Lecture 20 - Cluster Analysis

Introduction

- Classification involves using data to group places, events, things into types.
- In geography we are often interested classifying places into regions.
- A "gentrifying neighborhood" evokes multidimensional picture of a place.

Cluster Analysis vs. an Atlas

- Traditionally geographers would explore multivariate spatial data by producing an atlas.
- Each page of the atlas would describe a single variable (e.g. income, homeownership, third-wave coffee shop density, dog salons per capita…).
- We could to identify "gentrifying" neighborhoods by cross referencing maps.

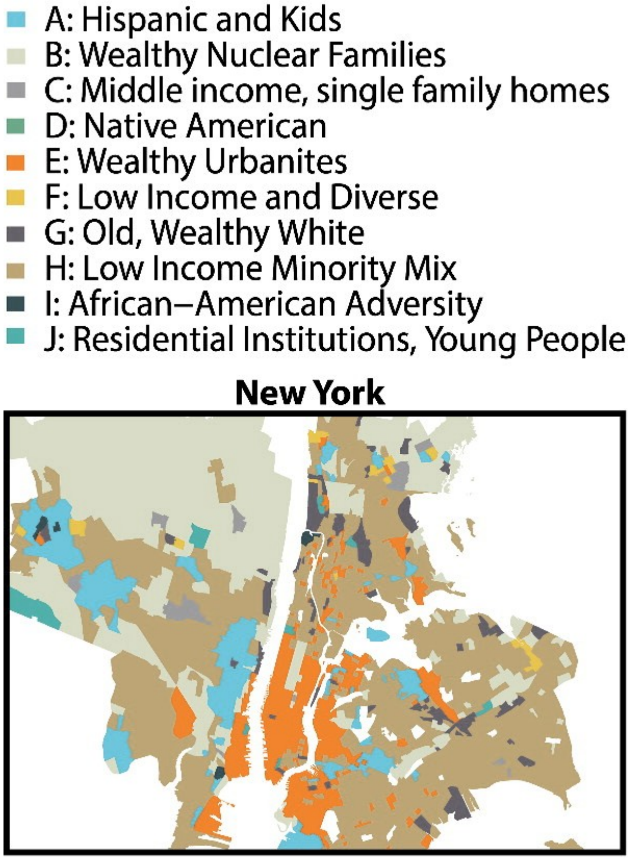
Cluster Analysis vs. an Atlas

- However, as our data grew in complexity the task of identifying interesting patterns in the data would become more complex.
- If we had 50 variables we would need to have an atlas with at least 50 pages.
- We would have to cross reference many maps. Identifying patterns would be difficult.

Cluster Analysis vs. an Atlas

- Cluster Analysis is a set of statistical techniques to let people "discover" groups in data.
- What you could do visually in 2 or 3 dimensions cluster analysis does in high dimensions.
- Each data point is labeled by group membership.
- Each cluster has an **attribute profile**…kind of like a "bookmarked" set of atlas pages that best describe places in that cluster.

Example


A: Hispanic and Kids
B: Wealthy Nuclear Families
C: Middle income, single family homes
D: Native American
E: Wealthy Urbanites
F: Low Income and Diverse
G: Old, Wealthy White
H: Low Income Minority Mix
I: African–American Adversity
J: Residential Institutions, Young People
New York

(Singleton and Spielman 2015)

Geographic Cluster Analysis

- Cluster analysis joins areas that are close together in “attribute space”.
- We might want to add a spatial constraint to this process.
- Cluster analysis with a spatial constraint is sometimes called regionalization.

Regionalization Example

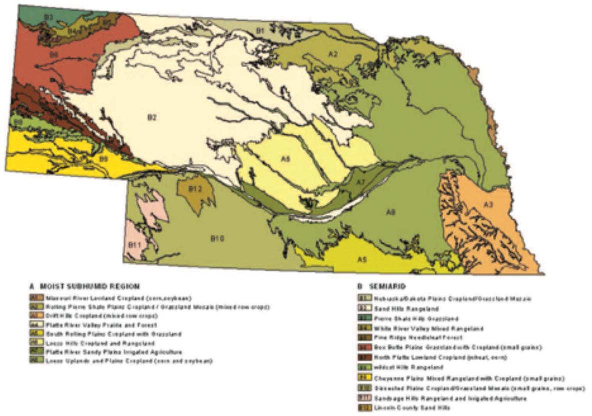
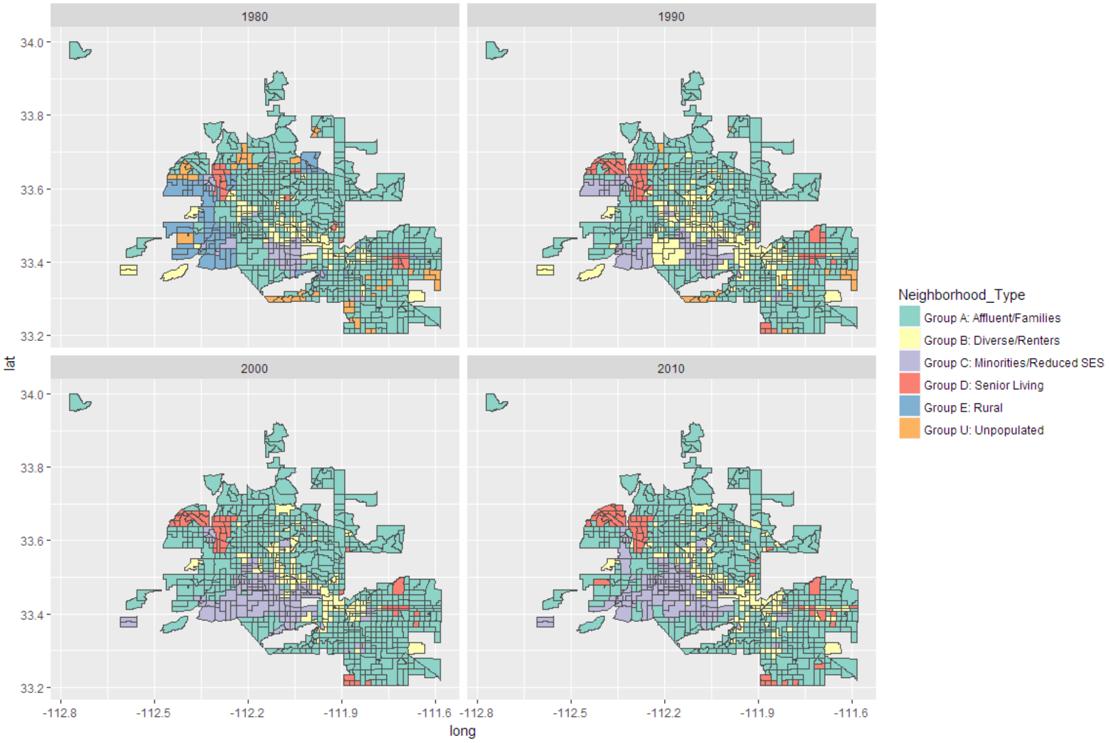

B3
B6
B1
A2
A3
B2
A8
B9
B12
A7
A6
A3
B10
B11
A5
A MOIST SUBHUMID REGION
A1 Missouri River Lowland Cropland (corn,soybean)
A2 Rolling Pierre Shale Plains Cropland / Grassland Mosaic (mixed row crops)
A3 Drift Hills Cropland (mixed row crops)
A4 Platte River Valley Prairie and Forest
A5 South Rolling Plains Cropland with Grassland
A6 Loess Hills Cropland and Rangeland
A7 Platte River Sandy Plains Irrigated Agriculture
A8 Loess Uplands and Plains Cropland (corn and soybean)
B SEMIARID
B1 Nebraska/Dakota Plains Cropland/Grassland Mosaic
B2 Sand Hills Rangeland
B3 Pierre Shale Hills Grassland
B4 White River Valley Mixed Rangeland
B5 Pine Ridge Needleleaf Forest
B6 Box Butte Plains Grassland with Cropland (small grains)
B7 North Platte Lowland Cropland (wheat, corn)
B8 Wildcat Hills Rangeland
B9 Cheyenne Plains Mixed Rangeland with Cropland (small grains)
B10 Dissected Plains Cropland/Grassland Mosaic (small grains, row crops)
B11 Sandsage Hills Rangeland and Irrigated Agriculture
B12 Lincoln County Sand Hills

Figure 8. Nebraska eco-region map consisting of the two highest of three hierarchical levels generated by the Spatial Pattern Analysis Model.

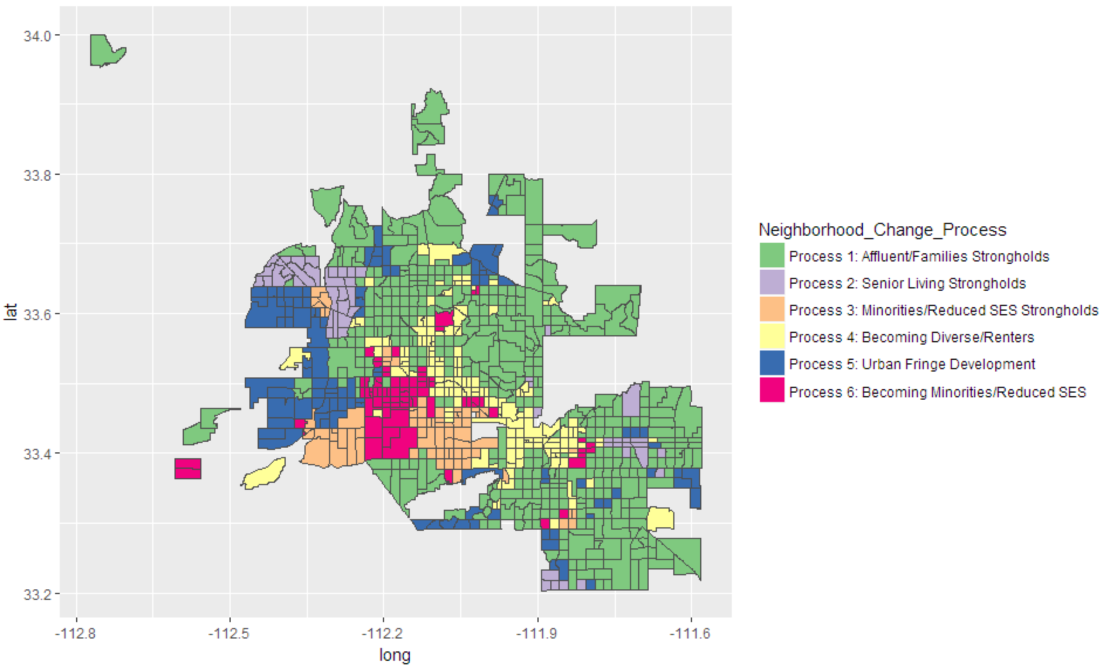
Space-Time Clustering

We can also use cluster analysis to describe how places change over time:



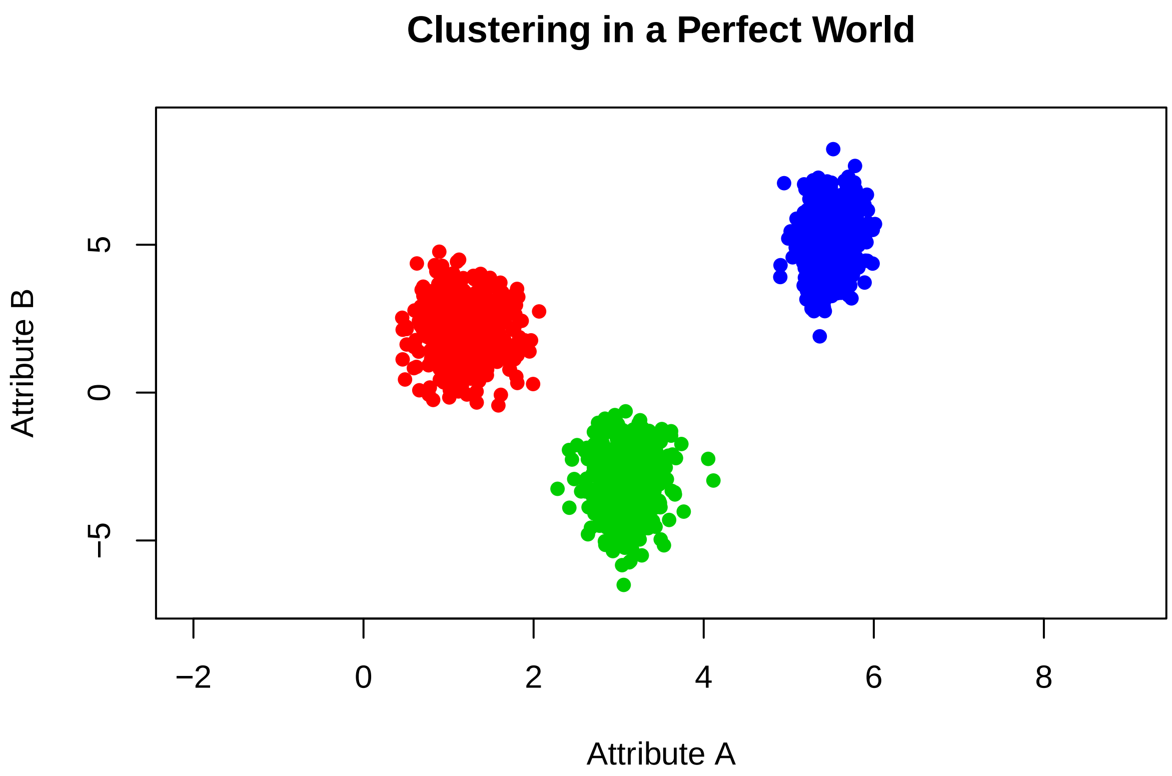
Space-Time Clustering

We can also use cluster analysis to describe how places change over time:


34.0
33.8
33.6
33.4
33.2
lat
-112.8
-112.5
-112.2
-111.9
-111.6
long
Neighborhood_Change_Process
Process 1: Affluent/Families Strongholds
Process 2: Senior Living Strongholds
Process 3: Minorities/Reduced SES Strongholds
Process 4: Becoming Diverse/Renters
Process 5: Urban Fringe Development
Process 6: Becoming Minorities/Reduced SES

Clusters in Attribute Space

- Clusters are sometimes visually obvious in high-density regions of the “attribute space”.
- High-density regions = lots of mutual nearest-neighbors.
- We can also describe each cluster’s members as being closer to an “exemplar” or “centroid” than any other.



Clustering Around Centroids: K-Means

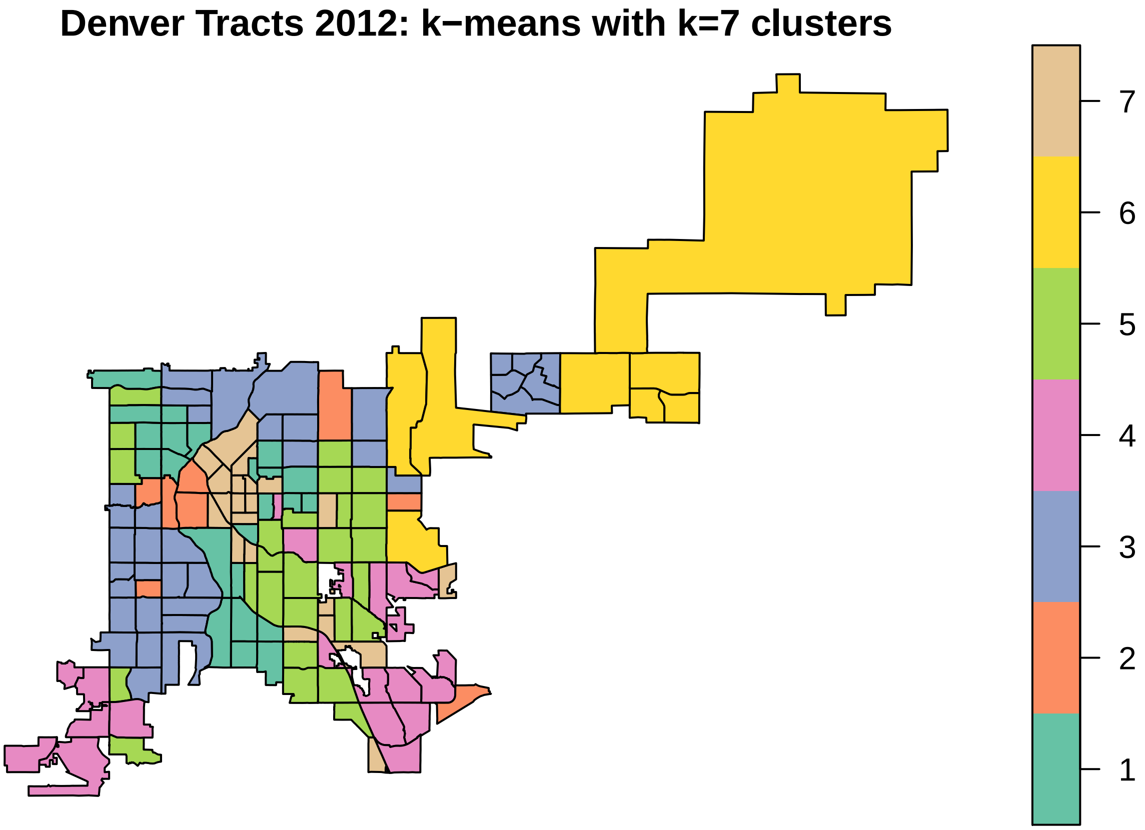
1. Randomly place k number of points (centroids) in the attribute space.
2. Each dot (observation) is assigned to the nearest centroid.
3. Centroid is recalculated as the mean of the points assigned to it.
4. Repeat steps 2 - 3 until “convergence” (centroids stop moving).

K-Means Example on “Real World” Data

```r
## remove geographic identifiers, x/y coords,
## and test variable (health insurance coverage) from cluster inputs
clust_vars = names(den)[!names(den) %in% c('GEOID', 'Nghbrhd', 'INTPTLA',
                                           'INTPTLO', 'Hlth_Un', 'Hlth_In')]

## generate clustering input dataframe
clust_dat = den@data[,clust_vars]

## standardize (z-score) cluster inputs
clust_dat_z = scale(clust_dat)
```

```
## perform clustering
set.seed(909)

# perform k-means and extract group labels
kmclust = kmeans(clust_dat_z, centers = 7)$cluster
```

```
## map the clusters in physical space
den_map = as(den,'sf')
den_map$kmeans_cluster = factor(kmclust)
plot(den_map['kmeans_cluster'],main = paste('Denver Tracts 2012: k-means with k=7 clusters'))
```



Clustering by (Dis)similarity

- A **dissimilarity matrix** is like a "mileage chart" for our data.
- An **affinity matrix** is like inverse of a mileage chart (i.e. measuring *proximity* by subtracting every distance from the max distance).
- Both measures support different clustering tasks.
- e.g. hierarchical vs. nearest-neighbors clustering

	Philadelphia	New York	Boston	Charleston
Philadelphia	0.00	1.39	4.76	8.61
New York	1.39	0.00	3.37	9.91
Boston	4.76	3.37	0.00	13.06
Charleston	8.61	9.91	13.06	0.00

Clustering by (Dis)similarity

- Dissimilarity/affinity matrices can be built from:
  - **Continuous** data (i.e. Euclidean or Manhattan distance)
  - **Categorical** data (i.e. Matching or Jaccard distance)
  - **Mixed-type** data (i.e. Gower distance)

Hierarchical Clustering

- Use dissimilarities to organize data into a **dendrogram**, a tree-like diagram.
- The “leaves” describe individual observations.
- The “stems” describe more specific clusters.
- The “branches” describe more general clusters.
- Clusters are recovered by “cutting” the dendrogram at a desired `k` or height.

Hierarchical Clustering: Linking/Sorting Strategies

- Distance-based: merge the groups *closest* on some criterion
- **Single linkage** (nearest-neighbor)
- **Complete linkage** (furthest-neighbor)
- **Average linkage** (centroid)
- Variance-based: **Ward’s Method**
- Each merge minimizes the “error sum of squares” (ESS), a measure of within-cluster dissimilarity.

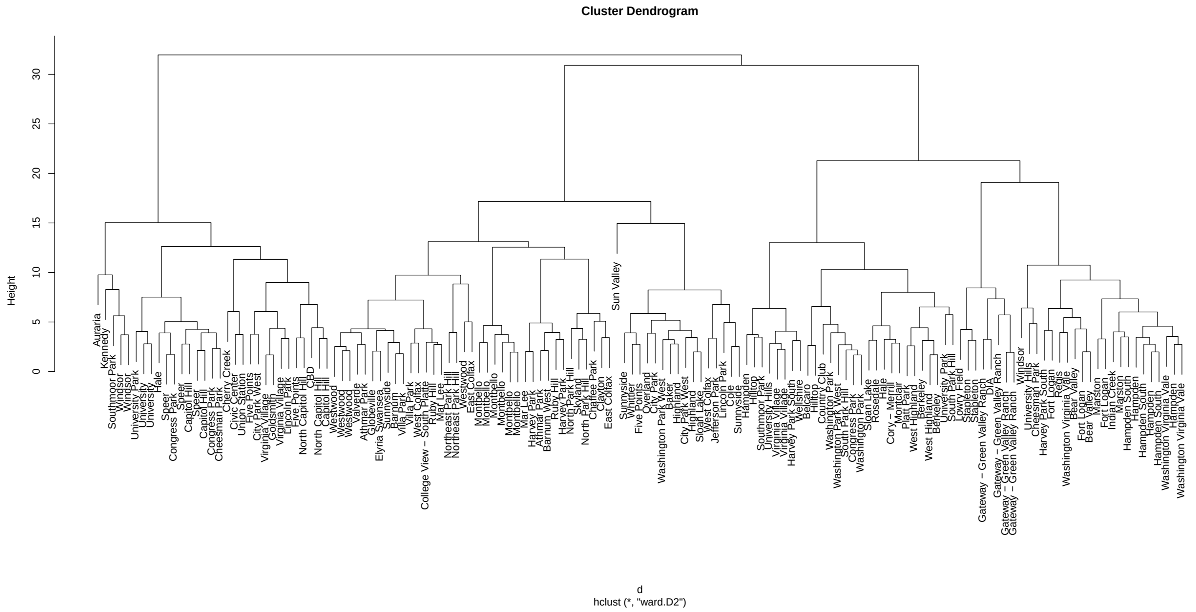
A Dendrogram of Denver Tracts

- Generate a euclidean distance matrix using R’s `dist` function.
- Generate a dendrogram from the distance matrix using R’s `hclust` function.
- Use the *Ward* linkage method (minimize within-cluster variance).

```
## add neighborhood ids to rownames for readability
rownames(clust_dat_z) = den$Nghbrhd

## generate distance matrix
d = dist(clust_dat_z)

## ward dendrogram
dend = hclust(d = d, method = 'ward.D2')
```

A Dendrogram of Denver Tracts

```r
## view the dendrogram
plot(dend)
```



Finding a Suitable k

- Clusters should be **internally consistent** and **well separated**.
- Often useful to consider variance-based and separation-based criteria.
- Can iterate k groups and measure each of these criteria to find a “best” solution.

Finding a Suitable k: Variance-Based Criteria

$$GOF = \frac{BSS}{TSS}$$

where

$$TSS = BSS + WSS$$

Sometimes called **Goodness of Variance Fit (GOF)**. - **Total Sum of Squares (TSS)**: sum of squared distances from data centroid - **Between Sum of Squares (BSS)**: sum of squared distances between all group centroids and the data centroid - **Within Sum of Squares (WSS)**: sum of squared distances between all group members and their centroid

Finding a Suitable k: Variance-Based Criteria

$$GOF = \frac{BSS}{TSS}$$

where

$$TSS = BSS + WSS$$

Look familiar? - This is kind of like an Rˆ2 diagnostic for clustering. - Instead of a “line of best fit”, we have cluster centroids. - Instead of “fitted values”, we have cluster labels. - The “explained” part (BSS) tells us how distinct from data centroid the cluster centroids are. - The “unexplained” part (WSS) tells us how much observations vary about their own centroid.

Finding a Suitable k: Separation-Based Criteria

- Clusters should be *well separated*: they should inhabit their own “high density” portions of the attribute space.
- Information provided by each cluster should be distinct, and shared as little as possible with other clusters.
- **Average Silhouette Width:** to what degree do clusters overlap?
- 0 = high overlap
- 1 = high separation
- -1 = incorrect labels.

Selecting k for Denver Tracts

1. Specify a desired range of cluster numbers (here $k = 3...10$).
2. Cut the dendogram at each `k` and…

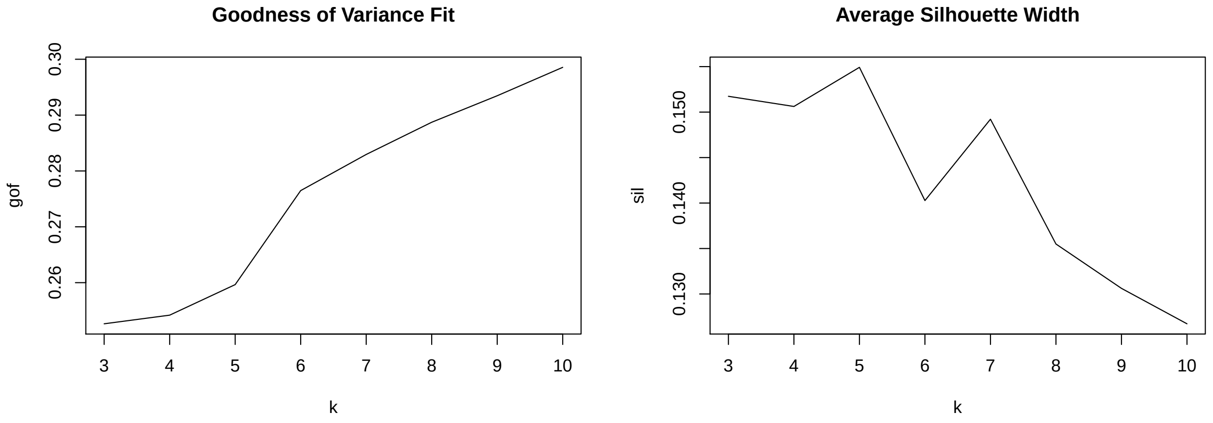
- Compute variance-based measure (Goodness of Variance Fit).
- Compute separation-based measure (Average Silhouette Width in R library `cluster`).

4. Compare the measures visually and identify an optimal solution.

```
## Specify a range of cluster numbers
krange = 3:10

# goodness of variance fit
gof = sapply(krange, function(k){

  kclust = cutree(dend, k)
  fastClusterGOF(dat = clust_dat, clust = kclust)

})

# average silhouette width
sil = sapply(krange, function(k){
  kclust = cutree(dend, k)
  mean(silhouette(x = kclust, dist = d)[,3])

})
```

Selecting k for Denver Tracts

```
## output diagnostics
cl_diag = cbind(k = krange, gof = gof, sil = sil)
par(mfrow=c(1,2))
plot(gof ~ k, data = cl_diag, type='l', main = 'Goodness of Variance Fit')
plot(sil ~ k, data = cl_diag, type='l', main = 'Average Silhouette Width')
```



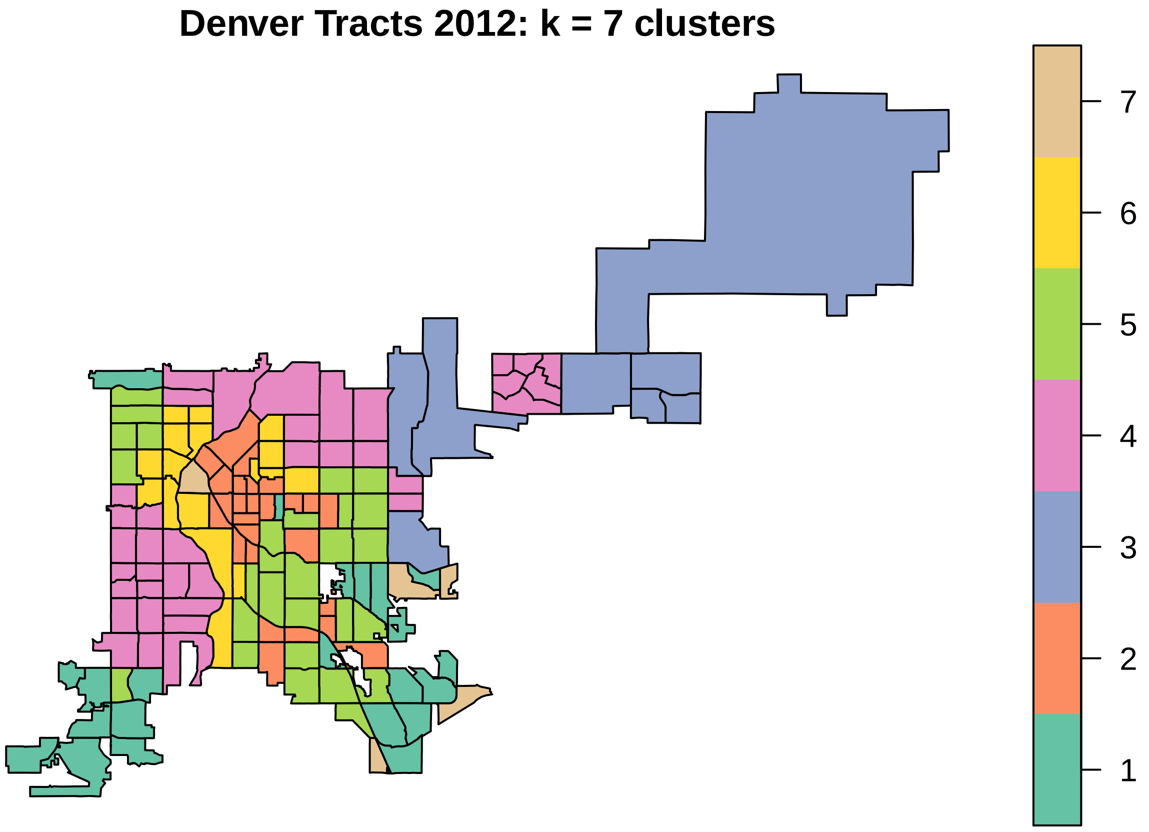
```
kable(round(data.frame(cl_diag), 2))
```

k	gof	sil
3	0.25	0.15
4	0.25	0.15
5	0.26	0.15
6	0.28	0.14
7	0.28	0.15
8	0.29	0.14
9	0.29	0.13
10	0.30	0.13
</lef	t>	

Map the Final Solution

```
## cut dendrogram at best k and assign it to our sf object
best_k = 7
den_map['cluster'] = factor(cutree(dend, best_k))
```

```
## plot the map
plot(den_map['cluster'],main = paste('Denver Tracts 2012: k =',best_k,'clusters'))
```



Interrogating the Clusters

- How well do the clusters match with prior expectations of data under analysis?
- e.g. We know "Downtown Denver" is distinct from the rest of the city.
- How well do the clusters suit the objectives of the analysis?
- e.g. Revealing different "socially vulnerable" groups.

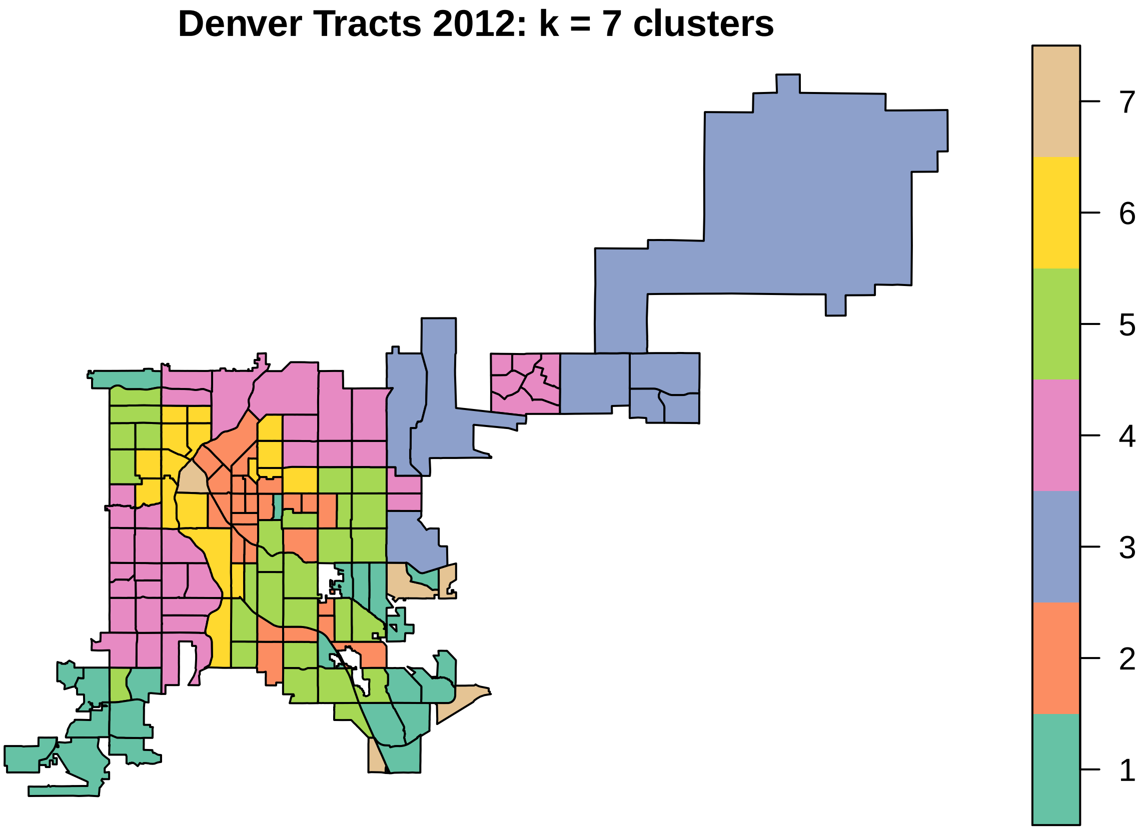
Interrogating the Clusters

Outcome measures or a "ground-truth" can be useful.

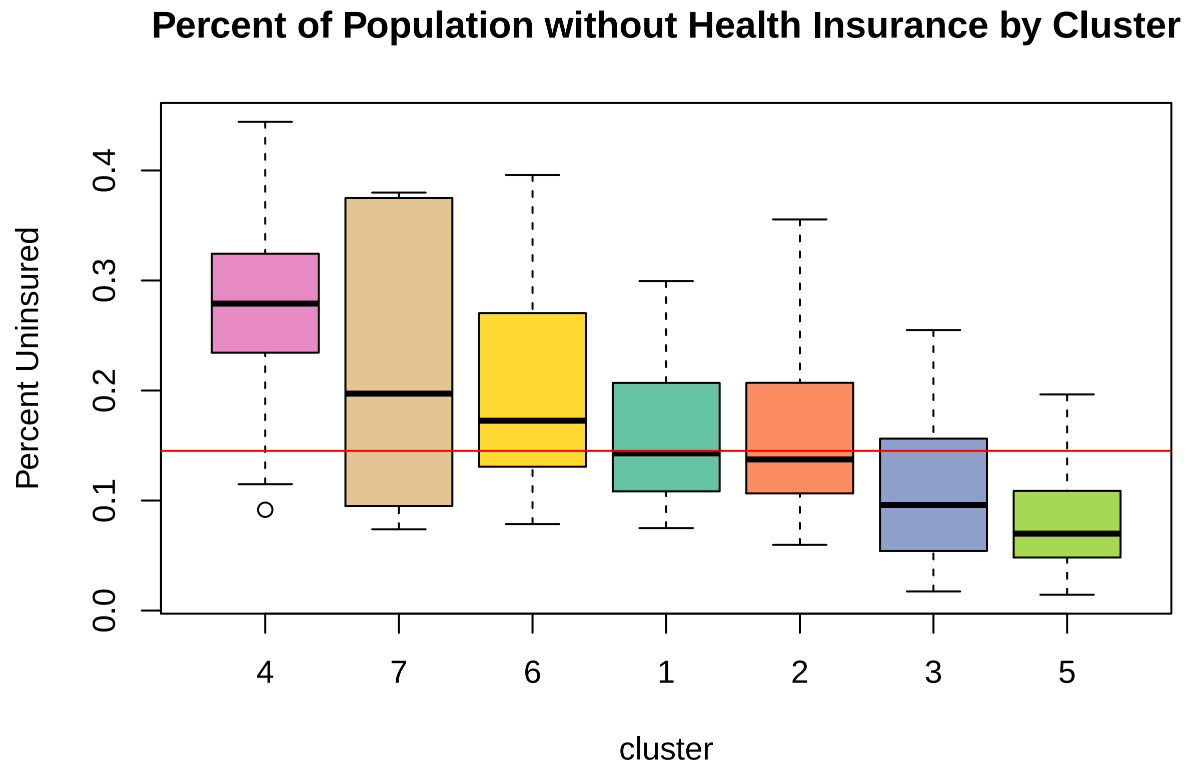
- Do the clusters align well with a particular outcome?
- e.g. Are flood losses concentrated more heavily in one cluster than others?
- Do the clusters match a "ground truth" well?
- e.g. Observations/categories from a field assessment.

Comparing the Denver Tract Clusters to an Outcome Measure

```
## re-plot map
plot(den_map['cluster'],main = paste('Denver Tracts 2012: k =',best_k,'clusters'))
```



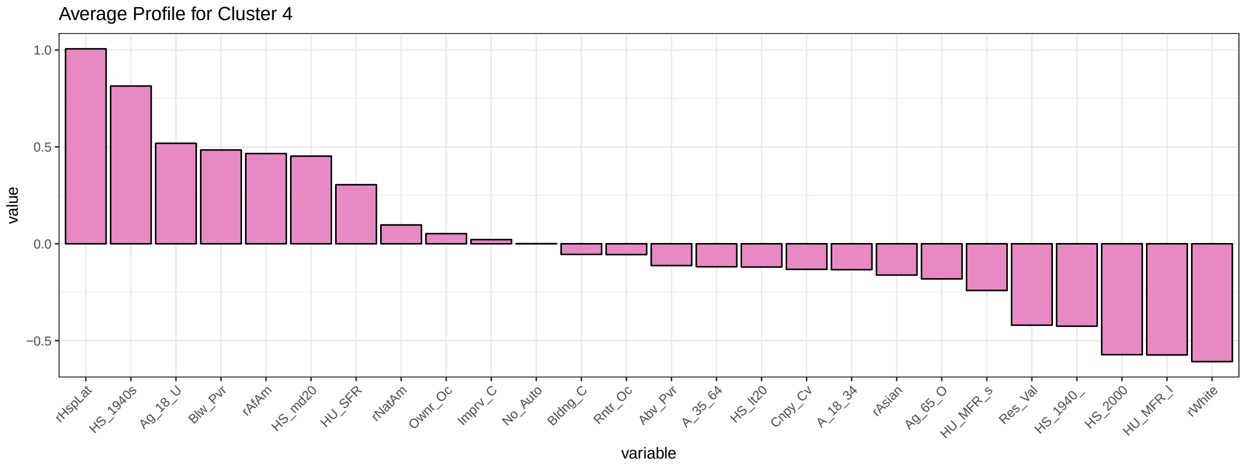
```
## assign cluster labels to full data
den@data$cluster = factor(cutree(dend, best_k))

## sort clusters by median of outcome variable, highest to lowest
health_uninsured_by_cluster = with(den@data, aggregate(Hlth_Un ~ cluster, FUN = 'median'))
health_uninsured_by_cluster = health_uninsured_by_cluster[order(health_uninsured_by_cluster$Hlth_Un, de
den$cluster = factor(den$cluster, levels = health_uninsured_by_cluster$cluster)

## plot outcome variable
cols = brewer.pal(best_k, 'Set2')[as.numeric(levels(den$cluster))]
with(den@data, plot(Hlth_Un ~ cluster, col = cols, main = 'Percent of Population without Health Insuranc
abline(h = median(den$Hlth_Un), col = 'red')
```



Profiling Clusters

An **average profile** plot tells us how far a above/below the data average a cluster is on variables of interest:

```r
## generate average profile of a cluster
den_cent = colMeans(clust_dat) # the data centroid
cl = levels(den$cluster)[1] # our target cluster
cl_cent = colMeans(clust_dat[den$cluster==cl,]) # the cluster centroid
avp = (cl_cent - den_cent) / den_cent # difference from data mean

## format the data for plotting
# plot vars greatest to smallest
avp_melt = melt(avp)
var_order = rownames(avp_melt)[order(avp_melt$value, decreasing = T)]
avp_melt$variable = factor(rownames(avp_melt), levels = var_order)
cl_col = cols[which(levels(den$cluster) == cl)] # for coloring barplot

ggplot(avp_melt, aes(x = variable, y = value)) +
  geom_bar(fill = cl_col, color = 'black', stat = 'identity') +
  theme_bw() +
  theme(axis.text.x=element_text(angle=45,hjust=1)) +
  ggtitle(paste('Average Profile for Cluster',cl))
```



Side Notes: "Built-in" Selection of k

Some methods handle selection of `k` themselves...

- **Mutual nearest-neighbors** (Community Detection)
- **Threshold distance neighbors** (DBSCAN)
- **Mutual similarity to an exemplar** (Affinity Propagation)

Tradeoff: Sometimes these methods generate a lot of "singletons" or noise.

Side Notes: Clustering Categorical Data

- Useful for grouping e.g. survey responses.
- Uses "model-based" clustering techniques like **Latent Class Analysis** (LCA).
- Model parameters are determined using criteria similar to logistic regression (i.e. maximum likelihood).
- Information-theoretic criteria (i.e. AIC, BIC) are used to find a suitable `k`.

Conclusion

- Cluster analysis provides geographers insight into latent conditions and processes in place.
- However, there is no "one size fits all" view of these phenomena.
- Clustering design depends on the *objectives* of the research (i.e. knowledge discovery vs. confirmatory analysis).
- Careful attention should be paid to:
- Variable selection
- Comparing cases
- Clustering method
- Interpretation