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Tune Hyperparameters for Classification Machine Learning Algorithms

by Jason Brownlee on December 13, 2019 in Python Machine Learning

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Last Updated on August 28, 2020

Machine learning algorithms have hyperparameters that allow you to tailor the behavior of the algorithm to your specific dataset.

Hyperparameters are different from parameters, which are the internal coefficients or weights for a model found by the learning algorithm. Unlike parameters, hyperparameters are specified by the practitioner when configuring the model.

Typically, it is challenging to know what values to use for the hyperparameters of a given algorithm on a given dataset, therefore it is common to use random or grid search strategies for different hyperparameter values.

The more hyperparameters of an algorithm that you need to tune, the slower the tuning process. Therefore, it is desirable to select a minimum subset of model hyperparameters to search or tune.

Not all model hyperparameters are equally important. Some hyperparameters have an outsized effect on the behavior, and in turn, the performance of a machine learning algorithm.

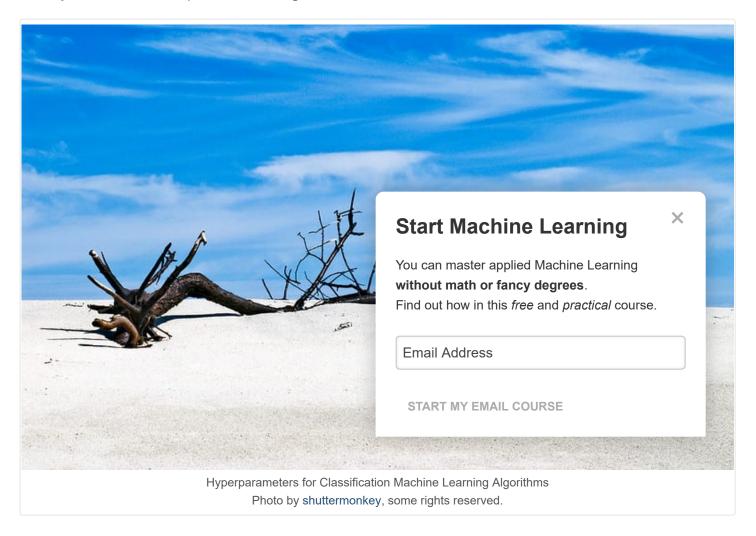
As a machine learning practitioner, you must know which hyperparameters to focus on to get a good result quickly.

In this tutorial, you will discover those hyperparameters that are most important for some of the top machine learning algorithms.

Kick-start your project with my new book Machine Learning Mastery With Python, including *step-by-step tutorials* and the *Python source code* files for all exam^r

Let's get started.

Update Jan/2020: Updated for changes in scikit-learn v0.22 API.



Classification Algorithms Overview

We will take a closer look at the important hyperparameters of the top machine learning algorithms that you may use for classification.

We will look at the hyperparameters you need to focus on and suggested values to try when tuning the model on your dataset.

The suggestions are based both on advice from textbooks on the algorithms and practical advice suggested by practitioners, as well as a little of my own experience.

The seven classification algorithms we will look at are as follows:

- 1. Logistic Regression
- 2. Ridge Classifier
- 3. K-Nearest Neighbors (KNN)
- 4. Support Vector Machine (SVM)
- 5. Bagged Decision Trees (Bagging)

- 6. Random Forest
- 7. Stochastic Gradient Boosting

We will consider these algorithms in the context of their scikit-learn implementation (Python); nevertheless, you can use the same hyperparameter suggestions with other platforms, such as Weka and R.

A small grid searching example is also given for each algorithm that you can use as a starting point for your own classification predictive modeling project.

Note: if you have had success with different hyperparameter values or even different hyperparameters than those suggested in this tutorial, let me know in the comments below. I'd love to hear about it.

Let's dive in.

Logistic Regression

Logistic regression does not really have any critical hy

Sometimes, you can see useful differences in perform

• solver in ['newton-cg', 'lbfgs', 'liblinear', 'sag', 'sag'

Regularization (penalty) can sometimes be helpful.

• penalty in ['none', 'l1', 'l2', 'elasticnet']

Note: not all solvers support all regularization terms.

• C in [100, 10, 1.0, 0.1, 0.01]

For the full list of hyperparameters, see:

sklearn.linear model.LogisticRegression API.

The example below demonstrates grid searching the key hyperparameters for LogisticRegression on a synthetic binary classification dataset.

Some combinations were omitted to cut back on the warnings/errors.

The C parameter controls the penality strength, which can also be effective.

```
# example of grid searching key hyperparametres for logistic regression
from sklearn.datasets import make_blobs
from sklearn.model_selection import RepeatedStratifiedKFold
from sklearn.model_selection import GridSearchCV
from sklearn.linear_model import LogisticRegression
# define dataset
X, y = make_blobs(n_samples=1000, centers=2, n_features=100, cluster_std=20)
# define models and parameters
model = LogisticRegression()
solvers = ['newton-cg', 'lbfgs', 'liblinear']
Start Machine Learning
```



Note: Your results may vary given the stochastic nature of the algorithm or evaluation procedure, or differences in numerical precision. Consider running the X **Start Machine Learning** outcome. You can master applied Machine Learning Running the example prints the best result as well as without math or fancy degrees. Best: 0.945333 using {'C': 0.01, 'penalty': ' Find out how in this free and practical course. 0.936333 (0.016829) with: {'C': 100, 'penalty 0.937667 (0.017259) with: {'C': 100, 4 0.938667 (0.015861) with: {'C': 100, 'penalty **Email Address** 5 0.936333 (0.017413) with: {'C': 10, 'penalty' 6 0.938333 (0.017904) with: {'C': 10, 'penalty' 7 0.939000 (0.016401) with: {'C': 10, 'penalty' 8 0.937333 (0.017114) with: {'C': 1.0, 'penalty START MY EMAIL COURSE 9 0.939000 (0.017195) with: {'C': 1.0, 10 0.939000 (0.015780) with: {'C': 1.0, 'penalty : LZ, solver: '12', 11 0.940000 (0.015706) with: {'C': 0.1, 'penalty': 'solver': 'newton-cg'} 12 0.940333 (0.014941) with: {'C': 0.1, 'penalty': 'l2', 'solver': 'lbfgs'} 13 0.941000 (0.017000) with: {'C': 0.1, 'penalty': 'l2', 14 0.943000 (0.016763) with: {'C': 0.01, 'penalty': 'l2', 'solver': 'newton-cg'} , 55101 . Newton-10103 (0.010703) with: {'C': 0.01, 'penalty': 'l2', 'solver': 'lbfgs'}

16 0.945333 (0.017651) with: {'C': 0.01, 'penalty': 'l2', 'solver': 'libline' , 'solver': 'liblinear'}

Ridge Classifier

Ridge regression is a penalized linear regression model for predicting a numerical value.

Nevertheless, it can be very effective when applied to classification.

Perhaps the most important parameter to tune is the regularization strength (*alpha*). A good starting point might be values in the range [0.1 to 1.0]

• alpha in [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0]

For the full list of hyperparameters, see:

sklearn.linear model.RidgeClassifier API.

The example below demonstrates grid searching the key hyperparameters for RidgeClassifier on a synthetic binary classification dataset.

Start Machine Learning

```
1 # example of grid searching key hyperparametres for ridge classifier
 2 from sklearn.datasets import make_blobs
   from sklearn.model_selection import RepeatedStratifiedKFold
 4 from sklearn.model_selection import GridSearchCV
 5 from sklearn.linear_model import RidgeClassifier
 6 # define dataset
 7 X, y = make_blobs(n_samples=1000, centers=2, n_features=100, cluster_std=20)
 8 # define models and parameters
 9 model = RidgeClassifier()
10 alpha = [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0]
11 # define grid search
12 grid = dict(alpha=alpha)
13 cv = RepeatedStratifiedKFold(n_splits=10, n_repeats=3, random_state=1)
14 grid_search = GridSearchCV(estimator=model, param_grid=grid, n_jobs=-1, cv=cv, scoring='accura
15 grid_result = grid_search.fit(X, y)
16 # summarize results
17 print("Best: %f using %s" % (grid_result.best_score arid result hest narams ))
18 means = grid_result.cv_results_['mean_test_sc
19 stds = grid_result.cv_results_['std_test_score
                                                    Start Machine Learning
20 params = grid_result.cv_results_['params']
21 for mean, stdev, param in zip(means, stds, pa
22
        print("%f (%f) with: %r" % (mean, stdev,
                                                     You can master applied Machine Learning
                                                     without math or fancy degrees.
Note: Your results may vary given the stochastic natural
                                                     Find out how in this free and practical course.
differences in numerical precision. Consider running the
outcome.
                                                      Email Address
Running the example prints the best result as well as
                                                      START MY EMAIL COURSE
    Best: 0.974667 using {'alpha': 0.1}
    0.974667 (0.014545) with: {'alpha': 0.1}
 3 0.974667 (0.014545) with: {'alpha': 0.2}
 4 0.974667 (0.014545) with: {'alpha': 0.3}
 5 0.974667 (0.014545) with: {'alpha': 0.4}
 6 0.974667 (0.014545) with: {'alpha': 0.5}
 7 0.974667 (0.014545) with: {'alpha': 0.6}
 8 0.974667 (0.014545) with: {'alpha': 0.7}
 9 0.974667 (0.014545) with: {'alpha': 0.8}
10 0.974667 (0.014545) with: {'alpha': 0.9}
11 0.974667 (0.014545) with: {'alpha': 1.0}
```

K-Nearest Neighbors (KNN)

The most important hyperparameter for KNN is the number of neighbors (*n neighbors*).

Test values between at least 1 and 21, perhaps just the odd numbers.

• **n_neighbors** in [1 to 21]

It may also be interesting to test different distance metrics (*metric*) for choosing the composition of the neighborhood.

metric in ['euclidean', 'manhattan', 'minkowski']

For a fuller list see:

sklearn.neighbors.DistanceMetric API

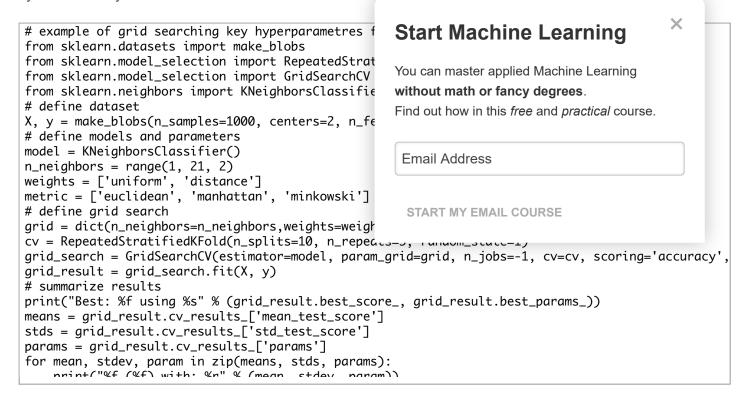
It may also be interesting to test the contribution of members of the neighborhood via different weightings (weights).

• weights in ['uniform', 'distance']

For the full list of hyperparameters, see:

sklearn.neighbors.KNeighborsClassifier API.

The example below demonstrates grid searching the key hyperparameters for KNeighborsClassifier on a synthetic binary classification dataset.



Note: Your results may vary given the stochastic nature of the algorithm or evaluation procedure, or differences in numerical precision. Consider running the example a few times and compare the average outcome.

Running the example prints the best result as well as the results from all combinations evaluated.

```
Best: 0.937667 using {'metric': 'manhattan', 'n_neighbors': 13,
                                                                          'weights': 'uniform'}
   0.833667 (0.031674) with: {'metric': 'euclidean', 'n_neighbors': 1,
                                                                              'weights': 'uniform'}
3
   0.833667 (0.031674) with: {'metric': 'euclidean'
                                                          'n_neighbors': 1,
                                                                              'weights': 'distance'}
                                                          'n_neighbors': 3,
   0.895333 (0.030081) with: {'metric': 'euclidean'
                                                                              'weights': 'uniform'}
   0.895333 (0.030081) with: {'metric':
                                            'euclidean'
                                                          'n_neighbors'
                                                                              'weights':
                                                                                          'distance'}
5
                                                                         : 3,
   0.909000 (0.021810) with: {'metric':
                                                          'n_neighbors': 5,
                                                                              'weights':
                                                                                          'uniform'}
6
                                            'euclidean'
   0.909000 (0.021810) with: {'metric': 'euclidean'
                                                                         : 5,
                                                                              'weights': 'distance'}
                                                          'n_neighbors'
  0.925333 (0.020774) with: {'metric': 'euclidean'
                                                          'n_neighbors': 7,
                                                                              'weights': 'uniform'}
8
9 0.925333 (0.020774) with: {'metric': 'euclidean',
                                                          'n_neighbors': 7,
                                                                              'weights': 'distance'}
10 0.929000 (0.027368) with: {'metric': 'euclidean', 'n_neighbors': 9, 11 0.929000 (0.027368) with: {'metric': 'euclidean' 'n_neighbors': 9
                                                          'n_neighbors': 9,
                                                                              'weights': 'uniform'}
12 ...
                                                        Start Machine Learning
```

Support Vector Machine (SVM)

The SVM algorithm, like gradient boosting, is very popular, very effective, and provides a large number of hyperparameters to tune.

Perhaps the first important parameter is the choice of kernel that will control the manner in which the input variables will be projected. There are many to choose from, but linear, polynomial, and RBF are the most common, perhaps just linear and RBF in practice.

kernels in ['linear', 'poly', 'rbf', 'sigmoid']

If the polynomial kernel works out, then it is a good idea to dive into the degree hyperparameter.

Another critical parameter is the penalty (*C*) that can to on the shape of the resulting regions for each class. A

• **C** in [100, 10, 1.0, 0.1, 0.001]

For the full list of hyperparameters, see:

sklearn.svm.SVC API.

The example below demonstrates grid searching the lassification dataset.



```
# example of grid searching key hyperparametres for SVC
from sklearn.datasets import make_blobs
from sklearn.model_selection import RepeatedStratifiedKFold
from sklearn.model_selection import GridSearchCV
from sklearn.svm import SVC
# define dataset
X, y = make_blobs(n_samples=1000, centers=2, n_features=100, cluster_std=20)
# define model and parameters
model = SVC()
kernel = ['poly', 'rbf', 'sigmoid']
C = [50, 10, 1.0, 0.1, 0.01]
gamma = ['scale']
# define grid search
grid = dict(kernel=kernel, C=C, gamma=gamma)
cv = RepeatedStratifiedKFold(n_splits=10, n_repeats=3, random_state=1)
grid_search = GridSearchCV(estimator=model, param_grid=grid, n_jobs=-1, cv=cv, scoring='accuracy',
grid_result = grid_search.fit(X, y)
# summarize results
print("Best: %f using %s" % (grid_result.best_score_, grid_result.best_params_))
means = grid_result.cv_results_['mean_test_score']
stds = grid_result.cv_results_['std_test_score']
params = grid_result.cv_results_['params']
for mean, stdev, param in zip(means, stds, params):
    nnin+("" ( ( ( ) wi+h · «n" « ( maan
```

Note: Your results may vary given the stochastic nature of the algorithm or evaluation procedure, or differences in numerical precision. Consider running the example a few times and compare the average outcome.

Running the example prints the best result as well as the results from all combinations evaluated.

```
Best: 0.974333 using {'C': 1.0, 'gamma': 'scale', 'kernel': 'poly'}
    0.973667 (0.012512) with: {'C': 50, 'gamma': 'scale', 'kernel': 'poly'}
                                                                  'kernel': 'rbf'}
    0.970667 (0.018062) with: {'C': 50, 'gamma': 'scale',
   0.945333 (0.024594) with: {'C': 50, 'gamma':
                                                        'scale',
                                                                   'kernel': 'sigmoid'}
                                              'gamma':
                                                                   'kernel': 'poly'}
 5 0.973667 (0.012512) with: {'C': 10,
                                                         'scale',
                                                        'scale',
    0.970667 (0.018062) with: {'C': 10,
                                                                   'kernel':
                                              'gamma':
    0.957000 (0.016763) with: {'C': 10, 'gamma': 'scale',
 7
                                                                   'kernel': 'sigmoid'}
   0.974333 (0.012565) with: {'C': 1.0, 'gamma': 'scale',
                                                                    'kernel': 'poly'}
 9 0.971667 (0.016948) with: {'C': 1.0, 'gamma': 'scale',
                                                                    'kernel':
10 0.966333 (0.016224) with: {'C': 1.0, 'gamma': 'scale', 'kernel': 'sigmoid'}
                                                                  , 'kernel':
11 0.972333 (0.013585) with: {'C': 0.1, 'gamma': 'scale'
12 0.974000 (0.013317) with: {'C': 0.1, 'gamma': 'scale', 'kernel': 'rbf'}
13 0.971667 (0.015934) with: {'C': 0.1, 'gamma': 'scale', 'kernel': 'sigmoid'}
14 0.972333 (0.013585) with: {'C': 0.01, 'gamma': 'scale', 'kernel': 'poly'}
13 0.971667 (0.015934) with: {'C': 0.1, '14 0.972333 (0.013585) with: {'C': 0.01,
15 0.973667 (0.014716) with: {'C': 0.01, 'gamma'
16 0.974333 (0.013828) with: {'C': 0.01,
                                                            Start Machine Learning
Bagged Decision Trees (Baggin
                                                            You can master applied Machine Learning
                                                            without math or fancy degrees.
The most important parameter for bagged decision tre
                                                            Find out how in this free and practical course.
Ideally, this should be increased until no further improve
                                                             Email Address
Good values might be a log scale from 10 to 1,000.
```

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• n_estimators in [10, 100, 1000]

For the full list of hyperparameters, see:

sklearn.ensemble.BaggingClassifier API

The example below demonstrates grid searching the key hyperparameters for BaggingClassifier on a synthetic binary classification dataset.

```
# example of grid searching key hyperparameters for BaggingClassifier
2 from sklearn.datasets import make_blobs
3 from sklearn.model_selection import RepeatedStratifiedKFold
4 from sklearn.model_selection import GridSearchCV
5 from sklearn.ensemble import BaggingClassifier
6 # define dataset
   X, y = make_blobs(n_samples=1000, centers=2, n_features=100, cluster_std=20)
  # define models and parameters
9 model = BaggingClassifier()
10 n_{estimators} = [10, 100, 1000]
11 # define grid search
12 grid = dict(n_estimators=n_estimators)
13 cv = RepeatedStratifiedKFold(n_splits=10, n_repeats=3, random_state=1)
14 grid_search = GridSearchCV(estimator=model, param_grid=grid, n_jobs=-1, cv=cv, scoring='accura@
15 grid_result = grid_search.fit(X, y)
16 # summarize results
17 print("Best: %f using %s" % (grid_result.best_score_, grid_result.best_params_))
18 means = grid_result.cv_results_['mean_test_score']
19 stds = grid_result.cv_results_['std_test_score']
20 params = grid_result.cv_results_['params']
21 for mean, stdev, param in zip(means, stds, pa
                                                   Start Machine Learning
       print("%f (%f) with: %r" % (mean, stdev,
```

Note: Your results may vary given the stochastic nature of the algorithm or evaluation procedure, or differences in numerical precision. Consider running the example a few times and compare the average outcome.

Running the example prints the best result as well as the results from all combinations evaluated.

```
1 Best: 0.873667 using {'n_estimators': 1000}
2 0.839000 (0.038588) with: {'n_estimators': 10}
3 0.869333 (0.030434) with: {'n_estimators': 100}
4 0.873667 (0.035070) with: {'n_estimators': 1000}
```

Random Forest

The most important parameter is the number of rando (*max_features*).

You could try a range of integer values, such as 1 to 2

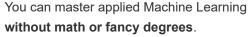
• max_features [1 to 20]

Alternately, you could try a suite of different default va

• max_features in ['sqrt', 'log2']

Another important parameter for random forest is the

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Ideally, this should be increased until no further improvement is seen in the model.

Good values might be a log scale from 10 to 1,000.

• n_estimators in [10, 100, 1000]

For the full list of hyperparameters, see:

sklearn.ensemble.RandomForestClassifier API.

The example below demonstrates grid searching the key hyperparameters for BaggingClassifier on a synthetic binary classification dataset.

```
# example of grid searching key hyperparameters for RandomForestClassifier
from sklearn.datasets import make_blobs
from sklearn.model_selection import RepeatedStratifiedKFold
from sklearn.model_selection import GridSearchCV
from sklearn.ensemble import RandomForestClassifier
# define dataset
X, y = make_blobs(n_samples=1000, centers=2, n_features=100, cluster_std=20)
# define models and parameters
model = RandomForestClassifier()
n_estimators = [10, 100, 1000]
max_features = ['sqrt', 'log2']
# define grid search
grid = dict(n_estimators=n_estimators,max_feature
cv = RepeatedStratifiedKFold(n_splits=10, n_repeated)
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```

Note: Your results may vary given the stochastic nature of the algorithm or evaluation procedure, or differences in numerical precision. Consider running the example a few times and compare the average outcome.

Running the example prints the best result as well as the results from all combinations evaluated

```
1 Best: 0.952000 using {'max_features': 'log2', 2 0.841000 (0.032078) with: {'max_features': 'sq 3 0.938333 (0.020830) with: {'max_features': 'sq 4 0.944667 (0.024998) with: {'max_features': 'sq 5 0.817667 (0.033235) with: {'max_features': 'lo 6 0.940667 (0.021592) with: {'max_features': 'lo 7 0.952000 (0.019562) with: {'max_features': 'lo
```

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Stochastic Gradient Boosting

Also called Gradient Boosting Machine (GBM) or nam

The gradient boosting algorithm has many parameters to tune.

There are some parameter pairings that are important to consider. The first is the learning rate, also called shrinkage or eta (*learning_rate*) and the number of trees in the model (*n_estimators*). Both could be considered on a log scale, although in different directions.

- learning_rate in [0.001, 0.01, 0.1]
- n_estimators [10, 100, 1000]

Another pairing is the number of rows or subset of the data to consider for each tree (*subsample*) and the depth of each tree (*max_depth*). These could be grid searched at a 0.1 and 1 interval respectively, although common values can be tested directly.

- **subsample** in [0.5, 0.7, 1.0]
- max_depth in [3, 7, 9]

For more detailed advice on tuning the XGBoost implementation, see:

How to Configure the Gradient Boosting Algorithm

For the full list of hyperparameters, see:

sklearn.ensemble.GradientBoostingClassifier API

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ost.

The example below demonstrates grid searching the key hyperparameters for GradientBoostingClassifier on a synthetic binary classification dataset.

```
# example of grid searching key hyperparameters for GradientBoostingClassifier
   from sklearn.datasets import make_blobs
   from sklearn.model_selection import RepeatedStratifiedKFold
   from sklearn.model_selection import GridSearchCV
    from sklearn.ensemble import GradientBoostingClassifier
 6
   # define dataset
   X, y = make_blobs(n_samples=1000, centers=2, n_features=100, cluster_std=20)
 7
 8 # define models and parameters
 9 model = GradientBoostingClassifier()
10 n_{estimators} = [10, 100, 1000]
11 learning_rate = [0.001, 0.01, 0.1]
12 subsample = [0.5, 0.7, 1.0]
13 max_depth = [3, 7, 9]
14 # define grid search
15 grid = dict(learning_rate=learning_rate, n_es
                                                                                                 x_de
                                                     Start Machine Learning
16 cv = RepeatedStratifiedKFold(n_splits=10, n_r
17 grid_search = GridSearchCV(estimator=model, p
                                                                                                 urad
                                                     You can master applied Machine Learning
18 grid_result = grid_search.fit(X, y)
19 # summarize results
                                                     without math or fancy degrees.
20 print("Best: %f using %s" % (grid_result.best
                                                     Find out how in this free and practical course.
21 means = grid_result.cv_results_['mean_test_sc
22 stds = grid_result.cv_results_['std_test_score
23 params = grid_result.cv_results_['params']
                                                      Email Address
24 for mean, stdev, param in zip(means, stds, pa
        print("%f (%f) with: %r" % (mean, stdev,
                                                       START MY EMAIL COURSE
Note: Your results may vary given the stochastic natural
differences in numerical precision. Consider running the
outcome.
```

Running the example prints the best result as well as the results from all combinations evaluated.

```
Best: 0.936667 using {'learning_rate': 0.01, 'max_depth': 3, 'n_estimators': 1000,
                                                                                        'subsample':
                                                       'max_depth': 3, 'n_estimators': 10, 'subsamm
   0.803333 (0.042058) with: {'learning_rate': 0.001,
   0.783667 (0.042386) with: {'learning_rate': 0.001,
                                                       'max_depth': 3,
                                                                       'n_estimators': 10,
                                                                                            'subsamr
  0.711667 (0.041157) with: {'learning_rate': 0.001,
                                                       'max_depth': 3, 'n_estimators': 10, 'subsamm
  0.832667 (0.040244) with: {'learning_rate': 0.001,
                                                       'max_depth': 3, 'n_estimators': 100, 'subsar
   0.809667 (0.040040) with: {'learning_rate': 0.001,
                                                                       'n_estimators': 100, 'subsan
                                                        'max_depth': 3,
   0.741333 (0.043261) with: {'learning_rate': 0.001,
                                                        'max_depth': 3,
                                                                        'n_estimators': 100,
                                                                                             'subsar
  0.881333 (0.034130) with: {'learning_rate': 0.001,
8
                                                       'max_depth': 3,
                                                                       'n_estimators': 1000, 'subso
9 0.866667 (0.035150) with: {'learning_rate': 0.001,
                                                       'max_depth': 3,
                                                                       'n_estimators': 1000, 'subso
10 0.838333 (0.037424) with: {'learning_rate': 0.001,
                                                        'max_depth': 3,
                                                                       'n_estimators': 1000, 'subso
                                                        'max_depth': 7,
                                                                       'n_estimators': 10,
11 0.838333 (0.036614) with: {'learning_rate': 0.001,
                                                                                            'subsamr
12 0.821667 (0.040586) with: {'learning_rate': 0.001,
                                                        'max_depth': 7,
                                                                       'n_estimators': 10,
                                                                                            'subsamr
13 0.729000 (0.035903) with: {'learning_rate': 0.001,
                                                        'max_depth': 7,
                                                                       'n_estimators': 10,
                                                                                            'subsamp
14 0.884667 (0.036854) with: {'learning_rate': 0.001,
                                                        'max_depth': 7,
                                                                        'n_estimators': 100,
15 0.871333 (0.035094) with: {'learning_rate': 0.001,
                                                        'max_depth': 7,
                                                                        'n_estimators': 100,
                                                                                             'subsar
16 0.729000 (0.037625) with: {'learning_rate': 0.001,
                                                       'max_depth': 7,
                                                                       'n_estimators': 100,
                                                                                             'subsan
17 0.905667 (0.033134) with: {'learning_rate': 0.001,
                                                       'max_depth': 7, 'n_estimators': 1000, 'subso
18 ...
```

Further Reading

This section provides more resources on the topic if you are looking to go deeper.

- scikit-learn API
- · Caret List of Algorithms and Tuning Parameters

Summary

In this tutorial, you discovered the top hyperparameters and how to configure them for top machine learning algorithms.

Dev

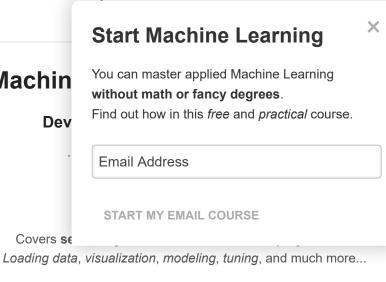
Covers se

Do you have other hyperparameter suggestions? Let me know in the comments below.

Do you have any questions?

Ask your questions in the comments below and I will do my best to answer.





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Jason Brownlee, PhD is a machine learning specialist who teaches developers how to get results with modern machine learning methods via hands-on tutorials.

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44 Responses to *Tune Hyperparameters for Classification Machine Learning Algorithms*



Dazhi December 13, 2019 at 6:07 am #

REPLY 5

Thanks for the useful post! A quick question here: why do you set n_repeats=3 for the cross validation? As far as I understand, the cv will split the data into folds and calculate the metrics on each fold and take the average. Is it necessary to repeat this process for 3 times?



Jason Brownlee December 13, 2019 at 6:29

Excellent question.

Repeats help to smooth out the variance in some r datasets. Repeated CV compared to 1xCV can oft model.

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Doug Dean December 13, 2019 at 7:09 am #

Thanks for the great article.

Changing the parameters for the ridge classifier did not change the outcome. Is that because of the synthetic dataset or is there some other problem with the example?



Jason Brownlee December 13, 2019 at 1:40 pm #

REPLY 🦴

Yes, likely because the synthetic dataset is so simple.

Jonathan Mackenzie December 13, 2019 at 10:20 am #



I normally use TPE for my hyperparameter optimisation, which is good at searching over large parameter spaces. Hyperas and hyperopt even let you do this in parallel! https://github.com/maxpumperla/hyperas

Also, keras recently introduced their own HO tool called keras-tuner, which looks easy to use:

https://github.com/keras-team/keras-tuner



Jason Brownlee December 13, 2019 at 1:42 pm #

REPLY

Thanks for sharing.



Oren December 13, 2019 at 11:50 am #

REPLY 🦴

Dear Jason,

How about an article about generalization abilities of ML models? For instance, we train and tune a specific learning algorithm on a data set (train + validation set) from a distributon X and apply it to some data that

origins from another distribution Y. In practise, the learn how to counteract the problem besides basic stuff like

Best regards



Jason Brownlee December 13, 2019 at 1:44

Thanks for the suggestion.

Yes, I have tens of tutorials on the topic. Perhaps shttps://machinelearningmastery.com/introduction-togeneralization-error/

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Rich Larrabee December 21, 2019 at 9:23 am #



Thanks for the article Jason. I have a follow-up question. Which one of these models is best when the classes are highly imbalanced (fraud for example)? And why?

Thanks.

Rich

Jason Brownlee December 22, 2019 at 6:05 am #



There is no best model in general. I recommend testing a suite of different techniques for imbalanced classification and discovering what works best for your specific dataset.



adip32 January 5, 2020 at 10:49 pm #

REPLY +

xgboost not included? why only 7 algorithms?

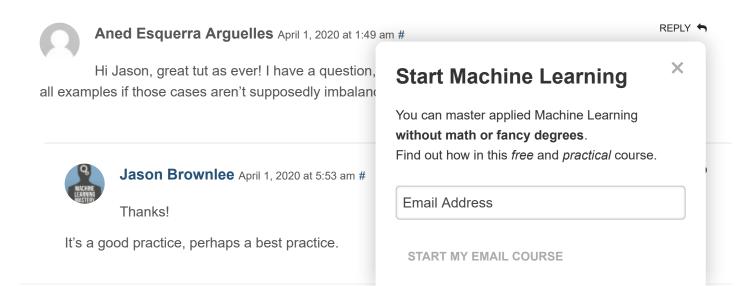


Jason Brownlee January 6, 2020 at 7:12 am #



This are the popular algorithms in sklearn.

For tuning xgboost, see the suite of tutorials, perhaps starting here: https://machinelearningmastery.com/start-here/#xgboost





John White April 30, 2020 at 9:12 am #

REPLY 🦴

Hi Jason!

Question on tuning RandomForest. For my hypertuning results, the best parameters' precision_score is very similar to the spot check. I am having a hard time understanding how is this possible.

From the spot check, results proved the model already has little skill, slightly better than no skill, so I think it has potential. However the best parameters says otherwise.

I am currently trying to tune a binary RandomForestClassifier using RandomizedSearchCV (... refit='precision'). Precision being: make scorer(precision score, average = 'weighted'). Dataset is balanced.

Jason Brownlee April 30, 2020 at 11:37 am #



Perhaps the difference in the mean results is no statistically significant. So the numbers look different, but the behavior is not different on average.



John White April 30, 2020 at 12:13 pm #

Ah I see. Is there a way to get to the bottom of this? I am currently looking into feature selection as given here: https://machinelearningmastery.com/feature-selection-with-real-and-categorical-data/



Jason Brownlee April 30, 2020 at 1:32 pm #

REPLY 🖴

X

Yes, here is some advice on how to use hypothesis tests to compare results: https://machinelearningmastery.com/statistical-significance-tests-for-comparing-machine-learning-algorithms/

Or perhaps you can change your test harness, e.g. more repeats, more folds, to help better expose differences between algorithms.



John White April 30, 2020 at 1:42 pm #

Thank you. I'll start there. When I was models, they also returned similar very similar just the similar: slightly better than no skill.

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Jason Brownlee May 1, 2020 at 6:2

It is possible that your problem is not predictable in its current form/framing.



John White May 9, 2020 at 5:13 am #

I am going to try out different models. Features are correlated and important through different feature selection and feature importance tests. Also coupled with industry knowledge, I also know the features can help determine the target variable (problem). I won't give up!



Jason Brownlee May 9, 2020 at 6:25 am #

Sounds great!



Skylar May 16, 2020 at 5:04 am #

Hi Jason,

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REPLY +

Nice post, very clear! You mainly talked about algorithms for classification problems, do you also have the summary for regression? Or it is more or less similar? Thanks!



Jason Brownlee May 16, 2020 at 6:24 am #

REPLY 🦴

Thanks!

Not at this stage, perhaps soon.



Skylar May 16, 2020 at 2:32 pm #

That would be great, I will definitely ke



Jason Brownlee May 17, 2020 at 6

Thanks.

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sukhpal June 1, 2020 at 1:10 am #

sir what technique we apply after hyper-parameter optimization to furthur refine the results



Jason Brownlee June 1, 2020 at 6:25 am #



REPLY <

See this:

http://machinelearningmastery.com/machine-learning-performance-improvement-cheat-sheet/



Vinayak Shanawad July 10, 2020 at 6:42 pm #



Thank you so much.

1. Why do you set random state=1 for the cross validation?

cv = RepeatedStratifiedKFold(n_splits=10, n_repeats=3, random_state=1)

As per my understanding, in test_train_split with different random state we get different accuracies and to avoid that we will do cross validation.

2. Is it necessary to set the random state=1 for the crc

3. In your all examples above, from gridsearch results we are getting accuracy of Training data set. Is that right?

summarize results

print("Best: %f using %s" % (grid result.best score, grid result.best params))

I think from grid result which is our best model and using that calculate the accuracy of Test data set.

Jason Brownlee July 11, 2020 at 6:07 am #

REPLY 🦴

The random seed is fixed to ensure we get the same result each time the code is run – helpful

for tutorials.

You can set any value you like:

https://machinelearningmastery.com/faq/single-faq

We are not using a train/test split, we are using reperformance of each config.

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Mihai July 16, 2020 at 11:22 pm #

Regarding the parameters for Random Forest

0.22: The default value of n_estimators changed from 10 to 100 in 0.22." – In your code you have up to 1000, in case you want to update your code ©



Jason Brownlee July 17, 2020 at 6:17 am #

REPLY 🦴

Thanks.

More is better to a limit, when it comes to RF.



Amilkar August 11, 2020 at 12:20 am #

REPLY 숙

I love your tutorials. I think you do a great job. I have learned so much from you. I've been considering buying one of your books, but you a so many that I don't know which one to buy. I have come to realize how important hyperparameter tuning is and I have noticed that each model is different and I need a summarized source of information that gives me a general idea of what hyperparameters to try for each model and techniques to do the process as fast and efficiently as possible. I've heard about Bayesian hyperparameter optimization techniques. Would be great if I could learn how to do this with scikitlearn. Also, I'm particularly interested in XGBoost because I've read in your blogs that it tends to perform really well. Which one of your books would you recommend me to learn how to do hyperparameter tuning fast and efficiently using python (special mention on XGBoost if Start Machine Learning



Jason Brownlee August 11, 2020 at 6:34 am #

REPLY 👆

REPLY <

X

Thanks!

I recommend using the free tutorials and only get a book if you need more information or want to systematically work through a topic.



Hi Jason, thanks for the post. Regarding this the same results in each split and repetition? Or where

Jason Brownlee August 16, 2020 at 5:48 am

When random_state is set on the cv object hyperparameter configuration is evaluated on the state of the state

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Sreeram August 16, 2020 at 11:52 pm #

why Repeated Stratified K fold is used?





Jason Brownlee August 17, 2020 at 5:47 am #

REPLY 🦴

It is a best practice for evaluating models on classification tasks.



jenny November 18, 2020 at 12:52 pm #

REPLY 🦴

what are the best classification algorithms to use in the popular (fashion mnist) dataset and also which hyperparameters are preferable?



Jason Brownlee November 18, 2020 at 1:08 pm #

REPLY 🦴

A CNN.



Binnan November 19, 2020 at 3:14 pm #

REPLY

Hi Jason, it's a great article!

I am just wondering that since grid search implement through cross-validation, once the optimal combination of hyperparameters are selected, is it necessary to perform cross-validation again to test the model performance with optimal parameters?



Jason Brownlee November 20, 2020 at 6:42 am #

REPLY 🖛

No, but you can if you like to confirm the f



Hadi Sabahi June 12, 2021 at 12:01 am #

Hi Jason, thanks for your post, I have a quest tune a classifier, we should find its Operating Point, wh intersection with Y=-X. The ROC curve is calculated us corresponding hyperparameters of the Operating Point My question is that why do you use (scoring='accuracy In other words, why don't you consider sensitivity and curve?

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Jason Brownlee June 12, 2021 at 5:35 am #



I recommend optimizing the ROC AUC and use roc curve as a diagnostic.

Leave a Reply

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Email (will not be published) (required)

Website

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and I help developers get results with machine learning.

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