Originally meant for preprocessing, this notebook is used to generate data sets that serve as experimental groups in order to study the effects of unsupervised discretization. As our chosen training data is all continuous, discretization is deployed to determine the effect on training data. It begins by exploring techniques for discretization (Part 1), and then establishes two approaches for optimizing the number of bins in a given discretized variable, the first being cumulative variance and the second cumulative entropy present in the variable. The cumulative values for the variable are based on that found in each of the bins for a variable. The relative value of these measures were used to establish the best number of bins for a given a binning technique for a given continuous variable (with further details in Part 2). Finally, specific ensembles of the different techniques were established to test the effectiveness combining binning approaches based on one of two different measures: overall change to correlation between variables and overall change to mutual information (with further detail in Part 3).

Part 1: Exploration of Discretization Techniques

Import Dependencies

In [6]:
```
from sklearn.preprocessing import KBinsDiscretizer
from sklearn.feature_selection import mutual_info_regression
from sklearn.metrics import mutual_info_score
from scipy.stats import entropy
import seaborn as sns
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from collections import defaultdict
import warnings
import pickle

warnings.filterwarnings('ignore')
np.random.seed(42)
```

Retrieves Data

In [127…
```
df = pd.read_csv('preprocessed_data.csv').iloc[:,1:10]
class_var = df['class']
df.head()
```

Out[127…

	alpha	delta	u	g	r	i	z	class	re
0	135.689107	32.494632	23.87882	22.27530	20.39501	19.16573	18.79371	GALAXY	0.6
1	144.826101	31.274185	24.77759	22.83188	22.58444	21.16812	21.61427	GALAXY	0.7
2	142.188790	35.582444	25.26307	22.66389	20.60976	19.34857	18.94827	GALAXY	0.6
3	338.741038	-0.402828	22.13682	23.77656	21.61162	20.50454	19.25010	GALAXY	0.9
4	345.282593	21.183866	19.43718	17.58028	16.49747	15.97711	15.54461	GALAXY	0.1

In [128…

```
df.dtypes
```

Out[128…

```
alpha       float64
delta       float64
u           float64
g           float64
r           float64
i           float64
z           float64
class        object
redshift    float64
dtype: object
```

Explores discretization techniques for the same variable "u" to explore the distibution changes due to the deployed technique. The techniques explored include equal bin width (the range of values included in the bin are the same), equal bin frequency (the width will vary to ensure that all of the bins have the same number of data objects), and kmeans (which uses distance measures to create k bins of data based on the central value of each bin, yields both varying width and frequency between bins in a given variable).

In [129…

```
u = pd.DataFrame(df.u)
u.head()
```

Out[129…

	u
0	23.87882
1	24.77759
2	25.26307
3	22.13682
4	19.43718

double checks that outliers removed in outlier_analysis.ipynb

In [133…

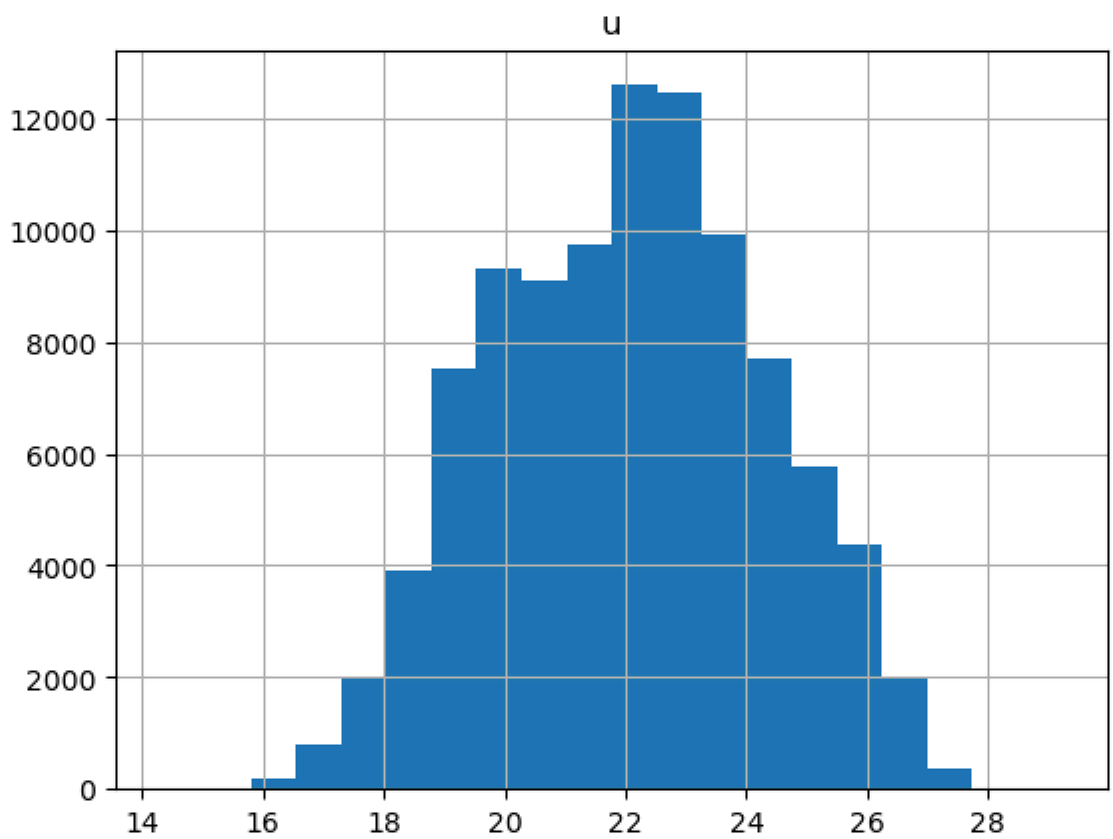
```
u.nsmallest(1,'u')
```

Out[133...

	u
54011	14.31105

Histogram prior to unsupervised discretization techniques.

In [134...
```
u.hist(bins = 20)
plt.show()
```

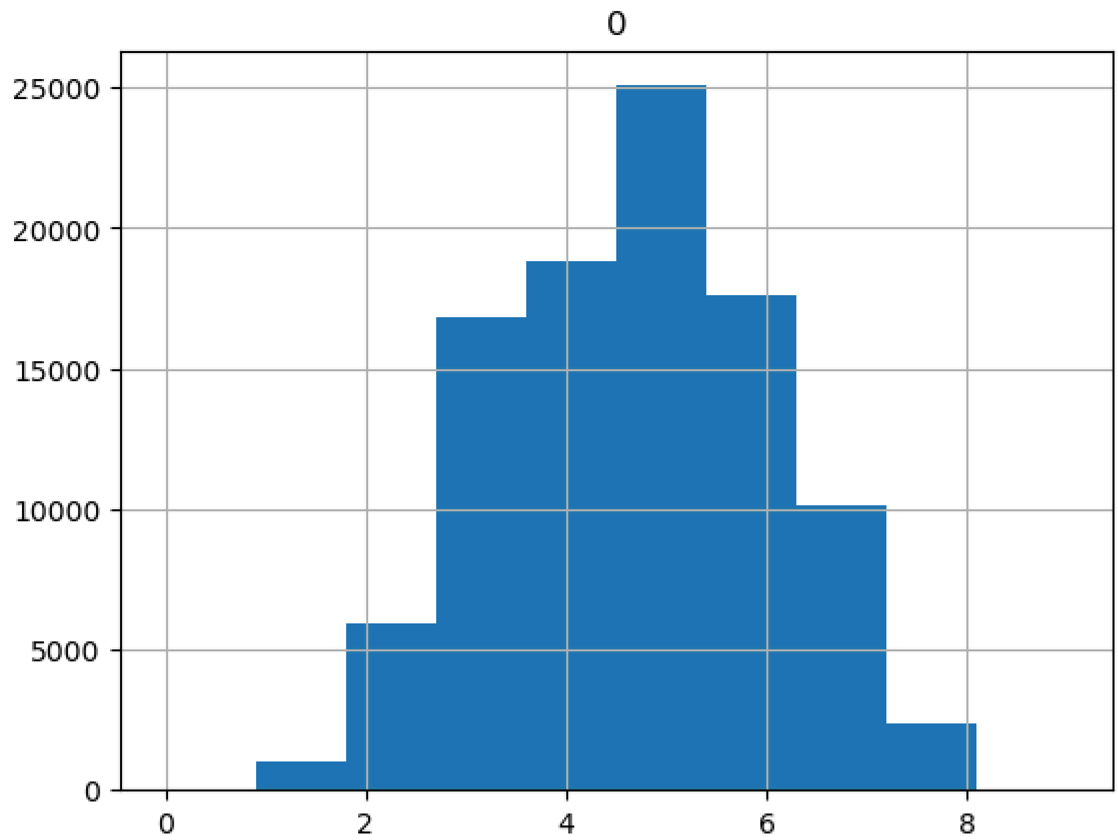


Sets up and fits the discretizer with uniform discretization (bins of same width).

In [ ]:
```
dc = KBinsDiscretizer(n_bins=10, encode='ordinal', strategy='uniform')
dc.fit(u)
Xu = dc.transform(u)
print(Xu)
```

Displays histogram after uniform discretization

In [137...
```
Xd = pd.DataFrame(Xu)
Xd.hist(bins = 10)
plt.show()
```



In [138…
```
print(dc.bin_edges_)
```

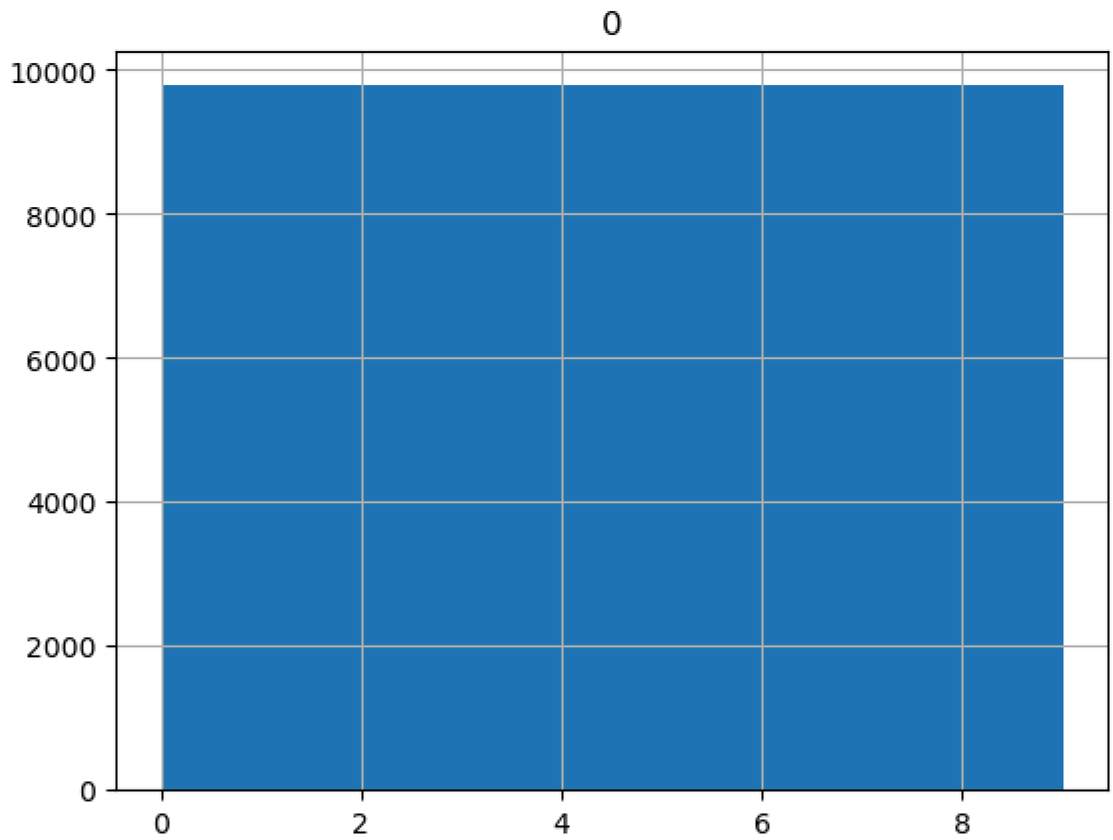
```
[array([14.31105 , 15.803383, 17.295716, 18.788049, 20.280382, 21.772715,
        23.265048, 24.757381, 26.249714, 27.742047, 29.23438 ])          ]
```

Sets up and fits the discretizer with quantil discretization (bins of same number of data objects).

In [ ]:
```
dc = KBinsDiscretizer(n_bins=10, encode='ordinal', strategy='quantile');
dc.fit(u)
Xu = dc.transform(u)
print(Xu)
```

Displays histogram after quantile discretization

In [141…
```
Xd = pd.DataFrame(Xu)
Xd.hist(bins=10)
plt.show()
```



In [142…
```
print(dc.bin_edges_)
```

```
[array([14.31105 , 19.119002, 19.949052, 20.721462, 21.528726, 22.15742 ,
        22.72338 , 23.31888 , 24.070266, 25.093166, 29.23438 ])          ]
```

Sets up and fits the discretizer with kmeans discretization (bins of variable frequency and width).

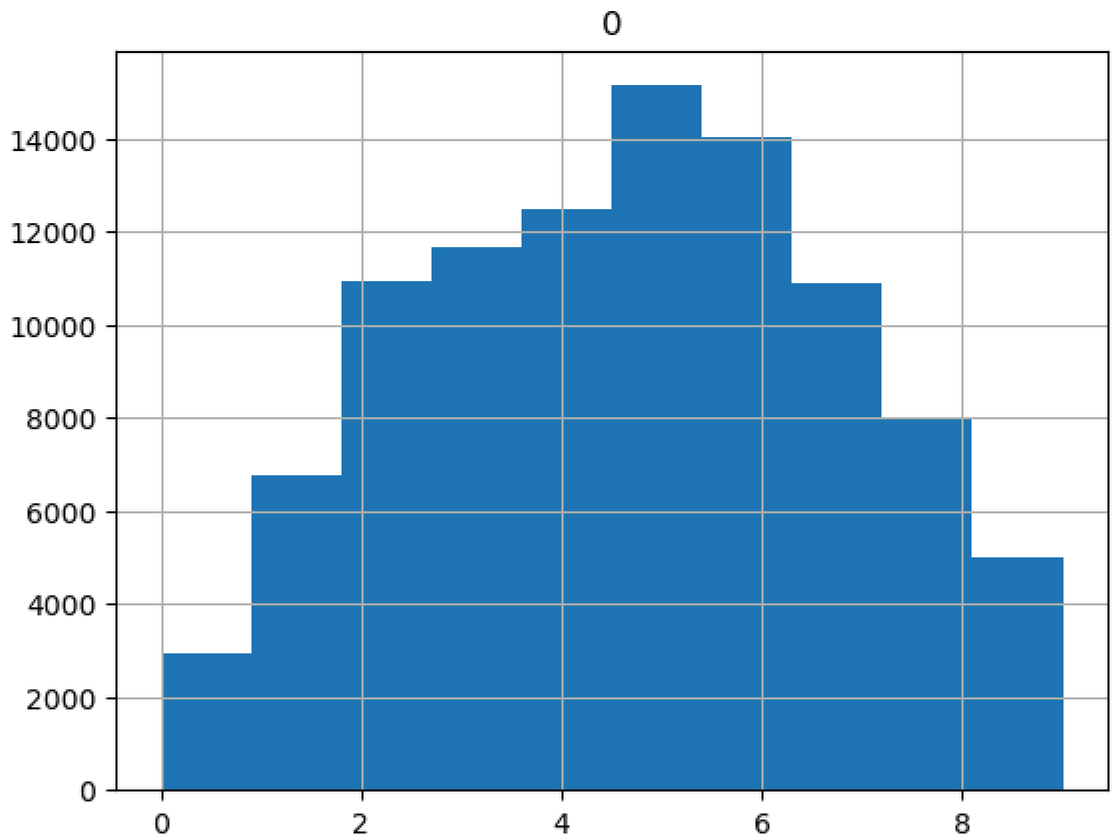
In [143…
```
dc = KBinsDiscretizer(n_bins=10, encode='ordinal', strategy='kmeans');
```

In [144…
```
dc.fit(u)
Xu = dc.transform(u).astype(int)
Xu.astype(int).dtype
```

```
[[7]
 [8]
 [8]
 ...
 [4]
 [8]
 [5]]
```

Displays histogram after kmeans discretization

In [146…
```
Xd = pd.DataFrame(Xu)
Xd.hist(bins=10)
plt.show()
```



In [147…
```
print(dc.bin_edges_)
```

```
[array([14.31105   , 18.01466338, 19.11349395, 20.03590366, 20.98019309,
        21.91386403, 22.79690257, 23.71600339, 24.70441566, 25.7664468 ,
        29.23438   ])                                                      ]
```

Part2: K-optimization:

Each of the above techniques is assessed on each continuous training variable in order to find the best k-value for each variable per discretization technique. Each technique exploits an inherent measure for identifying the optimal number of bins (k) across techniques deployed on each continuous variable. These measures ultimately define groups of test datasets. The first is variance in each of the variables post discretization. It is assessed iteratively per k-value candidate by calculating a weighted sum of the individual variances of the bins fitted to the variable. The distribution of weighted sum variances are evaluated to find the k-value associated with an inititial inflection point (hueristically the location of where the "second derivitive" values change sign from negative to positive). The sum is weighted because variance is in part defined by the inverse of the number of instances in the distribution it is found for which leads to smaller bin sizes having a disproportionate impact on the overal variance measure. The second measure is entropy which is a measure of the "randomness" of the data withing the bins which is also found for the entire binned variable by summing the measure in each bin . Because it is not dependent on the number of instances in the bin, it does not need to be weighted. In a similar fashion to variance, the inflection point of the distribution entropy for k candidates was utilized to identify the ideal k-value for a given variable and given technique but the inflection point reflects a change from postitive to negative. Ultimately per optimization measure, a set of three candidate-discretizations are generated for each continuous variable- one for each binning technique- so that each has a specifically tailored number of bins.

functions for assessing variance and entropy

In [148…
```
def wt_sum_variance(df: pd.DataFrame)->float:
    """
        establishes cumulative variance for binning
        of a variable
    """
    # stores weighted variances of bins
    bin_wt_variances = []

    # list of bin number identifiers that are to be iterated through to find
    bins = df.iloc[:,1].unique()

    for bin in bins:
        # get bin members
        bin_members = df[df.iloc[:, 1] == bin].iloc[:, 0]
        # appends bin_wt_variances with next value
        bin_wt_variances.append((bin_members.shape[0]/df.shape[0])*bin_membe

    return sum(bin_wt_variances)
```

In [149…
```
def sum_entropy(df: pd.DataFrame)-> float:
    bin_entropies = []

    bins = df.iloc[:,1].unique()

    for bin in bins:
        bin_members = df[df.iloc[:,1] == bin]. iloc[:,0]

        p = bin_members.shape[0]/df.shape[0]
        bin_entropies.append(-p*np.log2(p))

    return sum(bin_entropies)
```

Functions to assess k-values associated with inflection points for bin number optimization measures.

In [ ]:
```
def best_k_index_variance(variances: list) -> int:
    """
        finds the correct location of the inflection pt
        in the change in variance
    """
    # second derivative of variance
    acceleration = np.diff(np.diff(variances))
```

```
    for k in range(1, len(acceleration)):
        # finds inflection in variance
        if acceleration[k-1] < 0 and acceleration[k] > 0:
            # "+2" addresses indicial shift when finding f''
            return k + 2
    return -1  # if no inflection point, return indicator
```

very similar definition for finding elbow/inflection in the distribution of entropies for k-candidates

In [ ]:
```
def best_k_index_entropy(entropies: list) -> int:
    """
        finds the correct location of the inflection pt
        in the change in entropies
    """
    # second derivative of entropy
    acceleration = np.diff(np.diff(entropies))
    for k in range(1, len(acceleration)):
        # finds inflection in variance
        if acceleration[k-1] > 0 and acceleration[k] < 0:
            # "+2" addresses indicial shift when finding f''
            return k + 2
    return -1  # if no inflection point, return indicator
```

K-value optimizations:

The following cells deploy the above functions on a range of candidate k-values. The range maximum is determined using the variance and absolute frequency of all instances in the predictive variables. The frequency is inherently constant across variables but the variance is specific to each. The minimum is the number of classes in the predicted variable. The resulting candidated variable discretizations were appended to a data frame respective to the measure used for optimization.

finds optimal k's for binned candidate variables relative to variance and appends them to a data frame iterated through in part 3.

In [152…
```
# minimum k candidate range
minK = len(df["class"].unique())

# chunks of k candidates to test: prevents running all potential k's if secc

chunk = 10

# predictor df
variance_predict_vars = df.columns[df.dtypes == "float64"]
variance_predict_df = df[variance_predict_vars]
variance_predict_df.drop(list(variance_predict_df.filter(regex = 'ID')), axi

# predictor variables list
colNames = variance_predict_df.columns

for col in colNames:
```

```
    x = variance_predict_df[col]

    # ensures that the
    maxK = min(int(minK * (len(x)//x.var())), 1000)
    print(f"{col}_maxK: {maxK}")
    k_candidates = np.arange(minK,maxK,1, dtype= int)

    # dictionaries: key = k-value, value = labels
    width_dict = defaultdict(list)
    freq_dict = defaultdict(list)
    kmeans_dict = defaultdict(list)

    # lists: store variances for each bin type
    width_variances = []
    freq_variances = []
    kmeans_variances = []

    for i in range(minK, maxK, chunk):

        # protects from out of bounds at end of loop range
        end_i = min(i+chunk, maxK)

        for k in range(i, end_i):

            # discretizer objects per k
            DC_width = KBinsDiscretizer(n_bins=k, encode='ordinal', strategy

            # populates the dictionaries
            width_dict[k] = DC_width.fit_transform(x.values.reshape(-1, 1)).

            # creates dfs for variance evaluation
            width_df = pd.DataFrame({'column': x,
                                     'bins': width_dict[k]})

            # populates variance lists
            width_variances.append(wt_sum_variance(width_df))


        best_width_i = best_k_index_variance(width_variances)

        if best_width_i == -1 :
            continue

        best_k_width = k_candidates[best_width_i]
        print(f"{col} width k: {best_k_width}")
        variance_predict_df[f"{col}_width"] = width_dict[best_k_width]

        break

    for i in range(minK, maxK, chunk):

        # protects from outof bounds at end of loop range
        end_i = min(i+chunk, maxK)

        for k in range(i, end_i):
```

```
            DC_freq = KBinsDiscretizer(n_bins=k, encode='ordinal', strategy=

            # populates the dictionaries
            freq_dict[k] = DC_freq.fit_transform(x.values.reshape(-1, 1)).as

            # creates dfs for variance evaluation
            freq_df = pd.DataFrame({'column': x,
                                    'bins': freq_dict[k]})

            # populates variance lists
            freq_variances.append(wt_sum_variance(freq_df))

        best_freq_i = best_k_index_variance(freq_variances)

        if best_freq_i == -1 :
            continue


        best_k_freq = k_candidates[best_freq_i]
        print(f"{col} frequency k: {best_k_freq}")
        variance_predict_df[f"{col}_freq"] = freq_dict[best_k_freq]

        break

    for i in range(minK, maxK, chunk):

        # protects from outof bounds at end of loop range
        end_i = min(i+chunk, maxK)

        for k in range(i, end_i):

            DC_kmeans = KBinsDiscretizer(n_bins=k, encode='ordinal', strateg

            # populates the dictionaries
            kmeans_dict[k] = DC_kmeans.fit_transform(x.values.reshape(-1, 1)

            # creates dfs for variance evaluation
            kmeans_df = pd.DataFrame({'column': x,
                                    'bins': kmeans_dict[k]})

            # populates variance lists
            kmeans_variances.append(wt_sum_variance(kmeans_df))

        best_kmeans_i = best_k_index_variance(kmeans_variances)

        if best_kmeans_i == -1 :
            continue


        best_k_kmeans = k_candidates[best_kmeans_i]
        print(f"{col} kmeans k: {best_k_kmeans}")
        variance_predict_df[f"{col}_kmeans"] = kmeans_dict[best_k_kmeans]

        break
```

```
variance_predict_df.head()
```

```
alpha_maxK: 30
alpha width k: 8
alpha frequency k: 12
alpha kmeans k: 10
delta_maxK: 759
delta width k: 8
delta frequency k: 11
delta kmeans k: 10
u_maxK: 1000
u width k: 28
u frequency k: 49
u kmeans k: 16
g_maxK: 1000
g width k: 17
g frequency k: 41
g kmeans k: 19
r_maxK: 1000
r width k: 9
r frequency k: 51
r kmeans k: 20
i_maxK: 1000
i width k: 6
i frequency k: 38
i kmeans k: 17
z_maxK: 1000
z width k: 6
z frequency k: 68
z kmeans k: 14
redshift_maxK: 1000
redshift width k: 18
redshift frequency k: 34
redshift kmeans k: 12
```

Out[152…

	alpha	delta	u	g	r	i	z	redshift	al
0	135.689107	32.494632	23.87882	22.27530	20.39501	19.16573	18.79371	0.634794	
1	144.826101	31.274185	24.77759	22.83188	22.58444	21.16812	21.61427	0.779136	
2	142.188790	35.582444	25.26307	22.66389	20.60976	19.34857	18.94827	0.644195	
3	338.741038	-0.402828	22.13682	23.77656	21.61162	20.50454	19.25010	0.932346	
4	345.282593	21.183866	19.43718	17.58028	16.49747	15.97711	15.54461	0.116123	

5 rows × 32 columns

code finds the best k relative to entropy inflection point.

In [178…

```
def best_k_index_entropy(entropies: list) -> int:
    """
        finds the correct location of the inflection pt
        in the change in entropies
```

```
    """
    # second derivative of variance
    acceleration = np.diff(np.diff(entropies))
    # starting at one corrects for first indicial shift due to diff array
    for k in range(1, len(acceleration)):
        # finds inflection in variance
        if acceleration[k-1] > 0 and acceleration[k] < 0:
            # "+2" addresses second indicial shift
            return k + 2
    # safety: if inflection can't be found, uses smallest change
    return np.argmin(acceleration) + 2
```

finds optimal k's for binned candidate variables relative to entropy and appends them to a data frame iterated through in part 3.

In [154…

```
# minimum k candidate range
minK = len(df["class"].unique())


# predictor df
entropy_predict_vars = df.columns[df.dtypes == "float64"]
entropy_predict_df = df[entropy_predict_vars]
entropy_predict_df.drop(list(entropy_predict_df.filter(regex = 'ID')), axis

# predictor variables list
colNames = entropy_predict_df.columns

for col in colNames:
    x = entropy_predict_df[col]

    # ensures that there are sufficient candidates without being excessive
    maxK = min(int(minK * (len(x)//x.var())), 100)
    print(f"{col}_maxK: {maxK}")
    k_candidates = np.arange(minK,maxK,1, dtype= int)

    # dictionaries: key = k-value, value = labels
    width_dict = defaultdict(list)
    freq_dict = defaultdict(list)
    kmeans_dict = defaultdict(list)

    # lists: store variances for each bin type
    width_entropies = []
    freq_entropies = []
    kmeans_entropies = []



    for k in range(i, maxK):

        # discretizer objects per k
        DC_width = KBinsDiscretizer(n_bins=k, encode='ordinal', strategy='ur
        DC_freq = KBinsDiscretizer(n_bins=k, encode='ordinal', strategy='qua
        DC_kmeans = KBinsDiscretizer(n_bins=k, encode='ordinal', strategy='k

        # populates the dictionaries
```

```
        width_dict[k] = DC_width.fit_transform(x.values.reshape(-1, 1)).asty
        freq_dict[k] = DC_freq.fit_transform(x.values.reshape(-1, 1)).astype
        kmeans_dict[k] = DC_kmeans.fit_transform(x.values.reshape(-1, 1)).as

        # creates dfs for variance evaluation
        width_df = pd.DataFrame({'column': x,
                                'bins': width_dict[k]})
        freq_df = pd.DataFrame({'column': x,
                            'bins': freq_dict[k]})
        kmeans_df = pd.DataFrame({'column': x,
                        'bins': kmeans_dict[k]})

        # populates entropy lists
        width_entropies.append(sum_entropy(width_df))
        freq_entropies.append(sum_entropy(freq_df))
        kmeans_entropies.append(sum_entropy(kmeans_df))


    best_width_i = best_k_index_entropy(width_entropies)
    best_freq_i = best_k_index_entropy(freq_entropies)
    best_kmeans_i = best_k_index_entropy(kmeans_entropies)



    best_k_width = k_candidates[best_width_i]
    best_k_freq = k_candidates[best_freq_i]
    best_k_kmeans = k_candidates[best_kmeans_i]


    print(f"{col} width k: {best_k_width}")
    print(f"{col} frequency k: {best_k_freq}")
    print(f"{col} kmeans k: {best_k_kmeans}")


    entropy_predict_df[f"{col}_width"] = width_dict[best_k_width]
    entropy_predict_df[f"{col}_freq"] = freq_dict[best_k_freq]
    entropy_predict_df[f"{col}_kmeans"] = kmeans_dict[best_k_kmeans]



entropy_predict_df.head()
```

```
alpha_maxK: 30
alpha width k: 9
alpha frequency k: 5
alpha kmeans k: 10
delta_maxK: 100
delta width k: 9
delta frequency k: 5
delta kmeans k: 11
u_maxK: 100
u width k: 12
u frequency k: 5
u kmeans k: 12
g_maxK: 100
g width k: 6
g frequency k: 5
g kmeans k: 17
r_maxK: 100
r width k: 6
r frequency k: 5
r kmeans k: 7
i_maxK: 100
i width k: 6
i frequency k: 5
i kmeans k: 11
z_maxK: 100
z width k: 7
z frequency k: 5
z kmeans k: 8
redshift_maxK: 100
redshift width k: 15
redshift frequency k: 44
redshift kmeans k: 6
```

Out[154…

	alpha	delta	u	g	r	i	z	redshift	al
0	135.689107	32.494632	23.87882	22.27530	20.39501	19.16573	18.79371	0.634794	
1	144.826101	31.274185	24.77759	22.83188	22.58444	21.16812	21.61427	0.779136	
2	142.188790	35.582444	25.26307	22.66389	20.60976	19.34857	18.94827	0.644195	
3	338.741038	-0.402828	22.13682	23.77656	21.61162	20.50454	19.25010	0.932346	
4	345.282593	21.183866	19.43718	17.58028	16.49747	15.97711	15.54461	0.116123	

5 rows × 32 columns

Part3: Correlation/Mutual Information Optimization for experimental groups

---

The data frames of binned candidates for representation of the original continuous predictive variables are utilized to exhaustively evaluate their combinations so that each combination has a single binned version of the original predicitve variables represented once. Two different approaches are used to evaluate each combination. The first is the maximum reduction of correlation between variables, relative to the correlation that exists between the original continuous predictors. The second is the minimum increase in mutual information between variables relative to the continuous predictors. In both cases it is theorized that it is beneficial to have both of these measures be as small as possible for the transformed data that the models will train on as they measure the amount to which each variable is similar to other variables. While some machine learning algorithms can handle training on variables with high levels of similarity others cannot and in some cases it can cause greater complexity in the models. Correlation reflects the covariation of the variables it is measured between (cite probability text) but is resticted to linear variation. Mutual Information is a more generalized meausure of similairty between variables.It includes linear relationships but also includes nonlinear relationships. It tends to increase with discretization suggesting artificial relationships between variables due to the higher level of shared values due to the bins created.

In [155…

```
variance_predict_df.head()
```

Out[155…

	alpha	delta	u	g	r	i	z	redshift	al
0	135.689107	32.494632	23.87882	22.27530	20.39501	19.16573	18.79371	0.634794	
1	144.826101	31.274185	24.77759	22.83188	22.58444	21.16812	21.61427	0.779136	
2	142.188790	35.582444	25.26307	22.66389	20.60976	19.34857	18.94827	0.644195	
3	338.741038	-0.402828	22.13682	23.77656	21.61162	20.50454	19.25010	0.932346	
4	345.282593	21.183866	19.43718	17.58028	16.49747	15.97711	15.54461	0.116123	

5 rows × 32 columns

In [156…

```
entropy_predict_df.head()
```

Out[156…

	alpha	delta	u	g	r	i	z	redshift	al
0	135.689107	32.494632	23.87882	22.27530	20.39501	19.16573	18.79371	0.634794	
1	144.826101	31.274185	24.77759	22.83188	22.58444	21.16812	21.61427	0.779136	
2	142.188790	35.582444	25.26307	22.66389	20.60976	19.34857	18.94827	0.644195	
3	338.741038	-0.402828	22.13682	23.77656	21.61162	20.50454	19.25010	0.932346	
4	345.282593	21.183866	19.43718	17.58028	16.49747	15.97711	15.54461	0.116123	

5 rows × 32 columns

User functions for Mutual Information Matrices generatation: used in test group 1_b and test group 2_b and control_b

- continuous_mi is heuristic and is not restricted to maximum of one. It is only used with the original data to visualize it and compare it to the binned data ensembles

In [34]:
```
def continuous_mi(df: pd.DataFrame) -> np.ndarray:
    cols = df.columns
    length = len(cols)
    mi_matrix = np.zeros((length, length))

    for i in range(length):
        for j in range(length):

            # conditionally makes diagonals one (simplifies evaluation of ch
            if i == j:
                mi_matrix[i,j] = 1
            else:
                mi = mutual_info_regression(df[[cols[i]]], df[cols[j]])[0]
                norm_mi = mi/np.sqrt(np.var(df[cols[i]])*np.var(df[cols[j]])
                mi_matrix[i,j] = norm_mi

    return mi_matrix
```

In [37]:
```
def discrete_mi(df: pd.DataFrame) -> np.ndarray:
    cols = df.columns
    length = len(cols)
    mi_matrix = np.zeros((length, length))

    for i in range(length):
        for j in range(length):
            mi = mutual_info_score(df[cols[i]], df[cols[j]])

            norm_mi = mi/np.sqrt(entropy(np.bincount(df[cols[i]]))*entropy(r
            mi_matrix[i,j] = norm_mi

    return mi_matrix
```

Experiment:

experimental groups:

- 1_a variance optimized bin size; correlation optimized technique ensemble
- 1_b variance optimized bin size; mutual information optimized technique ensemble
- 1_c randomized bin sizes and ensemple
- 2_a entropy optimized bin size; correlation optimized technique ensemble
- 2_b entropy optimized bin size; mutual information optimized technique ensemble
- 2_c randomized bin sizes and ensemple (equals 1_c)
- control: original continuous predictors

The **experimental design**:

- train on each test group, and compare to training on the control group

Outcome:

- the greatest success relative to the control group will determine if (a) discretization matters at all in the efficacy of training different classifier models and (b) if optimization using variance measures has any impact on the efficacy.

Predetermined hypothesis:

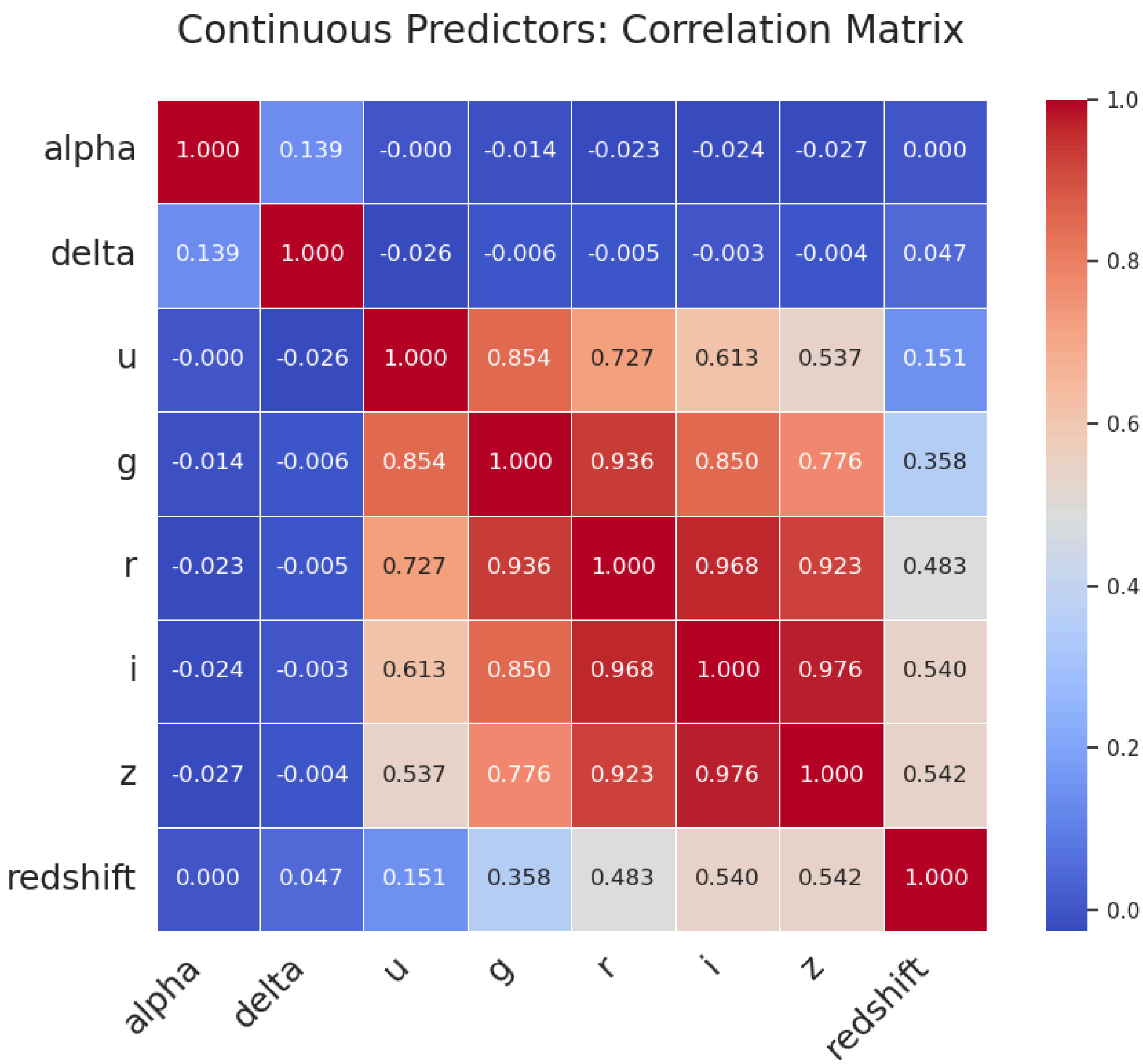
- answers: do you think discretization will improve on the effectiveness of the models overall and if so do you think the prescribed discretization technique will be more or less effective than random discretization?

Control group prep

The heat-mapped correlation matrix of the continuous versions of the predictive variables.

In [54]:
```
# separates continuous predictors from discretized
# contPred_df = df.drop('class',axis=1)
# contPred_df.to_csv("../Dataset/Control_Group.csv", index= False)

contPred_df = pd.read_csv("../Dataset/Control_Group.csv")
var_corr_matrix = contPred_df.corr()

var_corr_matrix.style\
    .format(precision = 3)\
    .format_index(str.upper, axis = 0)\
    .format_index(str.upper, axis = 1)\
    .background_gradient(cmap='coolwarm')



plt.figure(figsize=(10, 8))

sns.heatmap(var_corr_matrix, annot=True, fmt=".3f", cmap='coolwarm', square=
plt.title("Continuous Predictors: Correlation Matrix\n",
          fontsize = 20
          )
plt.xticks(rotation=45, ha='right',
           fontsize = 18
           )
plt.yticks(rotation=0,
           fontsize = 18
           )
plt.tight_layout()

# To save the plot
```

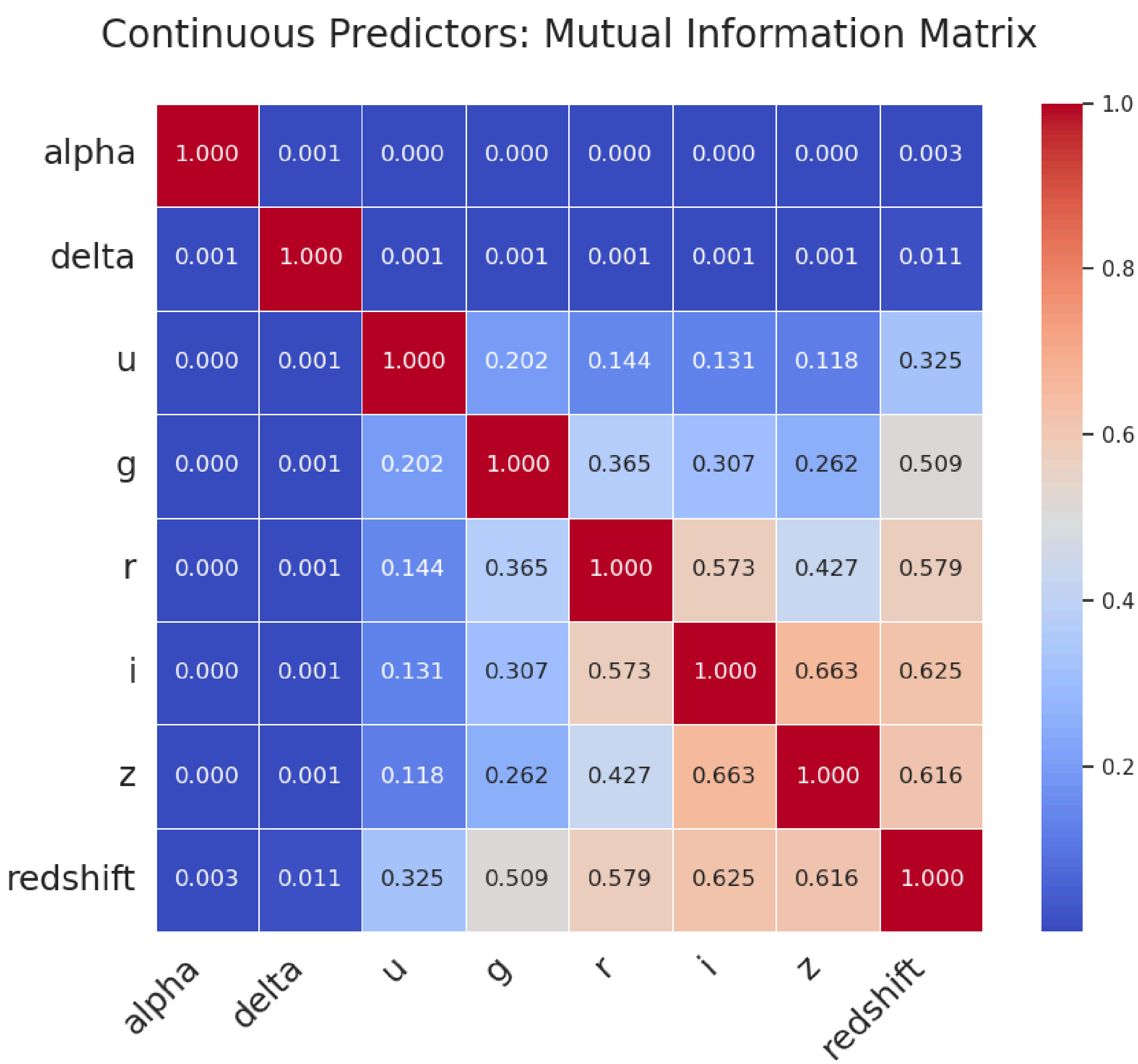
```
plt.savefig("../IMGs/continuousPredictors_corrheatmap.png", dpi=300)
plt.show()
```



Heat map of Mutual Info of original continuous predictors

In [60]:
```
cols = contPred_df.columns

# because numpy matrix, adds var names back in
best_df_mi_matrix = pd.DataFrame(continuous_mi(contPred_df), index= cols, co
best_df_mi_matrix

best_df_mi_matrix.style\
    .format(precision = 3)\
    .format_index(str.upper, axis = 0)\
    .format_index(str.upper, axis = 1)\
    .background_gradient(cmap='coolwarm')

plt.figure(figsize=(10, 8))

sns.heatmap(best_df_mi_matrix, annot=True, fmt=".3f", cmap='coolwarm', squar
plt.title("Continuous Predictors: Mutual Information Matrix\n",
```

```
           fontsize = 20
           )
plt.xticks(rotation=45, ha='right',
            fontsize = 18
            )
plt.yticks(rotation=0,
            fontsize = 18
            )
plt.tight_layout()

# To save the plot
plt.savefig("../IMGs/continuousPredictors_miheatmap.png", dpi=300)
plt.show()
```



Test group 1 prep

Test Group 1 consists of data frames of optimized discretizations of continuous predictive variables. The number of bins is based on variance measures. The bin type ensembles are based on both reduction of correlation across variables (1_a) and reduction of mutual information across variables (1_b). Both correlation and mutual information measure the level of dependency between variables but correlation reveals variation that is linear only while mutual information can have relationships that are nonlinear as well as linear. (1_c) tests random selection of bin sizes and tehcnique ensembles.

Test Group 1_a

Based in variance metrics, creates list of "mosaic" data frames that reflect all the combinations of the discretized predictive variables relative to the techniques used to create them. The bins are based on the optimization through correlation reduction.

In [ ]:
```
# separates original discretized predictors from continuous
var_discPred_df = variance_predict_df.iloc[:,8:variance_predict_df.shape[1]]

# strips the variable identifier from the matrix
var_corr_matrix = var_corr_matrix.values

# builds name lists based on names of continuous variables s.t. each list ha
contVar_names = contPred_df.columns

discVar_names = list(var_discPred_df.columns)

# assigns appropriate names to distinguishing variables
alpha_names, delta_names, u_names, g_names, r_names, i_names, z_names, redsh

mosaics_list = []



# iteratively combine binning type var per continuous names with each other
for a in alpha_names:
    for d in delta_names:
        for u in u_names:
            for g in g_names:
                for r in r_names:
                    for i in i_names:
                        for z in z_names:
                            for red in redshift_names:
                                group_names = [a,d,u,g,r,i,z,red]
                                df = var_discPred_df[group_names]
                                df_cols = df.columns
                                # print(df.head(3))
                                disc_cor_mat = df.corr().values
                                # messed up commented line below: should be
                                # diffCor_mat = -(corr_matrix - cor_mat)
                                diffCor_mat = -(disc_cor_mat - var_corr_matr
                                # print(diffCor_mat)
                                summed_corDiff = np.sum(diffCor_mat)
                                # print(cumm_diffCor)
```

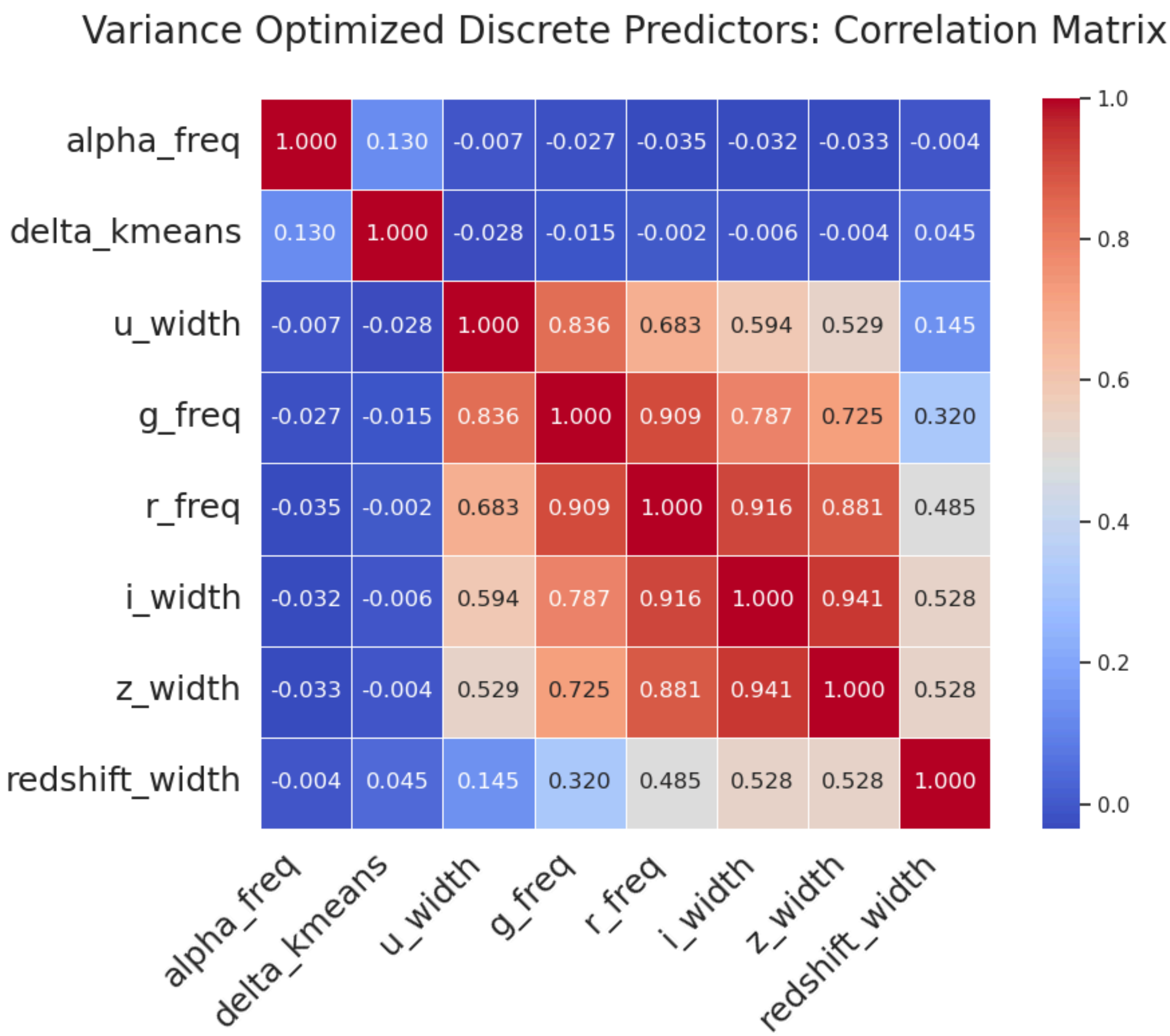
```
                                obj = {
                                      'variable_names' : df_cols,
                                    #   'df' : df,
                                      'cor_mat' : disc_cor_mat,
                                      'diffCor_mat' : diffCor_mat,
                                      'summed_corDiff' : summed_corDiff
                                    }
                                mosaics_list.append(obj)
```

Gets the combinations of the optimized discretized variables from mosaics list that reduce the correlation the to the greatest degree and the the combination that actually increases the overall correlation.

In [ ]:
```
sorted_mosaics_list = sorted(mosaics_list, key = lambda x: x["summed_corDiff

CorChange_best_df = var_discPred_df[sorted_mosaics_list[len(sorted_mosaics_l


CorChange_best_df.head()

# Creates Test Group 1_a df
CorChange_best_df.to_csv("../Dataset/TestGroup_1a.csv", index= False)
```

Heat map of best variance optimized ensemble by correlation

In [56]:
```
CorChange_best_df1 = pd.read_csv("../Dataset/TestGroup_1a.csv")
best_df_corr_matrix = CorChange_best_df.corr()

best_df_corr_matrix.style\
    .format(precision = 3)\
    .format_index(str.upper, axis = 0)\
    .format_index(str.upper, axis = 1)\
    .background_gradient(cmap='coolwarm')

plt.figure(figsize=(10, 8))

sns.heatmap(best_df_corr_matrix, annot=True, fmt=".3f", cmap='coolwarm', squ
plt.title("Variance Optimized Discrete Predictors: Correlation Matrix\n",
          fontsize = 20
          )
plt.xticks(rotation=45, ha='right',
           fontsize = 18
           )
plt.yticks(rotation=0,
           fontsize = 18
           )
plt.tight_layout()

# To save the plot
plt.savefig("../IMGs/VarDiscrete_Predictors_corrheatmap.png", dpi=300)
plt.show()
```



Test Group 1_b

Based in variance metrics, creates list of "mosaic" data frames that reflect all the combinations of the discretized predictive variables relative to the techniques used to create them. The bins are based on the optimization through mutual information reduction.

In [163…

```
test_df = variance_predict_df.iloc[:,[8,11,14,17,20]]

print(test_df.head())

discrete_mi(test_df)
```

```
   alpha_width  delta_width  u_width  g_width  r_width
0            3            4       17       10        5
1            3            3       19       11        6
2            3            4       20       11        5
3            7            1       14       12        6
4            7            3        9        4        1
```

Out[163…
```
array([[1.        , 0.12454808, 0.00762735, 0.01234982, 0.01719893],
       [0.12454808, 1.        , 0.00376838, 0.00549696, 0.00833369],
       [0.00762735, 0.00376838, 1.        , 0.31583494, 0.22122235],
       [0.01234982, 0.00549696, 0.31583494, 1.        , 0.45679059],
       [0.01719893, 0.00833369, 0.22122235, 0.45679059, 1.        ]])
```

In [165…
```
# separates original discretized predictors from continuous
var_discPred_df = variance_predict_df.iloc[:,8:variance_predict_df.shape[1]]

# creates continuous mutual information matrix
var_mi_matrix = continuous_mi(contPred_df)
print(var_mi_matrix)

# builds name lists based on names of continuous variables s.t. each list ha
contVar_names = contPred_df.columns

discVar_names = list(var_discPred_df.columns)

# assigns appropriate names to distinguishing variables
alpha_names, delta_names, u_names, g_names, r_names, i_names, z_names, redsh

mosaics_list = []



# iteratively combine binning type variables per continuous names with each
for a in alpha_names:
    for d in delta_names:
        for u in u_names:
            for g in g_names:
                for r in r_names:
                    for i in i_names:
                        for z in z_names:
                            for red in redshift_names:

                                group_names = [a,d,u,g,r,i,z,red]
                                df = var_discPred_df[group_names]
                                df_cols = df.columns

                                # creates mutual info matrix for current gro
                                disc_mi_mat = discrete_mi(df)
                                diff_mi_mat = -(disc_mi_mat - var_mi_matrix)
                                summed_diff_mi = np.sum(diff_mi_mat)
                                obj = {
                                      'variable_names' : df_cols,
                                      'mi_mat' : disc_mi_mat,
                                      'diff_mi_mat' : diff_mi_mat,
                                      'summed_diff_mi' : summed_diff_mi
                                    }
                                mosaics_list.append(obj)
```

```
[[1.00000000e+00 7.01323172e-04 1.49121897e-04 1.95513517e-04
  3.10078540e-04 2.76432393e-04 2.28539242e-04 2.79542736e-03]
 [7.01323097e-04 1.00000000e+00 5.72637164e-04 9.96757989e-04
  1.32499352e-03 1.39910537e-03 1.26720697e-03 1.08914675e-02]
 [1.49106938e-04 5.72636314e-04 1.00000000e+00 2.01773197e-01
  1.43647401e-01 1.31277346e-01 1.18126407e-01 3.25216354e-01]
 [1.95522910e-04 9.96802529e-04 2.01777586e-01 1.00000000e+00
  3.64779670e-01 3.06518987e-01 2.61594313e-01 5.09232912e-01]
 [3.10103004e-04 1.32478034e-03 1.43654998e-01 3.64776701e-01
  1.00000000e+00 5.73004077e-01 4.26609126e-01 5.79062048e-01]
 [2.76446582e-04 1.39926281e-03 1.31276566e-01 3.06517845e-01
  5.73010297e-01 1.00000000e+00 6.63453112e-01 6.24924951e-01]
 [2.28495914e-04 1.26736641e-03 1.18134419e-01 2.61592910e-01
  4.26613219e-01 6.63453501e-01 1.00000000e+00 6.16019739e-01]
 [2.79546554e-03 1.08915551e-02 3.25202140e-01 5.09224195e-01
  5.79054920e-01 6.24920170e-01 6.16006492e-01 1.00000000e+00]]
```

In [166…

```python
mi_mosaics_copy = mosaics_list.copy()

# don't want to run the above cell ever again:
with open('../Dataset/mi_mosaics_variance.pkl', 'wb') as f:
    pickle.dump(mi_mosaics_copy, f)
```

gets best combination of binned variables per mutual information

In [ ]:

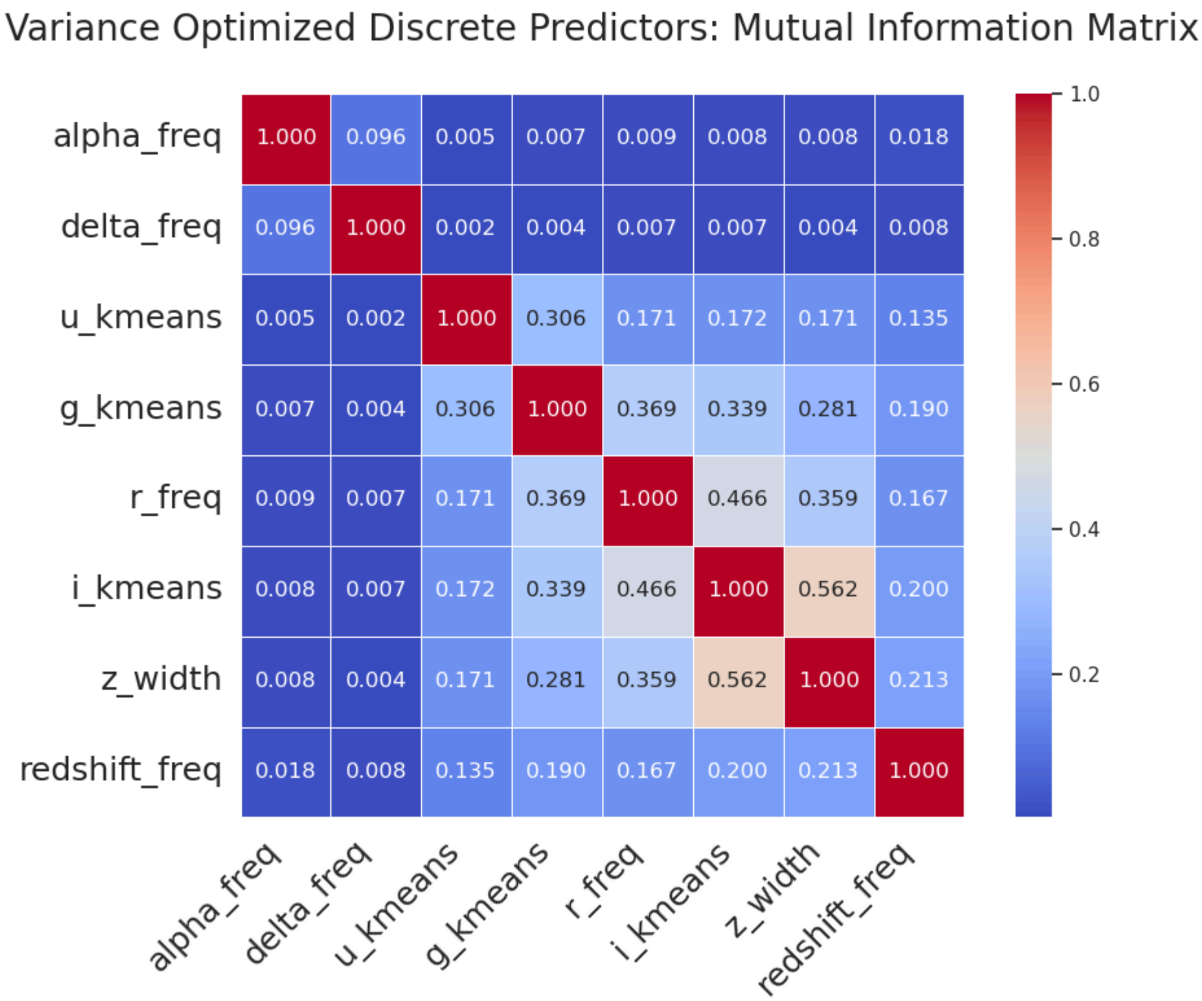
```python
sorted_mosaics_list = sorted(mosaics_list, key = lambda x: x["summed_diff_mi

miChange_best_df = var_discPred_df[sorted_mosaics_list[len(sorted_mosaics_li

# Creates Test Group 1b df
miChange_best_df.to_csv("../Dataset/TestGroup_1b.csv", index=False)
```

Heat map of best variance optimized ensemble by Mutual Info

In [57]:

```python
miChange_best_df = pd.read_csv("../Dataset/TestGroup_1b.csv")

cols = miChange_best_df.columns

# because numpy matrix, adds var names back in
best_df_mi_matrix = pd.DataFrame(discrete_mi(miChange_best_df), index= cols,
best_df_mi_matrix

best_df_mi_matrix.style\
    .format(precision = 3)\
    .format_index(str.upper, axis = 0)\
    .format_index(str.upper, axis = 1)\
    .background_gradient(cmap='coolwarm')



plt.figure(figsize=(10, 8))

sns.heatmap(best_df_mi_matrix, annot=True, fmt=".3f", cmap='coolwarm', squar
plt.title("Variance Optimized Discrete Predictors: Mutual Information Matrix
          fontsize = 20
```

```
            )
plt.xticks(rotation=45, ha='right',
           fontsize = 18
           )
plt.yticks(rotation=0,
           fontsize = 18
           )
plt.tight_layout()

# To save the plot
plt.savefig("../IMGs/VarDiscrete_Predictors_miheatmap.png", dpi=300)
plt.show()
```



Test group 1_c:

Random selection of number of bins and binning techniques for transformation of each continuous predictive variable.

In [187…

```
kmin = 3
kmax = 60
varNames = df.columns

randomPredict_df = pd.DataFrame()
```

```
for var in varNames:
        choice = np.random.randint(1,4)
        x = df[var]
        if choice == 1:
                DC_width = KBinsDiscretizer(n_bins=np.random.randint(kmin,km
                discVar = DC_width.fit_transform(x.values.reshape(-1, 1)).as
                randomPredict_df[f"{var}_width"] = discVar

        elif choice == 2:
                DC_freq = KBinsDiscretizer(n_bins=np.random.randint(kmin,kma
                discVar = DC_freq.fit_transform(x.values.reshape(-1, 1)).ast
                randomPredict_df[f"{var}_freq"] = discVar
        else:
                DC_kmeans = KBinsDiscretizer(n_bins=np.random.randint(kmin,k
                discVar = DC_kmeans.fit_transform(x.values.reshape(-1, 1)).a
                randomPredict_df[f"{var}_kmeans"] = discVar

randomPredict_df.to_csv("../Dataset/TestGroup_1c.csv", index=False)
```

Test group 2 prep

Test Group 2 consists of data frames of optimized discretizations of continuous predictive variables. The number of bins is based on entropy measures. The bin type ensembles are based on both reduction of correlation across variables (2_a) and reduction of mutual information across variables (2_b). Both correlation and mutual information measure the level of dependency between variables but correlation reveals variation that is linear only while mutual information can have relationships that are nonlinear as well as linear. (2_c) tests random selection of bin sizes and tehcnique ensembles.

Shows all versions of each discretized predictive variable

In [171…

```
entropy_predict_df.head()
```

Out[171…

	alpha	delta	u	g	r	i	z	redshift	al
0	135.689107	32.494632	23.87882	22.27530	20.39501	19.16573	18.79371	0.634794	
1	144.826101	31.274185	24.77759	22.83188	22.58444	21.16812	21.61427	0.779136	
2	142.188790	35.582444	25.26307	22.66389	20.60976	19.34857	18.94827	0.644195	
3	338.741038	-0.402828	22.13682	23.77656	21.61162	20.50454	19.25010	0.932346	
4	345.282593	21.183866	19.43718	17.58028	16.49747	15.97711	15.54461	0.116123	

5 rows × 32 columns

Test Group 2_a

Based in entropy metrics, creates list of "mosaic" data frames that reflect all the combinations of the discretized predictive variables relative to the techniques used to create them. The bins are based on the optimization through correlation reduction.

In [173…

```
# separate original discretized predictors from continuous
ent_discPred_df = entropy_predict_df.iloc[:,8:entropy_predict_df.shape[1]]
ent_contPred_df = entropy_predict_df.iloc[:,0:8]

# strips the variable identifier from the matrix
ent_corr_matrix = var_corr_matrix

# build name lists based on names of continuous variables s.t. each list has
contEnt_names = ent_contPred_df.columns

discEnt_names = list(ent_discPred_df.columns)

# assigns appropriate names to distinguishing variables
alpha_names, delta_names, u_names, g_names, r_names, i_names, z_names, redsh

ent_mosaics_list = []



# iteratively combine binning type var per continuous names with each other
for a in alpha_names:
    for d in delta_names:
        for u in u_names:
            for g in g_names:
                for r in r_names:
                    for i in i_names:
                        for z in z_names:
                            for red in redshift_names:
                                group_names = [a,d,u,g,r,i,z,red]
                                df = ent_discPred_df[group_names]
                                df_cols = df.columns
                                disc_cor_mat = df.corr().values

                                diffCor_mat = -(disc_cor_mat - ent_corr_matr
                                summed_corDiff = np.sum(diffCor_mat)

                                obj = {
                                      'variable_names' : df_cols,
                                      'cor_mat' : disc_cor_mat,
                                      'diffCor_mat' : diffCor_mat,
                                      'summed_corDiff' : summed_corDiff
                                    }

                                ent_mosaics_list.append(obj)
```

```
  # transform df into cor matrix
  # find and store difference between the continuous corr matrix and the mos
  # order the mosaic dfs by greatest to least cumulative cor distance
```

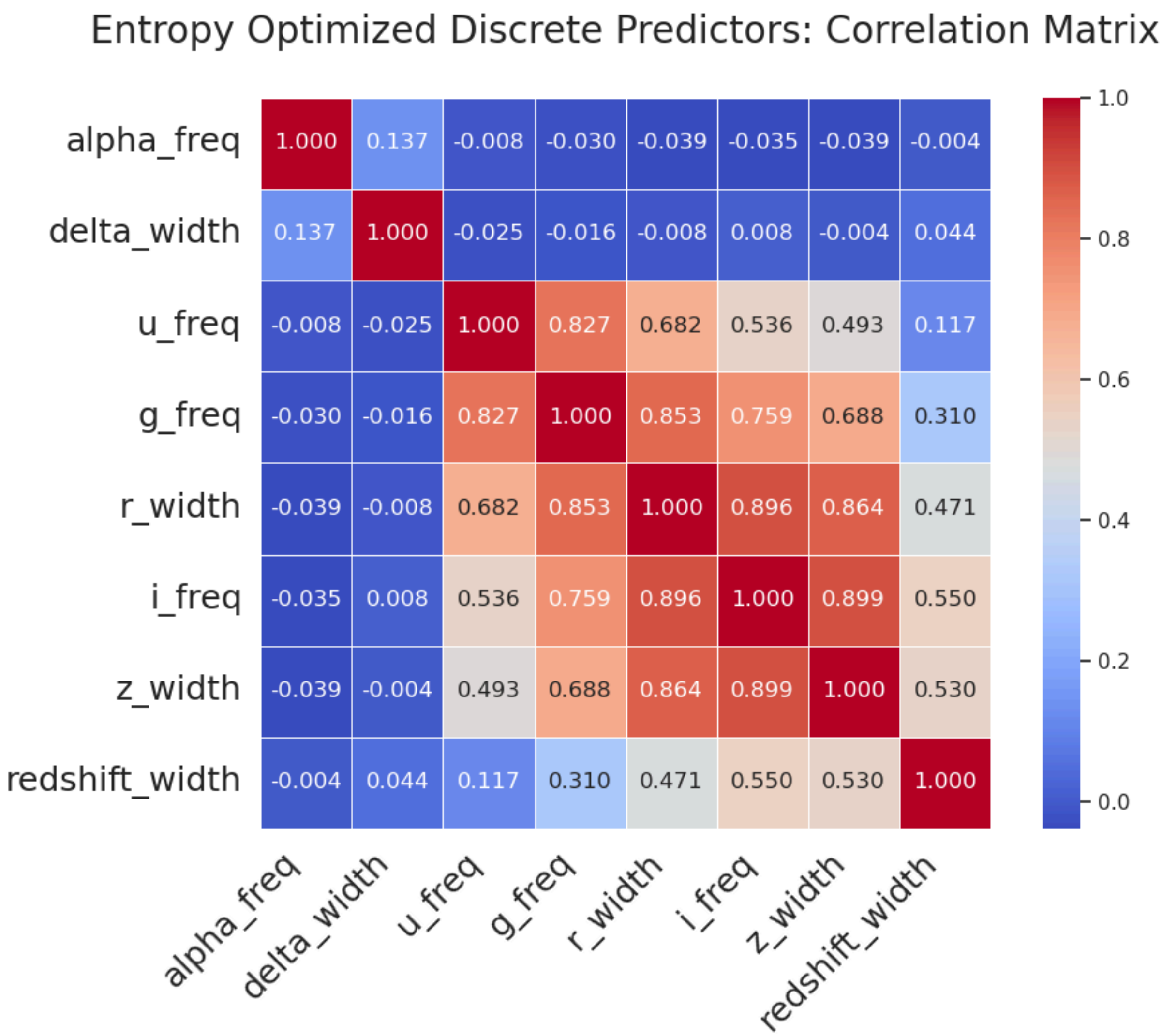
In [186…

```
sorted_mosaics_list = sorted(ent_mosaics_list, key = lambda x: x["summed_cor

corChange_best_df = ent_discPred_df[sorted_mosaics_list[len(sorted_mosaics_l
# CorChange_worst_df = discPred_df[sorted_mosaics_list[0]['variable_names']]

# Creates Test Group 2a df
corChange_best_df.to_csv("../Dataset/TestGroup_2a.csv", index= False)
```

Heat map of best entropy optimized ensemble by Correlation

In [58]:

```
CorChange_best_df2 = pd.read_csv("../Dataset/TestGroup_2a.csv")

best_df_corr_matrix = CorChange_best_df2.corr()

best_df_corr_matrix.style\
    .format(precision = 3)\
    .format_index(str.upper, axis = 0)\
    .format_index(str.upper, axis = 1)\
    .background_gradient(cmap='coolwarm')

plt.figure(figsize=(10, 8))

sns.heatmap(best_df_corr_matrix, annot=True, fmt=".3f", cmap='coolwarm', squ
plt.title("Entropy Optimized Discrete Predictors: Correlation Matrix\n",
          fontsize = 20
          )
plt.xticks(rotation=45, ha='right',
           fontsize = 18
           )
plt.yticks(rotation=0,
           fontsize = 18
           )
plt.tight_layout()

# To save the plot
plt.savefig("../IMGs/EntDiscrete_Predictors_corrheatmap.png", dpi=300)
plt.show()
```



Test Group 2_b

Based in entropy metrics, creates list of "mosaic" data frames that reflect all the combinations of the discretized predictive variables relative to the techniques used to create them. The bins are based on the optimization through mutual information reduction.

In [177…

```
# separate original discretized predictors from continuous
ent_discPred_df = entropy_predict_df.iloc[:,8:entropy_predict_df.shape[1]]

# creates continuous mutual information matrix
ent_mi_matrix = continuous_mi(contPred_df)
print(ent_mi_matrix)

# build name lists based on names of continuous variables s.t. each list has
contEnt_names = contPred_df.columns

discEnt_names = list(ent_discPred_df.columns)

# assigns appropriate names to distinguishing variables
alpha_names, delta_names, u_names, g_names, r_names, i_names, z_names, redsh
```

```
mosaics_list = []



# iteratively combine binning type var per continuous names with each other
for a in alpha_names:
    for d in delta_names:
        for u in u_names:
            for g in g_names:
                for r in r_names:
                    for i in i_names:
                        for z in z_names:
                            for red in redshift_names:

                                group_names = [a,d,u,g,r,i,z,red]
                                df = ent_discPred_df[group_names]
                                df_cols = df.columns

                                # creates mutual info matrix for current gro
                                disc_mi_mat = discrete_mi(df)
                                diff_mi_mat = -(disc_mi_mat - ent_mi_matrix)
                                summed_diff_mi = np.sum(diff_mi_mat)
                                obj = {
                                      'variable_names' : df_cols,
                                      'mi_mat' : disc_mi_mat,
                                      'diff_mi_mat' : diff_mi_mat,
                                      'summed_diff_mi' : summed_diff_mi
                                    }
                                mosaics_list.append(obj)
```

```
[[1.00000000e+00 7.01323072e-04 1.49128249e-04 1.95510635e-04
  3.10080791e-04 2.76423274e-04 2.28489277e-04 2.79544529e-03]
 [7.01323080e-04 1.00000000e+00 5.72697954e-04 9.96813105e-04
  1.32496975e-03 1.39916935e-03 1.26709348e-03 1.08910569e-02]
 [1.49101373e-04 5.72611046e-04 1.00000000e+00 2.01776236e-01
  1.43651595e-01 1.31278240e-01 1.18117073e-01 3.25210024e-01]
 [1.95510267e-04 9.96800852e-04 2.01773068e-01 1.00000000e+00
  3.64779945e-01 3.06519095e-01 2.61592968e-01 5.09243336e-01]
 [3.10120800e-04 1.32489884e-03 1.43642276e-01 3.64775266e-01
  1.00000000e+00 5.73005387e-01 4.26615328e-01 5.79096774e-01]
 [2.76427270e-04 1.39915036e-03 1.31275310e-01 3.06516148e-01
  5.73006556e-01 1.00000000e+00 6.63452062e-01 6.24918292e-01]
 [2.28480536e-04 1.26706608e-03 1.18108908e-01 2.61597701e-01
  4.26613694e-01 6.63454102e-01 1.00000000e+00 6.15975828e-01]
 [2.79538139e-03 1.08913526e-02 3.25221265e-01 5.09265913e-01
  5.79099040e-01 6.24934833e-01 6.15978440e-01 1.00000000e+00]]
```

In [179…

```
mi_mosaics_copy = mosaics_list.copy()

# don't want to run the above cell ever again either:
with open('../Dataset/mi_mosaics_entropy.pkl', 'wb') as f:
    pickle.dump(mi_mosaics_copy, f)
```

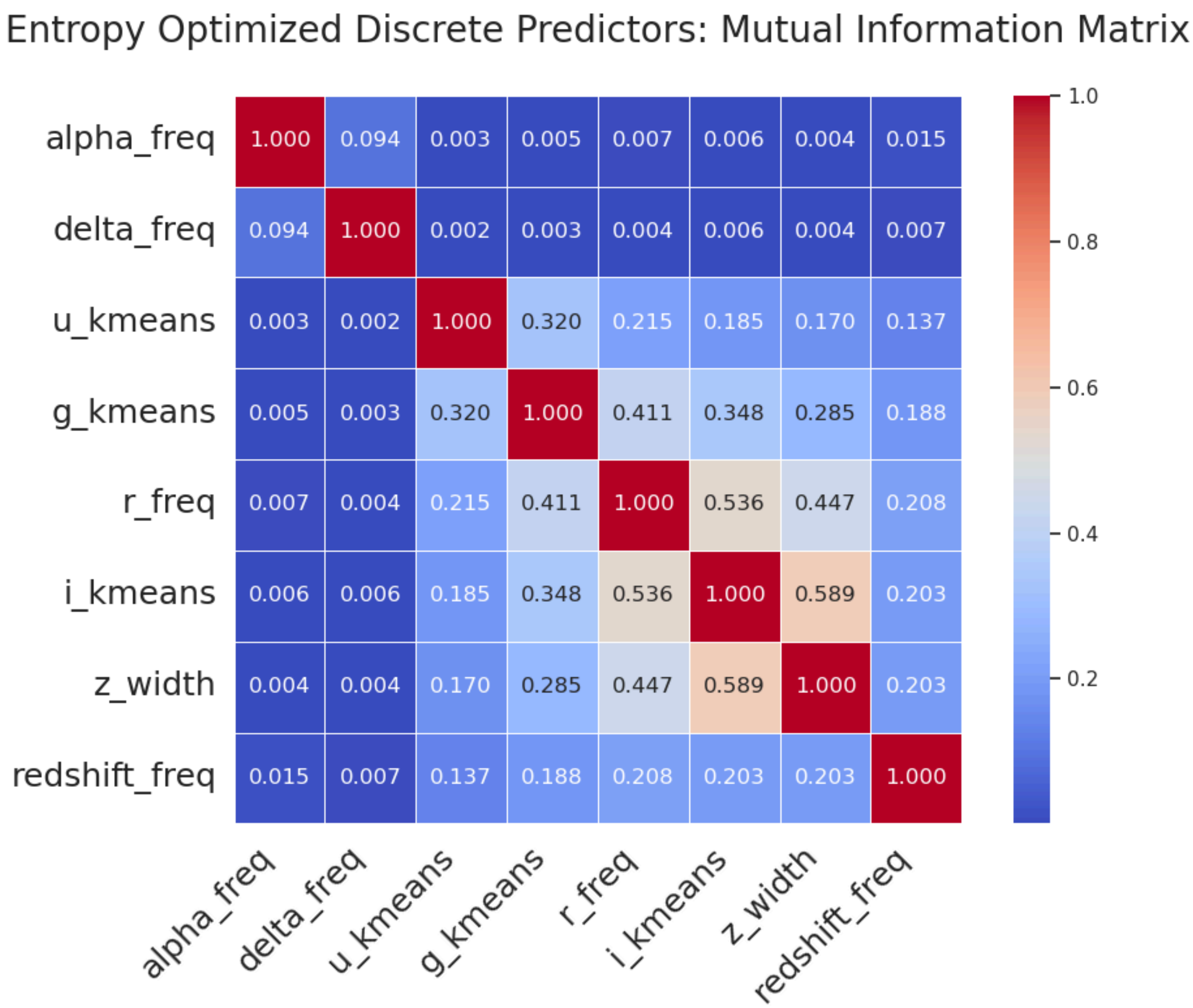
In [185…

```
sorted_mosaics_list = sorted(mosaics_list, key = lambda x: x["summed_diff_mi
```

```
miChange_best_df = ent_discPred_df[sorted_mosaics_list[len(sorted_mosaics_li


# Creates Test Group 2b df
miChange_best_df.to_csv("../Dataset/TestGroup_2b.csv", index= False)
```

Heat map of best entropy optimized ensemble by Mutual Info

In [59]:
```
miChange_best_df = pd.read_csv("../Dataset/TestGroup_2b.csv")

cols = miChange_best_df.columns

# because numpy matrix, adds var names back in
best_df_mi_matrix = pd.DataFrame(discrete_mi(miChange_best_df), index= cols,
best_df_mi_matrix

best_df_mi_matrix.style\
    .format(precision = 3)\
    .format_index(str.upper, axis = 0)\
    .format_index(str.upper, axis = 1)\
    .background_gradient(cmap='coolwarm')

plt.figure(figsize=(10, 8))

sns.heatmap(best_df_mi_matrix, annot=True, fmt=".3f", cmap='coolwarm', squar
plt.title("Entropy Optimized Discrete Predictors: Mutual Information Matrix\
          fontsize = 20
          )
plt.xticks(rotation=45, ha='right',
           fontsize = 18
           )
plt.yticks(rotation=0,
           fontsize = 18
           )
plt.tight_layout()

# To save the plot
plt.savefig("../IMGs/EntDiscrete_Predictors_miheatmap.png", dpi=300)
plt.show()
```



Test Group 2_c: intentionally the same as 1_c

In [184…

```
randomPredict_df.to_csv("../Dataset/TestGroup_2c.csv",index = False)
```