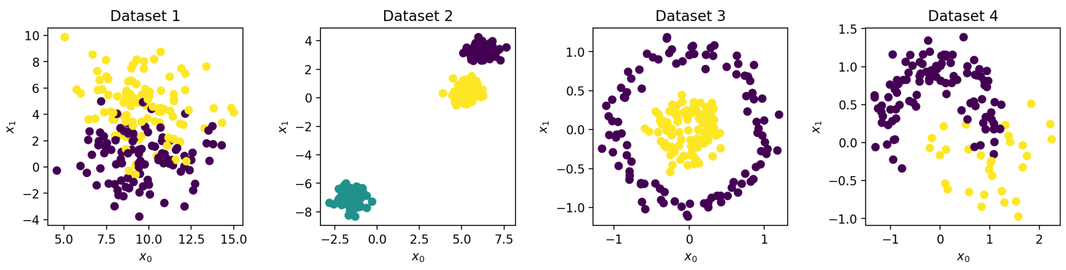
Classification - Assignment 7

Data and Package Import

In [1]:
```
%matplotlib inline
import numpy as np
import pandas as pd
import pylab as plt
```

In [2]:
```
from sklearn.datasets import make_blobs, make_moons, make_circles
np.random.seed(4)

noisiness = 1

X_blob, y_blob = make_blobs(n_samples = 200, centers = 2, cluster_std = 2 * noisiness, n_feat

X_mc, y_mc = make_blobs(n_samples = 200, centers = 3, cluster_std = 0.5 * noisiness, n_featu

X_circles, y_circles = make_circles(n_samples = 200, factor = 0.3, noise = 0.1 * noisiness)

X_moons, y_moons = make_moons(n_samples = 200, noise = 0.25 * noisiness)

N_include = 30
idxs = []
Ni = 0
for i, yi in enumerate(y_moons):
    if yi == 1 and Ni < N_include:
        idxs.append(i)
        Ni += 1
    elif yi == 0:
        idxs.append(i)

y_moons = y_moons[idxs]
X_moons = X_moons[idxs]

fig, axes = plt.subplots(1, 4, figsize = (15, 3), dpi = 200)

all_datasets = [[X_blob, y_blob], [X_mc, y_mc], [X_circles, y_circles], [X_moons, y_moons]]

labels = ['Dataset 1', 'Dataset 2', 'Dataset 3', 'Dataset 4']
for i, Xy_i in enumerate(all_datasets):
    Xi, yi = Xy_i
    axes[i].scatter(Xi[:, 0], Xi[:, 1], c = yi)
    axes[i].set_title(labels[i])
    axes[i].set_xlabel('$x_0$')
    axes[i].set_ylabel('$x_1$')

fig.subplots_adjust(wspace = 0.4);
```



In [3]:
```
df = pd.read_csv('data/perovskite_data.csv')
X_perov = df[['nA', 'nB', 'nX', 'rA (Ang)', 'rB (Ang)', 'rX (Ang)', 't', 'tau']].values
y_perov = df['exp_label'].values
```

1. k-nearest Neighbors Model

1-NN

Calculate the accuracy of a 1-nearest Neighbors model for the training data.

A 1-nearest Neighbors model considers a point as its own nearest neighbors.

> Accuracy will be just 1. 1-NN simple memorizes the label of each data point.

Will this be a reliable indicator of its accuracy for testing data?

Briefly explain your answer.

> No. Even though the accuracy is 1, this cannot be a reliable indicator, since we know that this score is due to a simple memorization.

Weighted Neighbors Classification

Instead of selecting the k-nearest neighbors to vote, we could design an algorithm where all neighbors get to vote, but their vote is weighted inversely to their distance from the point of interest:

$y_i = \sum_j y_j/(||x_i - x_j||)$

where j is an index over all training points.

The class will be assigned as follows:

- class 1 if $y_i \geq 0$
- class -1 if $y_i < 0$

In [4]:
```python
def distance(x1, x2):
    return np.linalg.norm(x1 - x2, 2)
```

In [5]:
```python
def get_neighbor(x, x_list):
    dist_pairs = []
    for i, xi in enumerate(x_list):
        dist = distance(x, xi)
        dist_pairs.append([dist, i])
    return dist_pairs
```

Write a function that assigns a class to a point.

The function should take the followings as arguments:

- a single point x
- a list of training points x_list
- a list of training labels y_list

You may want to use functions above. You will also need to add a statement to avoid dividing by zero if the point is in the training set. If the distance between 2 points is zero, then the label from the same point in the training set should be used (e.g. if

In [6]:
```
def assign_class(x, x_list, y_list):
    neighbors = get_neighbor(x, x_list)
    vote = 0

    for i, xi in enumerate(neighbors):
        if neighbors[i][0] == 0:
            vote = y_list[i]
            break
        vote += y_list[i] / neighbors[i][0]

    if vote >= 0:
        assignment = 1
    else:
        assignment = -1

    return assignment
```

Write a function that returns the prediction for a given list of testing points.

The function should take the followings as arguments:

- a list of testing points X
- a list of training points X_train
- a list of training labels y_train

In [7]:
```
def weighted_neighbors(X, X_train, y_train):
    y_hat = []
    for x in X:
        assign = assign_class(x, X_train, y_train)
        y_hat.append(assign)
    return y_hat
```

Train the model for the perovskite dataset using a random selection of 75% of the data as training data.

In [8]:
```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X_perov, y_perov, test_size = 0.25)
y_predict = weighted_neighbors(X_perov, X_train, y_train)
```

Compute the accuracy and precision of the prediction.

In [9]:
```
from sklearn.metrics import accuracy_score, precision_score

acc = accuracy_score(y_perov, y_predict)
prec = precision_score(y_perov, y_predict)

print('Accuracy: {}'.format(acc))
print('Precision: {}'.format(prec))
```

```
Accuracy: 0.9635416666666666
Precision: 0.9506172839506173
```

Train a 5-NN model using the same training data.

In [10]:
```
from sklearn.neighbors import KNeighborsClassifier

knn = KNeighborsClassifier(n_neighbors = 5)

knn.fit(X_train, y_train)
y_predict = knn.predict(X_perov)
```

Compute the accuracy and precision.

In [11]:
```
acc = accuracy_score(y_perov, y_predict)
prec = precision_score(y_perov, y_predict)

print('Accuracy: {}'.format(acc))
print('Precision: {}'.format(prec))
```

```
Accuracy: 0.9322916666666666
Precision: 0.9391025641025641
```

2. Multi-dimensional Classification

Simple logistic regression

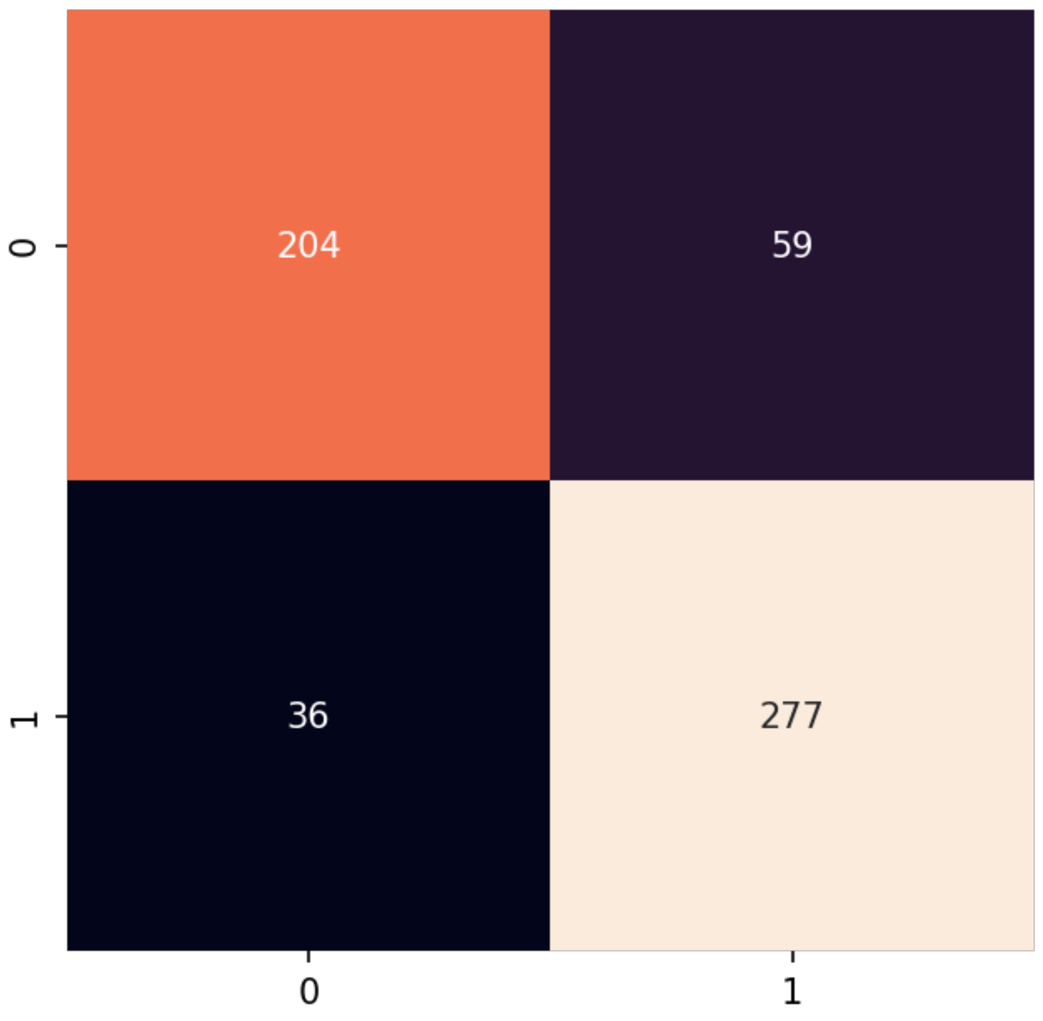
Train a logistic regression model using all columns except the `tau` column of the perovskite dataset.

You may use some functions that have been already built in the previous assignments.

In [12]:
```
from sklearn.linear_model import LogisticRegression

X = X_perov[:, :-1]

logreg = LogisticRegression(penalty = 'none') # no regularization
logreg.fit(X, y_perov);
```

Plot the confusion matrix.

In [13]:
```
from sklearn.metrics import confusion_matrix
import seaborn as sns

y_predict = logreg.predict(X)
cm = confusion_matrix(y_perov, y_predict)

fig, ax = plt.subplots(figsize = (5, 5), dpi = 150)
sns.heatmap(cm, annot = True, ax = ax, cbar = False, fmt = 'd');
```



Compute the accuracy, precision and recall.

In [14]:
```
from sklearn.metrics import recall_score

acc = accuracy_score(y_perov, y_predict)
prec = precision_score(y_perov, y_predict)
rec = recall_score(y_perov, y_predict)

print('Accuracy: {}'.format(acc))
print('Precision: {}'.format(prec))
print('Recall: {}'.format(rec))
```

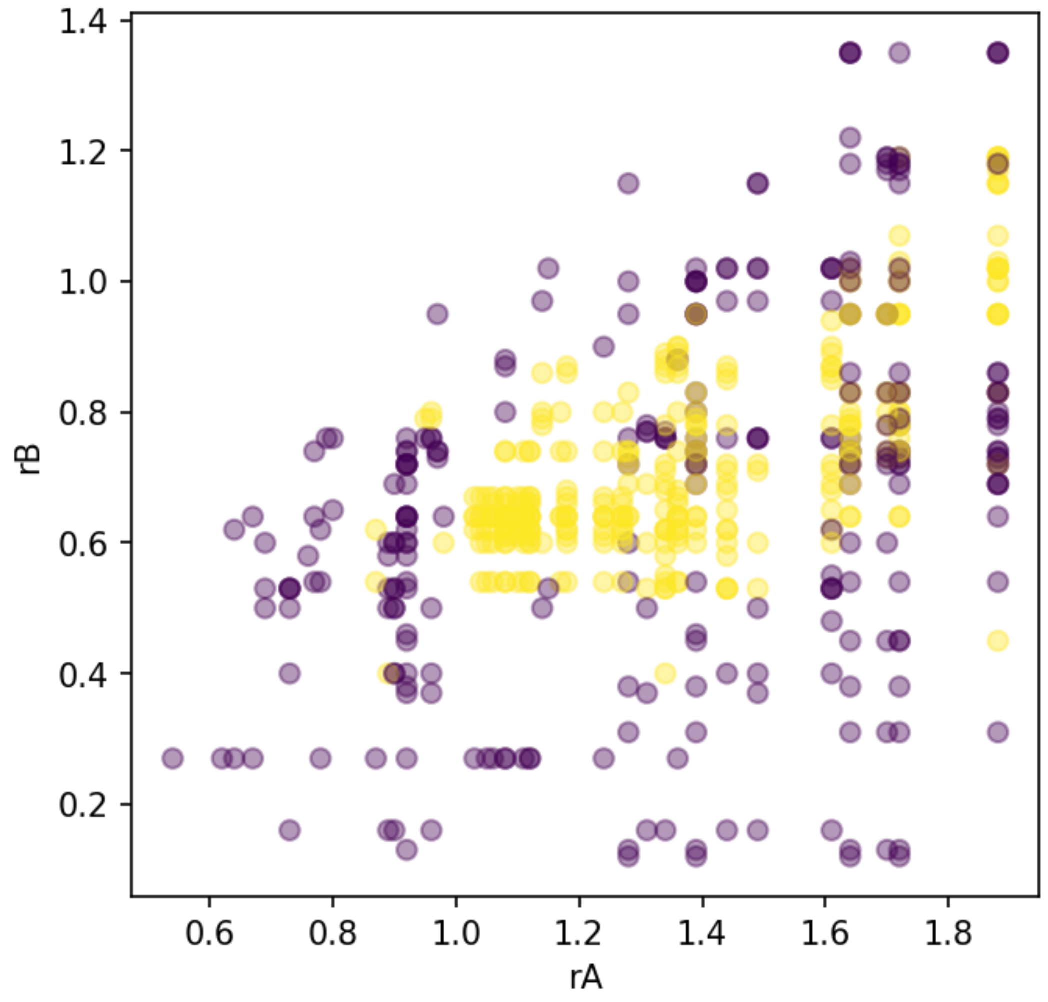
```
Accuracy: 0.8350694444444444
Precision: 0.8244047619047619
Recall: 0.8849840255591054
```

6745 Only: Customizing non-linear boundaries

In this problem, you will create a single custom feature that improves the separation performance as much as possible.

Plot the `y_perov` as a function of `rA (Ang)` and `rB (Ang)`.

In [15]:
```
rA = X_perov[:, 3]
rB = X_perov[:, 4]

fig, ax = plt.subplots(figsize = (5, 5), dpi = 150)
ax.scatter(rA, rB, c = y_perov, alpha = .4)
ax.set_xlabel('rA')
ax.set_ylabel('rB');
```



Build a baseline model based on logistic regression.

Report the accuracy and precision of the baseline model.

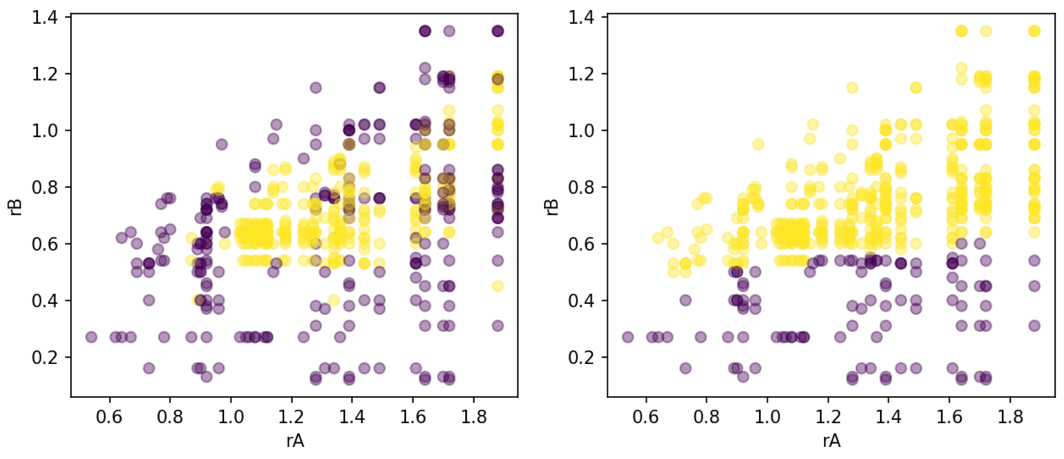
In [16]:
```
logreg = LogisticRegression(penalty = 'none')

logreg.fit(X_perov[:, [3, 4]], y_perov)
y_predict = logreg.predict(X_perov[:, [3, 4]])
```

```
acc = accuracy_score(y_perov, y_predict)
prec = precision_score(y_perov, y_predict)

print('Accuracy: {}'.format(acc))
print('Precision: {}'.format(prec))
```

```
Accuracy: 0.6631944444444444
Precision: 0.6263269639065817
```

Plot the prediction of the baseline model.

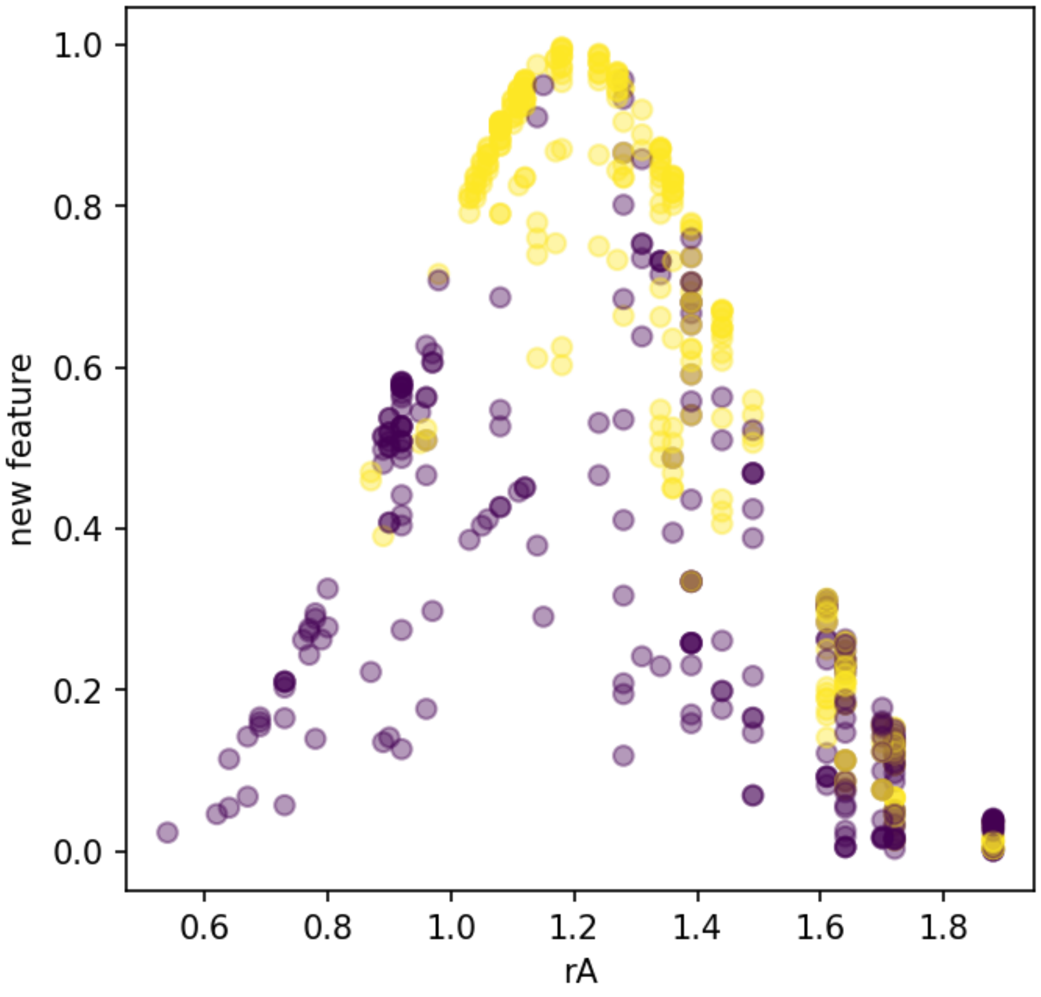
In [17]:
```
fig, axes = plt.subplots(1, 2, figsize = (10, 4), dpi = 150)

axes[0].scatter(rA, rB, c = y_perov, alpha = .4)
axes[0].set_xlabel('rA')
axes[0].set_ylabel('rB')

axes[1].scatter(rA, rB, c = y_predict, alpha = .4)
axes[1].set_xlabel('rA')
axes[1].set_ylabel('rB');
```



Create a new feature based on a non-linear combination of `rA (Ang)` and `rB (Ang)` .

Plot the new feature as a function of `rA (Ang)` .

In [18]:
```
X_new = np.exp((rA - 1.2)**2 + (rB - 0.6)**2)**(-6.9)
X_new = X_new.reshape(-1, 1)

fig, ax = plt.subplots(figsize = (5, 5), dpi = 150)
ax.scatter(rA, X_new, alpha = .4, c = y_perov)
ax.set_xlabel('rA')
ax.set_ylabel('new feature');
```



Build a new model that includes `rA (Ang)` , `rB (Ang)` and your new feature.

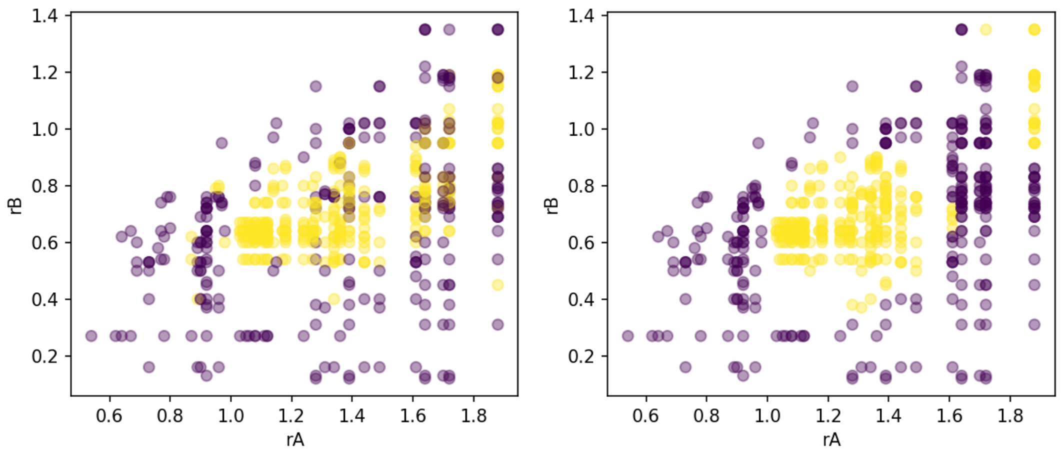
Report the accuracy and precision.

In [19]:
```
X_new_matrix = np.append(X_perov[:, [3, 4]], X_new, 1)

logreg.fit(X_new_matrix, y_perov)
y_predict = logreg.predict(X_new_matrix)

acc = accuracy_score(y_perov, y_predict)
prec = precision_score(y_perov, y_predict)

print('Accuracy: {}'.format(acc))
print('Precision: {}'.format(prec))
```

```
Accuracy: 0.8038194444444444
Precision: 0.8597122302158273
```

Plot the result of your new model.

In [20]:
```
fig, axes = plt.subplots(1, 2, figsize = (10, 4), dpi = 150)

axes[0].scatter(rA, rB, c = y_perov, alpha = .4)
axes[0].set_xlabel('rA')
axes[0].set_ylabel('rB')

axes[1].scatter(rA, rB, c = y_predict, alpha = .4)
axes[1].set_xlabel('rA')
axes[1].set_ylabel('rB');
```



Briefly explain how you decided on the feature.

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3. Comparison of Classification Model

In this problem, you will compare the classification performance of three different models using the perovskite dataset.

Choose three different classification models and import them.

These could be models discussed in the lectures, or others that you have learned about elsewhere.

In [21]:
```
from sklearn.ensemble import RandomForestClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.neighbors import KNeighborsClassifier

rf = RandomForestClassifier()
logreg = LogisticRegression(solver = 'saga')
knn = KNeighborsClassifier()
```

Make a hyperparameter grid for each model.

You should optimize at least one hyperparameter for each model.

In [22]:
```
param_rf = {'n_estimators': [50, 100, 150], 'max_depth': [2, 3, 4]}
param_logreg = {'penalty': ['l1', 'l2', 'none']}
param_knn = {'n_neighbors': [2, 3, 4, 5]}
```

Optimize hyperparameters.

First, you select a validation set using hold-out (`train_test_split`). Optimize hyperparameters using `GridSearchCV` on the training set.

In [23]:
```
from sklearn.model_selection import GridSearchCV
import warnings

warnings.simplefilter('ignore')

X_train, X_test, y_train, y_test = train_test_split(X_perov, y_perov, test_size = .25)

rf_search = GridSearchCV(rf, param_rf, cv = 3)
logreg_search = GridSearchCV(logreg, param_logreg, cv = 3)
knn_search = GridSearchCV(knn, param_knn, cv = 3)

rf_search.fit(X_train, y_train)
logreg_search.fit(X_train, y_train)
knn_search.fit(X_train, y_train)

rf_best = rf_search.best_estimator_
logreg_best = logreg_search.best_estimator_
knn_best = knn_search.best_estimator_
```

Compare the accuracy by predicting the results of the validation set.

In [24]:
```
print('Accuracy of Random Forest: {}'.format(accuracy_score(y_test, rf_best.predict(X_test))))
print('Accuracy of Logistic Regression: {}'.format(accuracy_score(y_test, logreg_best.predict(
print('Accuracy of k-Nearest Neighbors: {}'.format(accuracy_score(y_test, knn_best.predict(X_
```

```
Accuracy of Random Forest: 0.9166666666666666
Accuracy of Logistic Regression: 0.6597222222222222
Accuracy of k-Nearest Neighbors: 0.9444444444444444
```

Briefly describe your conclusions based on the results.

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