

Lec 16 - scikit-learn classification

Statistical Computing and Computation

Sta 663 | Spring 2022

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OpenIntro - Spam

We will start by looking at a data set on spam emails from the OpenIntro project. A full data dictionary can be found [here](#). To keep things simple this week we will restrict our exploration to including only the following columns: `spam`, `exclaim_mess`, `format`, `num_char`, `line_breaks`, and `number`.

- `spam` - Indicator for whether the email was spam.
- `exclaim_mess` - The number of exclamation points in the email message.
- `format` - Indicates whether the email was written using HTML (e.g. may have included bolding or active links).
- `num_char` - The number of characters in the email, in thousands.
- `line_breaks` - The number of line breaks in the email (does not count text wrapping).
- `number` - Factor variable saying whether there was no number, a small number (under 1 million), or a big number.

```
email = pd.read_csv('data/email.csv')[['spam', 'exclaim_mess', 'format', 'num_char', 'line_breaks', 'number']]

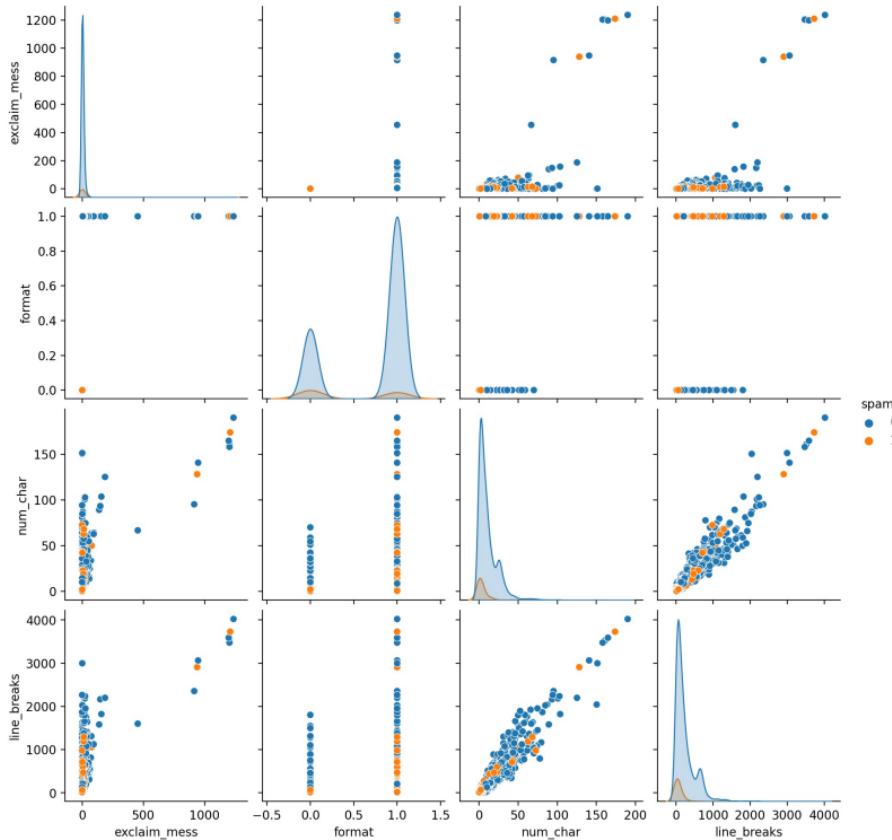
##      spam exclaim_mess format num_char line_breaks number
## 0        0            0      1    11.370       202    big
## 1        0            1      1    10.504       202   small
## 2        0            6      1     7.773       192   small
## 3        0           48      1    13.256       255   small
## 4        0            1      0     1.231        29  none
## ...
## 3916     1            0      0     0.332        12  small
## 3917     1            0      0     0.323        15  small
## 3918     0            5      1     8.656       208  small
## 3919     0            0      0    10.185       132  small
## 3920     1            1      0     2.225        65  small
##
## [3921 rows x 6 columns]
```

Given that `number` is categorical, we will take care of the necessary dummy coding via `pd.get_dummies()`,

```
email_dc = pd.get_dummies(email)
email_dc
```

```
##      spam exclaim_mess format num_char line_breaks number_big number_none number_small
```

```
sns.pairplot(email, hue='spam')
```



Model fitting

```
from sklearn.linear_model import LogisticRegression

y = email_dc.spam
X = email_dc.drop('spam', axis=1)

m = LogisticRegression(fit_intercept = False).fit(X, y)

m.feature_names_in_
## array(['exclaim_mess', 'format', 'num_char', 'line_breaks', 'number_big', 'number_none', 'number_small'], dt
m.coef_
## array([[ 0.00982, -0.61893,  0.0545 , -0.00556, -1.21224, -0.69336, -1.92076]])
```

A quick comparison

```
glm(spam ~ . - 1, data = d, family=binomial)

##
## Call: glm(formula = spam ~ . - 1, family = binomial, data =
## 
## Coefficients:
##   exclaim_mess      format     num_char  line_breaks    nu
##   0.009587     -0.604782     0.054765   -0.005480    -1
##   numbernone  numbersmall
##   -0.706843     -1.950440
## 
## Degrees of Freedom: 3921 Total (i.e. Null); 3914 Residual
## Null Deviance: 5436
## Residual Deviance: 2144 AIC: 2158
```

```
m.feature_names_in_
## array(['exclam_mess', 'format', 'num_char', 'line_breaks', '']
m.coef_
## array([[ 0.00982, -0.61893,  0.0545, -0.00556, -1.21224, -0.
```

Why are these different?

```
sklearn.linear_model.LogisticRegression
```

•

This class implements regularized logistic regression using the ‘liblinear’ library, ‘newton-cg’, ‘sag’, ‘saga’ and ‘lbfgs’ solvers. **Note that regularization is applied by**

Penalty parameter

`LogisticRegression()` has a parameter called `penalty` that applies `l1` (lasso), `l2` (ridge), `elasticnet` or `none` with `l2` being the default. To make matters worse, the regularization is controlled by the parameter `c` which defaults to 1 (not 0) - also `c` is the inverse regularization strength (e.g. different from `alpha` for ridge and lasso models).

$$\min_{w, c} \frac{1 - \rho}{2} w^T w + \rho |w|_1 + C \sum_{i=1}^n |\log(\exp(-y_i (X_i^T w + c)) + 1)|,$$

```
m = LogisticRegression(fit_intercept = False, penalty="none").fit(X, y)
m.feature_names_in_
## array(['exclaim_mess', 'format', 'num_char', 'line_breaks', 'number_big', 'number_none', 'number_small'], dt_
m.coef_
## array([[ 0.00958, -0.60606,  0.05505, -0.00549, -1.26347, -0.70637, -1.95091]])
```

Solver parameter

It is also possible specify the solver to use when fitting a logistic regression model, to complicate matters somewhat the choice of the algorithm depends on the penalty chosen:

- newton-cg - [l2, none]
- lbgfs - [l2, none]
- liblinear - [l1, l2]
- sag - [l2, none]
- saga - [elasticnet, l1, l2, none]

Also there can be issues with feature scales for some of these solvers:

Note: ‘sag’ and ‘saga’ fast convergence is only guaranteed on features with approximately the same scale. You can preprocess the data with a scaler from `sklearn.preprocessing`.

Prediction

Classification models have multiple prediction methods depending on what type of output you would like,

```
m.predict(x)
```

```
m.predict_proba(X)
```

```

## array([[0.91318,  0.08682],
##        [0.956   ,  0.044  ],
##        [0.95796,  0.04204],
##        [0.94091,  0.05909],
##        [0.68747,  0.31253],
##        [0.68439,  0.31561],
##        [0.93424,  0.06576],
##        [0.96366,  0.03634],
##        [0.89589,  0.10411],
##        [0.94186,  0.05814],
##        [0.9326  ,  0.0674 ],
##        [0.89604,  0.10396],
##        [0.91236,  0.08764],

```

```
m.predict_log_proba(x)
```

```

## array([[ -0.09082, -2.44394],
##        [-0.04499, -3.12364],
##        [-0.04295, -3.16909],
##        [-0.06091, -2.82873],
##        [-0.37474, -1.16305],
##        [-0.37922, -1.15326],
##        [-0.06802, -2.72176],
##        [-0.03702, -3.3147 ],
##        [-0.10994, -2.26229],
##        [-0.0599 , -2.84487],
##        [-0.06978, -2.69706],
##        [-0.10977, -2.26371],
##        [-0.09172, -2.43457],

```

Scoring

Classification models also include a `score()` method which returns the model's accuracy,

```
m.score(X, y)  
## 0.90640142820709
```

Other scoring options are available via the `metrics` submodule

```
from sklearn.metrics import accuracy_score, roc_auc_score, f1_score, confusion_matrix  
  
accuracy_score(y, m.predict(X))  
## 0.90640142820709  
  
roc_auc_score(y, m.predict_proba(X)[:,1])  
## 0.7606622771440706  
  
f1_score(y, m.predict(X))  
## 0.0
```

confusion_matrix(y, m.predict(X), labels=m.classes_)	## array([[3554, 0], [367, 0]])
--	---------------------------------

Scoring visualizations - confusion matrix

```
from sklearn.metrics import ConfusionMatrixDisplay  
cm = confusion_matrix(y, m.predict(X), labels=m.classes_)  
  
disp = ConfusionMatrixDisplay(cm).plot()  
plt.show()
```



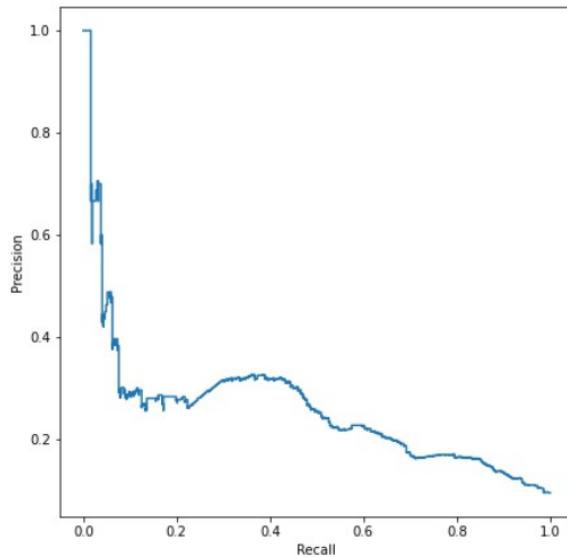
Scoring visualizations - ROC curve

```
from sklearn.metrics import auc, roc_curve, RocCurveDisplay

fpr, tpr, thresholds = roc_curve(y, m.predict_proba(X)[:,1])
roc_auc = auc(fpr, tpr)
disp = RocCurveDisplay(fpr=fpr, tpr=tpr, roc_auc=roc_auc,
                      estimator_name='Logistic Regression').plot()
plt.show()
```

Scoring visualizations - Precision Recall

```
from sklearn.metrics import precision_recall_curve, PrecisionRecallDisplay  
  
precision, recall, _ = precision_recall_curve(y, m.predict_proba(X)[:,1])  
disp = PrecisionRecallDisplay(precision=precision, recall=recall).plot()  
plt.show()
```



Another visualization

```
def confusion_plot(truth, probs, threshold=0.5):

    d = pd.DataFrame(
        data = {'spam': y, 'truth': truth, 'probs': probs}
    )

    # Create a column called outcome that contains the labeling outcome for the given threshold
    d['outcome'] = 'other'
    d.loc[(d.spam == 1) & (d.probs >= threshold), 'outcome'] = 'true positive'
    d.loc[(d.spam == 0) & (d.probs >= threshold), 'outcome'] = 'false positive'
    d.loc[(d.spam == 1) & (d.probs < threshold), 'outcome'] = 'false negative'
    d.loc[(d.spam == 0) & (d.probs < threshold), 'outcome'] = 'true negative'

    # Create plot and color according to outcome
    plt.figure(figsize=(12,4))
    plt.xlim((-0.05,1.05))
    sns.stripplot(y='truth', x='probs', hue='outcome', data=d, size=3, alpha=0.5)
    plt.axvline(x=threshold, linestyle='dashed', color='black', alpha=0.5)
    plt.title("threshold = %.2f" % threshold)
    plt.show()
```

```
truth = pd.Categorical.from_codes(y, categories = ('not spam', 'spam'))  
probs = m.predict_proba(X)[:,1]  
confusion_plot(truth, probs, 0.5)
```



```
confusion_plot(truth, probs, 0.25)
```



Demo 1 - DecisionTreeClassifier

Demo 2 - SVC

MNIST handwritten digits

```
from sklearn.datasets import load_digits  
  
digits = load_digits(as_frame=True)
```

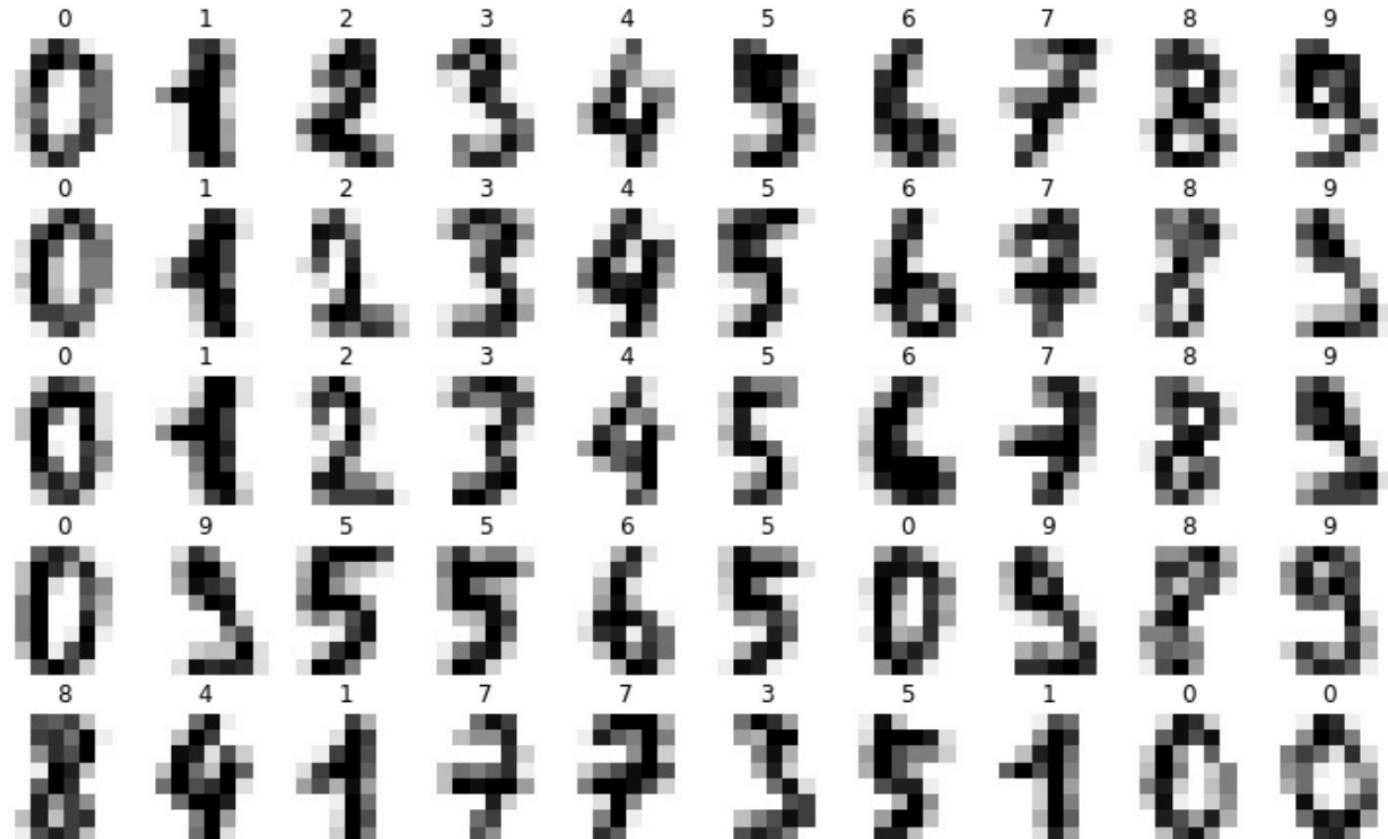
```
X = digits.data  
X  
  
##      pixel_0_0  pixel_0_1  pixel_0_2  pixel_0_3  pixel_0_4  
## 0        0.0      0.0      5.0     13.0      9.0  
## 1        0.0      0.0      0.0     12.0     13.0  
## 2        0.0      0.0      0.0      4.0     15.0  
## 3        0.0      0.0      7.0     15.0     13.0  
## 4        0.0      0.0      0.0      1.0     11.0  
## ...     ...      ...      ...      ...  
## 1792    0.0      0.0      4.0     10.0     13.0  
## 1793    0.0      0.0      6.0     16.0     13.0  
## 1794    0.0      0.0      1.0     11.0     15.0  
## 1795    0.0      0.0      2.0     10.0      7.0  
## 1796    0.0      0.0     10.0     14.0      8.0  
##  
## [1797 rows x 64 columns]
```

```
y = digits.target  
y  
  
## 0      0  
## 1      1  
## 2      2  
## 3      3  
## 4      4  
## ..  
## 1792   9  
## 1793   0  
## 1794   8  
## 1795   9  
## 1796   8  
## Name: target, Length: 1797, dtype: int64
```

digit description

```
## .. _digits_dataset:  
##  
## Optical recognition of handwritten digits dataset  
## -----  
##  
## **Data Set Characteristics:**  
##  
## :Number of Instances: 1797  
## :Number of Attributes: 64  
## :Attribute Information: 8x8 image of integer pixels in the range 0..16.  
## :Missing Attribute Values: None  
## :Creator: E. Alpaydin (alpaydin '@' boun.edu.tr)  
## :Date: July; 1998  
##  
## This is a copy of the test set of the UCI ML hand-written digits datasets  
## https://archive.ics.uci.edu/ml/datasets/Optical+Recognition+of+Handwritten+Digits  
##  
## The data set contains images of hand-written digits: 10 classes where  
## each class refers to a digit.  
##  
## Preprocessing programs made available by NIST were used to extract  
## normalized bitmaps of handwritten digits from a preprinted form. From a  
## total of 43 people, 30 contributed to the training set and different 13  
## to the test set. 32x32 bitmaps are divided into nonoverlapping blocks of  
## 4x4 and the number of on pixels are counted in each block. This generates  
## an input matrix of 8x8 where each element is an integer in the range  
## 0..16. This reduces dimensionality and gives invariance to small  
## distortions.  
##  
## For info on NIST preprocessing routines, see M. D. Garris, J. L. Blue, G.
```

Example digits



Doing things properly - train/test split

To properly assess our modeling we will create a training and testing set of these data, only the training data will be used to learn model coefficients or hyperparameters, test data will only be used for final model scoring.

```
X_train, X_test, y_train, y_test = train_test_split(  
    X, y, test_size=0.33, shuffle=True, random_state=1234  
)
```

Multiclass logistic regression

Fitting a multiclass logistic regression model will involve selecting a value for the `multi_class` parameter, which can be either `multinomial` for multinomial regression or `ovr` for one-vs-rest where k binary models are fit.

```
mc_log_cv = GridSearchCV(  
    LogisticRegression(penalty='none', max_iter = 5000),  
    param_grid = {"multi_class": ["multinomial", "ovr"]},  
    cv = KFold(10, shuffle=True, random_state=12345),  
    n_jobs = 4  
).fit(X_train, y_train)  
  
mc_log_cv.best_estimator_  
  
## LogisticRegression(max_iter=5000, multi_class='multinomial', penalty='none')  
  
mc_log_cv.best_score_  
  
## 0.943477961432507  
  
for p, s in zip(mc_log_cv.cv_results_["params"], mc_log_cv.cv_results_["mean_test_score"]):  
    print(p, "Score:", s)
```

Model coefficients

```
pd.DataFrame(  
    mc_log_cv.best_estimator_.coef_  
)  
  
##      0         1         2         3         4       ...        59        60        61        62        63  
## 0  0.0 -0.133584 -0.823611  0.904385  0.163397 ...  1.211092 -0.444343 -1.660396 -0.750159 -0.184264  
## 1  0.0 -0.184931 -1.259550  1.453983 -5.091361 ... -0.792356  0.384498  2.617778  1.265903  2.338324  
## 2  0.0  0.118104  0.569190  0.798171  0.943558 ...  0.281622  0.829968  2.602947  2.481998  0.788003  
## 3  0.0  0.239612 -0.381815  0.393986  3.886781 ...  1.231867  0.439466  1.070662  0.583209 -1.027194  
## 4  0.0 -0.109904 -1.160712 -2.175923 -2.580281 ... -0.937843 -1.710608 -0.651175 -0.656791 -0.097263  
## 5  0.0  0.701265  4.241974 -0.738130  0.057049 ...  2.045636 -0.001139 -1.412535 -2.097753 -0.210256  
## 6  0.0 -0.103487 -1.454058 -1.310946 -0.400937 ... -1.407609  0.249136  2.466801  1.005207 -0.624921  
## 7  0.0  0.088562  1.386086  1.198007  0.467463 ... -2.710461 -3.176521 -2.635078 -0.710317 -0.099948  
## 8  0.0 -0.347408 -0.306168 -1.933009  1.074249 ...  0.872821  1.722070 -2.302814 -1.602654 -0.679128  
## 9  0.0 -0.268228 -0.811336  1.409475  1.480082 ...  0.205230  1.707472 -0.096190  0.481356 -0.203353  
##  
## [10 rows x 64 columns]  
  
mc_log_cv.best_estimator_.coef_.shape  
  
## (10, 64)  
  
mc_log_cv.best_estimator_.intercept_
```

Confusion Matrix

Within sample

```
accuracy_score(  
    y_train,  
    mc_log_cv.best_estimator_.predict(X_train)  
)  
  
## 1.0  
  
confusion_matrix(  
    y_train,  
    mc_log_cv.best_estimator_.predict(X_train)  
)  
  
## array([[125,     0,     0,     0,     0,     0,     0,     0,  
##         [  0, 118,     0,     0,     0,     0,     0,     0,  
##         [  0,     0, 119,     0,     0,     0,     0,     0,  
##         [  0,     0,     0, 123,     0,     0,     0,     0,  
##         [  0,     0,     0,     0, 110,     0,     0,     0,  
##         [  0,     0,     0,     0,     0, 114,     0,     0,  
##         [  0,     0,     0,     0,     0,     0, 124,     0,  
##         [  0,     0,     0,     0,     0,     0,     0, 124,  
##         [  0,     0,     0,     0,     0,     0,     0,     0,
```

Out of sample

```
accuracy_score(  
    y_test,  
    mc_log_cv.best_estimator_.predict(X_test)  
)  
  
## 0.9579124579124579  
  
confusion_matrix(  
    y_test,  
    mc_log_cv.best_estimator_.predict(X_test),  
    labels = digits.target_names  
)  
  
## array([[53,     0,     0,     0,     0,     0,     0,     0,     0,     0,  
##         [  0,  64,     0,     0,     0,     0,     0,     0,     0,     0,  
##         [  0,     2,  56,     0,     0,     0,     0,     0,     0,     0,  
##         [  0,     0,     1,  58,     0,     1,     0,     0,     0,     0,  
##         [  1,     0,     0,     0,  69,     0,     0,     0,     1,     0,  
##         [  0,     0,     0,     1,     1,  64,     2,     0,     0,     0,  
##         [  1,     1,     0,     0,     0,     0,  55,     0,     0,     0,  
##         [  0,     0,     0,     0,     2,     0,     0,  53,     0,     0], 24, 29
```

Report

```
print( classification_report(  
    y_test,  
    mc_log_cv.best_estimator_.predict(X_test)  
) )  
  
##          precision    recall  f1-score   support  
##  
##      0       0.96     1.00     0.98      53  
##      1       0.89     1.00     0.94      64  
##      2       0.95     0.97     0.96      58  
##      3       0.98     0.97     0.97      60  
##      4       0.96     0.97     0.97      71  
##      5       0.97     0.94     0.96      68  
##      6       0.96     0.96     0.96      57  
##      7       1.00     0.96     0.98      55  
##      8       0.96     0.84     0.89      55  
##      9       0.96     0.96     0.96      53  
##  
##        accuracy                           0.96      594  
##        macro avg       0.96     0.96     0.96      594  
##        weighted avg       0.96     0.96     0.96      594
```

ROC & AUC?

These metrics are slightly awkward to use in the case multiclass problems since they depend on the probability predictions to calculate.

```
roc_auc_score(  
    y_test, mc_log_cv.best_estimator_.predict_proba(X_test)  
)
```

```
## ValueError: multi_class must be in ('ovo', 'ovr')
```

```
roc_auc_score(  
    y_test, mc_log_cv.best_estimator_.predict_proba  
    multi_class = "ovr"  
)
```

```
## 0.9979624274858663
```

```
roc_auc_score(  
    y_test, mc_log_cv.best_estimator_.predict_proba  
    multi_class = "ovo"  
)
```

```
roc_auc_score(  
    y_test, mc_log_cv.best_estimator_.predict_proba  
    multi_class = "ovr", average = "weighted"  
)
```

```
## 0.9979869175119241
```

```
roc_auc_score(  
    y_test, mc_log_cv.best_estimator_.predict_proba  
    multi_class = "ovo", average = "weighted"  
)
```

Prediction

```
mc_log_cv.best_estimator_.predict(X_test)
```

```

## array([7, 1, 7, 6, 0, 2, 4, 3, 6, 3, 7, 8, 7, 9, 4, 3, 1, 7,
##        8, 1, 3, 9, 1, 3, 9, 6, 9, 5, 2, 1, 9, 2, 1, 3, 8, 7,
##        6, 4, 6, 2, 3, 4, 7, 5, 0, 9, 1, 0, 5, 6, 7, 6, 3, 8,
##        5, 9, 3, 9, 3, 1, 2, 0, 8, 2, 8, 5, 2, 4, 6, 8, 3, 9,
##        6, 3, 2, 3, 2, 6, 5, 2, 9, 4, 7, 0, 1, 0, 4, 3, 1, 2,
##        1, 2, 3, 9, 1, 3, 2, 9, 3, 4, 3, 4, 1, 0, 1, 8, 5, 0,
##        4, 7, 3, 8, 6, 3, 8, 6, 4, 7, 0, 6, 6, 8, 3, 8, 3, 8,
##        8, 1, 1, 7, 1, 7, 1, 6, 4, 5, 5, 5, 3, 1, 0, 4, 4, 6,
##        1, 1, 4, 3, 0, 5, 9, 5, 5, 7, 5, 0, 6, 1, 5, 7, 9, 0,
##        1, 5, 2, 1, 6, 4, 2, 1, 1, 9, 4, 3, 9, 6, 5, 0, 4, 7])

```

```
mc_log_cv.best_estimator_.predict_proba(X_test),
```

Exercise 1

Using these data fit a `DecisionTreeClassifier` to these data, you should employ `GridSearchCV` to tune some of the parameters (`max_depth` at a minimum) - see the full list [here](#).

Does this model perform better or worse than the multinomial regression model we just used?

```
from sklearn.datasets import load_digits
digits = load_digits(as_frame=True)

X, y = digits.data, digits.target
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.33, shuffle=True, random_state=1234
)
```

Examining the coeffs

```
coef_img = mc_log_cv.best_estimator_.coef_.reshape(10,8,8)

fig, axes = plt.subplots(nrows=2, ncols=5, figsize=(10, 5), layout="constrained")
axes2 = [ax for row in axes for ax in row]

for ax, image, label in zip(axes2, coef_img, range(10)):
    ax.set_axis_off()
    img = ax.imshow(image, cmap=plt.cm.gray_r, interpolation="nearest")
    txt = ax.set_title(f"{label}")

plt.show()
```