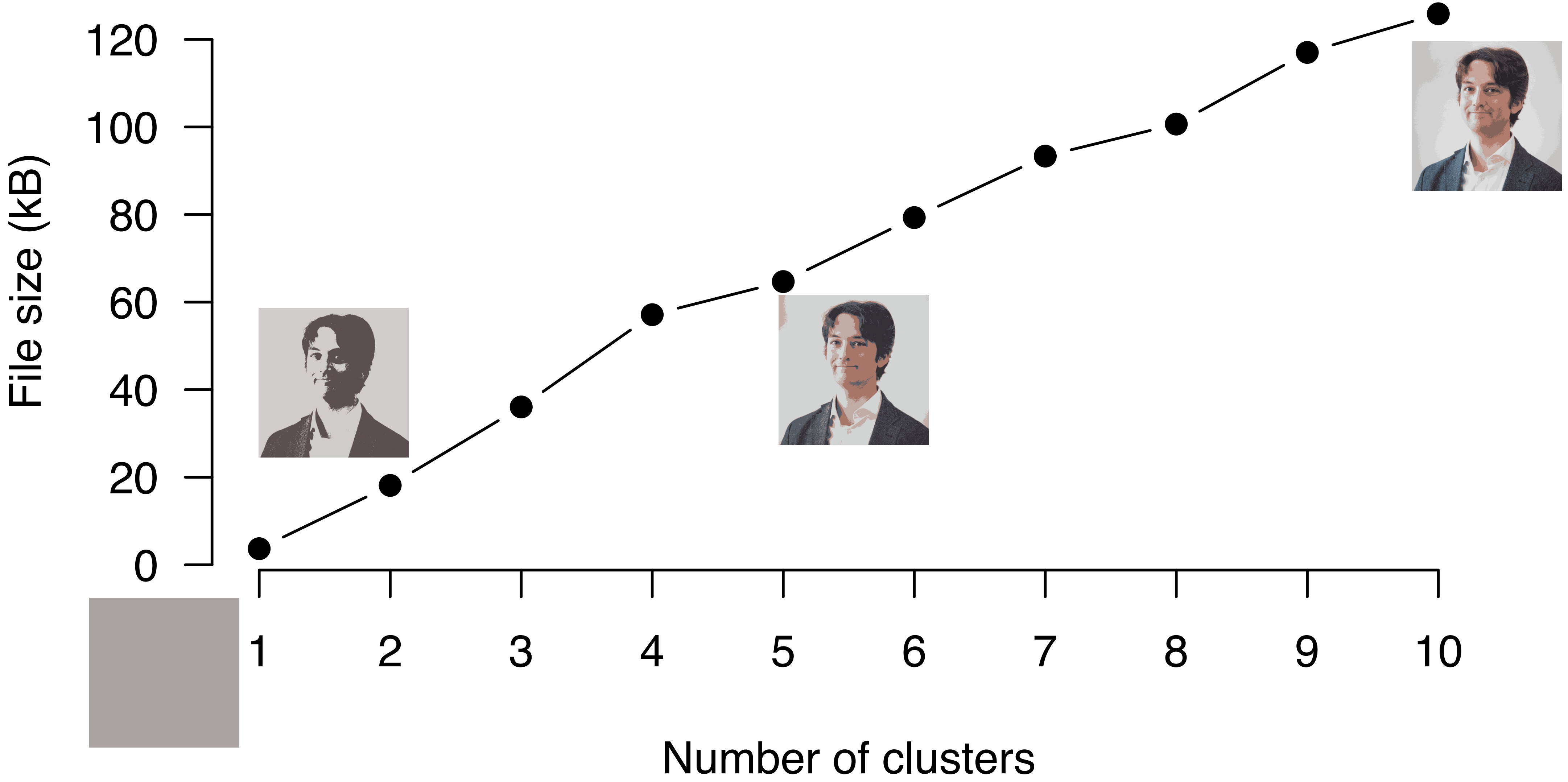
- Cluster shape parameters (the variance-covariance matrix) *can* be constrained to be *equal* across clusters
- Can also be *different* across clusters
- More flexible, complex model
- Think: **bias-variance tradeoff**

How to evaluate clustering results

1. Use of external information
2. Visual exploration
3. Stability assessment / sensitivity analysis
4. Internal validation indexes
5. **Testing for clustering structure**

Much more info & helpful advice: Clustering strategy & method selection (ch 31 of Handbook of clustering), https://arxiv.org/pdf/1503.02059.pdf

File size increases with number clusters



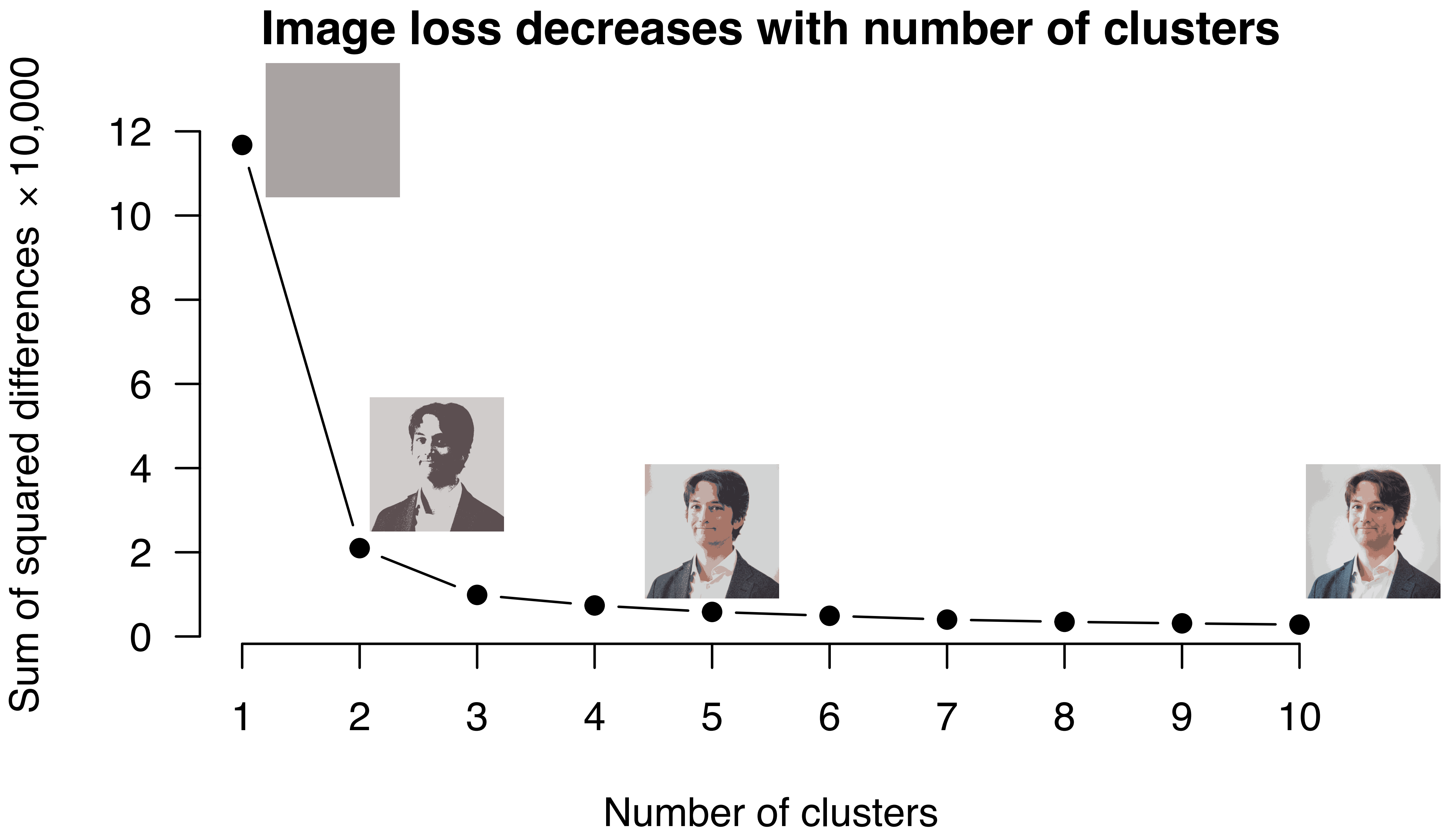
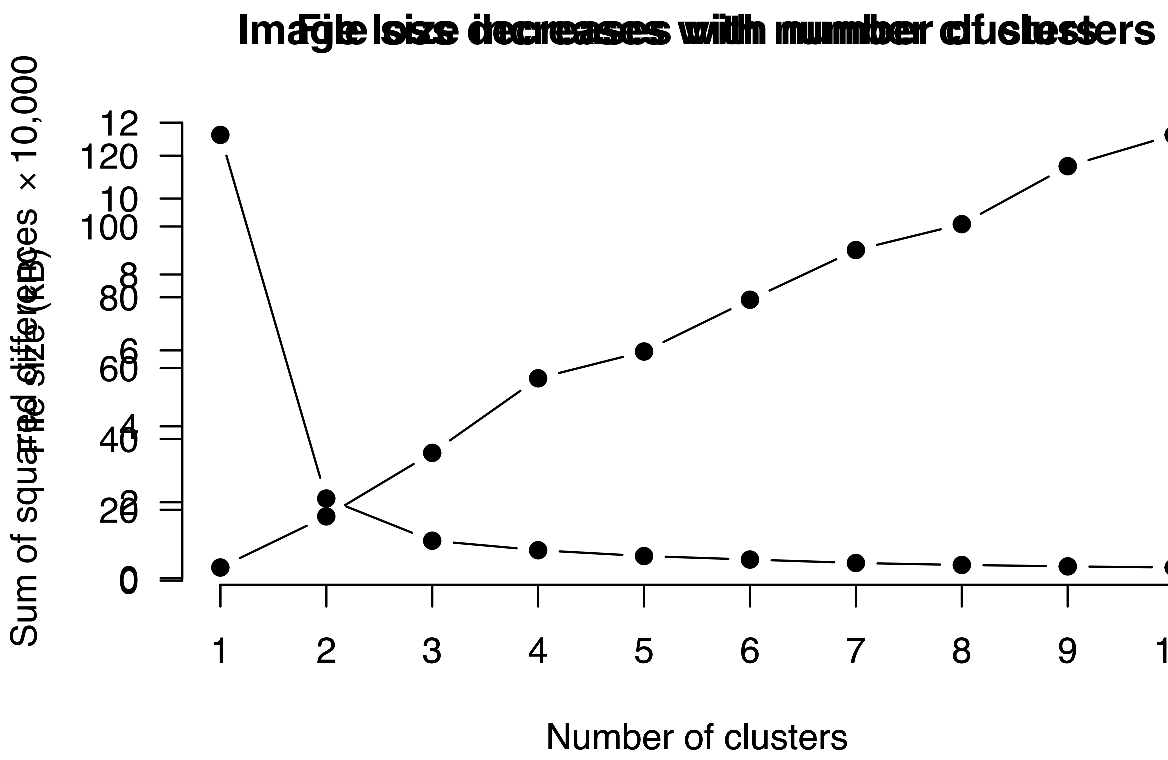


Image loss decreases with number of clusters
Sum of squared differences ×10,000
0
2
4
6
8
10
12
1
2
3
4
5
6
7
8
9
10
Number of clusters



- More clusters gives **better "fit"** in terms of reconstruction of the image
  (compression is less "lossy")
- More clusters gives **bigger file size**
  (solution is more complex, takes more bytes to store)
- So the **model loss and model complexity trade off against each other**
- This is a common theme in (unsupervised) machine learning and you should remember this for model-based clustering lecture

Model fit

- The likelihood says how well the model fits to the data
- It forms the basis of information criteria (lower is better)
  - Can be used to compare different clustering models and pick the best one

$$BIC = -2 \cdot \log(\ell) + m \cdot \log(n)$$

- ℓ : Likelihood, $p(\text{data} \mid \theta)$
- $-2 \cdot \log(\ell)$: *"Deviance"*
- m : Number of parameters
- n : Number of observations/examples

Model fit

- Tradeoff between fit and complexity

$$\underbrace{-2 \cdot \log(\ell)}_{\text{“Reconstruction loss”}} + \underbrace{m \cdot \log(n)}_{\approx\text{“File size”*}}$$

- Think: bias and variance tradeoff
  - Variance also has to do with “clustering stability”

- Better fit *and* lower complexity = better cluster solution

*Approximation for BIC, different choices possible

More model fit criteria

- BIC: “Schwarz/Bayesian information criterion”
- AIC: “Another/Akaike information criterion”

  (same as BIC but penalty is m)
- AIC3: The same as AIC but penalty is $\frac{3}{2}m$
- ICL: “Integrated information criterion” (Biernacki et al. 2000)

(Same as BIC but reconstruction loss includes the assigned clusters)

- *(Others based on):*
  - *Minimum description length (MDL)*
  - *Bayesian marginal likelihood*

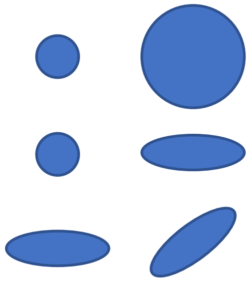
Model-based clustering in R

- `mclust` implements multivariate model-based clustering
- Provides an easy interface to fit several parameterizations
- Model comparison with BIC
- Plotting functionality

```
> library(mclust)

    __  ___________    __  _____________
   /  |/  / ____/ /   / / / / ___/_  __/
  / /|_/ / /   / /   / / / /\__ \ / /
 / /  / / /___/ /___/ /_/ /___/ // /
/_/  /_/\____/_____/\____//____//_/    version 5.4.6
```

Model-based clustering in R

- Mclust uses an identifier for each possible parametrization :
- **E** for **e**qual, **V** for **v**ariable, **I** for identity matrix:
    - Volume (size of the clusters in data space):
    - Shape (circle or ellipse)
    - Orientation (the angle of the ellipse)

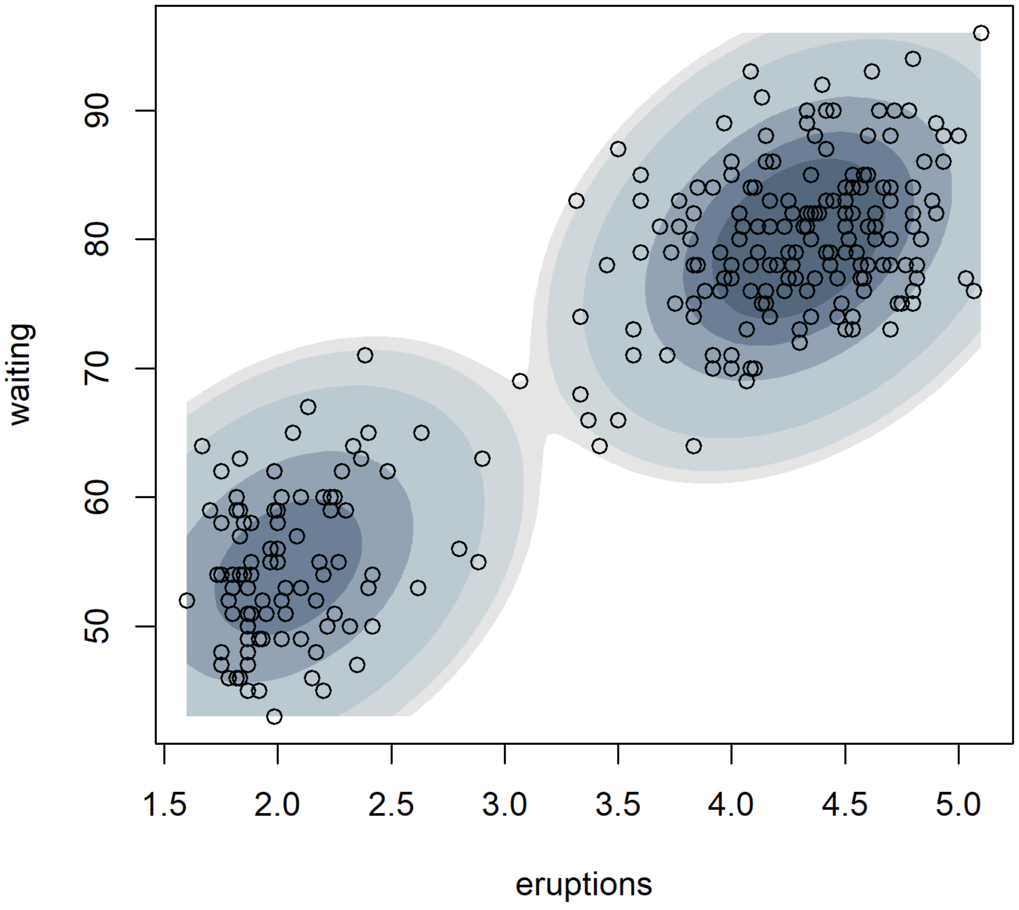


- E.g. an “EEE” model has equal volume, shape and orientation
- A VVV model has variable volume, shape, and orientation
- A VVE model has variable volume and shape but equal orientation

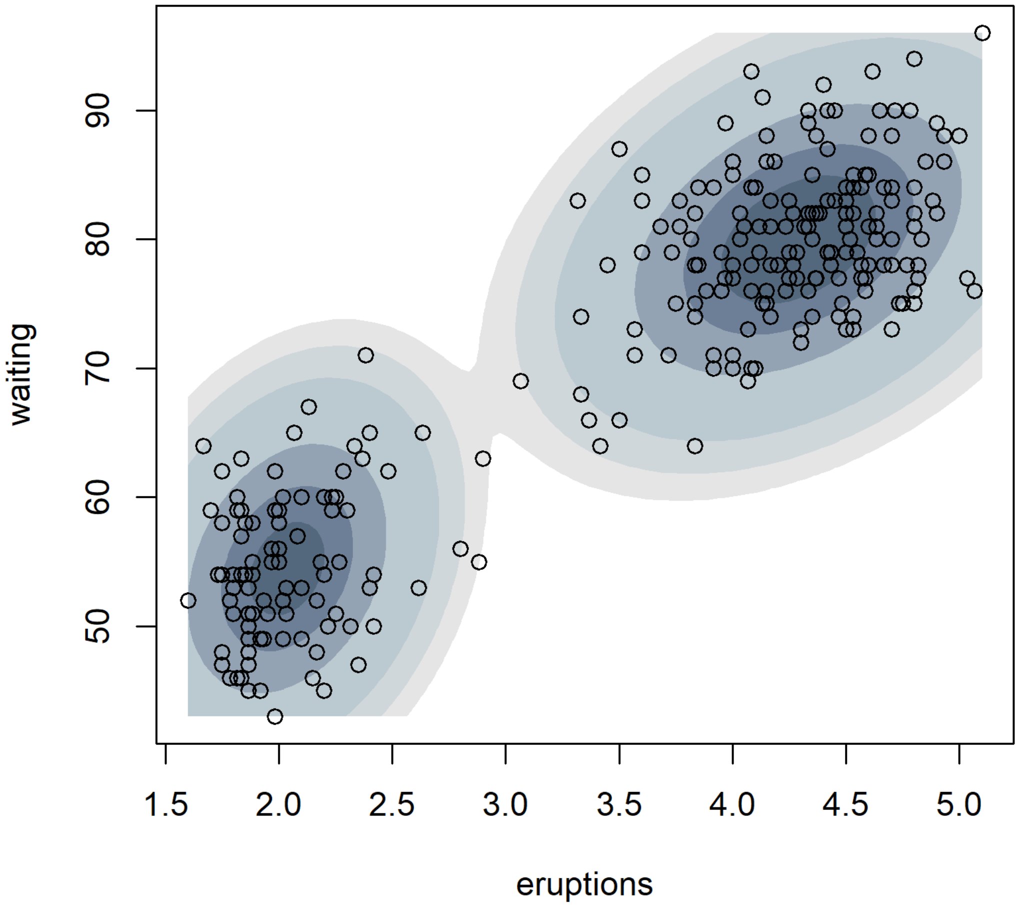
Model-based clustering in R:

EEE vs. VVV

Equal volume, shape, orientation



Variable volume, shape, orientation



TOP SECRET SLIDE

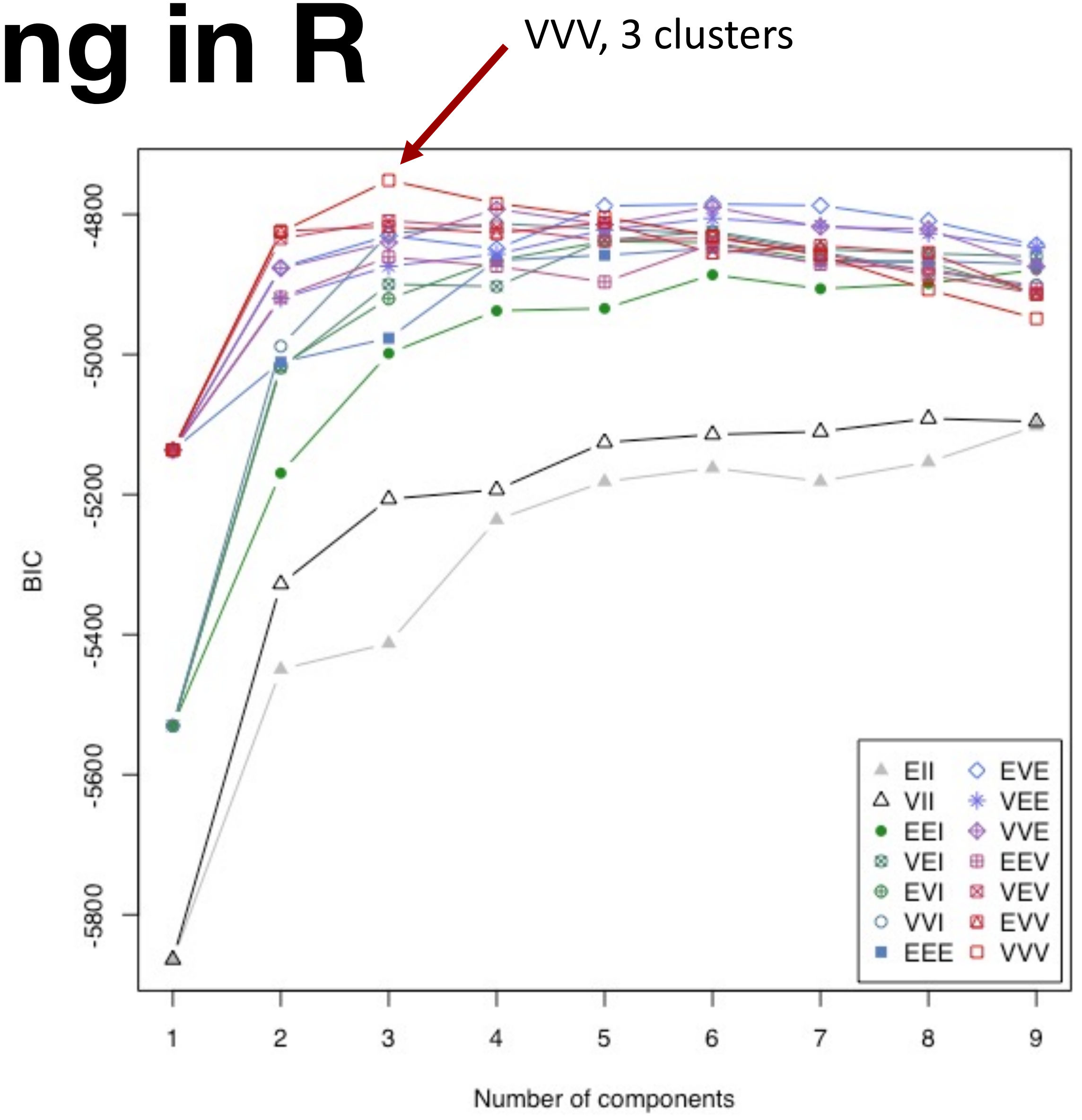
K-MEANS IS A GMM WITH THE FOLLOWING MODEL:

- All prior class proportions are 1/K;
- **`EII`** model: equal volume, only circles;
- All posteriors are either 0 or 1 (“classification likelihood”).

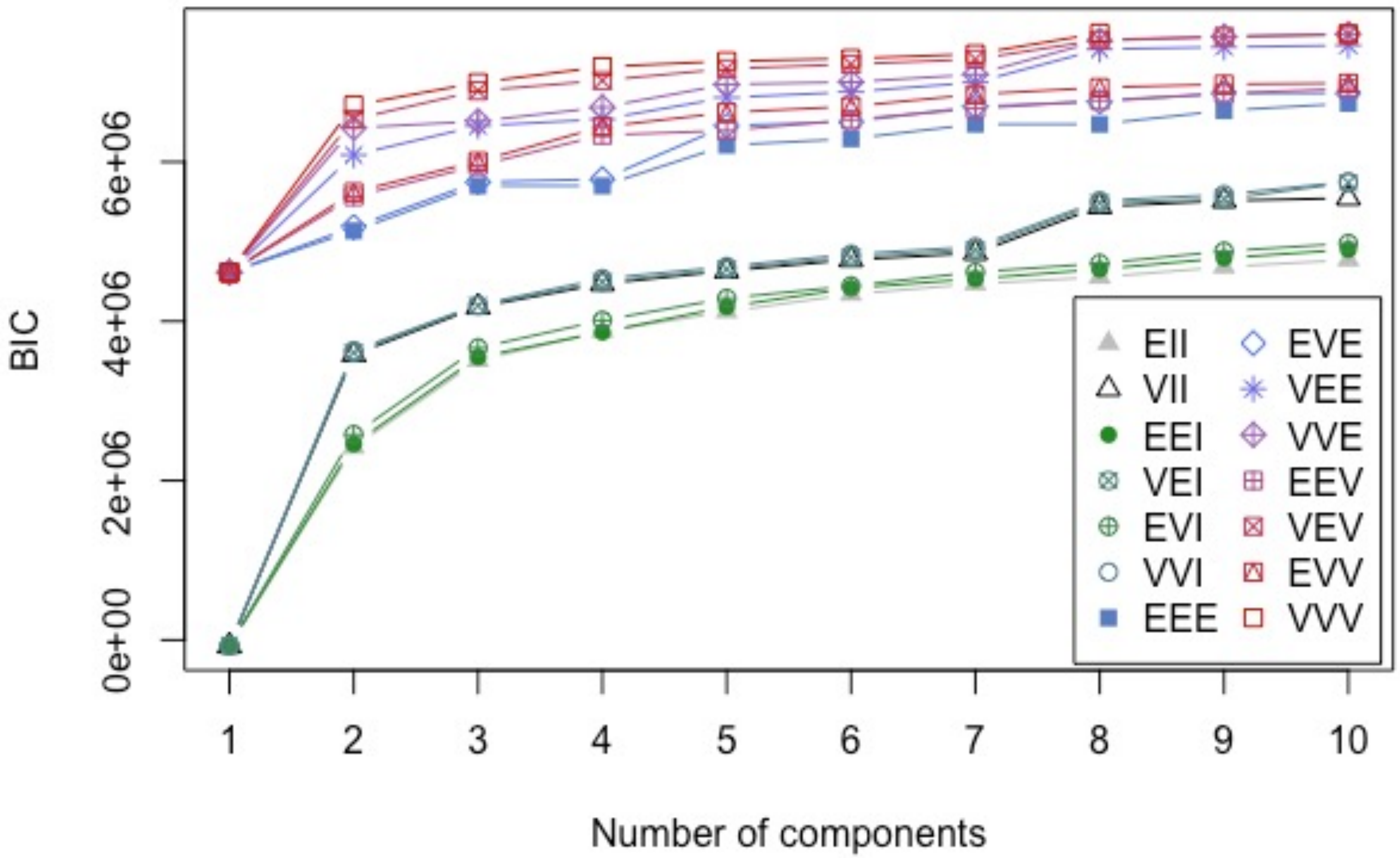
Model-based clustering in R

- How `mclust` optimizes hyperparameters:
  - Fit all the models with up to 9 clusters (or more, your choice!)
  - Compute the BIC (or ICL) of each model
  - Choose the model with the best BIC

- R assignment: using mclust



Model selection using BIC for image example



```
> fit_mc <- Mclust(im_ar, G = 1:10)
fitting ...
  |=======================================================| 100%
> summary(fit_mc)
----------------------------------------------------
Gaussian finite mixture model fitted by EM algorithm
----------------------------------------------------
Mclust VVV (ellipsoidal, varying volume, shape, and orientation)
model with 8 components:

 log-likelihood      n df     BIC     ICL
        3808542 640000 79 7616028 7530927

Clustering table:
     1      2      3      4      5      6      7      8
151032  48661 155542  34602  82621  49494  41665  76383
```

Merging *components* to get *clusters*

- GMM obviously has trouble with clusters that are not ellipses
- Secret weapon: **merging**

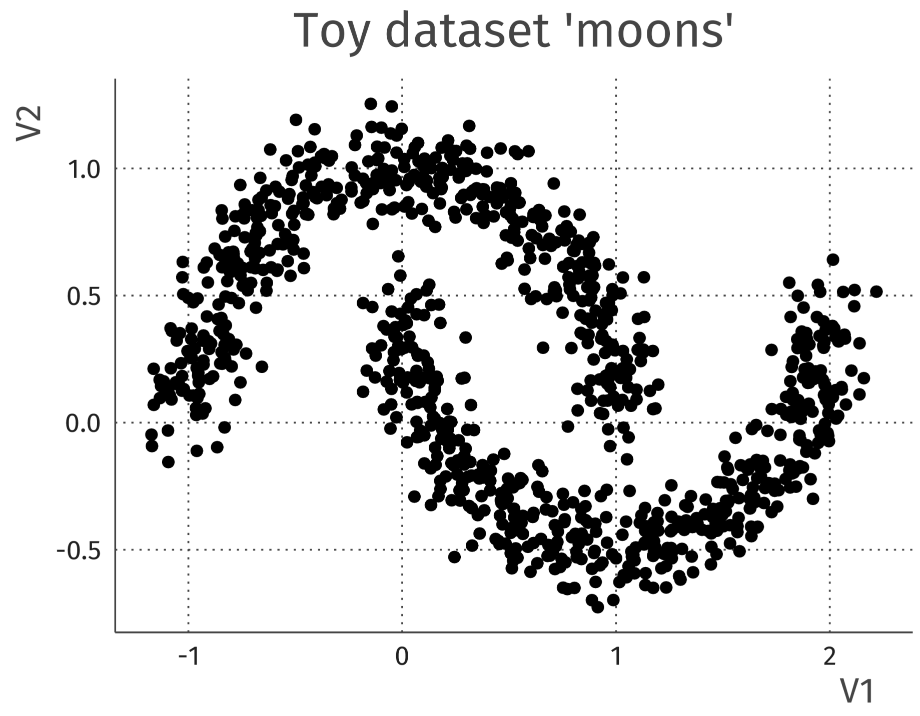
Powerful idea:

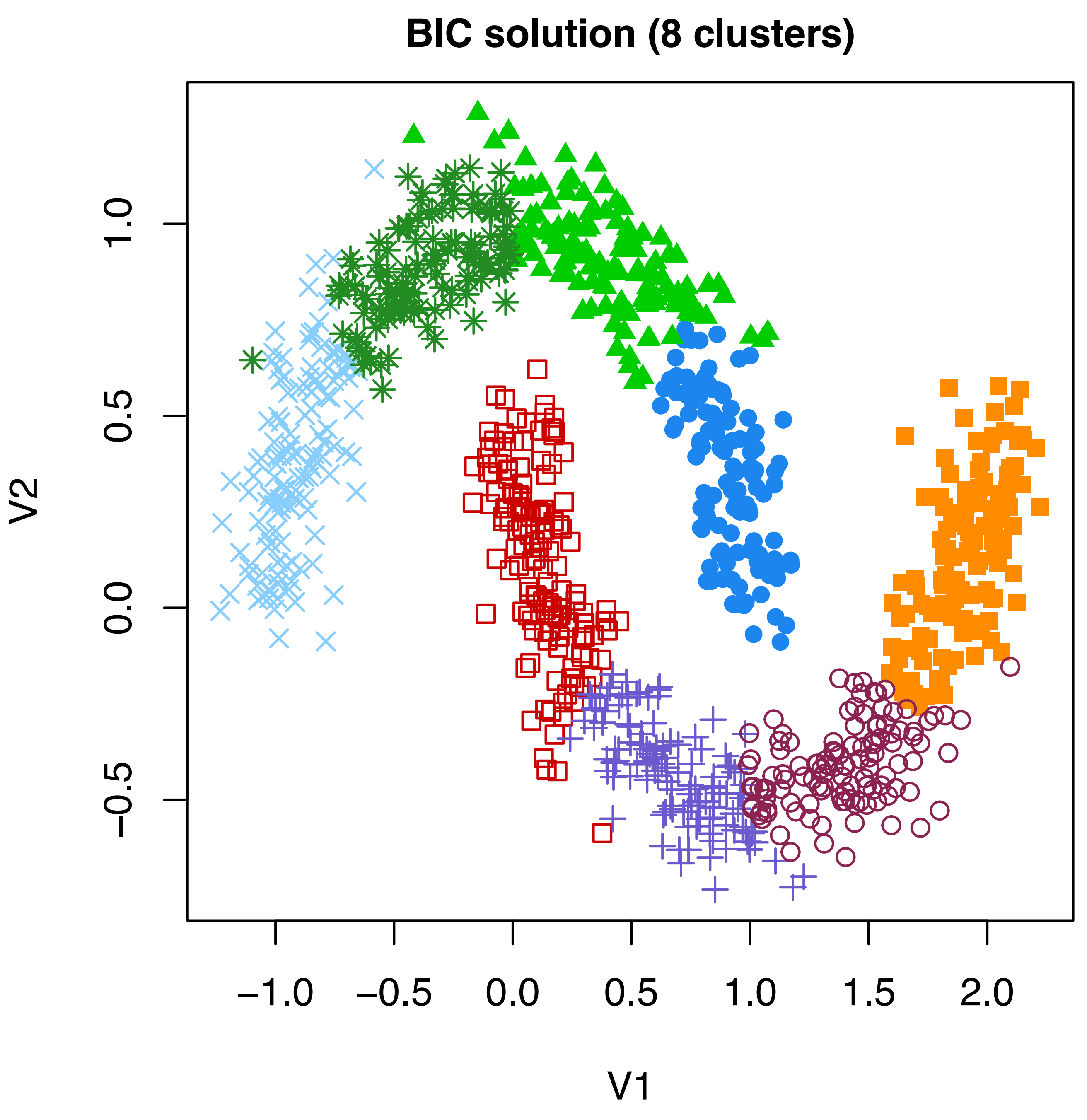
- Start out with the usual Gaussian mixture solution;
- **merge** “similar” *components* to create non-Gaussian *clusters.*

Note: we’re distinguishing “components” from “clusters” now.

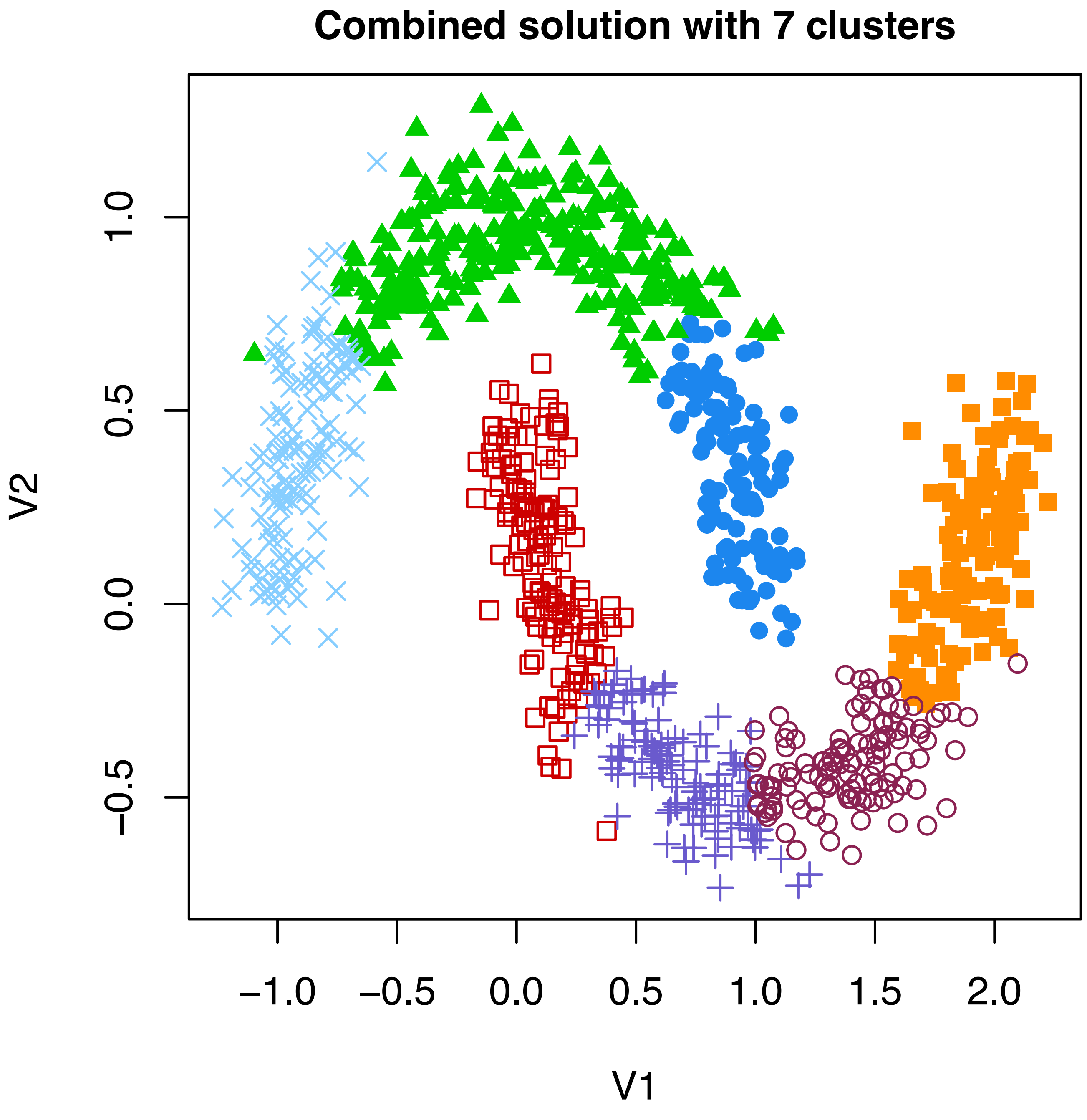
Merging components to get clusters

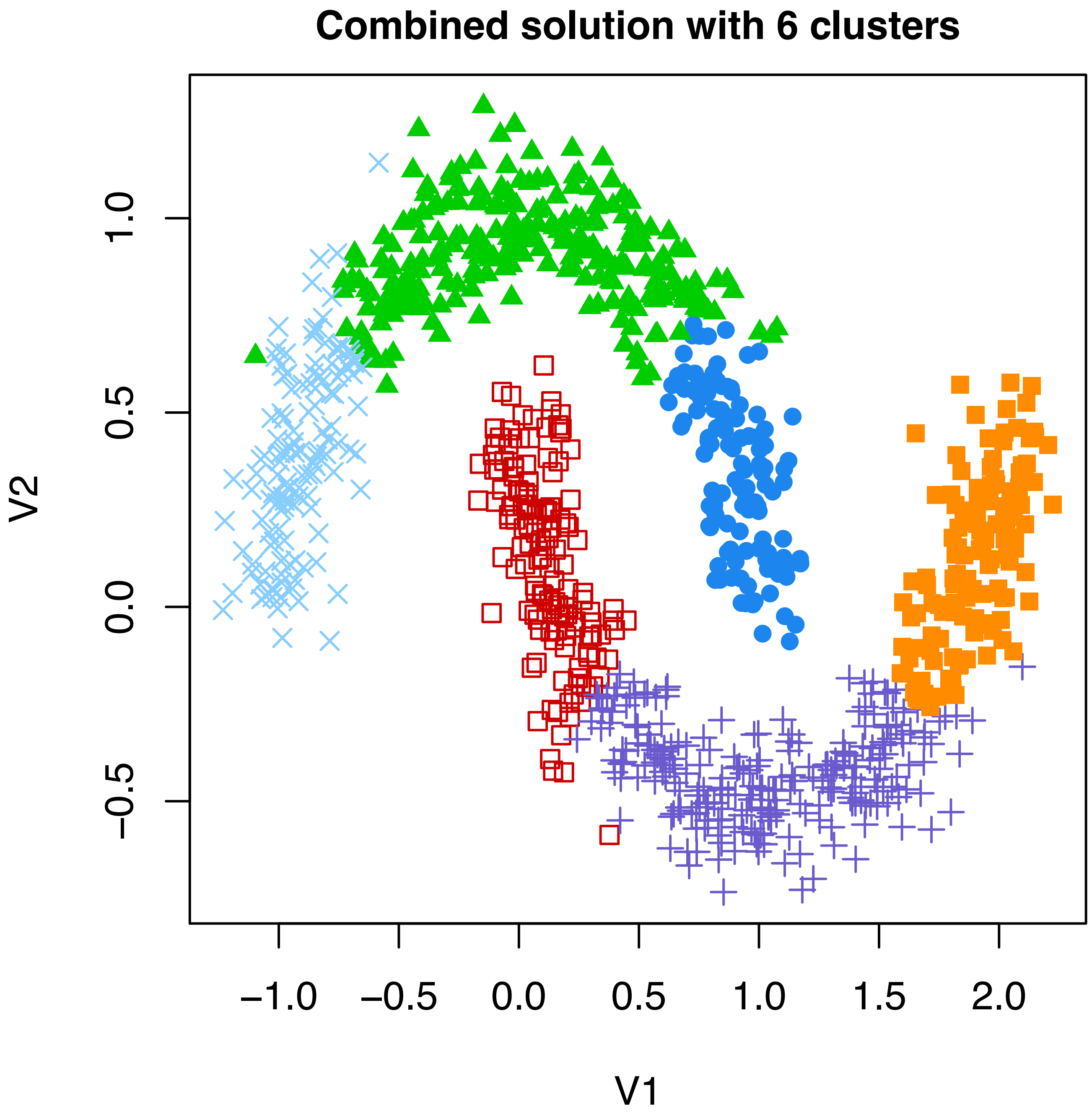
```
library(mclust)

output <- clustCombi(data = x)
plot(output)
```



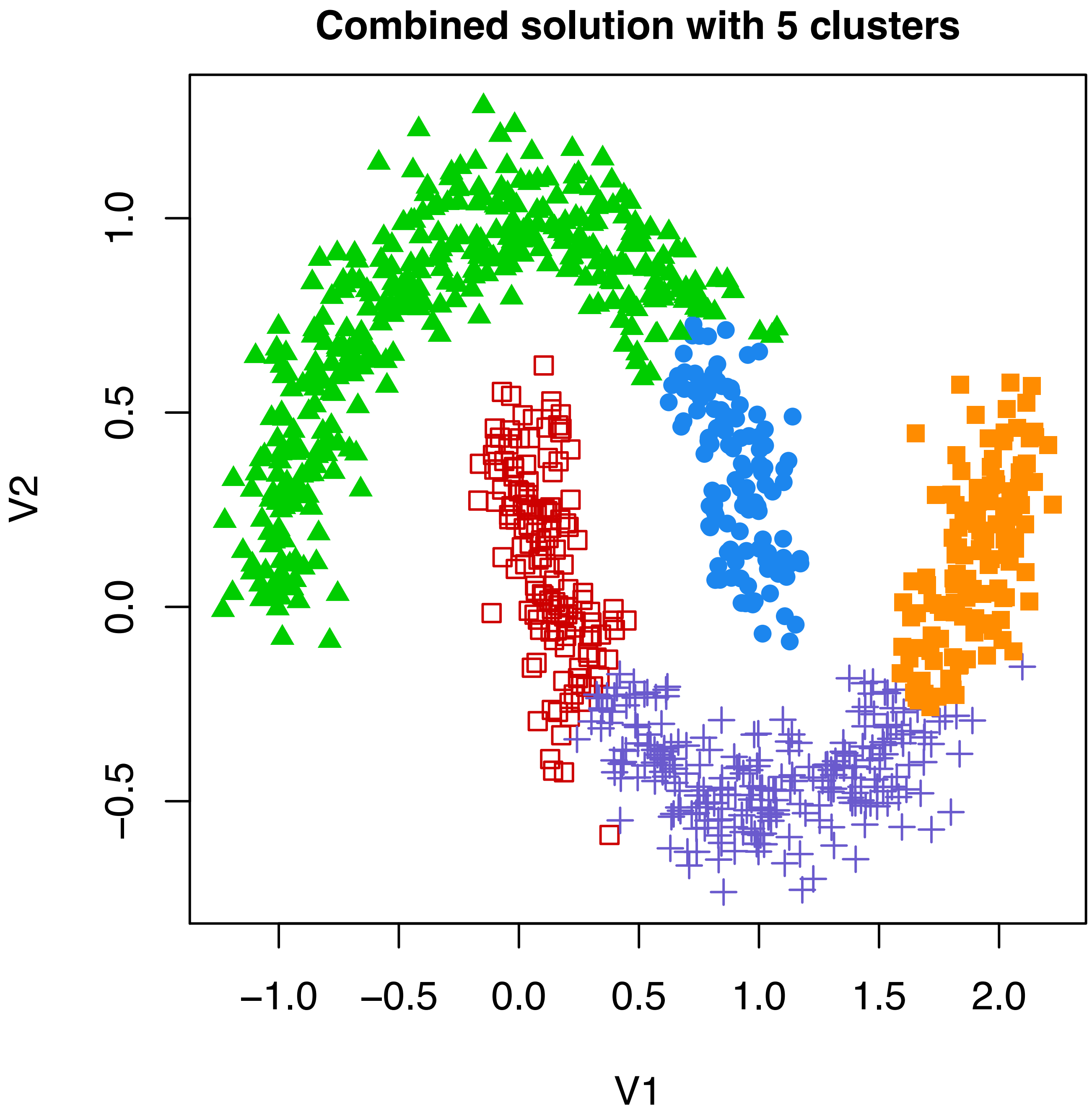


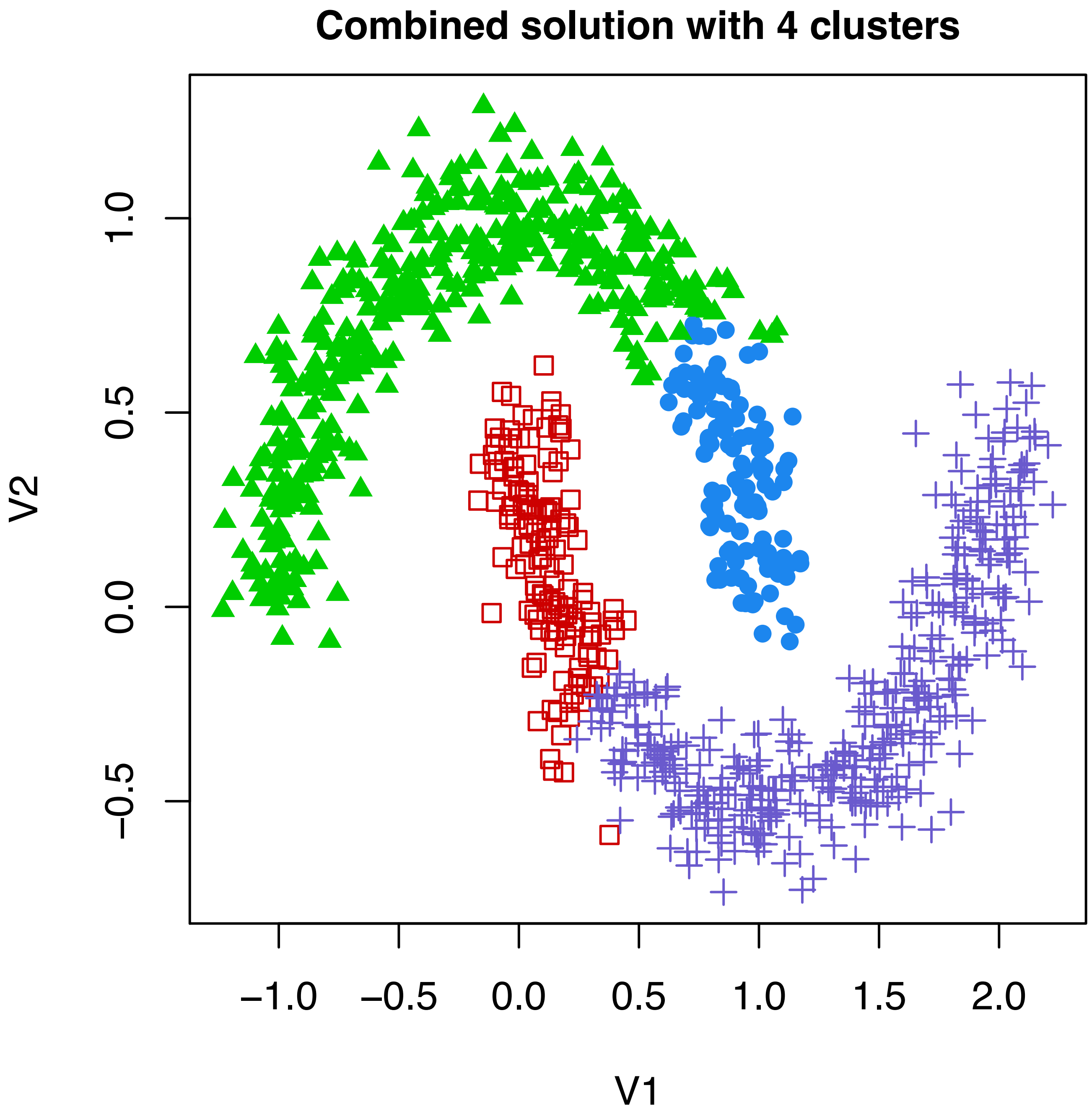
BIC solution (8 clusters)
V2
V1
1.0
0.5
0.0
−0.5
−1.0
0.0
0.5
1.0
1.5
2.0


Combined solution with 7 clusters
V2
1.0
0.5
0.0
−0.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
V1



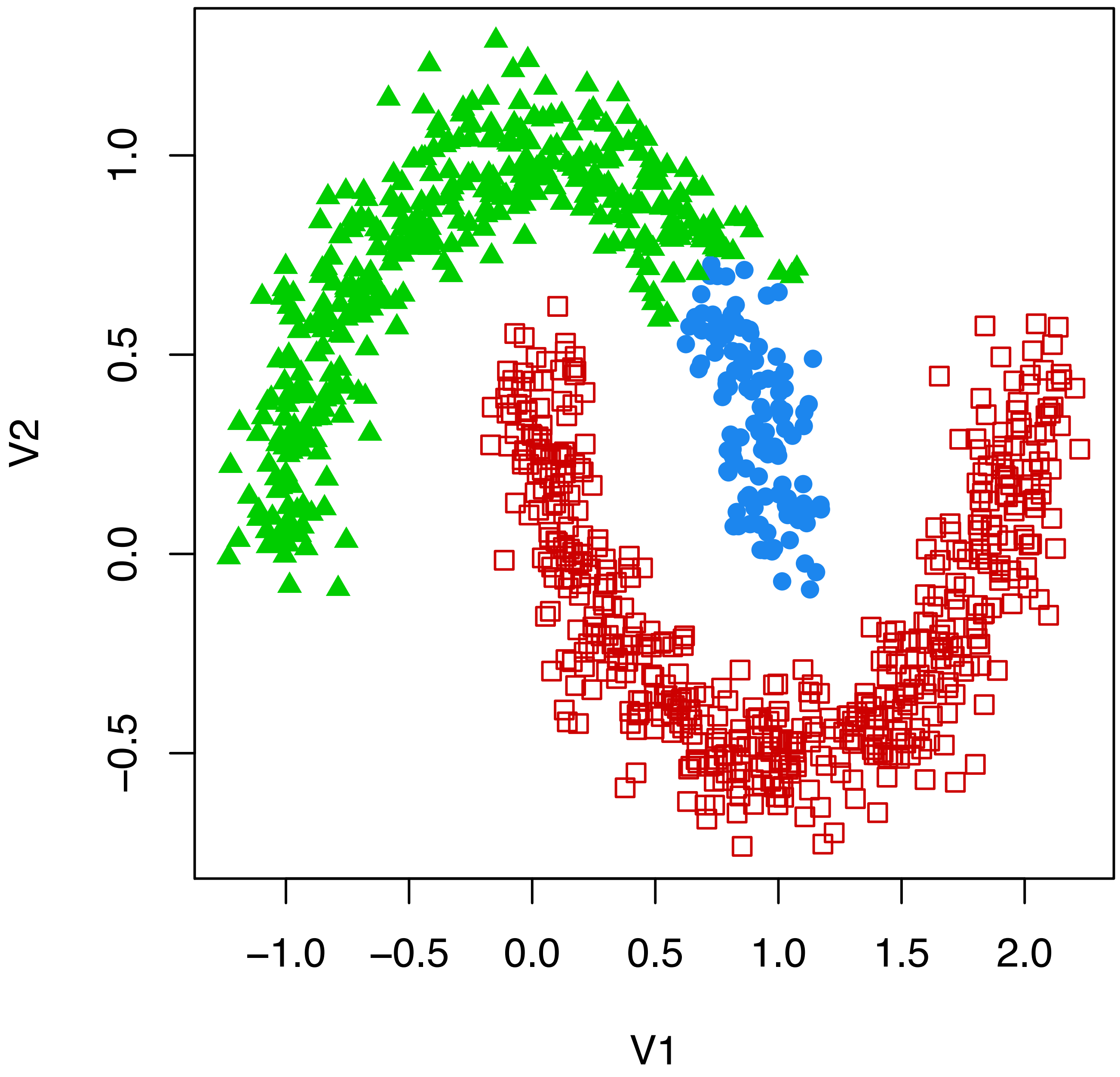
Combined solution with 6 clusters
V2
1.0
0.5
0.0
−0.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
V1

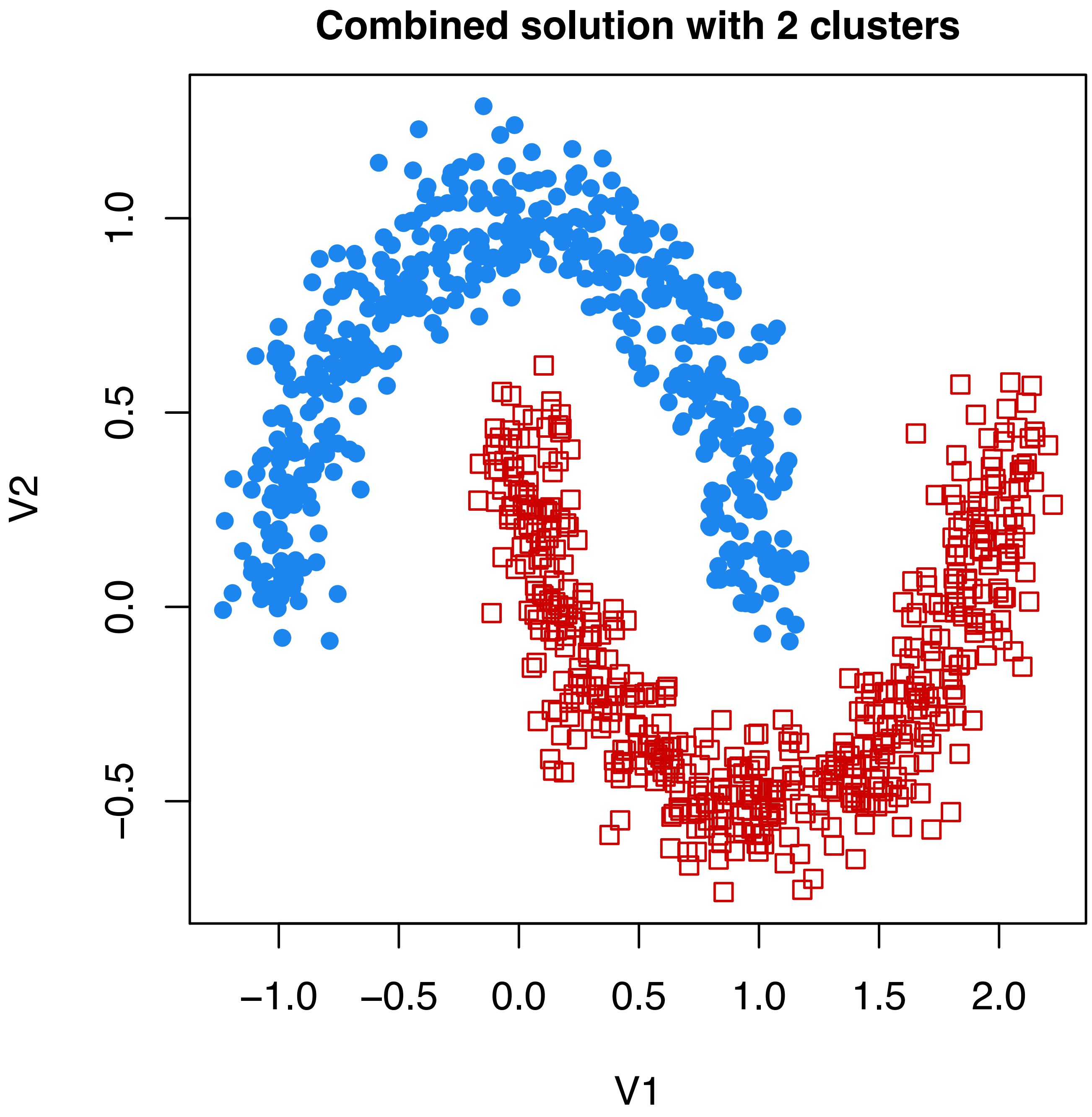

Combined solution with 5 clusters
V1
V2
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
−0.5
0.0
0.5
1.0

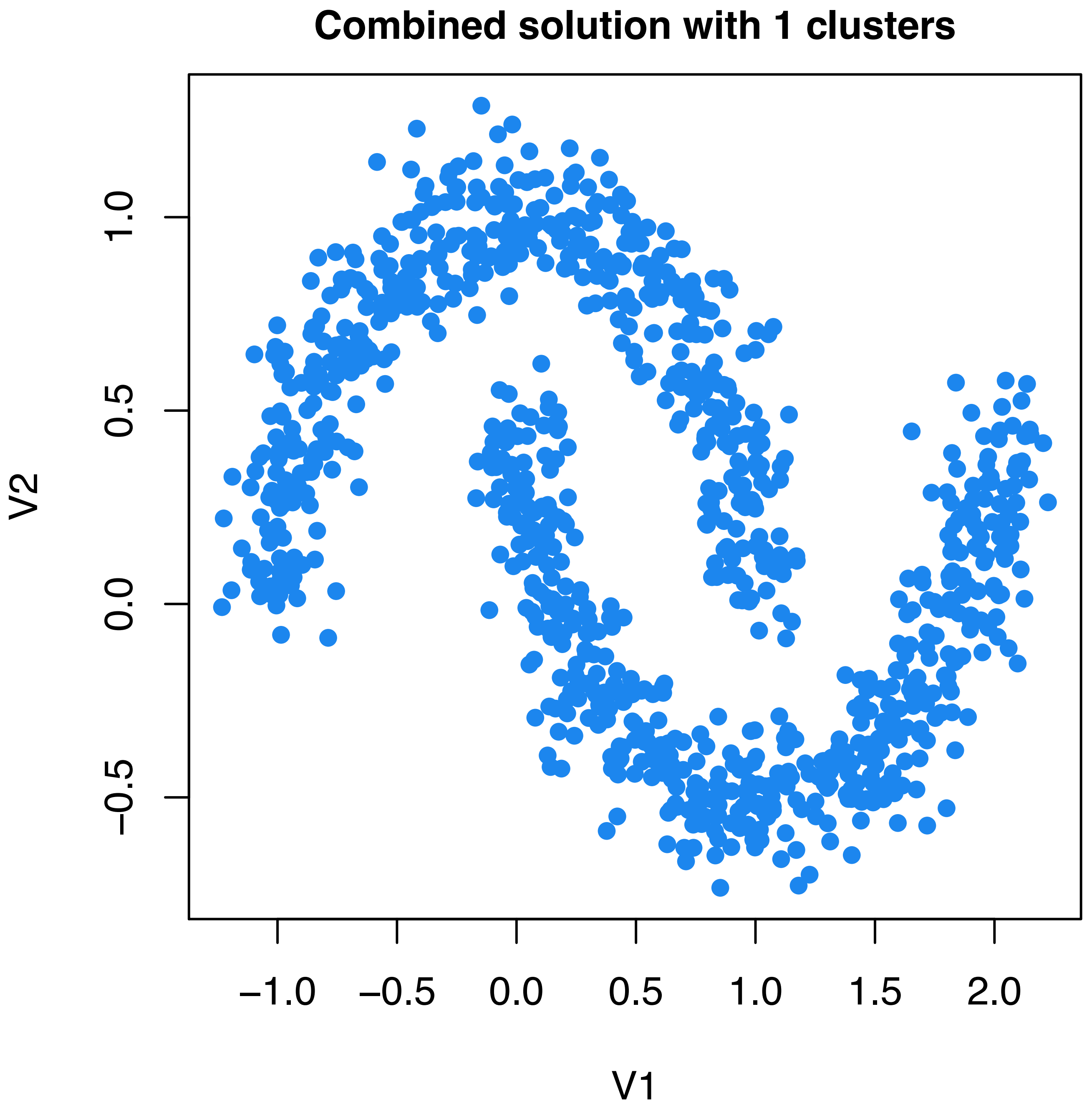


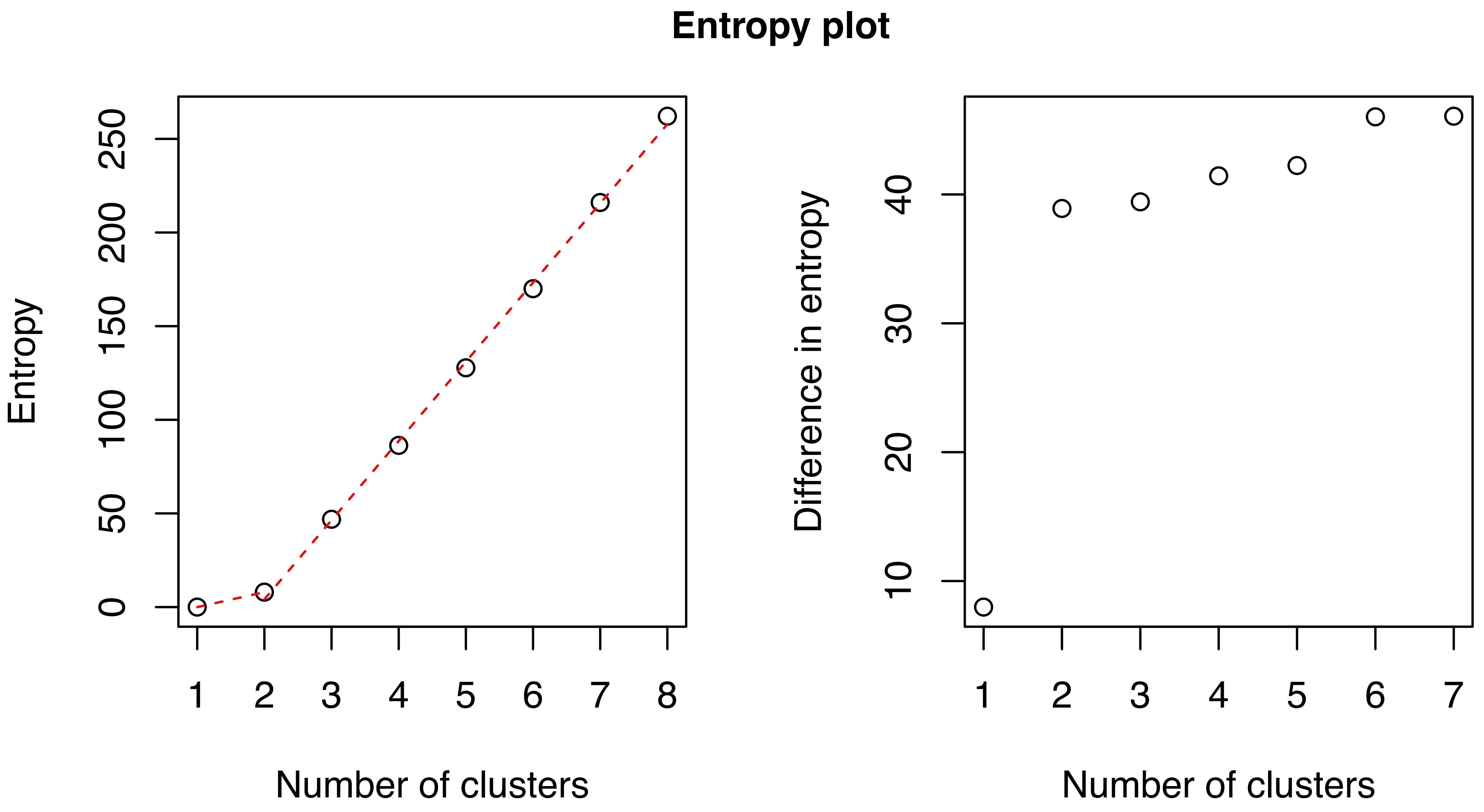
Combined solution with 4 clusters
1.0
0.5
0.0
−0.5
V2
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
V1

Combined solution with 3 clusters




Combined solution with 2 clusters
V2
V1
1.0
0.5
0.0
−0.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0


Combined solution with 1 clusters
V2
1.0
0.5
0.0
−0.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
V1



Entropy plot
Entropy
0
50
100
150
200
250
1 2 3 4 5 6 7 8
Number of clusters
Difference in entropy
10
20
30
40
1 2 3 4 5 6 7
Number of clusters

Clustering other types of things

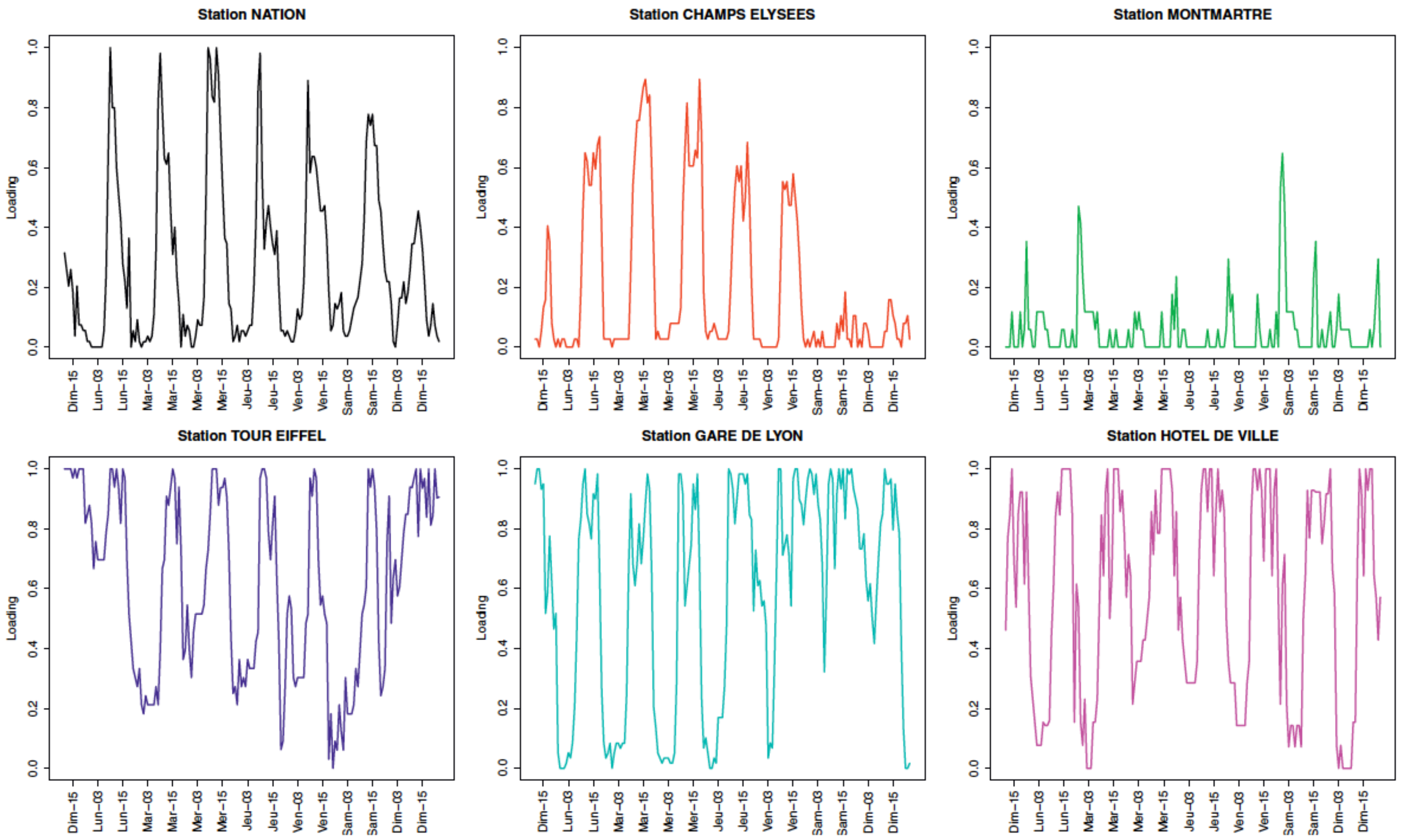
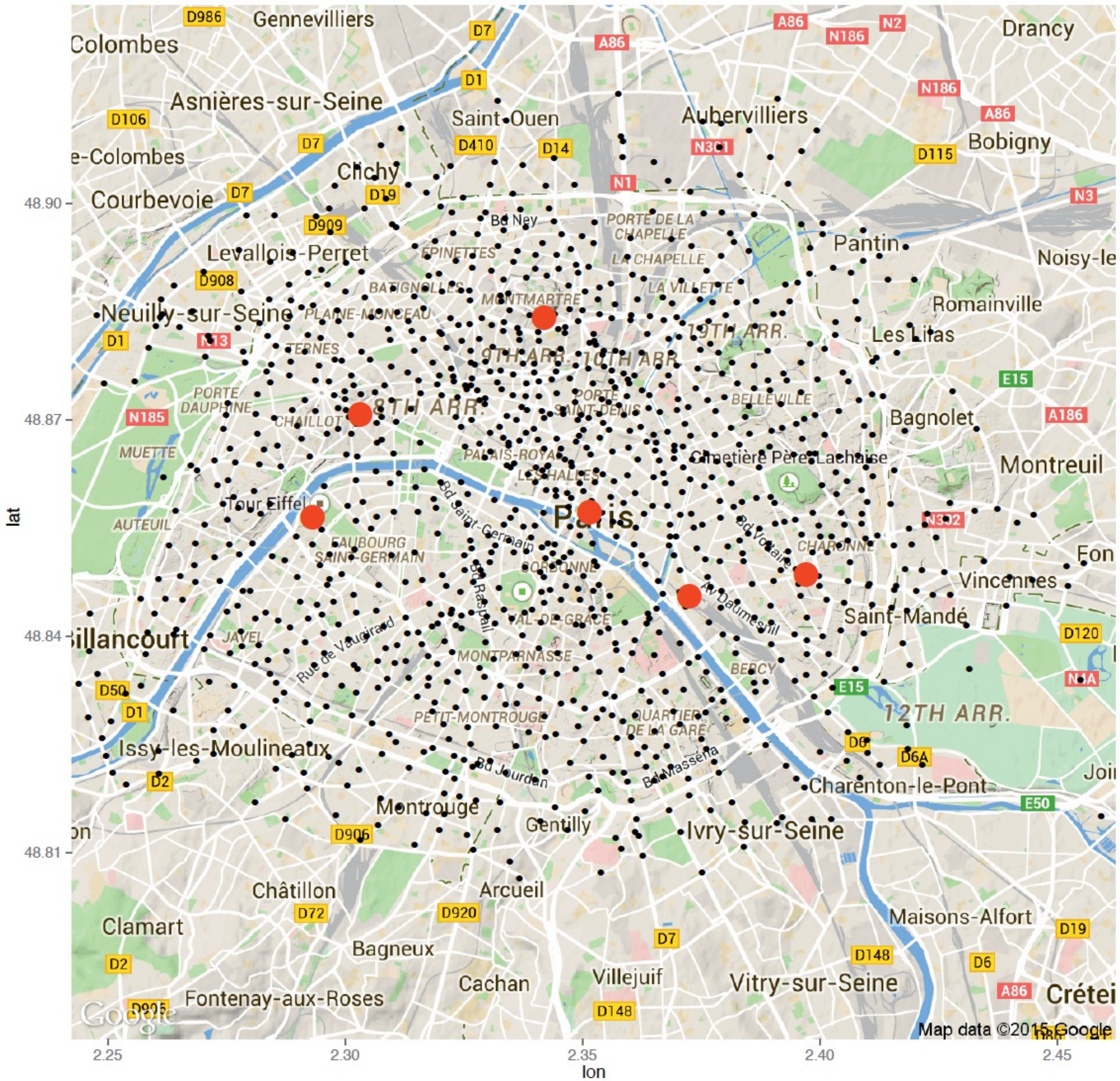


Figure 12.1 Loading profiles of some Vélib stations. A loading value equal to 1 means that the station is full of bikes whereas a value equal to 0 indicates a station without available bikes.

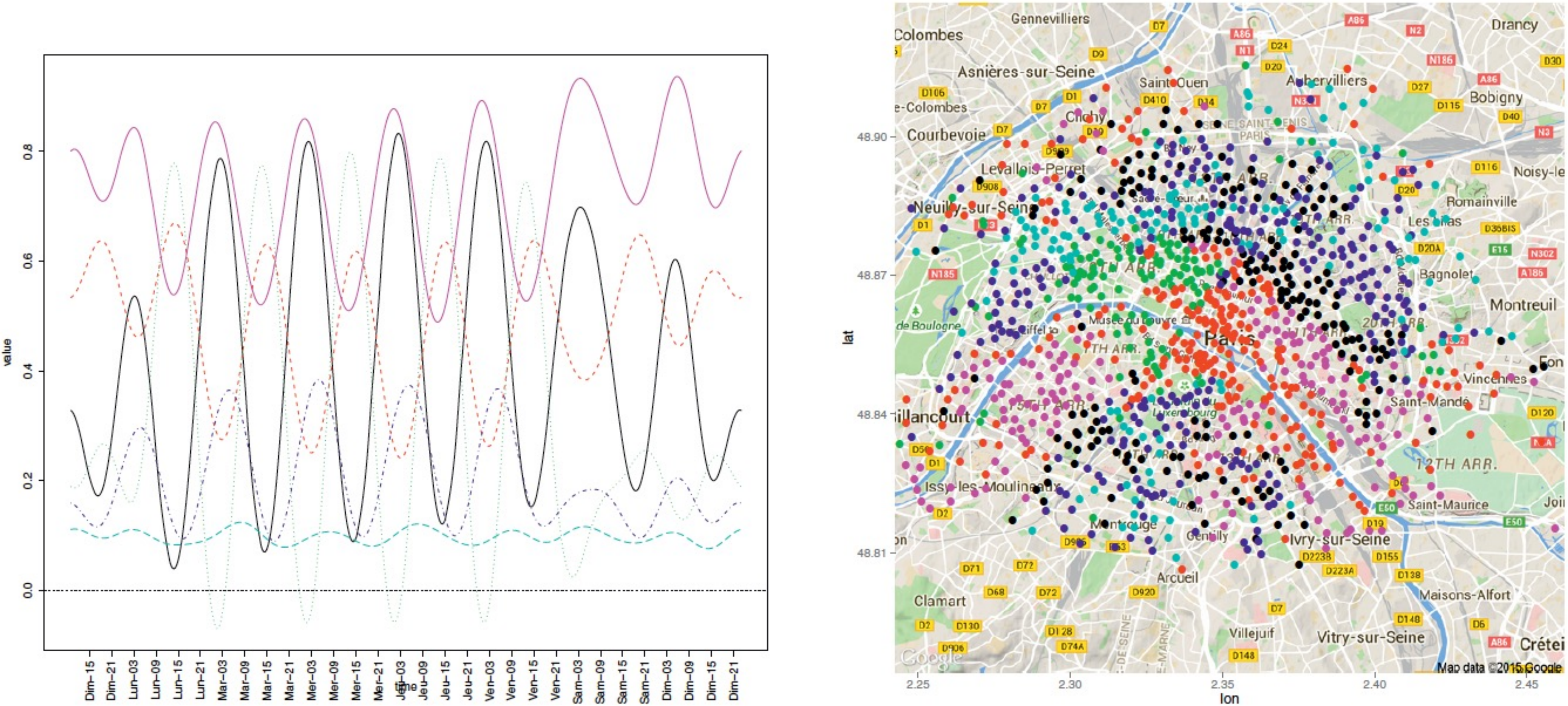
Bouveyron et al. 2018



lat
48.90
48.87
48.84
48.81
lon
2.25
2.30
2.35
2.40
2.45
Colombes
Gennevilliers
Asnières-sur-Seine
Saint-Ouen
Aubervilliers
Drancy
Bobigny
Clichy
Courbevoie
Levallois-Perret
Pantin
Neuilly-sur-Seine
Romainville
Les Lilas
Bagnolet
Montreuil
Paris
Tour Eiffel
Vincennes
Saint-Mandé
Issy-les-Moulineaux
Montrouge
Gentilly
Ivry-sur-Seine
Charenton-le-Pont
Châtillon
Arcueil
Clamart
Bagneux
Cachan
Villejuif
Vitry-sur-Seine
Maisons-Alfort
Fontenay-aux-Roses
Map data ©2015 Google

“functional data” clustering in R

```
# Loading libraries and data
library(funFEM)
data(velib)

# Transformation of the raw data as curves
basis = create.fourier.basis(c(0, 181) , nbasis =25)
fdobj = smooth.basis (1:181 ,t(velib$data),basis)$fd

# Clustering with funFEM
res = funFEM(fdobj ,K=6)
```



(a) Cluster mean functions

(b) Map of clustered stations

Figure 12.6 Cluster mean functions and map of clustered stations by funFEM on the Vélib data set.

Conclusion

- **Model-based clustering:**
  1. Pretend we believe in a model;
  2. Estimate the model.
- Algorithm is defined by the model;
- Easy to think about assumptions;
- Flexible in using other data types;
- Common model: GMM (implementation `mclust` in R);
- Secret weapon: component merging.