Displays for Statistics 5401

Lecture 42

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(not given)

Christopher Bingham, Instructor
612-625-1024

Class Web Page
http://www.stat.umn.edu/~kb/classes/5401

K-means clustering

K-means clustering is useful when you are clustering cases from a N by p data matrix **X** and have some idea about the number K of clusters to find.

The formal <u>ideal goal</u> is the following

> Find clusters $U_1, U_2, U_3, \ldots, U_k$ that minimize $\sum_{1\leq j\leq K} SSE_j(U_1, U_2, \ldots, U_k)$ where $SSE_j(U_1, U_2, U_3, \ldots, U_k)$ is the error SS in an ANOVA of x_j using the clusters as groups.

Another way to state this is:

> Find clusters $U_1, U_2, U_3, \ldots, U_k$ that <u>minimize</u> $tr(\mathbf{E}(U_1, U_2, \ldots, U_k))$ where **E** is the error matrix from a MANOVA using the clusters as groups

Now, if $\mathbf{H}(U_1, U_2, \ldots, U_k)$ is the between groups MANOVA matrix, $\mathbf{E}(U_1, U_2, \ldots, U_k) + \mathbf{H}(U_1, U_2, \ldots, U_k) = \sum(\mathbf{x}_j - \overline{\mathbf{x}})(\mathbf{x}_j - \overline{\mathbf{x}})'$ doesn't depend on the clustering. This means the ideal goal is equivalent to

> Find clusters $U_1, U_2, U_3, \ldots, U_k$ so as to <u>maximize</u> $tr(\mathbf{H}(U_1, U_2, \ldots, U_k))$

Such an assignment to clusters is the maximum likelihood assignment assuming clusters correspond to populations with $MVN(\boldsymbol{\mu}_j, \sigma^2\mathbf{I}_p)$ distributions, i = 1, ..., K.

This suggests the goal is best adapted to spherical clusters which is in fact the case.

A <u>simpler</u> goal, that would be satisfied by a clustering which minimizes $tr(\mathbf{E}(U_1, U_2, \ldots, U_k))$ is the following:

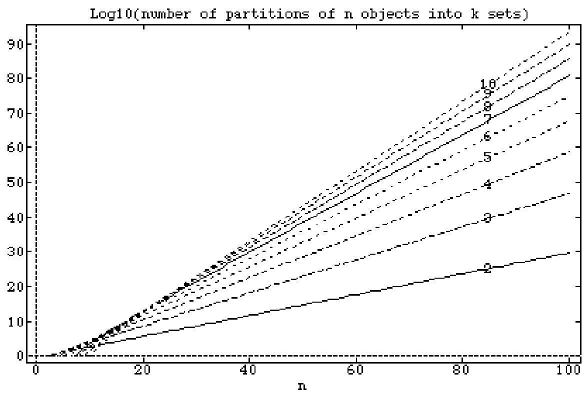
> Divide the N data points into k clusters $U_1, U_2, U_3, \ldots, U_k$ with means $\overline{\mathbf{x}}_{U_1}, \overline{\mathbf{x}}_{U_2}, \ldots, \overline{\mathbf{x}}_{U_k}$ such that
> $$U_j = \{\mathbf{x}_\ell \mid \|\mathbf{x}_\ell - \overline{\mathbf{x}}_{U_j}\| = \min_i \|\mathbf{x}_\ell - \overline{\mathbf{x}}_{U_i}\|\}$$

That is, each cluster consists of all the points that are nearest to its centroid.

However, a clustering can satisfy this, but not be the clustering that minimizes $tr(\mathbf{E}(U_1, U_2, \ldots, U_k))$.

Even this condition is almost impossible to solve by brute force because there are just too many ways to split into clusters.

When N is even moderately large, to find the "best" of all clusterings, using any criterion, is a tall order since there are approximately $N^k/k!$ such sets.



The ***K-means algorithm*** is an iterative method for, you hope, coming close to the optimal.

In the following, for any set of cases V, $\bar{\mathbf{x}}_V$ is the sample mean of the cases in V

- You start with K *initial* trial clusters $U_1, \ldots, U_k$, chosen in some way, possibly randomly, and compute $\bar{\mathbf{x}}_{U_j}^{\pm i}$, $j = 1,\ldots,K$.

When $\mathbf{x}_i$ is not in U_j, $\bar{\mathbf{x}}_{U_j}^{+i} \equiv \bar{\mathbf{x}}_{\{U_j,i\}}$
When $\mathbf{x}_i$ is in U_j, $\bar{\mathbf{x}}_{U_j}^{-i} \equiv \bar{\mathbf{x}}_{\{U_j - i\}}$.

Then, repeat the following until there is no change.

- Examine $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ sequentially.
  If $\mathbf{x}_i \in U_\ell$, compute the distances
  $d_j = \|\mathbf{x}_i - \bar{\mathbf{x}}_{U_j}^{+i}\|$, $j \neq \ell$, $d_\ell = \|\mathbf{x}_i - \bar{\mathbf{x}}_{U_\ell}^{-i}\|$
- Define J by $d_J = \min\{d_j\}$. If $J \neq \ell$, reallocate $\mathbf{x}_i$ to U_ℓ and update means.

Eventually you will complete a cycle through $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ without reallocating any points. Then you stop.

That is, reallocating any point would put it closer to another cluster's centroid than to the centroid of the other points in its cluster.

This differs from the description in Johnson & Wichern. They suggest computing distances

$$d_j = \|\mathbf{x}_i - \bar{\mathbf{x}}_{U_j}\|,\ j = 1,\ldots,K$$

and reallocating $\mathbf{x}_i$ to the nearest group, the group with d_j. Their method performs worse as measured by tr $\mathbf{E}(U_1,\ldots,U_K)$,.

It's easy to use the distances to the unadjusted means $\bar{\mathbf{x}}_{U_\ell}$ and $\bar{\mathbf{x}}_{U_j}$ to compute the distances to the adjusted means $\bar{\mathbf{x}}_{U_\ell}^{-i}$ and $\bar{\mathbf{x}}_{U_j}^{+i}$.

When $\mathbf{x}_i \in U_\ell$,

$$\boxed{\|\mathbf{x}_i - \bar{\mathbf{x}}_{U_\ell}^{-i}\|^2 = (n_\ell/(n_\ell - 1))\|\mathbf{x}_i - \bar{\mathbf{x}}_{U_\ell}\|^2}$$

and for $j \neq \ell$

$$\boxed{\|\mathbf{x}_i - \bar{\mathbf{x}}_{U_j}^{+i}\|^2 = (n_j/(n_j + 1))\|\mathbf{x}_i - \bar{\mathbf{x}}_{U_j}\|^2}$$

Here n_j, $j = 1,\ldots,K$ are the cluster sizes at the point in the algorithm when you examining $\mathbf{x}_i$.

Example of use of kmeans() for doing k-means clustering

Try to cluster the utility company data using K-means. Keywords **kmax** and **kmin** specify that clustering will first be done with K = 8, followed by K = 7, 6, ..., 3.

```
Cmd> stuff <- kmeans(data,kmax:8,kmin:3)
Cluster analysis by reallocation of objects using Trace W
criterion
Variables are standardized before clustering
Initial allocation is random
  k     Initial       Final Reallocations
  8      112.13      48.275      13
  8      48.275      45.473       2
  8      45.473       45.21       1
  8       45.21      43.191       2
  8      43.191      43.191       0   Criterion for K = 8
Merging clusters 3 and 7; criterion = 49.35
  k     Initial       Final Reallocations
  7       49.35       48.98       1
  7       48.98       48.98       0   Criterion for K = 7
Merging clusters 1 and 5; criterion = 58.154
  k     Initial       Final Reallocations
  6      58.154      58.154       0   Criterion for K = 6
Merging clusters 2 and 5; criterion = 67.406
  k     Initial       Final Reallocations
  5      67.406      67.406       0   Criterion for K = 5
Merging clusters 2 and 4; criterion = 80.383
  k     Initial       Final Reallocations
  4      80.383      80.383       0   Criterion for K = 4
Merging clusters 1 and 3; criterion = 101.71
  k     Initial       Final Reallocations
  3      101.71      101.71       0   Criterion for K = 3
```

Later clusters start by merging two clusters. As you see, they converge to a solution with less effort than with K = 8.

kmeans() first uses the k-means algorithm for K = 8. Then it merges the two closest clusters using the weighted distances $\{n_i n_j/(n_i+n_j)\}\|\bar{\mathbf{x}}_i - \bar{\mathbf{x}}_j\|^2$. This ensures that $\mathrm{tr}(\mathbf{E}(U_1, U_2,\ldots, U_{k-1}))$ is minimized over the k(k-1)/2 clusterings obtainable by merging two clusters.

```
Cmd> compnames(stuff) # the result is a structure
(1) "classes"     N by kmax-kmin+1 matrix
(2) "criterion"   vector of length k

Cmd> kmeansclass <- stuff$classes

Cmd> print(kmeansclass,format:"4.0f") # classes
MATRIX:    8    7     6    5    4    3  Clusters
  (1,1)    5    5    1    1    1    1
  (2,1)    7    6    5    2    2    2
  (3,1)    1    1    1    1    1    1
  (4,1)    3    3    3    3    3    1
  (5,1)    4    4    4    4    2    2
  (6,1)    1    1    1    1    1    1
  (7,1)    6    6    5    2    2    2
  (8,1)    8    7    6    5    4    3
  (9,1)    1    1    1    1    1    1
 (10,1)    3    3    3    3    3    1
 (11,1)    8    7    6    5    4    3
 (12,1)    6    6    5    2    2    2
 (13,1)    3    3    3    3    3    1
 (14,1)    5    5    1    1    1    1
 (15,1)    6    6    5    2    2    2
 (16,1)    8    7    6    5    4    3
 (17,1)    2    2    2    2    2    2
 (18,1)    5    5    1    1    1    1
 (19,1)    5    5    1    1    1    1
 (20,1)    3    3    3    3    3    1
 (21,1)    6    6    5    2    2    2
 (22,1)    7    3    3    3    3    1
```

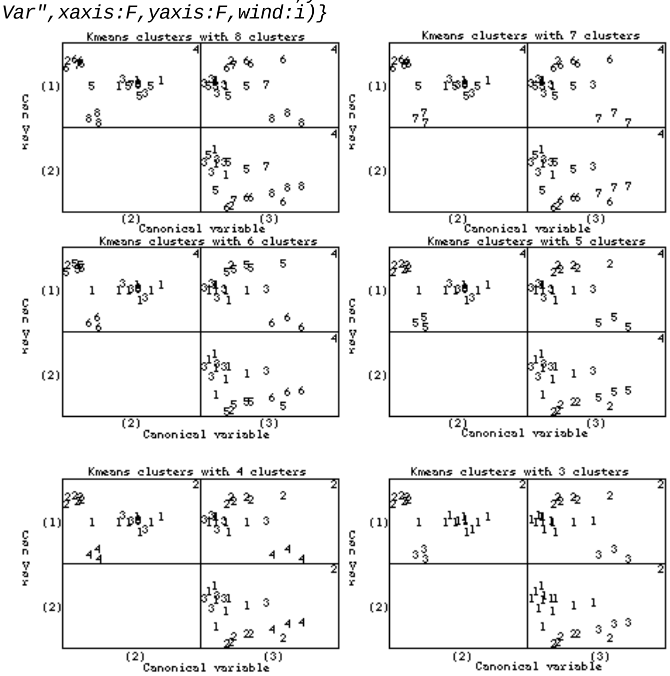
Note K decreases from left to right.


```
Cmd> split(run(22), kmeansclass[,5]) # 4 cluster membership
component: comp1  Cases in cluster 1
(1)           1          3          6          9         14
(6)          18         19
component: comp2  Cases in cluster 2
(1)           2          5          7         12         15
(6)          17         21
component: comp3  Cases in cluster 3
(1)           4         10         13         20         22
component: comp4  Cases in cluster 4
(1)           8         11         16

Cmd> split(run(22), avelnkclass[,3]) # compare w/ aver linkage
component: comp1  Cases in cluster 1
 (1)           1          3          4          6          9
 (6)          10         13         14         18         19
(11)          20         22
component: comp2  Cases in cluster 2
(1)            8         11         16
component: comp3  Case in cluster 3
(1)            5
component: comp4  Cases in cluster 4
(1)            2          7         12         15         17
(6)           21

Cmd> tabs(,avelnkclass[,3],kmeansclass[,5]) # confusion matrix
(1,1)          0          7          5          0  Ave Link 1
(2,1)          0          0          0          3  Ave Link 2
(3,1)          1          0          0          0  Ave Link 3
(4,1)          6          0          0          0  Ave Link 4

Cmd> tabs(,avelnkclass[,4],kmeansclass[,4]) # same, K = 5
(1,1)          7          0          5          0          0
(2,1)          0          0          0          0          3
(3,1)          0          0          0          1          0
(4,1)          0          5          0          0          0
(5,1)          0          1          0          0          0

Cmd> junk <- kmeans(data,avelnkclass[,3],start:"class")
Cluster analysis by reallocation of objects using Trace W
criterion
Variables are standardized before clustering
Initial allocation is predefined
  k    Initial      Final Reallocations
  4     88.734     88.734       0
```

No reallocations, but tr **E** > K-means tr **E**

Plots of clusters using canonical variables

```
Cmd> for(i,run(6)){plotmatrix(z,symbols:kmeansclass[,i],\
  upper:T,title:paste("Kmeans clusters with",9-i,"clusters"),\
  xlab:"Canonical variable",ylab:"Can
Var",xaxis:F,yaxis:F,wind:i)}
```



By default **kmeans()** uses random starting clusters.

I did 200 **kmeans()** clustering with K = 4, each using a different random start.

```
Cmd> M <- 200; CRITERION <- rep(0,M)

Cmd> for(i,run(M)){ # cluster and save criterion
     CRITERION[i] <- kmeans(data,kmax:4)$criterion;;}

Cmd> unique(round(CRITERION,3)) # 8 different criterion found
(1)     80.383      92.01     90.883     91.781      96.11
(6)     88.734     99.207      92.52  Different values found

Cmd> sum(round(CRITERION,3) == unique(round(CRITERION,3))')
(1,1)        184          3          3          5          2
(1,6)          1          1          1 Counts of each value
```

Most of the time, it found the identical clustering. 184 times it hit 80.383, and never was greater than 92.52.

J&W don't say how they did the clustering in their example, but it is not optimal. **kmeans()** can improve on it

```
Cmd> junk <- kmeans(data,jwclass,start:"class",kmax:4)
Cluster analysis by reallocation of objects using Trace W
criterion
Variables are standardized before clustering
Initial allocation is predefined
  k    Initial      Final Reallocations
  4      85.84     80.383       4
  4     80.383     80.383       0
```

The starting value for the criterion is 85.84, worse than what **kmeans()** accomplished.

I wrote a macro to do J&W type K-means clustering. It does worse than **kmeans()**.

```
Cmd> dataS <- standardize(data) # macro does not standardize

Cmd> CRITERION1 <- rep(0, M)

Cmd> for(i,run(M)){
     CRITERION1[i] <-\
        reverse(kmeansmac1(dataS,k:4,silent:T)$criterion)[1];;}

Cmd> describe(hconcat(CRITERION,CRITERION1),\
     mean:T,stddev:T,min:T,max:T,median:T)
component: min    Minima from kmeans() and and J&W kmeans
(1)     80.383     80.383
component: median Medians from kmeans() and and J&W kmeans
(1)     80.383     93.752
component: max    Max from kmeans() and and J&W kmeans
(1)     99.207      123.7
component: mean   Maxima from kmeans() and and J&W kmeans
(1)     81.354     93.566
component: stddev
(1)     3.3726     9.3496

Cmd> min(abs(CRITERION1-85.84)) # never hit 85.84
(1)      0.375
```

Not once did I get 85.84 and the mean and median are worse than from **kmeans()**. Now do K-means clustering of can. vars.

```
Cmd> zclasses <- kmeans(z,kmax:4)$classes
Cluster analysis by reallocation of objects using Trace W
criterion
Variables are standardized before clustering
Initial allocation is random
  k    Initial      Final Reallocations
  4     57.628     8.8961      15
  4     8.8961     8.8961       0

Cmd> @junk <- kmeans(data,zclasses,start:"class")
  k    Initial      Final Reallocations
  4     88.734     88.734       0
```


Example with artificial data set with 4 known "clusters".

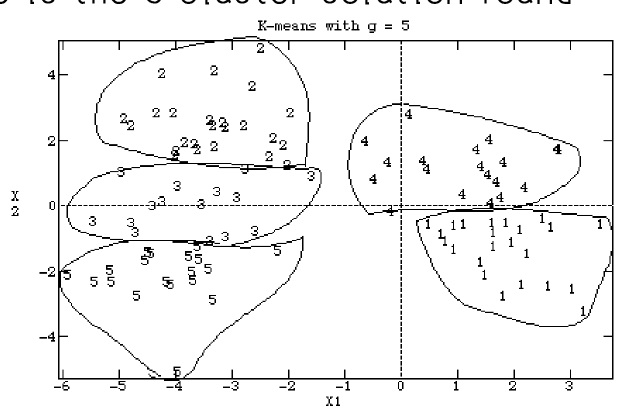
```
Cmd> results <- kmeans(x1,kmax:5,kmin:3) # K-means analysis
Cluster analysis by reallocation of objects using Trace W
criterion
Variables are standardized before clustering
Initial allocation is random
  k      Initial        Final Reallocations
  5       190.45       45.582      77
  5       45.582       35.884      19
  5       35.884       28.866      14
  5       28.866       28.386       5
  5       28.386       28.386       0
Merging clusters 3 and 5; criterion = 38.985
  k      Initial        Final Reallocations
  4       38.985       35.321       6
  4       35.321       35.252       1
  4       35.252       35.252       0
Merging clusters 1 and 4; criterion = 53.093
  k      Initial        Final Reallocations
  3       53.093       50.767       2
  3       50.767       50.748       1
  3       50.748       50.748       0
```

This first found a 5 group clustering (**kmax:5**), taking four cycles through the cases before no more points to move on cycle 5. Then in merged clusters 3 and 5, the pair with the smallest value of

$$(n_i n_j/(n_i+n_j))\|\bar{\mathbf{y}}_i - \bar{\mathbf{y}}_j\|^2$$

This minimizes the tr **E** criterion after merging.

Here is the 5 cluster solution found

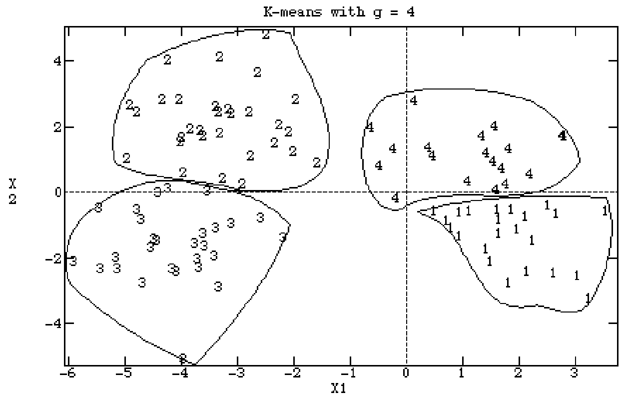


Here is the confusion matrix with the "true" clusters:

```
Cmd> tabs(,groups,results$classes[,1])
(1,1)          3          0          0         17          0 Group 1
(2,1)         20          0          0          2          0 Group 2
(3,1)          0         24          6          0          0 Group 3
(4,1)          0          0          9          0         19 Group 4
```

Groups 1 and 2 are almost entirely in k-means clusters 4 and 1, respectively; group 3 is 75% in k-means cluster 2 and group 4 is 68% in k-means cluster 5, with kmeans cluster 3 overlapping both groups 3 and 4.

The 4 cluster solution:

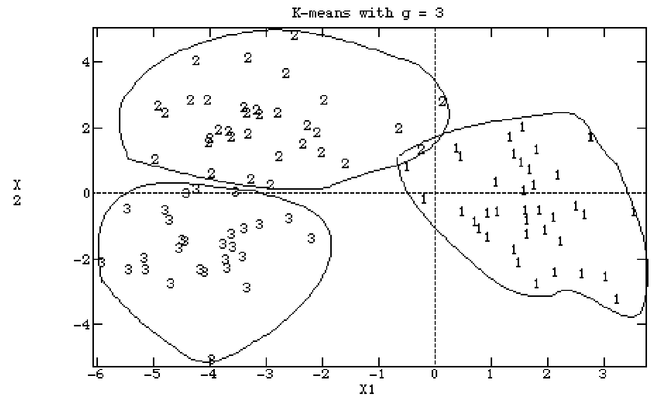


with confusion matrix

```
Cmd> tabs(,groups,results$classes[,2])
(1,1)          3          0          0         17 Group 1
(2,1)         20          0          0          2 Group 2
(3,1)          0         29          1          0 Group 3
(4,1)          0          1         27          0 Group 4
```

This does a remarkably good job each cluster almost coinciding with a sample.

The three cluster solution merges the two clusters on the right.



Confusion matrix

```
Cmd> tabs(,groups,results$classes[,3])
(1,1)         17          3          0 Group 1
(2,1)         22          0          0 Group 2
(3,1)          0         29          1 Group 3
(4,1)          0          1         27 Group 4
```

By carefully comparing the solutions, you can verify that this process is <u>not hierarchical</u>. For example, although the new cluster 1 is primarily a merging of clusters 4 and 1, some of cluster 4 ended up in cluster 2.