CA4 - Eirik H?yheim

April 9, 2021

1 CA4 - Eirik Høyheim

1.1 Imports

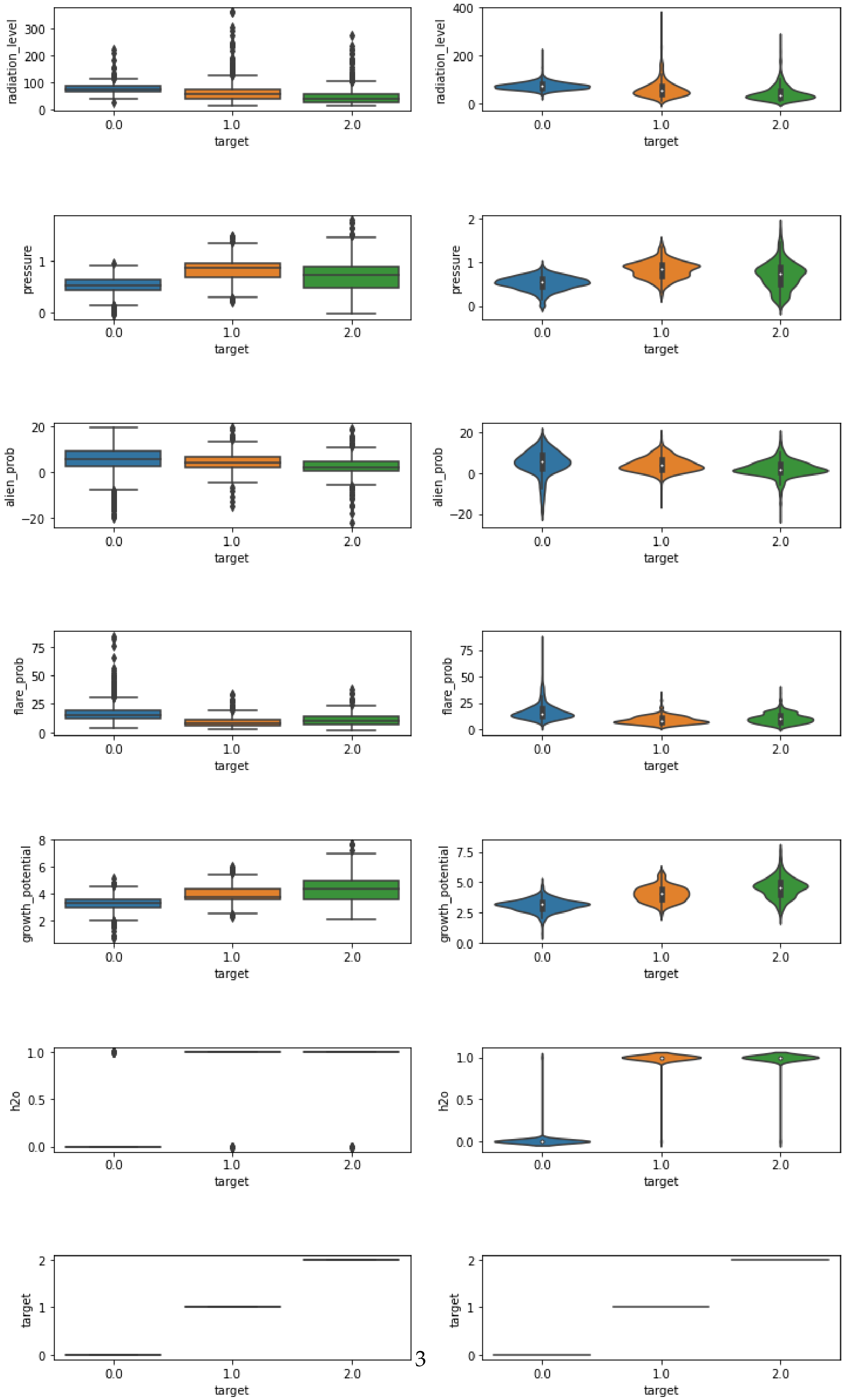
[1]:
```
import pandas as pd
import numpy as np
import copy
import time
import matplotlib.pyplot as plt
import seaborn as sns


from sklearn.model_selection import train_test_split
from sklearn.preprocessing import LabelEncoder, StandardScaler
from sklearn.impute import SimpleImputer

from sklearn.pipeline import make_pipeline
from sklearn.decomposition import KernelPCA, PCA
from sklearn.model_selection import GridSearchCV, cross_val_score
from sklearn.metrics import confusion_matrix

from sklearn.svm import SVC
from sklearn.linear_model import LogisticRegression
from sklearn.ensemble import RandomForestClassifier

from sklearn.metrics import roc_curve, auc
from sklearn.model_selection import StratifiedKFold
from numpy import interp
```

[2]:
```
train_raw = pd.read_csv("data/train.csv")
test_raw = pd.read_csv("data/test.csv")

class_le = LabelEncoder()
train_raw["target"] = class_le.fit_transform(train_raw["target"].values)  #␣
 ↪Changes names of targets to numbers
```

```
imr = SimpleImputer(missing_values=np.nan, strategy="median")  # Initialize the␣
 ↪imputer, will change NaNs to column median
imr = imr.fit(train_raw.values)  # fit all values into the imputer
train_no_nan = copy.copy(imr.transform(train_raw.values)) # change all NaN␣
 ↪values to the column median

train_no_nan = pd.DataFrame(train_no_nan, columns=train_raw.columns)  #␣
 ↪Transforming numpy array into pandas dataframe for easier visualization

X = copy.copy(train_no_nan.iloc[:, :-1]) # Seperates the data, X: all columns␣
 ↪but not target
y = copy.copy(train_no_nan.iloc[:, -1])  # y: all targets (0, 1, 2)

X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, stratify=y, random_state=1)
```

1.2 Visualization

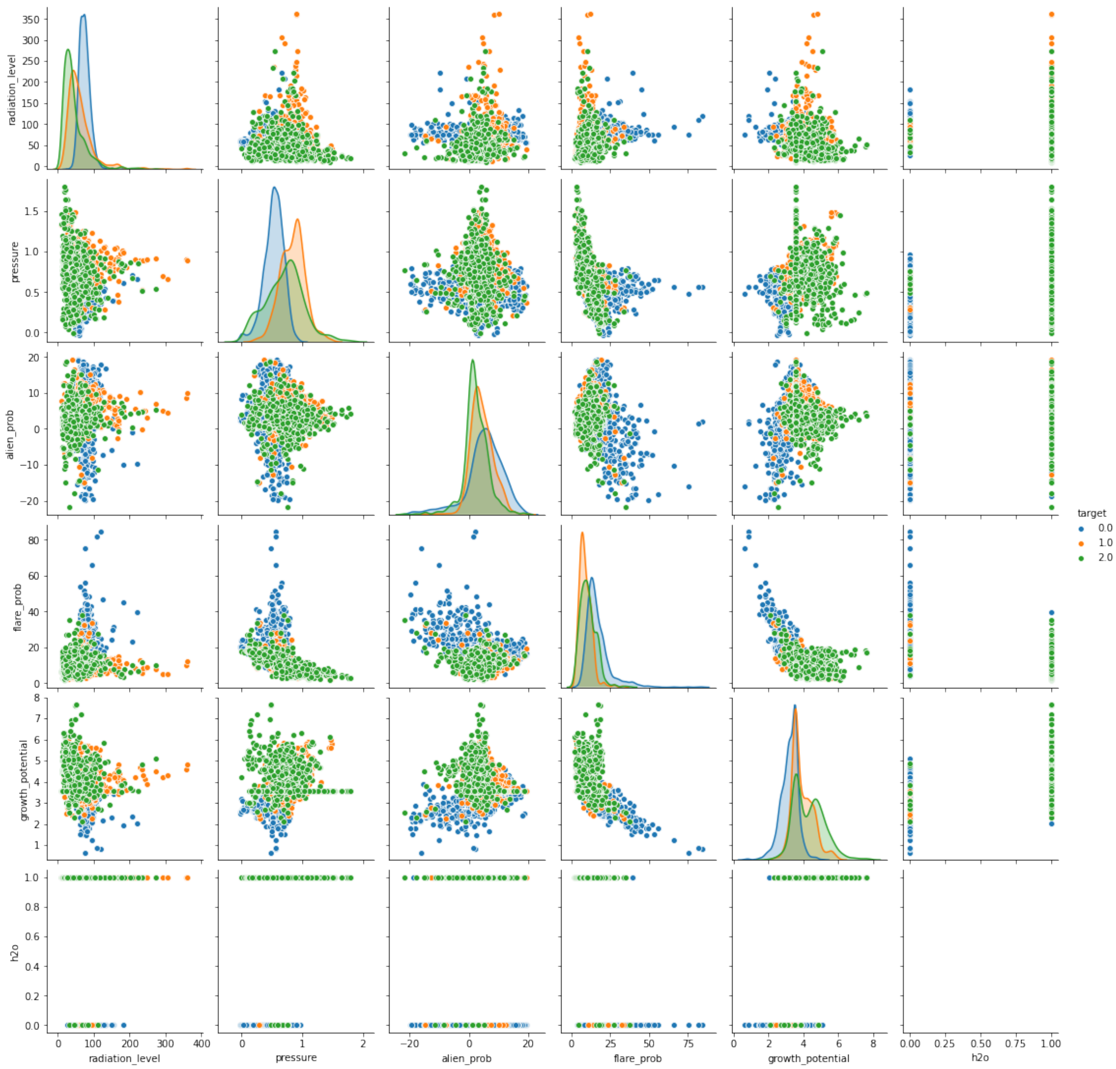
[3]:
```
columns = train_no_nan.columns  # all columns in train_no_nan
fig, ax = plt.subplots(len(columns), 2, figsize=(12,20))  # prepairs subplots␣
 ↪for all columns
plt.subplots_adjust(bottom=.2, top=1, hspace=1)
for index, col in enumerate(columns):
    sns.boxplot(ax=ax[index, 0], y=train_no_nan[col], x=train_no_nan["target"])␣
 ↪ # plots a boxplot for all columns with seperation on targets
    sns.violinplot(ax=ax[index, 1], data=train_no_nan, y=train_raw[col],␣
 ↪x=train_no_nan["target"])  # plots a violin polot for all columns with␣
 ↪seperation on targets
```


radiation_level
pressure
alien_prob
flare_prob
growth_potential
h2o
target
0.0
1.0
2.0

We can see that the `h2o` feature makes it easier to seperate class 0 from 1 and 2 because the majority of all plantes that does not have water, is non-habitable. There is also some features that seems to have alot of consentrated points, as in feature `flare_prob` and `radiation_level`. `alien_prob` is on a "weird" scale, since it goes from about -20 to 20, and not positive procent points.

[4]:
```
sns.pairplot(train_no_nan, hue="target")
plt.show()
```

```
C:\Users\eirik\Anaconda3\lib\site-packages\seaborn\distributions.py:369:
UserWarning: Default bandwidth for data is 0; skipping density estimation.
  warnings.warn(msg, UserWarning)
C:\Users\eirik\Anaconda3\lib\site-packages\seaborn\distributions.py:369:
UserWarning: Default bandwidth for data is 0; skipping density estimation.
  warnings.warn(msg, UserWarning)
C:\Users\eirik\Anaconda3\lib\site-packages\seaborn\distributions.py:369:
UserWarning: Default bandwidth for data is 0; skipping density estimation.
  warnings.warn(msg, UserWarning)
```



Non of the features is linearly seperable out of the box. `flare_prob` and `radiation_level` seems to be very skeewed, which fits with the observations we did in the box- and violin plots.

1.3 Pipline with kernel, SVM using Kernel PCA

[5]:
```
pipe_svc = make_pipeline(StandardScaler(),
                         KernelPCA(),
                         SVC(random_state=1))  # Pipline containing a Standard Scaler, Kernal PCA and SVM.

param_range  = np.arange(2.5, 2.9, 0.1) # For regularization parameter C.
param_range2 = np.arange(3.3, 4, 0.1) # For scaling parameter gamma in rbf-kernel for SVC.
param_range3 = np.arange(5, 7, 1)  # for n_components pca
param_range4 = np.arange(0.001, 0.04, 0.01) # for gamma KPCA
```

```
param_grid   = [{'kernelpca__n_components': param_range3,
                 'kernelpca__kernel':['rbf'],
                 'kernelpca__gamma': param_range4,
                 'svc__C': param_range,
                 'svc__kernel': ['linear']},
                {'kernelpca__n_components': param_range3,
                 'kernelpca__kernel':['rbf'],
                 'kernelpca__gamma': param_range4,
                 'svc__C': param_range,
                 'svc__gamma': param_range2,
                 'svc__kernel': ['rbf']}
    ]  # param_grid containing all parameters that I want to change to get the␣
 ↪most optimal solution for the SVM algorithm

# Inner loop
gs = GridSearchCV(estimator  = pipe_svc,
                  param_grid = param_grid,
                  scoring    = 'accuracy',
                  cv         = 10,
                  n_jobs     = -1)  # Searching through all possible␣
 ↪combinations from param_grid. Cross-validation with 10 folds


t1 = time.time()
gs = gs.fit(X_train, y_train)  # Fit the training data to grid search to find␣
 ↪the parameters that gives the highest score
t2 = time.time()

print(f"Best score: {gs.best_score_}")
print(f"Best params:\n{gs.best_params_}")  # Printing out the best parameters␣
 ↪for further use
print(f"Time: {(t2-t1):.3f}s")
```

```
Best score: 0.8724221105527639
Best params:
{'kernelpca__gamma': 0.030999999999999996, 'kernelpca__kernel': 'rbf',
'kernelpca__n_components': 6, 'svc__C': 2.5, 'svc__gamma': 3.6, 'svc__kernel':
'rbf'}
Time: 214.269s
```

[6]:

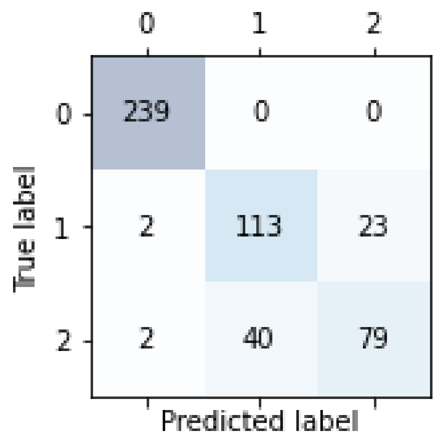
```
clf = gs.best_estimator_
clf.fit(X_train, y_train)
print(f"Test accuracy: {clf.score(X_test, y_test):.3f}")  # Looking at how the␣
 ↪model preformed against the test set
```

```
Test accuracy: 0.865
```

[7]:
```python
# Cross-validation
pipe_svc = make_pipeline(StandardScaler(),
                         KernelPCA(n_components=6, kernel='rbf', gamma=0.031),
                         SVC(random_state=1, kernel='rbf', C=2.7, gamma=3.4)) ␣
 ↪# a pipline containing the best parameters found in the grid search

scores = cross_val_score(estimator=pipe_svc,
                        X=X_train,
                        y=y_train,
                        cv=10,      # 10 cross-validation
                        n_jobs=-1)  # uses all CPUs when running

print(f"CV accuracy: {np.mean(scores):.3f} +/- {np.std(scores):.3f}")  # going␣
 ↪through a cross valdiation with the best parameters to see how stable the␣
 ↪model is
```

```
CV accuracy: 0.872 +/- 0.028
```

[8]:
```python
# Confusion matrix
y_pred = clf.predict(X_test)  # What my model think the target of X_test data␣
 ↪is
confmat = confusion_matrix(y_true=y_test, y_pred=y_pred)   # Creating a␣
 ↪confusion matrix by compairing true target against predicted target

fig, ax = plt.subplots(figsize=(2.5, 2.5))
ax.matshow(confmat, cmap=plt.cm.Blues, alpha=0.3)
for i in range(confmat.shape[0]):
    for j in range(confmat.shape[1]):
        ax.text(x=j, y=i, s=confmat[i, j], va='center', ha='center')

plt.xlabel('Predicted label')
plt.ylabel('True label')

plt.tight_layout()
plt.show()
```



As we can see, the model was not able to predict 0 (non-habitable) right only four times. The model was not as efficient of seperating between class 1 (potentially-habitable) and class 2 (very-habitable). It guessed 23 times that the class was 2 when it was 1, and 40 times 1 when the class was 2. Overall, the model guessed more right than wronge, but in the future it would be a good idea to do some feature enginering to seperate label 1 and 2 to make it easier for the model to seperate between the two classes.

1.4 Pipeline with regularization, Logistic Regression using L1 and L2 regularization

[9]:
```
pipe_lr = make_pipeline(StandardScaler(),
                        PCA(),
                        LogisticRegression(random_state=1))  # Pipeline␣
 ↪containing Standard Scaler, PCA and Logitsic Regression

param_range  = np.arange(0.1, 6, 0.1) # For regularization parameter C.


param_grid   = [
    {'pca__n_components': [None, 5, 6],
     'logisticregression__C': param_range,
     'logisticregression__penalty': ['l2'],
     'logisticregression__solver': ['newton-cg', 'lbfgs', 'saga', 'sag']},
    {'pca__n_components': [None, 5, 6],
     'logisticregression__C': param_range,
     'logisticregression__penalty': ['l1'],
     'logisticregression__solver': ['liblinear']}
    ]  # param_grid containing all parameters that I want to change to get the␣
 ↪most optimal solution for the SVM algorithm

gs = GridSearchCV(estimator  = pipe_lr,
                  param_grid = param_grid,
                  scoring    = 'accuracy',
```

```
                  cv          = 10
                  n_jobs      = -1)  # Searching through all possible␣
 ↪combinations from param_grid. Cross-validation with 10 fold


t1 = time.time()
gs = gs.fit(X_train, y_train)  # Fit the training data to grid search to find␣
 ↪the parameters that gives the highest score
t2 = time.time()

print(f"Best score: {gs.best_score_}")
print(f"Best params:\n{gs.best_params_}")
print(f"Time: {(t2-t1):.3f}s")
```

```
Best score: 0.8558492462311558
Best params:
{'logisticregression__C': 0.8, 'logisticregression__penalty': 'l2',
'logisticregression__solver': 'newton-cg', 'pca__n_components': None}
Time: 321.635s
```

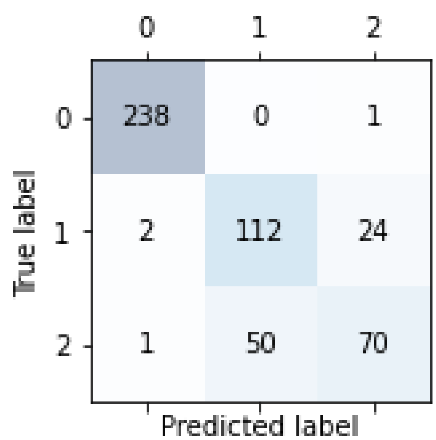
[10]:
```
clf = gs.best_estimator_
clf.fit(X_train, y_train)
print(f"Test accuracy: {clf.score(X_test, y_test):.3f}")
```

```
Test accuracy: 0.843
```

[11]:
```
# cross validation
pipe_lr = make_pipeline(StandardScaler(),
                        PCA(n_components=None),
                        LogisticRegression(penalty='l1',
                                           random_state=1,
                                           C=0.3,
                                           solver='liblinear'))  # a pipline␣
 ↪containing the best parameters found in the grid search
scores = cross_val_score(estimator=pipe_lr,
                        X=X_train,
                        y=y_train,
                        cv=10,      # 10 cross-validation
                        n_jobs=-1)

print(f"CV accuracy: {np.mean(scores):.3f} +/- {np.std(scores):.3f}")  # going␣
 ↪through a cross valdiation with the best parameters to see how stable the␣
 ↪model is
```

```
CV accuracy: 0.852 +/- 0.023
```

[12]:
```python
# confusion matrix
y_pred = clf.predict(X_test)
confmat = confusion_matrix(y_true=y_test, y_pred=y_pred)

fig, ax = plt.subplots(figsize=(2.5, 2.5))
ax.matshow(confmat, cmap=plt.cm.Blues, alpha=0.3)
for i in range(confmat.shape[0]):
    for j in range(confmat.shape[1]):
        ax.text(x=j, y=i, s=confmat[i, j], va='center', ha='center')

plt.xlabel('Predicted label')
plt.ylabel('True label')

plt.tight_layout()
plt.show()
```



Logistic regression missclassified class 1 and 2 more than SVM. It also had a worse score than SVM.

1.5 Bonus, Random Forest with PCA

[13]:
```python
pipe_forest = make_pipeline(
    PCA(),
    RandomForestClassifier(random_state=1, n_jobs=-1, n_estimators=1000)
)

param_range  = np.arange(14, 20, 1) # For max_depth

param_range2 = np.arange(2, 3, 1)  # for min_samples_split

param_range3 = np.arange(1, 2, 1)  # for min_samples_leaf
```

```
param_grid   = [
    {'randomforestclassifier__max_depth': param_range,
     'pca__n_components': [5, 6],
     'randomforestclassifier__min_samples_split': param_range2,
     'randomforestclassifier__min_samples_leaf': param_range3,
     'randomforestclassifier__oob_score': [True],
     'randomforestclassifier__criterion': ['gini', 'entropy']
    }
]



gs = GridSearchCV(estimator=pipe_forest,
                  param_grid=param_grid,
                  scoring='accuracy',
                  cv=5,  # fewer cross-validations to reduce time usage
                  n_jobs=-1)

t1 = time.time()
gs = gs.fit(X_train, y_train)
t2 = time.time()

print(gs.best_score_)
print(gs.best_params_)
print(f"Time: {(t2-t1):.3f}s")
```

```
0.8865064671729576
{'pca__n_components': 6, 'randomforestclassifier__criterion': 'gini',
'randomforestclassifier__max_depth': 17,
'randomforestclassifier__min_samples_leaf': 1,
'randomforestclassifier__min_samples_split': 2,
'randomforestclassifier__oob_score': True}
Time: 194.008s
```

[14]:
```
clf = gs.best_estimator_
clf.fit(X_train, y_train)
print(f"Test accuracy: {clf.score(X_test, y_test):.3f}")
```

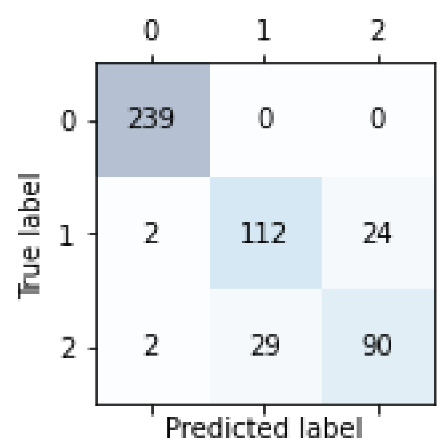
```
Test accuracy: 0.886
```

[15]:
```
# Cross val
pipe_forest = make_pipeline(
    KernelPCA(kernel='linear',
              n_components=6),
    RandomForestClassifier(random_state=1, n_jobs=-1, n_estimators=2000,␣
 ↪max_depth=17, oob_score=True, criterion='gini')
)
scores = cross_val_score(estimator=pipe_forest,
```

```
                        X=X_train,
                        y=y_train,
                        cv=10,
                        n_jobs=-1)
print(f"CV accuracy: {np.mean(scores):.3f} +/- {np.std(scores):.3f}")
```

```
CV accuracy: 0.887 +/- 0.025
```

[16]:
```
# Confusion matrix
y_pred = clf.predict(X_test)
confmat = confusion_matrix(y_true=y_test, y_pred=y_pred)

fig, ax = plt.subplots(figsize=(2.5, 2.5))
ax.matshow(confmat, cmap=plt.cm.Blues, alpha=0.3)
for i in range(confmat.shape[0]):
    for j in range(confmat.shape[1]):
        ax.text(x=j, y=i, s=confmat[i, j], va='center', ha='center')

plt.xlabel('Predicted label')
plt.ylabel('True label')

plt.tight_layout()
plt.show()
```



Random forrest predicted the same amount to be class zero as SVM, but managed to predict more classes right when label was 1 and 2 compared to both SVM and Logistic Regression.

1.6 Submission to Kaggle

1.6.1 Best model of SVM and Logistic regression

The model with the highest training score and test score was SVM.

[17]:
```python
pipe_svc = make_pipeline(StandardScaler(),
                         KernelPCA(n_components=6, kernel='rbf', gamma=0.031),
                         SVC(random_state=1, kernel='rbf', C=2.7, gamma=3.4))
pipe_svc.fit(X, y)


imr = SimpleImputer(missing_values=np.nan, strategy="median")
imr = imr.fit(test_raw.values)
test = copy.copy(imr.transform(test_raw.values))


y_predictions = pipe_svc.predict(test)
my_submission = {"Id": [], "Predicted": []}
for pred_id, pred in enumerate(y_predictions):
    my_submission["Id"].append(pred_id)
    my_submission["Predicted"].append(int(pred))

submission_ready = pd.DataFrame(my_submission)
submission_ready.to_csv("submissions/svc_rbf__kpca_rbf__strategy_median",␣
 ↪index=False)
```

Score on Kaggle public leaderboard: **0.88554**

1.6.2 Random Forest

[18]:
```
pipe_forest = make_pipeline(
    KernelPCA(kernel='linear',
             n_components=6),
    RandomForestClassifier(random_state=1, n_jobs=-1, n_estimators=2000,␣
 ↪max_depth=17, oob_score=True, criterion='gini')
)
pipe_forest.fit(X, y)


imr = SimpleImputer(missing_values=np.nan, strategy="median")
imr = imr.fit(test_raw.values)
test = copy.copy(imr.transform(test_raw.values))


y_predictions = pipe_forest.predict(test)
my_submission = {"Id": [], "Predicted": []}
for pred_id, pred in enumerate(y_predictions):
    my_submission["Id"].append(pred_id)
    my_submission["Predicted"].append(int(pred))

submission_ready = pd.DataFrame(my_submission)
submission_ready.to_csv("submissions/random_forest__pca__strategy_median",␣
 ↪index=False)
```

Score on Kaggle public leaderboard: **0.89608**
This was my highest score on the public leaderboard.

1.7 ROC-curve

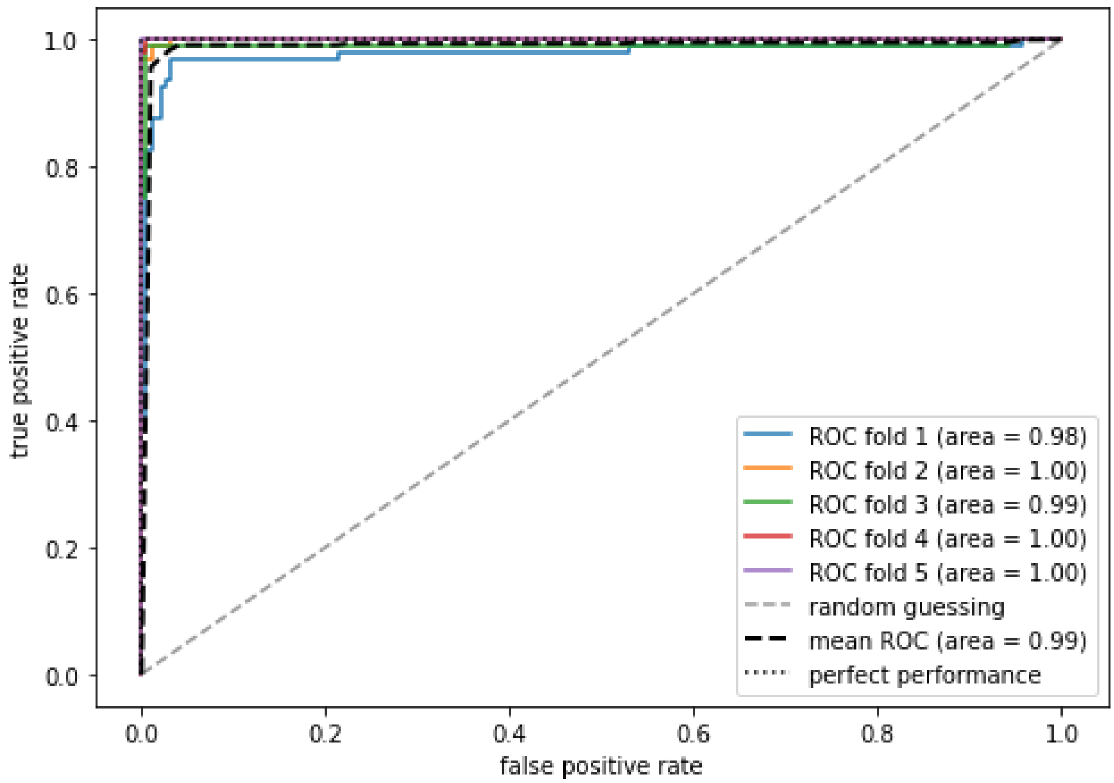
[19]:
```
X_train = X_train[y_train != 1].values  # Removing all ones from the data (1␣
 ↪represent potentially-habitable)
y_train = y_train[y_train != 1].values
```

All code below taken from lecture 6, part 2b and https://github.com/rasbt/python-machine-learning-book-3rd-edition/blob/master/ch06/ch06.ipynb with some modifications to fit the data

[20]:
```
# Set up pipeline with scale, decomposer and classifyer
pipe_lr = make_pipeline(StandardScaler(),
                        PCA(n_components=None),
                        LogisticRegression(penalty='l1',
                                           random_state=1,
                                           C=0.3,
                                           solver='liblinear'))
# Reduced variable set
X_train2 = X_train[:, :]

# Cross-validation specification
cv = list(StratifiedKFold(n_splits=5).split(X_train, y_train))
```

```
fig = plt.figure(figsize=(7, 5))

mean_tpr = 0.0
mean_fpr = np.linspace(0, 1, 100)
all_tpr = []

# Loop through folds of CV
for i, (train, test) in enumerate(cv):
    probas = pipe_lr.fit(X_train2[train],
                         y_train[train]).predict_proba(X_train2[test]) #␣
 ↪Predict probability of classes

    # False Positive and True Positive Rates (thresholds for the decision␣
 ↪function)
    fpr, tpr, thresholds = roc_curve(y_train[test],
                                     probas[:, 1],
                                     pos_label=2)
    # Add to mean True Predictive Rate in a smoothed variant (interpolated)
    mean_tpr += interp(mean_fpr, fpr, tpr)
    roc_auc = auc(fpr, tpr)
    plt.plot(fpr,
             tpr,
             label='ROC fold %d (area = %0.2f)'
                   % (i+1, roc_auc))

plt.plot([0, 1],
         [0, 1],
         linestyle='--',
         color=(0.6, 0.6, 0.6),
         label='random guessing')

# Average True Positive Rate
mean_tpr /= len(cv)
mean_tpr[0] = 0.0
mean_tpr[-1] = 1.0
# Average AUC
mean_auc = auc(mean_fpr, mean_tpr)
plt.plot(mean_fpr, mean_tpr, 'k--',
         label='mean ROC (area = %0.2f)' % mean_auc, lw=2)
plt.plot([0, 0, 1],
         [0, 1, 1],
         linestyle=':',
         color='black',
         label='perfect performance')

plt.xlim([-0.05, 1.05])
```

```
plt.ylim([-0.05, 1.05])
plt.xlabel('false positive rate')
plt.ylabel('true positive rate')
plt.legend(loc="lower right")

plt.tight_layout()
plt.show()
```



As we can see from the ROC-curve, there are almost no false positivs and almost a "perfect" (no false positivs) ROC-curve. This indicates that it is fearly easy to seperate class 0 (non-habitable) and class 2 (very-habitable).