sklearn.model_selection.GridSearchCV

class `sklearn.model_selection.GridSearchCV`(*estimator*, *param_grid*, *scoring=None*, *n_jobs=None*, *iid='warn'*, *refit=True*, *cv='warn'*, *verbose=0*, *pre_dispatch='2*n_jobs'*, *error_score='raise-deprecating'*, *return_train_score=False*) [source]

Exhaustive search over specified parameter values for an estimator.

Important members are fit, predict.

GridSearchCV implements a “fit” and a “score” method. It also implements “predict”, “predict_proba”, “decision_function”, “transform” and “inverse_transform” if they are implemented in the estimator used.

The parameters of the estimator used to apply these methods are optimized by cross-validated grid-search over a parameter grid.

Read more in the User Guide.

Parameters:

estimator : *estimator object.*

This is assumed to implement the scikit-learn estimator interface. Either estimator needs to provide a `score` function, or `scoring` must be passed.

param_grid : *dict or list of dictionaries*

Dictionary with parameters names (string) as keys and lists of parameter settings to try as values, or a list of such dictionaries, in which case the grids spanned by each dictionary in the list are explored. This enables searching over any sequence of parameter settings.

scoring : *string, callable, list/tuple, dict or None, default: None*

A single string (see The scoring parameter: defining model evaluation rules) or a callable (see Defining your scoring strategy from metric functions) to evaluate the predictions on the test set.

For evaluating multiple metrics, either give a list of (unique) strings or a dict with names as keys and callables as values.

NOTE that when using custom scorers, each scorer should return a single value. Metric functions returning a list/array of values can be wrapped into multiple scorers that return one value each.

See Specifying multiple metrics for evaluation for an example.

If None, the estimator’s score method is used.

n_jobs : *int or None, optional (default=None)*

Number of jobs to run in parallel. `None` means 1 unless in a **`joblib.parallel_backend`** context. `-1` means using all processors. See Glossary for more details.

pre_dispatch : *int, or string, optional*

Controls the number of jobs that get dispatched during parallel execution. Reducing this number can be useful to avoid an explosion of memory consumption when more jobs get dispatched than CPUs can process. This parameter can be:

- None, in which case all the jobs are immediately created and spawned. Use this for lightweight and fast-running jobs, to avoid delays due to on-demand spawning of the jobs
- An int, giving the exact number of total jobs that are spawned
- A string, giving an expression as a function of n_jobs, as in '2*n_jobs'

iid : *boolean, default='warn'*

If True, return the average score across folds, weighted by the number of samples in each test set. In this case, the data is assumed to be identically distributed across the folds, and the loss minimized is the total loss per sample, and not the mean loss across the folds. If False, return the average score across folds. Default is True, but will change to False in version 0.22, to correspond to the standard definition of cross-validation.

Changed in version 0.20: Parameter `iid` will change from True to False by default in version 0.22, and will be removed in 0.24.

cv : *int, cross-validation generator or an iterable, optional*

Determines the cross-validation splitting strategy. Possible inputs for cv are:

- None, to use the default 3-fold cross validation,
- integer, to specify the number of folds in a `(Stratified)KFold`,
- CV splitter,
- An iterable yielding (train, test) splits as arrays of indices.

For integer/None inputs, if the estimator is a classifier and `y` is either binary or multiclass, **`StratifiedKFold`** is used. In all other cases, **`KFold`** is used.

Refer User Guide for the various cross-validation strategies that can be used here.

Changed in version 0.20: `cv` default value if None will change from 3-fold to 5-fold in v0.22.

refit : *boolean, string, or callable, default=True*

Refit an estimator using the best found parameters on the whole dataset.

For multiple metric evaluation, this needs to be a string denoting the scorer that would be used to find the best parameters for refitting the estimator at the end.

Where there are considerations other than maximum score in choosing a best estimator, `refit` can be set to a function which returns the selected `best_index_` given `cv_results_`.

The refitted estimator is made available at the `best_estimator_` attribute and permits using `predict` directly on this `GridSearchCV` instance.

Also for multiple metric evaluation, the attributes `best_index_`, `best_score_` and `best_params_` will only be available if `refit` is set and all of them will be determined w.r.t this specific scorer. `best_score_` is not returned if refit is callable.

See `scoring` parameter to know more about multiple metric evaluation.

Changed in version 0.20: Support for callable added.

verbose : *integer*

Controls the verbosity: the higher, the more messages.

error_score : *'raise' or numeric*

Value to assign to the score if an error occurs in estimator fitting. If set to 'raise', the error is raised. If a numeric value is given, FitFailedWarning is raised. This parameter does not affect the refit step, which will always raise the error. Default is 'raise' but from version 0.22 it will change to np.nan.

return_train_score : *boolean, default=False*

If `False`, the `cv_results_` attribute will not include training scores. Computing training scores is used to get insights on how different parameter settings impact the overfitting/underfitting trade-off. However computing the scores on the training set can be computationally expensive and is not strictly required to select the parameters that yield the best generalization performance.

Attributes:

cv_results_ : *dict of numpy (masked) ndarrays*

A dict with keys as column headers and values as columns, that can be imported into a pandas `DataFrame`.

For instance the below given table

param_kernel	param_gamma	param_degree	split0_test_score	…	rank_t…
'poly'	–	2	0.80	…	2
'poly'	–	3	0.70	…	4
'rbf'	0.1	–	0.80	…	3
'rbf'	0.2	–	0.93	…	1

will be represented by a `cv_results_` dict of:

```
{
'param_kernel': masked_array(data = ['poly', 'poly', 'rbf', 'rbf'],
                             mask = [False False False False]...)
'param_gamma': masked_array(data = [-- -- 0.1 0.2],
                            mask = [ True  True False False]...),
'param_degree': masked_array(data = [2.0 3.0 -- --],
                             mask = [False False  True  True]...),
'split0_test_score'  : [0.80, 0.70, 0.80, 0.93],
'split1_test_score'  : [0.82, 0.50, 0.70, 0.78],
'mean_test_score'    : [0.81, 0.60, 0.75, 0.85],
'std_test_score'     : [0.01, 0.10, 0.05, 0.08],
'rank_test_score'    : [2, 4, 3, 1],
'split0_train_score' : [0.80, 0.92, 0.70, 0.93],
'split1_train_score' : [0.82, 0.55, 0.70, 0.87],
'mean_train_score'   : [0.81, 0.74, 0.70, 0.90],
'std_train_score'    : [0.01, 0.19, 0.00, 0.03],
'mean_fit_time'      : [0.73, 0.63, 0.43, 0.49],
'std_fit_time'       : [0.01, 0.02, 0.01, 0.01],
'mean_score_time'    : [0.01, 0.06, 0.04, 0.04],
'std_score_time'     : [0.00, 0.00, 0.00, 0.01],
'params'             : [{'kernel': 'poly', 'degree': 2}, ...],
}
```

NOTE

The key `'params'` is used to store a list of parameter settings dicts for all the parameter candidates.

The `mean_fit_time`, `std_fit_time`, `mean_score_time` and `std_score_time` are all in seconds.

For multi-metric evaluation, the scores for all the scorers are available in the `cv_results_` dict at the keys ending with that scorer's name (`'_<scorer_name>'`) instead of `'_score'` shown above. ('split0_test_precision', 'mean_train_precision' etc.)

best_estimator_ : *estimator or dict*

Estimator that was chosen by the search, i.e. estimator which gave highest score (or smallest loss if specified) on the left out data. Not available if `refit=False`.

See `refit` parameter for more information on allowed values.

best_score_ : *float*

Mean cross-validated score of the best_estimator

For multi-metric evaluation, this is present only if `refit` is specified.

best_params_ : *dict*

Parameter setting that gave the best results on the hold out data.

For multi-metric evaluation, this is present only if `refit` is specified.

best_index_ : *int*

The index (of the `cv_results_` arrays) which corresponds to the best candidate parameter setting.

The dict at `search.cv_results_['params'][search.best_index_]` gives the parameter setting for the best model, that gives the highest mean score (`search.best_score_`).

For multi-metric evaluation, this is present only if `refit` is specified.

scorer_ : *function or a dict*

Scorer function used on the held out data to choose the best parameters for the model.

For multi-metric evaluation, this attribute holds the validated `scoring` dict which maps the scorer key to the scorer callable.

n_splits_ : *int*

The number of cross-validation splits (folds/iterations).

refit_time_ : *float*

Seconds used for refitting the best model on the whole dataset.

This is present only if `refit` is not False.

See also:

`ParameterGrid`

generates all the combinations of a hyperparameter grid.

`sklearn.model_selection.train_test_split`

utility function to split the data into a development set usable for fitting a GridSearchCV instance and an evaluation set for its final evaluation.

`sklearn.metrics.make_scorer`

Make a scorer from a performance metric or loss function.

Notes

The parameters selected are those that maximize the score of the left out data, unless an explicit score is passed in which case it is used instead.

If n_jobs was set to a value higher than one, the data is copied for each point in the grid (and not n_jobs times). This is done for efficiency reasons if individual jobs take very little time, but may raise errors if the dataset is large and not enough memory is available. A workaround in this case is to set `pre_dispatch`. Then, the memory is copied only `pre_dispatch` many times. A reasonable value for `pre_dispatch` is `2 * n_jobs`.

Examples

```
>>> from sklearn import svm, datasets
>>> from sklearn.model_selection import GridSearchCV
>>> iris = datasets.load_iris()
>>> parameters = {'kernel':('linear', 'rbf'), 'C':[1, 10]}
>>> svc = svm.SVC(gamma="scale")
>>> clf = GridSearchCV(svc, parameters, cv=5)
>>> clf.fit(iris.data, iris.target)
...
GridSearchCV(cv=5, error_score=...,
       estimator=SVC(C=1.0, cache_size=..., class_weight=..., coef0=...,
                     decision_function_shape='ovr', degree=..., gamma=...,
                     kernel='rbf', max_iter=-1, probability=False,
                     random_state=None, shrinking=True, tol=...,
                     verbose=False),
       iid=..., n_jobs=None,
       param_grid=..., pre_dispatch=..., refit=..., return_train_score=...,
       scoring=..., verbose=...)
>>> sorted(clf.cv_results_.keys())
...
['mean_fit_time', 'mean_score_time', 'mean_test_score',...
 'param_C', 'param_kernel', 'params',...
 'rank_test_score', 'split0_test_score',...
 'split2_test_score', ...
 'std_fit_time', 'std_score_time', 'std_test_score']
```

Methods

`decision_function`(self, X)	Call decision_function on the estimator with the best found parameters.
`fit`(self, X[, y, groups])	Run fit with all sets of parameters.
`get_params`(self[, deep])	Get parameters for this estimator.
`inverse_transform`(self, Xt)	Call inverse_transform on the estimator with the best found params.
`predict`(self, X)	Call predict on the estimator with the best found parameters.
`predict_log_proba`(self, X)	Call predict_log_proba on the estimator with the best found parameters.
`predict_proba`(self, X)	Call predict_proba on the estimator with the best found parameters.
`score`(self, X[, y])	Returns the score on the given data, if the estimator has been refit.
`set_params`(self, **params)	Set the parameters of this estimator.
`transform`(self, X)	Call transform on the estimator with the best found parameters.

`__init__`(*self, estimator, param_grid, scoring=None, n_jobs=None, iid='warn', refit=True, cv='warn', verbose=0, pre_dispatch='2*n_jobs', error_score='raise-deprecating', return_train_score=False*) [source]

`decision_function`(*self, X*) [source]

Call decision_function on the estimator with the best found parameters.

Only available if `refit=True` and the underlying estimator supports `decision_function`.

Parameters: **X** : *indexable, length n_samples*

Must fulfill the input assumptions of the underlying estimator.

`fit`(*self, X, y=None, groups=None, **fit_params*) [source]

Run fit with all sets of parameters.

Parameters: **X** : *array-like, shape = [n_samples, n_features]*

Training vector, where n_samples is the number of samples and n_features is the number of features.

y : *array-like, shape = [n_samples] or [n_samples, n_output], optional*

Target relative to X for classification or regression; None for unsupervised learning.

groups : *array-like, with shape (n_samples,), optional*

Group labels for the samples used while splitting the dataset into train/test set. Only used in conjunction with a “Group” cv instance (e.g., GroupKFold).

****fit_params** : *dict of string -> object*

Parameters passed to the `fit` method of the estimator

get_params(*self*, *deep=True*) [source]

Get parameters for this estimator.

Parameters:	**deep** : *boolean, optional* If True, will return the parameters for this estimator and contained subobjects that are estimators.
Returns:	**params** : *mapping of string to any* Parameter names mapped to their values.

inverse_transform(*self*, *Xt*) [source]

Call inverse_transform on the estimator with the best found params.

Only available if the underlying estimator implements `inverse_transform` and `refit=True`.

Parameters:	**Xt** : *indexable, length n_samples* Must fulfill the input assumptions of the underlying estimator.

predict(*self*, *X*) [source]

Call predict on the estimator with the best found parameters.

Only available if `refit=True` and the underlying estimator supports `predict`.

Parameters:	**X** : *indexable, length n_samples* Must fulfill the input assumptions of the underlying estimator.

predict_log_proba(*self*, *X*) [source]

Call predict_log_proba on the estimator with the best found parameters.

Only available if `refit=True` and the underlying estimator supports `predict_log_proba`.

Parameters:	**X** : *indexable, length n_samples* Must fulfill the input assumptions of the underlying estimator.

predict_proba(*self*, *X*) [source]

Call predict_proba on the estimator with the best found parameters.

Only available if `refit=True` and the underlying estimator supports `predict_proba`.

Parameters:	**X** : *indexable, length n_samples* Must fulfill the input assumptions of the underlying estimator.

score(*self*, *X*, *y=None*) [source]

Returns the score on the given data, if the estimator has been refit.

This uses the score defined by `scoring` where provided, and the `best_estimator_.score` method otherwise.

Parameters:	**X** : *array-like, shape = [n_samples, n_features]* Input data, where n_samples is the number of samples and n_features is the number of features. **y** : *array-like, shape = [n_samples] or [n_samples, n_output], optional* Target relative to X for classification or regression; None for unsupervised learning.
Returns:	**score** : *float*

set_params(*self*, ***params*) [source]

Set the parameters of this estimator.

The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

Returns:	self

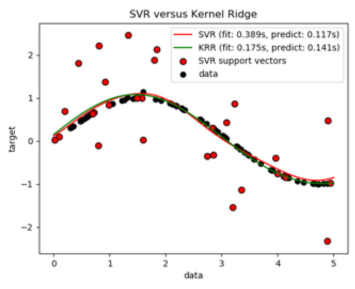
transform(*self*, *X*) [source]

Call transform on the estimator with the best found parameters.

Only available if the underlying estimator supports `transform` and `refit=True`.

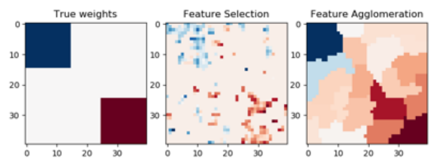
Parameters:	**X** : *indexable, length n_samples* Must fulfill the input assumptions of the underlying estimator.

Examples using `sklearn.model_selection.GridSearchCV`



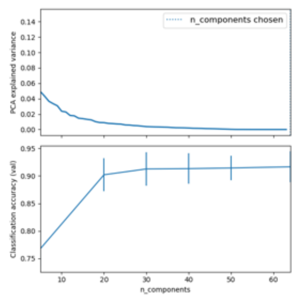
Comparison of kernel ridge regression and SVR

Faces recognition example using eigenfaces and SVMs



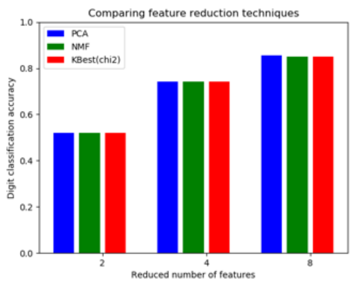
Feature agglomeration vs. univariate selection

Concatenating multiple feature extraction methods

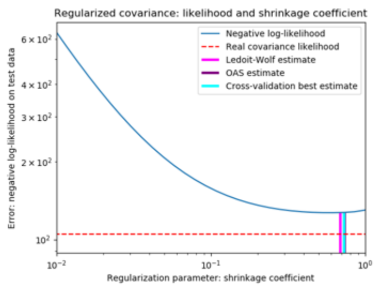


Pipelining: chaining a PCA and a logistic regression

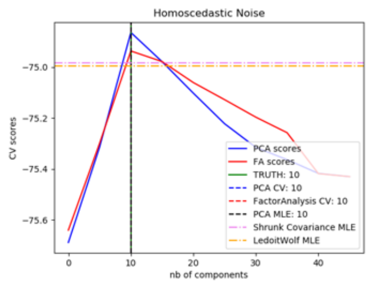
Column Transformer with Mixed Types



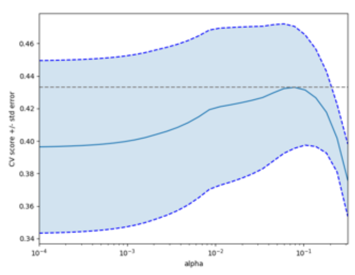
Selecting dimensionality reduction with Pipeline and GridSearchCV



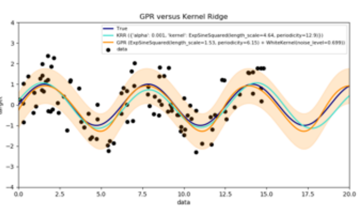
Shrinkage covariance estimation: LedoitWolf vs OAS and max-likelihood



Model selection with Probabilistic PCA and Factor Analysis (FA)



Cross-validation on diabetes Dataset Exercise

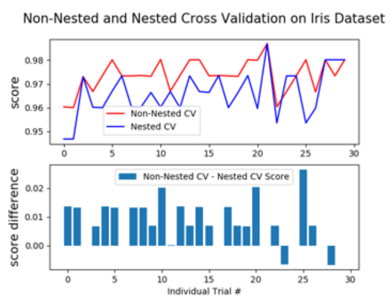


Comparison of kernel ridge and Gaussian process

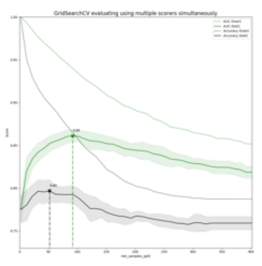
Parameter estimation using grid search with cross-regression

validation

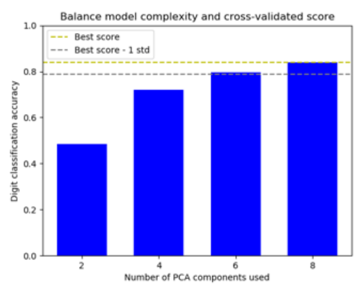
Comparing randomized search and grid search for hyperparameter estimation



Nested versus non-nested cross-validation

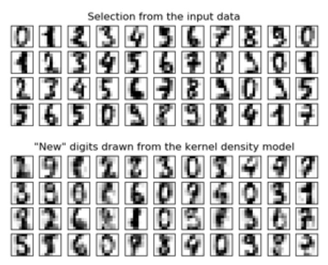


Demonstration of multi-metric evaluation on cross_-val_score and GridSearchCV

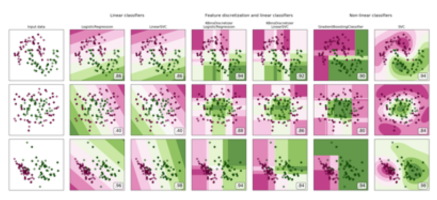


Balance model complexity and cross-validated score

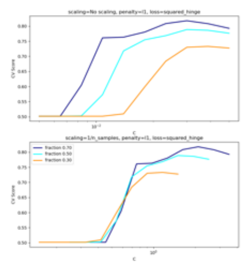
Sample pipeline for text feature extraction and evaluation



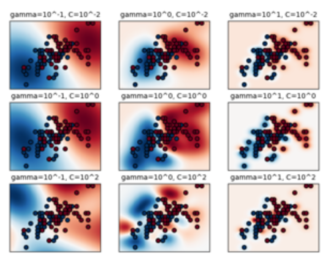
Kernel Density Estimation



Feature discretization



Scaling the regularization parameter for SVCs



RBF SVM parameters