DATA 608 Meetup 11: Clustering

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Week Summary

- Spring Break Next Week!
- Data Story 6 is available due week after spring break
- Last Data Story will be on Shiny Apps
- Talking about clustering today

NY Open Statistical Computing Meetup

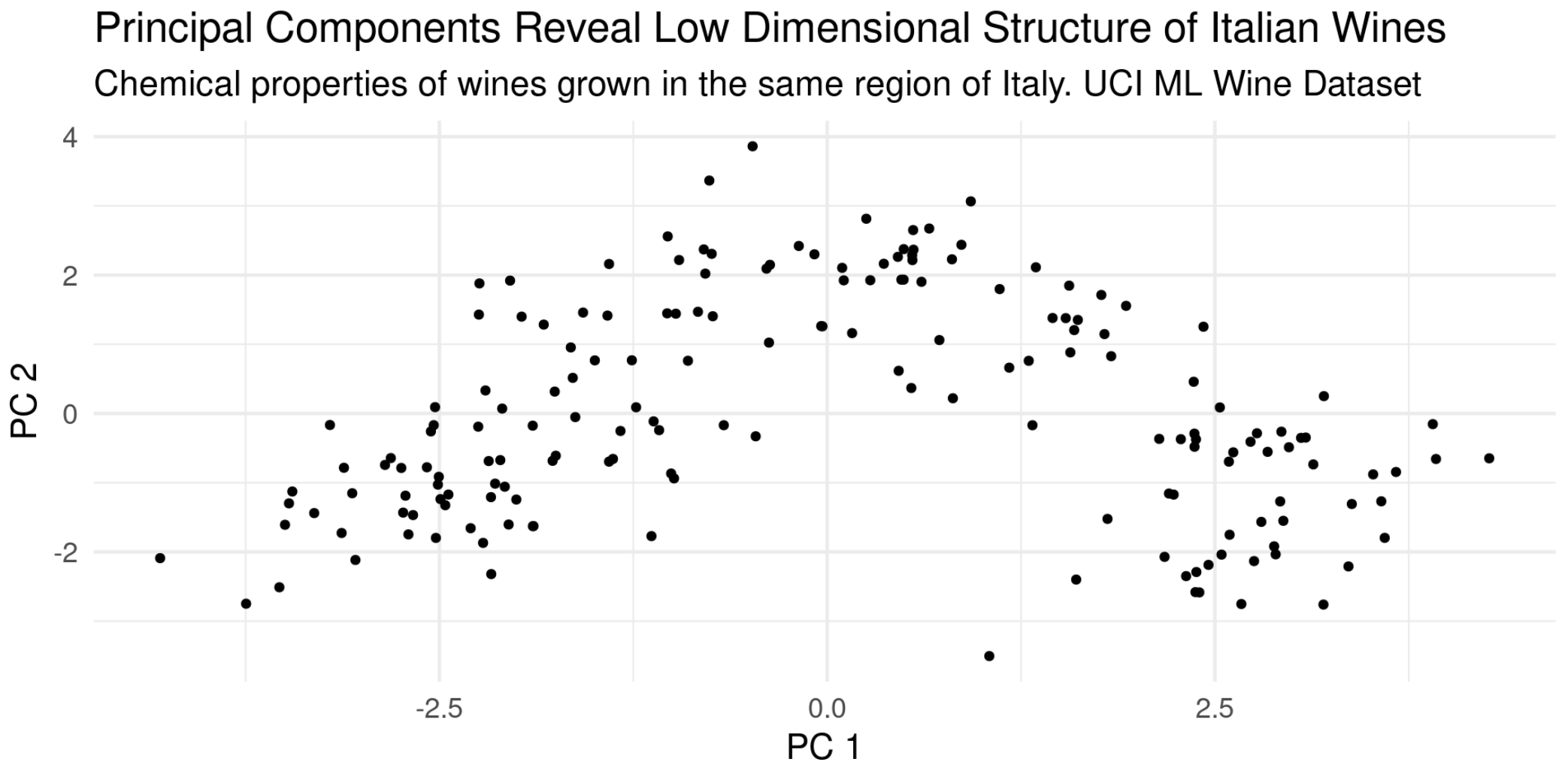
- April 8th 6:30-8:30+
- Great Networking/Learning Opportunity

Clustering and Dim. Reduction

- We can gain insight when we notice data points cluster together

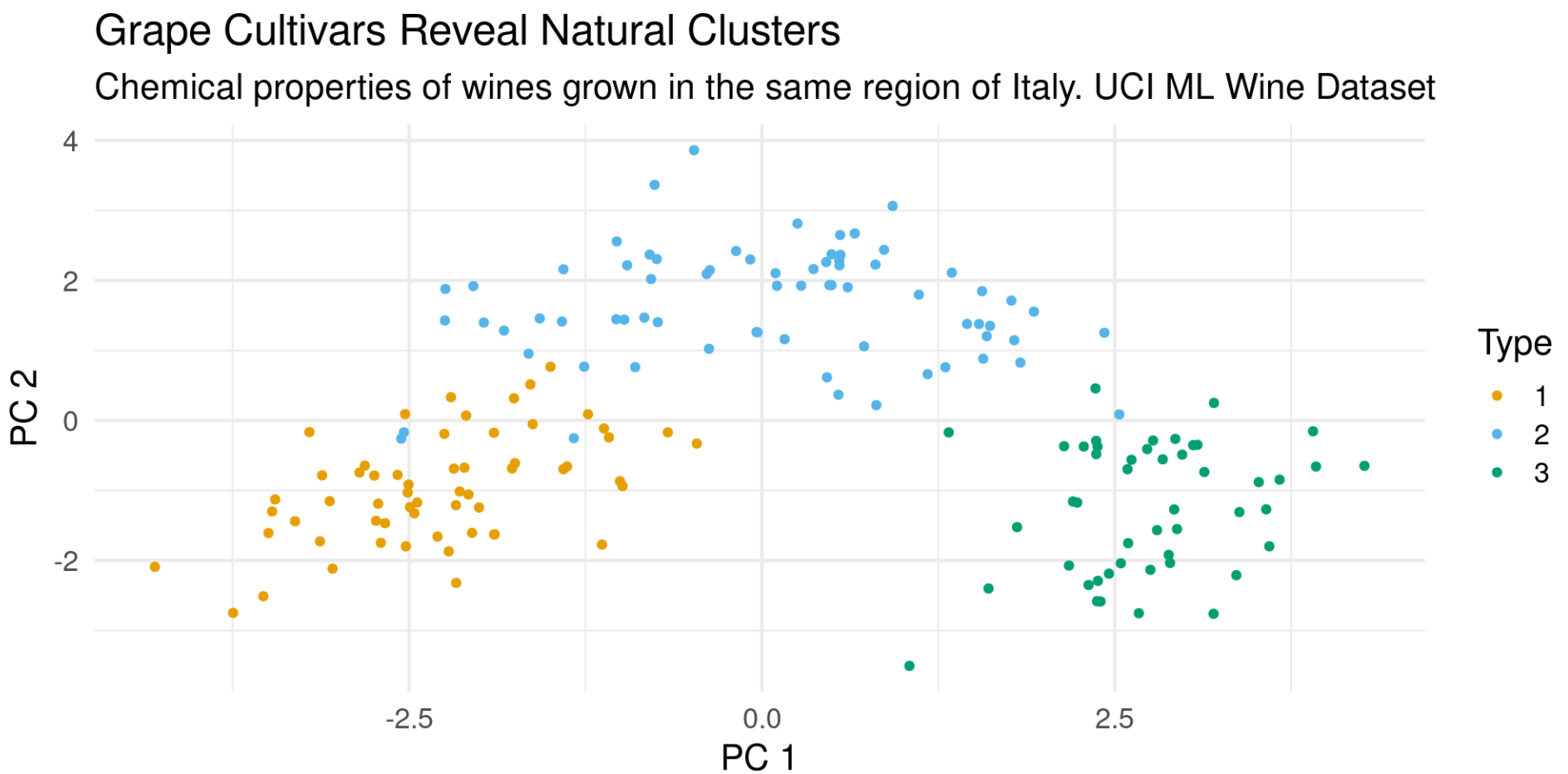
Alcohol	Malic	Ash	Alcalinity	Magnesium	Phenols	Flavanoids	Nonflavanoid
14.23	1.71	2.43	15.6	127	2.80	3.06	0.2
13.20	1.78	2.14	11.2	100	2.65	2.76	0.2
13.16	2.36	2.67	18.6	101	2.80	3.24	0.3
14.37	1.95	2.50	16.8	113	3.85	3.49	0.2
13.24	2.59	2.87	21.0	118	2.80	2.69	0.3
14.20	1.76	2.45	15.2	112	3.27	3.39	0.3
14.39	1.87	2.45	14.6	96	2.50	2.52	0.3
14.06	2.15	2.61	17.6	121	2.60	2.51	0.3
14.83	1.64	2.17	14.0	97	2.80	2.98	0.2
13.86	1.35	2.27	16.0	98	2.98	3.15	0.2

Clustering and Dim. Reduction

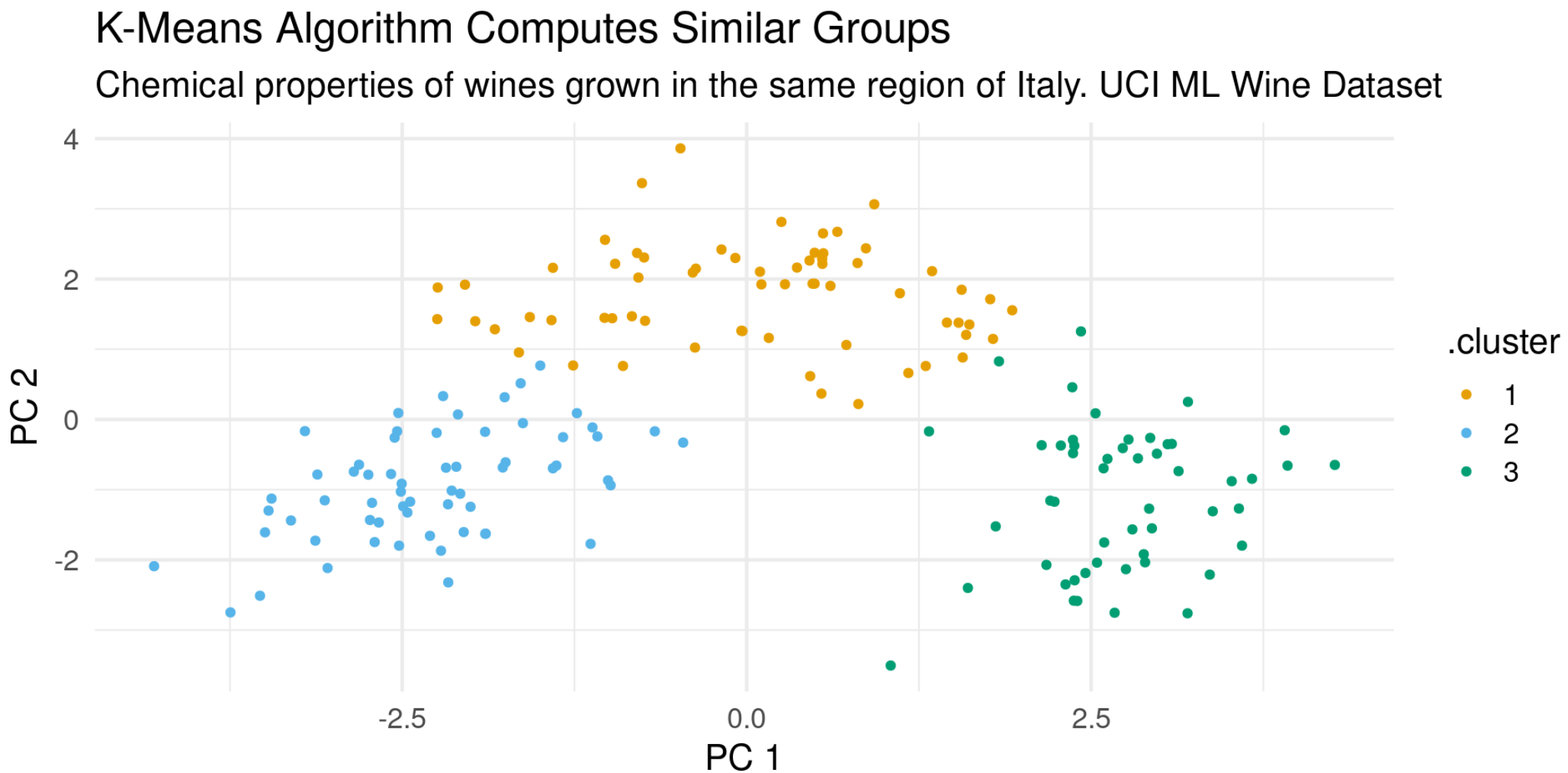


Clustering and Dim. Reduction

- Color by the grape type



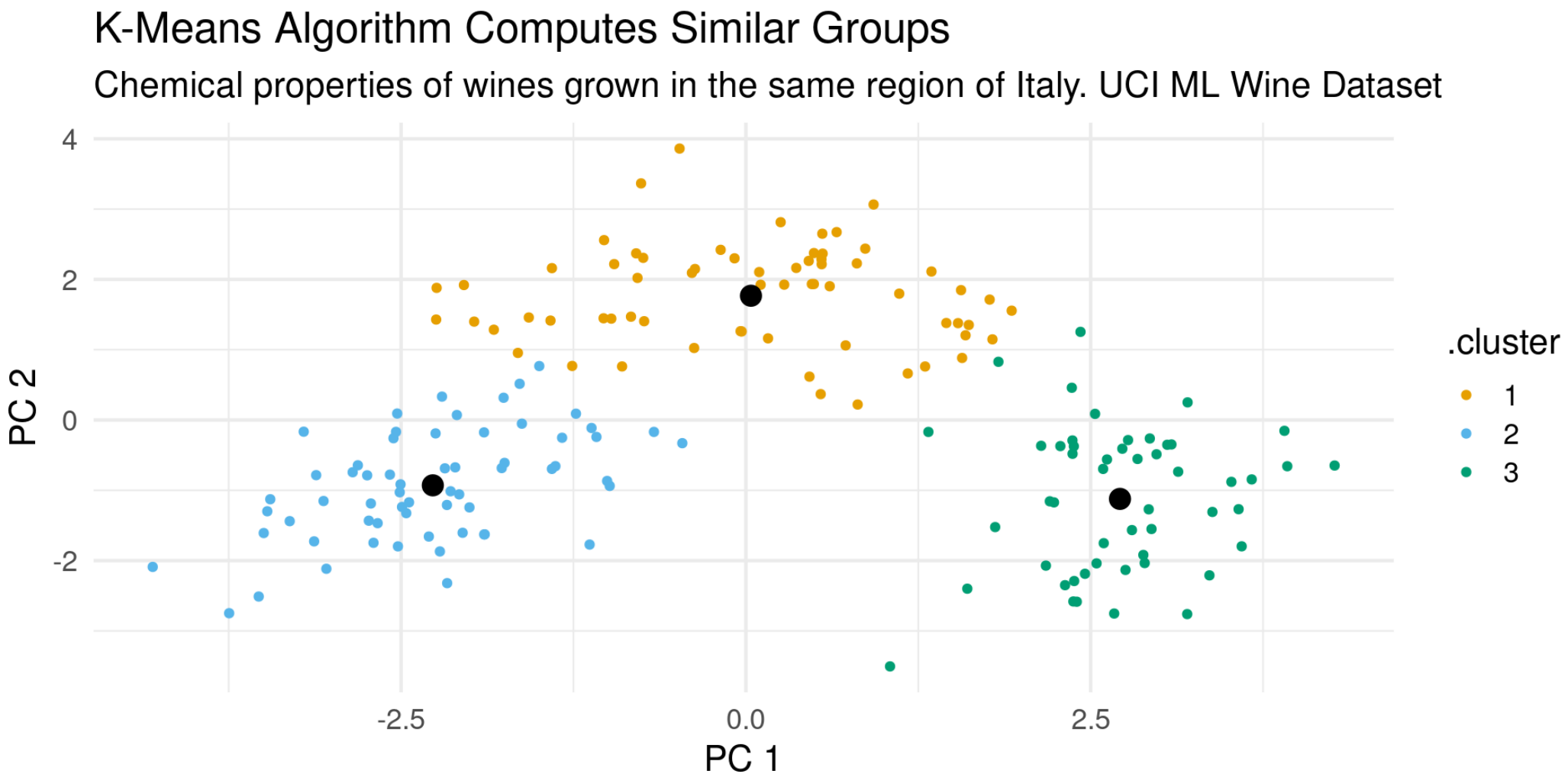
Automatic Clustering



k-means method

- Most common clustering method
- Needs two things:
  - Measure of distance between points
  - Number of Clusters to find
- Each cluster characterized by a center
- Points clustered to closest center

k-means method



Implementing k-means in R

- kmeans in stats package

```
wine_clusters = pca_fit|>
    augment(wine_df) |> select(-Type) |>
  select(.fittedPC1:.fittedPC13) |>
  kmeans(centers=3,nstart = 10)

wine_clusters
```

```
K-means clustering with 3 clusters of sizes 65, 62, 51

Cluster means:
   .fittedPC1 .fittedPC2   .fittedPC3  .fittedPC4  .fittedPC5  .fittedPC6
1  0.03685265  1.7672542  0.185615130  0.08001400 -0.07067870  0.12944063
2 -2.26979079 -0.9294322  0.001523733 -0.13511700  0.13453261 -0.21766922
3  2.71238444 -1.1224849 -0.238420685  0.06228125 -0.07346875  0.09964414
    .fittedPC7   .fittedPC8  .fittedPC9 .fittedPC10  .fittedPC11  .fittedPC12
1 -0.002320739 -0.017964647 -0.03216049  0.02293882  0.013900922  0.004371673
2  0.051963343  0.024894027  0.05014407 -0.07446923 -0.021230820 -0.007417378
3 -0.060213318 -0.007367207 -0.01997059  0.06129547  0.008093155  0.003445464
   .fittedPC13
1  0.008595707
```

2 -0.050476861
3 0.050408713

Key arguments

- `centers` species the number of clusters to find
- `nstart` is number of times to initialize algorithm
- `algorithm` several choices the default choice is usually very robust
- `iter.max` is the number of iterations to try

Key Outputs

- Clustering Vector: Identifies each point by cluster. Is attached to original data frame by augmnet

```
1 wine_clusters$cluster
```

```
  [1] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 [38] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 3 1 1 1 1 1 1 1 1 1 1 1
 [75] 1 1 1 1 1 1 1 1 1 3 1 1 1 1 1 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1
[112] 1 1 1 1 1 1 1 3 1 1 2 1 1 1 1 1 1 1 1 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
[149] 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
```

Key Outputs

- Cluster Means: These are the cluster centers

```
1 wine_clusters$centers
```

```
   .fittedPC1 .fittedPC2   .fittedPC3  .fittedPC4  .fittedPC5  .fittedPC6
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2 -0.050476861
3  0.050408713
```

Key Outputs

- Error Measurements
  - `withinss` sum of squares within clusters
  - `betweenss` between cluster sum of squares
  - `tot.withinss/totss` measure of how much clusters explain variance

```
  1 wine_clusters$withinss
```

```
[1] 558.6971 385.6983 326.3537
```

```
  1 wine_clusters$totss
```

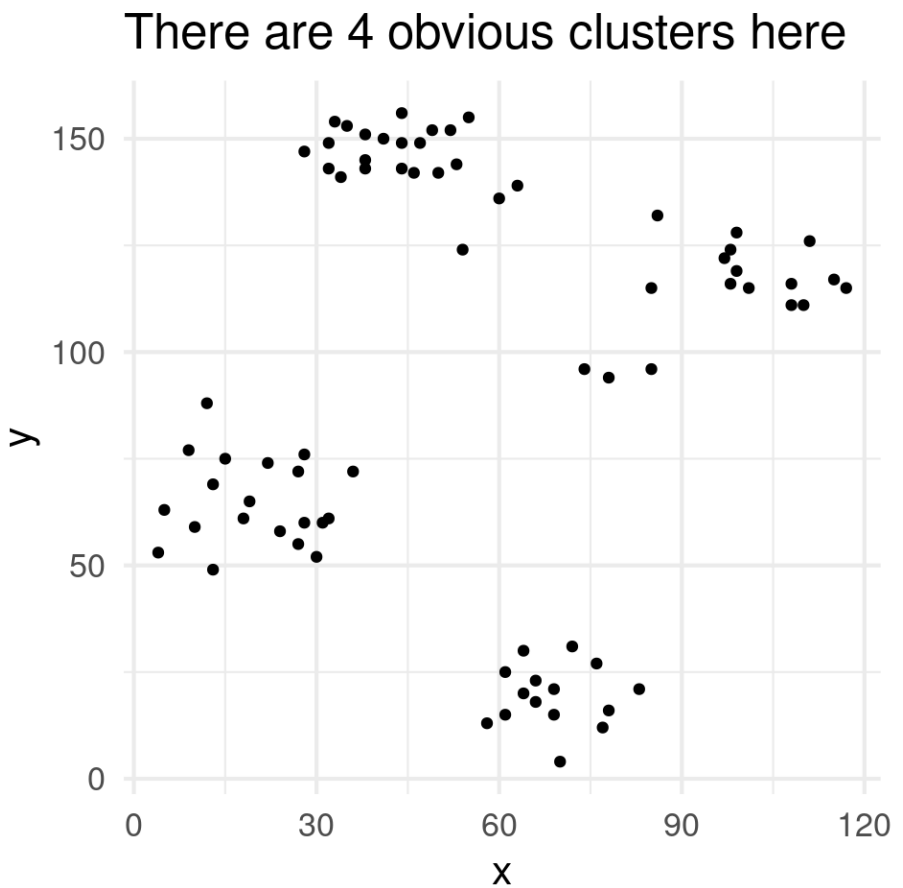
```
[1] 2301
```

```
  1 wine_clusters$tot.withinss/wine_clusters$totss
```

```
[1] 0.5522595
```

How many clusters?

- What happens when we increase the number of centers?



How many clusters?

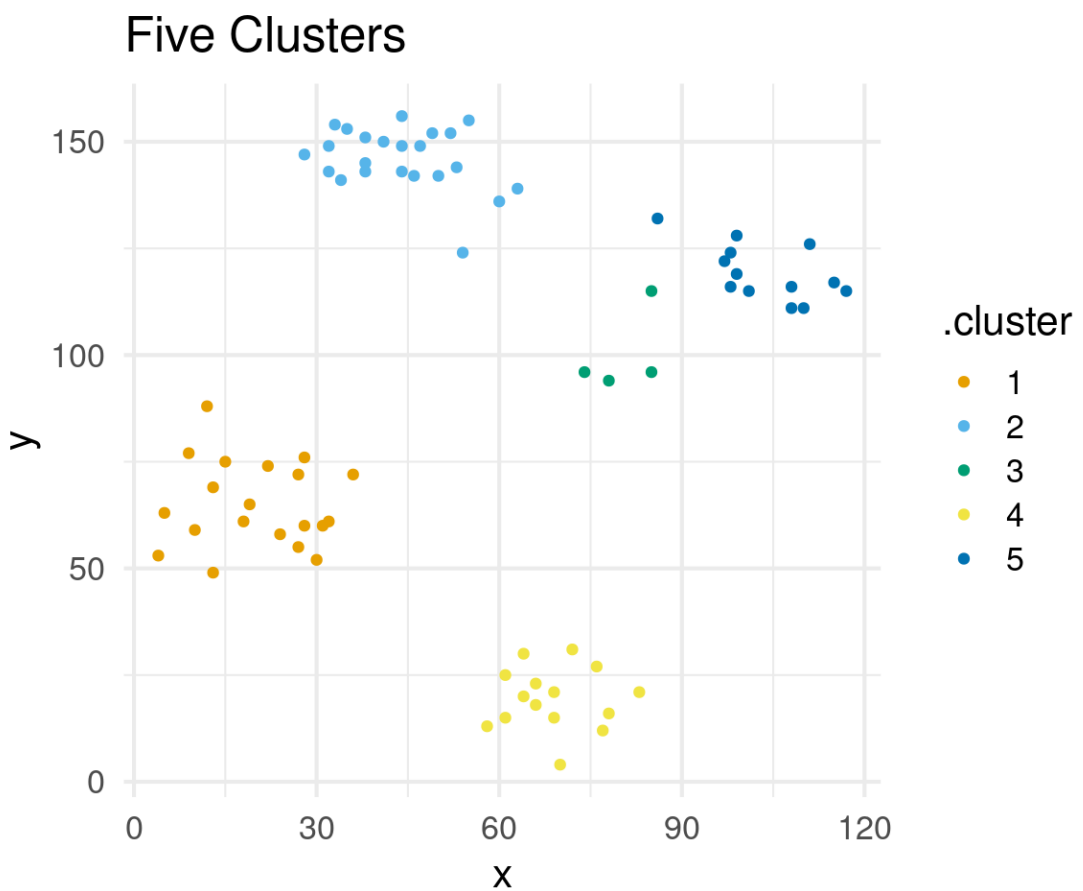
- 3 Clusters

How many clusters?

- 4 Clusters

How many clusters?

- 5 Clusters

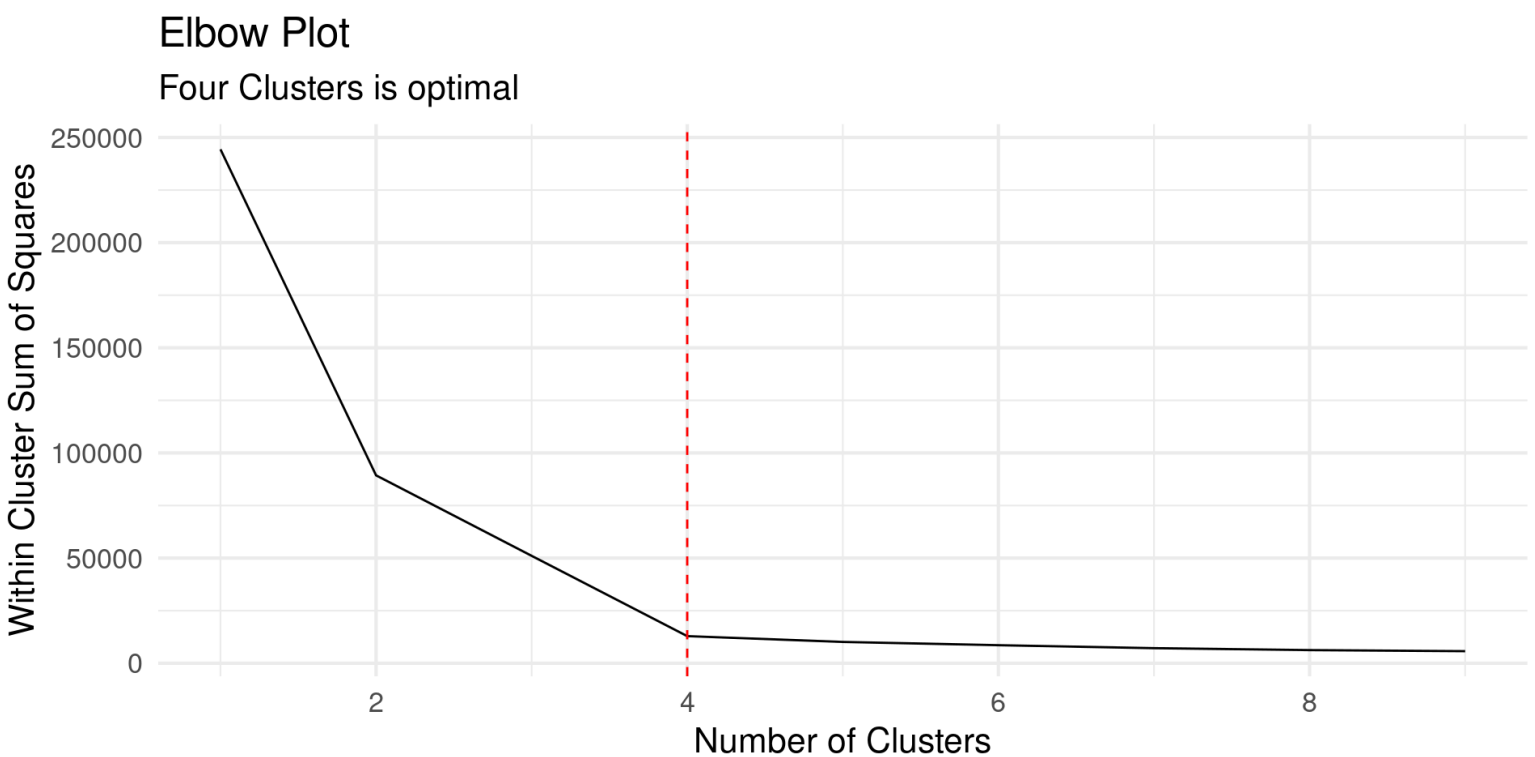


How many clusters?

- 10 Clusters

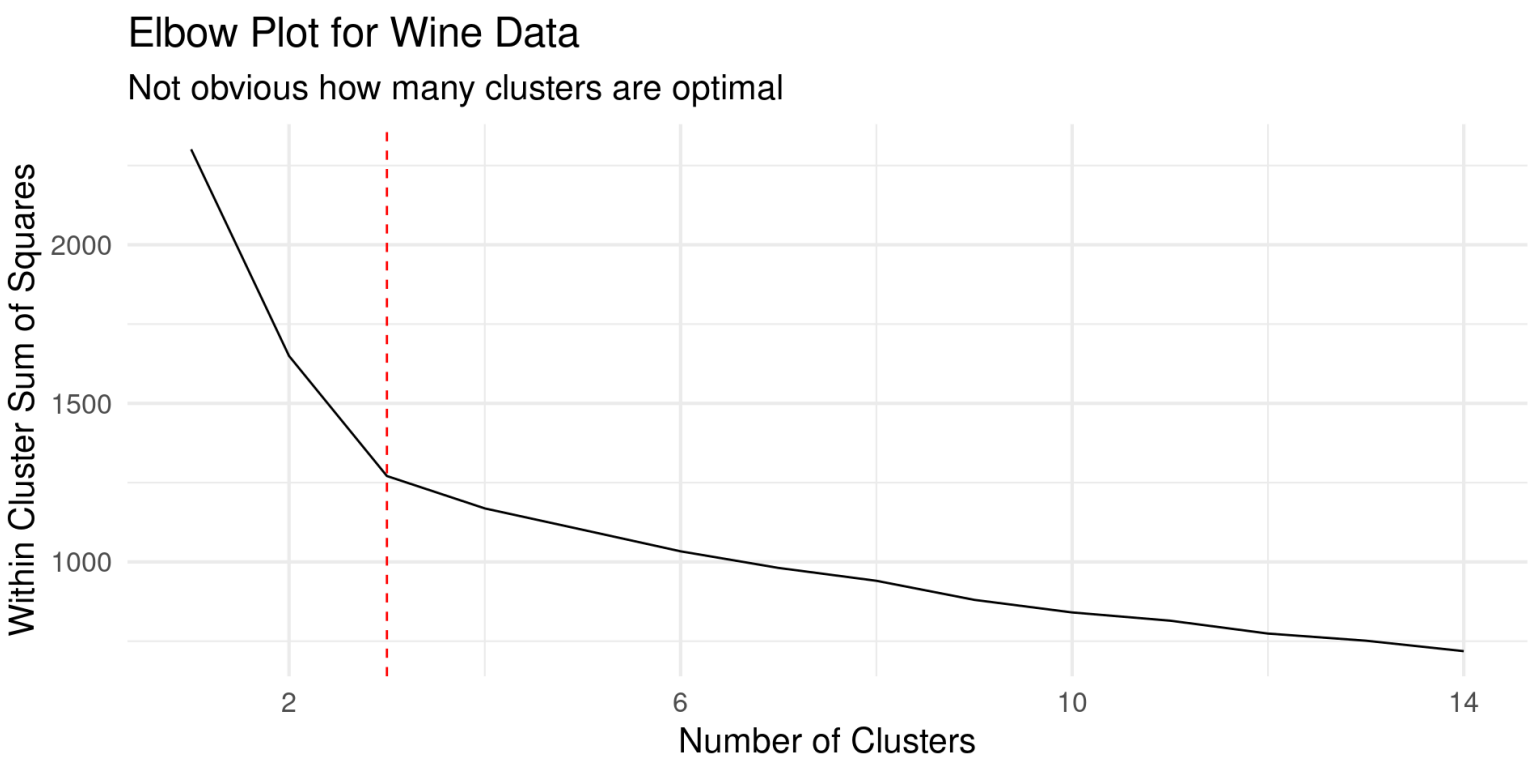
Quantitative Tools for Cluster Number

- Many methods for choosing the number of clusters!
- Elbow method: Look for `elbow` in plot of within cluster variance



Quantitative Tools for Cluster Number

- Many methods for choosing the number of clusters!
- Elbow method: Look for `elbow` in plot of within cluster variance



Quantitative Tools for Cluster Number

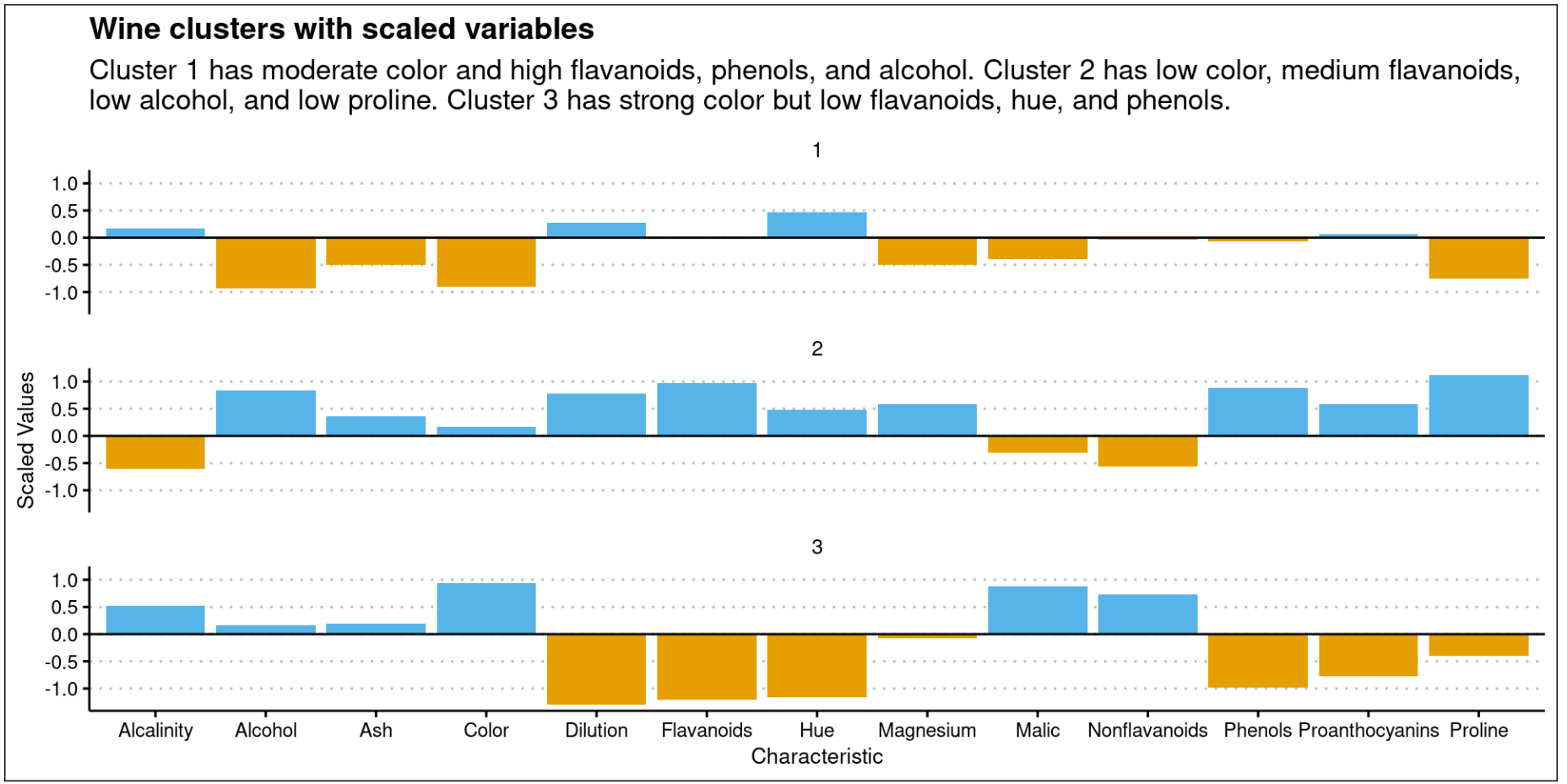
- Use `map` to apply k-means to many times

```
kvec = seq(2:10)

wcss = map(kvec,.f = function(k) {
    kmeans(ruspini, centers = k, nstart = 5)$tot.withinss
})
elbow_plot = tibble(clusters = kvec, wcss = wcss) |> unnest()
elbow_plot |> ggplot(aes(kvec, wcss)) +
  geom_line() +
  geom_vline(xintercept = 4, color = "red", linetype = 2) +
  theme_minimal(base_size = 16) +
  scale_x_continuous(breaks=c(2,4,6,8,10)) +
  labs(title = "Elbow Plot",
       subtitle = "Four Clusters is optimal",
       y = "Within Cluster Sum of Squares",
       x = "Number of Clusters")
```

Interpreting Clusters

- Goal of clustering is often to gain insight.



Interpreting Clusters

- Takes some tricky to understand code to transform the PCA coordinates:

```
wine_df_2 = wine_df |> select(-Type)
centers_df = t(t(wine_clusters$centers %*% t(pca_fit$rotation)) *
             pca_fit$scale + pca_fit$center) |>
  as_tibble() |>
  bind_rows(wine_df_2) |>
  scale() |>
  as_tibble() |>
  head(n=3) |>
  mutate(center = seq(1:3))
```

- `t(t(wine_clusters$centers %*% t(pca_fit$rotation)) * pca_fit$scale + pca_fit$center)` coordinate transformation
- `scale` enables visualization of variables together

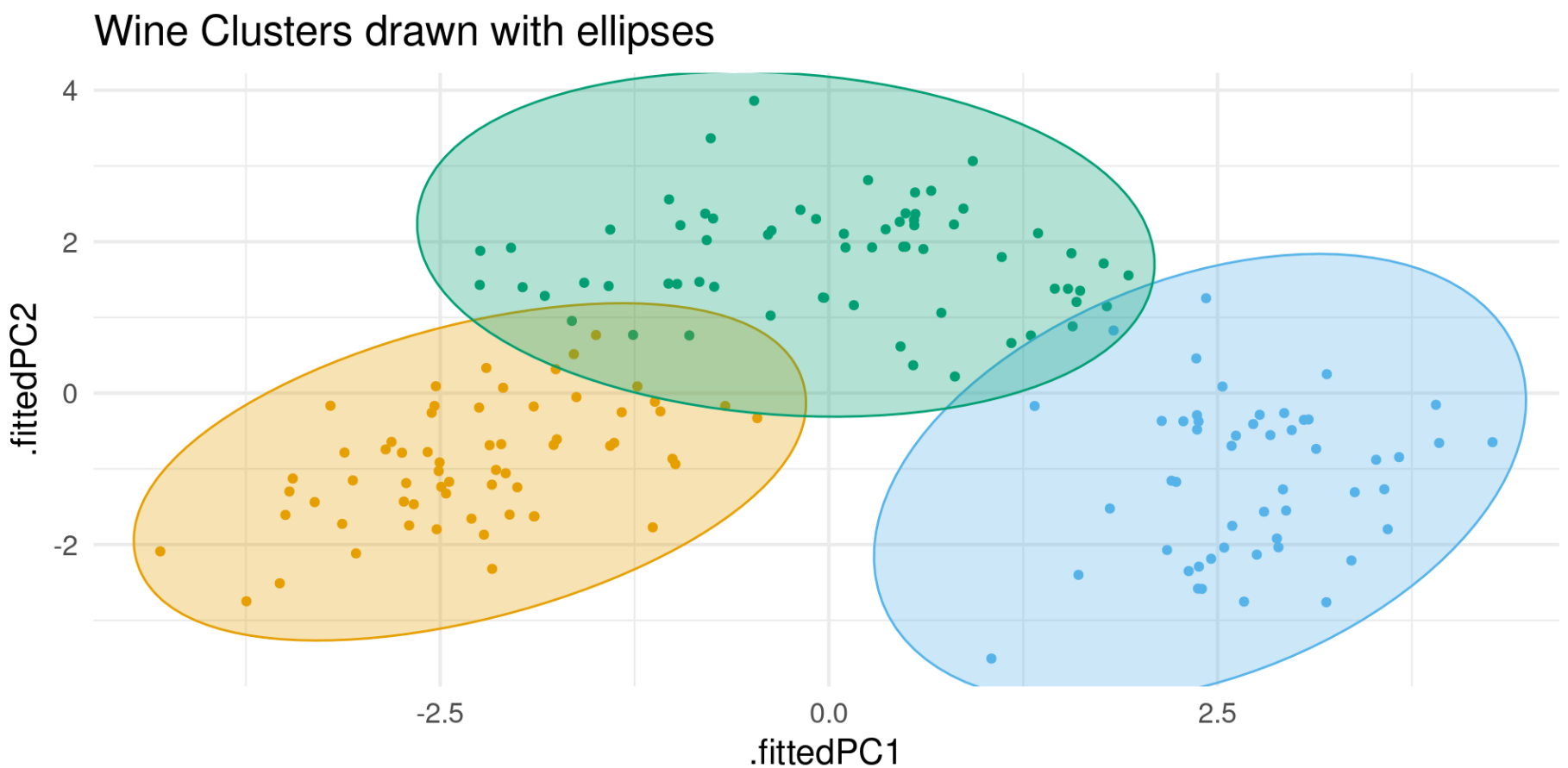
Interpreting Clusters

```
centers_df |> pivot_longer(
  cols = Alcohol:Proline,
  names_to = "type") |>
  mutate(sign= value>0) |>
  ggplot(aes(x=type,y=value)) +
  geom_col(aes(fill=sign)) +
  scale_fill_discrete(guide = "none") +
  geom_hline(yintercept = 0) +
  facet_wrap(~center,nrow=3) +
```

- There could be many ways of visualizing this
- Here chose column plot, colored by sign with a horizontal line to denote where 0 is across the facets
- I found this a little better than a dot plot for some reason

Annotating Clusters

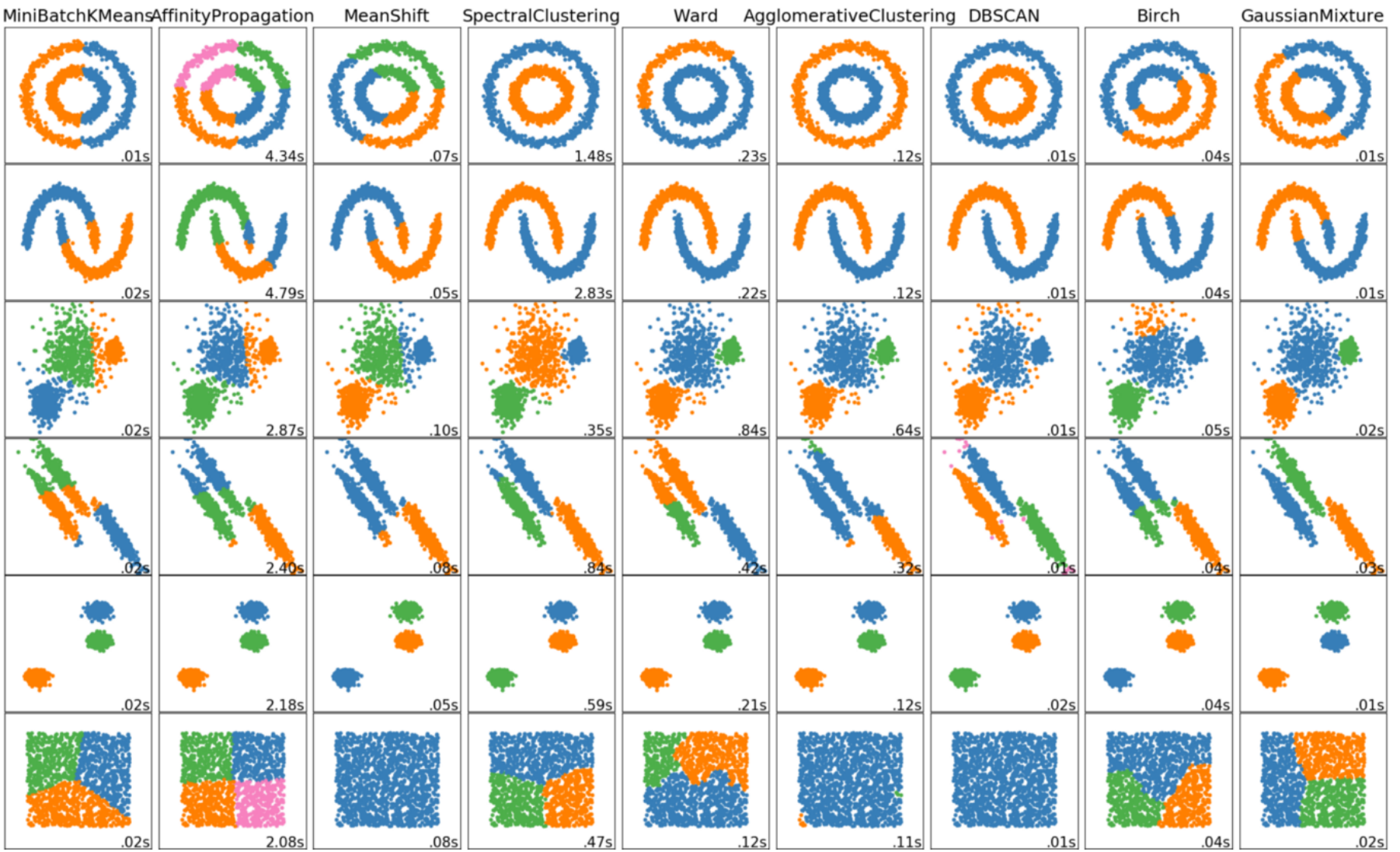
- `geom_mark_ellipse` to draw circles around clusters



k-means tips and pitfalls

- Algorithm not guaranteed to converge
  - Can get wrong answes if `nstart` too low
  - Can get stuck in local minima
- Very sensitive to outliers and largest scale of data
  - Always scale data first or used on scaled coordinates
- Assumes Spherical, Balanced Clusters
- Will find clusters when there are none

Other Clustering Algorithms



George Seif

Thanks!