In [1]:
```
%matplotlib inline
import matplotlib.pyplot as plt
import matplotlib as mpl
from cycler import cycler

plt.style.use('default')

font_size = 12

mpl.rcParams['axes.prop_cycle'] = cycler('color', ['#003057', '#EAAA00
', '#4B8B9B', '#B3A369', '#377117', '#1879DB', '#8E8B76', '#002233', '#
F5D580'])
mpl.rcParams['axes.titlesize'] = font_size
mpl.rcParams['axes.titleweight'] = 'ultralight'
mpl.rcParams['axes.labelsize'] = font_size
mpl.rcParams['axes.labelweight'] = 'ultralight'

mpl.rcParams['xtick.labelsize'] = font_size
mpl.rcParams['xtick.direction'] = 'in'

mpl.rcParams['ytick.labelsize'] = font_size
mpl.rcParams['ytick.left'] = True
mpl.rcParams['ytick.direction'] = 'in'

mpl.rcParams['lines.linewidth'] = 2
mpl.rcParams['lines.linestyle'] = '--'
#mpl.rcParams['lines.marker'] = 'o'

mpl.rcParams['figure.titlesize'] = font_size
mpl.rcParams['figure.titleweight'] = 'bold'
mpl.rcParams['figure.figsize'] = (8, 6)
mpl.rcParams['figure.dpi'] = 300
mpl.rcParams['figure.autolayout'] = True

mpl.rcParams['savefig.dpi'] = 300
mpl.rcParams['savefig.format'] = 'svg'
mpl.rcParams['savefig.transparent'] = True

mpl.rcParams['font.size'] = font_size
mpl.rcParams['font.family'] = 'sans-serif'
mpl.rcParams['font.sans-serif'] = 'Helvetica'
mpl.rcParams['font.style'] = 'normal'

mpl.rcParams['mathtext.default'] = 'regular'

mpl.rcParams['legend.fontsize'] = font_size - 3
```

In [2]:
```
import numpy as np
clrs = np.array(['#003057', '#EAAA00', '#4B8B9B', '#B3A369', '#377117',
'#1879DB', '#8E8B76', '#F5D580', '#002233'])
```

Perovskite dataset

We will work with a real dataset, taken from the paper "[New tolerance factor to predict the stability of perovskite oxides and halides (https://advances.sciencemag.org/content/5/2/eaav0693)](https://advances.sciencemag.org/content/5/2/eaav0693)" by Bartel et al. Perovskites are a very useful class of oxide materials that can have very high catalyic activities, and have recently shown promise in solar cells. However, not all combinations of elements will form a perovskite structure, and it is very useful to be able to predict whether or not an elemental composition will form a perovskite. This helps determine whether or not a material can be synthesized before going into the lab.

This dataset contains a list of chemical formulas, along with some chemical features of the elements (radius and oxidation state), and whether or not they will form a stable perovskite crystal structure:

In [3]:
```
import pandas as pd

df = pd.read_csv('data/perovskite_data.csv')

df.head(10)
```

Out[3]:

	ABX3	A	B	X	nA	nB	nX	rA (Ang)	rB (Ang)	rX (Ang)	t	tau	exp_label
0	AgBiO3	Ag	Bi	O	1	5	-2	1.28	0.76	1.40	0.88	4.07	-1
1	AgBrO3	Ag	Br	O	1	5	-2	1.28	0.31	1.40	1.11	6.43	-1
2	AgCaCl3	Ag	Ca	Cl	1	2	-1	1.28	1.00	1.81	0.78	6.00	-1
3	AgCdBr3	Ag	Cd	Br	1	2	-1	1.28	0.95	1.96	0.79	5.58	-1
4	AgClO3	Ag	Cl	O	1	5	-2	1.28	0.12	1.40	1.25	15.17	-1
5	AgCoF3	Ag	Co	F	1	2	-1	1.28	0.74	1.33	0.89	3.96	1
6	AgCuF3	Ag	Cu	F	1	2	-1	1.28	0.73	1.33	0.90	3.94	1
7	AgMgCl3	Ag	Mg	Cl	1	2	-1	1.28	0.72	1.81	0.86	4.60	-1
8	AgMgF3	Ag	Mg	F	1	2	-1	1.28	0.72	1.33	0.90	3.94	1
9	AgMnF3	Ag	Mn	F	1	2	-1	1.28	0.83	1.33	0.85	4.16	1

In [4]:
```
feature_columns = ['nA', 'nB', 'nX', 'rA (Ang)', 'rB (Ang)', 'rX (An
g)', 't', 'tau']

X_perov = df[feature_columns].values
y_perov = df['exp_label'].values

print(X_perov.shape, y_perov.shape)
```

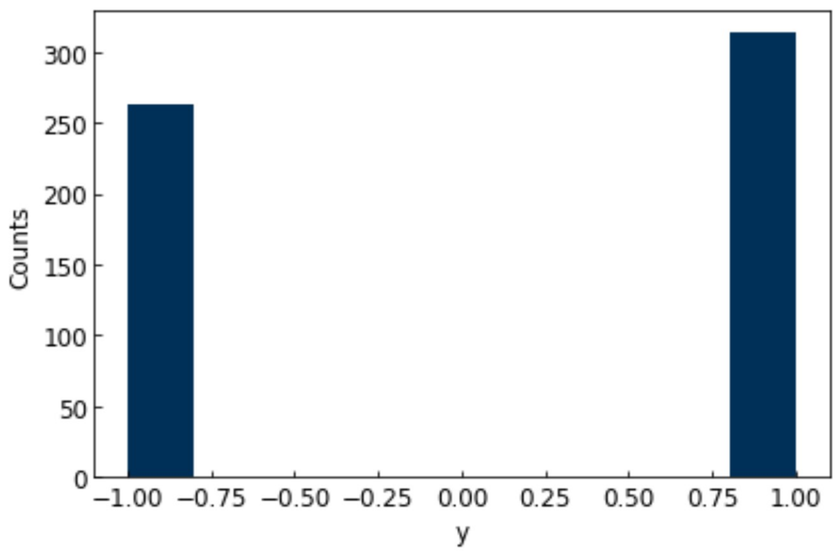
```
(576, 8) (576,)
```

A few things to note on this dataset:

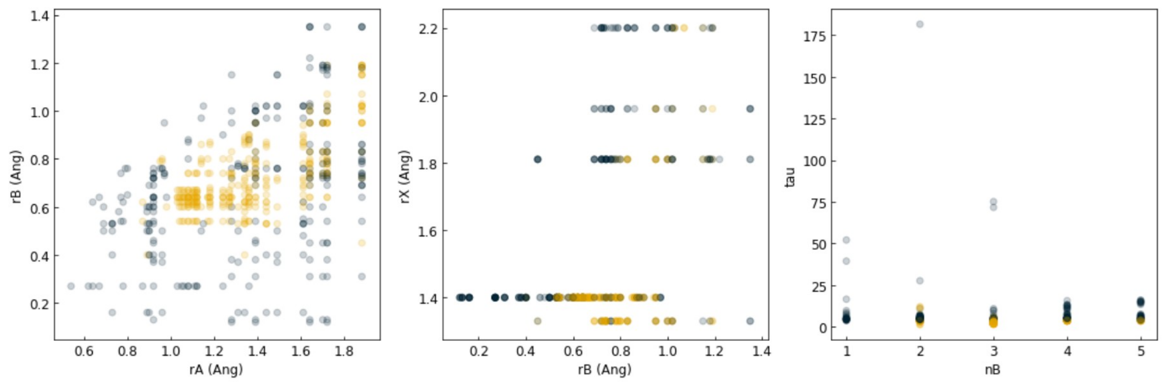
- We only take the continuous variables to form our feature matrix, X.
- The `A`, `B`, `X` columns determine which elements are in the structure, `nA`, `nB`, `nX` columns are the formal oxidation state of each element, and `rA`, `rB`, and `rX` columns are the radii of each element (in Angstrom).
- There are also two additional columns, `t` and `tau`, which are "derived features" that are described in the original publication.
- The outputs, y, are in [-1, 1] and are not perfectly evenly distributed.

In [5]:
```
fig, axes = plt.subplots()
axes.hist(y_perov)
axes.set_xlabel('y')
axes.set_ylabel('Counts')
plt.show()
```

```
/Users/SihoonChoi/opt/anaconda3/lib/python3.7/site-packages/matplotli
b/font_manager.py:1241: UserWarning: findfont: Font family ['sans-ser
if'] not found. Falling back to DejaVu Sans.
  (prop.get_family(), self.defaultFamily[fontext]))
/Users/SihoonChoi/opt/anaconda3/lib/python3.7/site-packages/matplotli
b/figure.py:2369: UserWarning: This figure includes Axes that are not
compatible with tight_layout, so results might be incorrect.
  warnings.warn("This figure includes Axes that are not compatible "
```



In [6]:
```
fig, axes = plt.subplots(1, 3, figsize = (15, 5))

axes[0].scatter(X_perov[:, 3], X_perov[:, 4], c = clrs[y_perov], alpha
= 0.2)
axes[0].set_xlabel(feature_columns[3])
axes[0].set_ylabel(feature_columns[4])

axes[1].scatter(X_perov[:, 4], X_perov[:, 5], c = clrs[y_perov], alpha
= 0.2)
axes[1].set_xlabel(feature_columns[4])
axes[1].set_ylabel(feature_columns[5])

axes[2].scatter(X_perov[:, 1], X_perov[:, 7], c = clrs[y_perov], alpha
= 0.2)
axes[2].set_xlabel(feature_columns[1])
axes[2].set_ylabel(feature_columns[7]);
```



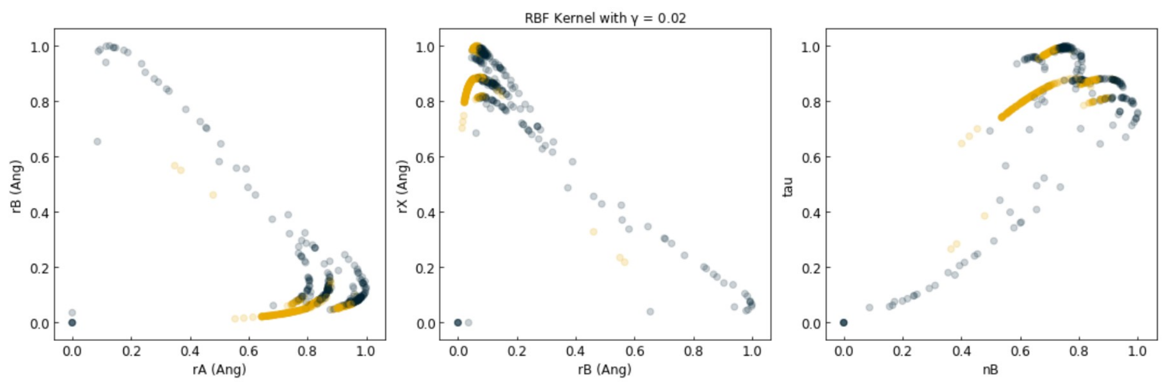
Kernel-based Models

In [7]:
```
from sklearn.metrics.pairwise import rbf_kernel
from sklearn.metrics import accuracy_score, confusion_matrix
```

In [8]:
```
X_kernel = rbf_kernel(X_perov, X_perov, gamma = 0.02)
```

In [9]:
```
fig, axes = plt.subplots(1, 3, figsize = (15, 5))

axes[0].scatter(X_kernel[:, 3], X_kernel[:, 4], c = clrs[y_perov], alph
a = 0.2)
axes[0].set_xlabel(feature_columns[3])
axes[0].set_ylabel(feature_columns[4])

axes[1].scatter(X_kernel[:, 4], X_kernel[:, 5], c = clrs[y_perov], alph
a = 0.2)
axes[1].set_xlabel(feature_columns[4])
axes[1].set_ylabel(feature_columns[5])

axes[2].scatter(X_kernel[:, 1], X_kernel[:, 7], c = clrs[y_perov], alph
a = 0.2)
axes[2].set_xlabel(feature_columns[1])
axes[2].set_ylabel(feature_columns[7])

axes[1].set_title('RBF Kernel with $\gamma$ = 0.02');
```

```
/Users/SihoonChoi/opt/anaconda3/lib/python3.7/site-packages/matplotli
b/figure.py:2369: UserWarning: This figure includes Axes that are not
compatible with tight_layout, so results might be incorrect.
  warnings.warn("This figure includes Axes that are not compatible "
```



In [10]:
```
def add_intercept(X):
    intercept = np.ones((X.shape[0],1))
    X_intercept = np.append(intercept,X,1)
    return X_intercept
```

In [11]:
```
def linear_classifier(X, w):
    X_intercept = add_intercept(X)
    p = np.dot(X_intercept, w)
    return np.array(p > 0, dtype = int)
```

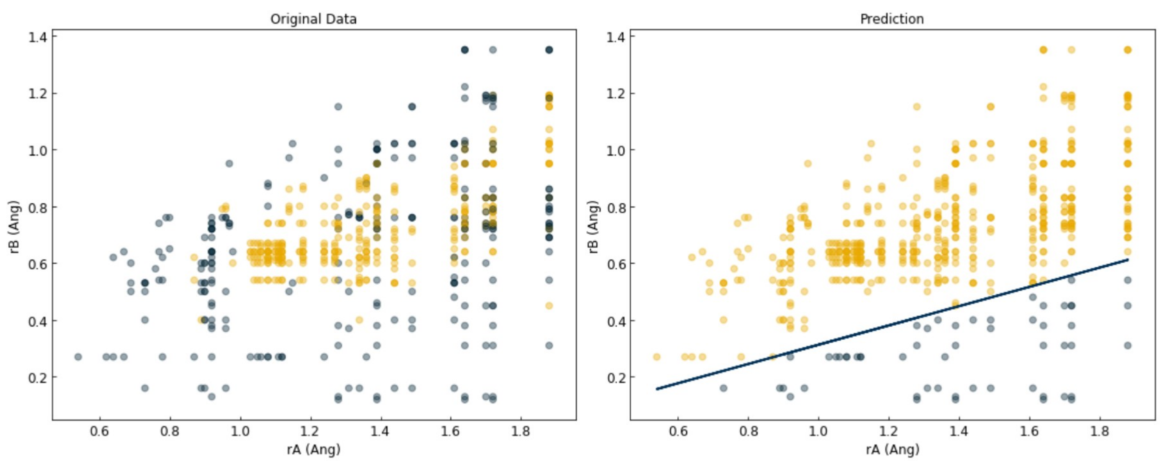
In [12]:
```
def regularized_cost(w, X = X_perov, y = y_perov, alpha = 1):
    X_intercept = add_intercept(X)
    Xb = np.dot(X_intercept, w)
    cost = sum(np.maximum(0, 1 - y*Xb))
    cost += alpha*np.linalg.norm(w[1:], 2)
    return cost
```

In [13]:
```
from scipy.optimize import minimize
```

In [14]:
```
w_guess = np.array([-10, -4, -10])
result = minimize(regularized_cost, w_guess, args = (X_perov[:, 3:5], y
_perov, 1))
w_svm = result.x
```

In [15]:
```
prediction = linear_classifier(X_perov[:, 3:5], w_svm)
prediction = 2 * prediction - 1

fig, axes = plt.subplots(1, 2, figsize = (15, 6))
axes[0].scatter(X_perov[:, 3], X_perov[:, 4], c = clrs[y_perov], alpha
= .4)
axes[0].set_xlabel(feature_columns[3])
axes[0].set_ylabel(feature_columns[4])

axes[1].scatter(X_perov[:, 3], X_perov[:, 4], c = clrs[prediction], alp
ha = .4)
axes[1].set_xlabel(feature_columns[3])
axes[1].set_ylabel(feature_columns[4])

m = -w_svm[1] / w_svm[2]
b = -w_svm[0] / w_svm[2]
axes[1].plot(X_perov[:, 3], m * X_perov[:, 3] + b, ls = '-')

axes[0].set_title('Original Data')
axes[1].set_title('Prediction');
```

```
/Users/SihoonChoi/opt/anaconda3/lib/python3.7/site-packages/matplotli
b/figure.py:2369: UserWarning: This figure includes Axes that are not
compatible with tight_layout, so results might be incorrect.
  warnings.warn("This figure includes Axes that are not compatible "
```



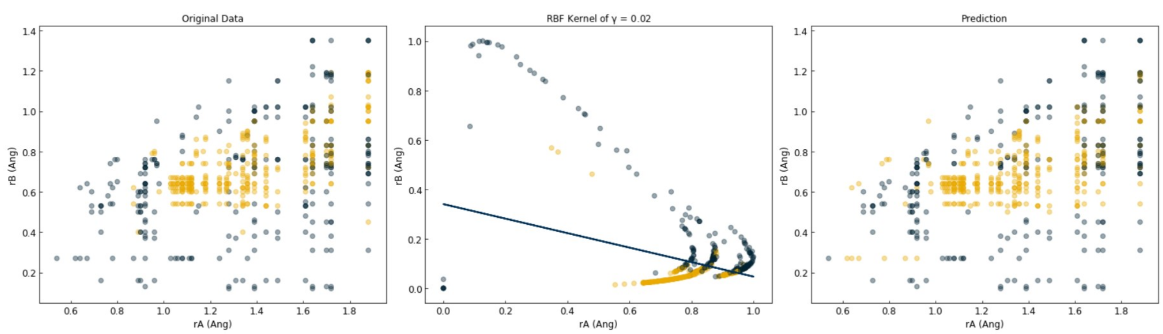
In [16]:
```
print(accuracy_score(y_perov, prediction))
```

```
0.6302083333333334
```

In [17]:
```
w_guess = np.array([-10, -4, -10])
result = minimize(regularized_cost, w_guess, args = (X_kernel[:, 3:5],
y_perov, 1))
w_svm = result.x
```

In [18]:
```
prediction = linear_classifier(X_kernel[:, 3:5], w_svm)
prediction = 2 * prediction - 1

fig, axes = plt.subplots(1, 3, figsize = (21, 6))
axes[0].scatter(X_perov[:, 3], X_perov[:, 4], c = clrs[y_perov], alpha
= .4)
axes[0].set_xlabel(feature_columns[3])
axes[0].set_ylabel(feature_columns[4])

axes[1].scatter(X_kernel[:, 3], X_kernel[:, 4], c = clrs[y_perov], alph
a = .4)
axes[1].set_xlabel(feature_columns[3])
axes[1].set_ylabel(feature_columns[4])

axes[2].scatter(X_perov[:, 3], X_perov[:, 4], c = clrs[prediction], alp
ha = .4)
axes[2].set_xlabel(feature_columns[3])
axes[2].set_ylabel(feature_columns[4])

m = -w_svm[1] / w_svm[2]
b = -w_svm[0] / w_svm[2]
axes[1].plot(X_kernel[:, 3], m * X_kernel[:, 3] + b, ls = '-')

axes[0].set_title('Original Data')
axes[1].set_title('RBF Kernel of $\gamma$ = 0.02')
axes[2].set_title('Prediction');
```

```
/Users/SihoonChoi/opt/anaconda3/lib/python3.7/site-packages/matplotli
b/figure.py:2369: UserWarning: This figure includes Axes that are not
compatible with tight_layout, so results might be incorrect.
  warnings.warn("This figure includes Axes that are not compatible "
```



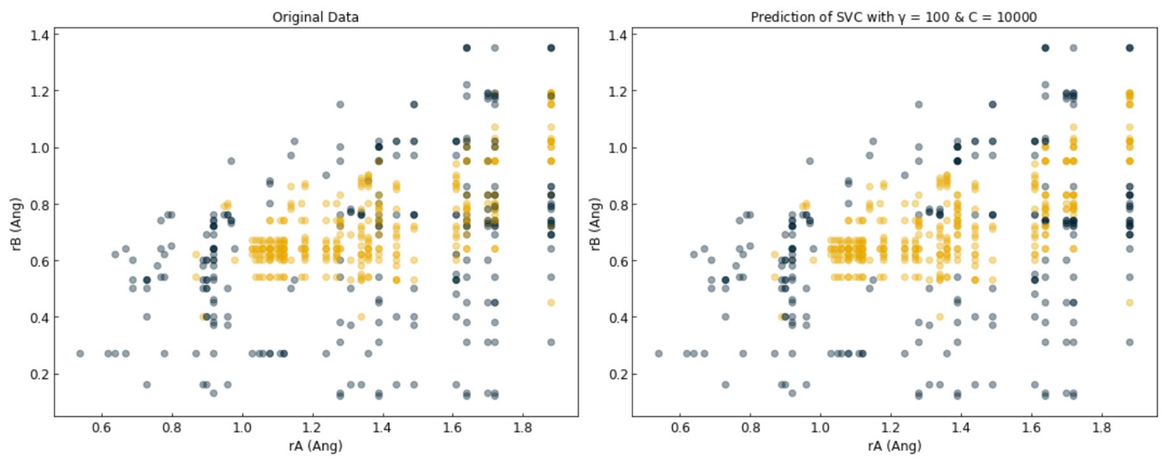
In [19]:
```
print(accuracy_score(y_perov, prediction))
```

```
0.8472222222222222
```

In [20]:
```
from sklearn.svm import SVC
```

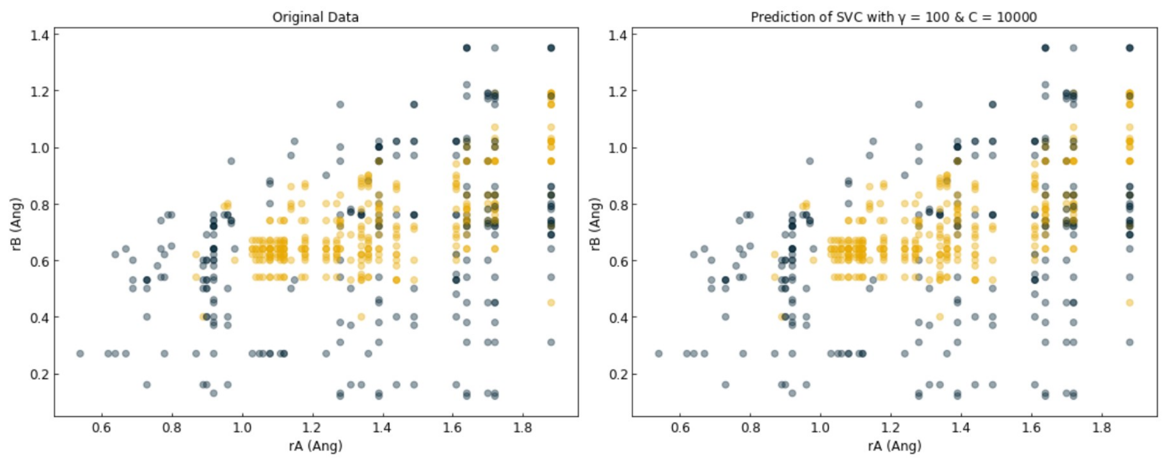
In [21]:
```
model = SVC(kernel = 'rbf', gamma = 100, C = 1000)
model.fit(X_perov[:, 3:5], y_perov)
y_predict = model.predict(X_perov[:, 3:5])

print(model.score(X_perov[:, 3:5], y_perov))

fig, axes = plt.subplots(1, 2, figsize = (15, 6))
axes[0].scatter(X_perov[:, 3], X_perov[:, 4], c = clrs[y_perov], alpha
= .4)
axes[0].set_xlabel(feature_columns[3])
axes[0].set_ylabel(feature_columns[4])

axes[1].scatter(X_perov[:, 3], X_perov[:, 4], c = clrs[y_predict], alph
a = .4)
axes[1].set_xlabel(feature_columns[3])
axes[1].set_ylabel(feature_columns[4])

axes[0].set_title('Original Data')
axes[1].set_title('Prediction of SVC with $\gamma$ = 100 & C = 10000');
```

```
0.9253472222222222

/Users/SihoonChoi/opt/anaconda3/lib/python3.7/site-packages/matplotli
b/figure.py:2369: UserWarning: This figure includes Axes that are not
compatible with tight_layout, so results might be incorrect.
  warnings.warn("This figure includes Axes that are not compatible "
```



In [22]:
```
model = SVC(kernel = 'rbf', gamma = 100, C = 1000)
model.fit(X_perov, y_perov)
y_predict = model.predict(X_perov)

print(model.score(X_perov, y_perov))

fig, axes = plt.subplots(1, 2, figsize = (15, 6))
axes[0].scatter(X_perov[:, 3], X_perov[:, 4], c = clrs[y_perov], alpha
= .4)
axes[0].set_xlabel(feature_columns[3])
axes[0].set_ylabel(feature_columns[4])

axes[1].scatter(X_perov[:, 3], X_perov[:, 4], c = clrs[y_predict], alph
a = .4)
axes[1].set_xlabel(feature_columns[3])
axes[1].set_ylabel(feature_columns[4])

axes[0].set_title('Original Data')
axes[1].set_title('Prediction of SVC with $\gamma$ = 100 & C = 10000');
```

```
0.9965277777777778

/Users/SihoonChoi/opt/anaconda3/lib/python3.7/site-packages/matplotli
b/figure.py:2369: UserWarning: This figure includes Axes that are not
compatible with tight_layout, so results might be incorrect.
  warnings.warn("This figure includes Axes that are not compatible "
```



Comparing Model Performance

We can use a train/test split to check for over-fitting:

In [23]:
```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X_perov, y_perov, t
est_size=0.33)
```

Now, we can work only with the training set to optimize the hyperparameters of the model. Similar to the case of regression, we can take advantage of `GridSearchCV` :

In [24]:
```
from sklearn.model_selection import GridSearchCV
from sklearn.utils import shuffle

X_train, y_train = shuffle(X_train, y_train) #Shuffle everything just f
or good measure

sigmas = np.array([1e-3, 1e-2, 1e-1, 1, 10, 100])
gammas = 1. / 2 / sigmas**2

alphas = np.array([1e-6, 1e-5, 1e-4, 1e-3, 1e-2, 1e-1, 1])
Cs = 1 / alphas

parameter_ranges = {'C': Cs, 'gamma': gammas}

svc = SVC(kernel = 'rbf')

svc_search = GridSearchCV(svc, parameter_ranges, cv = 3)
svc_search.fit(X_train, y_train)
svc_search.best_estimator_, svc_search.best_score_
```

```
/Users/SihoonChoi/opt/anaconda3/lib/python3.7/site-packages/sklearn/m
odel_selection/_search.py:814: DeprecationWarning: The default of the
`iid` parameter will change from True to False in version 0.22 and wi
ll be removed in 0.24. This will change numeric results when test-set
sizes are unequal.
  DeprecationWarning)
```

Out[24]:
```
(SVC(C=99999.99999999999, cache_size=200, class_weight=None, coef0=0.
0,
     decision_function_shape='ovr', degree=3, gamma=0.005, kernel='rb
f',
     max_iter=-1, probability=False, random_state=None, shrinking=Tru
e,
     tol=0.001, verbose=False), 0.922077922077922)
```

Let's investigate the performance of this model on the validation set:

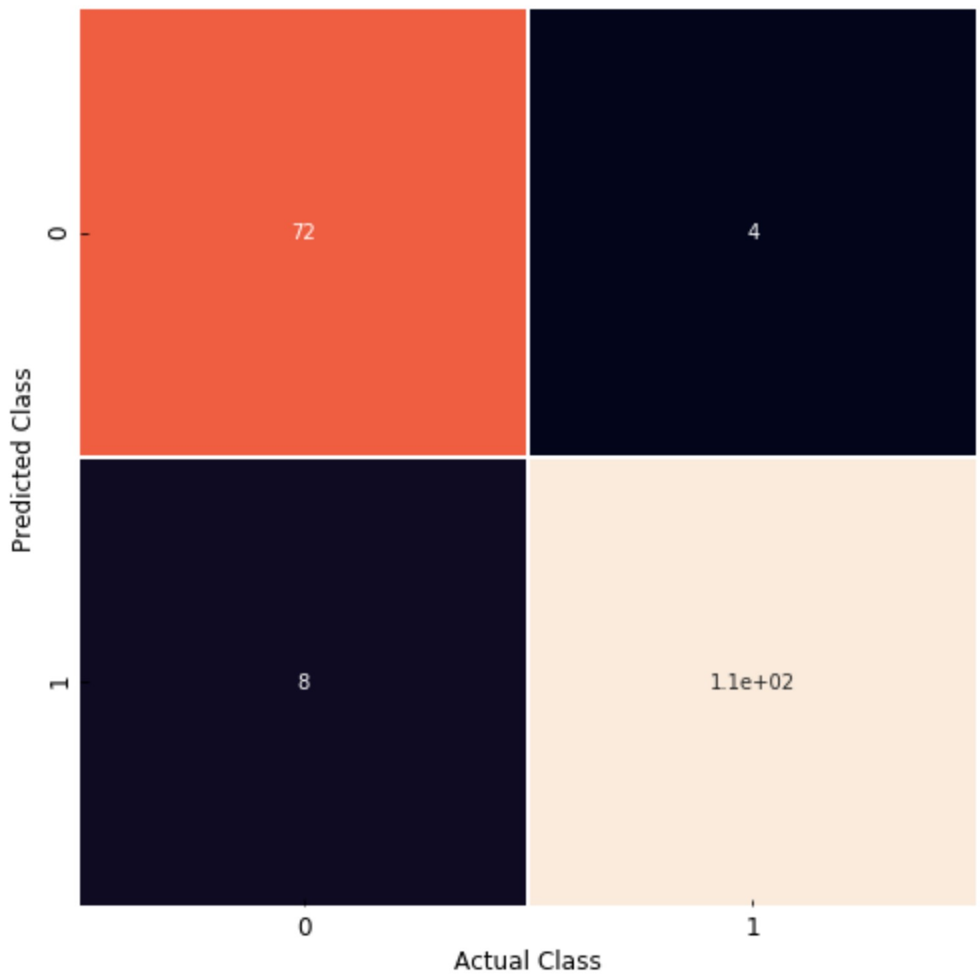
In [25]:
```
best_svc = svc_search.best_estimator_

y_predict = best_svc.predict(X_test)

best_svc.score(X_test, y_test)
```

Out[25]:
```
0.93717277486911
```

We see that it works pretty well. We can also visualize the performance using a confusion matrix:

In [26]:
```
from sklearn.metrics import confusion_matrix
import seaborn as sns

cm = confusion_matrix(y_test, y_predict)

fig, ax = plt.subplots(figsize = (7, 7))
sns.heatmap(cm, annot = True, linewidth = .45, cbar = False)
ax.set_xlabel('Actual Class')
ax.set_ylabel('Predicted Class');
```

```
/Users/SihoonChoi/opt/anaconda3/lib/python3.7/site-packages/matplotli
b/font_manager.py:1241: UserWarning: findfont: Font family ['sans-ser
if'] not found. Falling back to DejaVu Sans.
  (prop.get_family(), self.defaultFamily[fontext]))
/Users/SihoonChoi/opt/anaconda3/lib/python3.7/site-packages/matplotli
b/figure.py:2369: UserWarning: This figure includes Axes that are not
compatible with tight_layout, so results might be incorrect.
  warnings.warn("This figure includes Axes that are not compatible "
```



Exercise: Calculate the accuracy, precision, and recall for the best SVC model on the perovskite dataset.

In [27]:
```
from sklearn.tree import DecisionTreeClassifier

dtree=DecisionTreeClassifier()
dtree.fit(X_train,y_train)
y_predict = dtree.predict(X_train)

cm_train = confusion_matrix(y_train, y_predict)
```

We see that the model performs very well on the training set. However, what we really want to check is the test set:

In [28]:
```
y_predict = dtree.predict(X_test)
cm_test = confusion_matrix(y_test, y_predict)
```

In [29]:
```
fig, axes = plt.subplots(1, 2, figsize = (12, 6))
sns.heatmap(cm_train, annot = True, cbar = False, linewidth = .5, ax =
axes[0], fmt = 'd')
sns.heatmap(cm_test, annot = True, cbar = False, linewidth = .5, ax = a
xes[1], fmt = 'd')

axes[0].set_xlabel('Actual Class')
axes[0].set_ylabel('Predicted Class')
axes[0].set_title('Performance on the Training Set')

axes[1].set_xlabel('Actual Class')
axes[1].set_ylabel('Predicted Class')
axes[1].set_title('Performance on the Test Set');
```

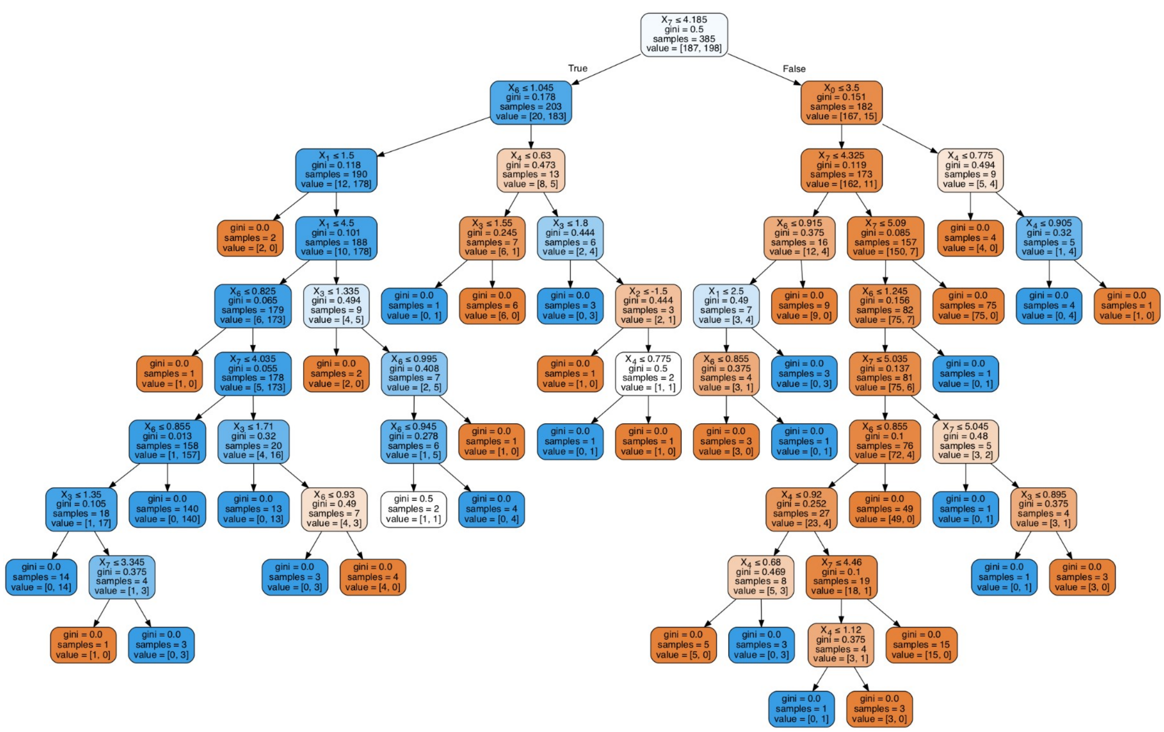
```
/Users/SihoonChoi/opt/anaconda3/lib/python3.7/site-packages/matplotli
b/figure.py:2369: UserWarning: This figure includes Axes that are not
compatible with tight_layout, so results might be incorrect.
  warnings.warn("This figure includes Axes that are not compatible "
```

We see that the performance is worse, but not too bad. Let's visualize the model to get some intuition about how it is working:

In [30]:
```
from sklearn.externals.six import StringIO
from IPython.display import Image
from sklearn.tree import export_graphviz
import pydotplus

dot_data = StringIO()
export_graphviz(dtree, out_file = dot_data,
                filled = True, rounded = True,
                special_characters = True)
graph = pydotplus.graph_from_dot_data(dot_data.getvalue())
Image(graph.create_png())
```

```
/Users/SihoonChoi/opt/anaconda3/lib/python3.7/site-packages/sklearn/e
xternals/six.py:31: DeprecationWarning: The module is deprecated in v
ersion 0.21 and will be removed in version 0.23 since we've dropped s
upport for Python 2.7. Please rely on the official version of six (ht
tps://pypi.org/project/six/).
  "(https://pypi.org/project/six/).", DeprecationWarning)
```

Out[30]:



We see that the tree is very complicated! However, we see that we can "read" the tree and make intuitive sense of how the model works. This is one of the greatest strengths of the decision tree. We can also control the complexity of the tree by limiting its maximum depth:

In [31]:
```
dtree = DecisionTreeClassifier(max_depth = 3)
dtree.fit(X_train,y_train)
y_predict = dtree.predict(X_train)

cm_train = confusion_matrix(y_train, y_predict)
```

We see that the training performance is slightly poorer if the max depth is limited. However, the test performance is comparable:

In [32]:
```
y_predict = dtree.predict(X_test)
cm_test = confusion_matrix(y_test, y_predict)
```

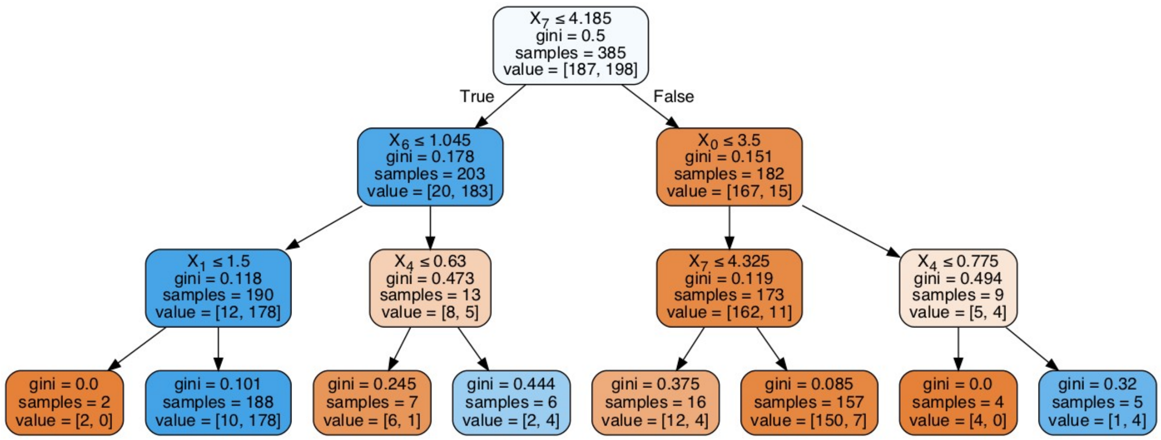
In [33]:
```
fig, axes = plt.subplots(1, 2, figsize = (12, 6))
sns.heatmap(cm_train, annot = True, cbar = False, linewidth = .5, ax =
axes[0], fmt = 'd')
sns.heatmap(cm_test, annot = True, cbar = False, linewidth = .5, ax = a
xes[1], fmt = 'd')

axes[0].set_xlabel('Actual Class')
axes[0].set_ylabel('Predicted Class')
axes[0].set_title('Performance on the Training Set')

axes[1].set_xlabel('Actual Class')
axes[1].set_ylabel('Predicted Class')
axes[1].set_title('Performance on the Test Set');
```

```
/Users/SihoonChoi/opt/anaconda3/lib/python3.7/site-packages/matplotli
b/figure.py:2369: UserWarning: This figure includes Axes that are not
compatible with tight_layout, so results might be incorrect.
  warnings.warn("This figure includes Axes that are not compatible "
```

We can also visualize the tree:

In [34]:
```
from sklearn.externals.six import StringIO
from IPython.display import Image
from sklearn.tree import export_graphviz
import pydotplus

dot_data = StringIO()
export_graphviz(dtree, out_file = dot_data,
                filled = True, rounded = True,
                special_characters = True)
graph = pydotplus.graph_from_dot_data(dot_data.getvalue())
Image(graph.create_png())
```

Out[34]:



Discussion: Which variable is most important for determining whether or not a material will form a perovskite?