Clustering and the k-means Algorithm

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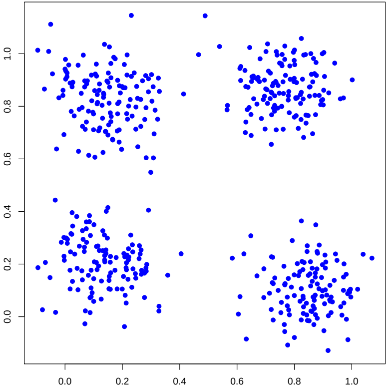
- Goal: segment the data into k groups

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

Example data



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

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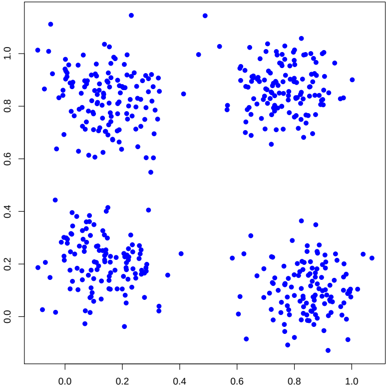

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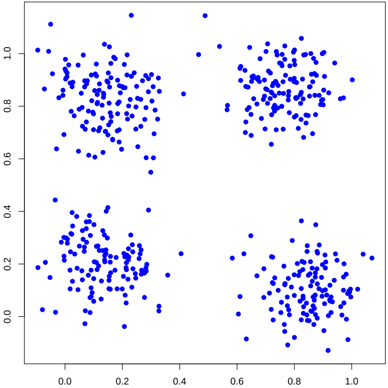
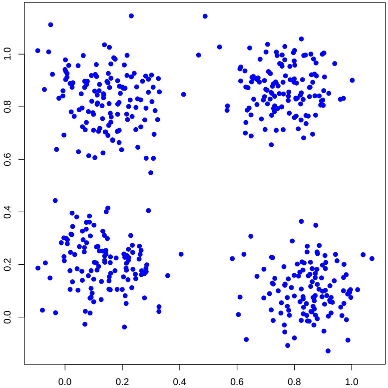


- What is a good distance function here?
- Squared Euclidean distance is reasonable

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

Example data



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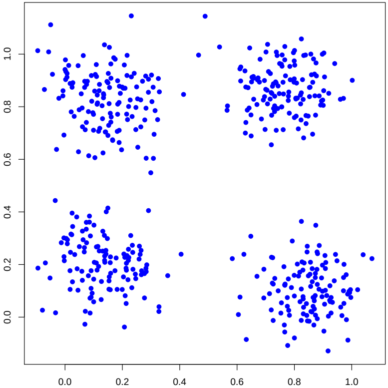

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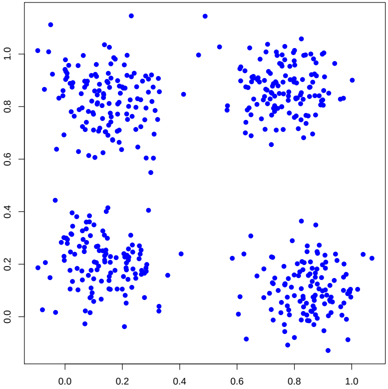

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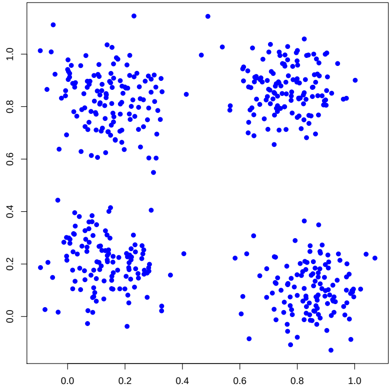
- What should *k* be?
- Automatically choosing *k* is complicated; for now, 4.

k-means



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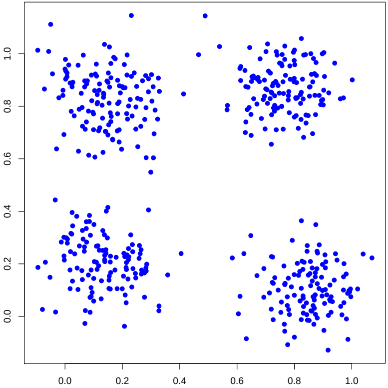

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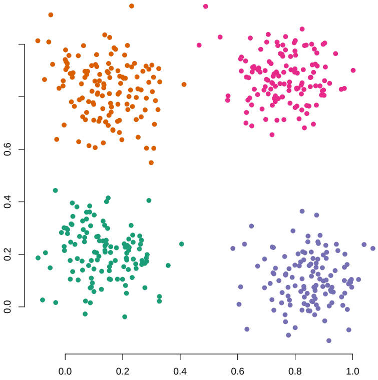

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- The goal of *k*-means is to assign data to clusters and define these clusters with their means.

k-means algorithm

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

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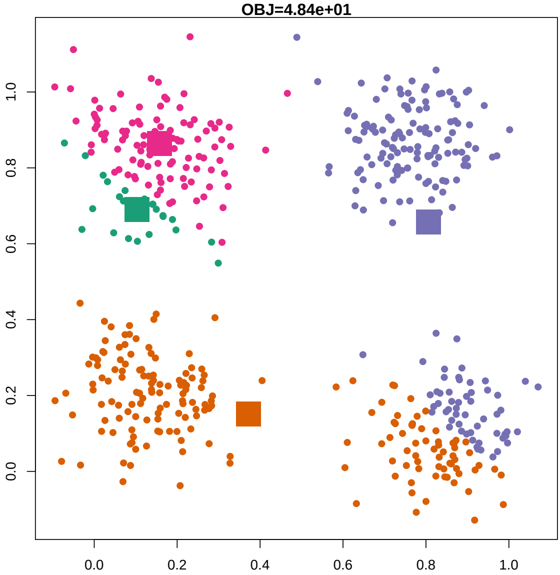

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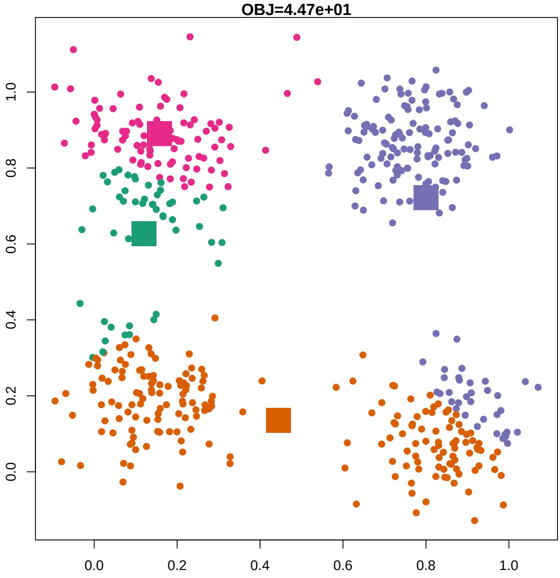

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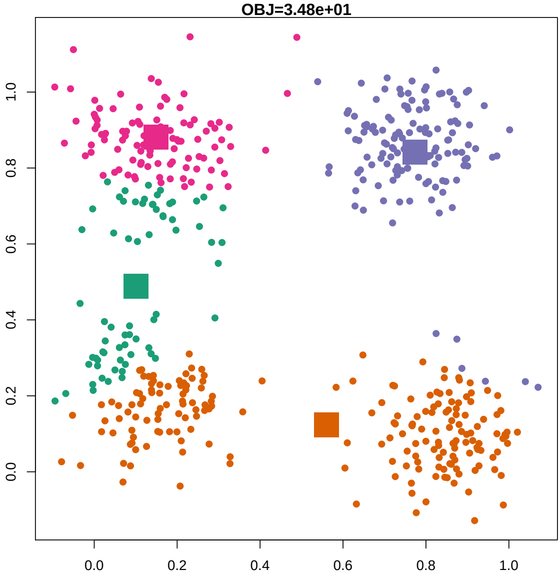

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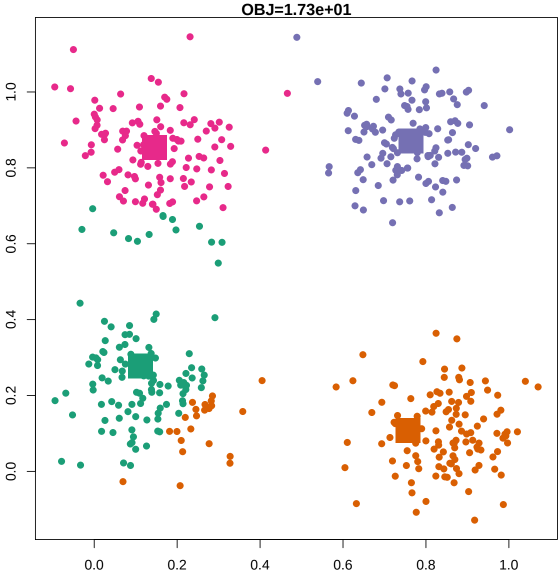

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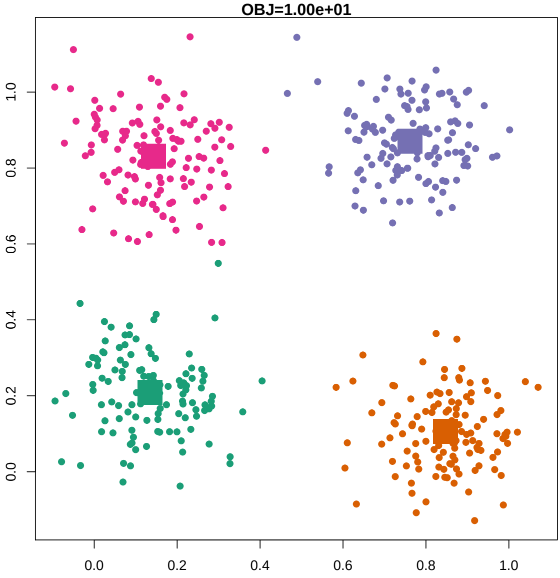

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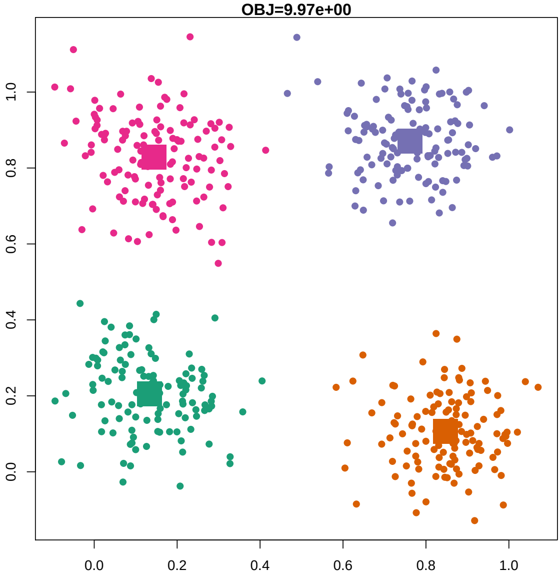

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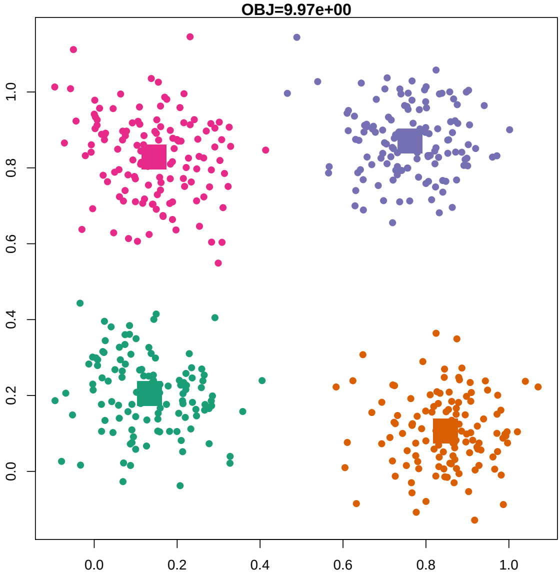

Objective function

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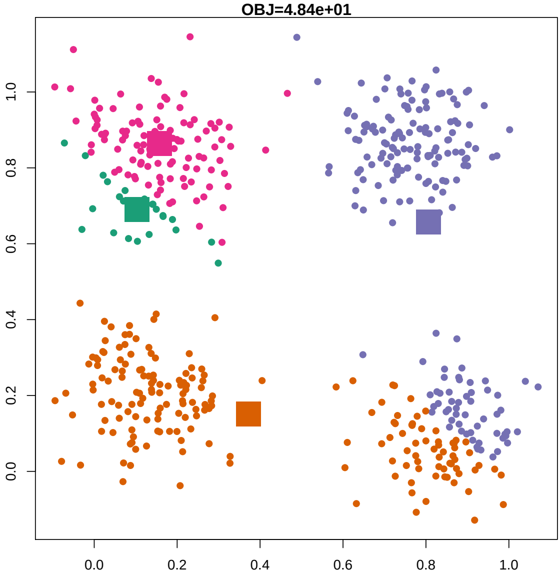
- The k-means objective function is the sum of the squared distances of each point to each assigned mean

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

k-means example (look at the objective)



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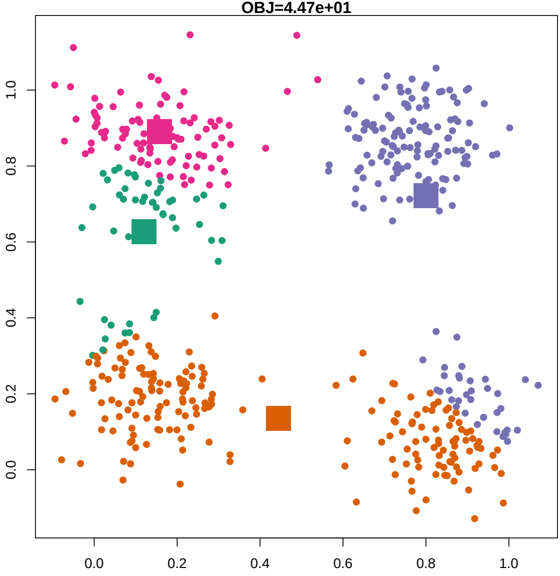

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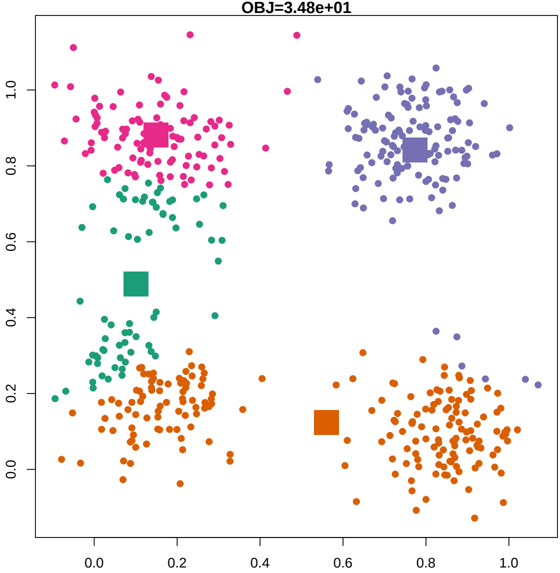

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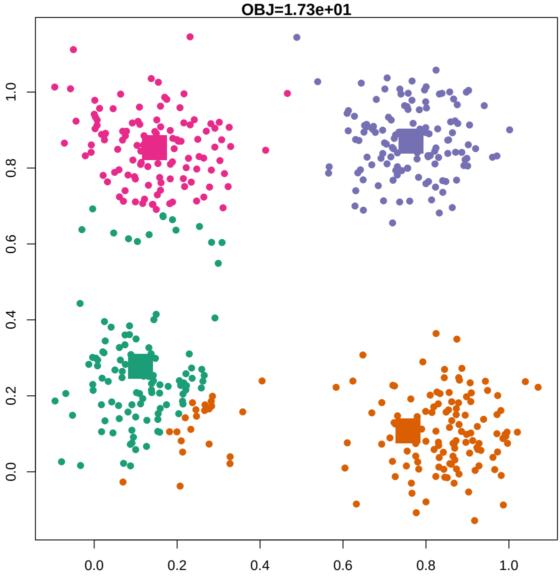

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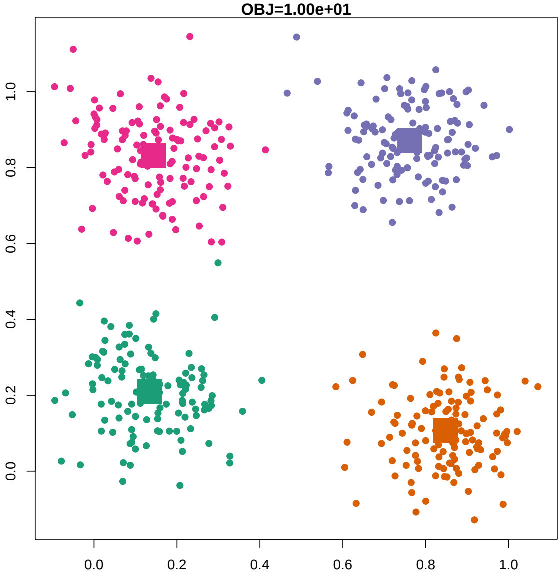

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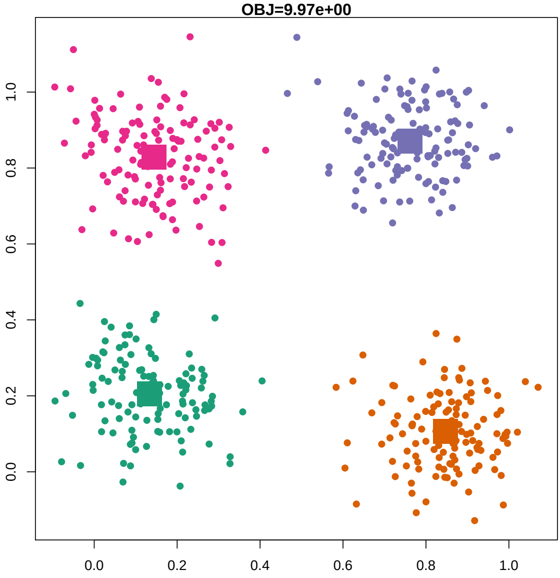

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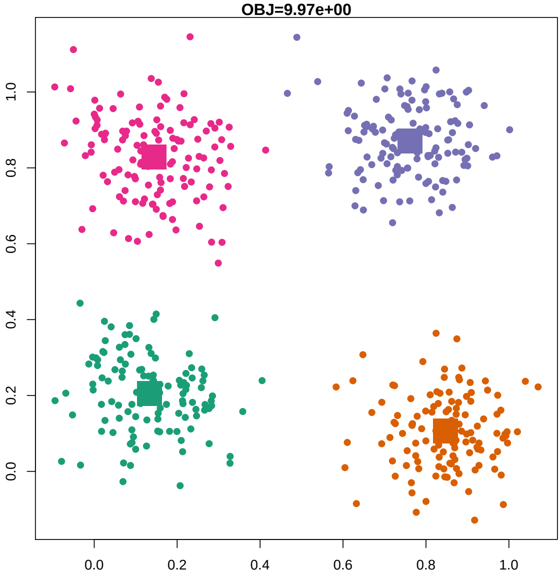

Coordinate descent

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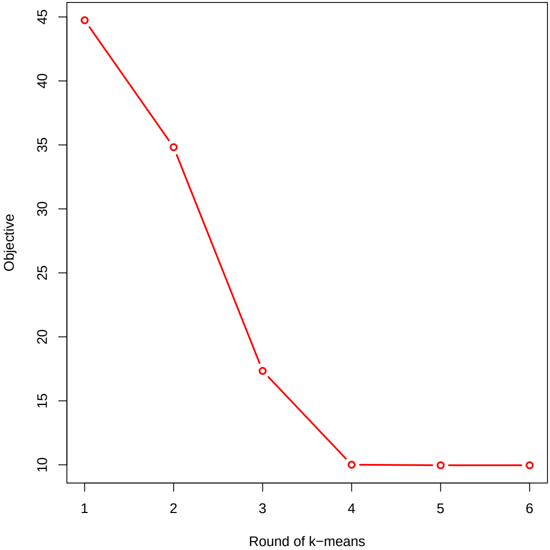
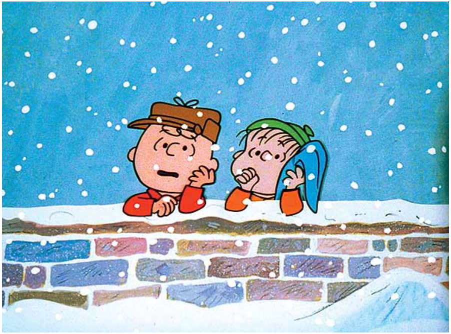
- It finds a *local minimum*. (Multiple restarts are often necessary.)

Objective for the example data



Compressing images



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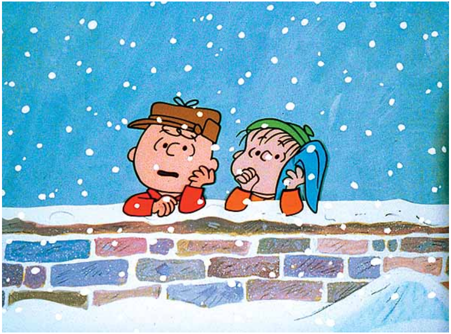

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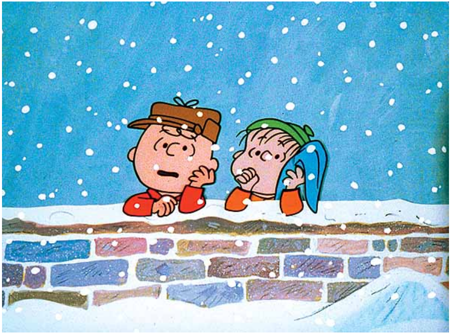

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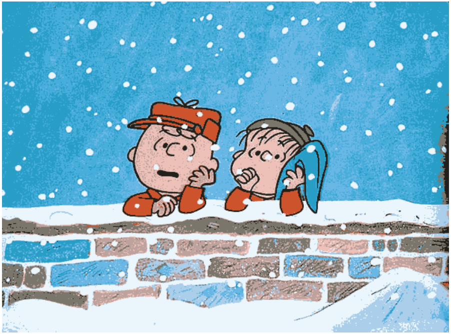
- How can we use k-means to compress this image?

Vector quantization



- Replace each pixel $\mathbf{x}_n$ with its assignment $\mathbf{m}_{z_n}$ (“paint by numbers”).

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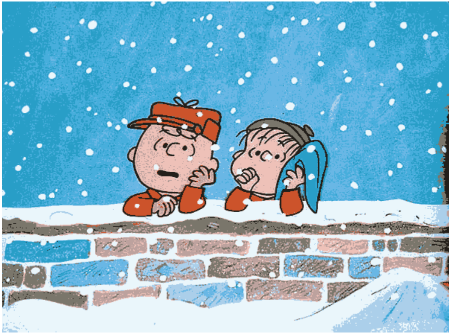

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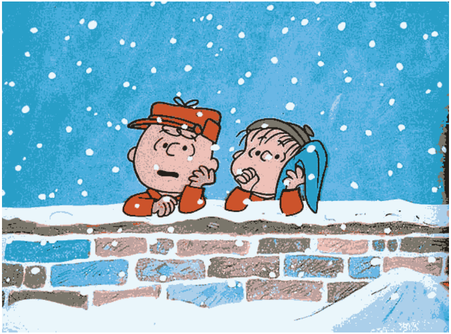

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- With $k = 100$, we need 7 bits per pixel plus 100×3 bits ≈ 897K.

Charlie Brown and Linus VQ

2 means

Charlie Brown and Linus VQ

4 means

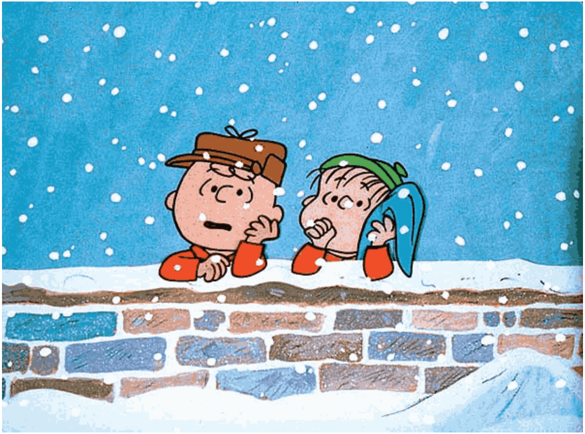
Charlie Brown and Linus VQ

8 means

Charlie Brown and Linus VQ

16 means

Charlie Brown and Linus VQ



32 means

Charlie Brown and Linus VQ

64 means

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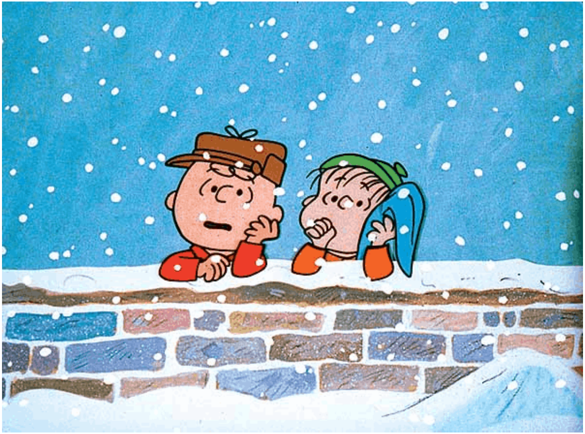

128 means

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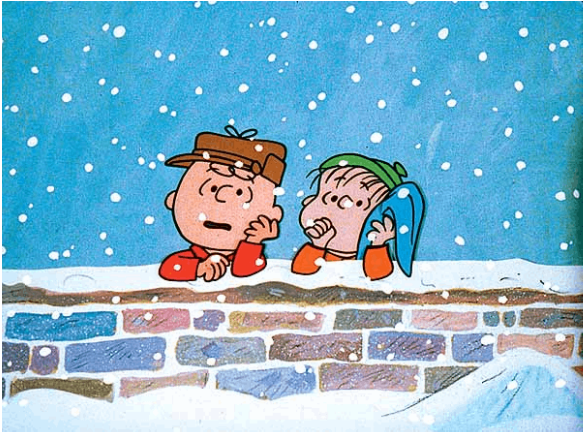
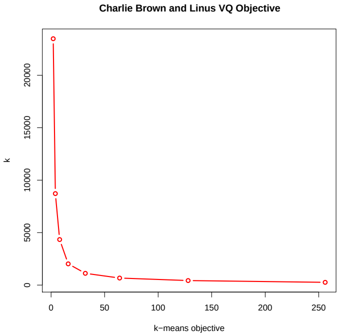


256 means

Measure of distortion



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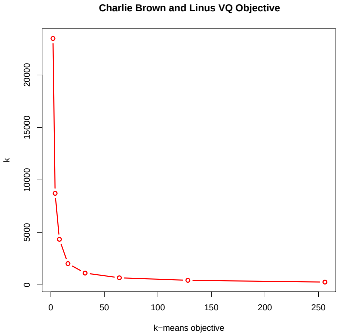

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- For more clusters, the picture is less distorted.

k-medoids

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- *No need to define the mean.*
- Each of the clusters is associated with its most typical example

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   2. For each cluster, find the data point in that cluster that is closest to the other points in that cluster

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

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$$z_n = \arg \min_{i \in \{1,\ldots,k\}} d(\mathbf{x}_n, \mathbf{m}_i)$$

   2. For each cluster, find the data point in that cluster that is closest to the other points in that cluster

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

   3. Set each cluster center equal to their closest data points

$$m_k = \mathbf{x}_{i_k}$$

k-medoids algorithm

1. Initialization
   - Data are $\mathbf{x}_{1:N}$
   - Choose initial cluster identities $\mathbf{m}_{1:k}$
2. Repeat
   1. Assign each data point to its closest center

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   3. Set each cluster center equal to their closest data points

$$m_k = \mathbf{x}_{i_k}$$

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

Choosing k

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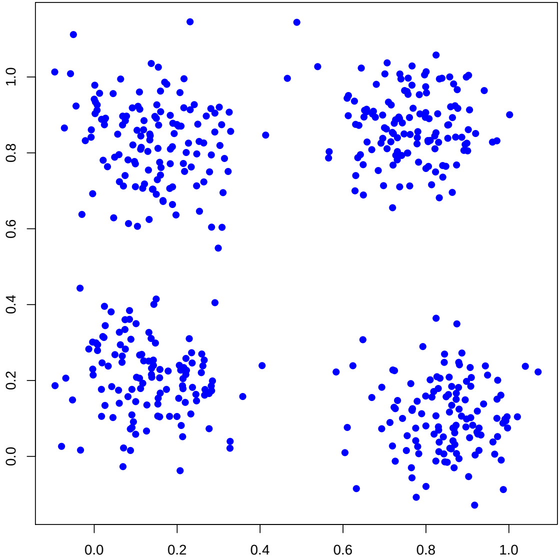
  - Clustering customers for k salespeople in a business
- Usually, we seek the “natural” clustering, but what does this mean?
- It is not well-defined.

What happens as *k* increases?



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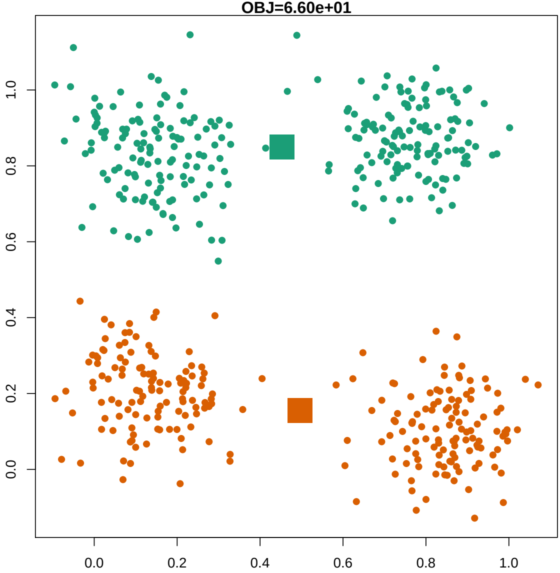

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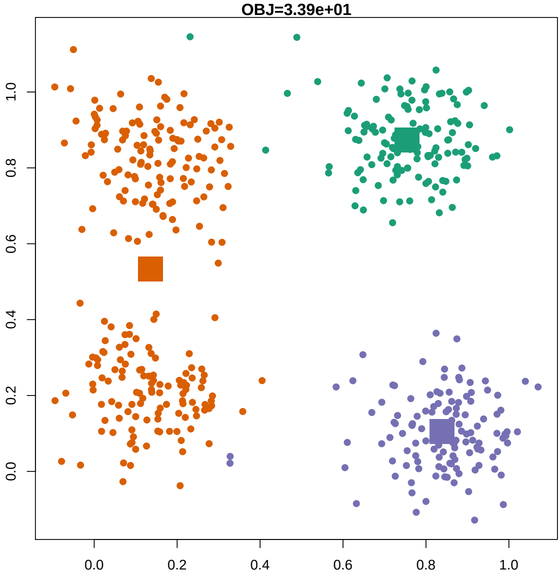

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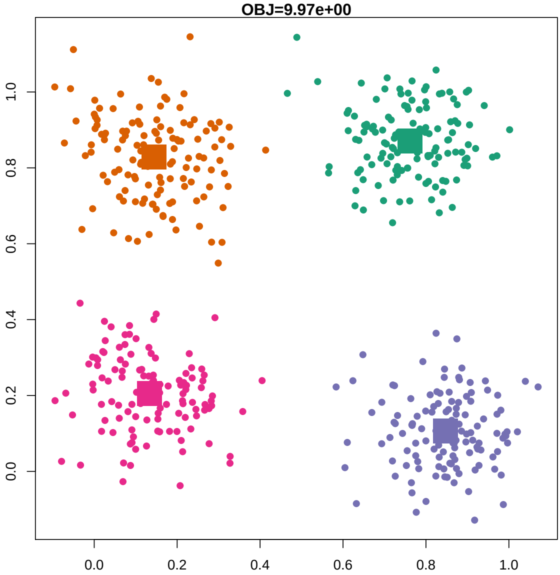

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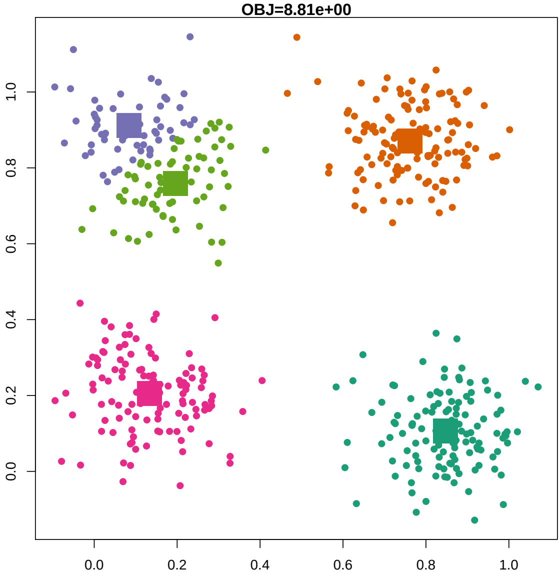

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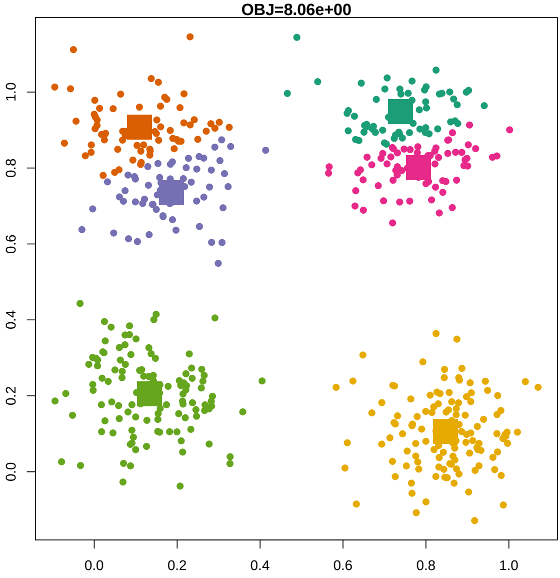

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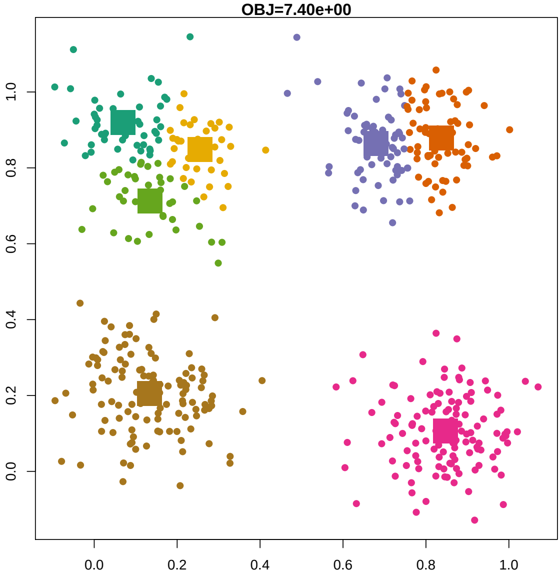

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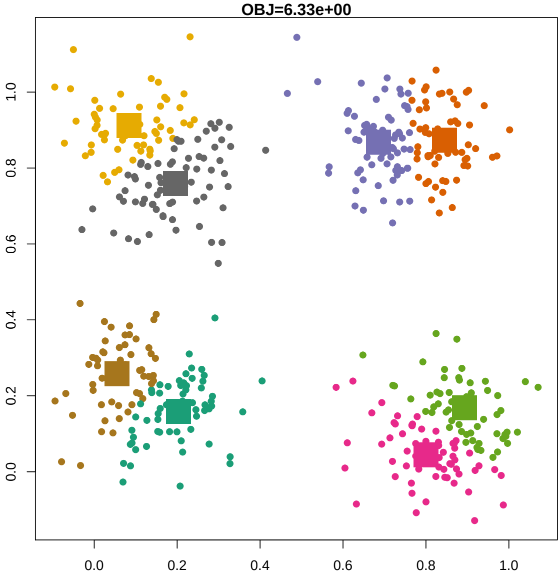
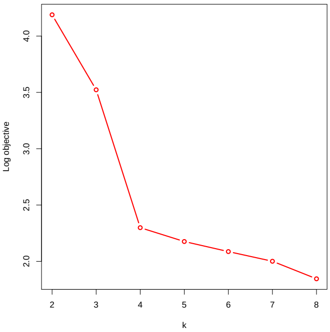
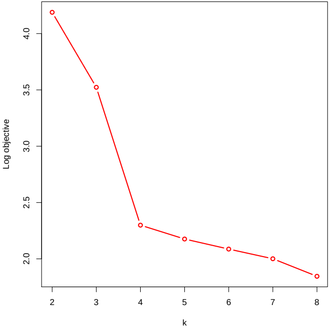


Heuristic: A kink in the objective



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

Heuristic: A kink in the objective



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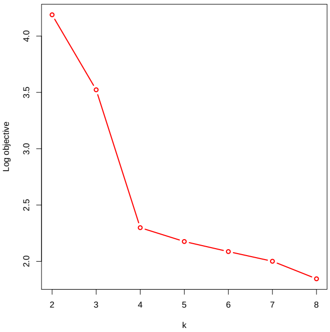

- Notice the “kink” in the objective between 3 and 5.
- This suggests that 4 is the right number of clusters.
- Tibshirani (2001) presents a method for finding this kink.

Archeology

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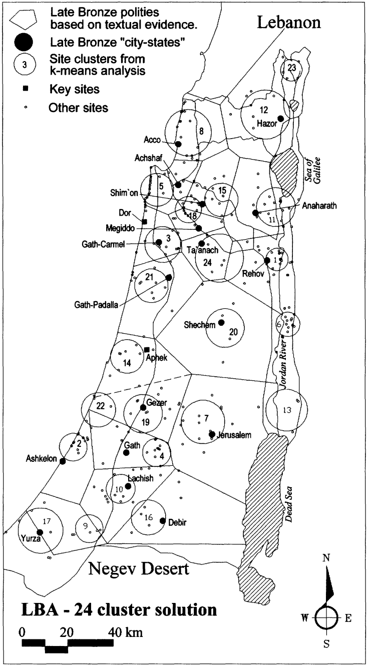
- Cluster the location of archeological sites in Israel
- Make inferences about political history based on the clusters
- Choose k very carefully, with a complicated computational technique.



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

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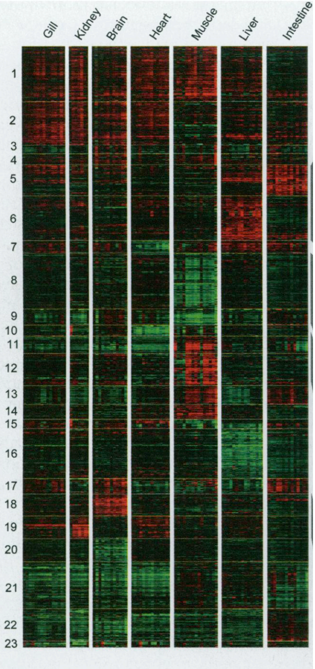
- (No mention of how $k = 23$ was chosen.)


Gill
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Education

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- I.e., the levels of encouragement are corrected for
- 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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- Draw the conclusion that patterns exist. What's wrong with this?
- 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