Lecture 16: Analysing and Visualizing Data I

In [1]: %load_ext rmagic

Today's lecture topics:

• Bivariate Analysis: visualizing population clusters and variable relations

• Multivariate Analysis: Visualization

. Multivariate analysis: Clustering

1. Bivariate Analysis: visualizing population clusters and variable relations

Consider a population for which one has only two variables.

As example, we will simulate grade data for a student population, for which one has the midterm grade and the final grade.

The maximal score should be 100.

To simulate continous variable, one can use the function

```
rnorm(n, mean, sd)
```

returning a numeric vector of real numbers

- which is normally distributed around mean
- has standard deviation std

Since the numbers generated by rnorm may fall outside our allowed range (0 to 100), we need take care of these bad values. We can correct these bad values using the **bracket operator** and **logical indexing**:

```
X[X < some_value] = some_other_value</pre>
```

Since we may reuse this code more than one time, let's package it into a function:

```
In [3]: %%R

simulate.grades = function(n, score.mean, score.sd, score.max) {
          grades = rnorm(n, mean=score.mean, sd=score.sd)
          grades[grades < 0] = 0
          grades[grades > score.max] = score.max
          return(grades)
}
```

We can now simulate our grades, and check their values by plotting the variable histograms, using the command

```
hist(X, main, xlim)
```

which takes

- · a continous variable X
- an argument main specifying the histogram title
- an argument ${\tt xlim}$ containing the axis upper and lower values

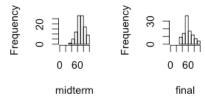
The function

```
par(mfrow=c(n,m))
```

allows us to diplay our plots on a $n \times m$ grid of plots (similar to subplots function in matplotlib).

par(mfrow=c(1,2))
hist(midterm, main='Midterm grade distribution', xlim=c(0,100))
hist(final, main='Final grade distribution', xlim=c(0,100))

idterm grade distriFinal grade distribu



Row and column analysis

At this point, we have roughly two possible types of analysis:

Population (or row) Analysis:

We can investigate whether our variables split our population in natural group called **clusters**. This is an analysis of the rows.

Example: Are the student grades splitting the class into students of different strenght? We may use these cluster to establish letter grades for instance.

Variable (or column) Analysis:

We can investigate whether our **variables** are **related** to each other, or wether they are **indenpendent**. This is an analysis of the columns.

Example: Is the final score strongly dependent on the midterm score? Can we find a functional relationship between these two scores?

Scatter plots

A scatter plot of our variables will give us indications for these two types of analysis:

- possible clusters in the rows (population)
- possible relations between the columns (variables)

Definition:

A scatter plot of two numeric vectors $X=(x_1,\ldots,x_n)$ and $Y=(y_1,\ldots,y_n)$ with the same number n of elements is a graph with two axes representing the two variable ranges and displaying n points with coordinates $(x_1,y_1),\ldots,(x_n,y_n)$.

Suppose we have

- a population Ω we wish to study
- two continous variables $X,Y:\Omega\longrightarrow\mathbb{R}$ of interest for our study
- a population sample $S = \{s_1, \dots, s_m\} \subset \Omega$

The values of our variables on the population sample gives us two vectors:

$$X=(x_1,\ldots,x_m), \quad ext{where} \quad x_i=X(s_i)$$

$$Y = (y_1, \dots, y_m), \quad ext{where} \quad y_i = Y(s_i)$$

In a scatter plot each sample individual $s_i \in S$ is represented as a point in \mathbb{R}^2 with coordinates (x_i,y_i) .

Looking at the **geometry** of the **cloud of points** plotted **in the scatter plot** in the xy-plane:

$$(x_1,y_1),\,(x_2,y_2),\ldots,\,(x_m,y_m)\in\mathbb{R}^2$$

will give us indications on

- · the variable relations
- · the population clusters

Important remark: Of course, we will only obtain indications this way. This is particularly true if we don't have values for the whole populations but only for a sample of the population. It may be the case that the clusters and relations we see for a given sample disappear after add more individual to our sample!!!

In R, the function that allows us to display **scatter plots** of two numeric vectors is the <u>plot function (http://www.r-tutor.com/elementary-statistics/quantitative-data/scatter-plot)</u>:

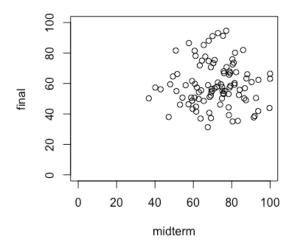
```
plot(X, Y, xlim, ylim, main, xlab, ylab)
```

that takes

- two numeric vectors X and Y
- two numeric vectors xlim and ylim containing the axis upper-and-lower bounds
- legend strings main for the title, xlab, ylab for the x-and-y axis legends

Remark: The appearance or not of clusters in the scatter plot may depends on the scale chosen for the x-and-y axis!

Let us display a scatter plot of our two grade variables:



From this scatter plots, we see a single cluster of points centered on

```
(mean (midterm), mean (final))
```

but **no particular relationship between the two exam scores** (i.e. a student may have performed well at the midterm and badly at the final in a completely independent way).

This type of cloud is characteristic of normally distributed independent variables. So not much to report.

Simulating variable relationships

A better model for grade simulation can be achieved by considering as before that

· the two exam scores are normally distributed around two different means

but now we will add the following assumptions to our model:

- · students work harder for the final exam
- final grades are generally lower than midterm grades
- · relative student performances should be somewhat the same for both exams

Mathematically, we can choose a linear model to represent the assumption aboves:

$$F = \alpha M - \beta + \epsilon$$

where

- $oldsymbol{\cdot}$ lpha is a **positive proportionality factor** representing the relative amount of work put into the final in comparison with the midterm
- eta is a **positive** number modelling the fact that the **final is harder than the midterm**
- $oldsymbol{\epsilon}$ is a normally distributed error term accounting for the fact that particular students may not follows perfectly our model

Let us simulate grades according to this model. We will do that in three steps:

- simulate the midterm grades as before
- use our model $F=\alpha imes M-\beta$ to simulate the final grades
- add an normally distributed error term ϵ to the final grades

Good practice wants us to package our linear simulation in a function:

Without adding the error term ϵ , a scatter plot makes the variable relation cristal clear.

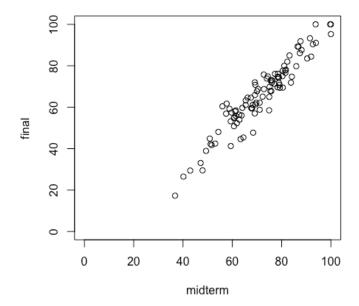
Increasing the error term tends to mask the functional realtionship between our two variables, but it is still visible:

```
In [7]: %%R -r 96

n = 100; alpha = 1.2; beta = 20; error = 5; score.max = 100

final = simulate.final(midterm, alpha, beta, error, score.max)

plot(midterm, final, xlim=c(0, 100), ylim=c(0, 100))
```



Simulating population clusters

Now suppose, we want to add to our grade model the fact that student from different majors may perform differently in the class exams.

Suppose we have two majors:

- · LITT for litterature majors
- · DOUB for double majors in CS and statistics

For a "Computing with Data" class, one may expect the DOUB major to perform the better and the LITT major.

Let's try to built this feature into our simulated grade data.

First, we simulate midterm grades with different means and standard deviations for the two groups:

```
In [8]: %%R
max_score = 100

L_number = 30; L_mean = 40; L_sd = 5
D_number = 80; D_mean = 80; D_sd = 5

L_midterm = simulate.grades(L_number, L_mean, L_sd, max_score)
D_midterm = simulate.grades(D_number, D_mean, D_sd, max_score)
```

Second, we use our linear model with different parameters for the two groups:

```
In [9]: %%R
    L_alpha = 0.5; L_beta = 10; L_error = 15
    D_alpha = 1.2; D_beta = 10; D_error = 5

L_final = simulate.final(L_midterm, L_alpha, L_beta, L_error, max_score)
    D_final = simulate.final(D_midterm, D_alpha, D_beta, D_error, max_score)
```

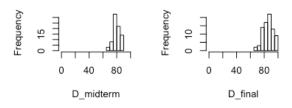
The historgram plots for the exam scores for each section already reveal a certain clustering in the data:

Histogram of D_midterr

Histogram of L_midtern

Histogram of D_final

Histogram of L_final



Third, we create a data frame for each major with a column for the section names, and we concatenate the two data frames into a single one using the row bind function:

```
Final Midterm Section
1 6.411672 44.46837 LITT
2 17.169801 34.76351 LITT
3 31.799930 49.85669 LITT
4 0.000000 38.08184 LITT
```

```
5 6.514070 48.27073 LITT 6 21.634841 47.56106 LITT
```

Invoked with an integer n, the function

```
sample(n)
```

return a vector with the first n integers randomly permuted entries.

Let us use this trick to shuffle the LITT and DOUB sections in our data frame grade.

Remark: The function nrow (df) and nool (df) return respectively the number of rows and the number of columns of the data frame df.

We can now display the scatter plot of our two variables.

To verify that the clusters correspond to the majors, we'd like to plot our points in two different colors depending on the section.

The function plot takes a character vector

```
col=color_vector
```

containing the colors with which each point is to be plotted.

To construct this color vector, we can first contruct a vector with the

Since the data frame column corresponding to the section is a factor with two possible integer values:

- 1 for 'LITT'
- 2 for 'DOUB'

we can construct our color vector using the bracket operator on the vector containing our two colors:

Latus nose this color vector as the --1 argument to plat and add a legand using the functions

```
point_colors = my_colors[grades$Section]

print(point_colors)

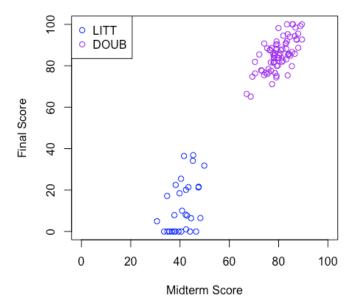
[1] "blue" "blue" "purple" "purple" "purple" "purple" "purple" "purple" "purple" "blue"
[9] "purple" "purple" "blue" "purple" "blue" "purple" "purple" "purple" "blue"
[25] "purple" "purple" "blue" "blue" "purple" "
```

Let us pass this color vector as the cold argument to piot and add a legend using the function.

legend(location, legend=levels(grades\$Section), col=my colors, pch=1)

where

- the location argument can be 'topleft', 'toprigth', 'bottomleft', 'bottomrigth'
- the legend corresponds to the category names
- the col is a character vector containing the category colors
- the pch=1 is a necessary argument that you should not worry about now



Conclusion:

The scatter plot shows us what we put into the data. Namely:

- two student clusters corresponding to two sections "LITT" and "DOUB"
- a seemingly linear relationship between the final grade and the midterm grade

The **linear variable relation** is more pronounced on the "DOUB" clusters. This is due to the fact that we cranked up the **error** term for the "LITT" student (L_ERROR = 15 while D_ERROR = 5).

EXERCISE: Try to see how the **population clusters** and the **variable relation** survive modification of the various parameters we entered into the model. This will give you sense of the care with with you should draw conclusion with real data.

2. Multivariate Analysis: Visualization

With two variables, it's possible to visualize population clusters and variable relations on a single scatter plot, since it involves to plot points on the variable plane.

With three variables we can still use a scatter plot, although we now need to plot our points in a 3 dimensional space, which renders the interpretation slightly more challenging.

With more than three variables the only way to visualize the scatter plot (which involves plotting in a n-dimensional space, where n is the number of variables) is to plot 2-dimensional projections of the n-dimensional scatter plot. This means that we can plot all the scatter plots for each pair of variables. The visual situation is however more challenging to interpret, and we will need to use other tools for that, as we will see.

To get started, let's add a variable to our simulated grade data and plot the 3D scatter plot.

The variable we will add is an homework grade. To keep simulation simple, we will generate a homework grade for the whole class, without making any distinction between the two sections.

The lattice library and the cloud function

Name109 87.89609 81.53302 81.43087

Name110 21.25706 47.48521 69.34250

The lattice library offers advance plotting capabilities in R. To load it, type in

```
library(lattice)
```

The display 3D scatter plots of 3 continous variables, say X, Y, and Z, stored in a data frame myFrame, we will use the lattice function

```
cloud(Z \sim X + Y, data=myFrame, group=cat, auto.key=T)
```

• The first argument is an R formula. For now, you only need to understand that

DOUB

LITTT

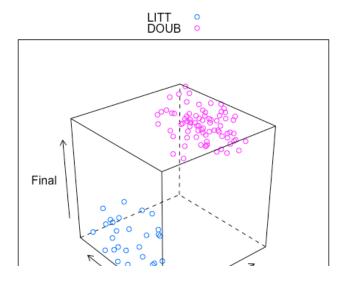
```
Z ~ X + Y
```

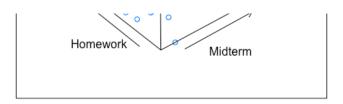
means that Z will be plotted on the z-axis, while X and Y will be plotted on the xy-plane.

- The second argument data is the data frame from which the quantitative variables X,Y, and Z will be retrieved from.
- The **third argument** group is a **categorical variable** from the data frame myFrame indicating that the points from different categories should be displayed with different colors.
- The last argument auto. key is a Boolean argument indicating a legend describing which color corresponds to which category should be
 plotted.

Let us display a 3D scatter plot of our variables Final, Midterm and Homework and plot them with different colors depending on the Section variable.

Remark: In the notebook, one needs to store the output of cloud into a variable, which we will need to print in order for the plot to appears.





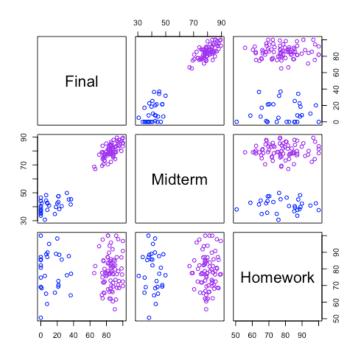
One still clearly seet the two clusters of LITT and DOUB majors. The linear relationship between the variables is however not clearly perceptible on the plot.

The scatter plot matrix

Another way to display variable relations and population clusters for more than 2 variables is to plot a scatter plot matrix containing a scatter plot of each pair of variables.

One can again pass our color vector to the col argument.

```
In [18]: | %%R -r 96 -w 500 -h 500
          plot(grades[,c(1,2,3)], col=point colors)
```



The two section clusters are very visible in each of the scatter plots.

At contrast with our 3D scatter plot, one can still see the linear relation ship between the midterm score and the final score that we build into our data.

Although still very useful for three variables, we begin to get a sense that more sophisticated methods will be needed as the number of variable increases... That's what we are going to learn next.

3. Multivariate analysis: Clustering

Let us add a fourth variable to our simulated grade data:

```
In [19]: %%R
         quiz = simulate.grades(L_number + D_number, score.mean=30, score.sd=5, max_score)
         grades$Quiz = quiz
         grades = grades[,c('Final', 'Midterm', 'Homework', 'Quiz', 'Section')]
         print(head(grades))
                   Final Midterm Homework
                                                Quiz Section
                8.167408 42.28068 89.86770 27.85688
         Name2 0.000000 39.39495 85.75620 26.71910
```

LITT

```
      Name3
      91.891964
      83.39170
      100.00000
      34.79697
      DOUB

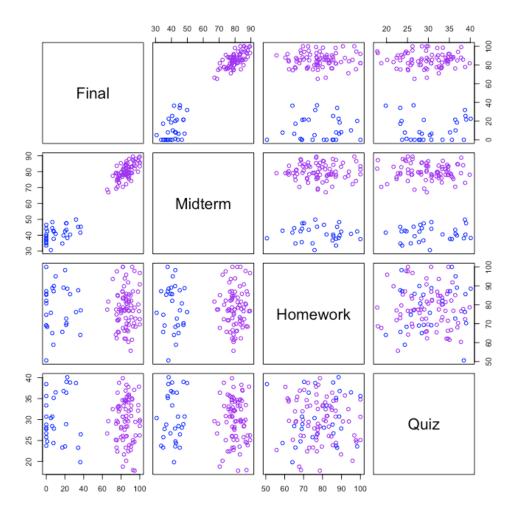
      Name4
      87.820700
      79.03601
      60.37647
      37.78026
      DOUB

      Name5
      1.018811
      42.47156
      68.35079
      24.79602
      LITT

      Name6
      83.712879
      81.23105
      66.23481
      34.65286
      DOUB
```

We can still display a scatter plot matrix:

```
In [20]: %%R -r 96 -w 700 -h 700
plot(grades[,c(1,2,3,4)], col=point_colors)
```



We still see some clustering appearing for some variables, but for others (Quiz and Homework) the clustering does not seem to be present.

As the number of variable grows, we need to use other methods to retrieve clusters from the data.

The distance matrix

Consider n variables X_1,\ldots,X_n for a population sample of m individual.

All the variable values for all the sample individuals can be arranged into a matrix

$$egin{pmatrix} x_{11} & x_{12} & \cdots & x_{1n} \ x_{21} & x_{22} & \cdots & x_{2n} \ dots & & dots \ x_{m1} & x_{2m} & \cdots & x_{mn} \end{pmatrix} \qquad ext{where} \qquad x_{ij} = X_i(s_j) \quad ext{(value of the variable} \quad X_i \quad ext{for the individual} \quad s_j \)$$

In other word, this matrix is the data frame stripped from its row and column labels.

The **points** v_1,\ldots,v_m represented in a **scatter plots** are just the **row vectors** of this value matrix:

$$egin{array}{lcl} v_1 &=& (x_{11},x_{12},\ldots,x_{1n}) \ v_2 &=& (x_{21},x_{22},\ldots,x_{2n}) \ &dots \ v_m &=& (x_{m1},x_{m2}\ldots,x_{mn}) \end{array}$$

In R, a **matrix** is a represented by a **vector** with the **hidden dimension vector** set up with the corresponding number of rows and columns, in the same way a **class** is a **list** with the **hidden class string** set up to the **class name**.

This hidden dimension vector is accessed and set up through the function

```
dim(x)
```

Changing the dimension of a vector makes R interpret the resulting object as an instance of the class matrix.

One can extract the value matrix from a data frame using the conversion funtion

```
as.matrix(x)
```

The distance matrix of a matrix $A=(x_{ij})$ is the matrix containing all the distances between the matrix row vectors v_1,v_2,\ldots,v_m :

$$\mathrm{dist}(A) \quad = \quad egin{pmatrix} d(v_1,v_1) & d(v_1,v_2) & \cdots & d(v_1,v_n) \ d(v_2,v_1) & d(v_2,v_2) & \cdots & d(v_2,v_n) \ dots & & dots \ d(v_m,v_1) & d(v_m,v_2) & \cdots & d(v_m,v_n) \end{pmatrix}$$

where

$$d(v_i,v_j) = \sum_{k=1}^m \sqrt{(x_{ik}^2 - x_{jk}^2)}$$

is the euclidean distance between the row vectors v_i and v_i .

In R, one computes the distance matrix using the function

```
dist(x)
```

The distance matrix contains all the necessary information to perform clustering.

```
In [23]: %%R
scores_dist = dist(scores)
```

Hierachical Clustering Analysis

The function

```
hclust(distance_matrix)
```

takes a distance matrix and returns an object of the class holust, which contains a hierachical groups of the population.

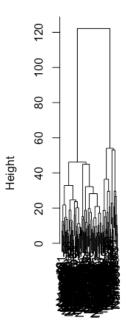
This hierachical groups are computed as follows by hclust:

- it starts by groupping indiduals (i.e. rows) two by two by smallest distance
- then it computes a distance between this pairs of two and group these pairs again two by two by smallest distance
- · this algorithm continues until there is no group is left for groupping

The hierarchy that results can be further plotted as a dendrogram using the plot funciton.

```
%%R -r 96 -w 200 -h 600
In [24]:
         hclusters = hclust(scores_dist)
         plot(hclusters, main='Dendrogram of the class scores')
```

ndrogram of the class



```
scores_dist
hclust (*, "complete")
```

We see from the dendrogram that we can obtain a different number of cluster by cutting the dendogram at a given height.

In our example,

- cutting at a distance between 60 and 120, then two cluster emerges that most probably correspond to the two majors.
- cutting at a distance of 40, will produce several additional clusters revealing more structure in the data.

Of course, if the distance between the two cluster is small it may indicate that the cluster structure is not very strong. In our example, only the two main clusters seems to be real.

To retrieve a given number of cluster, one uses the function

```
cutree(hcluster_object, number_of_clusters)
```

which returns a integer vector where each element is an integer telling which cluster the corresponding individual in our population belongs to. This labels of this vectors are the individual names.

```
clusters = cutree(hclusters, 2)
print(clusters)
  Name1
          Name2
                   Name3
                           Name4
                                    Name5
                                            Name 6
                                                     Name7
                                                              Name8
                                                                      Name 9
                                                                              Name 10
                               2.
                                        1
Name11
         Name12
                  Name13
                          Name14
                                   Name15
                                           Name16
                                                    Name17
                                                             Name18
                                                                     Name19
                                                                              Name20
              2
                               2
                                        2
                                                         2
                                                                  2
                                                 1
Name21
         Name22
                  Name23
                          Name24
                                   Name25
                                           Name26
                                                    Name27
                                                             Name28
                                                                     Name29
                                                                              Name30
              2
                       2
                                                 2
                                                                           2
      1
                               1
                                        2
                                                         1
                                                                  1
                                                                                   2
                                                                              Name40
Name31
         Name32
                  Name33
                          Name34
                                   Name35
                                            Name36
                                                    Name37
                                                             Name38
                                                                     Name39
                      2
                               2.
                                        2
                                                         2
      2
              1
                                                2
                                                                 1
                  Name43
                          Name44
                                                    Name47
Name41
         Name42
                                   Name45
                                                                     Name49
                               2
              2
                       2
                                        2
                                                 2
                                                         2
                                                                  2
                                                                           2
      1
 Name51
         Name52
                  Name53
                          Name54
                                   Name55
                                            Name56
                                                    Name57
                                                             Name58
                                                                     Name59
      1
              2
                       2
                               2
                                        2
                                                 2
                                                         2
                                                                  1
                                                                           2
Name61
         Name62
                                                    Name67
                                                                     Name69
                  Name63
                          Name64
                                   Name65
                                            Name66
                                                             Name68
      2
              1
                       2
                               1
                                        1
                                                 2
                                                         2
                                                                  1
                                                                           2
                                                                                   2
Name71
         Name72
                  Name73
                          Name74
                                   Name75
                                            Name76
                                                    Name77
                                                             Name78
                                                                     Name79
                                                                              Name80
      1
              1
                       2
                               2
                                        2
                                                 2
                                                         2
                                                                  1
                                                                           2
Name81
         Name82
                  Name83
                          Name84
                                   Name85
                                            Name86
                                                    Name87
                                                             Name88
                                                                     Name89
                                                                              Name 90
              2
                                                          2
                  Name 93
                                                    Name 97
Name 91
         Name 92
                          Name 94
                                   Name 95
                                           Name 96
                                                             Name 98
                                                                     Name 99 Name 100
              2
                       2
                                        1
                                                 2
                                                          2
                                                                           2
Name101 Name102 Name103 Name104 Name105 Name106 Name107 Name108 Name109 Name110
              2
                       2
                                1
                                        2
                                                 2
                                                          2
                                                                  2
```

We can now separate the rows or our initial data frame into two categories, corresponding to the returned clusters and check that they represent the two majors:

```
In [26]: %%R
    cluster1.names = names(clusters[clusters == 1])
    students1 = grades[cluster1.names,]
    print(students1)
```

Final Midterm Homework Ouiz Section 8.167408 42.28068 89.86770 27.85688 85.75620 26.71910 0.000000 39.39495 Name2 LITT 1.018811 42.47156 68.35079 24.79602 Name5 6.514070 48.27073 88.78673 30.72553 Name11 LITT Name16 36.858106 45.34581 77.06705 26.46216 LITT Name20 7.650583 42.83610 58.85665 24.38272 LITT Name21 34.135075 45.21806 87.68278 23.27935 LITT Name24 18.456039 39.82039 89.04705 36.80462 LITT 10.040498 40.85245 Name27 95.02425 36.48378 LITT 0.000000 36.72109 85.28308 28.81202 Name28 LITT 6.411672 44.46837 65.03373 28.43104 Name 32 T.TTT Name38 31.799930 49.85669 76.14792 38.71780 LITT 4.950563 30.65106 75.76314 30.35330 Name41 LITT Name51 0.000000 35.67982 68.99259 27.74343 LITT Name58 21.393468 43.39615 72.68805 36.41388 LITT 7.888644 37.72932 87.15932 35.16833 Name62 LITT Name64 21.634841 47.56106 70.26098 39.00863 Name65 25.473728 40.41483 85.59218 38.85771 LITT 0.000000 33.52930 Name 68 87.13033 23.74760 T.TTT Name71 36.444332 41.61503 64.06714 19.82498 LITT Name72 22.496625 38.23300 88.47793 40.10673 LITT Name78 20.099845 42.41015 98.29730 23.59381 LITT 0.000000 38.08184 50.60226 38.46387 Name81 LITT Name84 0.000000 44.07351 69.15280 30.70273 LITT 0.000000 46.53951 80.71281 28.06864 Name94 T.TTT Name95 0.000000 37.58013 100.00000 35.61793 Name98 0.000000 34.87726 74.72632 25.78762 LITT Name101 17.169801 34.76351 65.66622 23.32371 Name104 0.000000 40.49539 82.10907 33.37872 LITT Name110 21.257056 47.48521 69.34250 28.89553 LITT

```
In [26]:

In [26]:

In [26]:

In [26]:

In [26]:
```