Clustering and the k-means Algorithm

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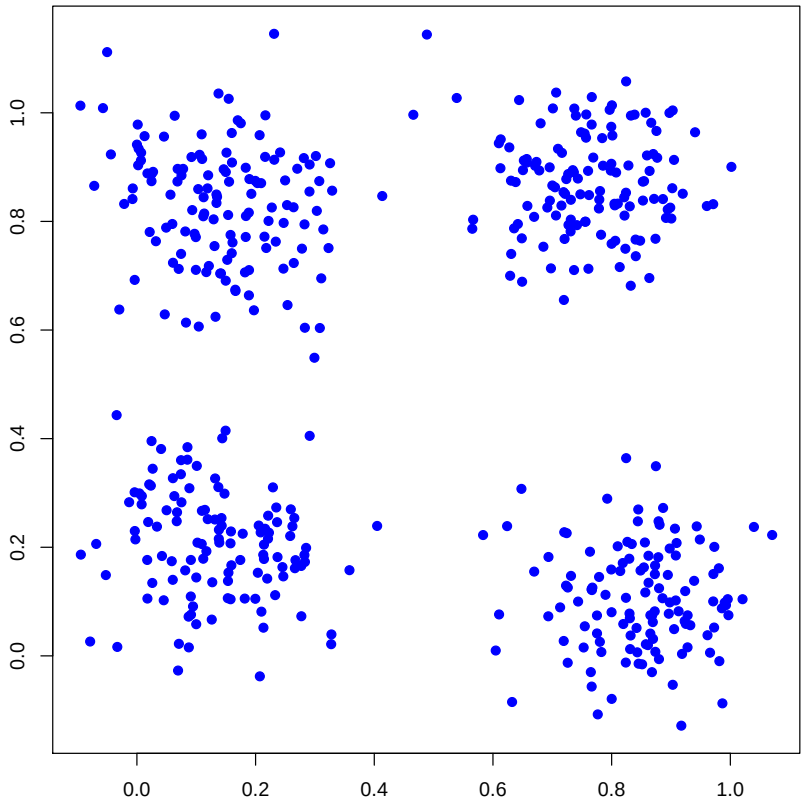
- Define a *distance function* between data, $d(\mathbf{x}_n, \mathbf{x}_m)$.
- Goal: segment the data into k groups

$$\{z_1, \ldots, z_N\} \quad \text{where} \quad z_i \in \{1, \ldots, K\}.$$

Example data



500 2-dimensional data points: $\mathbf{x}_n = \langle x_{n,1}, x_{n,2} \rangle$

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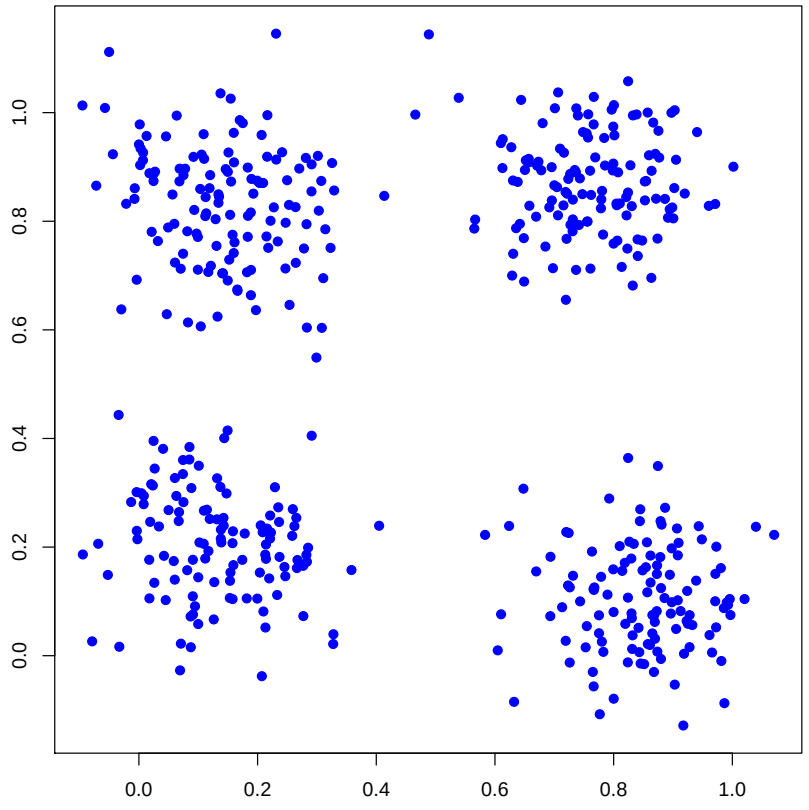

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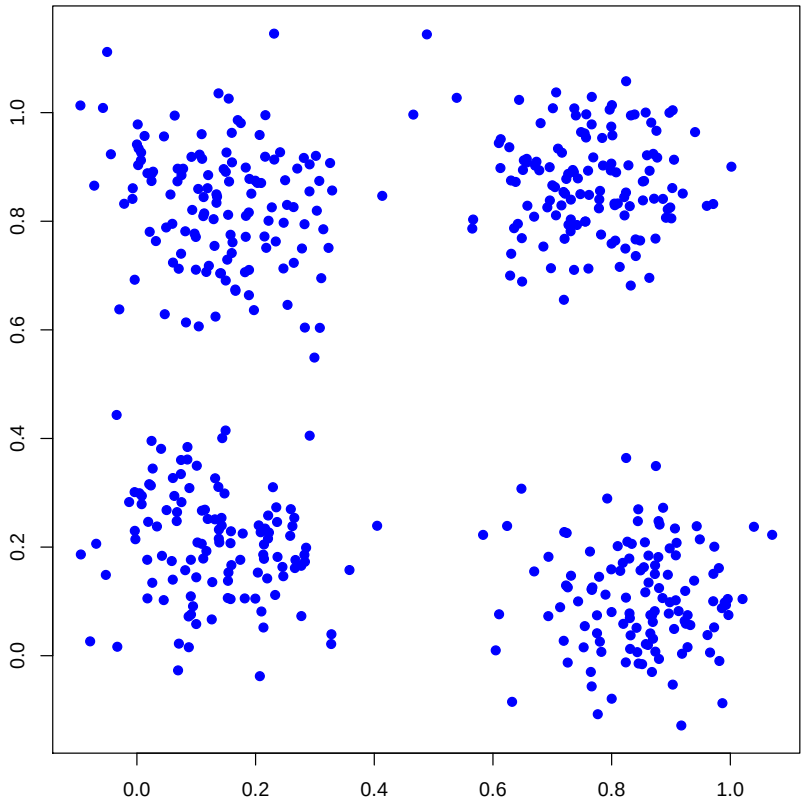
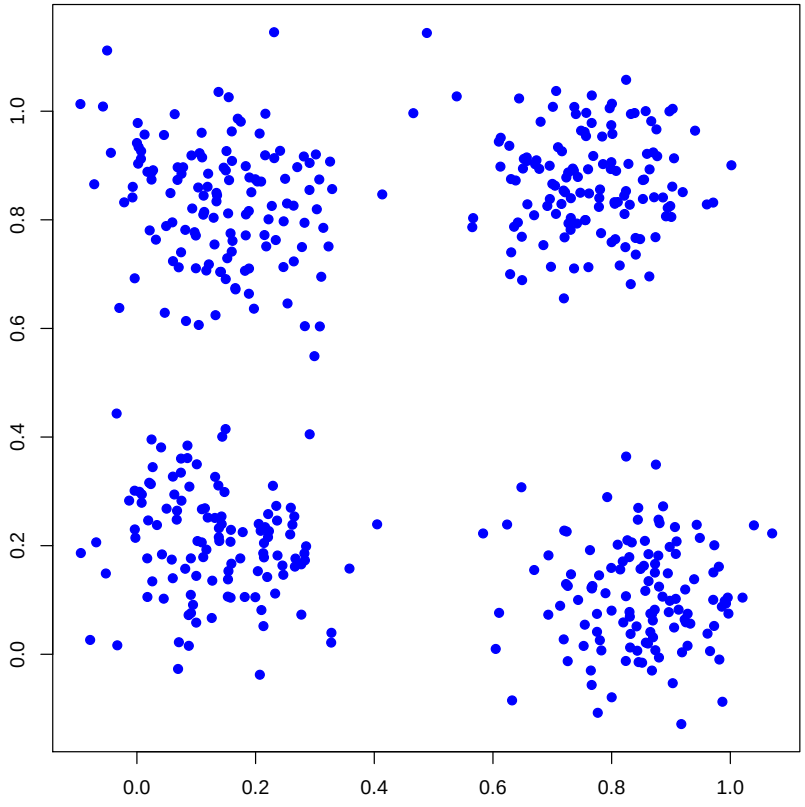


- What is a good distance function here?
- Squared Euclidean distance is reasonable

$$d(\mathbf{x}_n, \mathbf{x}_m) = \sum_{i=1}^{p} (x_{n,i} - x_{m,i})^2 = \|x_n - x_m\|^2$$

Example data



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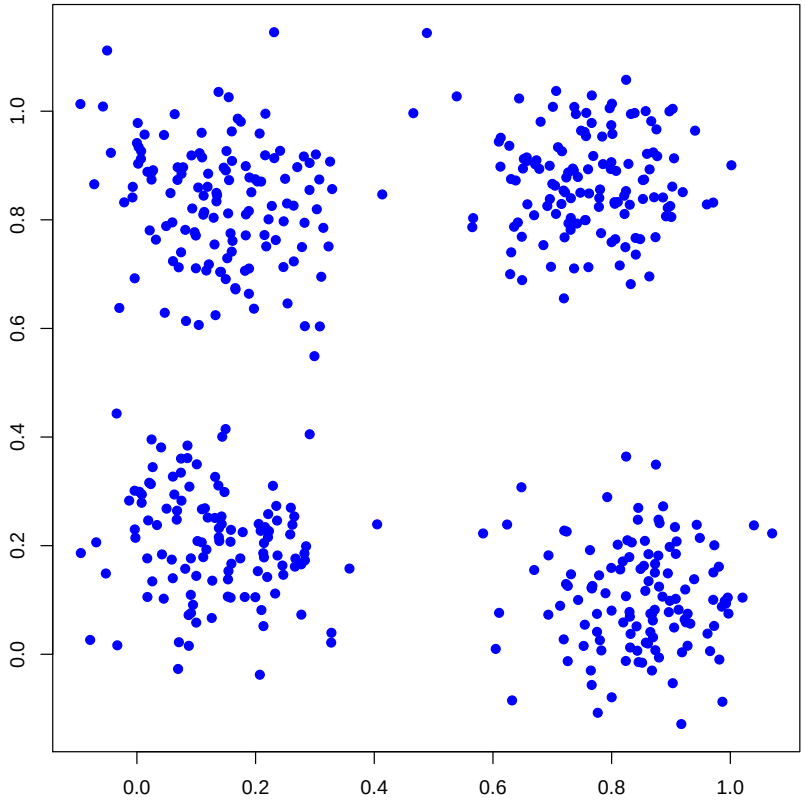

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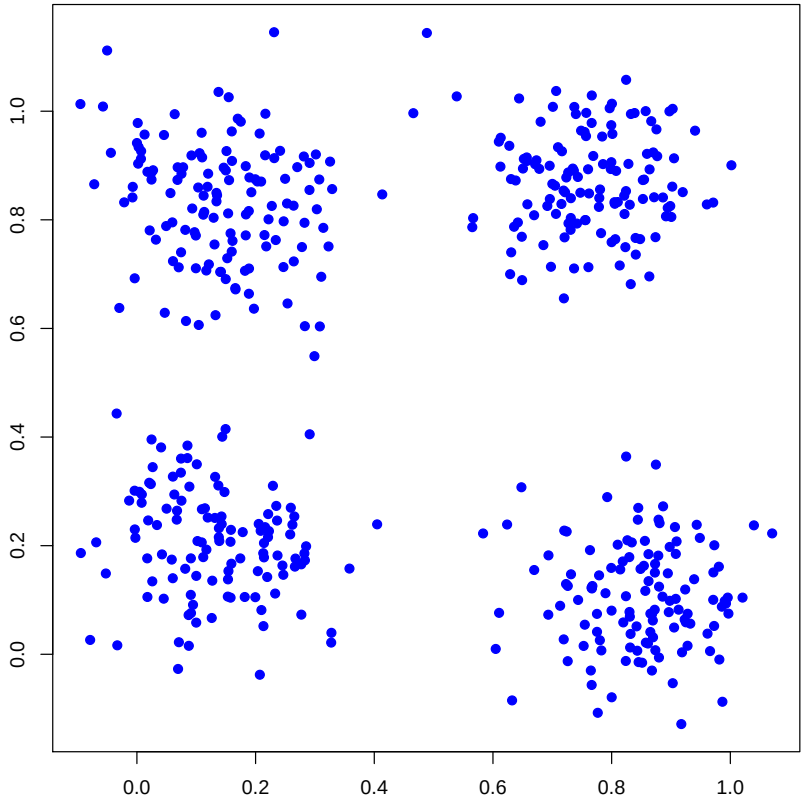

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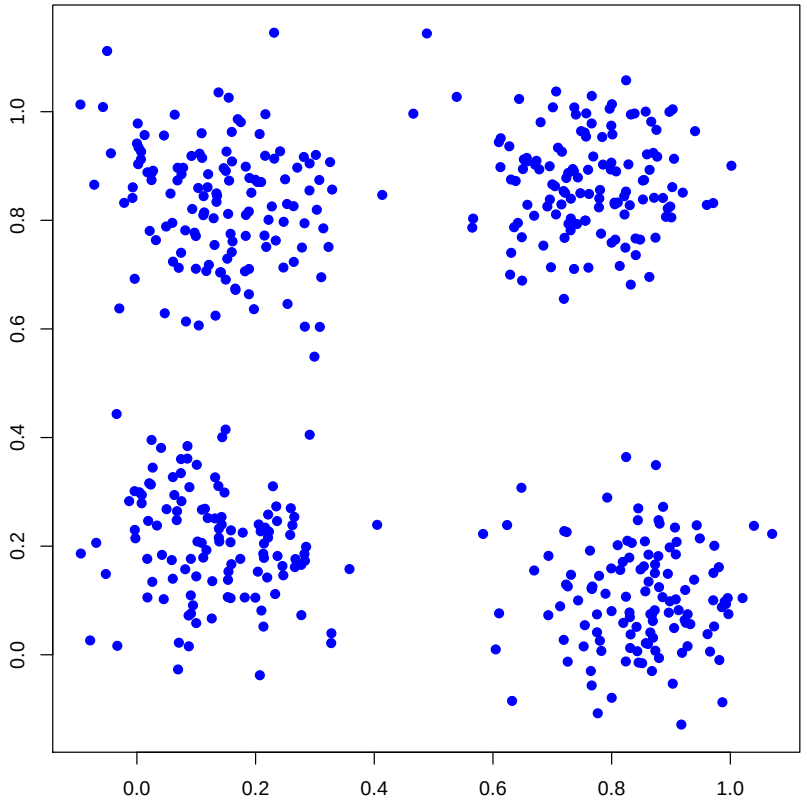
- What should k be?
- Automatically choosing k is complicated; for now, 4.

k-means



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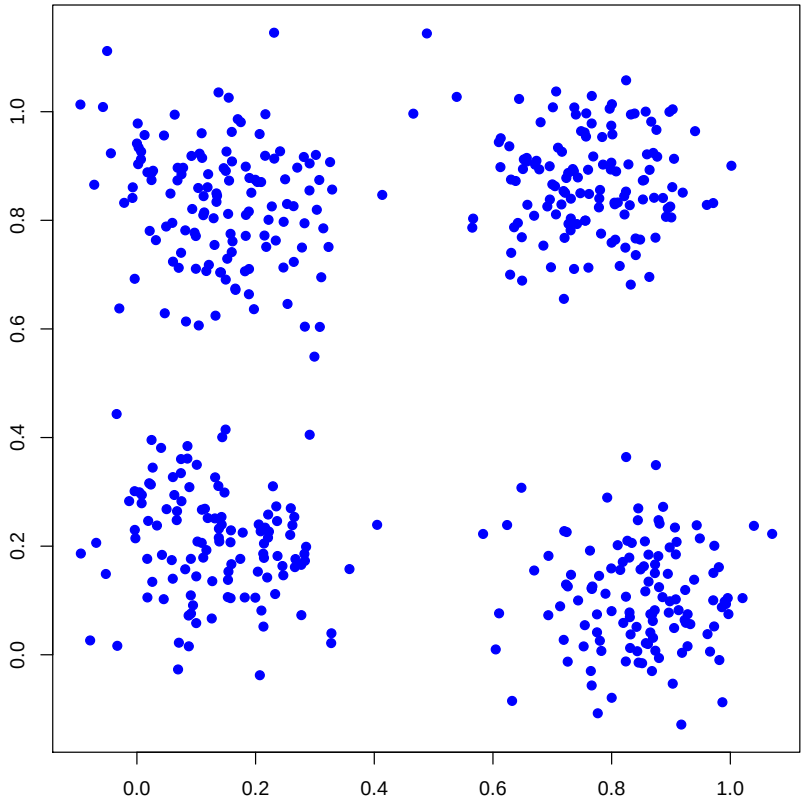

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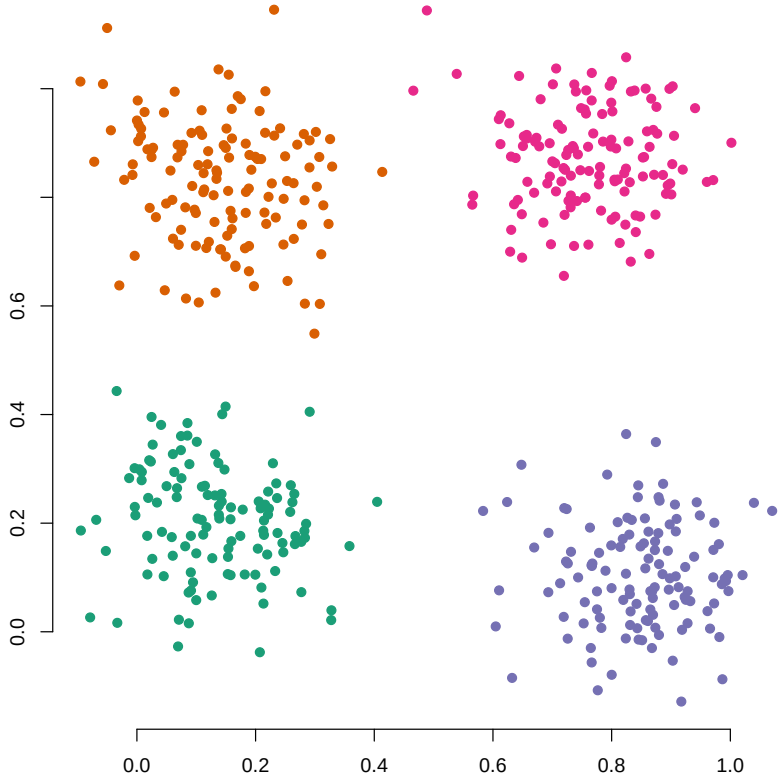

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- The goal of *k*-means is to assign data to clusters and define these clusters with their means.

k-means algorithm

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3. Until assignments $\mathbf{z}_{1:N}$ do not change

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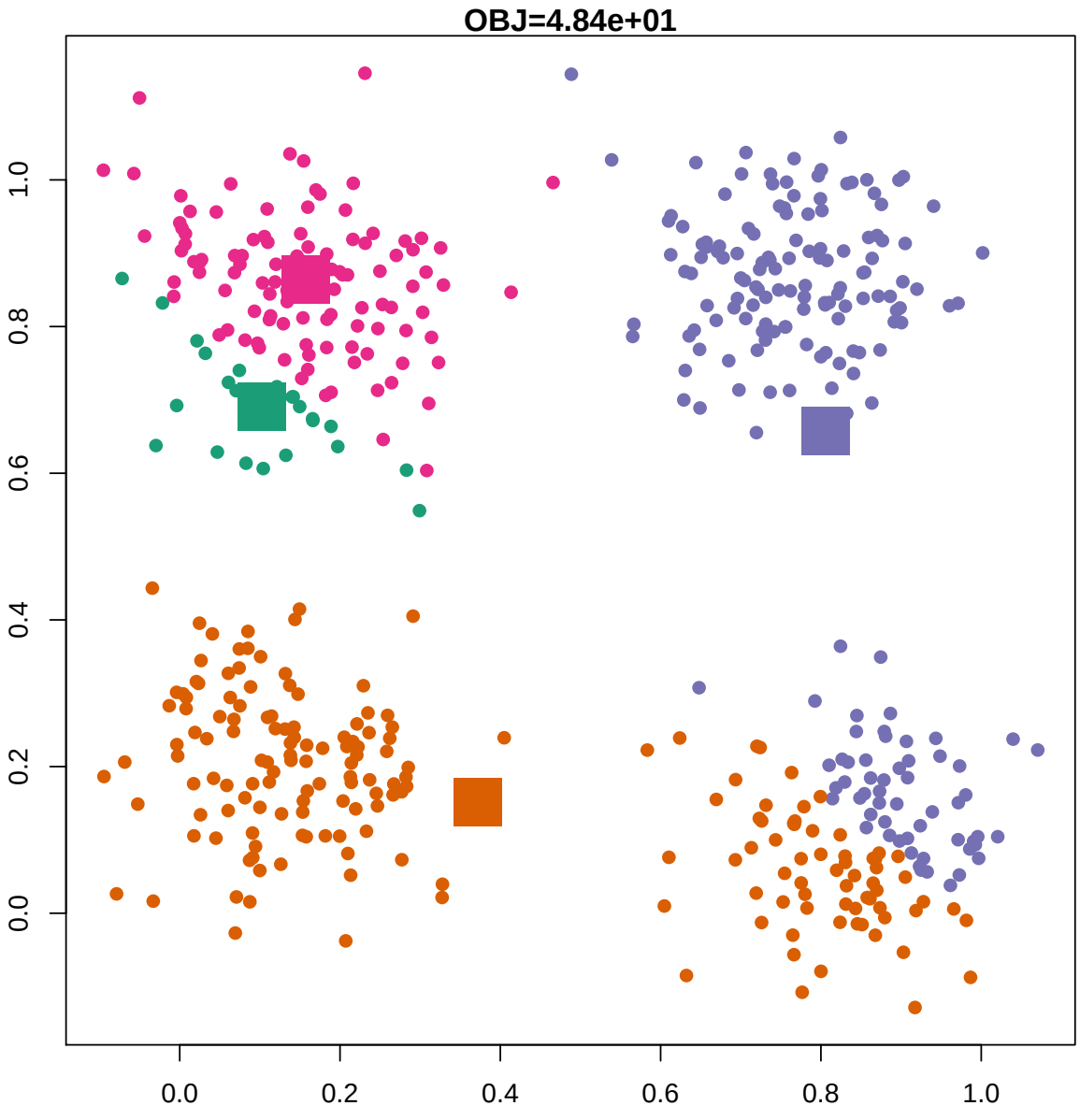

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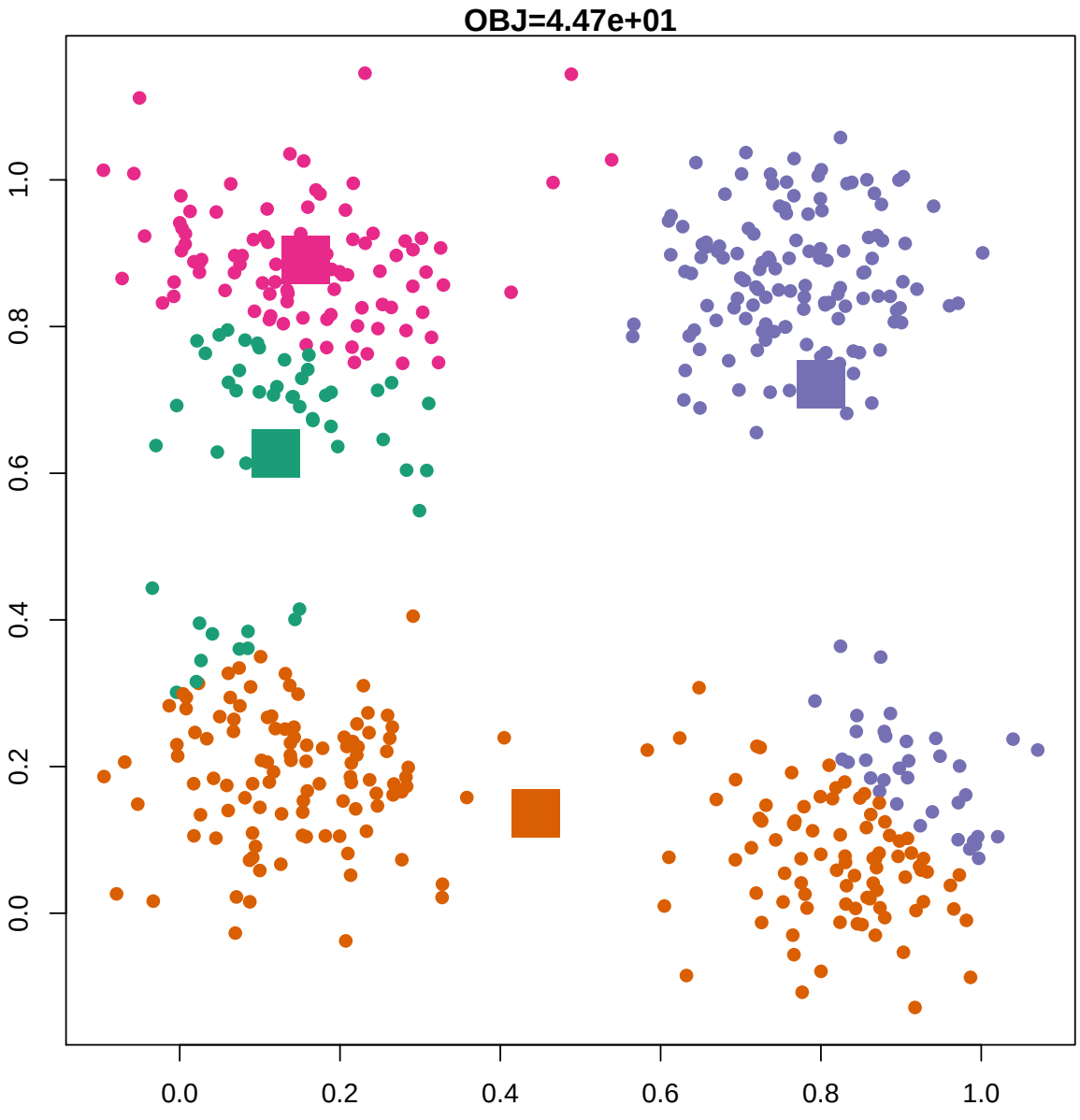

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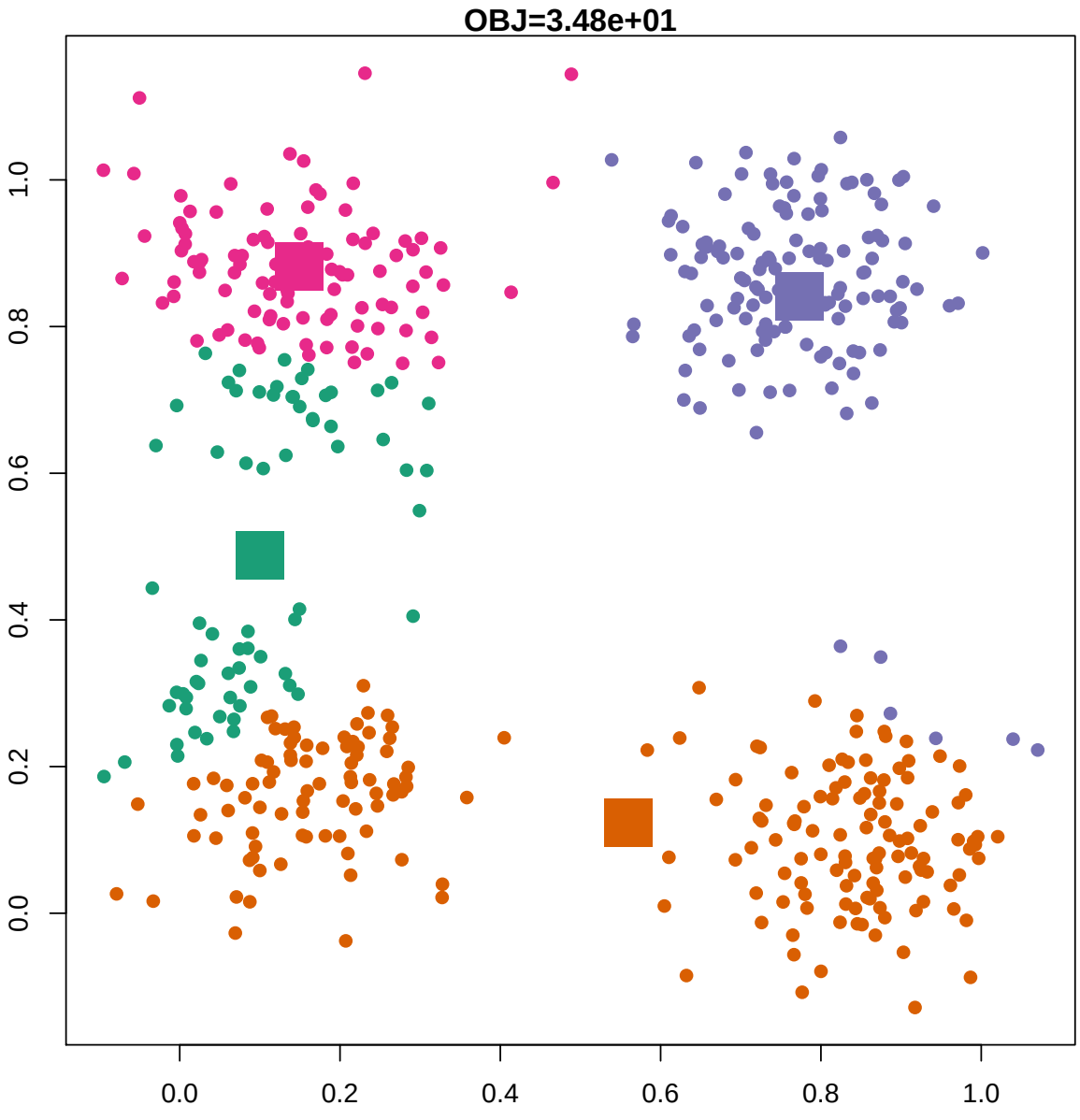

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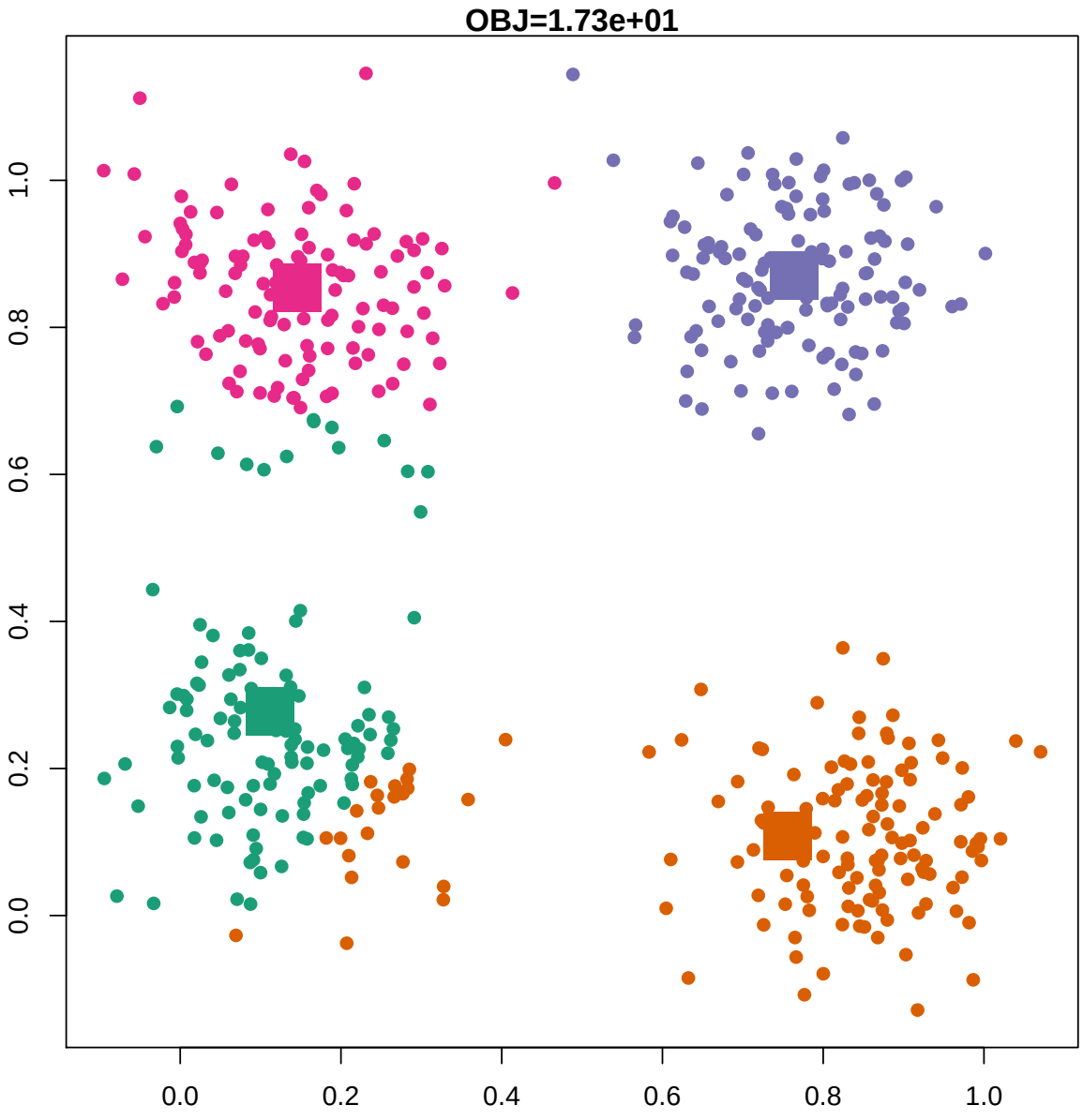

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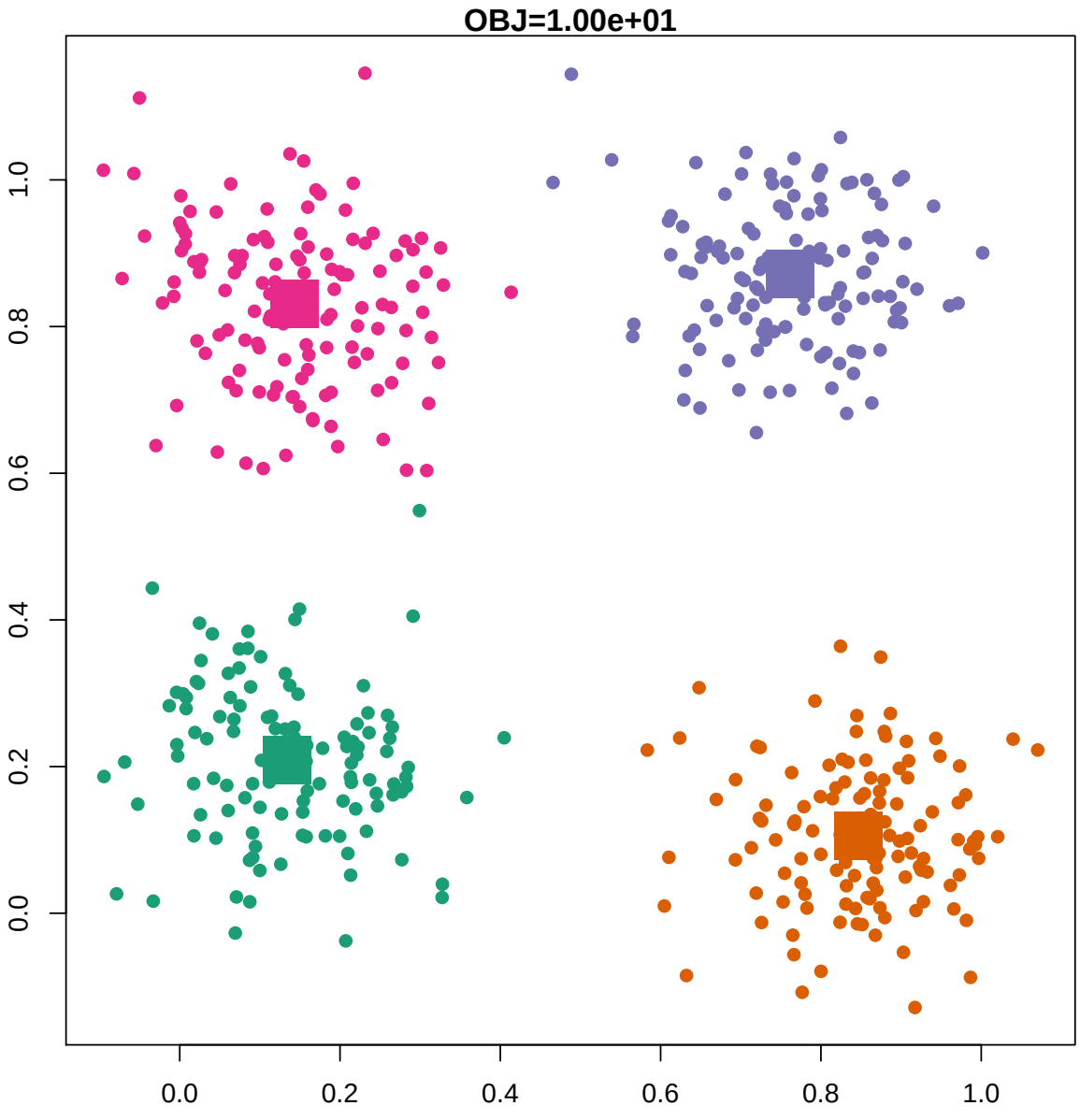

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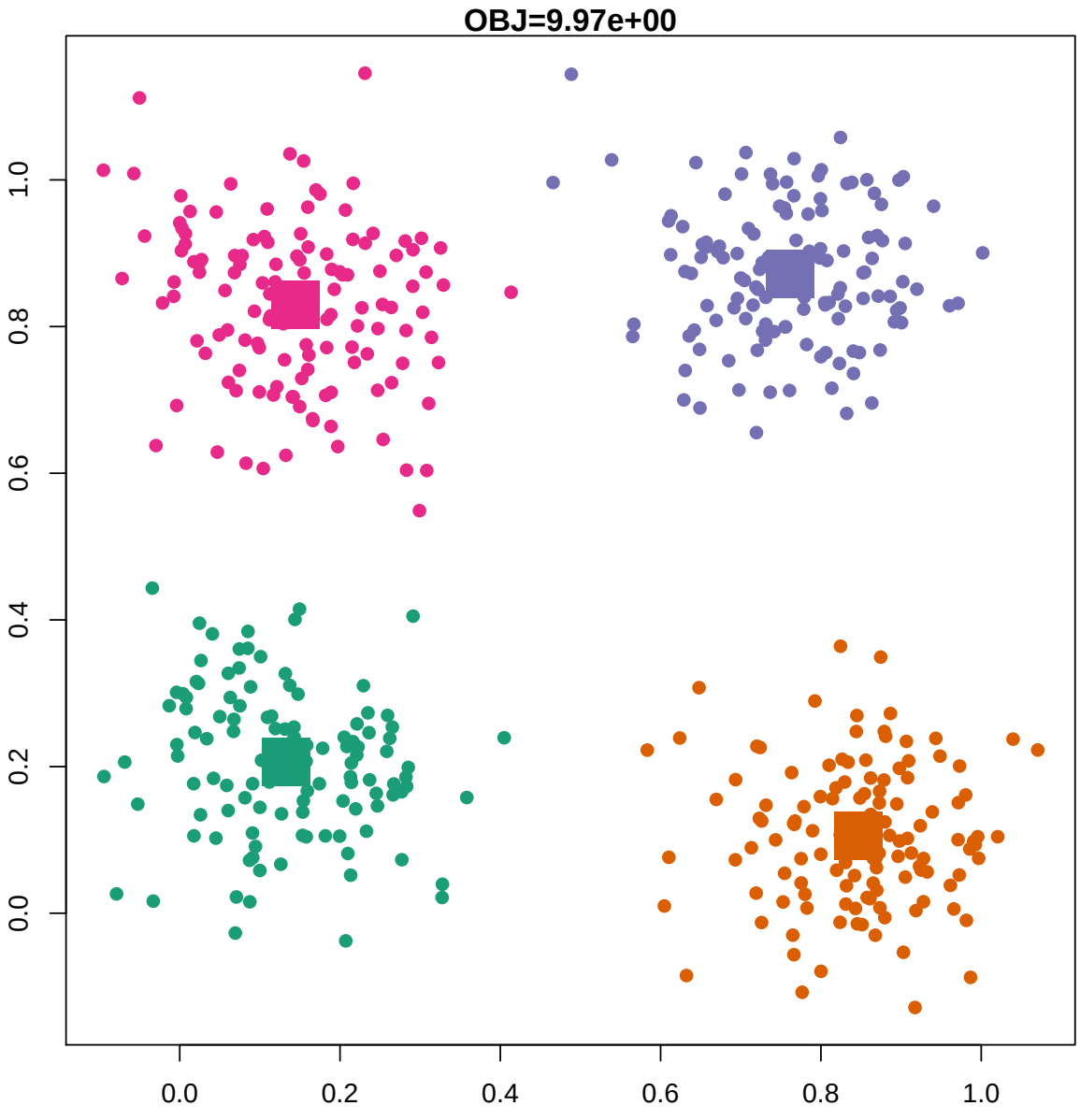

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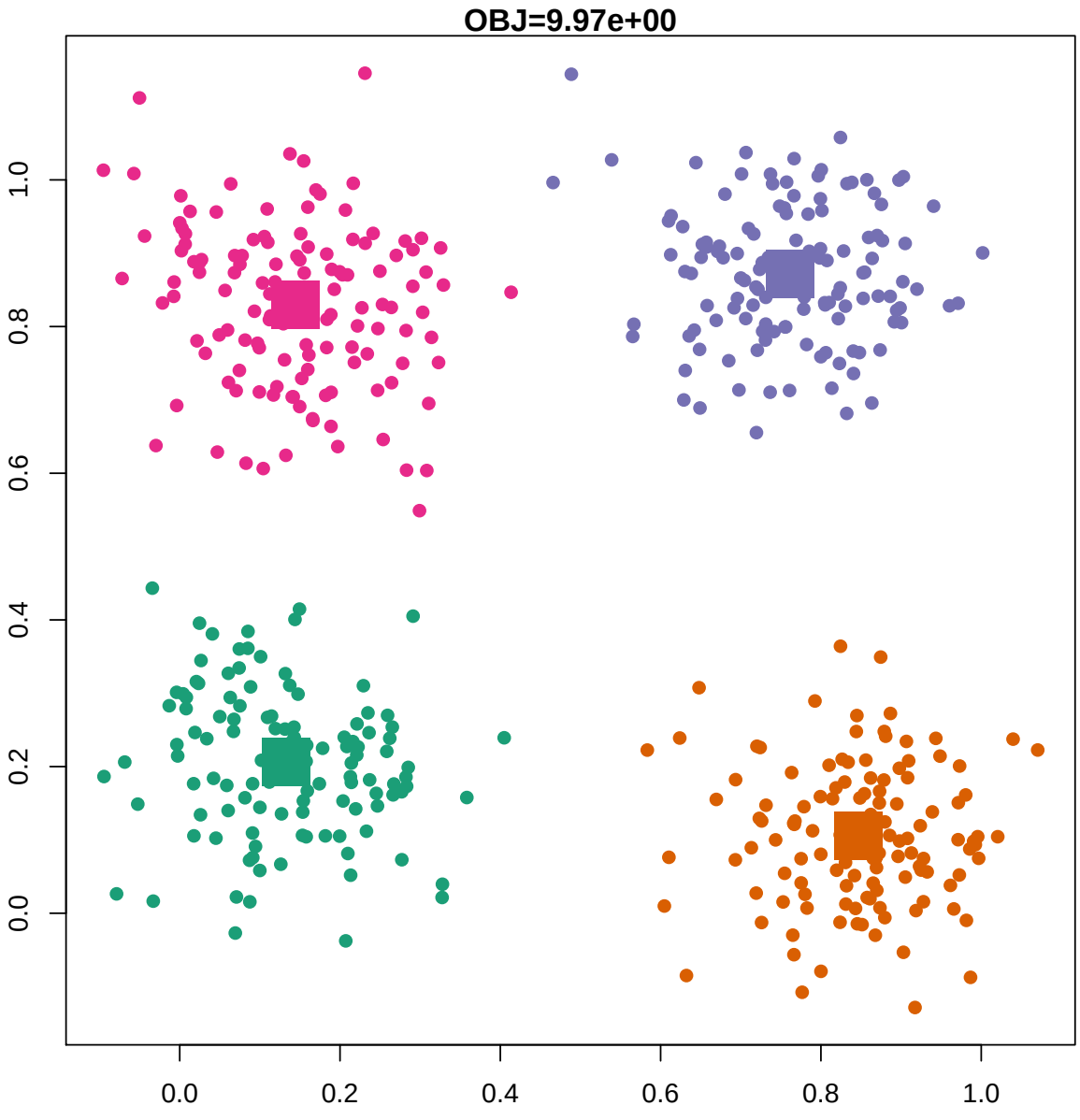

Objective function

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- The k-means objective function is the sum of the squared distances of each point to each assigned mean

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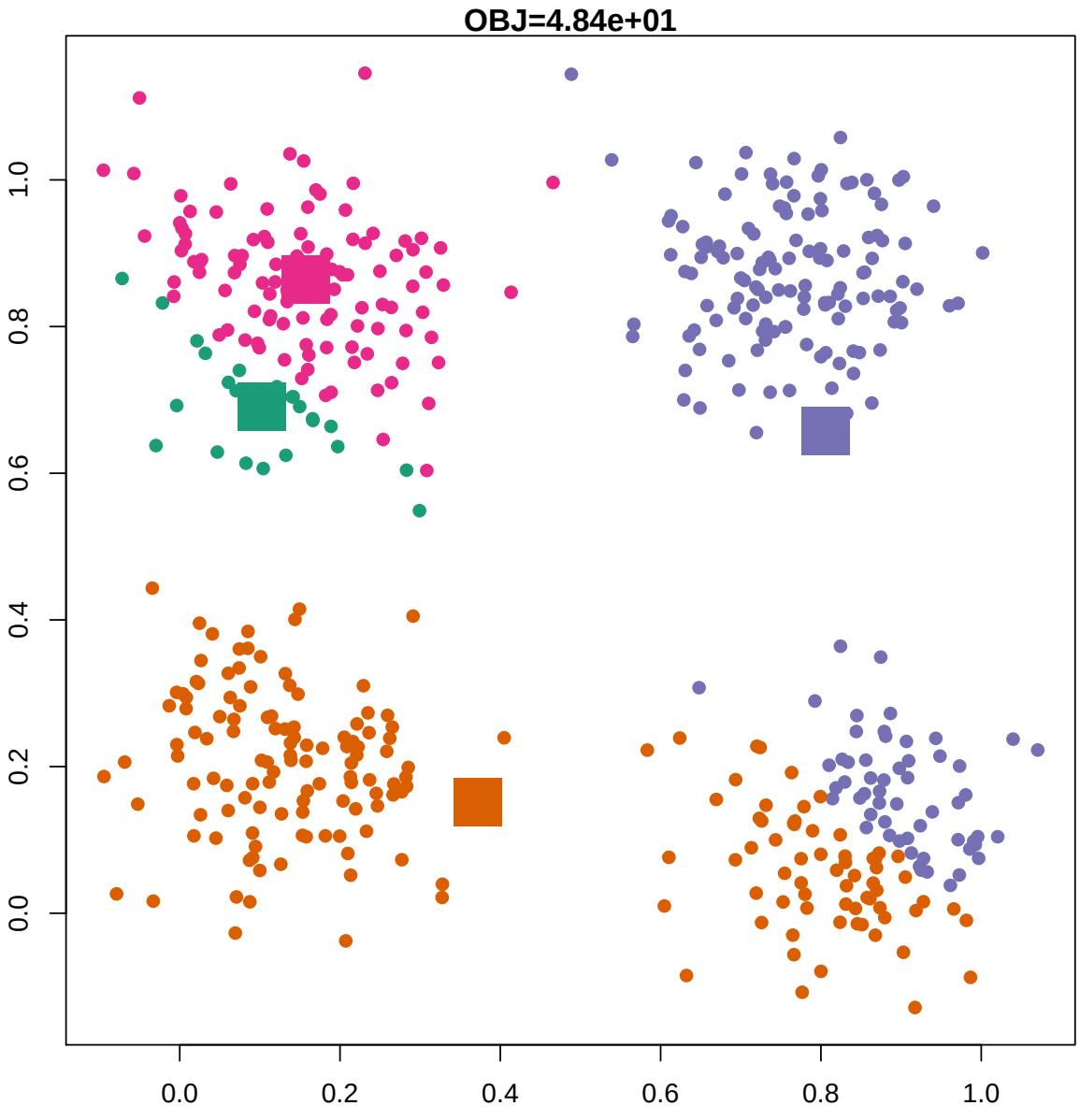
k-means example (look at the objective)



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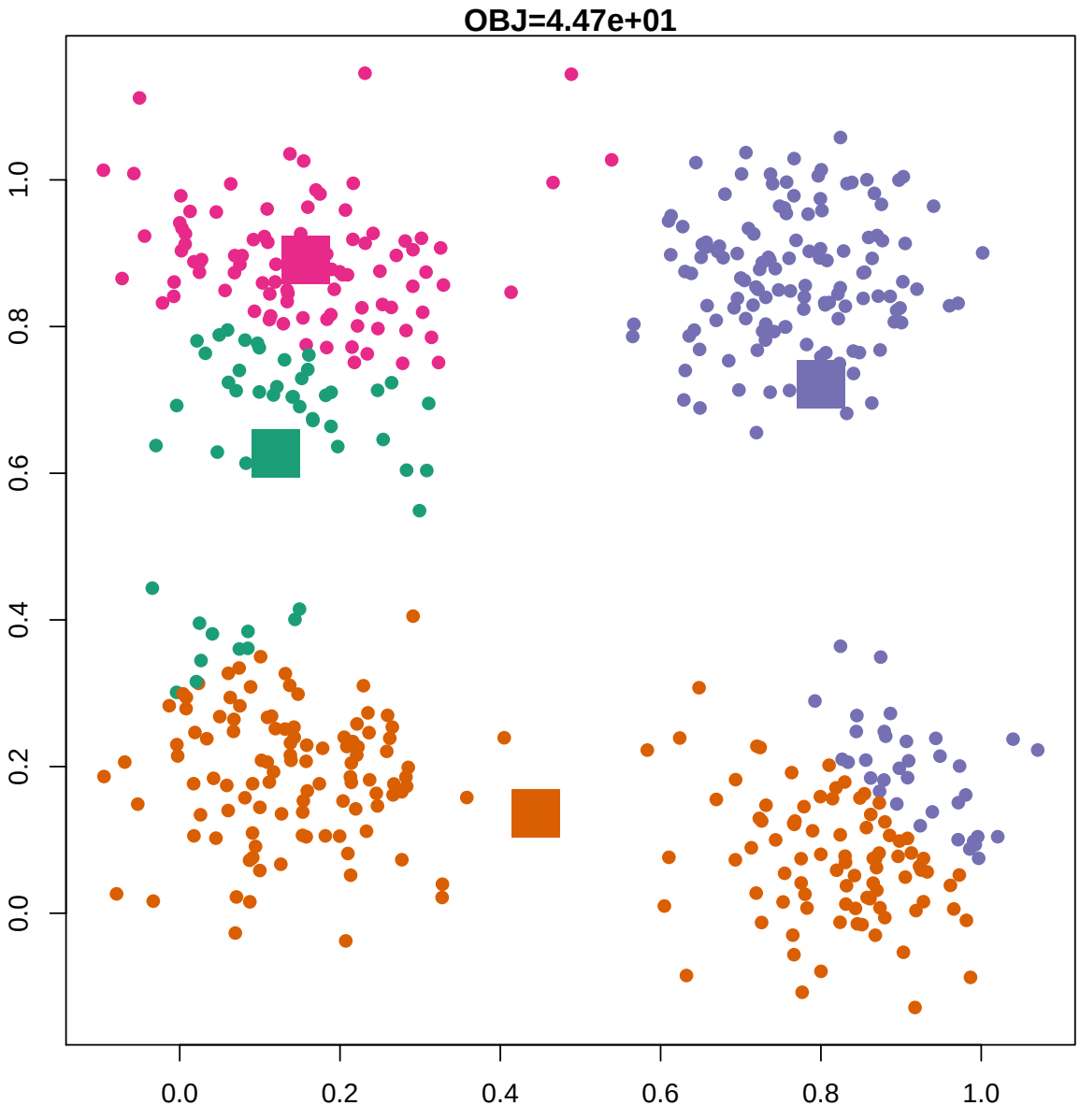

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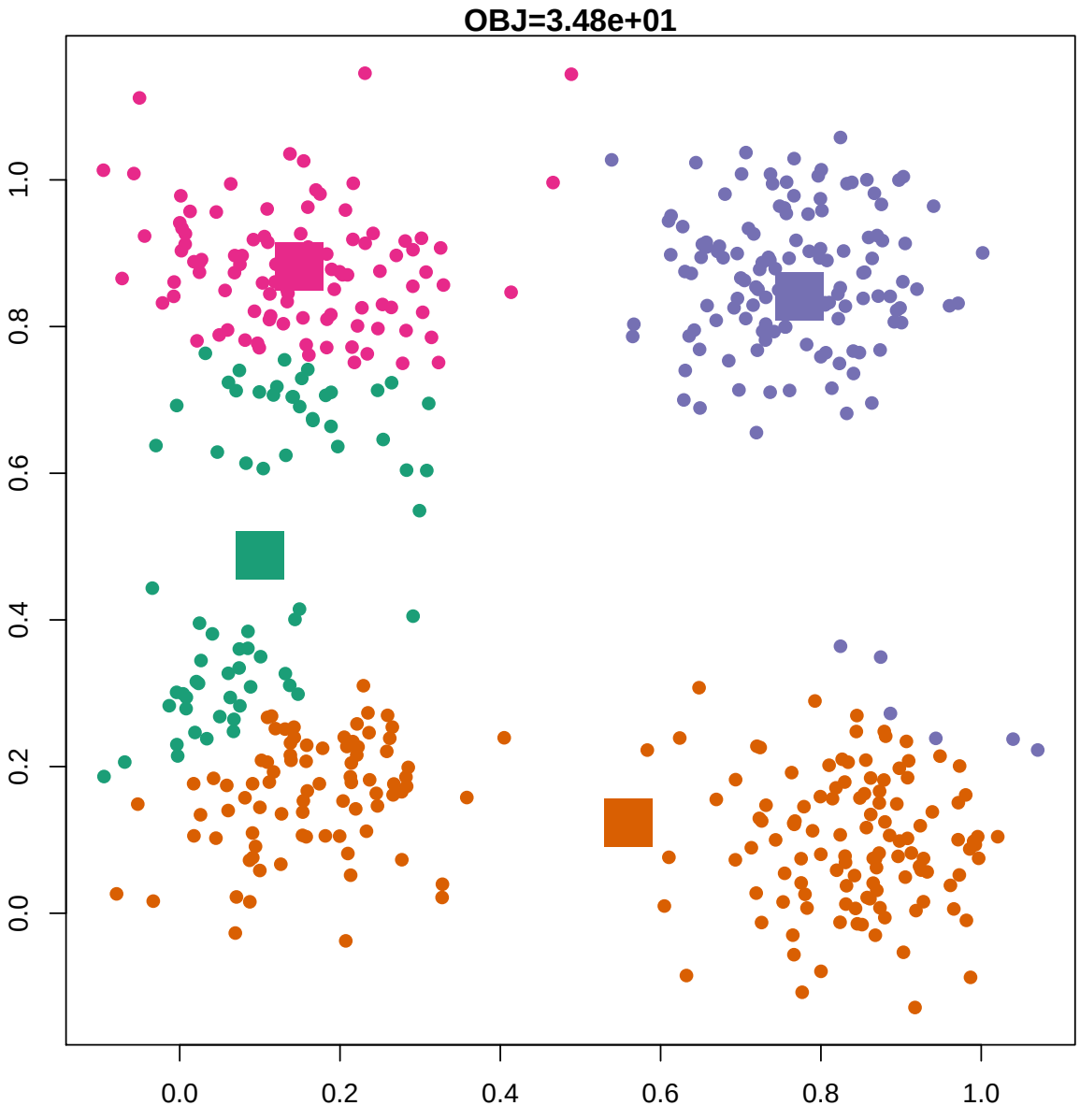

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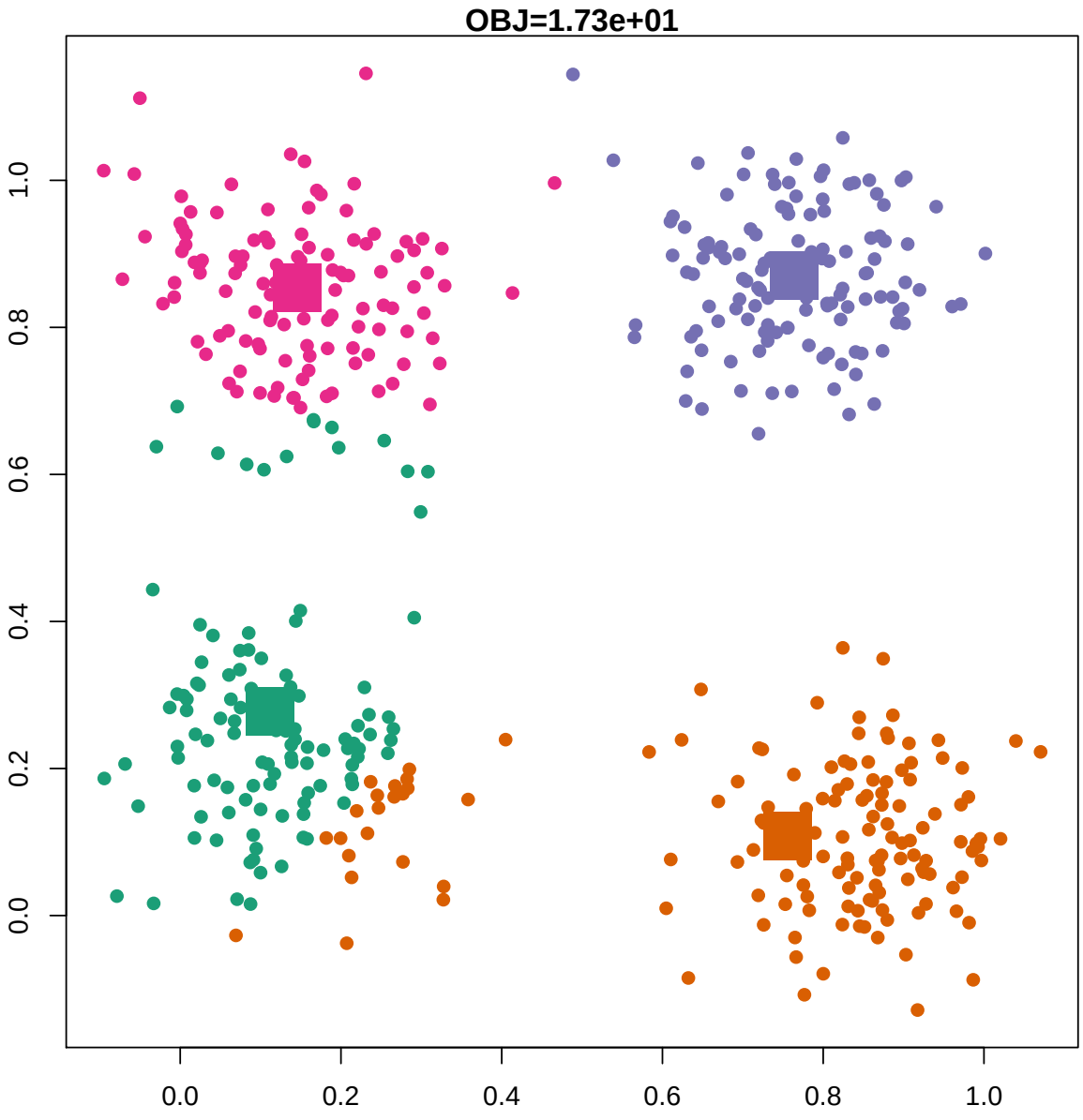

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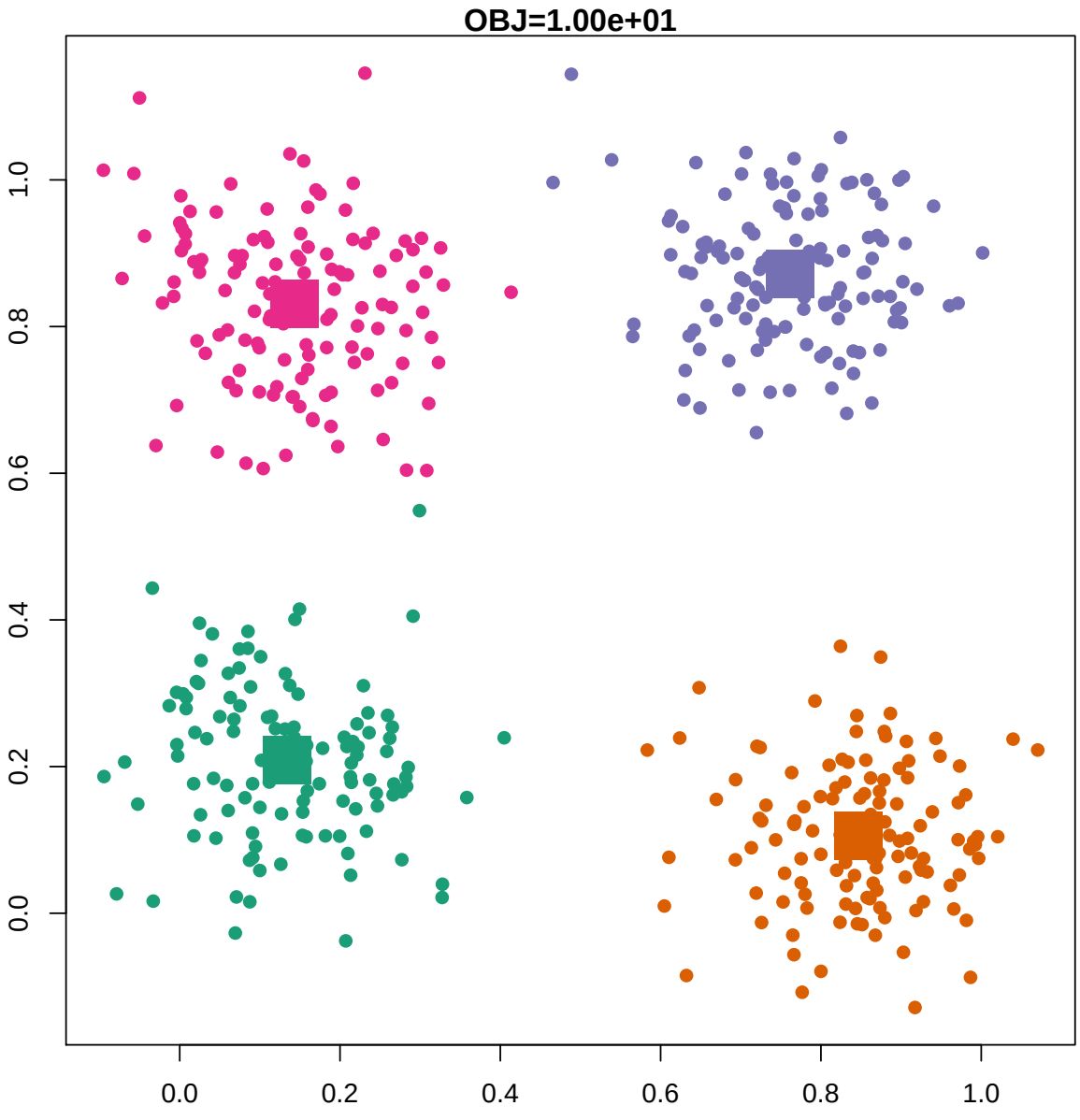

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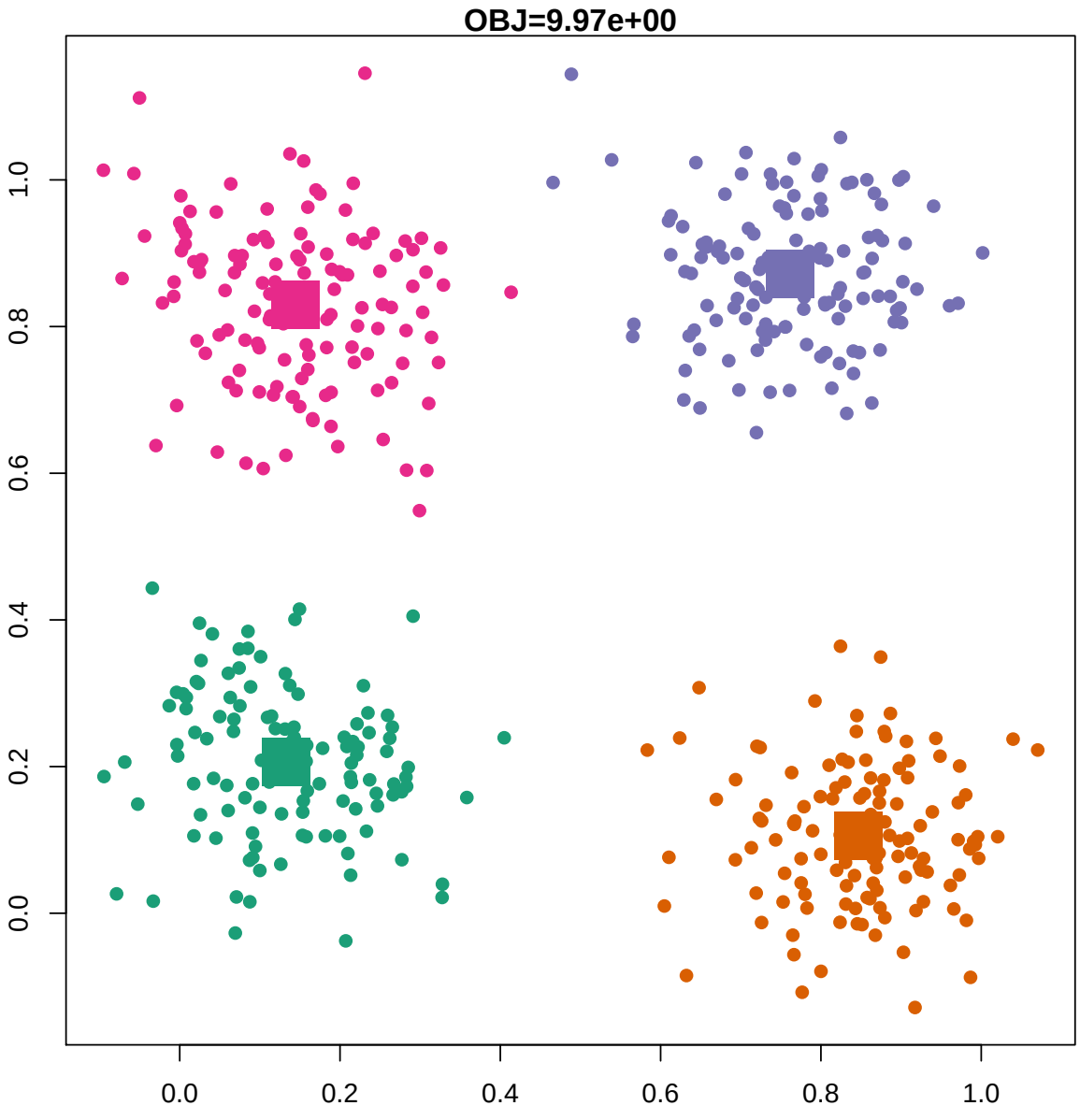

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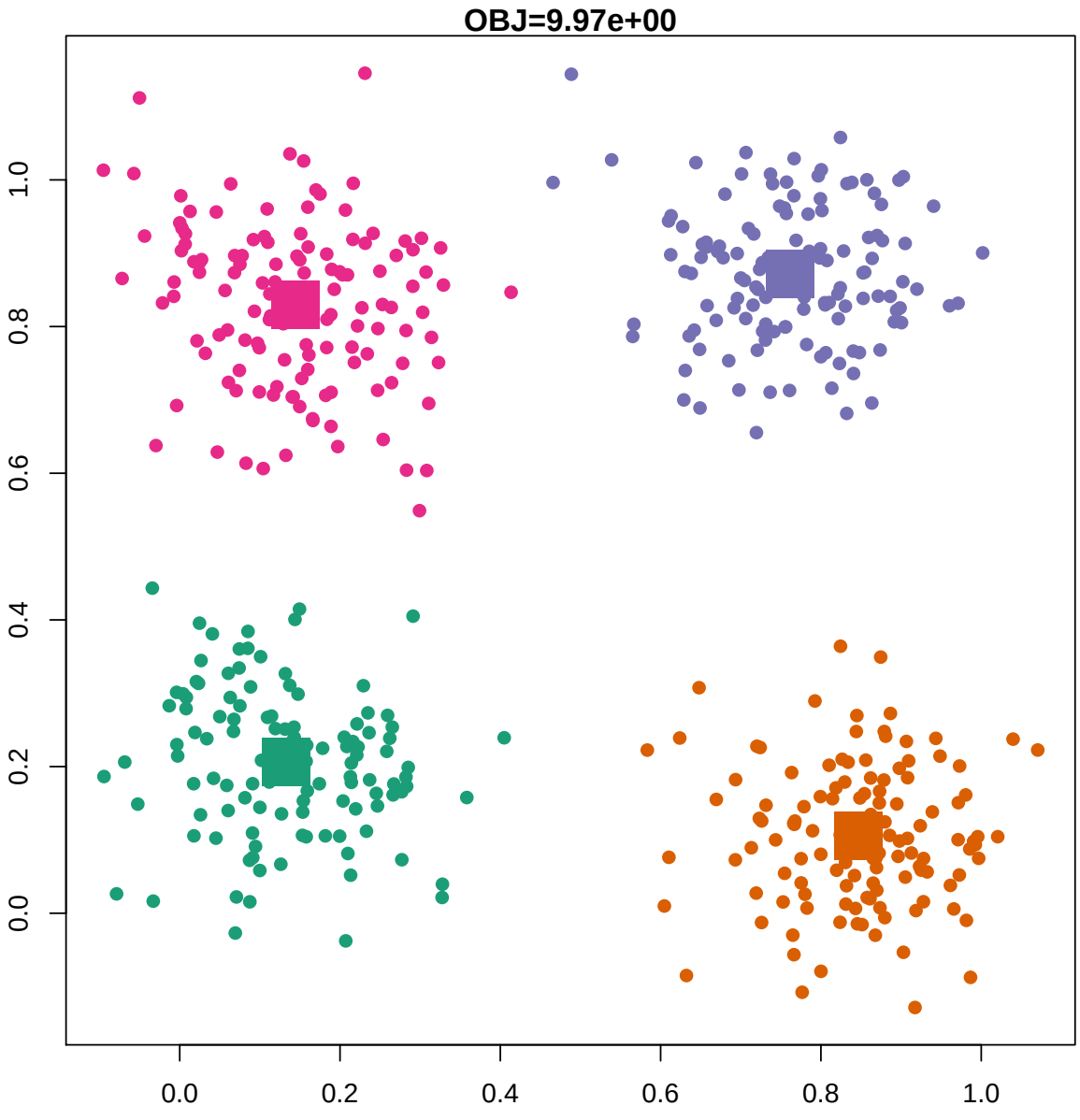

Coordinate descent

$$F(z_{1:N}, \mathbf{m}_{1:k}) = \frac{1}{2} \sum_{n=1}^{N} ||\mathbf{x}_n - \mathbf{m}_{z_n}||^2$$

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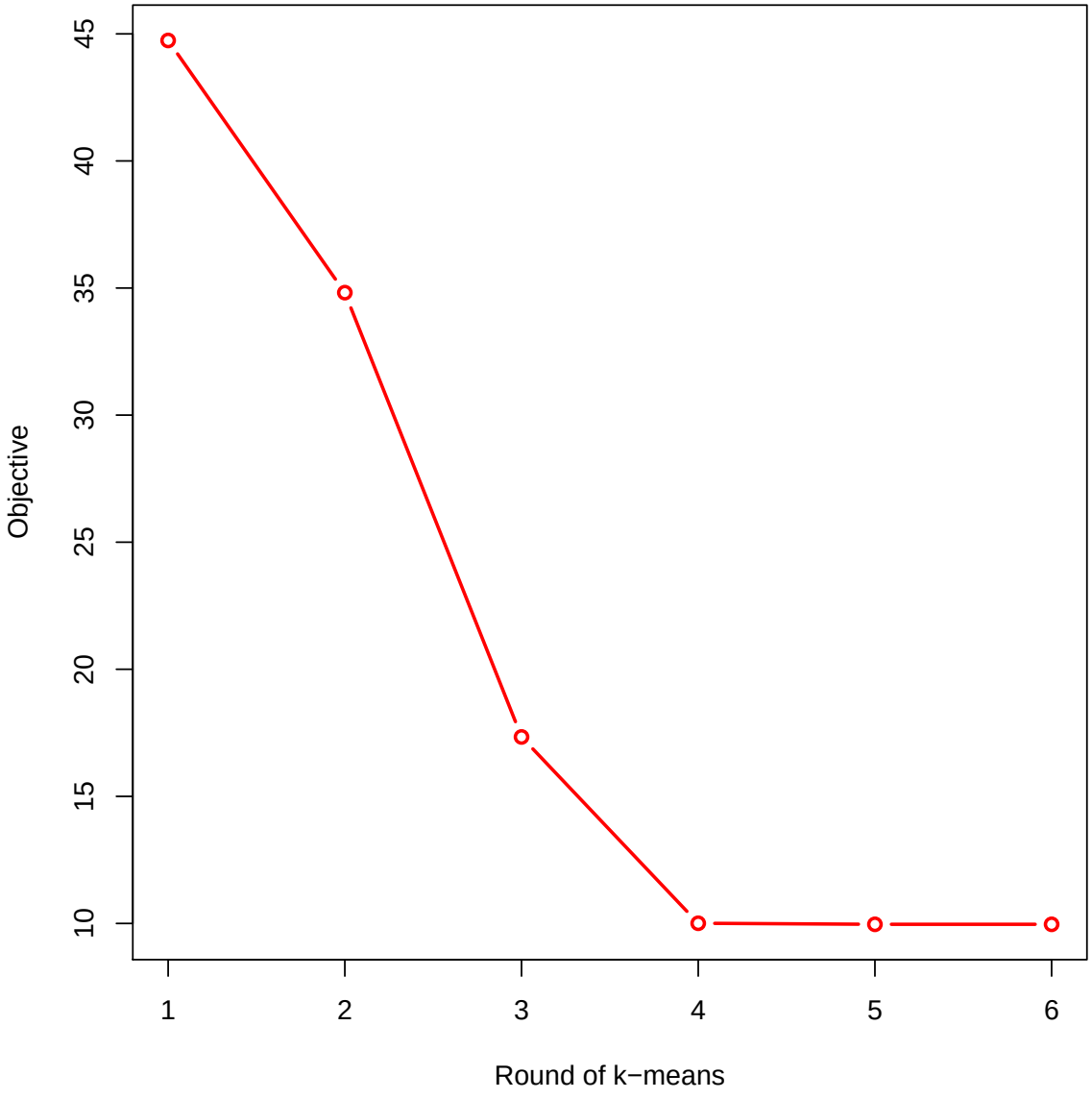
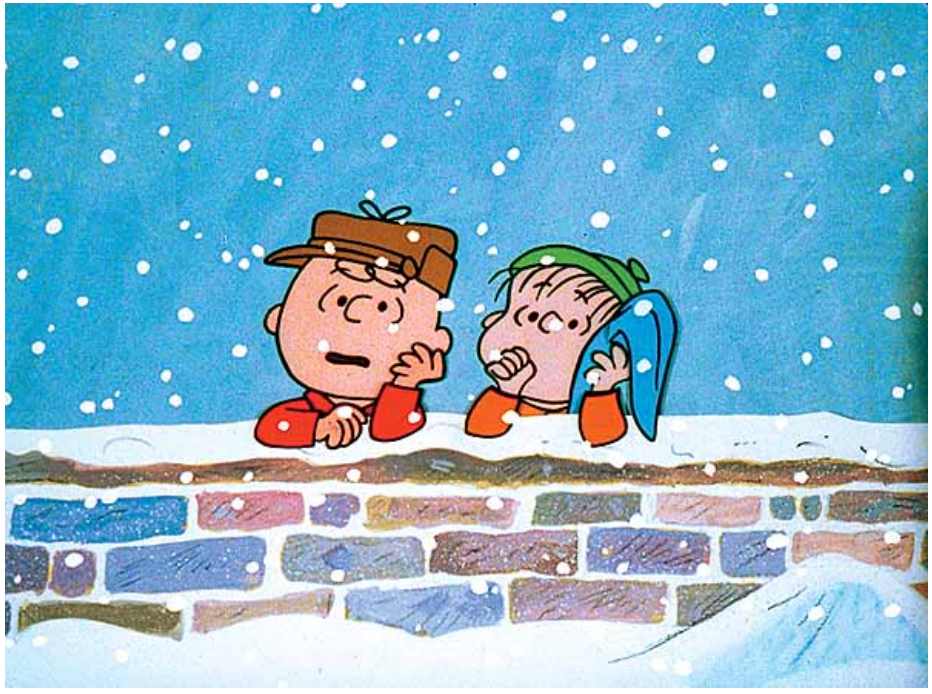
- Thus, k-means is a *coordinate descent* algorithm.
- It finds a *local minimum*. (Multiple restarts are often necessary.)

Objective for the example data



Compressing images



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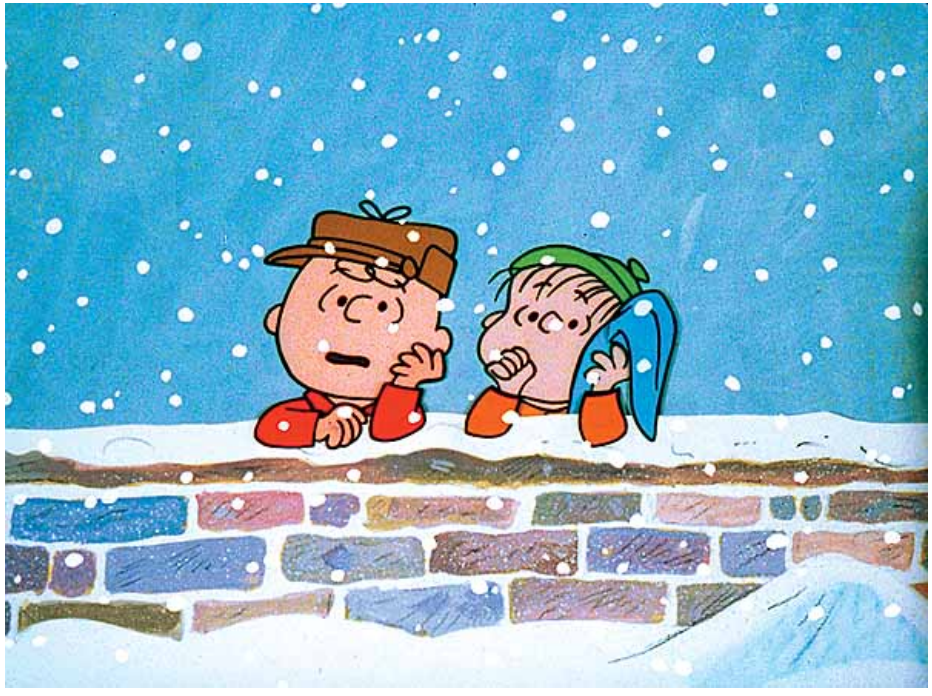

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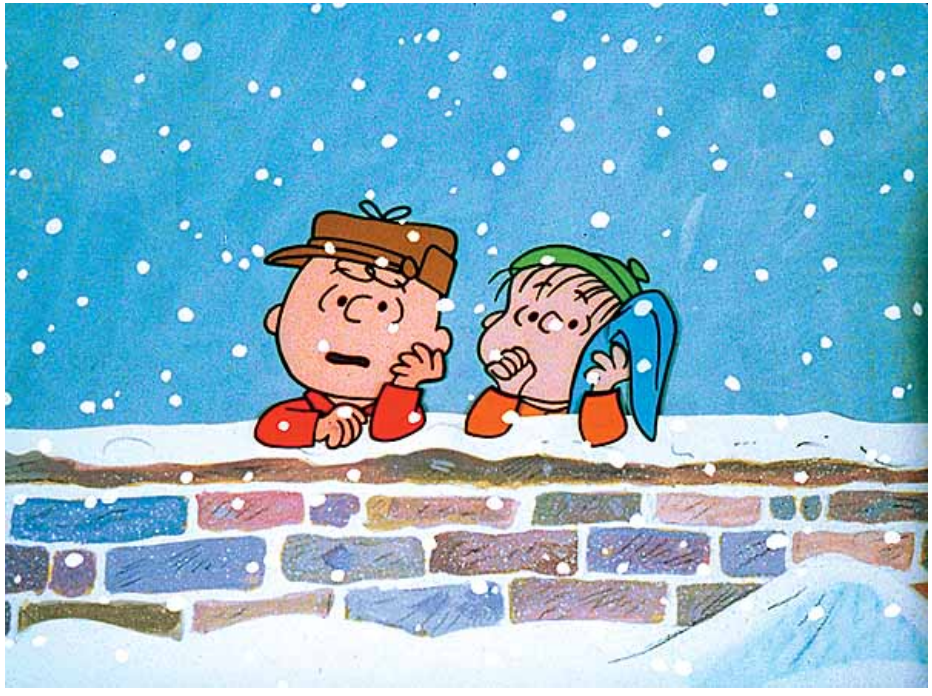

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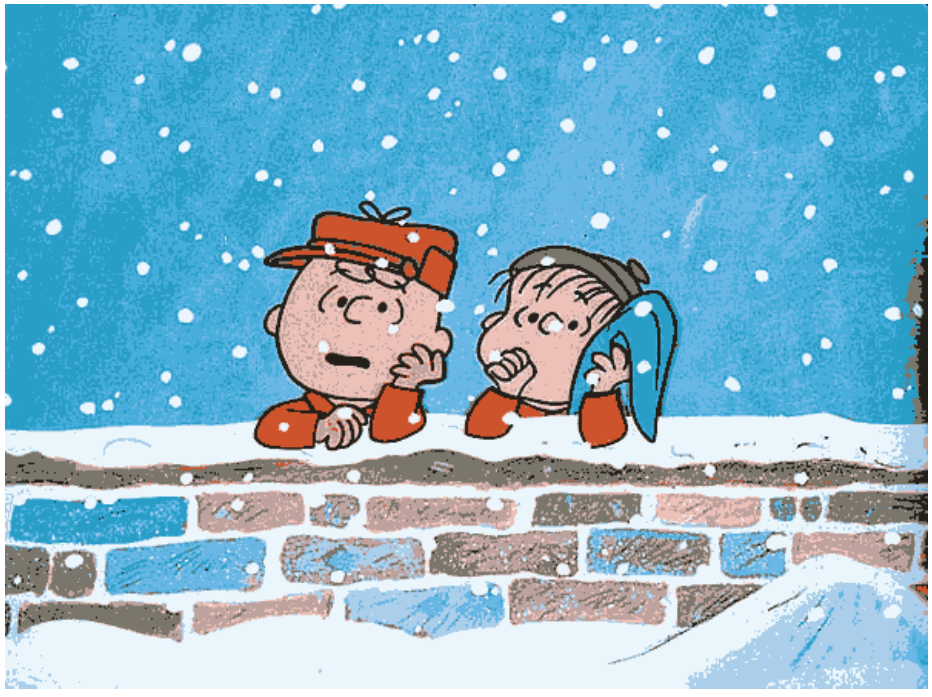
- How can we use *k*-means to compress this image?

Vector quantization



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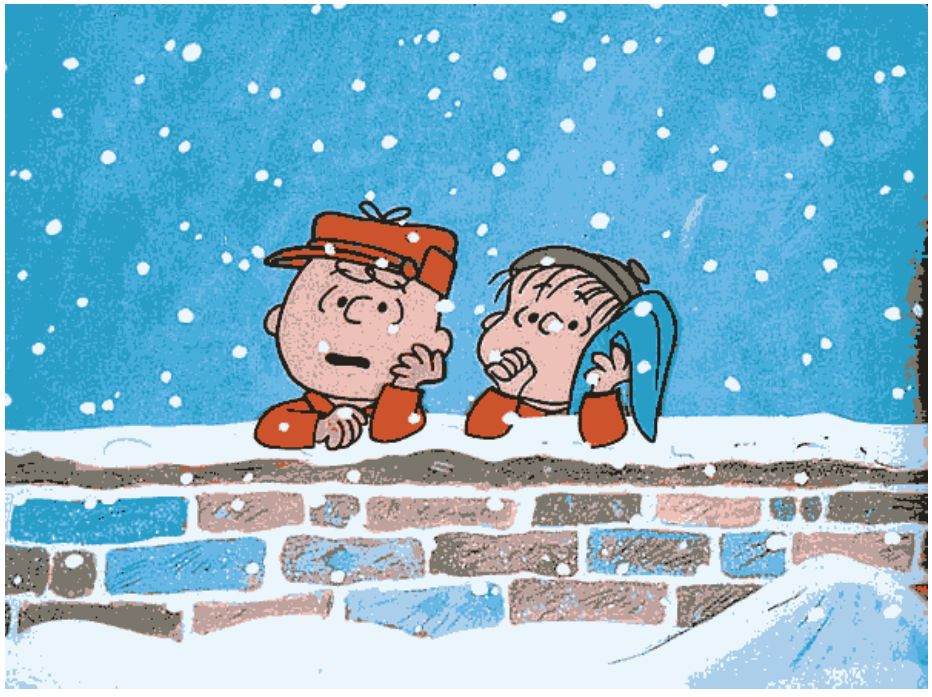
Vector quantization



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- With $k = 100$, we need 7 bits per pixel plus 100×3 bits $\approx$ 897K.

Charlie Brown and Linus VQ

2 means

Charlie Brown and Linus VQ

4 means

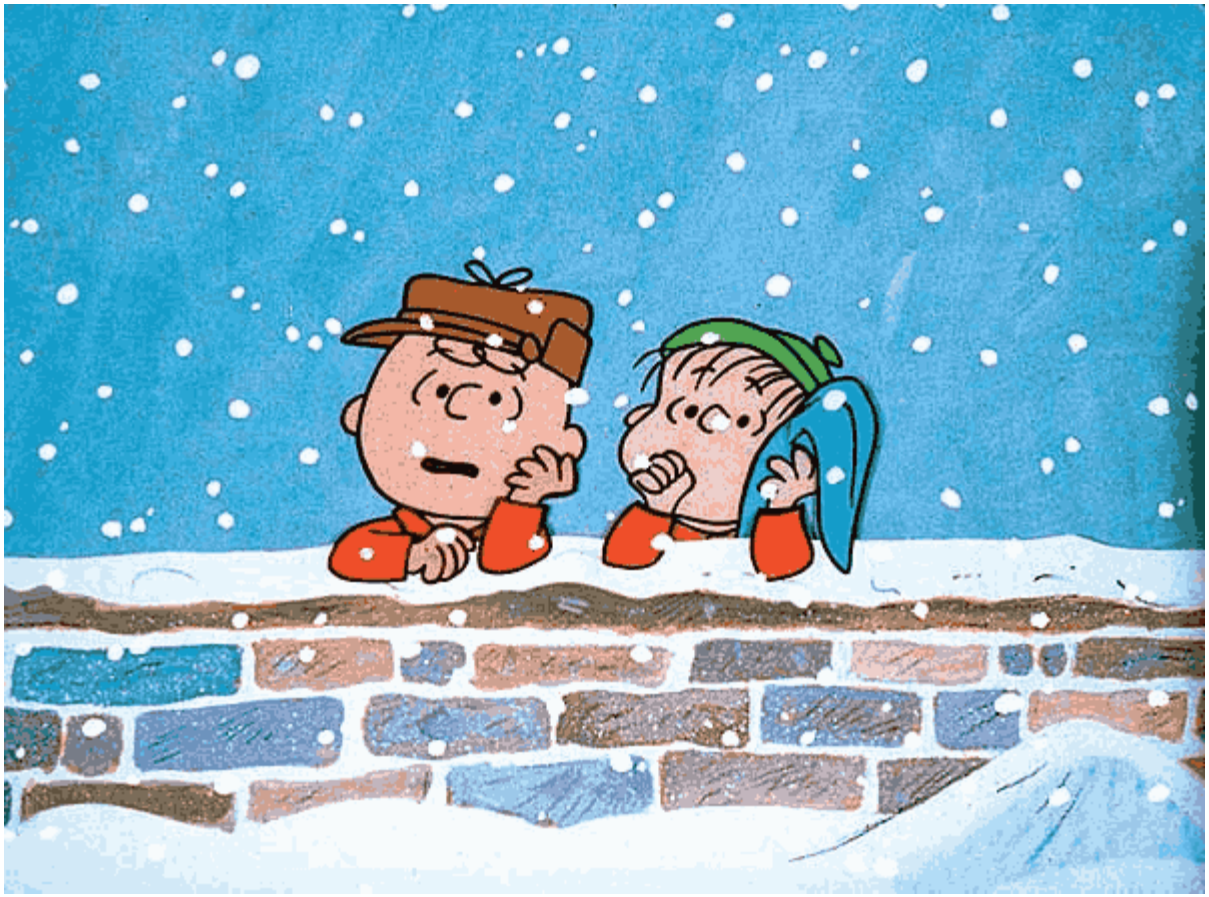
Charlie Brown and Linus VQ

8 means

Charlie Brown and Linus VQ

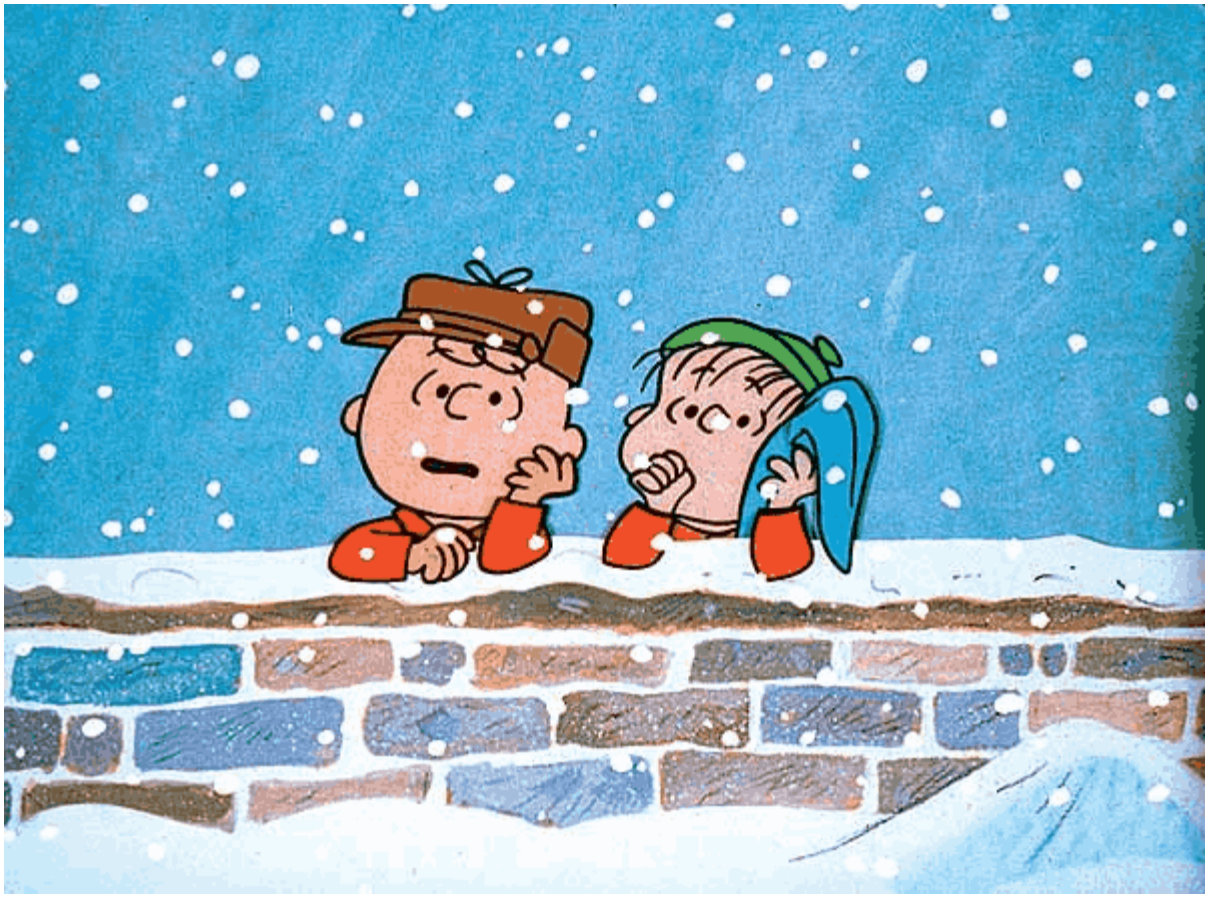
16 means

Charlie Brown and Linus VQ



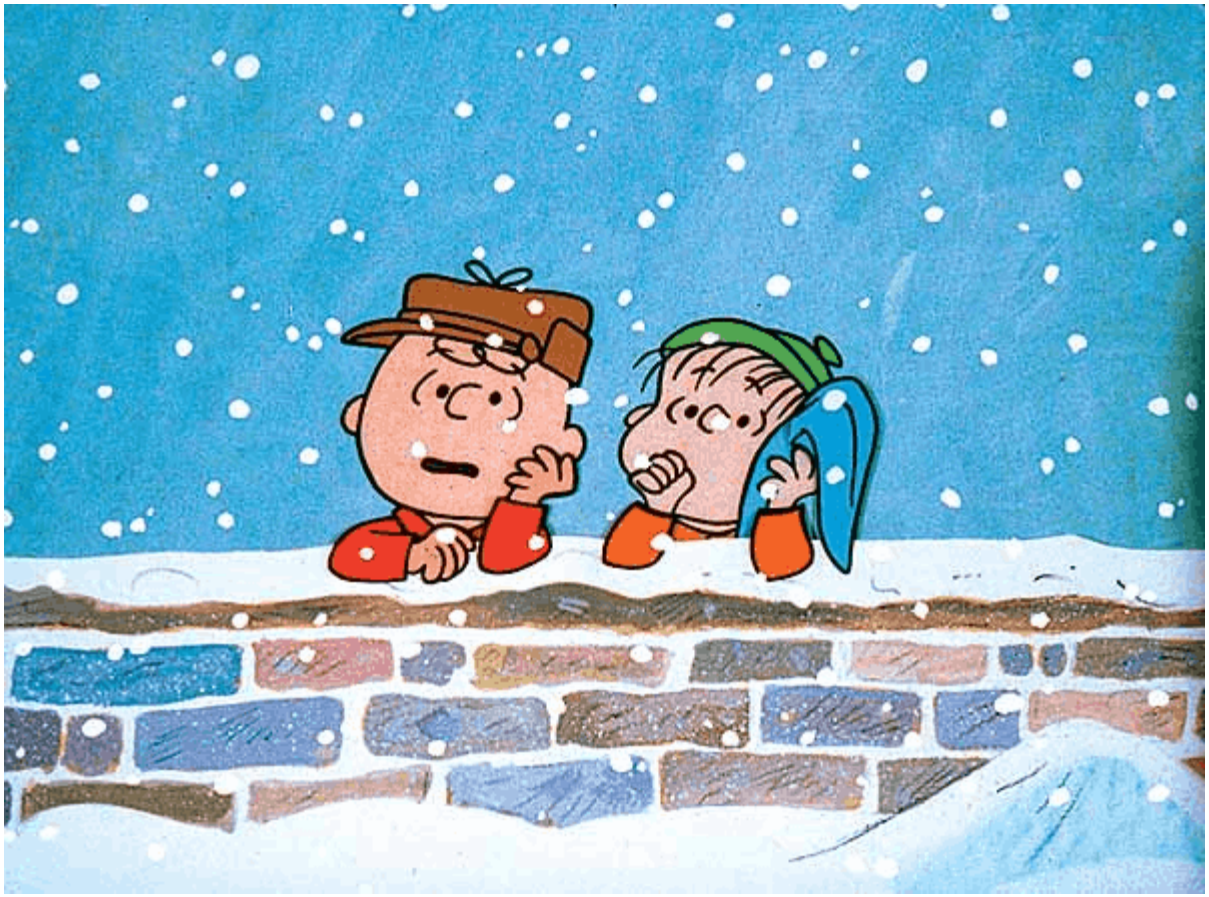
32 means

Charlie Brown and Linus VQ



64 means

Charlie Brown and Linus VQ



128 means

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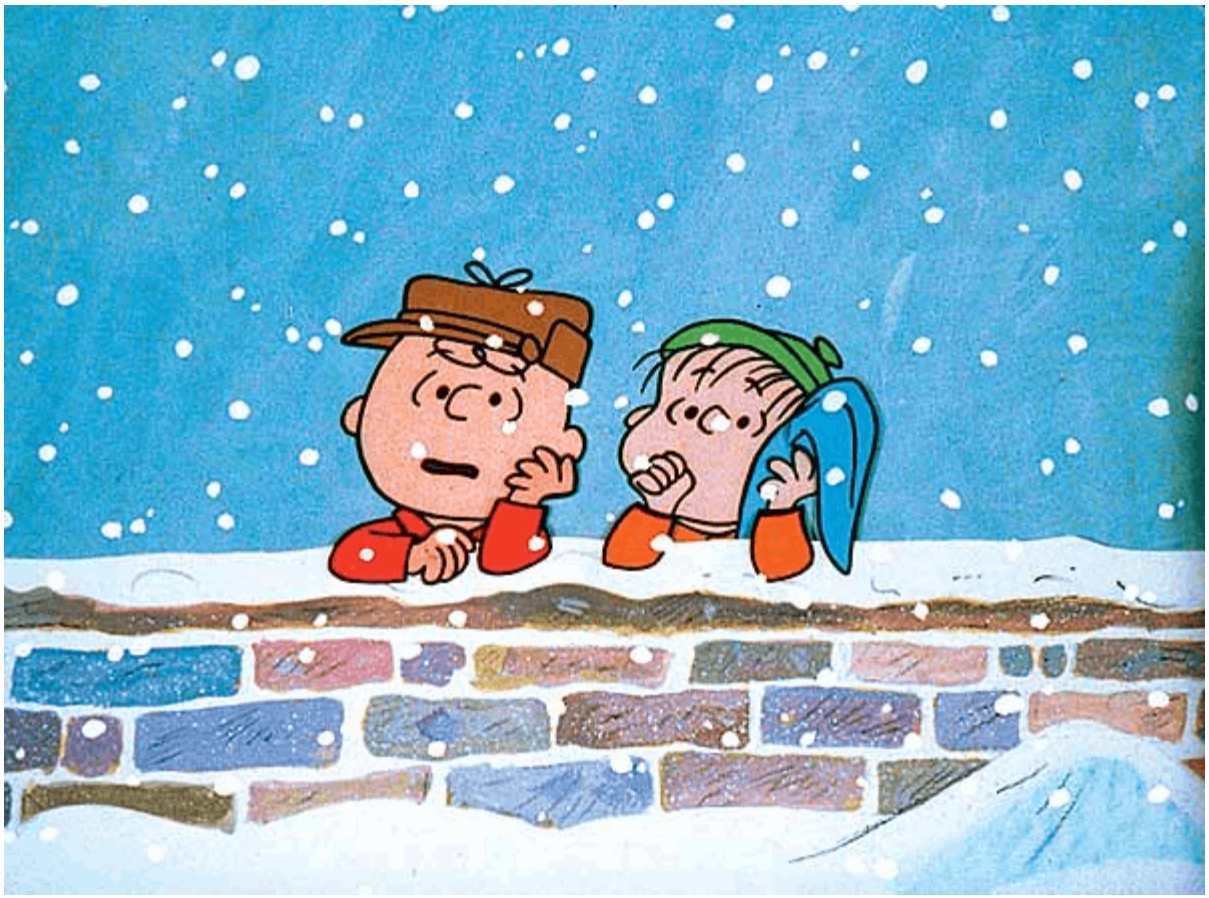
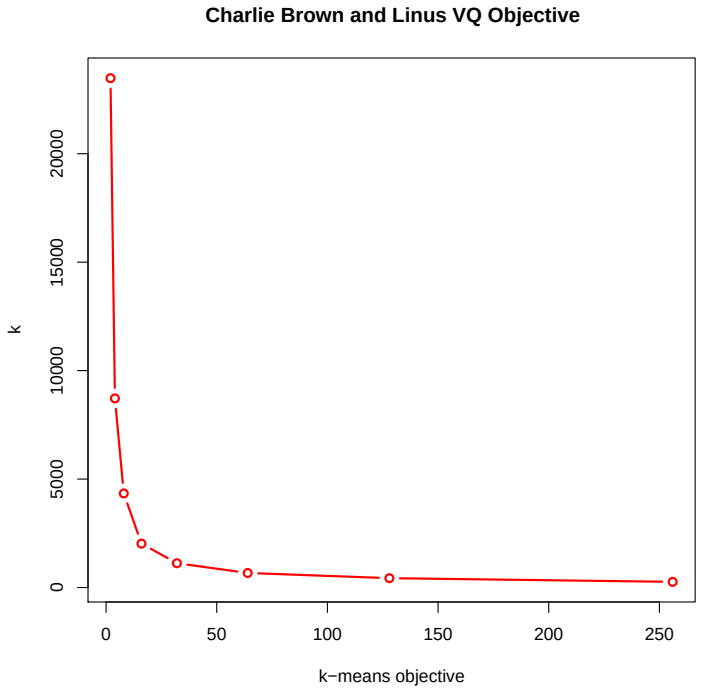


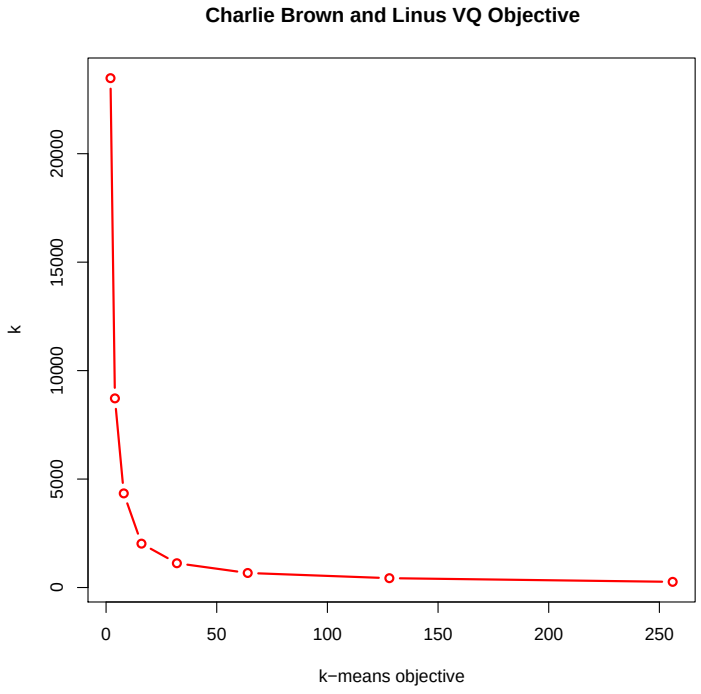
256 means

Measure of distortion



- The objective gives a measure of how distorted the compressed picture is relative to the original picture

Measure of distortion



- The objective gives a measure of how distorted the compressed picture is relative to the original picture
- For more clusters, the picture is less distorted.

k-medoids

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- Each of the clusters is associated with its most typical example

k-medoids algorithm

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$$i_k = \arg\min_{\{n : z_n = k\}} \sum_{\{m : z_m = k\}} d(\mathbf{x}_n, \mathbf{x}_m)$$

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3. Until assignments $\mathbf{z}_{1:N}$ do not change

Choosing k

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- Sometimes, the problem determines k
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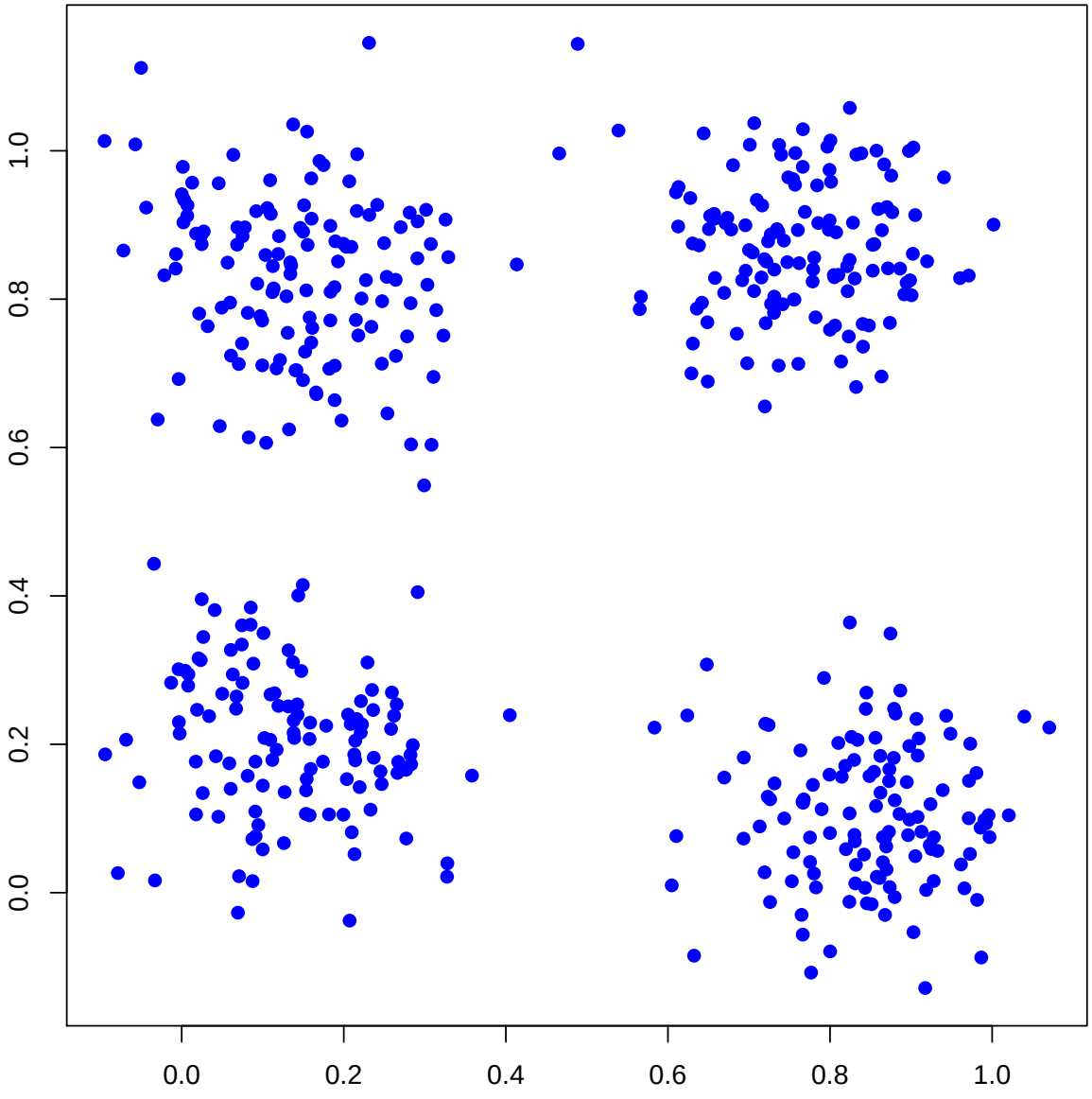
  - Clustering customers for k salespeople in a business
- Usually, we seek the “natural” clustering, but what does this mean?
- It is not well-defined.

What happens as k increases?



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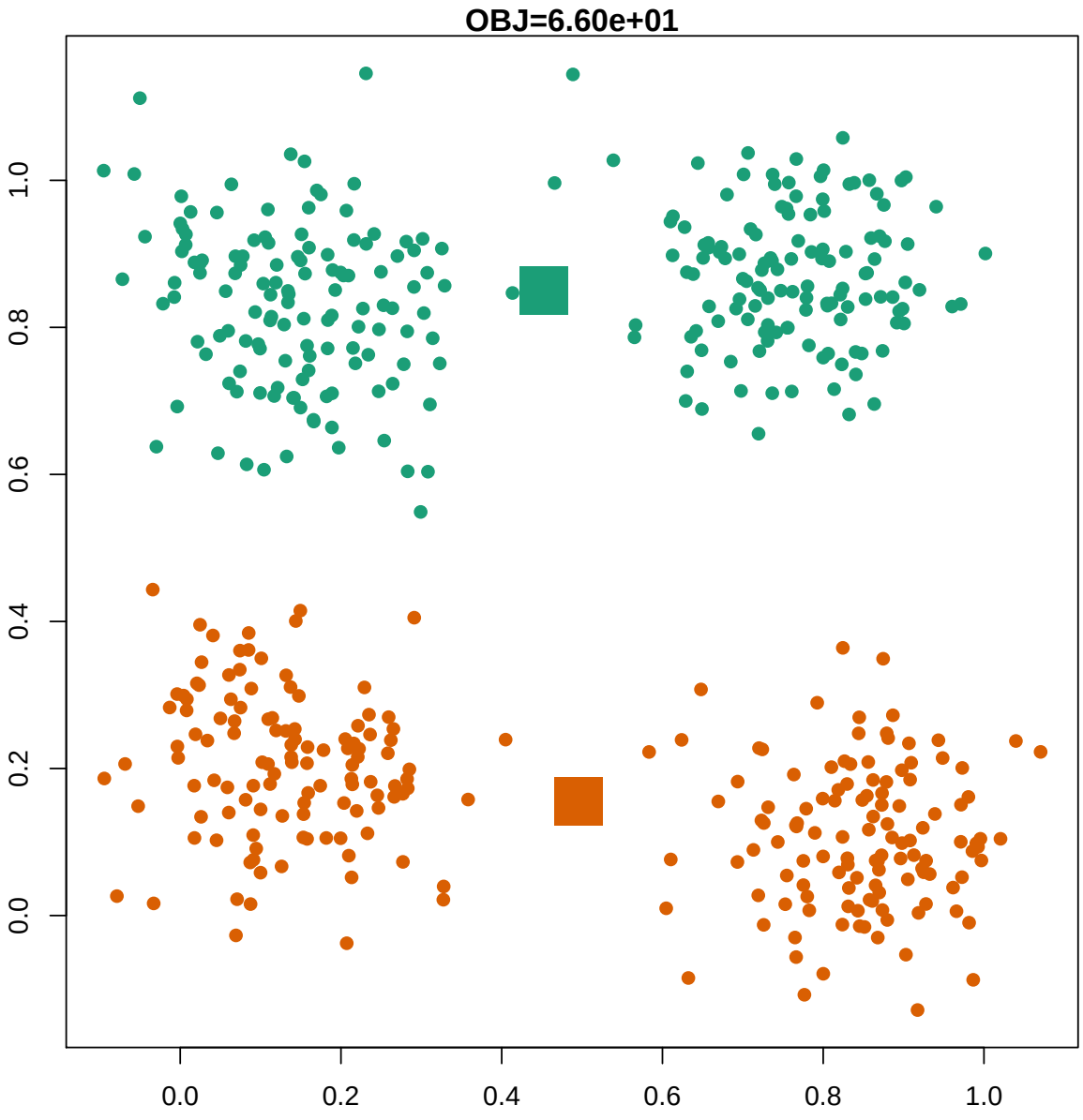

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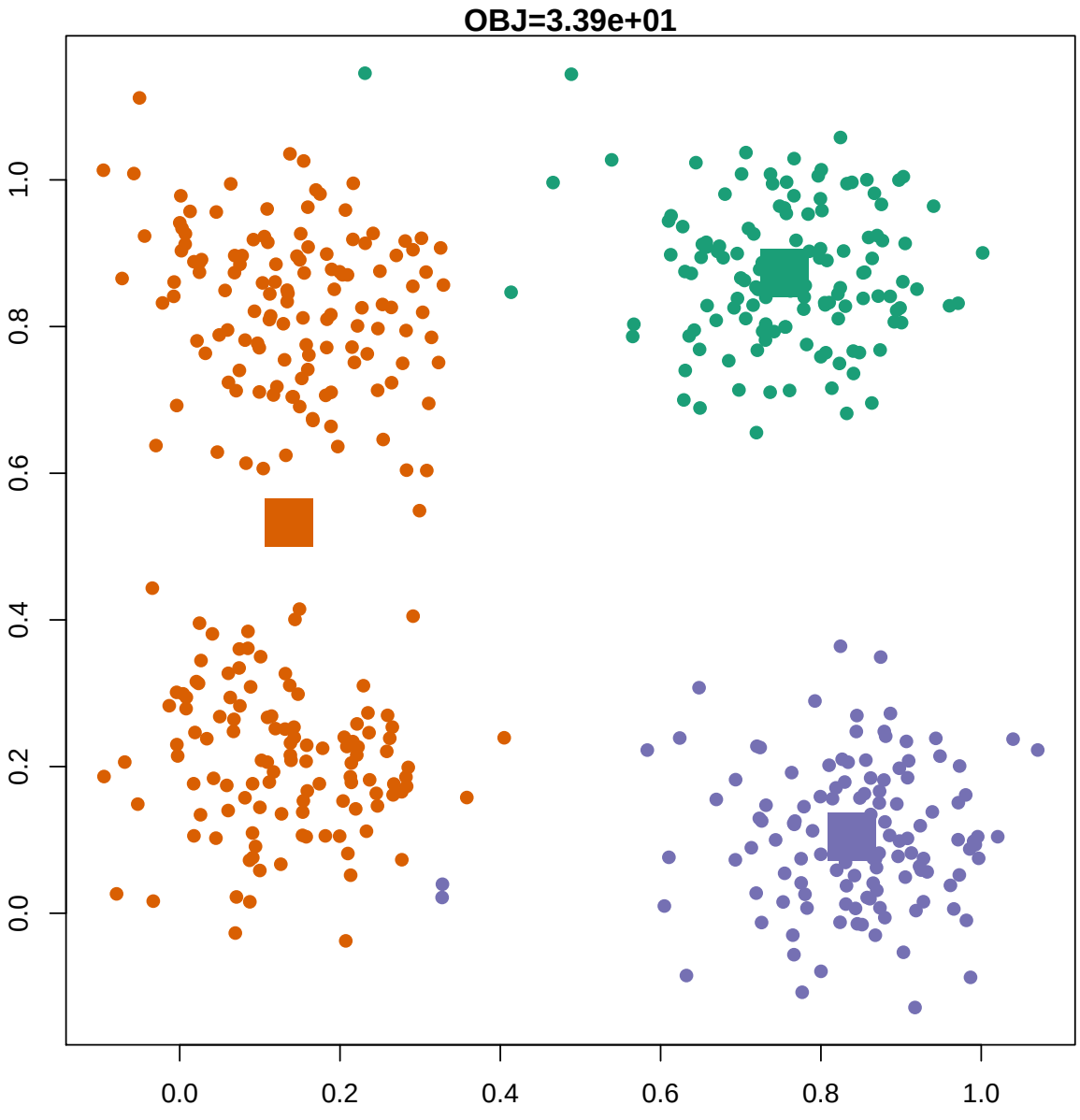

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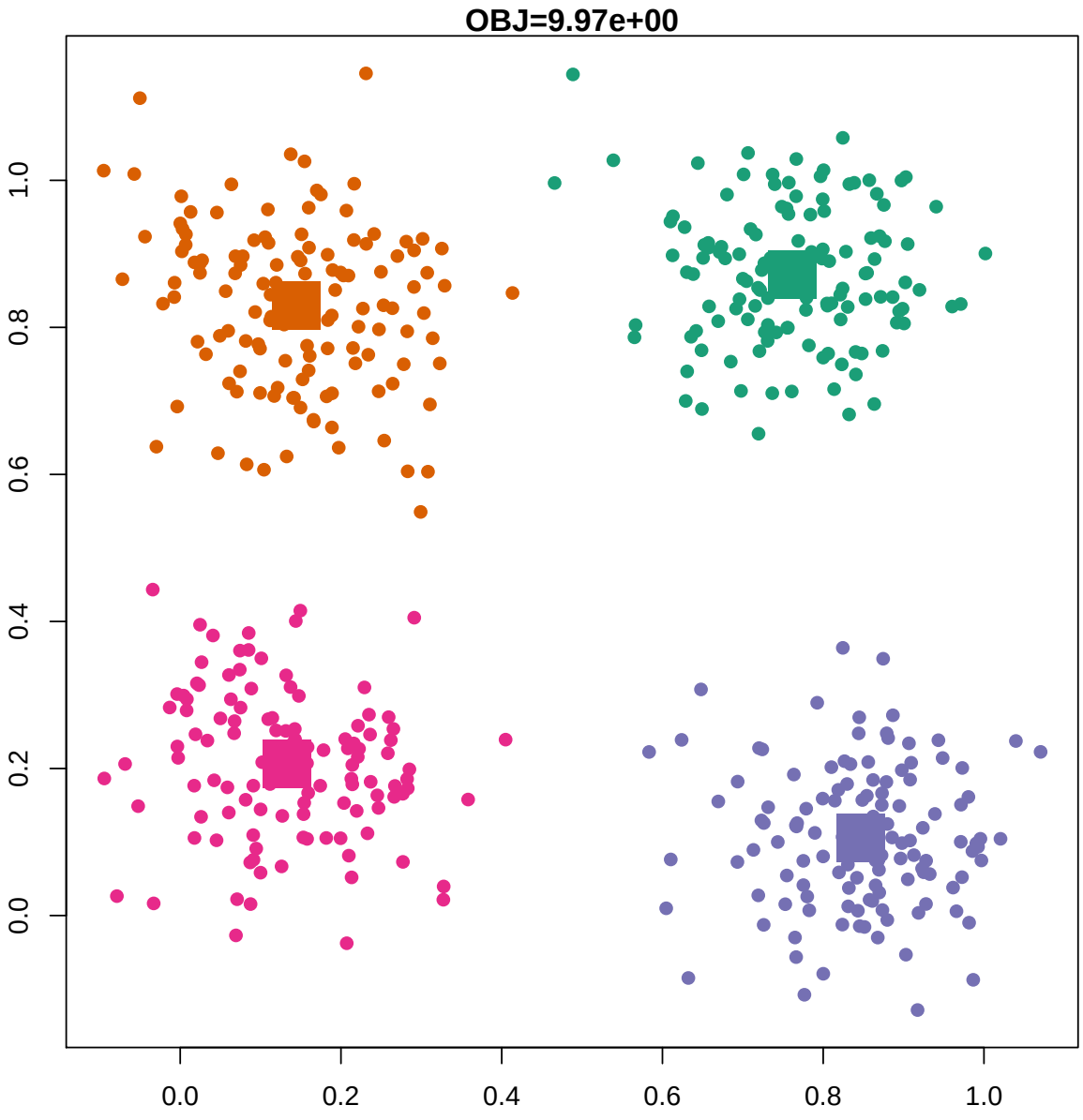

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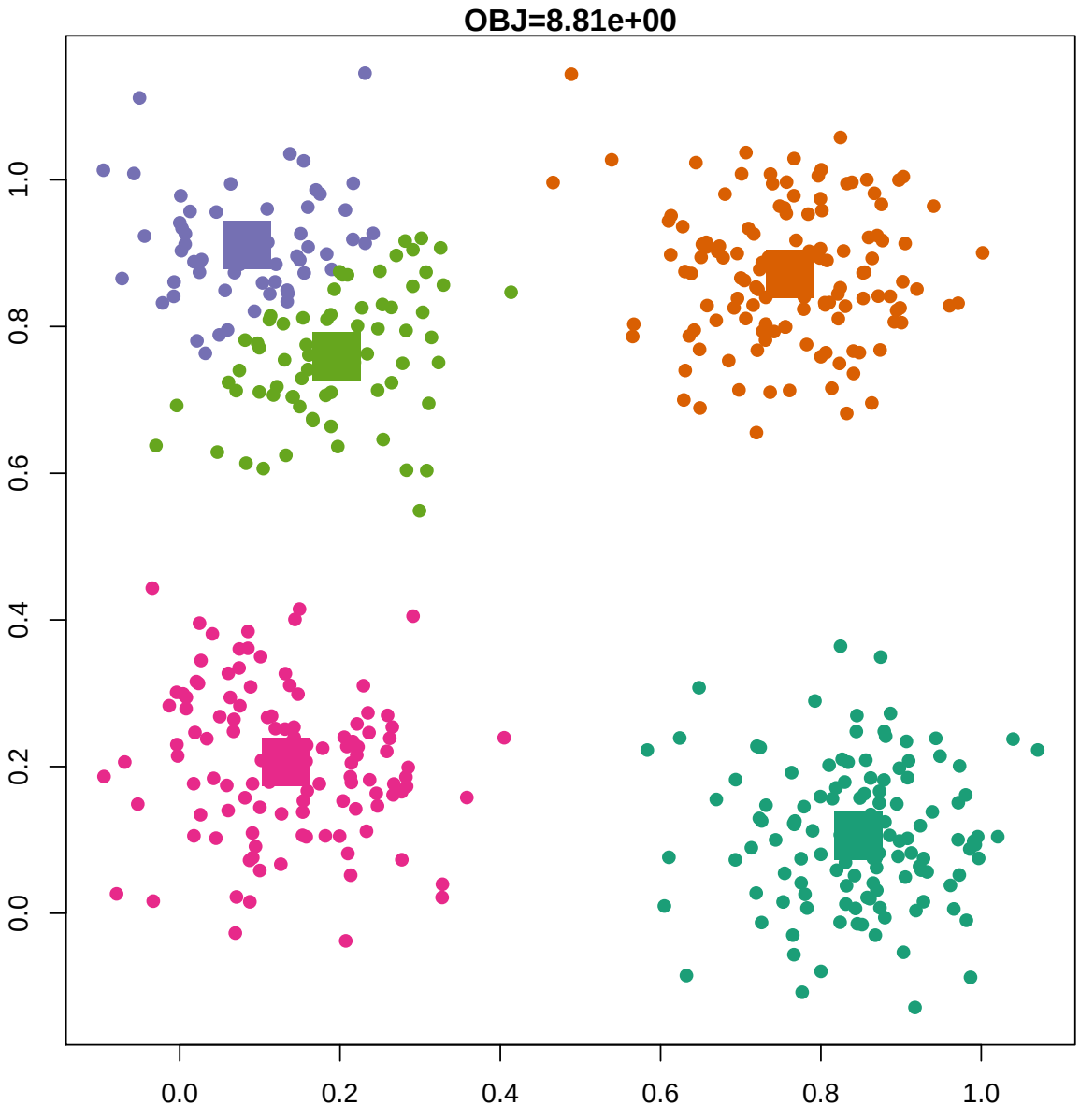

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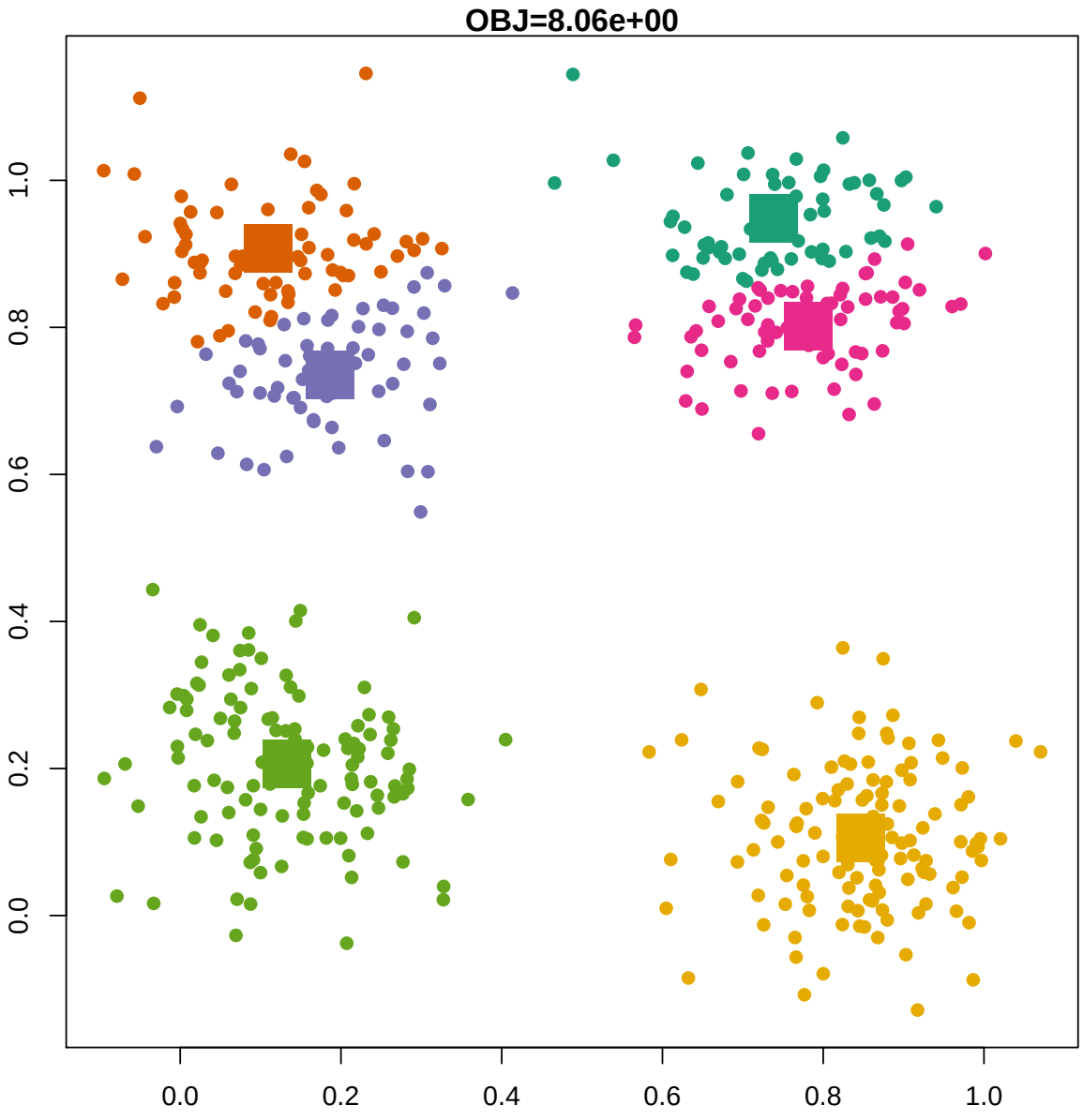

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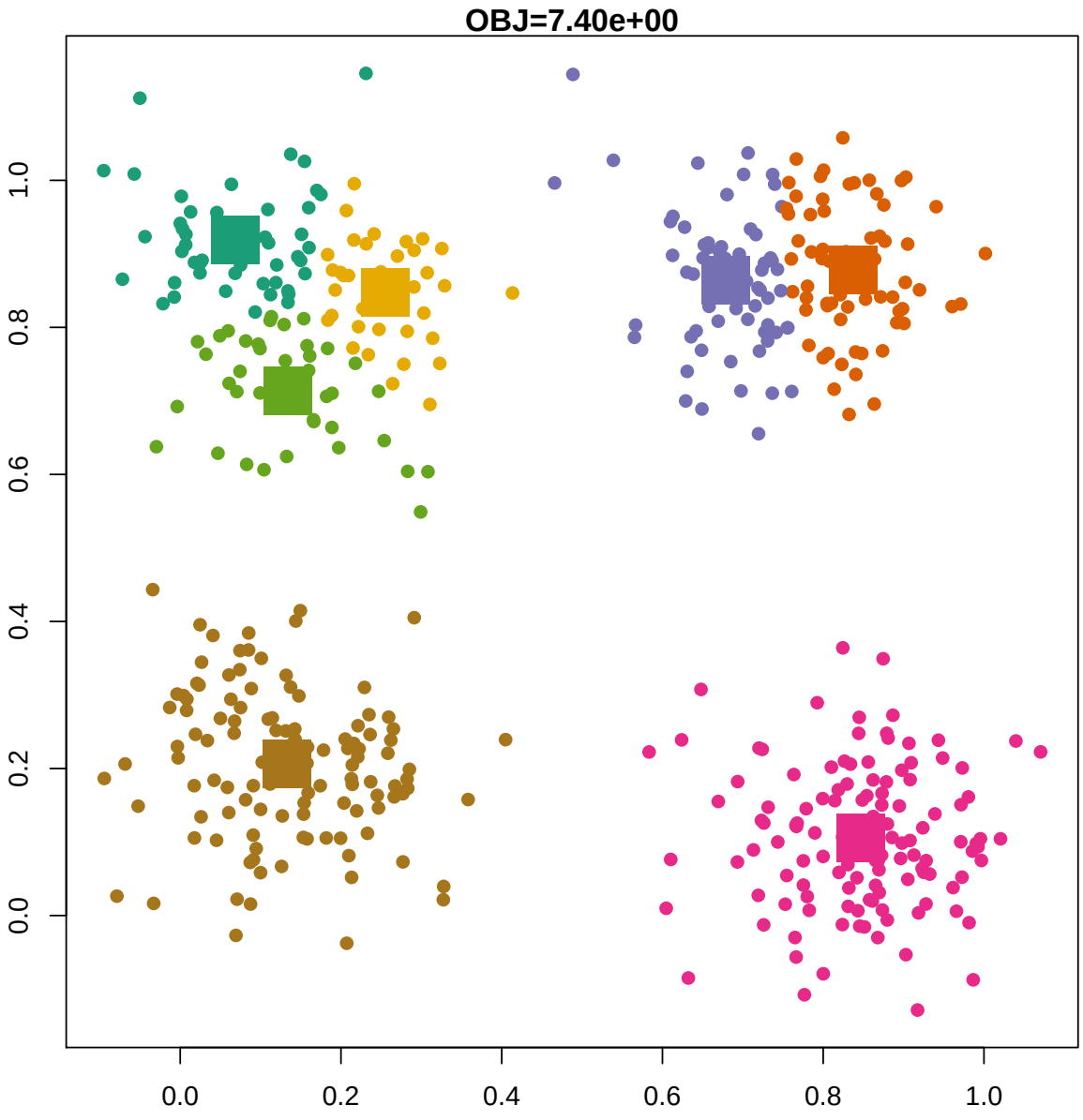

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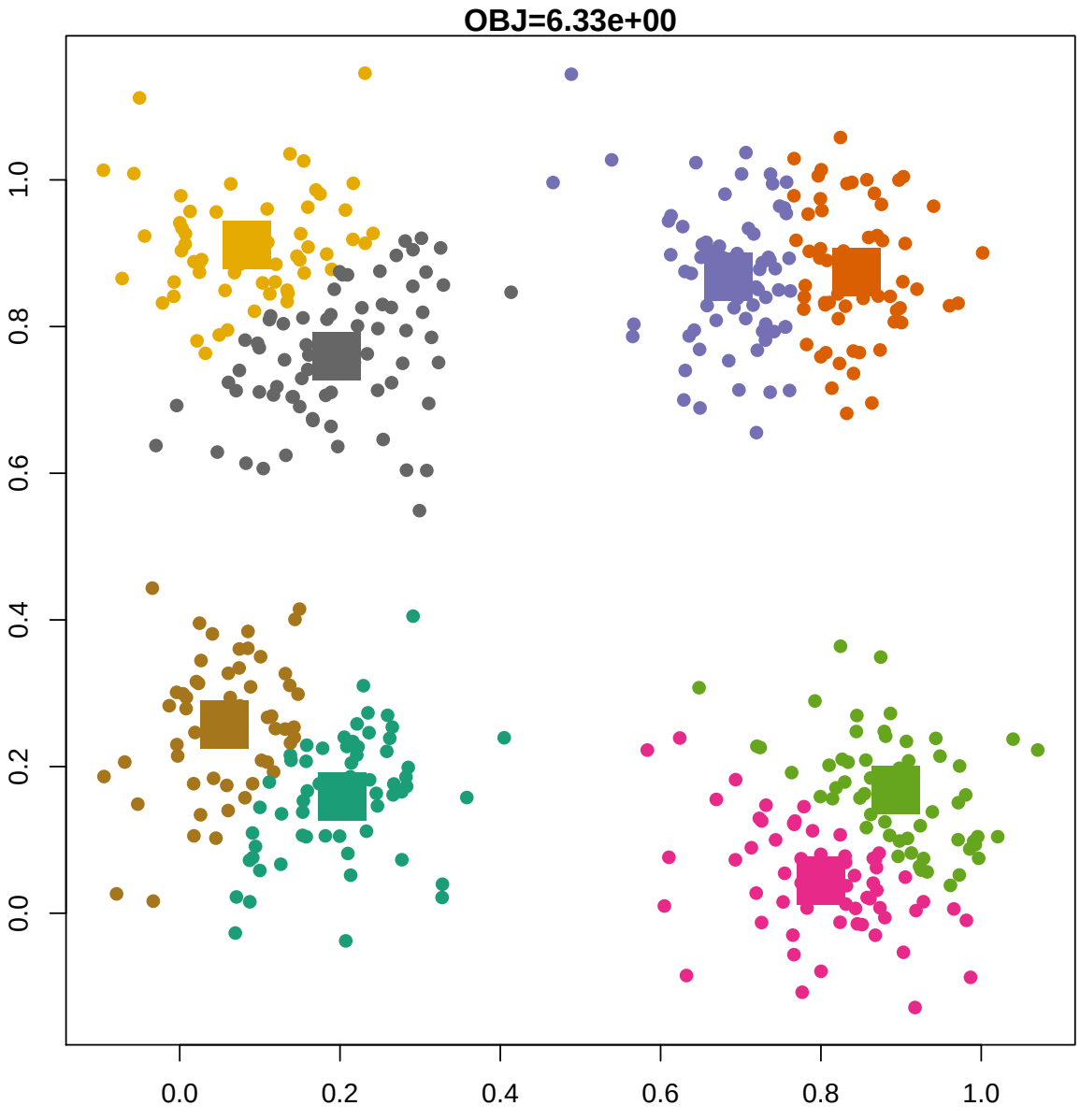
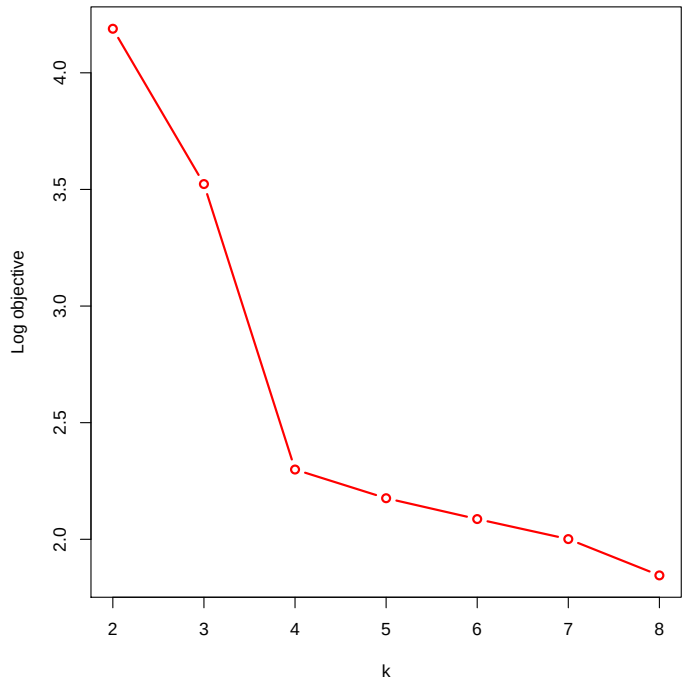


Heuristic: A kink in the objective



- Notice the “kink” in the objective between 3 and 5.

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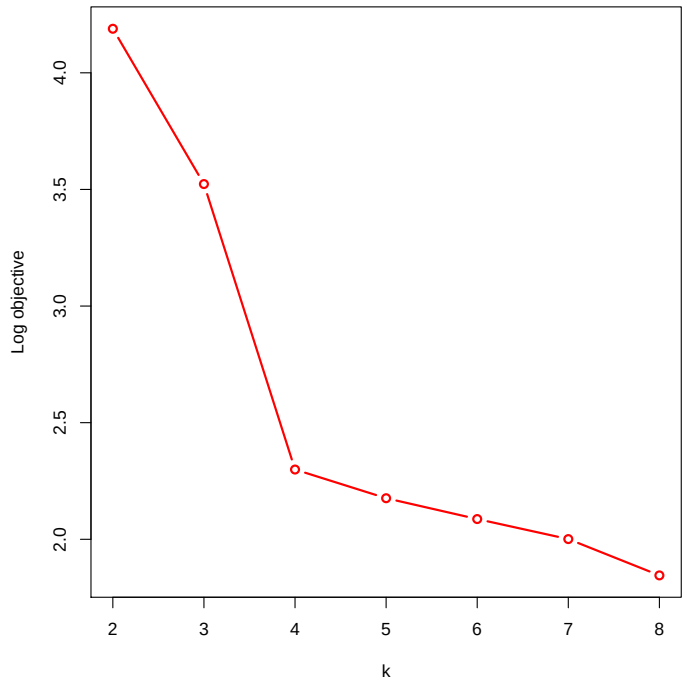

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- This suggests that 4 is the right number of clusters.

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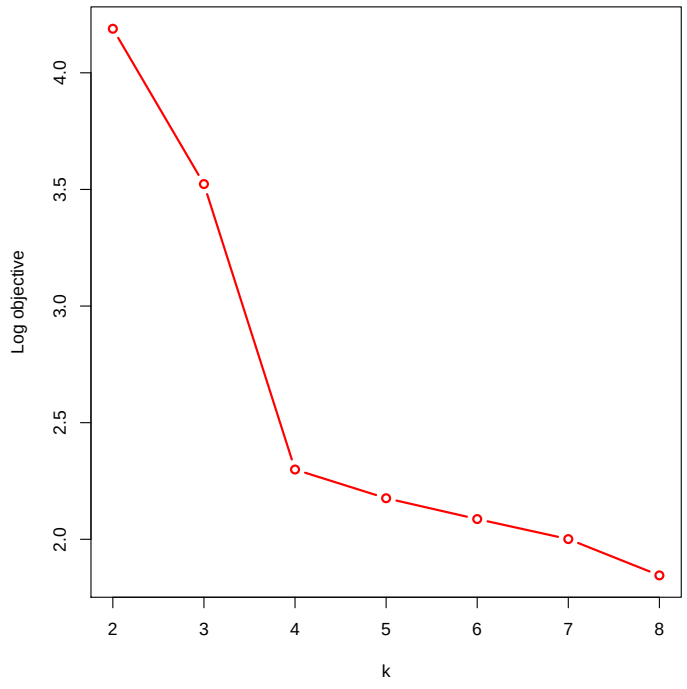

- Notice the “kink” in the objective between 3 and 5.
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- Tibshirani (2001) presents a method for finding this kink.

Archeology

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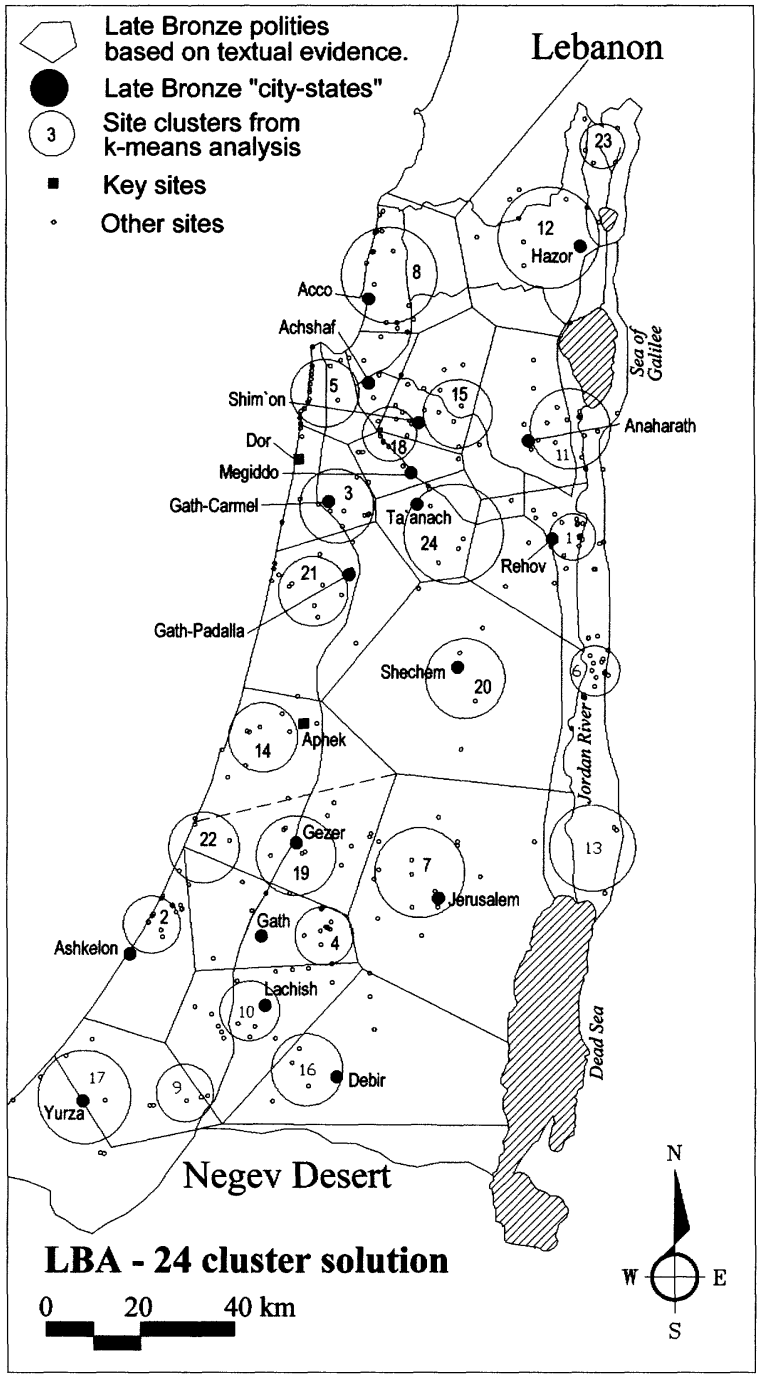
- Choose k very carefully, with a complicated computational technique.


Late Bronze polities based on textual evidence.
Late Bronze "city-states"
Site clusters from k-means analysis
Key sites
Other sites
Lebanon
Acco
Achshaf
Shim`on
Dor
Megiddo
Gath-Carmel
Hazor
Anaharath
Ta'anach
Rehov
Gath-Padalla
Shechem
Aphek
Gezer
Jerusalem
Gath
Ashkelon
Lachish
Debir
Yurza
Sea of Galilee
Jordan River
Dead Sea
Negev Desert
LBA - 24 cluster solution
0 20 40 km
N
W
E
S

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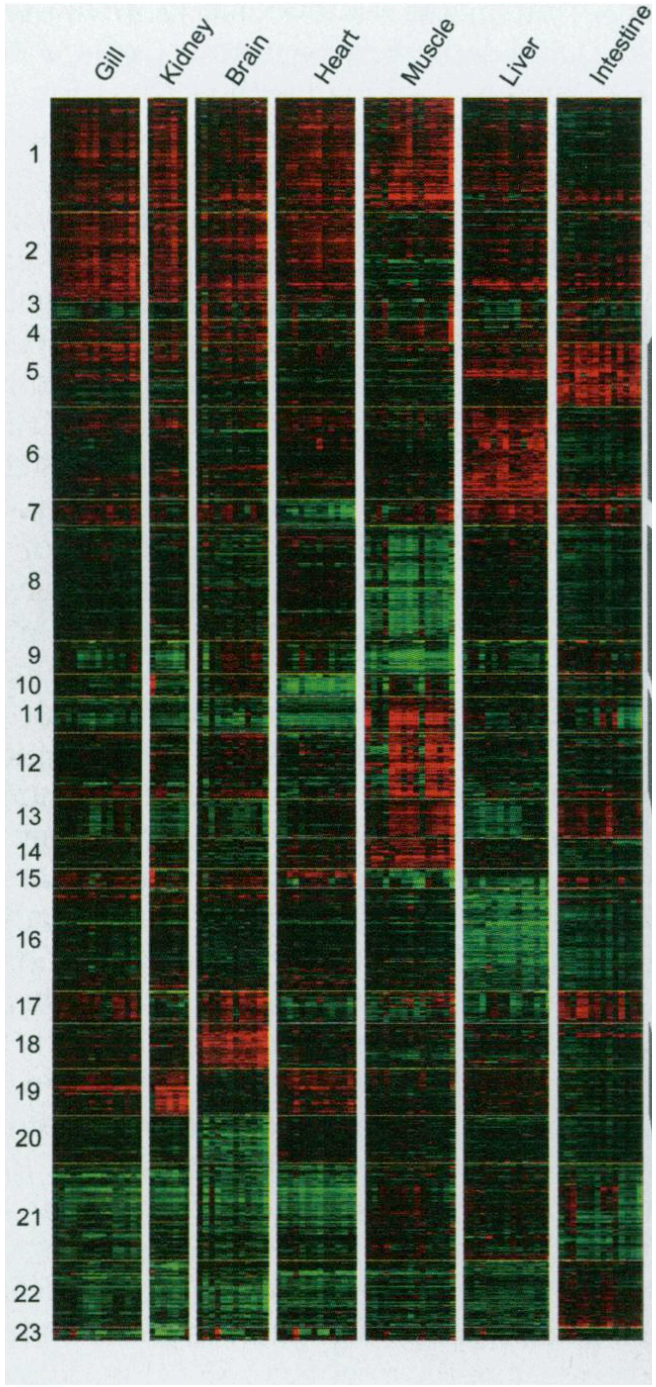
- (No mention of how $k = 23$ was chosen.)


Gill
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Education

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- Chose the number of clusters to get nice results

TABLE 3. Five-Cluster Solution: *Z* scores on Each Clustering Variable

	Cluster 1	Cluster 2	Cluster 3	Cluster 4	Cluster 5
Teacher caring	−.5	−.5 to .5	−.5 to .5	−.5	1.0
Peers' academic support	1.0	−.5	1.0	−.5	−.5 to .5
Parents' academic support	.5	−1.0	−.5 to .5	−.5 to .5	1.0

TABLE 4. Means and Standard Deviations for Each Cluster on Grade 8 Motivational Variables

	Academic Self-Efficacy		Intrinsic Valuing of Education		Teacher-Rated Effort	
Cluster	*M*	SD	*M*	SD	*M*	SD
1. All positive	3.59	.48[a]	2.99	.55[a]	3.74	.26[a]
2. Peer negative, parents very negative	2.44	.66[b]	2.16	.51[b]	3.05	.61[b]
3. Peer positive	3.01	.73[c]	2.43	.66[b]	3.26	.66[b]
4. Negative teacher and peer	2.47	.63[b]	2.24	.51[b]	3.17	.59[b]
5. Positive teacher and parents	3.19	.65[c]	2.89	.62[a]	3.54	.47[a]

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- k-means will find patterns everywhere!

TABLE 2. Percentage distribution of participants, by cluster, and behavioral patterns defining each cluster

Cluster type and behavioral patterns	%
Light substance dabblers—infrequent or no current use of substances† None have had sex	24.4
Abstainers—none have ever used substances† or had sex	22.7
Sex dabblers—all have had sex Median no. of partners=1 60% used a condom at last sex Infrequent use of substances†	14.5
Drinkers—all consumed alcohol in past 12 mos. 49% report binge drinking Infrequent or no illicit drug use None have had sex	7.4
Smokers—all smoke cigarettes daily Infrequent use of alcohol/illicit drugs 62% have had sex	7.3
Alcohol-and-sex dabblers—all drink occasionally; all have had sex Infrequent tobacco/illicit drug use	5.4
Binge drinkers—all binge frequently Infrequent cigarette, marijuana and other drug use 60% binge ≥1 time/wk. 45% have had sex	4.4
Heavy dabblers—all smoke, drink and binge drink with moderate frequency 45% use marijuana; few use other illicit drugs 91% have had sex	3.6
Combination sex and drug use—all have had sex; all used alcohol/illicit drug at last sex	3.4
Marijuana users—all use marijuana frequently; few have used other illicit drugs 94% use alcohol 79% smoke cigarettes 74% have had sex	1.7
Multiple partners—all report ≥14 sexual partners 75% report low or moderate use of substances†	1.3
Sex for drugs or money—all have had sex for drugs or money 50% report low or moderate use of substances† Median no. of partners=3	1.2
High marijuana use and sex—all use marijuana frequently; all have had sex All used alcohol/other drug at last sex 82% have had >1 partner (median=6)	1.1
Marijuana and other drug users—95% report heavy marijuana use; all use other illicit drugs 68% have had sex 28% used alcohol/other drug at last sex	0.6
Injection-drug users—all have injected drugs 82% have had sex Median no. of partners=4	0.6
Males who have sex with males—all are males who have had sex with another male 78% have had multiple partners (median=5) 40% used marijuana in past 30 days 50% use alcohol ≥1 time/mo. 17% have had sex for drugs or money	0.3

Summary