

# HW#3 || MDS Eigen Decomposition using pairwise distances of US cities

Saket Choudhary

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```
> library(graphics)
> library(ggplot2)
```

## Read Data:

```
> distanceMatrix <- read.csv("distance_matrix.csv", header=T)
> distanceMatrix
```

	BOST	NY	DC	MIAM	CHIC	SEAT	SE	LA	DENV
1	0	206	429	1504	963	2976	3095	2979	1949
2	206	0	233	1308	802	2815	2934	2786	1771
3	429	233	0	1075	671	2684	2799	2631	1616
4	1504	1308	1075	0	1329	3273	3053	2687	2037
5	963	802	671	1329	0	2013	2142	2054	996
6	2976	2815	2684	3273	2013	0	808	1131	1307
7	3096	2934	2799	3053	2142	808	0	379	1235
8	2979	2786	2631	1687	2054	1131	379	0	1059
9	1949	1771	1616	2037	996	1307	1235	1059	0

## 1 MDS

Coordinates of points are given by:

```
> rownames(mds) <- colnames(distanceMatrix)
> colnames(mds) <- c("X1", "X2")
> print(mds)
```

	X1	X2
BOST	-1388.4759	401.09561
NY	-1235.5455	281.49474
DC	-1110.4073	156.62867
MIAM	-1108.0546	-1273.17629
CHIC	-435.5452	288.46936
SEAT	1601.4477	651.49498
SE	1708.7378	76.02141
LA	1335.1428	-1065.44210
DENV	546.1006	78.38664

## 2 EigenValue Decomposition

### 2.1 Using similarity matrix

```
> similarityMatrix <- apply(distanceMatrix, 1, function(x) exp(-x^2/3000.0^2))
> similarityMatrix
```

	[,1]	[,2]	[,3]	[,4]	[,5]	[,6]	[,7]
BOST	1.0000000	0.9952960	0.9797587	0.7777617	0.9020900	0.3737889	0.3447196
NY	0.9952960	1.0000000	0.9939860	0.8268797	0.9310269	0.4145882	0.3842415
DC	0.9797587	0.9939860	1.0000000	0.8794991	0.9512040	0.4491365	0.4187467

```

> mds <- cmdscale(distanceMatrix)
> mdsPlot <- qplot(x=mds[,1],
+                 y=-mds[,2],
+                 label=colnames(distanceMatrix))
> mdsPlot +
+   geom_point(color='red') +
+   geom_text(hjust=-.15) +
+   xlab("X1") + ylab("X2") +
+   ggtitle("MDS plot using 2 dimensions")

```

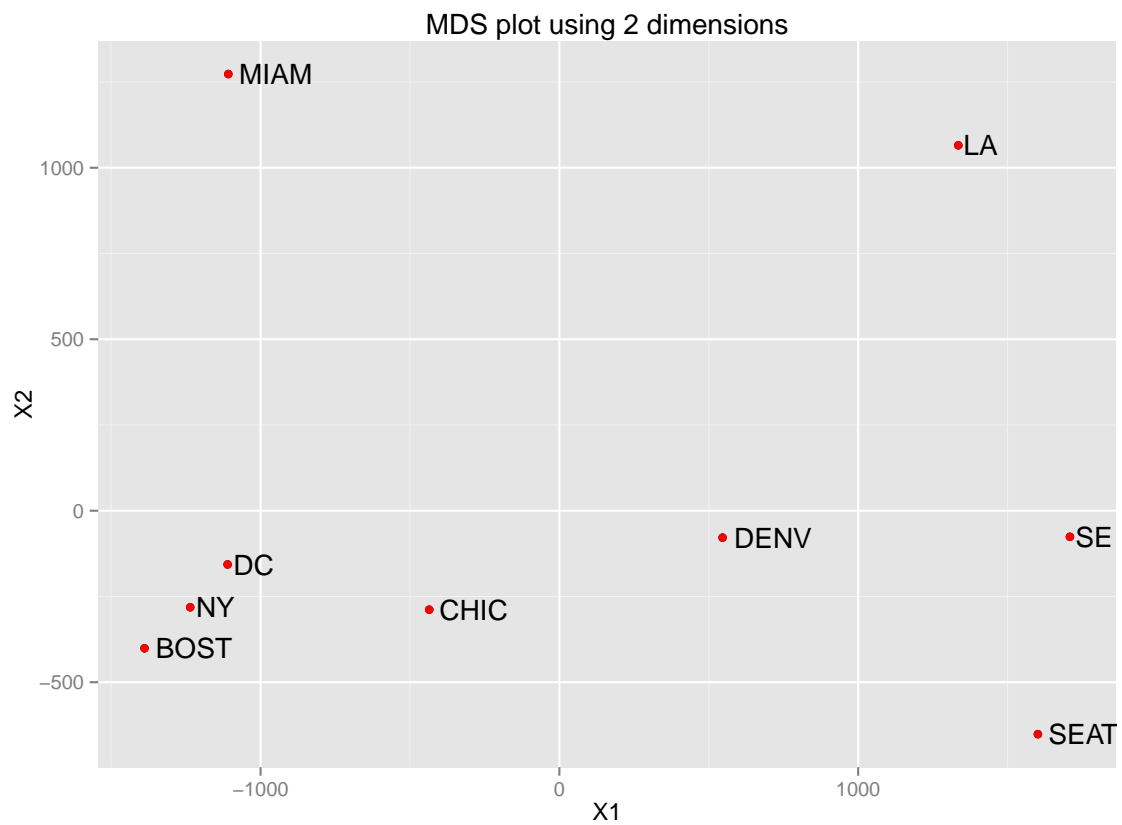


Figure 1: MDS plot(2D)

```

> similarityMatrix.prcomp <- prcomp(similarityMatrix, scale.=T)
> similarityMatrix.PCA <- similarityMatrix.prcomp$x[,1:2]
> similarityMatrix.plot <- qplot(x=similarityMatrix.PCA[,1],
+                               y=similarityMatrix.PCA[,2],
+                               label=colnames(distanceMatrix))
> similarityMatrix.plot +
+   geom_point(color='red') +
+   geom_text(hjust=-.15) +
+   xlab("PC1") + ylab("PC2")+
+   ggtitle("First 2 principle components of similarity Matrix")

```

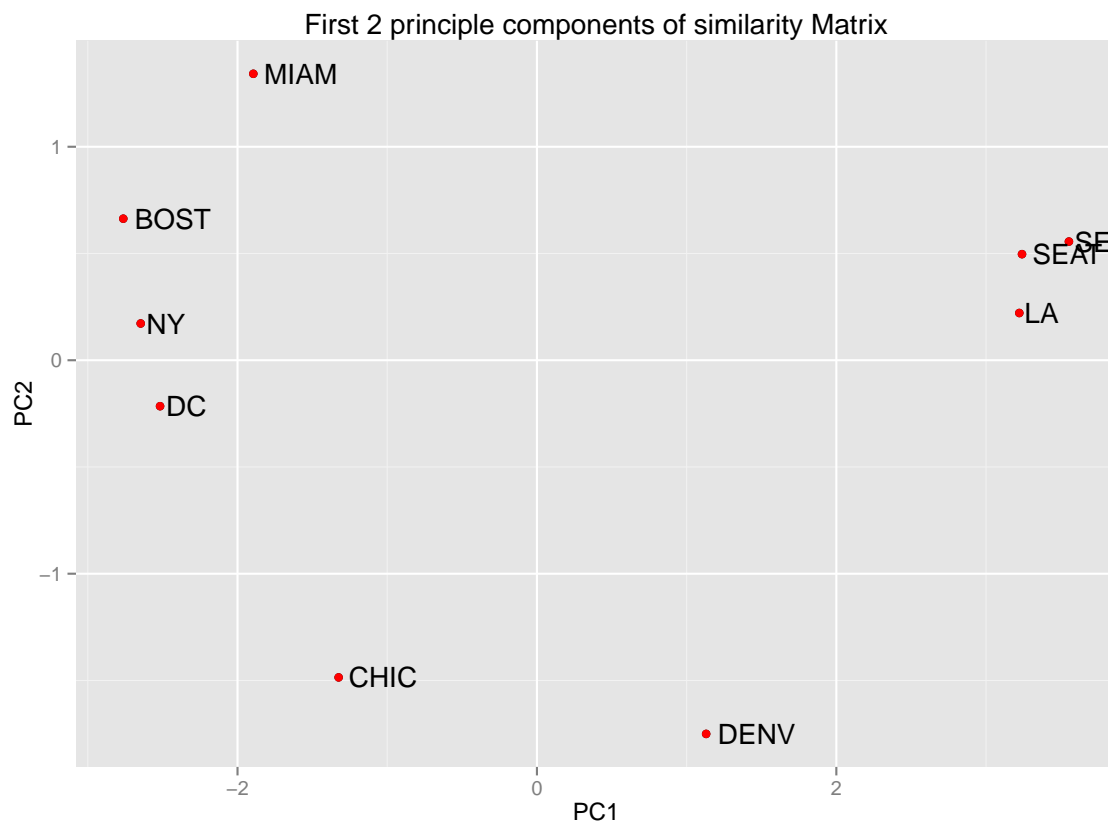


Figure 2: PCA using gaussian kernel(using similarity matrix)

```

MIAM 0.7777617 0.8268797 0.8794991 1.0000000 0.8218076 0.3041358 0.3549972
CHIC 0.9020900 0.9310269 0.9512040 0.8218076 1.0000000 0.6374745 0.6006181
SEAT 0.3737889 0.4145882 0.4491365 0.3041358 0.6374745 1.0000000 0.9300281
SE   0.3449568 0.3842415 0.4187467 0.3549972 0.6006181 0.9300281 1.0000000
LA   0.3730477 0.4221385 0.4634165 0.4483331 0.6257725 0.8675093 0.9841666
DENV 0.6556903 0.7057505 0.7481425 0.6306268 0.8956335 0.8271200 0.8441125
    [,8]    [,9]
BOST 0.3730477 0.6556903
NY   0.4221385 0.7057505
DC   0.4634165 0.7481425
MIAM 0.7289000 0.6306268
CHIC 0.6257725 0.8956335
SEAT 0.8675093 0.8271200
SE   0.9841666 0.8441125
LA   1.0000000 0.8828420
DENV 0.8828420 1.0000000

```

Perform PCA an similarityMatrix:

### 2.1.1 EigenValues

```
> print(similarityMatrix.prcomp$sdev)

[1] 2.763748e+00 1.011925e+00 5.609621e-01 1.317532e-01 6.715841e-02
[6] 3.342472e-02 6.485914e-03 1.019860e-03 1.743940e-16
```

### 2.1.2 EigenVectors

```
> print(similarityMatrix.prcomp$rotation[,1:2])

      PC1      PC2
[1,] -0.3552454 -0.15532942
[2,] -0.3556963 -0.17183709
[3,] -0.3555762 -0.18252044
[4,] -0.3372374 -0.03256753
[5,] -0.3160704 -0.47693301
[6,]  0.3425956 -0.25501975
[7,]  0.3540793 -0.19295181
[8,]  0.3348572 -0.03848530
[9,]  0.2287874 -0.76207529
```

### 2.1.3 Principle Components(Scaled and Centered)

```
> print(similarityMatrix.prcomp$x[,1:2])

      PC1      PC2
BOST -2.763048  0.6631076
NY    -2.646744  0.1721873
DC    -2.517306 -0.2152715
MIAM  -1.894466  1.3418267
CHIC  -1.324643 -1.4856597
SEAT   3.240198  0.4969233
SE     3.553513  0.5559057
LA     3.222135  0.2212970
DENV   1.130362 -1.7503165
```

## 2.2 Using distance matrix

Perform PCA an distanceMatrix:

### 2.2.1 EigenValues

```
> print(distanceMatrix.prcomp$sdev)

[1] 2.666684e+00 1.049368e+00 7.363066e-01 3.395746e-01 2.999203e-01
[6] 1.640774e-01 1.070771e-01 4.272792e-02 1.600394e-17
```

### 2.2.2 EigenVectors

```
> print(distanceMatrix.prcomp$rotation[,1:2])

      PC1      PC2
BOST  0.3609929  0.13053243
NY     0.3632938  0.14972372
DC     0.3651761  0.17155008
MIAM   0.2962816 -0.13553983
CHIC   0.2957988  0.54249894
SEAT  -0.3516124  0.16804789
SE     -0.3676068  0.08877045
LA     -0.3577376  0.10405688
DENV  -0.2057333  0.75596984
```

```

> distanceMatrix

  BOST  NY   DC MIAM CHIC SEAT  SE  LA DENV
1    0  206  429 1504  963 2976 3095 2979 1949
2  206    0  233 1308  802 2815 2934 2786 1771
3  429  233    0 1075  671 2684 2799 2631 1616
4 1504 1308 1075    0 1329 3273 3053 2687 2037
5  963  802  671 1329    0 2013 2142 2054  996
6 2976 2815 2684 3273 2013    0  808 1131 1307
7 3096 2934 2799 3053 2142  808    0  379 1235
8 2979 2786 2631 1687 2054 1131  379    0 1059
9 1949 1771 1616 2037  996 1307 1235 1059    0

> distanceMatrix.prcomp <- prcomp(distanceMatrix, scale.=T)
> distanceMatrix.PCA <- distanceMatrix.prcomp$x[,1:2]
> distanceMatrix.plot <- qplot(x=distanceMatrix.PCA[,1],
+                               y=distanceMatrix.PCA[,2],
+                               label=colnames(distanceMatrix))
> distanceMatrix.plot +
+   geom_point(color='red') +
+   geom_text(hjust=-.15) +
+   xlab("PC1") + ylab("PC2") +
+   ggtitle("First 2 principle components of distanceMatrix")

```

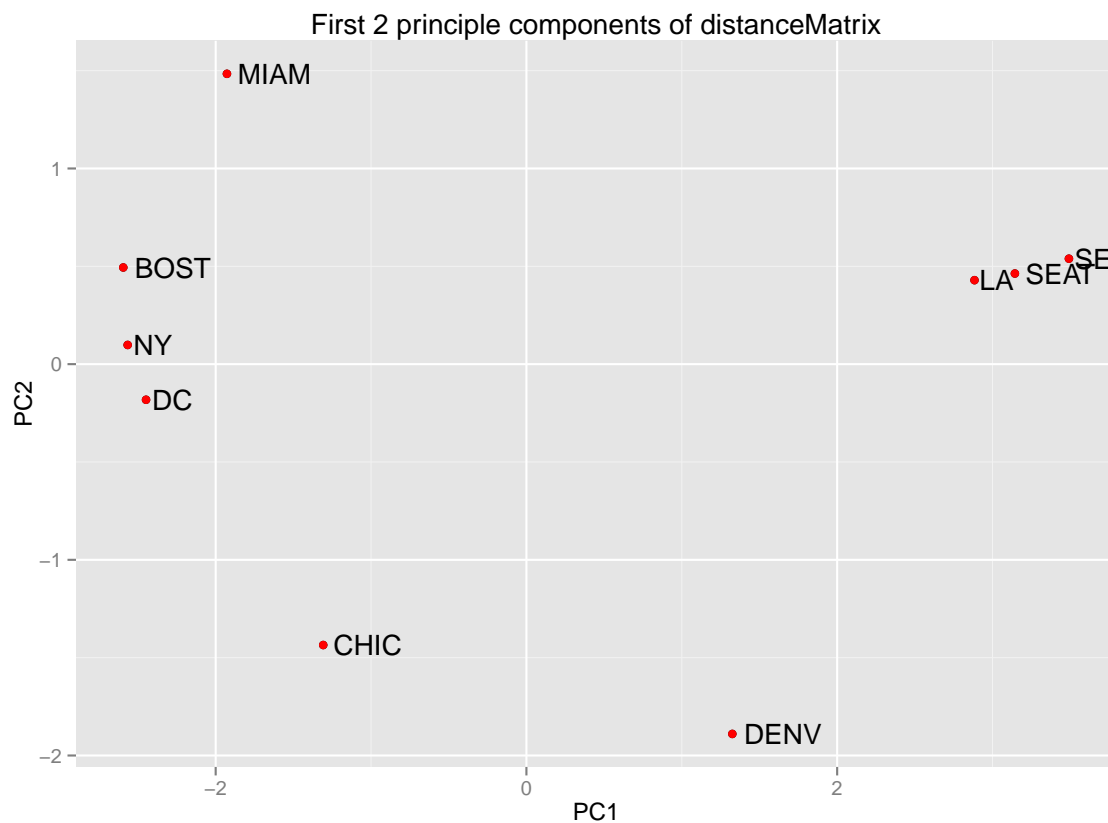


Figure 3: PCA without using gaussian kernel(using distance matrix)

### 2.2.3 Principle Components(Scaled and Centered)

```
> print(distanceMatrix.prcomp$x[,1:2])
```

	PC1	PC2
[1,]	-2.594727	0.49402847
[2,]	-2.566601	0.09812092
[3,]	-2.448209	-0.18194241
[4,]	-1.927579	1.48379129
[5,]	-1.307785	-1.43547852
[6,]	3.143991	0.46313051
[7,]	3.491687	0.53895796
[8,]	2.883923	0.42915851
[9,]	1.325301	-1.88976673

## 3 Discussion

As evident from Figure 1 and Figure 2, transforming original data from pairwise distances to pairwise similarities using gaussian kernel does not seem to have effect on the resulting PCA plots. The most probable reasoning is because the data is linearly separable in its original 9 dimensions. With the gaussian kernel trick each row being a 9-D vector is transformed to a infinite-dimensional space(a function for example satisfies all operations that a vector satisfies: addition/multiplication in 'higher' dimensions and with a gaussian kernel with fixed  $\sigma^2$  each original vector is sent to a 'higher' dimensional gaussian blob centered at that point. If any two points in original 9-D space were close, their gaussian transformation would lead to the resulting vectors having small angle in the 'higher' dimensional space), assuming that higher dimensions would guarantee linear separation. But in this case, linear separation is guaranteed in the original 9-dimensions itself.

### 3.1 Equivalence of MDS and PCA?

MDS and PCA are expected to have same results when eucliden distances are used. [Cox, Trevor F., and Michael AA Cox. Multidimensional scaling. CRC Press, 2000.]