K-Means Clustering in R: Plants Data

In this project, I use the k-means clustering algorithm in R to analyze the USDA's Plants data set, uncovering geographical structures of North America that are not immediately apparent from the raw data. I generate visualizations of the clustering results in R and Tableau. My analysis illustrates the relationship between the distribution of the plants and the geography of the states in the data set.

The data set comprises 34,781 plant genera and species, each associated with a list of states or provinces where the plant is found. Each record contains the plant's name along with the states it inhabits, identified by abbreviations.

Loading and Transforming Data Into Presence-Absence Matrix

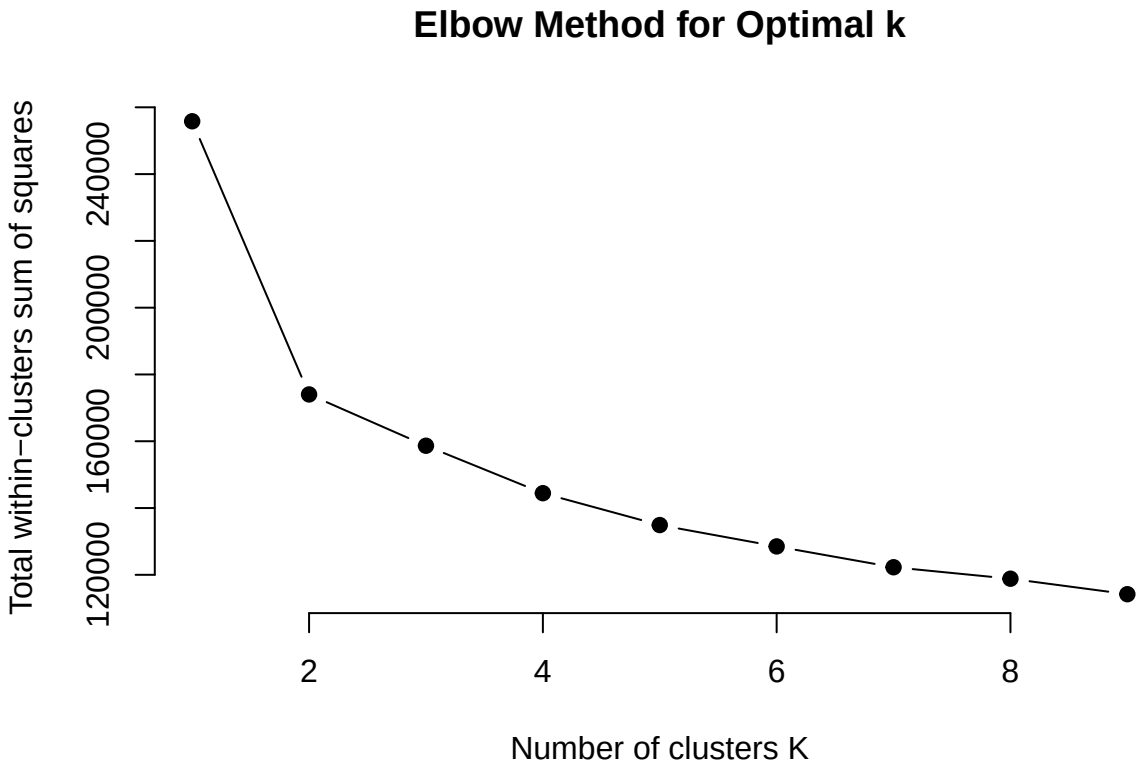
```
# Define the paths to the .names and .data files
data_file <- "/Users/arielseidman/Desktop/plants/plants.data"

# Read the raw data as a character vector
raw_data <- readLines(data_file)
raw_data <- iconv(raw_data, from = "UTF-8", to = "ASCII//TRANSLIT", sub = "")

# Below are the 69 unique "state" abbreviations in the data set
state_names <- c("al", "ak", "ar", "az", "ca", "co", "ct",
            "de", "dc", "fl", "ga", "hi", "id", "il",
            "in", "ia", "ks", "ky", "la", "me", "md",
            "ma", "mi", "mn", "ms", "mo", "mt", "ne",
            "nv", "nh", "nj", "nm", "ny", "nc", "nd",
            "oh", "ok", "or", "pa", "pr", "ri", "sc",
            "sd", "tn", "tx", "ut", "vt", "va", "vi",
            "wa", "wv", "wi", "wy", "ab", "bc", "mb",
            "nb", "lb", "nf", "nt", "ns", "nu", "on",
            "Prince Edward Island", "qc", "sk", "yt", "dengl", "fraspm")

# Initialize a matrix of zeros with 1 row per plant and 1 column per state
presence_matrix <- matrix(0, nrow = length(raw_data), ncol = length(state_names))

# Name the columns of the matrix using state names
colnames(presence_matrix) <- state_names

# Populate the matrix
for (i in 1:length(raw_data)) {
  # Split each line into the plant name and the list of states
  elements <- unlist(strsplit(raw_data[i], ","))

  # Extract the state names (discard the first element which is the plant name)
  plant_states <- elements[-1]

  # Trim white space and ensure consistent capitalization
  plant_states <- trimws(plant_states)
```

```r
  # Filter out any states that are not in the state_names list
  valid_states <- plant_states[plant_states %in% state_names]

  # Mark the corresponding columns with 1's
  presence_matrix[i, valid_states] <- 1
}
```

I will perform k-means clustering on the presence matrix. Before I can use the k-means algorithm, I must determine how many clusters to use (k).

Elbow Method for Choosing Value of K

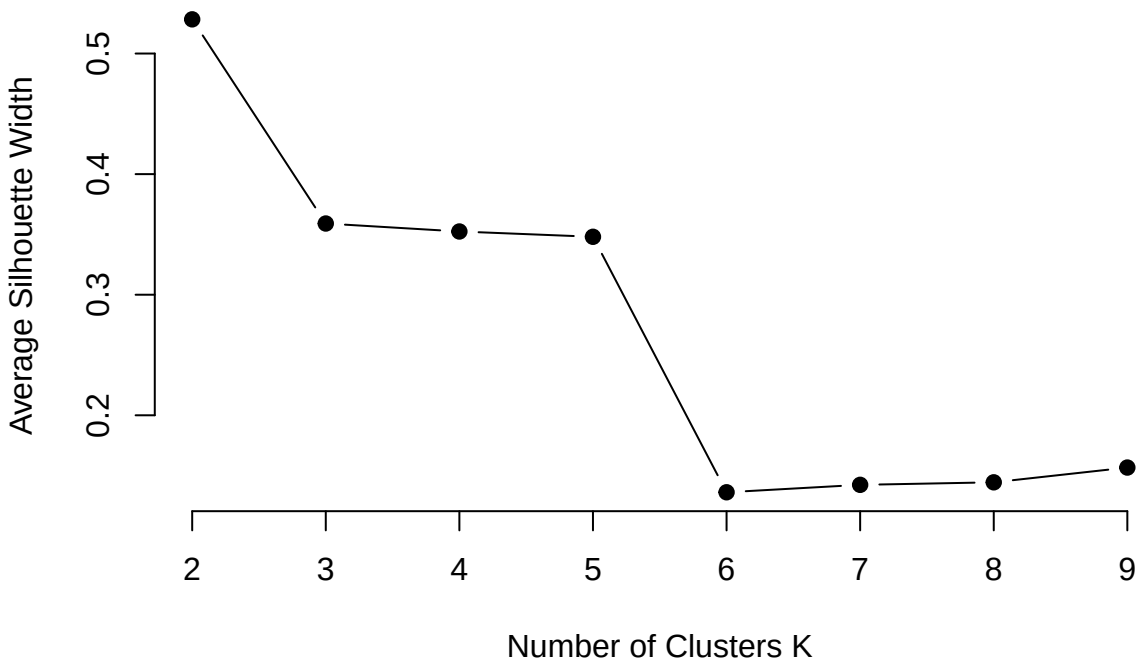
```r
# Initialize an empty vector to store within-cluster sum of squares (WSS) for each k
wss <- numeric()

# Range of k values to consider
k_range <- 1:9

# Calculate WSS for each k
for (k in k_range) {
  kmeans_result <- kmeans(presence_matrix, centers = k, nstart = 25, iter.max = 100)
  wss[k] <- kmeans_result$tot.withinss
}

# Plot WSS against the number of clusters
plot(k_range, wss, type = "b", pch = 19, frame = FALSE,
     xlab = "Number of clusters K",
     ylab = "Total within-clusters sum of squares",
     main = "Elbow Method for Optimal k")
```



The Elbow Method plot shows somewhat of a sharp bend at k=2. I will compare the results of the Elbow Method with results from the Silhouette Method.

Silhouette Method for Choosing Value of K

```
library(cluster)

# Sample a subset of the presence matrix to reduce data size

# (In order to keep the session from crashing, I am using a subset of the matrix instead
# of the full matrix)

# The subset is likely to be reasonably representative enough of the full matrix for
# evaluating general clustering trends due to the use of random sampling

set.seed(123)  # Set seed for reproducibility
sample_size <- 5000
sampled_data <- presence_matrix[sample(nrow(presence_matrix), sample_size), ]

# Initialize an empty vector to store average silhouette width for each k
k_range <- 2:9
sil_width <- numeric(length(k_range))

# Exclude k=1 from the range because silhouette width is undefined for k = 1 since
# silhouette analysis requires at least 2 clusters to compare

# Calculate silhouette width for each k
for (i in 1:length(k_range)) {
  k <- k_range[i]
  kmeans_result <- kmeans(sampled_data, centers = k, nstart = 25)
  sil <- silhouette(kmeans_result$cluster, dist(sampled_data))
  sil_width[i] <- mean(sil[, 3])
}

# Plot silhouette width against the number of clusters
plot(k_range, sil_width, type = "b", pch = 19, frame = FALSE,
     xlab = "Number of Clusters K",
     ylab = "Average Silhouette Width",
     main = "Silhouette Method for Optimal K")
```




```
optimal_k <- k_range[which.max(sil_width)]
cat("Optimal number of clusters:", optimal_k, "\n")
```

```
## Optimal number of clusters: 2
```

Based on my findings from the Elbow Method plot and the Silhouette Method plot, I will use a k value of 2.

Performing K-Means Clustering

In our case, each point in the 69-dimensional space represents one plant. K-means clustering assigns each point to the cluster that has the center closest to that point. The cluster centers are then updated based on the new assignment by averaging the positions of all the points in that cluster

```
set.seed(123)  # Set seed for reproducibility

# Perform k-means clustering with k = 2
kmeans_result <- kmeans(presence_matrix, centers = 2, nstart = 25, iter.max = 100)
```

Performing Principal Component Analysis (PCA)

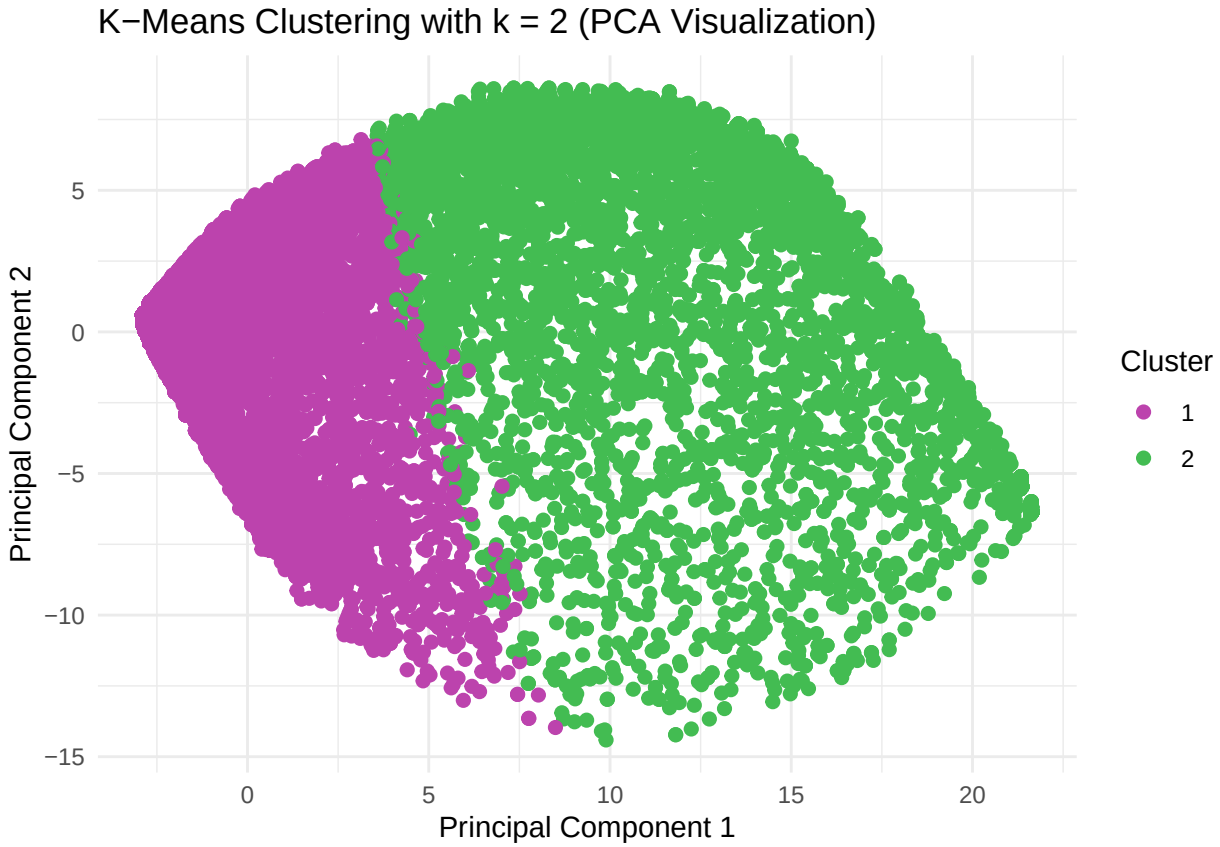
PCA is a dimensionality reduction technique that transforms the data into a new set of uncorrelated variables called principal components (PCs). These components capture the maximum variance in the data. In order to visualize the clustering results in 2D, I use PCA to reduce number of dimensions from 69 (there are 69 states, and there is 1 dimension per state) to 2.

```
# Identify columns with zero variance
zero_variance_cols <- apply(presence_matrix, 2, var) == 0

# Zero-variance columns are columns where all the values are the same (either all 0s or
# all 1s)

# Such columns do not contribute to distinguishing between different clusters
```

```r
# because they don't vary across the data

# Remove these columns from the matrix
filtered_matrix <- presence_matrix[, !zero_variance_cols]

# Print the number of columns removed
cat("Number of zero-variance columns removed:", sum(zero_variance_cols), "\n")
```

```
## Number of zero-variance columns removed: 1
```

```r
# Perform k-means clustering with k = 2
set.seed(123)
kmeans_result <- kmeans(filtered_matrix, centers = 2, nstart = 25, iter.max = 100)

# Perform PCA on the filtered matrix
pca_result <- prcomp(filtered_matrix, scale. = TRUE)

# Create a data frame with PCA results and cluster assignments
pca_data <- data.frame(pca_result$x[, 1:2], Cluster = as.factor(kmeans_result$cluster))

# Plot the PCA results with customized colors for clusters
library(ggplot2)
ggplot(pca_data, aes(x = PC1, y = PC2, color = Cluster)) +
  geom_point(size = 2) +
  scale_color_manual(values = c("#BC43AD", "#43BC52")) +
  labs(title = "K-Means Clustering with k = 2 (PCA Visualization)",
       x = "Principal Component 1",
       y = "Principal Component 2") +
  theme_minimal()
```



The plot indicates that the data set does not have two clusters that are very separated, as it appears more like a single group of points divided into two pieces rather than distinct, isolated clusters.

Probability Matrix

In this k-means clustering, we have a vector in 69-dimensional space for each cluster. Each element/dimension of a vector corresponds to one of the 69 states. Each element of the vector can be interpreted as the probability that a randomly selected plant from that cluster is found in the corresponding state. I will create a probability matrix which will show all of the information that the vectors contain; the matrix will show one probability value per state per cluster. The purpose of creating the matrix from the vectors is to put the information from the vectors in a format that is more suitable for building visualizations.

```
# Load required libraries
library(ggplot2)
library(tidyr)
library(dplyr)
```

```
##
## Attaching package: 'dplyr'
## The following objects are masked from 'package:stats':
##
##     filter, lag
## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```r
# Perform k-means clustering with k = 2
set.seed(123)
kmeans_result <- kmeans(presence_matrix, centers = 2, nstart = 25, iter.max = 100)

# Extract the cluster assignments from kmeans_result
cluster_assignments <- kmeans_result$cluster

# Number of clusters and states
num_clusters <- 2
num_states <- ncol(presence_matrix)

# Initialize a matrix to store probabilities (clusters x states)
prob_matrix <- matrix(0, nrow = num_clusters, ncol = num_states)
colnames(prob_matrix) <- colnames(presence_matrix)
rownames(prob_matrix) <- paste("Cluster", 1:num_clusters)

# Calculate the probability of each state having a "1" in each cluster
for (cluster in 1:num_clusters) {
  # Get the rows of the presence_matrix corresponding to the current cluster
  cluster_rows <- presence_matrix[cluster_assignments == cluster, ]

  # Calculate the probability of each state having a "1" in the current cluster
  prob_matrix[cluster, ] <- colMeans(cluster_rows)
}

# Calculate the overall average probability across all clusters and states
average_probability <- mean(presence_matrix)

# Output the result
cat("The average probability across the entire dataset is:", average_probability, "\n")
```

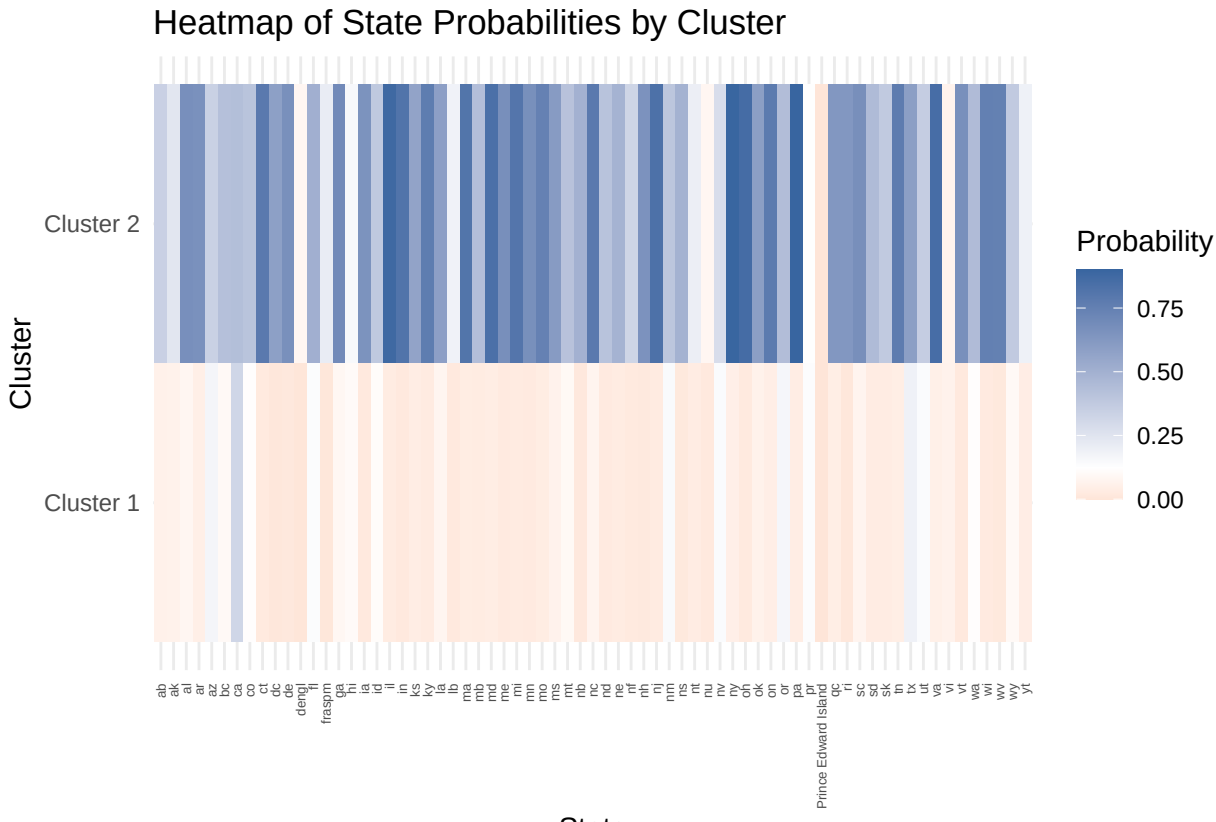
```
## The average probability across the entire dataset is: 0.1248858
```

Heat Map

I will create a heat map to visualize the probability matrix.

```r
# Load required libraries
library(ggplot2)
library(tidyr)
library(dplyr)

# Convert the matrix to a data frame and reshape it for ggplot2
prob_df <- as.data.frame(prob_matrix) %>%
  mutate(Cluster = rownames(prob_matrix)) %>%
  pivot_longer(cols = -Cluster, names_to = "State", values_to = "Probability")

# Create a custom color scale where white represents the average probability,
# blue represents above average, and orange represents below average
color_scale <- scale_fill_gradient2(
  low = "#D26217",      # Below average
  mid = "white",        # Average
  high = "#3865A0",     # Above average
  midpoint = average_probability, # Set the midpoint to the average probability
  name = "Probability"
```

```
)

# Plot the heat map using ggplot2
ggplot(prob_df, aes(x = State, y = Cluster, fill = Probability)) +
  geom_tile() +
  color_scale +
  labs(
    title = "Heatmap of State Probabilities by Cluster",
    x = "State",
    y = "Cluster"
  ) +
  theme_minimal() +
  theme(
    axis.text.x = element_text(angle = 90, vjust = 0.5, hjust = 1, size = 5),
    axis.text.y = element_text(angle = 0)
  )
```



The heat map illustrates how clustering reveals the geographic structure of the states; the closer two states are to each other geographically, the more similar their colors/probabilities are. To better visualize the relationship between the proximity of states and their respective colors, let's view the same information in the form of two choropleth maps (one map for each cluster).

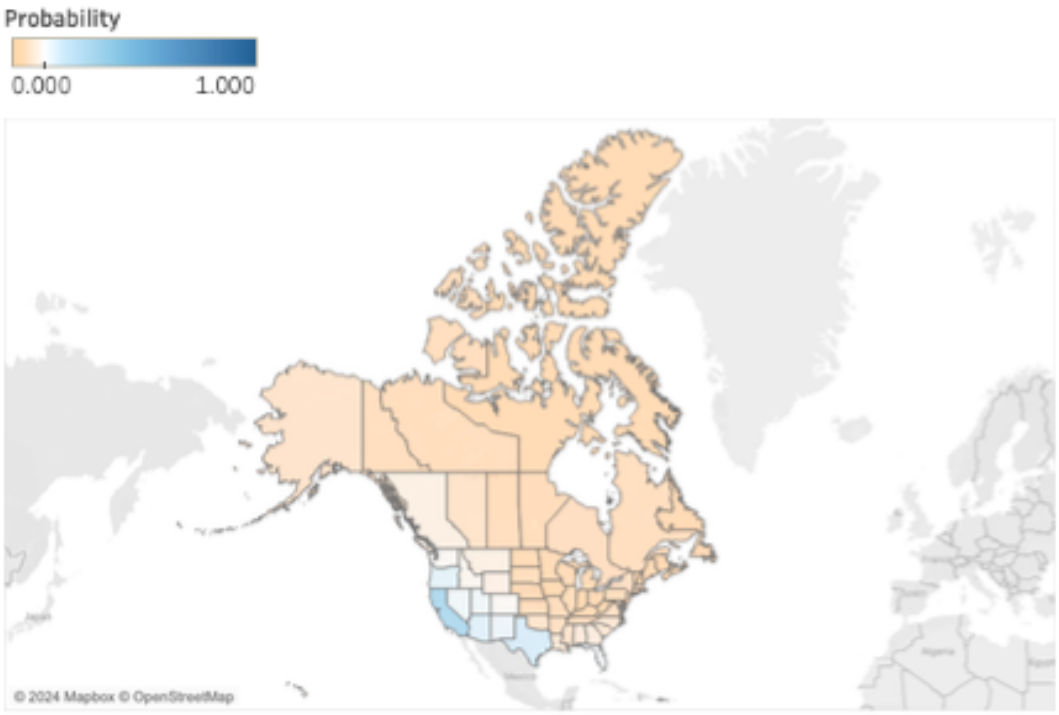
Using Choropleth Maps for Plants Data Set

Each vector in 69-dimensional space corresponds to a cluster. Each element of the vector corresponds to one of the 69 states. The value of each element is the probability that a plant chosen from that cluster at random is from that state.

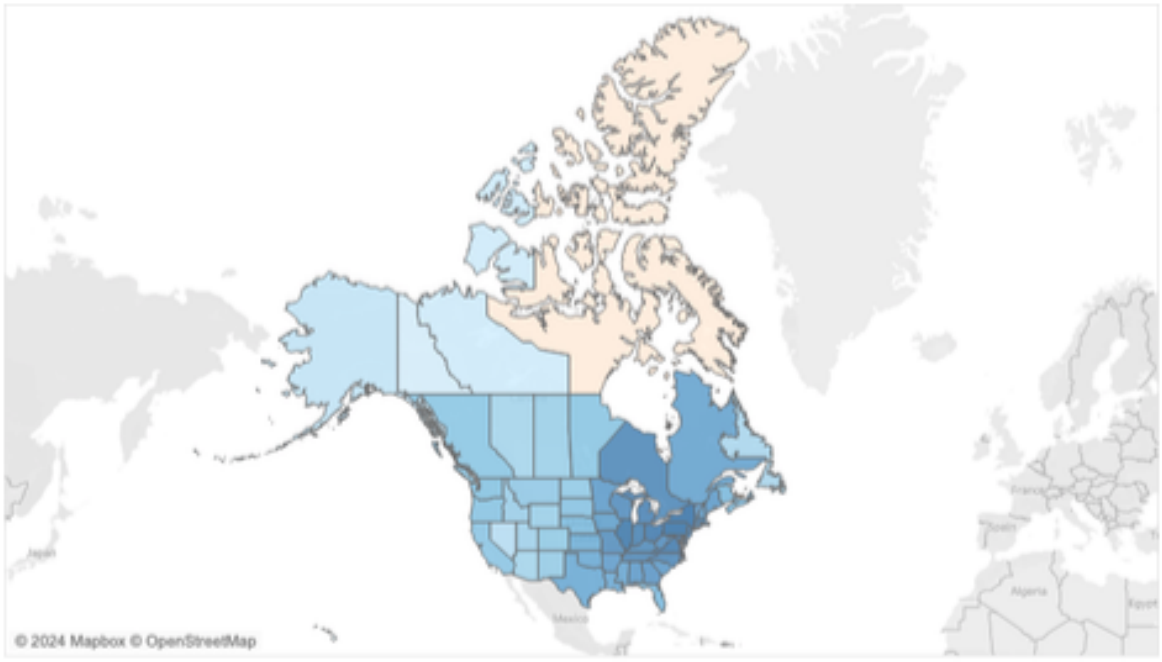
We can represent each cluster with a choropleth map by coloring each state on the map according to that state's probability value.

Transforming Probability Matrix for Choropleth Maps

```
# Load necessary libraries
library(tidyr)
library(dplyr)

# Convert the probability matrix into a data frame
prob_df <- as.data.frame(prob_matrix)

# Add cluster names as a column
prob_df$Cluster <- rownames(prob_matrix)

# Define a vector that maps each state to its respective country
country_mapping <- c(
  "ab" = "Canada", "bc" = "Canada", "mb" = "Canada", "nb" = "Canada", "lb" = "Canada",
  "nf" = "Canada", "nt" = "Canada", "ns" = "Canada", "nu" = "Canada", "on" = "Canada",
  "Prince Edward Island" = "Canada", "qc" = "Canada", "sk" = "Canada", "yt" = "Canada",
  "dengl" = "Denmark", "fraspm" = "France"
)

# Default all states to "United States" first
state_countries <- rep("United States", ncol(prob_df) - 1)
names(state_countries) <- colnames(prob_df)[-ncol(prob_df)]

# Overwrite specific states with their mapped countries
state_countries[names(country_mapping)] <- country_mapping

# Reshape the data into long format for Tableau
tableau_data <- prob_df %>%
  gather(key = "State", value = "Probability", -Cluster) %>%
  mutate(Country = state_countries[State])

# Save the reshaped data as a CSV file for Tableau
write.csv(tableau_data, "/Users/arielseidman/Desktop/plants/tableau_data.csv",
          row.names = FALSE)
```



Cluster 1



Cluster 2

Results

White on the maps represents the average probability of a random plant being found in a random state, which is about 0.1248858.

The choropleth maps show blue areas, orange areas, and white areas connecting them. This color gradient appears because plant distributions typically change gradually over large geographic areas.

The color transitions are not perfect gradients. Since the data set categorizes plant data by state, the colors vary state-by-state. If we had more specific location data (for example, plant data by county), the color transitions would be smoother. However, even with this state-level data, neighboring states still tend to have similar colors.

The color of each state represents the likelihood that a randomly selected plant from that cluster is from that state. If a state is blue, plants from that cluster are more likely to be found there than plants on average. Conversely, if a state is orange, plants in that cluster are less likely to be found there.

Cluster 1 is mostly orange with some blue in the West and Southwest United States, while Cluster 2 is mostly blue with some orange in Nunavut. This suggests that plants in Cluster 1 are more concentrated in the West and Southwest United States than in other areas, while plants in Cluster 2 are less concentrated in Nunavut than in other areas.

The k-means algorithm partially uncovers the geographic relationships between the states: although the data set lacks information about which states border each other, this information is revealed by the plant distributions across states and the clusters identified by k-means.

The main takeaway is that experimentation is important for finding the most suitable visual representation of a data set to uncover patterns and trends.