

Hierarchical Clustering

k -Means Clustering

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Clustering Task

- Clustering refers to grouping records, observations, or tasks into classes of similar objects
- Cluster is collection records similar to one another
- Records in one cluster dissimilar to records in other clusters
- Clustering is unsupervised data mining task
- Therefore, no target variable specified
- Clustering algorithms segment records and maximize homogeneity in subgroups
- Similarity to records outside cluster minimized

Clustering Task (*cont'd*)

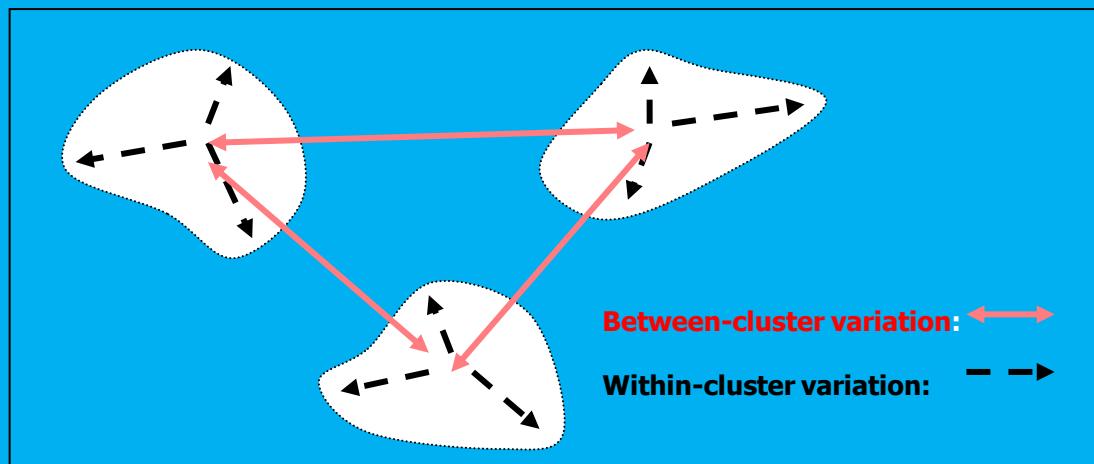
- For example, Claritas, Inc. provides demographic profiles of geographic areas, according to zip code
- PRIZM segmentation system clusters zip codes in terms of lifestyle types
- Recall clusters identified for 90210 Beverly Hills, CA
- Cluster 01: *Blue Blood Estates*
"Established executives, professionals, and 'old money' heirs that live in America's wealthiest suburbs..."
- Cluster 10: *Bohemian Mix*
- Cluster 02: *Winner's Circle*
- Cluster 07: *Money and Brains*
- Cluster 08: *Young Literati*

<http://www.claritas.com/MyBestSegments/Default.jsp?ID=20#>

Clustering Task (*cont'd*)

- Clustering Tasks in Business and Research
 - Target marketing for niche product, without large marketing budget
 - Segment financial behavior into benign and suspicious categories
 - Gene expression clustering, where genes exhibit similar characteristics
 - Clustering often performed as preliminary step in data mining process
 - Clustering results used as input to other data mining techniques

Clustering Task (*cont'd*)



- Clustering identifies groups of highly-similar records
- Algorithms construct clusters where between-cluster variation (BCV) large, as compared to within-cluster variation (WCV)
- Analogous to concept behind analysis of variance

Clustering Task (*cont'd*)

- Applying cluster analysis to enormous databases helpful
 - Reduces search space for downstream algorithms
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- Cluster analysis addresses similar issues encountered in classification
 - Similarity measurement
 - Recoding categorical variables
 - Standardizing and normalizing variables
 - Number of clusters

Distance Function

- How is similarity defined between an unclassified record and its neighbors?
- A distance metric is a real-valued function d used to measure the similarity between coordinates x , y , and z with properties:

1. $d(x, y) \geq 0$, and $d(x, y) = 0$ if and only if $x = y$
2. $d(x, y) = d(y, x)$
3. $d(x, z) \leq d(x, y) + d(y, z)$

- Property 1: Distance is always non-negative
- Property 2: Commutative, distance from “A to B” is distance from “B to A”
- Property 3: Triangle inequality holds, distance from “A to C” must be less than or equal to distance from “A to B to C”

Clustering Task (*cont'd*)

- Measuring Similarity
 - Euclidean Distance measures distance between records

$$d_{\text{Euclidean}}(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_i (x_i - y_i)^2}, \text{ where}$$

$\mathbf{x} = x_1, x_2, \dots, x_m$ and $\mathbf{y} = y_1, y_2, \dots, y_m$ represent m attribute values of two records

- Other distance measurements include City-Block Distance and Minkowski Distance

$$d_{\text{City-Block}}(\mathbf{x}, \mathbf{y}) = \sum_i |x_i - y_i|$$

$$d_{\text{Minkowski}}(\mathbf{x}, \mathbf{y}) = \left(\sum_i |x_i - y_i|^q \right)^{1/q}$$

Clustering Task (*cont'd*)

- “Different From” function measures similarity between categorical attributes

$$\text{different}(x_i, y_i) = \begin{cases} 0 & \text{if } x_i = y_i \\ 1 & \text{otherwise} \end{cases}$$

- Substitute *different(x,y)* for each categorical attribute in Euclidean Distance function
- Normalizing data enhances performance of clustering algorithms
- Use Min-max Normalization or Z-Score Standardization

$$\text{Min - Max Normalization} = \frac{X - \min(X)}{\max(X) - \min(X)}$$

$$\text{Z - Score Standardization} = \frac{X - \text{mean}(X)}{\text{standard deviation}(X)}$$

Hierarchical Clustering Methods

- Clustering algorithms either Hierarchical or Non-Hierarchical
- **Hierarchical**
 - Tree like cluster structure (dendogram) created through recursive partitioning (Divisive Methods) or combining (Agglomerative Methods) existing clusters
 - **Divisive Methods**
 - All records initialized into single cluster
 - At each iteration, most dissimilar record split off into separate cluster
 - Continues until each record represents single cluster

Hierarchical Clustering Methods

(cont'd)

- Agglomerative Methods
- Each observation initialized to become its own cluster
- At each iteration two closest clusters aggregated together
- Number of clusters reduced by one, each step
- Eventually, all records combined into single cluster
- Agglomerative more popular hierarchical method
- Therefore, focus remains on this approach
- Measuring distance between records straightforward once recoding and normalization applied
- However, how is distance between clusters determined?

Hierarchical Clustering Methods

(cont'd)

- Distance Between Clusters
 - Several criteria examined to determine distance between clusters, A and B
 - Single Linkage
 - Known as Nearest-Neighbor Approach
 - Minimum distance between any record in cluster A, and any record in cluster B
 - Cluster similarity based on most similar records from each cluster
 - Tends to form long, slender clusters
 - Sometime heterogeneous records clustered together

Hierarchical Clustering Methods

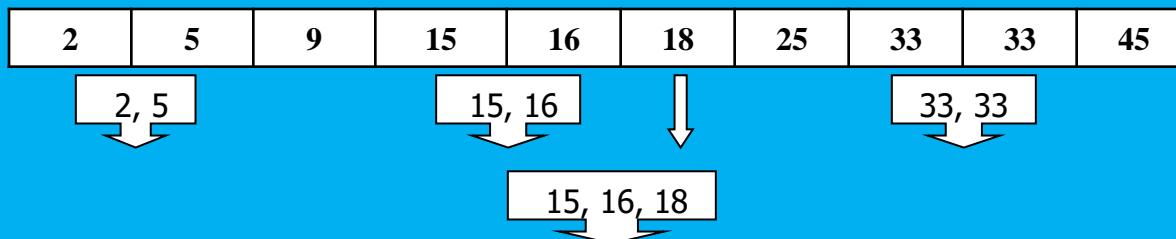
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- Measure is average distance of records in cluster A, from records in cluster B
- Resulting clusters have approximately equal within-cluster variability
- Next, linkage methods examined using small data set

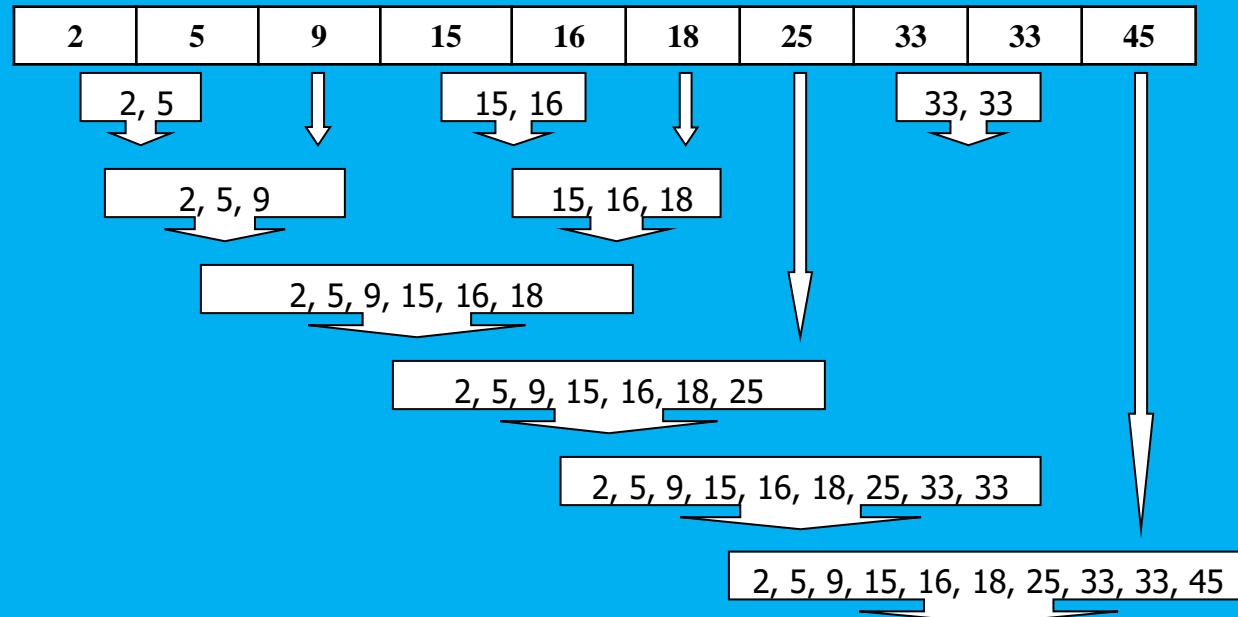
2 5 9 15 16 18 25 33 33 45

Single-Linkage Clustering

- To begin, each record assigned to its own cluster
- Single-linkage seeks minimum distance between any two records, in separate clusters
- Step 1: Minimum cluster distance is between clusters {33} and {33}. Distance = 0, clusters combined
- Step 2: Clusters {15} and {16} combined, where distance = 1
- Step 3: Cluster {15, 16} combined with cluster {18}
- Step 4: Clusters {2} and {5} combined



Single-Linkage Clustering (*cont'd*)



- Agglomeration continues similarly Steps 4 – 9
- Above, last cluster {2, 5, 9, 15, 16, 18, 25, 33, 33, 45} contains all records in data set

k-Means Clustering

- *k*-Means effective at finding clusters in data
- *k*-Means Algorithm
 - Step 1: Analyst specifies k = number of clusters to partition data
 - Step 2: k records randomly assigned to initial clusters
 - Step 3: For each record, find the nearest cluster center,
Each cluster center “owns” subset of records, we have
a partition of data set into k clusters, C_1, C_2, \dots, C_k
 - Step 4: For each of k clusters, find cluster centroid
Update cluster center location to centroid
 - Step 5: Repeats Steps 3 – 5 until convergence or termination

k-Means Clustering (*cont'd*)

- Nearest criterion in Step 3 typically Euclidean Distance
- Determining Cluster Centroid
 - Assume n data points $(a_1, b_1, c_1), (a_2, b_2, c_2), \dots, (a_n, b_n, c_n)$
 - Centroid of points is center of gravity of points
 - Located at point $(\sum a_i/n, \sum b_i/n, \sum c_i/n)$
 - For example, points $(1, 1, 1), (1, 2, 1), (1, 3, 1)$, and $(2, 1, 1)$ have centroid

$$\left(\frac{1+1+1+2}{4}, \frac{1+2+3+1}{4}, \frac{1+1+1+1}{4} \right) = (1.25, 1.75, 1.00)$$

k-Means Clustering (*cont'd*)

- *k*-Means algorithm terminates when centroids no longer change
- For *k* clusters, C_1, C_2, \dots, C_k , all records “owned” by cluster remain in cluster
- Convergence criterion may also cause termination
- For example, no significant reduction in SSE

$$SSE = \sum_{i=1}^k \sum_{p \in C_i} d(p, m_i)^2, \text{ where}$$

$p \in C_i$ = each data point in cluster i

m_i = represents centroid of cluster i

Example of k -Means Clustering at Work

- Assume $k = 2$ to cluster following data points

a	b	c	d	e	f	g	h
(1, 3)	(3, 3)	(4, 3)	(5, 3)	(1, 2)	(4, 2)	(1, 1)	(2, 1)

- Step 1: $k = 2$ specifies number of clusters to partition
- Step 2: Randomly assign $k = 2$ cluster centers
For example, $m_1 = (1, 1)$ and $m_2 = (2, 1)$

Example of k -Means Clustering at Work

First Pass (Copied from book)						
	Centroid		d1	d2		
m1			1	1		
m2			2	1		
Clustering						
	Point	d1	d2	Distance from m1	Distance from m2	Cluster Membership
	a	1	3			SE
	b	3	3			
	c	4	3			
	d	5	3			
	e	1	2			
	f	4	2			
	g	1	1			
	h	2	1			
SSE						
BCV						
BCV/WCV						

Example of k -Means Clustering at Work

First Pass (Copied from book)						
	Centroid		d1	d2		
m1		1	1			
m2		2	1			
Clustering						
Point	d1	d2	Distance from m1	Distance from m2	Cluster Membership	SE
a	1	3	2.00	2.24	C1	4
b	3	3	2.83	2.24	C2	5
c	4	3	3.61	2.83	C2	8
d	5	3	4.47	3.61	C2	13
e	1	2	1.00	1.41	C1	1
f	4	2	3.16	2.24	C2	5
g	1	1	0.00	1.00	C1	0
h	2	1	1.00	0.00	C2	0
SSE	36.00					
BCV	1					
BCV/WCV	0.028					
Centroid (Newly calculated)						
	Centroid		d1	d2		
m1		1	2			
m2		3.6	2.4			

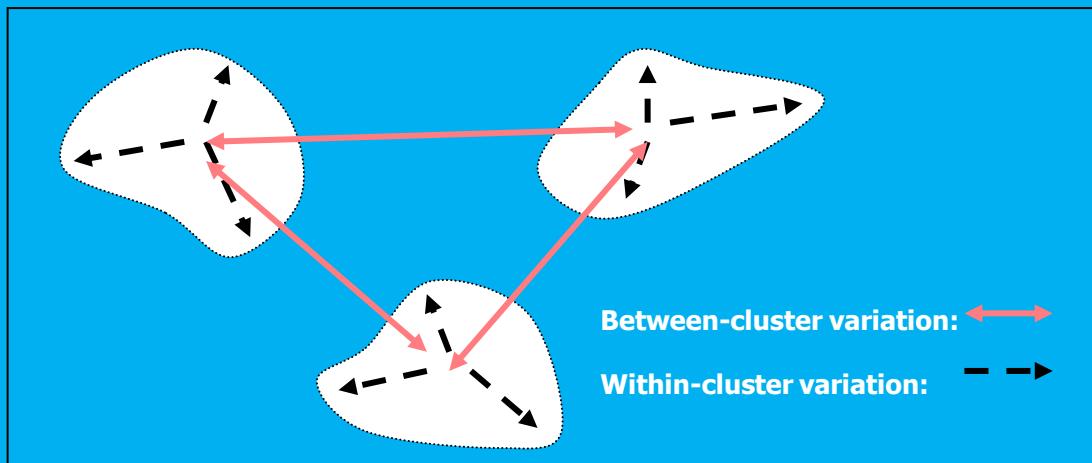
Example of k -Means Clustering at Work

Second Pass						
	Centroid					
	d1	d2				
m1	1	2				
m2	3.6	2.4				
Clustering						
Point	d1	d2	Distance from m1	Distance from m2	Cluster Membership	SE
a	1	3	1.00	2.67	C1	1
b	3	3	2.24	0.85	C2	0.72
c	4	3	3.16	0.72	C2	0.52
d	5	3	4.12	1.52	C2	2.32
e	1	2	0.00	2.63	C1	0
f	4	2	3.00	0.57	C2	0.32
g	1	1	1.00	2.95	C1	1
h	2	1	1.41	2.13	C1	2
SSE	7.88					
BCV	2.631					
BCV/WCV	0.334					
Centroid (Newly calculated)						
	d1	d2				
m1	1.25	1.75				
m2	4	2.75				

Example of k -Means Clustering at Work

Third Pass (Copied from book)						
	Centroid					
	d1	d2				
m1	1.25	1.75				
m2	4	2.75				
Clustering						
Point	d1	d2	Distance from m1	Distance from m2	Cluster Membership	SE
a	1	3	1.27	3.01	C1	1.625
b	3	3	2.15	1.03	C2	1.0625
c	4	3	3.02	0.25	C2	0.0625
d	5	3	3.95	1.03	C2	1.0625
e	1	2	0.35	3.09	C1	0.125
f	4	2	2.76	0.75	C2	0.5625
g	1	1	0.79	3.47	C1	0.625
h	2	1	1.06	2.66	C1	1.125
SSE	6.25					
BCV	2.926					
BCV/WCV	0.468					
Centroid (Newly calculated)						
	d1	d2				
m1	1.25	1.75				
m2	4	2.75				

Clustering Task (*Repeated slide*)



- Clustering identifies groups of highly-similar records
- Algorithms construct clusters where between-cluster variation (BCV) large, as compared to within-cluster variation (WCV)
- Analogous to concept behind analysis of variance

Example of k -Means Clustering at Work

- Assume $k = 2$ to cluster following data points

a	b	c	d	e	f	g	h
(1, 3)	(3, 3)	(4, 3)	(5, 3)	(1, 2)	(4, 2)	(1, 1)	(2, 1)

- Step 1: $k = 2$ specifies number of clusters to partition
 - Step 2: Randomly assign $k = 2$ cluster centers
For example, $m_1 = (1, 1)$ and $m_2 = (2, 1)$
- First Iteration
 - Step 3: For each record, find nearest cluster center
Euclidean distance from points to m_1 and m_2 shown

Point	a	b	c	d	e	f	g	h
Distance from m_1	2.00	2.83	3.61	4.47	1.00	3.16	0.00	1.00
Distance from m_2	2.24	2.24	2.83	3.61	1.41	2.24	1.00	0.00
Cluster Membership	C ₁	C ₂	C ₂	C ₂	C ₁	C ₂	C ₁	C ₂

Example of k -Means Clustering at Work (*cont'd*)

- Cluster m_1 contains {a, e, g} and m_2 has {b, c, d, f, h}
- Cluster membership assigned, now SSE calculated

$$\begin{aligned} SSE &= \sum_{i=1}^k \sum_{p \in C_i} d(p, m_i)^2 \\ &= 2^2 + 2.24^2 + 2.83^2 + 3.61^2 + 1^2 + 2.24^2 + 0^2 + 0^2 = 36 \end{aligned}$$

- Recall clusters constructed where between-cluster variation (BCV) large, as compared to within-cluster variation (WCV)

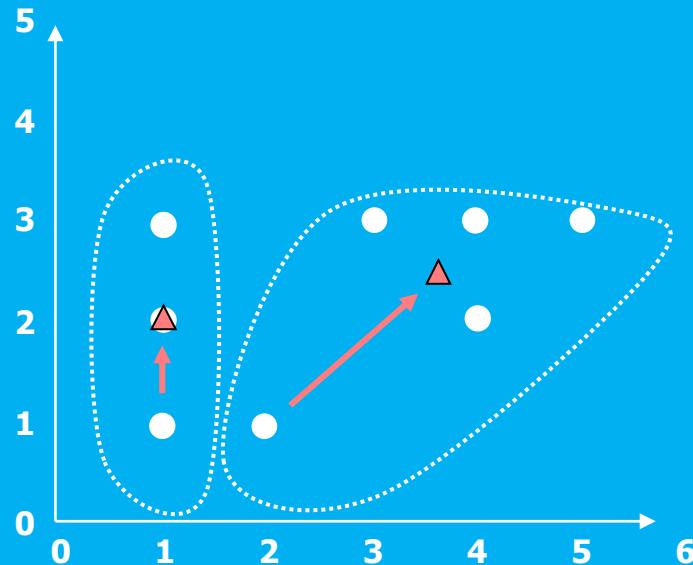
$$\frac{\text{BCV}}{\text{WCV}} = \frac{d(m_1, m_2)}{\text{SSE}} = \frac{1}{36} = 0.0278, \text{ where}$$

$d(m_1, m_2)$ = surrogate for BCV
 SSE = surrogate for WCV

- Ratio BCV/WCV expected to increase for successive iterations

Example of k -Means Clustering at Work (*cont'd*)

- Step 4: For k clusters, find cluster centroid, update location
- Cluster 1 = $[(1 + 1 + 1)/3, (3 + 2 + 1)/3] = (1, 2)$, Cluster 2 = $[(3 + 4 + 5 + 4 + 2)/5, (3 + 3 + 3 + 2 + 1)/5] = (3.6, 2.4)$
- Figure shows movement of clusters m_1 and m_2 (triangles) after first iteration of algorithm

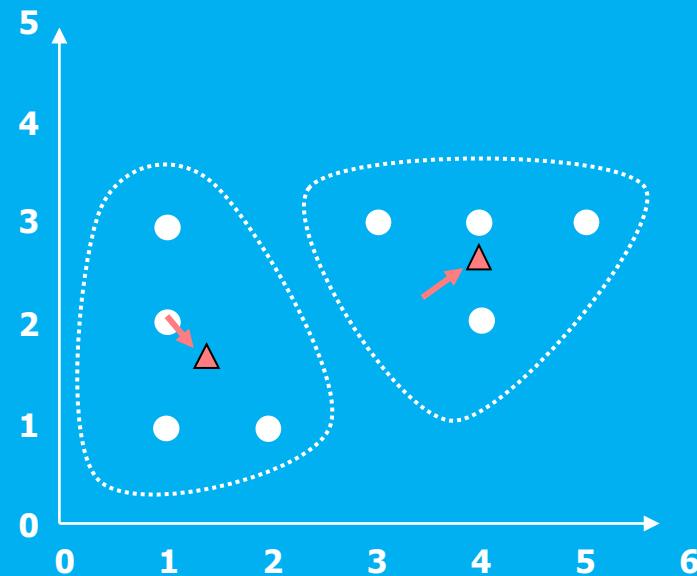


Example of k -Means Clustering at Work (*cont'd*)

- Step 5: Repeats Steps 3 – 4 until convergence or termination
- Second Iteration
 - Repeat procedure for Steps 3 – 4
 - Again, for each record find nearest cluster center $m_1 = (1, 2)$ or $m_2 = (3.6, 2.4)$
 - Cluster m_1 contains {a, e, g, h} and m_2 has {b, c, d, f}
 - SSE = 7.86, and BCV/WCV = 0.3346
 - Note 0.3346 has increased compared to First Iteration value = 0.0278
 - Between-cluster variation increasing with respect to Within-cluster variation

Example of k -Means Clustering at Work (*cont'd*)

- Cluster centroids updated to $m_1 = (1.25, 1.75)$ or $m_2 = (4, 2.75)$
- After Second Iteration, cluster centroids shown to move slightly



Example of k -Means Clustering at Work (*cont'd*)

- Third (Final) Iteration
 - Repeat procedure for Steps 3 – 4
 - Now, for each record find nearest cluster center $m_1 = (1.25, 1.75)$ or $m_2 = (4, 2.75)$
 - SSE = 6.23, and BCV/WCV = 0.4703
 - Again, BCV/WCV has increased compared to previous = 0.3346
 - This time, no records shift cluster membership
 - Centroids remain unchanged, therefore algorithm terminates

Example of k -Means Clustering at Work (*cont'd*)

- Summary
 - k -Means not guaranteed to find global minimum SSE
 - Instead, local minimum found
 - Invoking algorithm using variety of initial cluster centers improves probability of achieving global minimum
 - One approach places first cluster at random point, with remaining clusters placed far from previous centers (Moore)
 - What is appropriate value for k ?
 - Potential problem for applying k -Means
 - Analyst may have *a priori* knowledge of k

Example of k -Means Clustering at Work (*cont'd*)

- Outer loop to algorithm possible
- Cycles through different k values
- Results compared, selecting solution with smallest SSE

- What attributes to use as input?
- Some attributes likely more relevant than others
- Apply axis-stretching methods for quantifying attribute relevance discussed in Chapter 5