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Classic Iris dataset with 3 species.

We will build multi-class classifier and calibrate outputs.

1. perfect ML pipeline for small task

1.1. task

Task to use iris dataset for ML classification.

Задача состоит в использовании Iris flower датасета для задачи классификации.

Iris flower data set is sometimes called Anderson's Iris data set.

Этот датасет еще называют датасетом Андерсона, в честь Эдгора Андерсона, который среди своих заслуг в ботанике ввел термин introgressive hybridization, означающий обмен генами между двумя родственными, но различными видами.

This dataset is also called the Anderson dataset, in honor of Edgar Anderson, who, among his achievements in botany, introduced the term introgressive hybridization, meaning the exchange of genes between two related, but different species.

Dataset consist of 150 rows of iris flowers, 50 for each of 3 species. 4 columns for features and 1 for species.

1.2. Steps (not strict)

We will follow steps:

1. goal and ML problem formulation, metrics selection, validation strategy
2. data analysis for problem
3. common data transformation, feature engineering
4. model selection
5. data preparation, feature selection
6. selected model finetuning
7. model training
8. model validation
9. results analysis

1.3. Goal, problem, metric, strategy

Goal is to predict specie by 4 features.

Problem is multi-class classification for 3 classes.

All classes balanced, we will **metrics**: ROC AUC, macro precision and recall.

We have 150 observations, we should use them with maximum effeciency, that is why we use cross_validation **strategy** with LeaveOneOut folds. To choose model we split data to main and test parts as 10 percentage stratifyed.

1.3.1. Averaging techniques theory

Averaging techniques for metrics:

- macro - compute the metric independently for each class and then take the average - treating all classes equally
- weighted - weighted average for classes (score*num_occur_per_class)/totalnum
- micro - aggregate the contributions of all classes to compute the average metric - micro-average is preferable if you suspect there might be class imbalance

1.3.2. metrics exploration

```
def _check_model_scorings(est, X, Y, kfold):
    print( '{:40} {:5} {:5}'.format("metric", "mean_accuracy", "std" ))
    for k in metrics.get_scorer_names():
        # print(k)
        results = cross_validate(est, X, Y, cv=kfold, scoring=[k])
        r = results[f'test_{k}']
        if not all(np.isnan(r)):
            print( '{:40} {:5} {:5}'.format(k, round(r.mean(), 3), round(r.std(),2)) )
```

```
metric                                   mean_accuracy std
accuracy                                 0.973  0.02
adjusted_mutual_info_score               0.923  0.07
adjusted_rand_score                      0.921  0.07
balanced_accuracy                        0.973  0.02
completeness_score                        0.93  0.06
explained_variance                       0.962  0.04
f1_macro                                 0.973  0.03
f1_micro                                 0.973  0.02
f1_weighted                              0.973  0.03
fowlkes_mallows_score                    0.946  0.05
homogeneity_score                        0.927  0.06
jaccard_macro                             0.95  0.05
jaccard_micro                            0.949  0.05
jaccard_weighted                          0.95  0.05
matthews_corrcoef                        0.962  0.04
max_error                                 -0.6  0.49
mutual_info_score                        1.018  0.07
neg_log_loss                             -0.511  0.54
neg_mean_absolute_error                  -0.027  0.02
neg_mean_absolute_percentage_error       -0.023  0.02
neg_mean_squared_error                   -0.027  0.02
neg_mean_squared_log_error               -0.004   0.0
neg_median_absolute_error                  0.0   0.0
neg_root_mean_squared_error              -0.125  0.11
normalized_mutual_info_score             0.928  0.06
precision_macro                          0.977  0.02
precision_micro                          0.973  0.02
precision_weighted                       0.977  0.02
r2                                        0.96  0.04
rand_score                               0.966  0.03
recall_macro                             0.973  0.02
recall_micro                             0.973  0.02
recall_weighted                          0.973  0.02
roc_auc_ovo                              0.987  0.01
roc_auc_ovo_weighted                     0.987  0.01
roc_auc_ovr                              0.987  0.01
roc_auc_ovr_weighted                     0.987  0.01
v_measure_score                          0.928  0.06
```

1.4. data analysis for problem

```
import pandas as pd
from sklearn import datasets
import numpy as np
d = datasets.load_iris()
target_names = d['target_names']
print(target_names)
print(pd.DataFrame(d['data'], columns=d['feature_names']).describe())
print()
print("target:", np.unique(d['target']))
```

```
['setosa' 'versicolor' 'virginica']
       sepal length (cm)  sepal width (cm)  petal length (cm)  petal width (cm)
count         150.000000        150.000000         150.000000        150.000000
mean            5.843333          3.057333           3.758000          1.199333
std             0.828066          0.435866           1.765298          0.762238
min             4.300000          2.000000           1.000000          0.100000
25%             5.100000          2.800000           1.600000          0.300000
50%             5.800000          3.000000           4.350000          1.300000
75%             6.400000          3.300000           5.100000          1.800000
max             7.900000          4.400000           6.900000          2.500000
```

```
target: [0 1 2]
```

1.5. common data transformation

```
import pandas as pd
from sklearn import datasets
import numpy as np
from sklearn.model_selection import train_test_split
d = datasets.load_iris()
X = d['data']
y = d['target']
X_train, X_test_saved, y_train, y_test_saved = train_test_split(
    X, y, test_size=0.10, random_state=42, stratify=y)
X = X_train
y = y_train
```

1.6. model selection

We selected OneVsOneClassifier(estimator=LogisticRegression(multi_class='ovr'))

just for learning.

1.6.1. code

```
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import StratifiedKFold, KFold

from sklearn import linear_model
from sklearn.model_selection import cross_val_score, cross_validate
from sklearn.model_selection import StratifiedKFold, KFold

from sklearn.neural_network import MLPClassifier
from sklearn.neighbors import KNeighborsClassifier
from sklearn.svm import SVC
from sklearn.gaussian_process import GaussianProcessClassifier
from sklearn.gaussian_process.kernels import RBF
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import RandomForestClassifier, AdaBoostClassifier
from sklearn.naive_bayes import GaussianNB
from sklearn.discriminant_analysis import QuadraticDiscriminantAnalysis
# from sklearn.metrics import hinge_loss
from sklearn import metrics
from sklearn.multiclass import OneVsOneClassifier
import sklearn

def warn(*args, **kwargs):
    pass
import warnings
warnings.warn = warn


classifiers_binary = [
        KNeighborsClassifier(5),
        SVC(kernel="linear", C=0.025),  # очень долго
        SVC(gamma=2, C=1),  # слишком долго
        GaussianProcessClassifier(1.0 * RBF(1.0)), # не хватает памяти
        DecisionTreeClassifier(max_depth=5),
        RandomForestClassifier(max_depth=5, n_estimators=10, ),  # max_features=1
        MLPClassifier(alpha=1, max_iter=1000),
        AdaBoostClassifier(),
        GaussianNB(),
        QuadraticDiscriminantAnalysis()
]

def _select_metrics(est, X, Y, kfold):
    print( '{:40} {:5} {:5}'.format("metric", "mean_accuracy", "std" ))
    for k in metrics.get_scorer_names():
        # print(k)
        results = cross_validate(est, X, Y, cv=kfold, scoring=[k])
        r = results[f'test_{k}']
        if not all(np.isnan(r)):
            print( '{:40} {:5} {:5}'.format(k, round(r.mean(), 3), round(r.std(),2)) )

def _check_model_binary(est, X, Y, kfold):
    results = cross_validate(est, X, Y, cv=kfold, scoring=['accuracy', 'roc_auc'])
    print(est.__class__.__name__)
    print("Accuracy: %f" % results['test_accuracy'].mean())
    print("AUC: %f" % results['test_roc_auc'].mean())

def _check_model_multiclass_native(est, X, Y, kfold):
    """ https://scikit-learn.org/stable/modules/model_evaluation.html#scoring-parameter
    returns score per folds"""
    print(est)
    results = cross_validate(est, X, Y, cv=kfold,
                              scoring=['roc_auc_ovo', 'precision_macro',
                                       'recall_macro'])
    print("ROC_AUC: %f" % results['test_roc_auc_ovo'].mean())
    print("precision_macro: %f" % results['test_precision_macro'].mean())
```

```
    print("recall_macro: %f" % results['test_recall_macro'].mean())
    print()

def _check_model_multiclass_ovo(est, X, Y, kfold):
    """ https://scikit-learn.org/stable/modules/model_evaluation.html#scoring-parameter
    returns score per folds"""
    scoring=['accuracy', 'precision_macro',
                                  'recall_macro']
    results = cross_validate(est, X, Y, cv=kfold, scoring=scoring) #
    print(est)
    for x in scoring:
        print(x+ ": %f" % results['test_'+x].mean())
    print()


classifiers_multiclass_nativ = [
    sklearn.naive_bayes.BernoulliNB(),
    sklearn.tree.DecisionTreeClassifier(),
    sklearn.ensemble.RandomForestClassifier(max_depth=5, n_estimators=10, ),
    sklearn.tree.ExtraTreeClassifier(),
    sklearn.ensemble.ExtraTreesClassifier(),
    sklearn.naive_bayes.GaussianNB(),
    sklearn.neighbors.KNeighborsClassifier(),
    sklearn.linear_model.LogisticRegression(multi_class="multinomial"),
    sklearn.linear_model.LogisticRegressionCV(multi_class="multinomial")
    ]

classifiers_multiclass_ovo = [
    OneVsOneClassifier(sklearn.svm.LinearSVC(C=100.)),
    OneVsOneClassifier(sklearn.svm.SVC(kernel="linear", C=0.025)),  # очень долго
    OneVsOneClassifier(sklearn.svm.SVC(gamma=2, C=1)),  # слишком долго
    OneVsOneClassifier(sklearn.gaussian_process.GaussianProcessClassifier(1.0 * RBF(1.0))), # не хватает памяти
    OneVsOneClassifier(sklearn.neural_network.MLPClassifier(alpha=1, max_iter=1000)),
    OneVsOneClassifier(sklearn.ensemble.AdaBoostClassifier()),
    OneVsOneClassifier(sklearn.discriminant_analysis.QuadraticDiscriminantAnalysis()),
    OneVsOneClassifier(sklearn.ensemble.GradientBoostingClassifier()),
    OneVsOneClassifier(sklearn.gaussian_process.GaussianProcessClassifier()),
    OneVsOneClassifier(sklearn.linear_model.LogisticRegression(multi_class="ovr")),
    OneVsOneClassifier(sklearn.linear_model.LogisticRegressionCV(multi_class="ovr")),
    OneVsOneClassifier(sklearn.linear_model.SGDClassifier()),
    OneVsOneClassifier(sklearn.linear_model.Perceptron())
    ]


kfold = StratifiedKFold(n_splits=5)
# ----------- select metrics ------
# m = linear_model.LogisticRegressionCV(max_iter=10, multi_class='multinomial')
# m = linear_model.Lasso()
# m=KNeighborsClassifier(5)
# m = OneVsOneClassifier(sklearn.ensemble.AdaBoostClassifier())
# _select_metrics(m, X, y, kfold)
# ------------------ select model -----------
Xscal = sklearn.preprocessing.StandardScaler().fit_transform(X)

for est in classifiers_multiclass_nativ: # classifiers_multiclass_ovo:
    _check_model_multiclass_native(est, Xscal, y, kfold)

for est in classifiers_multiclass_ovo: # classifiers_multiclass_ovo:
    _check_model_multiclass_ovo(est, Xscal, y, kfold)
```

```
BernoulliNB()
ROC_AUC: 0.891358
precision_macro: 0.762554
recall_macro: 0.762963

DecisionTreeClassifier()
ROC_AUC: 0.961111
precision_macro: 0.952879
recall_macro: 0.948148

RandomForestClassifier(max_depth=5, n_estimators=10)
ROC_AUC: 0.995473
precision_macro: 0.966397
recall_macro: 0.962963

ExtraTreeClassifier()
ROC_AUC: 0.966667
precision_macro: 0.958333
recall_macro: 0.955556

ExtraTreesClassifier()
ROC_AUC: 0.995473
precision_macro: 0.959545
recall_macro: 0.955556

GaussianNB()
ROC_AUC: 0.994239
precision_macro: 0.965000
recall_macro: 0.962963

KNeighborsClassifier()
ROC_AUC: 0.995473
precision_macro: 0.969091
recall_macro: 0.962963
```

```
LogisticRegression(multi_class='multinomial')
ROC_AUC: 0.997531
precision_macro: 0.955000
recall_macro: 0.948148

LogisticRegressionCV(multi_class='multinomial')
ROC_AUC: 0.997942
precision_macro: 0.955000
recall_macro: 0.948148

OneVsOneClassifier(estimator=LinearSVC(C=100.0))
accuracy: 0.962963
precision_macro: 0.971212
recall_macro: 0.962963

OneVsOneClassifier(estimator=SVC(C=0.025, kernel='linear'))
accuracy: 0.903704
precision_macro: 0.908877
recall_macro: 0.903704

OneVsOneClassifier(estimator=SVC(C=1, gamma=2))
accuracy: 0.948148
precision_macro: 0.952879
recall_macro: 0.948148

OneVsOneClassifier(estimator=GaussianProcessClassifier(kernel=1**2 * RBF(length_scale=1)))
accuracy: 0.955556
precision_macro: 0.961852
recall_macro: 0.955556

OneVsOneClassifier(estimator=MLPClassifier(alpha=1, max_iter=1000))
accuracy: 0.948148
precision_macro: 0.955000
recall_macro: 0.948148

OneVsOneClassifier(estimator=AdaBoostClassifier())
accuracy: 0.955556
precision_macro: 0.959545
recall_macro: 0.955556

OneVsOneClassifier(estimator=QuadraticDiscriminantAnalysis())
accuracy: 0.962963
precision_macro: 0.968519
recall_macro: 0.962963

OneVsOneClassifier(estimator=GradientBoostingClassifier())
accuracy: 0.940741
precision_macro: 0.947424
recall_macro: 0.940741

OneVsOneClassifier(estimator=GaussianProcessClassifier())
accuracy: 0.955556
precision_macro: 0.958333
recall_macro: 0.955556

OneVsOneClassifier(estimator=LogisticRegression(multi_class='ovr'))
accuracy: 0.948148
precision_macro: 0.955000
recall_macro: 0.948148

OneVsOneClassifier(estimator=LogisticRegressionCV(multi_class='ovr'))
accuracy: 0.948148
precision_macro: 0.955000
recall_macro: 0.948148

OneVsOneClassifier(estimator=SGDClassifier())
accuracy: 0.925926
precision_macro: 0.938333
recall_macro: 0.925926

OneVsOneClassifier(estimator=Perceptron())
accuracy: 0.925926
precision_macro: 0.938333
recall_macro: 0.925926
```

1.7. data preparation

sklearn.linear_model.LogisticRegression uses L2-penalty by default, which is Ridge Regression.

As Hastie,Tibshirani and Friedman points out (page 82 of the pdf or at page 63 of the book) [1] Standardization of data is preffered.

```
X = sklearn.preprocessing.StandardScaler().fit_transform(X)
print(X[0:10])
```

```
>>> [[-1.37406347  0.32273255 -1.2292066  -1.31595957]
 [ 1.05870464 -0.12875858  0.82793667  1.43330011]
 [-1.73897869 -0.35450415 -1.34349233 -1.31595957]
 [ 0.45051261  0.77422368  0.94222241  1.43330011]
 [-1.00914826 -0.12875858 -1.2292066  -1.31595957]
 [-1.13078666  0.09698698 -1.28634947 -1.4468767 ]
```

```
 [ 0.69378943 -0.58024971  1.05650815  1.17146585]
 [-1.25242507 -0.12875858 -1.34349233 -1.18504244]
 [-0.15767942 -0.35450415  0.25650799  0.12412883]
 [-1.49570188  0.09698698 -1.28634947 -1.31595957]]
```

1.8. model finetuning and training

```
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import cross_validate
from sklearn.multiclass import OneVsOneClassifier
from sklearn.model_selection import LeaveOneOut


params = {'estimator__penalty': ['none', 'l2'], 'estimator__C': [0, 0.0001, 0.001,0.01,0.1]}
clf = GridSearchCV(OneVsOneClassifier(estimator=sklearn.linear_model.LogisticRegression(multi_class='ovr', n_jobs=2)),
                   params, cv=kfold)

results = clf.fit(X, y)
est = results.best_estimator_
print(est)
kfold = LeaveOneOut()
results = cross_val_score(results.best_estimator_, X, y, cv=kfold)
print("Accuracy: %f" % results.mean())
print(results)

scoring=['accuracy', 'precision_macro',
                                      'recall_macro']

results = cross_validate(est, X, y, cv=kfold, scoring=scoring) #

for x in scoring:
    print(x+ ": %f" % results['test_'+x].mean())
```

```
/usr/lib/python3.10/site-packages/sklearn/model_selection/_search.py:968: RuntimeWarning: invalid value encountered in cas
  results["rank_%s" % key_name] = np.asarray(
OneVsOneClassifier(estimator=LogisticRegression(C=0, multi_class='ovr',
                                                n_jobs=2, penalty='none'))
Accuracy: 0.970370
[1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 0. 1. 1. 1. 1.
 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 0. 1. 1. 1. 1.
 1. 0. 1. 1. 1. 1. 1. 1. 0. 1. 1. 1. 1. 1. 1.]
accuracy: 0.970370
precision_macro: 0.970370
recall_macro: 0.970370
```

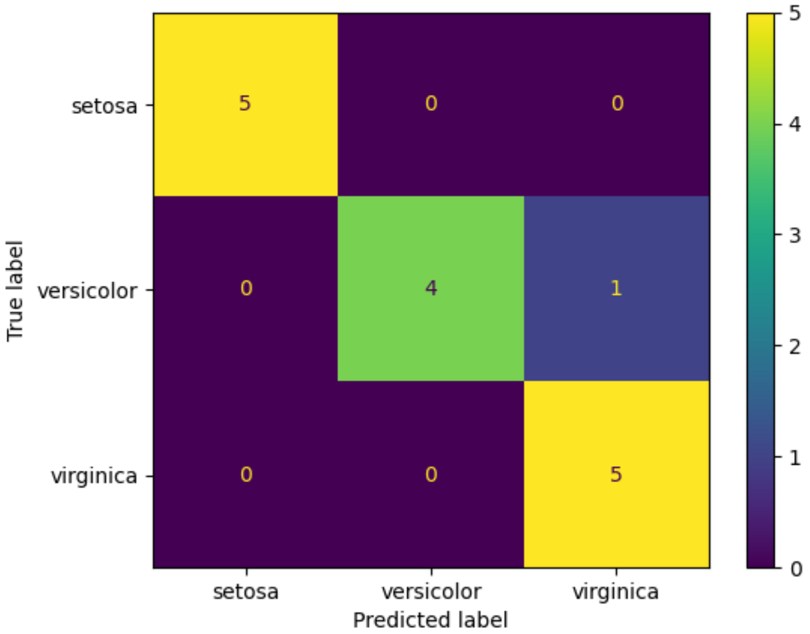
1.9. model validation

```
from sklearn.metrics import classification_report
from sklearn.metrics import confusion_matrix

est = OneVsOneClassifier(
    estimator=sklearn.linear_model.LogisticRegression(
        C=0, multi_class='ovr',
        n_jobs=2, penalty='none'))
est.fit(X,y)
X_test = sklearn.preprocessing.StandardScaler().fit_transform(X_test_saved)
y_pred = est.predict(X_test)
print(y_pred)
print(y_test_saved)
print(classification_report(y_test_saved, y_pred))
cm = confusion_matrix(y_test_saved, y_pred)
print("x-redicted:0,1,2", "y-true labels: 0, 1, 2 (from top to bottom)")
print(cm)
```

```
[1 2 2 1 2 0 0 0 2 1 0 2 1 2 0]
[1 2 2 1 2 0 0 0 2 1 0 2 1 1 0]
              precision    recall  f1-score   support

           0       1.00      1.00      1.00         5
           1       1.00      0.80      0.89         5
           2       0.83      1.00      0.91         5

    accuracy                           0.93        15
   macro avg       0.94      0.93      0.93        15
weighted avg       0.94      0.93      0.93        15

x-redicted:0,1,2 y-true labels: 0, 1, 2 (from top to bottom)
[[5 0 0]
 [0 4 1]
 [0 0 5]]
```

```
mkdir ./autoimgs
```

```
from sklearn.metrics import ConfusionMatrixDisplay
import matplotlib.pyplot as plt
disp = ConfusionMatrixDisplay(confusion_matrix=cm,
                              display_labels=target_names)
disp.plot()
plt.savefig('./autoimgs/confusion_matrix.png')
```



1.10. results analysis

results analysis:

- we get only one mistake at validation in "versicolor" specie.

1.11. model output calibration

We want to have confidence score for result of model inference on the prediction.

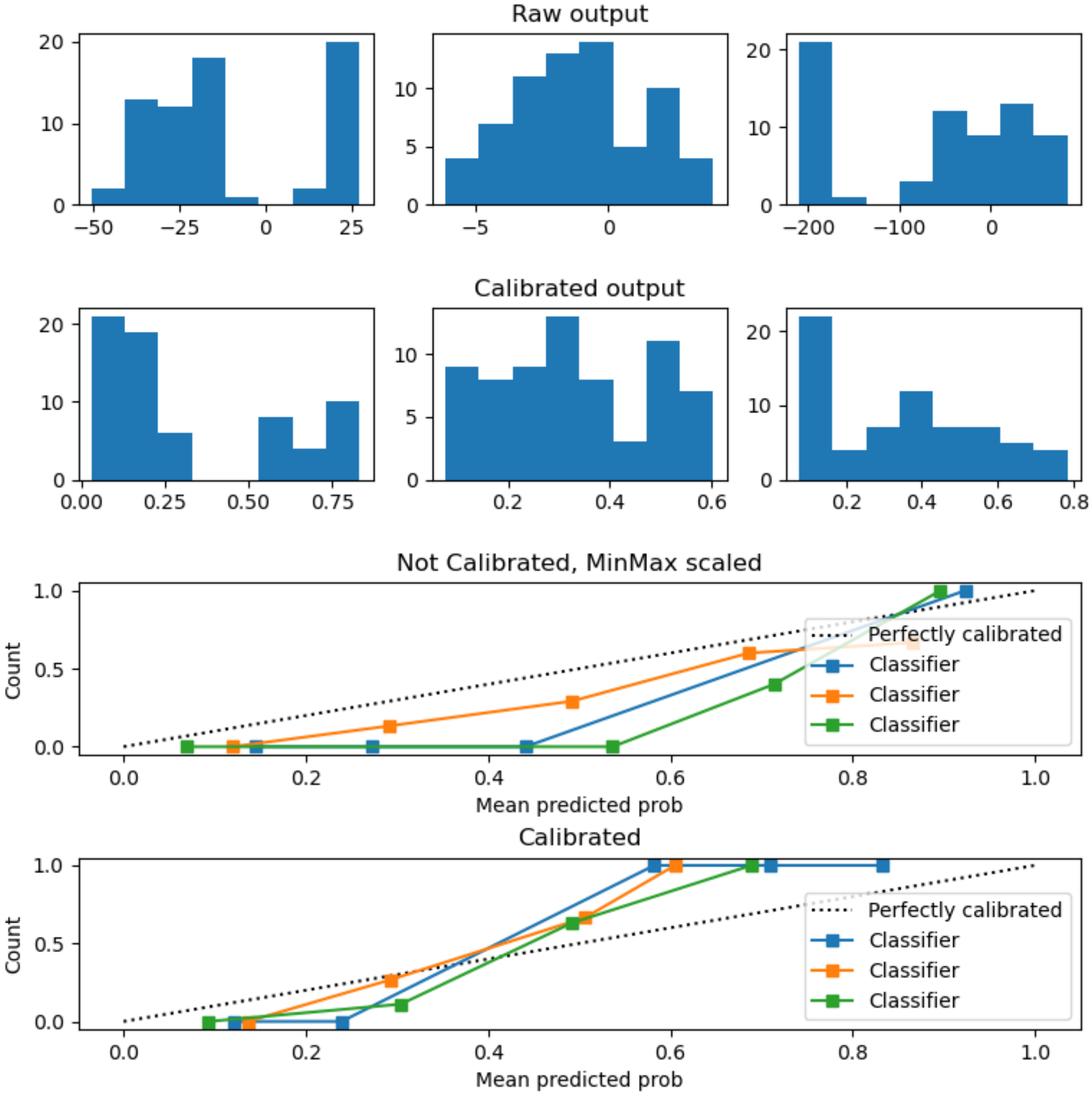
If we have 0.8 it will mean, approximately 80% actually belong to the positive class.

It allow making decisions under uncertainty.

OneVsRest has equal accuracy with OneVsOne. We take OneVsRest for clarity.

```
# print(est.predict_proba(X_test))
from sklearn.calibration import CalibratedClassifierCV
from sklearn.multiclass import OneVsRestClassifier
import matplotlib.pyplot as plt
from sklearn.calibration import CalibrationDisplay
from sklearn.preprocessing import MinMaxScaler

# ---- plot default and calibrated classifiers
fig = plt.figure(figsize=(9,9))
gs = fig.add_gridspec(4,3, hspace=0.6)
#                       left=2.1, right=0.1, bottom=0.1, top=0.9,
#                       wspace=0.9, hspace=0.1)
# | 1 | 2 | 3 |
# | 4 | 5 | 6 |
# | 7 | 7 | 7 |
# | 8 | 8 | 8 |
d1 = fig.add_subplot(gs[0,0])
d2 = fig.add_subplot(gs[0,1])
d3 = fig.add_subplot(gs[0,2])

d4 = fig.add_subplot(gs[1,0])
d5 = fig.add_subplot(gs[1,1])
d6 = fig.add_subplot(gs[1,2])

d7 = fig.add_subplot(gs[2,:])
d8 = fig.add_subplot(gs[3,:])
```

```
colors = plt.cm.get_cmap("Dark2")
markers = ["^", "v", "s", "o"]
# -- data preparation
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.50, random_state=42, stratify=y)

y_test # y_true
# covert to onevsrest
y_test_oneh = np.zeros((y_test.size, y_test.max() + 1))
y_test_oneh[np.arange(y_test.size), y_test] = 1
# print(y_test_oneh)


# -- default:
clf_default = OneVsRestClassifier(
    estimator=sklearn.linear_model.LogisticRegression(
        C=0, multi_class='ovr',
        n_jobs=2, penalty='none'))

clf_default.fit(X_train, y_train)
y_prob = clf_default.decision_function(X_test)
d1.hist(y_prob[:,0], bins='auto')
d2.hist(y_prob[:,1], bins='auto')
d3.hist(y_prob[:,2], bins='auto')
d2.set(title='Raw output')

y_prob = MinMaxScaler().fit_transform(y_prob)
CalibrationDisplay.from_predictions(y_test_oneh[:,0], y_prob[:,0],
                                            ax=d7)
CalibrationDisplay.from_predictions(y_test_oneh[:,1], y_prob[:,1],
                                            ax=d7)
CalibrationDisplay.from_predictions(y_test_oneh[:,2], y_prob[:,2],
                                            ax=d7)

d7.set(title='Not Calibrated, MinMax scaled', xlabel="Mean predicted prob", ylabel="Count")
# -- calibrated:
clf = OneVsRestClassifier(
    estimator=sklearn.linear_model.LogisticRegression(
        C=0, multi_class='ovr',
        n_jobs=2, penalty='none'))


cal_clf = CalibratedClassifierCV(clf, method="sigmoid",
                                 cv=StratifiedKFold(10)) # ,
cal_clf.fit(X_train, y_train)

# print(y_test)
y_prob = cal_clf.predict_proba(X_test)


d4.hist(y_prob[:,0], bins='auto')
d5.hist(y_prob[:,1], bins='auto')
d6.hist(y_prob[:,2], bins='auto')
d5.set(title='Calibrated output')
# plt.hist(y_prob, bins='auto')
# print(clf_probs)
# print(cal_clf_probs)


# display = CalibrationDisplay.from_predictions(
#         y_true
#         ,
#         y_test,
#     ax=d4
#         # n_bins=10,
#         # name='model',
#         # ax=ax_calibration_curve,
#         # color=colors(0),
#         # marker=markers[0],
# )
CalibrationDisplay.from_predictions(y_test_oneh[:,0], y_prob[:,0],
                                            ax=d8)
CalibrationDisplay.from_predictions(y_test_oneh[:,1], y_prob[:,1],
                                            ax=d8)
CalibrationDisplay.from_predictions(y_test_oneh[:,2], y_prob[:,2],
                                            ax=d8)
d8.set(title='Calibrated', xlabel="Mean predicted prob", ylabel="Count")
# plt.show()
plt.savefig('./autoimgs/calibrating.png')
# print(display)
```



1.11.1. link

- https://scikit-learn.org/stable/auto_examples/calibration/plot_compare_calibration.html#sphx-glr-auto-examples-calibration-plot-compare-calibration-py
- https://scikit-learn.org/stable/auto_examples/calibration/plot_calibration_multiclass.html#sphx-glr-auto-examples-calibration-plot-calibration-multiclass-py

1.12. old

```
from sklearn import datasets
from sklearn.linear_model import RidgeCV
from sklearn.model_selection import cross_validate
from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score
d = datasets.load_iris()
X = d['data']
y = d['target']
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.33, random_state=42)
c = RidgeCV()
c.fit(X_train, y_train)

accuracy_score(y_true, y_pred, normalize=False)
```

```
print(c.predict(X_test))
```

1.13. links

- ISO/IEC DIS 23053 - Machine Learning Framework
- 2022 [2205.02302] Machine Learning Operations (MLOps) Dominik Kreuzberger, Niklas Kühl, Sebastian Hirschl
- Probablistic Machine Learning, Kevin P. Murphy, MIT Press
- https://towardsdatascience.com/comprehensive-guide-on-multiclass-classification-metrics-af94cfb83fbd
- https://towardsdatascience.com/comprehensive-guide-to-multiclass-classification-with-sklearn-127cc500f362
- select sklearn algorithms for problems https://scikit-learn.org/stable/modules/multiclass.html

2. pandas, numpy - Small tasks Малые задачи

2.1. task 1

```
import pandas as pd
import numpy as np

import sklearn

print(np.arange(20))
a = np.random.randint(0, 20, size=10)
a = a.reshape((2,5))
b = np.eye(5)
b = b * 3
c = np.dot(a, b)
print(c.flatten())
```

```
[ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19]
[57.  0. 21. 30. 36. 30. 30. 45. 18.  3.]
```

2.2. task 2 DataFrame reshape

```
import pandas as pd
import numpy as np
df = pd.DataFrame({"a":[1,2,3]})
a = []

for x in range(12):
  s = np.random.randint(1,11, 3)
  df[str(x+1)] = s
print(df)
```

```
   a  1  2  3  4  5  6   7   8  9  10  11  12
0  1  9  5  1  7  2  4   6   8  2   1   6   2
1  2  7  9  6  2  8  7   3  10  5   7   5  10
2  3  5  6  1  1  8  1  10   3  8   4   7   1
```

We should transform v DataFrame to pivot table:

We will use DataFrame.melt: https://pandas.pydata.org/docs/user_guide/reshaping.html#reshaping

```
print(df)
print()
# print(v.pivot(index=["a"], columns=[1], values=[v.columns])) # , columns=["a"]
#
df2 = df.melt(id_vars=["a"])
df2["variable"] = df2.variable.astype(int)
print()
print(df2.sort_values(by=["a", "variable"]))
```

```
   a  1  2  3  4  5  6   7   8  9  10  11  12
0  1  9  5  1  7  2  4   6   8  2   1   6   2
1  2  7  9  6  2  8  7   3  10  5   7   5  10
2  3  5  6  1  1  8  1  10   3  8   4   7   1


    a  variable  value
0   1         1      9
3   1         2      5
6   1         3      1
9   1         4      7
12  1         5      2
15  1         6      4
18  1         7      6
21  1         8      8
24  1         9      2
```

```
27  1         10       1
30  1         11       6
33  1         12       2
1   2          1       7
4   2          2       9
7   2          3       6
10  2          4       2
13  2          5       8
16  2          6       7
19  2          7       3
22  2          8      10
25  2          9       5
28  2         10       7
31  2         11       5
34  2         12      10
2   3          1       5
5   3          2       6
8   3          3       1
11  3          4       1
14  3          5       8
17  3          6       1
20  3          7      10
23  3          8       3
26  3          9       8
29  3         10       4
32  3         11       7
35  3         12       1
```

2.2.1. learned RESHAPINGS guide https://pandas.pydata.org/docs/user_guide/reshaping.html

1. Resample for timeseries
    - 'M' - month boundary
    - 'A' - annual

```
loan_rev_data=data['Loan Amount']
loan_rev_data['date'] = pd.DatetimeIndex(data['Created Date'])
loan_rev_data = loan_rev_data.set_index('date')
monthly_loan_rev_data= loan_rev_data.resample('M').sum()
```

```
            Loan Amount
date
2014-10-31  13039283.00
2014-11-30  16097733.00
2014-12-31  29077334.00
```

2. pivot - rows to columns without aggregation

   Uses unique values from specified index / columns to form axes of the resulting DataFrame

   params: index, columns, values

```
import pandas as pd
df = pd.DataFrame({'foo': ['one', 'one', 'one', 'two', 'two','two'],
                   'bar': ['A', 'B', 'C', 'A', 'B', 'C'],
                   'baz': [1, 2, 3, 4, 5, 6],
                   'zoo': ['x', 'y', 'z', 'q', 'w', 't']})
print(df)
print()
print(df.pivot(index='foo', columns='bar', values='baz'))
```

```
   foo bar  baz zoo
0  one   A    1   x
1  one   B    2   y
2  one   C    3   z
3  two   A    4   q
4  two   B    5   w
5  two   C    6   t

bar  A  B  C
foo
one  1  2  3
two  4  5  6
```

   Possible misstakes example:

```
import pandas as pd
df = pd.DataFrame({"foo": ['one', 'one', 'two', 'two'],
                   "bar": ['A', 'A2', 'B', 'C'], # new columns should not have duplicates in one index
                   "baz": [1, 2, 3, 4]})
print(df.pivot(index='foo', columns='bar', values='baz'))
```

```
bar    A   A2    B    C
foo
```

```
one   1.0  2.0  NaN  NaN
two   NaN  NaN  3.0  4.0
```

- https://pandas.pydata.org/docs/user_guide/reshaping.html#reshaping
- https://pandas.pydata.org/docs/reference/api/pandas.DataFrame.pivot.html

3. stack (levels)

```
import pandas as pd
df_single_level_cols = pd.DataFrame([[0, 1], [2, 3]],
                                    index=['cat', 'dog'],
                                    columns=['weight', 'height'])
print(df_single_level_cols)
print()
print(df_single_level_cols.stack())
```

```
     weight  height
cat       0       1
dog       2       3

cat  weight    0
     height    1
dog  weight    2
     height    3
dtype: int64
```

4. melt - columns to rows
    1. ex1

```
import pandas as pd
df = pd.DataFrame(
    {
        "first": ["John", "Mary"],
        "last": ["Doe", "Bo"],
        "height": [5.5, 6.0],
        "weight": [130, 150],
    })
print(df)
print()
print(df.melt(id_vars=["first", "last"]))
```

```
  first last  height  weight
0  John  Doe     5.5     130
1  Mary   Bo     6.0     150

  first last variable  value
0  John  Doe   height    5.5
1  Mary   Bo   height    6.0
2  John  Doe   weight  130.0
3  Mary   Bo   weight  150.0
```

    2. ex2

```
import pandas as pd
df = pd.DataFrame({'A': {0: 'a', 1: 'b', 2: 'c'},
                   'B': {0: 1, 1: 3, 2: 5},
                   'C': {0: 2, 1: 4, 2: 6}})
print(df)
print()
print(pd.melt(df, id_vars=['A'], value_vars=['B']))
```

```
   A  B  C
0  a  1  2
1  b  3  4
2  c  5  6

   A variable  value
0  a        B      1
1  b        B      3
2  c        B      5
```

5. pivot_table - allow aggs
    1. ex1

```
import pandas as pd
import numpy as np
import datetime
df = pd.DataFrame(
    {
        "A": ["one", "one", "two", "three"] * 6,
        "B": ["A", "B", "C"] * 8,
        "C": ["foo", "foo", "foo", "bar", "bar", "bar"] * 4,
        "D": np.random.randn(24),
        "E": np.random.randn(24),
```

```
        "F": [datetime.datetime(2013, i, 1) for i in range(1, 13)]
        + [datetime.datetime(2013, i, 15) for i in range(1, 13)],
    })
print(df)
print()
print(pd.pivot_table(df, values="D", index=["A", "B"], columns=["C"]))
print()
print(pd.pivot_table(df, values="D", index=["B"], columns=["A", "C"], aggfunc=np.sum))
```

```
        A  B    C         D         E          F
0     one  A  foo -0.496471  0.783972 2013-01-01
1     one  B  foo  2.085890  0.095283 2013-02-01
2     two  C  foo -0.803101  1.063205 2013-03-01
3   three  A  bar -1.437647 -0.738354 2013-04-01
4     one  B  bar  1.698936 -0.153019 2013-05-01
5     one  C  bar  0.144399  0.121885 2013-06-01
6     two  A  foo -1.613003  0.807403 2013-07-01
7   three  B  foo  2.090471 -0.329079 2013-08-01
8     one  C  foo -1.268826  1.351324 2013-09-01
9     one  A  bar -0.490377 -0.635679 2013-10-01
10    two  B  bar -0.493791  1.150822 2013-11-01
11  three  C  bar  0.969203 -0.493382 2013-12-01
12    one  A  foo -0.701644  1.328246 2013-01-15
13    one  B  foo -0.012213 -0.926647 2013-02-15
14    two  C  foo  0.722384 -0.391392 2013-03-15
15  three  A  bar  1.241129  2.274940 2013-04-15
16    one  B  bar  1.171949 -0.101210 2013-05-15
17    one  C  bar  1.102122 -1.641848 2013-06-15
18    two  A  foo -0.009310  0.848572 2013-07-15
19  three  B  foo -0.984730  0.036997 2013-08-15
20    one  C  foo -0.944353 -1.265761 2013-09-15
21    one  A  bar  1.185517  0.252553 2013-10-15
22    two  B  bar  0.261429 -0.522052 2013-11-15
23  three  C  bar  0.004112  0.293106 2013-12-15

C             bar       foo
A     B
one   A  0.347570 -0.599057
      B  1.435442  1.036838
      C  0.623260 -1.106589
three A -0.098259       NaN
      B       NaN  0.552871
      C  0.486657       NaN
two   A       NaN -0.811156
      B -0.116181       NaN
      C       NaN -0.040358

A       one                three                two
C       bar       foo       bar       foo       bar       foo
B
A  0.695139 -1.198115 -0.196517       NaN       NaN -1.622313
B  2.870885  2.073677       NaN  1.105741 -0.232362       NaN
C  1.246521 -2.213179  0.973315       NaN       NaN -0.080716
```

2. ex2

```
import pandas as pd
import numpy as np
print(pd.pivot_table(df[["A", "B", "C", "D", "E"]], index=["A", "B"], columns=["C"]))
print()
print(pd.pivot_table(df, values="D", index=pd.Grouper(freq="M", key="F"), columns="C"))
print()
table = pd.pivot_table(df, index=["A", "B"], columns=["C"], values=["D", "E"])
print(table.to_string(na_rep=""))
print()
table = df.pivot_table(
    index=["A", "B"],
    columns="C",
    values=["D", "E"],
    margins=True,
    aggfunc=np.std)
print(table)
print()
print(table.stack())
```

```
                D                   E
C             bar       foo       bar       foo
A     B
one   A  0.347570 -0.599057 -0.191563  1.056109
      B  1.435442  1.036838 -0.127114 -0.415682
      C  0.623260 -1.106589 -0.759982  0.042781
three A -0.098259       NaN  0.768293       NaN
      B       NaN  0.552871       NaN -0.146041
      C  0.486657       NaN -0.100138       NaN
two   A       NaN -0.811156       NaN  0.827988
      B -0.116181       NaN  0.314385       NaN
      C       NaN -0.040358       NaN  0.335907

C                bar       foo
F
2013-01-31       NaN -0.599057
2013-02-28       NaN  1.036838
```

```
2013-03-31       NaN -0.040358
2013-04-30 -0.098259       NaN
2013-05-31  1.435442       NaN
2013-06-30  0.623260       NaN
2013-07-31       NaN -0.811156
2013-08-31       NaN  0.552871
2013-09-30       NaN -1.106589
2013-10-31  0.347570       NaN
2013-11-30 -0.116181       NaN
2013-12-31  0.486657       NaN

                D                   E
C             bar       foo       bar       foo
A     B
one   A  0.347570 -0.599057 -0.191563  1.056109
      B  1.435442  1.036838 -0.127114 -0.415682
      C  0.623260 -1.106589 -0.759982  0.042781
three A -0.098259            0.768293
      B            0.552871           -0.146041
      C  0.486657           -0.100138
two   A           -0.811156            0.827988
      B -0.116181            0.314385
      C           -0.040358            0.335907

                D                             E
C             bar       foo       All       bar       foo       All
A     B
one   A  1.185036  0.145079  0.879671  0.628075  0.384860  0.836517
      B  0.372636  1.483583  0.912645  0.036635  0.722614  0.449735
      C  0.677213  0.229437  1.080685  1.247147  1.850559  1.369230
three A  1.894181       NaN  1.894181  2.130720       NaN  2.130720
      B       NaN  2.174496  2.174496       NaN  0.258855  0.258855
      C  0.682422       NaN  0.682422  0.556131       NaN  0.556131
two   A       NaN  1.133982  1.133982       NaN  0.029111  0.029111
      B  0.534022       NaN  0.534022  1.182900       NaN  1.182900
      C       NaN  1.078681  1.078681       NaN  1.028556  1.028556
All      0.934619  1.220583  1.084208  0.993422  0.877783  0.909890

                    D         E
A     B C
one   A All  0.879671  0.836517
        bar  1.185036  0.628075
        foo  0.145079  0.384860
      B All  0.912645  0.449735
        bar  0.372636  0.036635
        foo  1.483583  0.722614
      C All  1.080685  1.369230
        bar  0.677213  1.247147
        foo  0.229437  1.850559
three A All  1.894181  2.130720
        bar  1.894181  2.130720
      B All  2.174496  0.258855
        foo  2.174496  0.258855
      C All  0.682422  0.556131
        bar  0.682422  0.556131
two   A All  1.133982  0.029111
        foo  1.133982  0.029111
      B All  0.534022  1.182900
        bar  0.534022  1.182900
      C All  1.078681  1.028556
        foo  1.078681  1.028556
All     All  1.084208  0.909890
        bar  0.934619  0.993422
        foo  1.220583  0.877783
```

6. pivot tables(old)

```python
melb_df.groupby(['Rooms', 'Type'])['Price'].mean() # иерархические индексы
melb_df.groupby(['Rooms', 'Type'])['Price'].mean().unstack() # раскладывает таблицу в столбцы
melb_df.pivot_table(
    values='Price',
    index='Rooms',
    columns='Type',
    fill_value=0
).round() # аналогично второму
```

7. crosstab - frequencies

frequency table of the factors unless an array of values and an aggregation function are passed.

```python
import pandas as pd
import numpy as np
foo, bar, dull, shiny, one, two = "foo", "bar", "dull", "shiny", "one", "two"
a = np.array([foo, foo, bar, bar, foo, foo], dtype=object)
b = np.array([one, one, two, one, two, one], dtype=object)
c = np.array([dull, dull, shiny, dull, dull, shiny], dtype=object)
print("frequencies:")
print(pd.crosstab(a, b))
print()
print(pd.crosstab(a, [b, c], rownames=["a"], colnames=["b", "c"]))
```

```
frequencies:
col_0  one  two
row_0
bar      1    1
foo      3    1

b    one        two
c   dull shiny dull shiny
a
bar    1     0    0     1
foo    2     1    1     0
```

8. cut - transform continuous variables to discrete or categorical variables

```
import pandas as pd
import numpy as np
ages = np.array([10, 15, 13, 12, 23, 25, 28, 59, 60])
print(pd.cut(ages, bins=3))
print()
print(pd.cut(ages, bins=[0, 18, 35, 70]))
```

```
[(9.95, 26.667], (9.95, 26.667], (9.95, 26.667], (9.95, 26.667], (9.95, 26.667], (9.95, 26.667], (26.667, 43.333], (
Categories (3, interval[float64, right]): [(9.95, 26.667] < (26.667, 43.333] < (43.333, 60.0]]

[(0, 18], (0, 18], (0, 18], (0, 18], (18, 35], (18, 35], (18, 35], (35, 70], (35, 70]]
Categories (3, interval[int64, right]): [(0, 18] < (18, 35] < (35, 70]]
```

9. dummies
    - pd.get_dummies(df, prefix="new_prefix")
    - pd.from_dummies(df, sep="_")
10. factorize - categories to numbers

```
import pandas as pd
import numpy as np
x = pd.Series(["A", "A", np.nan, "B", 3.14, np.inf])
labels, uniques = pd.factorize(x)
print(labels)
print(uniques)
```

```
[ 0  0 -1  1  2  3]
Index(['A', 'B', 3.14, inf], dtype='object')
```

11. explode

```
import pandas as pd
import numpy as np
keys = ["panda1", "panda2", "panda3"]
values = [["eats", "shoots"], ["shoots", "leaves"], ["eats", "leaves"]]
df = pd.DataFrame({"keys": keys, "values": values})
print(df)
print()
print(df["values"].explode())
print()
print(df.explode("values"))
```

```
     keys            values
0  panda1    [eats, shoots]
1  panda2  [shoots, leaves]
2  panda3    [eats, leaves]

0      eats
0    shoots
1    shoots
1    leaves
2      eats
2    leaves
Name: values, dtype: object

     keys  values
0  panda1    eats
0  panda1  shoots
1  panda2  shoots
1  panda2  leaves
2  panda3    eats
2  panda3  leaves
```

12. assign and explode - split values to rows

```
import pandas as pd
import numpy as np
df = pd.DataFrame([{"var1": "a,b,c,d", "var2": 1}, {"var1": "d,e,f", "var2": 2}])
print(df)
```

```
print()
print(df.assign(var1=df.var1.str.split(",")).explode("var1"))
```

```
      var1  var2
0  a,b,c,d     1
1    d,e,f     2

  var1  var2
0    a     1
0    b     1
0    c     1
0    d     1
1    d     2
1    e     2
1    f     2
```

Footnotes:

[1] https://web.stanford.edu/~hastie/Papers/ESLII.pdf

Created: 2023-04-26 Wed 17:59
Validate