DI2: prior-free and multi-item discretization of biomedical data and its applications

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Abstract

**Motivation:** A considerable number of data mining approaches for biomedical data analysis, including state-of-the-art associative models, require a form of data discretization. Although diverse discretization approaches have been proposed, they generally work under a strict set of statistical assumptions which are arguably insufficient to handle the diversity and heterogeneity of clinical and molecular variables within a given dataset. In addition, although an increasing number of symbolic approaches in bioinformatics are able to assign multiple items to values occurring near discretization boundaries for superior robustness, there are no reference principles on how to perform multi-item discretizations.

**Results:** In this study, an unsupervised discretization method, DI2, for variables with arbitrarily skewed distributions is proposed. DI2 provides robust guarantees of generalization by placing data corrections using the Kolmogorov-Smirnov test before statistically fitting distribution candidates. DI2 further supports multi-item assignments. Results gathered from biomedical data show its relevance to improve classic discretization choices.

**Software:** available at https://github.com/JupitersMight/DI2

**Keywords:** multi-item discretization; prior-free discretization; heterogeneous biomedical data

1 Introduction

Approaches to discretization of continuous variables have long been discussed alongside their pros and cons. Altman et al. [1] and Bennette et al. [2] both discuss the relevance and impact of categorizing continuous variables and reducing the cardinality of categorical variables. Liao et al. [3] compares various categorization techniques in the context of classification tasks in medical domains, without using domain knowledge of field experts. The relevance of discretization meets both descriptive and predictive ends, encompassing state-of-the-art approaches such as pattern-based biclustering [4] and associative models such as XGBoost [5].

In this work we present DI2, a Python library that extends non-parametric tests to find the best fitting distribution for a given variable and discretize it accordingly. DI2 offers three major contributions: i) corrections to the empirical distribution before statistical fitting to guarantee a more robust approximation of candidate distributions; ii) efficient statistical fitting of 100 state-of-the-art theoretical distributions; and, finally, iii) assignment of multiple items according to the proximity of values to the boundaries of discretization, a possibility supported by numerous
symbolic approaches [6, 4, 7]. The assignment of multiple items [8, 9], generally referred as multi-item discretization, conferes the possibility to avail the wealth of data structures and algorithms from the text processing and bioinformatics communities without the risks of the well-studied item-boundaries problem.

2 Background

Discretization methods have wide taxonomy[10] with a determinant division in: 1) supervised, where the method uses the class variable to bin the data, and, 2) unsupervised, where the method is independent of the class variable. DI2 places itself on the latter, it works independently on the class variable. Other characteristics of DI2 are: 1) static, where discretization of the variables takes place prior to an algorithm; 2) global, uses information about the variable as a whole to make the partitions and can still be applied with a scarce number of observations; 3) direct and splitting, splits the whole the range of values into $k$ intervals simultaneously; and 4) multivariate and univariate, DI2 can use either the whole dataset to create the intervals and discretize each variable or use each variable individually to create the respective intervals.

Some examples of unsupervised discretization methods are PD (Proportional Discretization), FFD (Fixed Frequency Discretization)[11], equal-width/frequency, k-means [12]. In this work, DI2 is compared with such classic discretization methods. These are illustrated in Figures I, II, and III.

![Figure I](image1.png)

**Figure I** Illustration of equal-frequency method with 9 points along an axis and 3 categories. This method is based on the frequency of the items, where each category has the same number of items, in order to set the intervals.

![Figure II](image2.png)

**Figure II** Illustration of equal-width method with 9 points along an axis and 3 categories. This method is based on the range taken by the items, where each category has the same width interval.

![Figure III](image3.png)

**Figure III** Illustration of K-means method with 9 points along an axis and 3 categories. This method is based in the k-means clustering, where each category is defined by a centroid.
2.1 DI2: normalization and feature scaling
While not mandatory, DI2 supports the following techniques: 1) min-max scaling,

\[ X' = \frac{X - X_{\text{min}}}{X_{\text{max}} - X_{\text{min}}} , \]  

where \( X \) is an ordered set of observed values; 2) z-score normalization, usually applied to samples normally distributed [13],

\[ X' = \frac{X - \mu}{\sigma} , \]  

where \( X \) is an ordered set of observed values; and 3) mean normalization,

\[ X' = \frac{X - \mu}{X_{\text{max}} - X_{\text{min}}} . \]  

2.2 DI2: statistical hypotheses
In order to discretize the data into intervals, DI2 provides two statistical hypothesis tests to be applied: 1) \( \chi^2 \) test [14], and 2) Kolmogorov-Smirnov goodness-of-fit test [15].

In the aforementioned tests the observed distribution is matched with a theoretical continuous distribution[1] provided by the SciPy open-source library [16] where the parameters are estimated through maximum likelihood estimation. The binning of the distributions for the \( \chi^2 \) test is based on the number of categories the user inputs and are built using the cumulative distribution function. The user can either choose the \( \chi^2 \) or the Kolmogorov-Smirnov goodness-of-fit as the primary fitting test. The theoretical continuous distribution with the lowest test statistic is picked as the best fit for the observed distribution.

2.3 DI2: outlier correction
The Kolmogorov-Smirnov goodness-of-fit test can optionally be used to remove up to 5% outlier points, from the observed distribution, according to the theoretical continuous distribution under assessment. Kolmogorov-Smirnov goodness-of-fit test returns a statistic (D statistic) that represents the maximum distance between the observed and the theoretical continuous distribution we are testing.

\[ D = \max \{ \max_{1 \leq j \leq n} \left\{ \frac{j}{n} - F(X_j) \right\}, \ \max_{1 \leq j \leq n} \left\{ F(X_j) - \frac{(j-1)}{n} \right\} \}, \]  

where \( n \) is the number of samples, \( j \) is the index of a given sample, and \( F \) is the frequency of sample \( X_j \). Using this statistic we can pin point where the farthest point between the distributions is and remove it. After up to 5% of the samples have been removed, the iteration with the best Kolmogorov-Smirnov statistic is picked (from 0 outliers removed to up to 5%). The data produced by outlier removal is then used to run the main statistical hypothesis test picked (\( \chi^2 \) or Kolmogorov-Smirnov). This correction guarantees the absence of penalizations caused by abrupt yet spurious deviations driven by the selected histogram granularity and help consolidate the choice of the theoretical continuous distribution.

[1]https://docs.scipy.org/doc/scipy/reference/stats.html
2.4 DI2: multi-item discretization
After selecting the theoretical continuous distribution that best fits the continuous variable, DI2 proceeds with the discretization. Given a desirable number of categories (bins), multiple cut-off points are generated using the inverse cumulative distribution function of the theoretical continuous distribution. The cut-off points guarantee an approximately uniform distribution of observation per category, although empirical-theoretical distribution differences can underlie imbalances.

DI2 supports multi-item assignments by identifying border values for each category, this is exemplified in Figure IV. To this end, the user can optionally also define a percentage (between 0 and 50% with 20% default) to affect the width of the borders. These borders take an intermediate value which symbolize that it belongs to both upper and lower category. Width extremes, 0% (50%) correspond to none (one) additional category assigned to every observation.

![Figure IV](Illustration example of discretization with 9 points along an axis and 3 categories considering border values (values which belong to 2 categories).)

3 Implementation
DI2 tool is fully implemented in Python and is provided as an open-source method at GitHub with well-annotated APIs and notebook tutorials for a practical illustration of its major functionalities. The algorithm workflow is shown in Algorithm 1 and the Kolmogorov-Smirnov correction is shown in Algorithm 2.

4 Results and Discussion
To illustrate some of the DI2 properties, we considered two published datasets: 1) the breast-tissue dataset [17], containing electrical impedance measurements in samples of freshly excised tissue from the breast, and 2) the yeast dataset [18], containing molecular statistics variables. Both of these are available at the UCI Machine Learning repository [19].

This section first discusses results on breast-tissue dataset, DI2 is executed with \( \chi^2 \) as the main statistical test, with and without Kolmogorov outlier removal, with single column discretization, and 5 categories per variable outputted. We will then present and discuss the fitting of the distribution with and without Kolmogorov outlier removal and the interval borders created compared with equal-frequency and equal-width.

We then consider yeast dataset, DI2 is executed with \( \chi^2 \) as the main statistical test, with and without Kolmogorov outlier removal, with single column and whole dataset discretization, and 5 categories per variable outputted. We will then present and discuss the distribution of the values by category with and without border values.
Algorithm 1: DI2 main algorithm

Input: dataset, number_of_bins
Optional input: statistical_test="chi2", multi_item_cutoff_margin=0.2, kolmogorov_opt=True, normalizer="min_max", distributions=[...], single_column_discretization=True
Output: The dataset discretized

```
if single_column_discretization then
    for column in dataset.columns do
        y_normalized = normalization(dataset[column], normalizer);
        main_operation(...);
    end
else
    for column in dataset.columns do
        y_normalized.append(normalization(dataset[column], normalizer));
    end
    main_operation(...);
end
```

Function main_operation(...):
```
best_dist, test_statistic, data_used;
for distribution in distributions do
    temp_statistic;
    if statistical_test == "chi2" then
        temp_data = kolmogorov_goodness_of_fit(y_normalized, distribution, kolmogorov_opt);
        temp_statistic = chi_squared_goodness_of_fit(temp_data, distribution, number_of_bins);
    else
        temp_statistic, temp_data = kolmogorov_goodness_of_fit(y_normalized, distribution, kolmogorov_opt);
    end
    if temp_statistic < test_statistic then
        test_statistic = temp_statistic;
        best_dist = distribution;
        data_used = temp_data;
    end
end
dataset[column] = discretize(best_dist, multi_item_cutoff_margin, data_used, dataset[column], number_of_bins, y_normalized);
```

and compare the different executions of DI2 with themselves and with K-means discretization category distribution.

Finally, still considering the yeast dataset, we will present the execution of multiple algorithms and the accuracy achieved with different DI2 discretization configurations and the other aforementioned discretization techniques.

4.1 breast-tissue dataset

The breast-tissue dataset contains 106 data instances and 9 continuous variables (I0, PA500, HFS, DA, AREA, A/DA, MAX IP, DR, P). The gathered results show the decisions placed by DI2 in the absence and presence of Kolmogorov-Smirnov optimization.

Table 1 shows the best fitting distribution for each continuous variable of the dataset. Variables "I0", "PA500", "A/DA", "DR", and "P" remained unchanged with a removal of up to 5% of outlier points. Variables "HFS" and "Area" produced better results in the $\chi^2$ test with the removal of outliers solidifying the distribution choice. Finally, the fitting choice changed for variables "DA" and "Max IP" under the $\chi^2$ test, revealing a more solid choice from the analysis of the residuals.
Algorithm 2: Kolmogorov outlier correction

**Input:** observed_distribution, theoretical_distribution, outlier_removal_flag  
**Output:** The statistic of Kolmogorov test and the corresponding data  
\[ N_5 = \text{size(data)} \times 0.05 \] if outlier_removal_flag else 1;  
results = [];  
\( i = 0; \)  
while \( i < N_5 \) do  
\( \text{Estimate Parameters( theoretical_distribution);} \)  
D_plus = D_minus = [];  
idx_max_d_plus = idx_max_d_minus = [];  
\( \text{calculate } \_d_{\text{minus}}(D_{\text{minus}}, \text{idx_max}_d_{\text{minus}}); \)  
\( \text{calculate } \_d_{\text{plus}}(D_{\text{plus}}, \text{idx_max}_d_{\text{plus}}); \)  
if len(results) == 0 then  
results = [\( \max(D_{\text{plus}}[\text{idx_max}_d_{\text{plus}}], D_{\text{minus}}[\text{idx_max}_d_{\text{minus}}]) \), data.copy()];  
else  
ks = \( \max(D_{\text{plus}}[\text{idx_max}_d_{\text{plus}}], D_{\text{minus}}[\text{idx_max}_d_{\text{minus}}]) \) if ks < results[0]  
then  
\( \text{results = [ks, data.copy()];} \)  
end  
end  
if D_plus[idx_max_d_plus] > D_minus[idx_max_d_minus] then  
delete data[idx_max_d_plus];  
else  
delete data[idx_max_d_minus];  
end  
++i;  
end  
return results;

| Variables | Without opt. | \( \chi^2 \) statistic | p-value < 0.05 | D statistic | With opt. | \( \chi^2 \) statistic | p-value < 0.05 | D statistic |
|-----------|-------------|------------------------|---------------|------------|-----------|------------------------|---------------|------------|
| I0 alpha  | 8.8         | True 0.12              |               |            | alpha     | 8.8         | True 0.11     |            |
| PA500 exponnorm  | 2.98       | True 0.07              |               |            | exponnorm | 2.98       | True 0.07     |            |
| HFS foldcauchy | 2.25       | True 0.07              |               |            | foldcauchy | 1.57       | True 0.07     |            |
| DA recipinvgauss | 1.6        | True 0.06              |               |            | chi2      | 1.01       | True 0.06     |            |
| Area frechet_r | 0.5        | True 0.07              |               |            | frechet_r | 0.25       | True 0.05     |            |
| A/DA mielek  | 1.17        | True 0.06              |               |            | mielek    | 1.17       | True 0.05     |            |
| Max IP johnsonsu | 4.72       | True 0.05              |               |            | alpha     | 1.09       | True 0.07     |            |
| DR johnsonsnb | 1.2         | True 0.05              |               |            | johnsonsnb | 1.2        | True 0.05     |            |
| P genextreme  | 5.13        | True 0.09              |               |            | genextreme | 5.13       | True 0.09     |            |

Considering variable "DA", Figures V.a and V.b show its Q-Q (quantile-quantile) plot, offering a view on the adequacy of the statistical fitting. In this context, we depict histograms for the observed data with 100 bins (blue dots) and the best theoretical distribution picked without and with Kolmogorov-Smirnov correction (red line). A moderate improvement from Figure V.a to V.b can be detected, with the observed quantiles (blue dots) being closer to the theoretical continuous quantiles (red line).

After the fitting stage, cut-off points are calculated to produce the final categories. Figure V.c compares different discretization options: equal-frequency, equal-width, and the two best fitting theoretical continuous distributions (without and with Kolmogorov-Smirnov optimization). Cut-off points are marked as red lines, and the border cut-off points in yellow. This analysis shows how critical discretization can be for determining the inclusion or exclusion of high density bins. The ability of DI2 to assign multiple items using borders can thus be explored by symbolic approaches to mitigate vulnerabilities inherent to the discretization process [20, 21].
4.2 yeast dataset

The yeast dataset contains 1484 data instances and 10 variables, including the sample identification, class, and 8 molecular statistics variables (mgc, gvh, alm, mit, erl, pox, vac, nuc). In the breast-tissue dataset we compared DI2 with two other unsupervised discretization, equal-frequency and equal-width. With this dataset we will compare DI2 with k-means.

Table 2 displays the results of the statistical tests produced by DI2 when applied to each variable independently and, the last row of the table, when applied to the
whole dataset together. Let’s use variable "mit" as an example for this dataset. Figure VI.a displays the distribution of values in the variable "mit" before outlier removal (brown and blue area of histogram) and after outlier removal (brown area of histogram).

Figures VI.b and VI.c compare the distribution of the categories of both discretization techniques (DI2 with outlier removal along different discretizations and k-means discretization), and also assess the impact of outlier removal had in categorizing in different executions of DI2 and k-means. Figure VII presents the border values under different DI2 discretization settings.

The performed analysis for the yeast dataset shows how critical the category border, previously discussed in more detail with the breast-tissue dataset, can be, determining the inclusion or exclusion of values. The ability of DI2 to assign multiple
VII.a. Categories between 0 and 2.

VII.b. Categories between 2 and 4.

Figure VII Variable “mit” categories distribution after DI2 discretization with different settings with border values. Single column discretization with Kolmogorov-Smirnov outlier removal (light blue columns), single column discretization without Kolmogorov-Smirnov outlier removal (dark blue columns), whole dataset discretization with Kolmogorov-Smirnov outlier removal (light purple columns), whole discretization without Kolmogorov-Smirnov outlier removal (dark purple columns).
Table 2: Best fitting distributions for each continuous variable, without and with Kolmogorov-Smirnov outlier removal.

| Variables | Without opt. | \(\chi^2\) statistic | p-value <0.05 | D statistic | With opt. | \(\chi^2\) statistic | p-value <0.05 | D statistic |
|-----------|-------------|------------------------|--------------|------------|-----------|------------------------|--------------|------------|
| mcg       | foldcauchy  | 3.72                   | True         | 0.08       | exponnorm | 3.18                   | True         | 0.02       |
| gvh       | genlogistic | 3.57                   | True         | 0.03       | genlogistic | 2.02                   | True         | 0.02       |
| alm       | genlogistic | 17.00                  | False        | 0.05       | genlogistic | 12.08                  | False        | 0.03       |
| mit       | exponnorm   | 19.23                  | False        | 0.05       | exponnorm | 6.11                   | True         | 0.03       |
| erl       | chi2        | 4.45                   | \(\times 10^{-14}\) | True       | chi2      | 4.23                   | \(\times 10^{-14}\) | True       |
| pox       | chi2        | 4.45                   | \(\times 10^{-14}\) | True       | gengamma | 4.23                   | \(\times 10^{-14}\) | True       |
| vac       | laplace     | 20.99                  | False        | 0.08       | pearson3  | 14.18                  | False        | 1.00       |
| nuc       | exponnorm   | 1116.63                | False        | 0.26       | mielke    | 795.28                 | False        | 0.26       |
| all variables | genhalflogistic | 45.69              | False        | 0.25       | genhalflogistic | 10.25              | False        | 0.21       |

items using borders can be explored by symbolic approaches to mitigate vulnerabilities inherent to the discretization process as discussed in the following subsection.

4.3 Predictive performance

To test the impact DI2 has when discretizing data we considered the yeast dataset, 5 categories per variable, and six supervised classification methods: Naive Bayes [22], Random Forest [23], SMO [24](Sequential Minimal Optimization), C4.5 [25], MLRM [26](Multinomial Logistic Regression Model), and FleBiC [27].

In Figure VIII the results for the aforementioned models are presented, with the exception of FleBiC which will be discussed later on. Each bar represents the average accuracy achieved with each discretization method, and the small bracket the standard deviation of the accuracy. In each model, DI2, with configurations of single column discretization and outlier removal, matched with the highest accuracy achieved by other discretization methods, and for the C4.5 model, DI2, with configurations of combined column discretization, achieved the highest accuracy compared with other discretization methods.

![Figure VIII](image_url)

In order to fully test out the potential of DI2, we now consider border values. From the aforementioned supervised classification methods only FleBiC is able to test this feature. FleBiC can be executed normally or with Random Forests (weight of decision 50% FleBiC, 50% Random Forests), which we will designate as FleBiC
Hybrid. In Figure IX the results of executing FleBiC and FleBiC Hybrid are presented. In terms of average accuracy, Figure IX.a., both FleBiC and FleBiC Hybrid predict with a higher average accuracy when using DI2 method than when using other discretization methods. Within the different settings of DI2, FleBiC Hybrid presents a higher accuracy when the predictive model considers border values. Finally in terms of sensitivity, Figure IX.b., we can see how considering border values affects the prediction of class NUC, making it possible to break through a ceiling on the prediction of class NUC when other discretization methods couldn’t.

5 Conclusion
This work proposed a new unsupervised method for data discretization, DI2, that takes into account data distribution, outliers within the data, and border values.
Results show that DI2 is a viable and coherent form of discretizing data. When compared with other well-known and frequently used unsupervised methods, DI2 brings out the same average accuracy in well-known and supervised classifiers. If we consider border values, which other unsupervised methods do not consider, and use a classifier that handles border values, FleBiC, then DI2 is able to improve the average accuracy previously achieved without border values.

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