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Code

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Basic Concepts

Spectral clustering aims at clustering observations based on their proximity information. It essentially consists of two steps. The first step is a feature embedding, or dimension reduction. We first construct the graph Laplacian $\mathbf{L}$ (or normalized version), which represent the proximity information, and perform eigen-decomposition of the matrix. This allows us to use a lower dimensional matrix to represent the proximity information of the original data. Once we have the low-dimensional data, we can perform the regular clustering algorithm, i.e., k-means on the new dataset.

An Example

Let's look at an example that regular k-means would fail.

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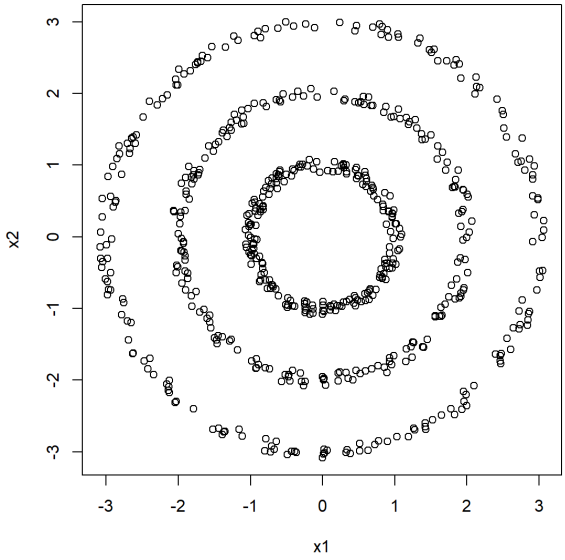
```
set.seed(1)

n = 200

r = c(rep(1, n), rep(2, n), rep(3, n)) + runif(n*3, -0.1, 0.1)
theta = runif(n) * 2 * pi

x1 = r * cos(theta)
x2 = r * sin(theta)
X = cbind(x1, x2)

plot(X)
```



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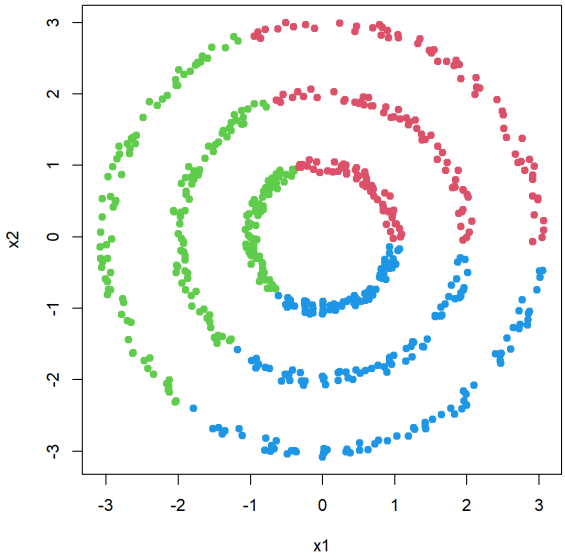
```
kmeanfit = kmeans(X, centers = 3)

plot(X, col = kmeanfit$cluster + 1, pch = 19)
```



Since k-means use Euclidean distance, it is not appropriate for such problems.

Adjacency Matrix

Maybe we should use a nonlinear way to describe the distance/closeness between subjects. For example, let's define two sample to be close if they are within the k-nearest neighbors of each other. We use $k = 10$, and create an adjacency matrix $\mathbf{W}$.

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```
library(FNN)

W = matrix(0, 3*n, 3*n)

# get neighbor index for each observation
nn = get.knn(X, k=10)

# write into W
for (i in 1:(3*n))
  W[i, nn$nn.index[i, ]] = 1

# W is not necessary symmetric
W = 0.5*(W + t(W))
# we may also use
# W = pmax(W, t(W))
```

Let's use a heatmap to display what the adjacency information look like. Please note that our data are ordered with clusters 1, 2 and 3.

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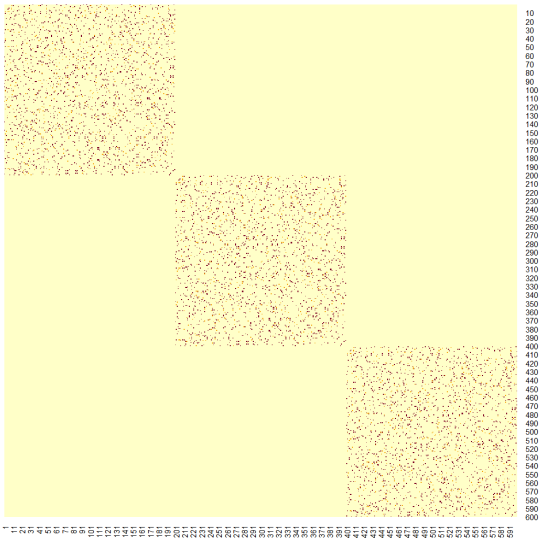
```
# plot the adjacency matrix
heatmap(W, Rowv = NA, Colv=NA, symm = TRUE, revC = TRUE)
```



Laplacian Matrix

The next step is to calculate the Laplacian

$$\mathbf{L} = \mathbf{D} - \mathbf{W},$$

where $\mathbf{D}$ is a diagonal matrix with its elements equation to the row sums (or column sums) of $\mathbf{W}$. We will then perform eigen-decomposition on $\mathbf{L}$ to extract/define some underlying features.

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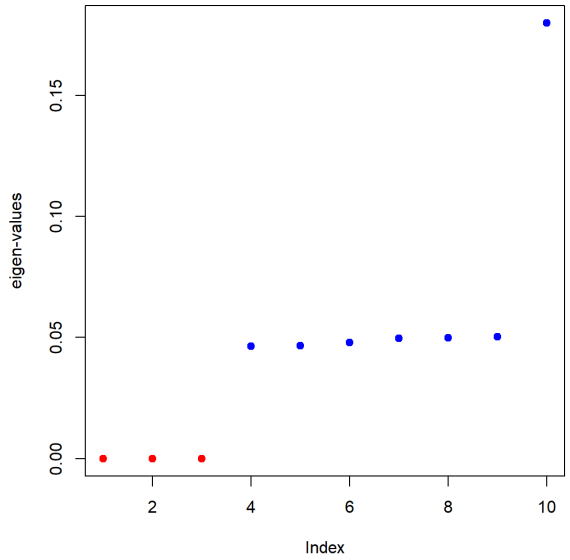
```
  # compute the degree of each vertex
  d = colSums(W)

  # the laplacian matrix
  L = diag(d) - W

  # eigen-decomposition
  f = eigen(L, symmetric = TRUE)

  # plot the smallest eigen-values
  # the smallest one will be zero --- why?
  plot(rev(f$values)[1:10], pch = 19, ylab = "eigen-values",
       col = c(rep("red", 3), rep("blue", 17)))
```



Feature Embedding

In fact the smallest eigen-value will always be zero. However, we can use the eigen-vectors associated with the second and third smallest eigen-values. They define some feature embedding or dimension reduction to represent the original data. Since we know the underlying model, two dimensions are enough (to separate three clusters). However, based on the eigen-value plot, there is a big gap between the third and the fourth one. Hence, we only need three. Further removing the smallest one, only two are needed.

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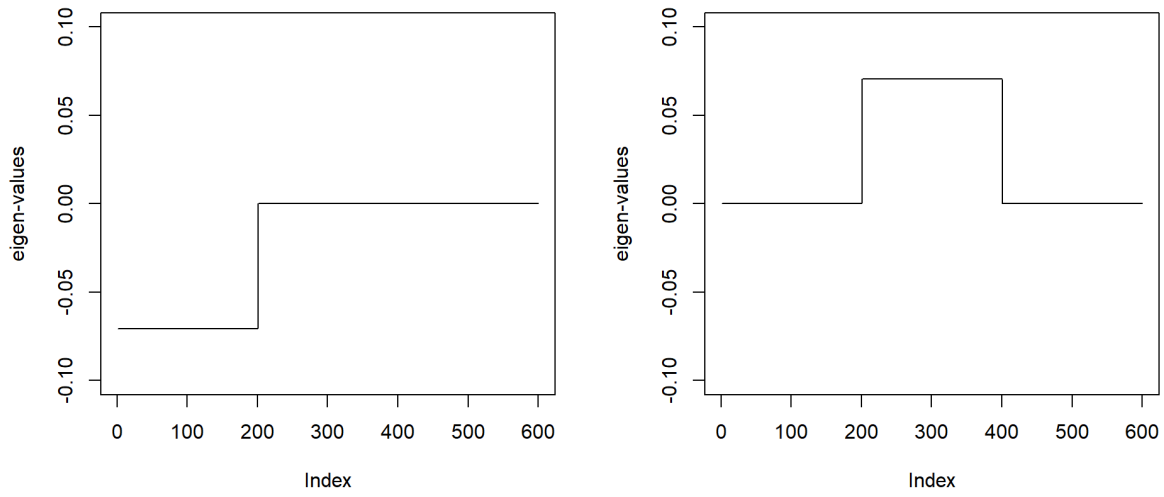
```
  par(mfrow=c(1,2))
  plot(f$vectors[, length(f$values)-1], type = "l", ylab = "eigen-values", ylim = c
(-0.1, 0.1))
  plot(f$vectors[, length(f$values)-2], type = "l", ylab = "eigen-values", ylim = c
(-0.1, 0.1))
```



Clustering with Embedded Features

We can then perform k-means on these two new features. And it will give us the correct clustering.

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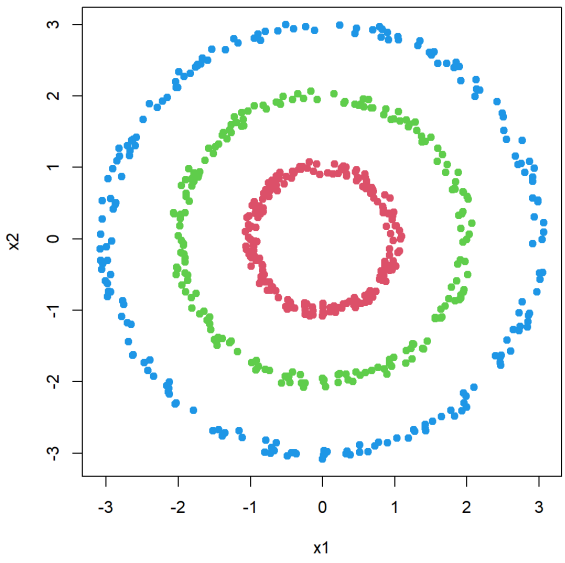
```
  par(mfrow=c(1,1))
  scfit = kmeans(f$vectors[, (length(f$values)-2) : (length(f$values)-1) ], centers
= 3, nstart = 20)
  plot(X, col = scfit$cluster + 1, pch = 19)
```



Another Laplacian

There are other choices of the Laplacian matrix. For example, a normalized graph Laplacian is defined as

$$\mathbf{L}_{\text{sym}} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2}$$

For our problem, it achieves pretty much the same effect.

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```
  # the normed laplacian matrix
  L = diag(nrow(W)) - diag(1/sqrt(d)) %*% W %*% diag(1/sqrt(d))

  # eigen-decomposition
  f = eigen(L, symmetric = TRUE)

  # perform clustering
  scfit = kmeans(f$vectors[, (length(f$values)-2) : (length(f$values)-1) ], centers
= 3, nstart = 20)
  plot(X, col = scfit$cluster + 1, pch = 19)
```