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ggESDA: An R Package for Exploratory Symbolic Data Analysis using ggplot2

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Abstract

This paper presents the ggESDA package, which we developed for exploratory symbolic data analysis in R. Based on ggplot2 Wickham (2009), the ggESDA package which is familiar programming structure with its parent provides a wide variety of graphical techniques such as histogram, 3D-scatterplot and radar plot. In addition, a general and customized transformation function classic2sym() is implemented for generating a symbolic data table from classical data frame by clustering algorithm, RSDA Rojas (2015) function and user-defined method, wait for edit......

Keywords: data visualization, symbolic data analysis, exploratory data analysis, **ggplot2** extensions, interval-valued data, R.

1. Introduction

"In Data Science the aim is to extract new knowledge from Standard, Big, and complex data. Often these data are unstructured with variables defined on different kinds of units. They can also be multi-sources (as mixtures of numerical and textual data, with images and networks)." Diday and Edwin (2018). The statement indicates that not only conventional data but the unstructured data, also known as symbolic data, is vital for data science. Rather than the classical data represented by a single value, symbolic data with measurements on p random variables can be p-dimensional statistical units such as hypercubes or histograms. The field of symbolic data analysis (SDA) Billard and Diday (2007) is to broaden the application aspects of statistical methodologies, extend traditional cognition of a form of data unit and build a brand-new analysis system of data science. Recent developments in the field of big data analytics have led to a renewed interest in complex structure data such as symbolic data. As shown in Figure 1, the number of researches in SDA represents an increasing trend from 1998 to 2020, which outstands the importance of it during the years.

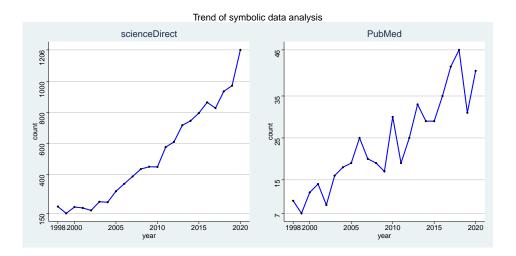


Figure 1: The number of "symbolic data analysis" or "interval-valued data" related articles in researches and applications according to PubMed and ScienceDirect online database over time from 1998 to 2020.

Among ScienceDirect, Engineering and Computer Science lead the subject areas obviously, shown in Figure 2.

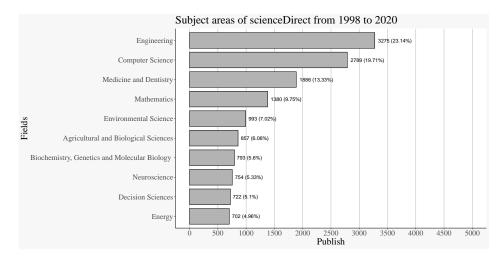


Figure 2: Top 10 researches and applications domains for SDA or interval-valued data (ScienceDirect) from 1998 to 2020

In practice, the symbolic data is often generated by aggregating massive datasets into intervals in order to make the management easy and appropriate. An interval-valued symbolic random variable X, taking values in interval, can be denoted such as $X = [a, b] \subset R^1$, where $a \leq b$, and $a, b \in R^1$. Let the random variable X, for instance, be the weight, then X = [50, 100] represents the interval covering the weight of people. With the advent of big data analytic, interval-valued data is becoming more common and accessible than ever. The researches for interval-valued data such as the sign test for COVID-19 data Sherwani, Shakeel, Saleem, Awan, Aslam, and Farooq (2021), the prediction via regularized artificial neural network Yang, Lin, and Zhang (2019), a bivariate Bayesian method for regression models Xu and Qin

(2021), etc.

Exploratory Data Analysis (EDA) Tukey (1977) is primarily used to see what data can reveal beyond the formal modeling or hypothesis testing task, provides an overview of raw datasets and obtains a general understanding about the variables and their relationships.

2. Basic usage of ggESDA

ggESDA is now available from the Github at https://github.com/kiangkiang/ggESDA. All reference manual documented by exported functions and introduction vignettes can also be download here. In the following section, we are going to illustrate the functionalities and syntaxes about ggESDA.

3. why SDA plot (weakness of classical plot)

3.1. sol overstike

For the conventional exploratory data analysis, it is always a severe challenge to deal with enormous datasets because conventional displays suffered from overstrikes of data points representing the value (scatterplot type displays) or overstrikes of line segments connecting values of neighboring variables. As a consequence, exploratory symbolic data analysis (SDA) becomes a preliminary yet essential tool for summarizing the main characteristics of a data set before appropriate statistical modeling can be applied. Besides escaping the problem mentioned above, SDA can effectively reduce observations in data, which will make the study focus on what we interesting instead of unnecessary information such as Figure 3.

In Figure 3, we can clearly visualize the scatter plot in the right hands, which is represented by symbolic data and aggregated by K-means MacQueen *et al.* (1967).

3.2. full information

In the past, we would like to use barplot to visualize the frequency of categorical data, but that was merely represented the distribution of full data in that category. It cannot lead researchers to explore more details in what they are interesting such as a particular part of data, so aggregation methods play a vital role to merge the data we interesting.

However, the conventional categorical data after merging will usually be represented by mode, which will be unmeaningful to visualize and cause the loss of information that may become larger when the data or the number of factors in that category is growing on. SDA will build a histogram by calculating each factor of the category of frequency as bins to solve this kind of problem as a result. In that way, a categorical variable will never be shown as a single value at all, instead, a complete information histogram will be substituted.

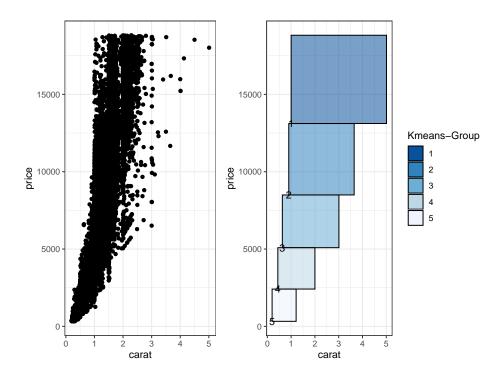


Figure 3: Compare classical data and symbolic data

4. classical data to symbolic data

4.1. datasets

We will apply the breast mass dataset, which is computed from a digitized image of a fine needle aspirate (FNA), to demonstrate how does a classical dataset transforms into a symbolic dataset. The breast mass dataset describe characteristics of the cell nuclei present in the image. It can be downloaded from the kaggle at https://www.kaggle.com/uciml/breast-cancer-wisconsin-data?select=data.csv. There are 569 observations and 32 variables in the dataset. We are going to store this dataset in breastData as data frame type in R, and the variables will be shown as follows:

> colnames(breastData)

[1]	"id"	"diagnosis"
[3]	"radius_mean"	"texture_mean"
[5]	"perimeter_mean"	"area_mean"
[7]	"smoothness_mean"	"compactness_mean"
[9]	"concavity_mean"	"concave points_mean"
[11]	"symmetry_mean"	"fractal_dimension_mean"
[13]	"radius_se"	"texture_se"
[15]	"perimeter_se"	"area_se"
[17]	"smoothness_se"	"compactness_se"
[19]	"concavity_se"	"concave points_se"

Except for the first two variables, they are all composed of mean, standard error, and "worst" in their own field respectively.

4.2. K-means

K-means clustering is a method of vector quantization, originally from signal processing, that aims to partition n observations into k clusters in which each observation belongs to the cluster with the nearest mean. In **ggESDA**, the algorithm will be based on the **stats** package, and the number of k is a parameter that user can define themself:

The id is unused in this case, so we remove it by dplyr. Then using classic2sym() to aggregate breastData. It will return several result sets include clustering result and interval-valued data, etc. The interval-valued data can be extracted by \$intervalData, and it will be presented by the package of RSDA type.

The groupby is a parameter that determine what kind of aggregation methods will be used. Whenever the K-means method is applied, the consequent k will become meaningful, whereas the other situation is not. It is also a default method when users have no input arguments in groupby.

4.3. Hierarchical

The second well-known clustering algorithm is called Hierarchical clustering Cecil C. Bridges (1966), also called hierarchical cluster analysis or HCA. It can be performed with a distance matrix calculated by raw data and used to present the distance of each cluster. In basic R package, it is also realized by **stats**, which the **ggESDA** is based on for implementing HCA:

```
\verb| > breastData.sym <- classic2sym(breastData, groupby = "hclust")|\\
```

> breastData.sym.i <- breastData.sym\$intervalData</pre>

Remark that the k parameter is not meaningful in the case without K-means clustering. In classic2sym(), the keywords of HCA is called hclust.

4.4. particular variable

Using a particular variable to merge different data is a common way for data analysis, too. **ggESDA** provides such as this concept in **classic2sym()** to analyze different factors of category variables, and merge the same factor into the symbolic data type:

In breastData, the only category variable is diagnosis, which means the diagnosis of breast tissues (M = malignant, B = benign). We put it as an input argument in groupby for merging different diagnosis results, and the interval-valued data of result sets will display its factor levels in row names.

4.5. user defined

In general, users may not always use the aggregation methods we provide, thus, besides generating a particular variable for the group, **ggESDA** facilitates the process through the min data and max data that user-defined.

For the demonstration, we will build both min data and max data using runif. Generate a uniform random variable to make sure that all min data are smaller than max data:

Then choose the customize argument in groupby, input which data are minData or maxData, and the transformation will be simply completed.

In order to simplify the process and make the preprocessing friendly, we develop these methods and let the people who want to analyze symbolic data easier. Overall, the conversion and essential concepts can be summarized in table 1.

Table 1. Sammary 101 014051015,()								
classic2sym()								
groupby Args.	Transformation	Data Type	Moment	Cluster Result	Require Other Args.			
kmeans	K-means	Numeric/Category	Smaller data	V	TRUE			
hclust	Hierarchical	Numeric/Category	Smaller data	V	FALSE			
variable name	Variables aggregation	Numeric/Category	Own the pre-clustering group	-	FALSE			
customize	User-defined	Numeric	Connect with other packages	-	TRUE			

Table 1: Summary for classic2sym()

5. Generalization and Extension

As far as generalization and extension are concerned, the package provides a simple way for making connections with other useful packages, so that the result of common statistical or machine learning methods on other packages may be visualized as well using ggESDA if it is interval-valued. The following will discuss these explicitly.

5.1. General principle

Generally, it is not merely the well-known packages in R that can make a plot using it. As long as keeping some principle, it will be easily performed:

- 1. Understand the data structure clearly if it is an object from other packages.
- 2. Extract the min data and max data from it or make some necessary transformation.
- 3. Classify the data you extract belong.
- 4. Reorganized it and use classic2sym() for the final transformation.
- 5. Visualize the front result using ggESDA.

Because of the interval-valued data, all SDA packages studying in the same field will store and deal with the min and max data. Hence, the transformation method in section 4.5 plays a important role. With the connection being built, it can be compatible with all other tools in R.

5.2. Example for generalization

For the demonstration, we consider two famous R packages for SDA, **HistDAWass** Irpino and Verde (2015) and **MAINT.Data** Duarte Silva and Brito (2011). Both of these make lots of contributions to the statistics of SDA, so we tend to make some analysis using these and plot the result with **ggESDA**.

HistDAWass

We use the principle in section 5.1 to process BLOOD data in **HistDAWass**, first. With the method **HistDAWass** provided, it will be more convenient to get min and max data:

```
> library(HistDAWass)
> # Get min and max data
> blood.min <- get.MatH.stats(BLOOD, stat = "min")</pre>
> blood.max <- get.MatH.stats(BLOOD, stat = "max")</pre>
> blood <- data.frame(blood.min, blood.max)</pre>
> # Reorganized and Build ggESDA obj.
> blood.sym <- classic2sym(blood, groupby = "customize",
                       minData = blood[, 2:4],
                       maxData = blood[, 6:8])
> # Make names
> blood.names <- get.MatH.main.info(BLOOD)$varnames
> blood.i <- blood.sym$intervalData
> colnames(blood.i) <- blood.names
> head(as.data.frame(blood.i), 5)
        Cholesterol
                         Hemoglobin
                                          Hematocrit
  [80.00 : 240.00] [12.00 : 15.00] [35.00 : 47.00]
2 [80.00 : 240.00] [10.50 : 14.00] [31.00 : 44.00]
3 [95.00 : 245.00] [10.50 : 14.00] [31.00 : 43.50]
4 [105.00 : 260.00] [10.50 : 14.00] [31.00 : 42.50]
5 [115.00 : 260.00] [10.80 : 13.60] [31.00 : 42.50]
```

After getting the necessary data, classifying data belonging is vital for reorganization, which means that differentiating the min data and max data. For instance, minData = blood[, 2:4] represents the min data are the columns of 2, 3, 4 in this case.

MAINT.Data

However, it is also a common way to store interval-valued data by median and range. In **MAINT.Data**, the data will exist in this form. Fortunately, a median-range form is not difficult to deal with. We can do the necessary conversion directly to get the data we expect:

```
# maxData = Aba[, 8:14])
> # Make names
> colnames(Aba.sym$intervalData) <- AbaloneIdt@VarNames
> Aba.i <- Aba.sym$intervalData %>%
+ cbind(Aba.obs = AbaloneIdt@ObsNames) %>%
+ column_to_rownames(var = "Aba.obs")
> head(Aba.i[, 1:4], 5)
```

		Length	Diameter	Height	Whole_weight
F-10-12	[0.34	: 0.78]	[0.26 : 0.63]	[0.06:0.23]	[0.21 : 2.66]
F-13-15	[0.39	: 0.82]	[0.30:0.65]	[0.10:0.25]	[0.27 : 2.51]
F-16-18	[0.40	: 0.74]	[0.32 : 0.60]	[0.10:0.24]	[0.35 : 2.20]
F-19-21	[0.49	: 0.72]	[0.36:0.58]	[0.12:0.21]	[0.68 : 2.12]
F-23-24	[0.45	: 0.80]	[0.38:0.63]	[0.14 : 0.22]	[0.64 : 2.53]

In brief, following the general principle in section 5.1 may facilitate the integration, extend utilize of **ggESDA** and generalize to all SDA studies.

6. Prominent SDA Packages

The most prominent packages on CRAN are commonly used for statistical or machine learning analyze. It can be briefly classified into two parts, one is focused on statistic analysis, and the other is general SDA packages including both analysis method and some graphical technology. Nevertheless, most of their graphical technology tends to use the basic graphics in R rather than **ggplot2**, or only visualizes univariate distribution which is difficult to present the relationship between variables.

On the contrary, **ggESDA** uses a high-level graphic system by **ggplot2** to solve the problem mentioned above and provides a variety of EDA methods in all kinds of the variate, which can be summarized as the table 2. The number in table 2 shows how many methods are provided in its field.

Available Summarize Statistic Machine learning Function UnivariateBivariate Multivariate Stat. Method Unsupervised Packag Version RSDA Rojas et al. (2015) R(4.1.0)classic.to.sym() 3 2 1 2 symbolicDA Dudek et al. (2013) R(4.1.0)2 1 1 HistDAWass Irpino (2015) R(4.1.0)4 3 1 data2hist() 1 MAINT.Data Silva & Brito (2011) R(4.1.0)7 Neto et al. (2011) 1 iRegression R(4.1.0)intReg Toomet (2012) R(3.6.0)1 ISDA.R Filho & Fagundes (2012) R(2.15.2)

GPCSIV

ggESDA

GraphPCA

Brahim (2013)

Jiang (2021)

Brahim & Kallyth (2014)

R(3.0.2)

R(4.1.0)

R(4.1.0)

Table 2: Compare with R packages

In python, we can also find the SDA package such as **iardacil** Umbleja, Ichino, and Yaguchi (2020) which is available from the Github at https://github.com/iardacil/SDA. The

classic2sym()

1

2

zoomstart software in **iardacil** is provided with SODAS software project Diday and Noirhomme-Fraiture (2008). It is a basic thinking for general radar plot, improved for distinct groups visualization by **ggESDA**, and implemented in R using **ggplot2**.

7. General design

The ggESDA object is composed of the interval-valued data, statistics data frame, clustering results, and other components from R6 class. Based on it, the developed graphical technology can extend three aspects by its variables, univariate, bivariate, and multivariate. The ggESDA aims to convert the traditional data into the ggESDA object and visualizes the symbolic data using ggplot2, which is shown in Figure 4.

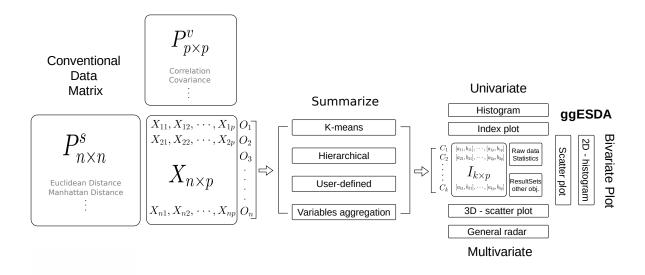


Figure 4: Package Structure and Diagram for the Transformation Flow

As illustrated in Figure 4, each row (observation) in the conventional data matrix $X_{p\times p}$ contains a vector of numeric values, $O_i=(x_1,x_2,\cdots,x_n)$, while each row of the interval-valued data matrix $I_{k\times p}$ contains a vector of intervals(ranges), $C_j=([a_{j1},b_{j1}],[a_{j2},b_{j2}],\cdots,[a_{jp},b_{jp}])$, called a CONCEPT (or UNIT). The CONCEPT describe the behavior of a group of observations. Thus, the aggregation method between them is an essential process in SDA.

8. Basic numerical summaries

The main content of EDA relates to the basic numerical summaries of data (e.g., the central tendency measures, and variation or variability measures) and the basic graphical summaries of data. For example, the five-number summary of numerical data (minimum, 25% quartiles, median, 70% quartiles, and maximum) is used to construct a boxplot. In the field of SDA, there are many algorithms to calculate descriptive statistics and frequency for interval-valued data, and we will illustrate the univariate and bivariate summaries respectively.

8.1. Univariate summaries

To build a statistic chart or analysis, descriptive statistics are necessary to be constructed, as well as the frequency occurring in each bin in a histogram chart. For a histogram chart, subdivisions of it into equidistant and non-equidistant will also be consider in this section.

Descriptive statistics

For the quantile in interval-valued data, summarizing it may seem to be obvious to separate data into a minimum and maximum data table, then calculate quantiles of both data tables to build a new interval-valued quantile data table.

In statistics, it may be more interesting to discuss mean and variance in a particular random variable Z; see Bertrand and Goupil (2000). The realization of Z for the observation W_u is the interval $Z(W_u) = [a_u, b_u]$, where $u = 1, 2, \dots, m$ and m is the number of concepts.

First of all, assume that each object is equally likely to be observed with probability $\frac{1}{m}$, and the empirical density function of Z is defined as:

$$f(\xi) = \frac{1}{m} \sum_{u:\xi \in Z(W_u)} (\frac{1}{b_u - a_u})$$
 (1)

where ξ is the individual descriptions.

The Equation (1) is also equivalently to:

$$f(\xi) = \frac{1}{m} \sum_{u \in E} \frac{I_u(\xi)}{\|Z(u)\|}, \xi \in \mathbb{R}$$

$$\tag{2}$$

where $I_u(.)$ is the indicator function that ξ is or is not in the interval Z(u), ||Z(u)|| is the length of that interval, and $E = \{w_1, w_2, \dots, w_m\}$.

Further, the symbolic sample mean from definition for Z is $\bar{Z} = \int_{-\infty}^{\infty} \xi f(\xi) d\xi$, which can be reduced as:

$$\bar{Z} = \frac{1}{m} \sum_{u \in E} \frac{a_u + b_u}{2} \tag{3}$$

Finally, after getting the sample mean, the symbolic sample variance can be defined as follow:

$$S^{2} = \int_{-\infty}^{\infty} (\xi - \bar{z})^{2} f(\xi) d\xi$$

$$= \int_{-\infty}^{\infty} \xi^{2} f(\xi) d\xi - \bar{z}$$
(4)

and substituting for $f(\xi)$ from Equation (2), we have

$$\int_{-\infty}^{\infty} \xi^{2} f(\xi) d\xi = \frac{1}{m} \sum_{u \in E} \int_{-\infty}^{\infty} \xi^{2} \frac{I_{u}(\xi)}{\|Z(u)\|} d\xi$$

$$= \frac{1}{m} \sum_{u \in E} \int_{a_{u}}^{b_{u}} \frac{\xi^{2}}{(b_{u} - a_{u})} d\xi$$

$$= \frac{1}{3m} \sum_{u \in E} (\frac{b_{u}^{3} - a_{u}^{3}}{b_{u} - a_{u}})$$
(5)

Hence,

$$S^{2} = \frac{1}{3m} \sum_{u \in E} (a_{u}^{2} + a_{u}b_{u} + b_{u}^{2}) - \frac{1}{4m^{2}} \left[\sum_{u \in E} (a_{u} + b_{u}) \right]^{2}$$
 (6)

Histogram Frequency

For the univariate histogram frequency, assume that we partition the interval $I = [\min_{u \in E} a_u, \max_{u \in E} b_u]$ into r subintervals, and all of them in the histogram are equal distance. That is, $I_g = [\zeta_{g-1}, \zeta_g), g = 1, 2, \dots, r$, then $||I_j|| = ||I_k||, j, k = 1, 2, \dots, r$. As a consequence, the observed frequency of the interval-valued variate Z for the histogram subinterval I_g from the definitions is

$$f_g = \sum_{u \in E} \frac{\|Z(u) \cap I_g\|}{\|Z(u)\|} \tag{7}$$

Moreover, for the interval-valued variate Z, we can pool the a_u and b_u from the interval of all observations, and sort it as a new vector $(x^{(1)}, x^{(2)}, x^{(2m)})$ to represent the cut of a histogram. The subinterval from the cut is then defined as $I'_g = [x^{(j)}, x^{(j+1)})$, where $j = 1, 2, \dots, 2m-1$, and apply the Equation (7) to get frequency. In most cases, $||I'_g||$ will not be equal to another, so we can get another histogram type, called non-equidistant-bin histogram.

8.2. Bivariate summaries

Many of the principles developed for the univariate case can be expanded to a general p-variate case, p > 1. We shall focus attention on obtaining joint histograms for p = 2. The following will reveal the statistics and bivariate histogram.

Descriptive statistics

For bivariates interval-valued variables, Z_1 and Z_2 , the observations u, where $u \in E$, on the rectangle $Z(u) = Z_1(u) \times Z_2(u)$ is $([a_{1u}, b_{1u}], [a_{2u}, b_{2u}])$. Assume the individual description vectors ξ are each uniformly distributed over the respective intervals $Z_1(u)$ and $Z_2(u)$. Define the empirical joint density function for (Z_1, Z_2) :

$$f(\xi_1, \xi_2) = \frac{1}{m} \sum_{u \in E} \frac{I_u(\xi_1, \xi_2)}{\|Z(u)\|}$$
(8)

where $I_u(\xi_1, \xi_2)$ is the indicator function that (ξ_1, ξ_2) is or is not in the rectangle Z_u and where ||Z(u)|| is the area of this rectangle.

There is three methods to calculate bivariate interval-valued variables covariance function. For the first one, it can be derived by Billard and Diday (2003) as following:

$$cov(Z_1, Z_2) = \frac{1}{4m} \sum_{u \in E} (b_{1u} + a_{1u})(b_{2u} + a_{2u}) - \frac{1}{4m^2} \left[\sum_{u \in E} (b_{1u} + a_{1u}) \right] \left[\sum_{u \in E} (b_{2u} + a_{2u}) \right]$$
(9)

Second, an alternative expression of the symbolic sample variance for Z in Equation (6) can be expressed as

$$S^{2} = \frac{1}{3m} \sum_{u \in E} \left[(a_{u} - \bar{Z})^{2} + (a_{u} - \bar{Z})(b_{u} - \bar{Z}) + (b_{u} - \bar{Z})^{2} \right]$$

The above equation can be generalized by Billard and Diday (2007) to formulate the form of the symbolic sample covariance for Z_j and $Z_{j'}$ as

$$cov(Z_j, Z_{j'}) = \frac{1}{3m} \sum_{i=1}^{m} G_j G_{j'} \left[Q_j Q_{j'} \right]^{1/2}, \quad j, j' = 1, 2, \cdots, p$$
(10)

where for J = j, j',

$$Q_{J} = (a_{iJ} - \bar{Z}_{J})^{2} + (a_{iJ} - \bar{Z}_{J})(b_{iJ} - \bar{Z}_{J}) + (b_{iJ} - \bar{Z}_{J})^{2},$$

$$G_{J} = \begin{cases} -1, & \text{if } \xi_{iJ}^{c} \leq \bar{Z}_{J} \\ 1, & \text{if } \xi_{iJ}^{c} > \bar{Z}_{J} \end{cases}$$

and ξ_{iJ}^c is the midpoint of the interval $[a_{iJ}, b_{iJ}]$.

Last, it was further demonstrated by Billard (2007) and Billard (2008) that the sample variance in Equation (6) is a function of the total sum of squares (SST) and that the SST can be decomposed into the sum of the internal (within) variation and the between variation. The total sum of products (SPT) is the sum of the within sum of products and the between sum of products. The Equation (6) was also extended to the bivariate case to obtain the sample covariance of Z_j and $Z_{j'}$ based on the decomposition of the SPT as

$$cov(Z_{j}, Z_{j'}) = \frac{1}{6m} \sum_{i=1}^{m} \left[2(a_{ij} - \bar{Z}_{j})(a_{ij'} - \bar{Z}_{j'}) + (a_{ij} - \bar{Z}_{j})(b_{ij'} - \bar{Z}_{j'}) + (b_{ij} - \bar{Z}_{j})(a_{ij'} - \bar{Z}_{j'}) + 2(b_{ij} - \bar{Z}_{j})(b_{ij'} - \bar{Z}_{j'}) \right]$$

$$(11)$$

The definitions and calculations of the symbolic sample covariance in Equations (9)???(11) are consistent with the results in the classic data case if $a_{ij} = b_{ij}$ for $i = 1, 2, \dots, m, j = 1, 2, \dots, p$. If j = j', the Equation (11) reduces to the sample variance of the interval-valued variable as given in Equation (6).

2D-Histogram

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