ml_algos_2

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1 Mudcard

- **How to choose the best model? or do we just try several techniques and pick the one with the best score?**
  - You have two models.
  - How do you decide which one is better?
  - Usually the model with the lower generalization error is better.
  - So you try many and pick the one with the best test score.
  - You can of course come up with other definitions but the field chooses based on the test scores.
- **Should we consider conditional probabilities when designing decision trees?**
  - I'm not sure what you mean. Could you clarify on Ed Discussion or come to the office hours?
- **How are trees made?**
  - the same way a linear or logistic regression model is made
  - the mathemical model that converts features to a prediction is a sequence of if-else statements, a tree
  - an optimization algorithm (usually a greedy algorithm) finds the best way to split the features for you (this is equivalent to gradient descent in linear and logistic regression)
  - the cost function is some measure of goodness which could be the RMSE in regression or accuracy in classification
  - sklearn does all of this for you
- **Ive read about the concept of data point 'leverage' before, and this measure seems similar to our discussion on how models treat feature outlier points. Are these concepts related in any way?**
  - not necessarily
  - a leverage point is not necessarily an outlier
  - it's usually a point which has a surprising target variable
  - e.g., in the make moons dataset, a blue point in the middle of the red points would be leveraged
- **Are there any algorithms that effectively choose the best subsets or paths?**
  - yes, sklearn does this for you
- **Is the output of the predict function in LogisticRegression calculated from predict_proba with critical probability = 0.5?**
  - yes

1.1 Supervised ML algorithms

By the end of this module, you will be able to - Summarize how decision trees, random forests, and support vector machines work - Describe how the predictions of these techniques behave in classification and regression - Describe which hyper-parameters should be tuned

1.1.1 A decision tree in regression

[1]:
```
import numpy as np
from sklearn.ensemble import RandomForestRegressor
np.random.seed(10)
def true_fun(X):
    return np.cos(1.5 * np.pi * X)

n_samples = 30

X = np.random.rand(n_samples)
y = true_fun(X) + np.random.randn(n_samples) * 0.1

X_new = np.linspace(0, 1, 1000)

reg = RandomForestRegressor(n_estimators=1,max_depth=1)
reg.fit(X[:, np.newaxis],y)
y_new = reg.predict(X_new[:, np.newaxis])
```

[2]:
```
help(RandomForestRegressor)
```

```
Help on class RandomForestRegressor in module sklearn.ensemble._forest:

class RandomForestRegressor(ForestRegressor)
 |  RandomForestRegressor(n_estimators=100, *, criterion='squared_error',
max_depth=None, min_samples_split=2, min_samples_leaf=1,
min_weight_fraction_leaf=0.0, max_features=1.0, max_leaf_nodes=None,
min_impurity_decrease=0.0, bootstrap=True, oob_score=False, n_jobs=None,
random_state=None, verbose=0, warm_start=False, ccp_alpha=0.0, max_samples=None)
 |
 |  A random forest regressor.
 |
 |  A random forest is a meta estimator that fits a number of classifying
 |  decision trees on various sub-samples of the dataset and uses averaging
 |  to improve the predictive accuracy and control over-fitting.
 |  The sub-sample size is controlled with the `max_samples` parameter if
 |  `bootstrap=True` (default), otherwise the whole dataset is used to build
 |  each tree.
 |
 |  Read more in the :ref:`User Guide <forest>`.
 |
 |  Parameters
```

```
  |  ----------
  |  n_estimators : int, default=100
  |      The number of trees in the forest.
  |
  |      .. versionchanged:: 0.22
  |         The default value of ``n_estimators`` changed from 10 to 100
  |         in 0.22.
  |
  |  criterion : {"squared_error", "absolute_error", "poisson"},
default="squared_error"
  |      The function to measure the quality of a split. Supported criteria
  |      are "squared_error" for the mean squared error, which is equal to
  |      variance reduction as feature selection criterion, "absolute_error"
  |      for the mean absolute error, and "poisson" which uses reduction in
  |      Poisson deviance to find splits.
  |      Training using "absolute_error" is significantly slower
  |      than when using "squared_error".
  |
  |      .. versionadded:: 0.18
  |         Mean Absolute Error (MAE) criterion.
  |
  |      .. versionadded:: 1.0
  |         Poisson criterion.
  |
  |      .. deprecated:: 1.0
  |          Criterion "mse" was deprecated in v1.0 and will be removed in
  |          version 1.2. Use `criterion="squared_error"` which is equivalent.
  |
  |      .. deprecated:: 1.0
  |          Criterion "mae" was deprecated in v1.0 and will be removed in
  |          version 1.2. Use `criterion="absolute_error"` which is equivalent.
  |
  |  max_depth : int, default=None
  |      The maximum depth of the tree. If None, then nodes are expanded until
  |      all leaves are pure or until all leaves contain less than
  |      min_samples_split samples.
  |
  |  min_samples_split : int or float, default=2
  |      The minimum number of samples required to split an internal node:
  |
  |      - If int, then consider `min_samples_split` as the minimum number.
  |      - If float, then `min_samples_split` is a fraction and
  |        `ceil(min_samples_split * n_samples)` are the minimum
  |        number of samples for each split.
  |
  |      .. versionchanged:: 0.18
  |         Added float values for fractions.
  |
```

```
|  min_samples_leaf : int or float, default=1
|      The minimum number of samples required to be at a leaf node.
|      A split point at any depth will only be considered if it leaves at
|      least ``min_samples_leaf`` training samples in each of the left and
|      right branches.  This may have the effect of smoothing the model,
|      especially in regression.
|
|      - If int, then consider `min_samples_leaf` as the minimum number.
|      - If float, then `min_samples_leaf` is a fraction and
|        `ceil(min_samples_leaf * n_samples)` are the minimum
|        number of samples for each node.
|
|      .. versionchanged:: 0.18
|         Added float values for fractions.
|
|  min_weight_fraction_leaf : float, default=0.0
|      The minimum weighted fraction of the sum total of weights (of all
|      the input samples) required to be at a leaf node. Samples have
|      equal weight when sample_weight is not provided.
|
|  max_features : {"sqrt", "log2", None}, int or float, default=1.0
|      The number of features to consider when looking for the best split:
|
|      - If int, then consider `max_features` features at each split.
|      - If float, then `max_features` is a fraction and
|        `round(max_features * n_features)` features are considered at each
|        split.
|      - If "auto", then `max_features=n_features`.
|      - If "sqrt", then `max_features=sqrt(n_features)`.
|      - If "log2", then `max_features=log2(n_features)`.
|      - If None or 1.0, then `max_features=n_features`.
|
|      .. note::
|          The default of 1.0 is equivalent to bagged trees and more
|          randomness can be achieved by setting smaller values, e.g. 0.3.
|
|      .. versionchanged:: 1.1
|          The default of `max_features` changed from `"auto"` to 1.0.
|
|      .. deprecated:: 1.1
|          The `"auto"` option was deprecated in 1.1 and will be removed
|          in 1.3.
|
|      Note: the search for a split does not stop until at least one
|      valid partition of the node samples is found, even if it requires to
|      effectively inspect more than ``max_features`` features.
|
|  max_leaf_nodes : int, default=None
```

```
|      Grow trees with ``max_leaf_nodes`` in best-first fashion.
|      Best nodes are defined as relative reduction in impurity.
|      If None then unlimited number of leaf nodes.
|
|  min_impurity_decrease : float, default=0.0
|      A node will be split if this split induces a decrease of the impurity
|      greater than or equal to this value.
|
|      The weighted impurity decrease equation is the following::
|
|          N_t / N * (impurity - N_t_R / N_t * right_impurity
|                              - N_t_L / N_t * left_impurity)
|
|      where ``N`` is the total number of samples, ``N_t`` is the number of
|      samples at the current node, ``N_t_L`` is the number of samples in the
|      left child, and ``N_t_R`` is the number of samples in the right child.
|
|      ``N``, ``N_t``, ``N_t_R`` and ``N_t_L`` all refer to the weighted sum,
|      if ``sample_weight`` is passed.
|
|      .. versionadded:: 0.19
|
|  bootstrap : bool, default=True
|      Whether bootstrap samples are used when building trees. If False, the
|      whole dataset is used to build each tree.
|
|  oob_score : bool, default=False
|      Whether to use out-of-bag samples to estimate the generalization score.
|      Only available if bootstrap=True.
|
|  n_jobs : int, default=None
|      The number of jobs to run in parallel. :meth:`fit`, :meth:`predict`,
|      :meth:`decision_path` and :meth:`apply` are all parallelized over the
|      trees. ``None`` means 1 unless in a :obj:`joblib.parallel_backend`
|      context. ``-1`` means using all processors. See :term:`Glossary
|      <n_jobs>` for more details.
|
|  random_state : int, RandomState instance or None, default=None
|      Controls both the randomness of the bootstrapping of the samples used
|      when building trees (if ``bootstrap=True``) and the sampling of the
|      features to consider when looking for the best split at each node
|      (if ``max_features < n_features``).
|      See :term:`Glossary <random_state>` for details.
|
|  verbose : int, default=0
|      Controls the verbosity when fitting and predicting.
|
|  warm_start : bool, default=False
```

```
|      When set to ``True``, reuse the solution of the previous call to fit
|      and add more estimators to the ensemble, otherwise, just fit a whole
|      new forest. See :term:`the Glossary <warm_start>`.
|
|  ccp_alpha : non-negative float, default=0.0
|      Complexity parameter used for Minimal Cost-Complexity Pruning. The
|      subtree with the largest cost complexity that is smaller than
|      ``ccp_alpha`` will be chosen. By default, no pruning is performed. See
|      :ref:`minimal_cost_complexity_pruning` for details.
|
|      .. versionadded:: 0.22
|
|  max_samples : int or float, default=None
|      If bootstrap is True, the number of samples to draw from X
|      to train each base estimator.
|
|      - If None (default), then draw `X.shape[0]` samples.
|      - If int, then draw `max_samples` samples.
|      - If float, then draw `max_samples * X.shape[0]` samples. Thus,
|        `max_samples` should be in the interval `(0.0, 1.0]`.
|
|      .. versionadded:: 0.22
|
|  Attributes
|  ----------
|  base_estimator_ : DecisionTreeRegressor
|      The child estimator template used to create the collection of fitted
|      sub-estimators.
|
|  estimators_ : list of DecisionTreeRegressor
|      The collection of fitted sub-estimators.
|
|  feature_importances_ : ndarray of shape (n_features,)
|      The impurity-based feature importances.
|      The higher, the more important the feature.
|      The importance of a feature is computed as the (normalized)
|      total reduction of the criterion brought by that feature.  It is also
|      known as the Gini importance.
|
|      Warning: impurity-based feature importances can be misleading for
|      high cardinality features (many unique values). See
|      :func:`sklearn.inspection.permutation_importance` as an alternative.
|
|  n_features_ : int
|      The number of features when ``fit`` is performed.
|
|      .. deprecated:: 1.0
|          Attribute `n_features_` was deprecated in version 1.0 and will be
```

```
|          removed in 1.2. Use `n_features_in_` instead.
|
|  n_features_in_ : int
|      Number of features seen during :term:`fit`.
|
|      .. versionadded:: 0.24
|
|  feature_names_in_ : ndarray of shape (`n_features_in_`,)
|      Names of features seen during :term:`fit`. Defined only when `X`
|      has feature names that are all strings.
|
|      .. versionadded:: 1.0
|
|  n_outputs_ : int
|      The number of outputs when ``fit`` is performed.
|
|  oob_score_ : float
|      Score of the training dataset obtained using an out-of-bag estimate.
|      This attribute exists only when ``oob_score`` is True.
|
|  oob_prediction_ : ndarray of shape (n_samples,) or (n_samples, n_outputs)
|      Prediction computed with out-of-bag estimate on the training set.
|      This attribute exists only when ``oob_score`` is True.
|
|  See Also
|  --------
|  sklearn.tree.DecisionTreeRegressor : A decision tree regressor.
|  sklearn.ensemble.ExtraTreesRegressor : Ensemble of extremely randomized
|      tree regressors.
|
|  Notes
|  -----
|  The default values for the parameters controlling the size of the trees
|  (e.g. ``max_depth``, ``min_samples_leaf``, etc.) lead to fully grown and
|  unpruned trees which can potentially be very large on some data sets. To
|  reduce memory consumption, the complexity and size of the trees should be
|  controlled by setting those parameter values.
|
|  The features are always randomly permuted at each split. Therefore,
|  the best found split may vary, even with the same training data,
|  ``max_features=n_features`` and ``bootstrap=False``, if the improvement
|  of the criterion is identical for several splits enumerated during the
|  search of the best split. To obtain a deterministic behaviour during
|  fitting, ``random_state`` has to be fixed.
|
|  The default value ``max_features="auto"`` uses ``n_features``
|  rather than ``n_features / 3``. The latter was originally suggested in
|  [1], whereas the former was more recently justified empirically in [2].
```

```
 |
 |  References
 |  ----------
 |  .. [1] L. Breiman, "Random Forests", Machine Learning, 45(1), 5-32, 2001.
 |
 |  .. [2] P. Geurts, D. Ernst., and L. Wehenkel, "Extremely randomized
 |         trees", Machine Learning, 63(1), 3-42, 2006.
 |
 |  Examples
 |  --------
 |  >>> from sklearn.ensemble import RandomForestRegressor
 |  >>> from sklearn.datasets import make_regression
 |  >>> X, y = make_regression(n_features=4, n_informative=2,
 |  …                         random_state=0, shuffle=False)
 |  >>> regr = RandomForestRegressor(max_depth=2, random_state=0)
 |  >>> regr.fit(X, y)
 |  RandomForestRegressor(…)
 |  >>> print(regr.predict([[0, 0, 0, 0]]))
 |  [-8.32987858]
 |
 |  Method resolution order:
 |      RandomForestRegressor
 |      ForestRegressor
 |      sklearn.base.RegressorMixin
 |      BaseForest
 |      sklearn.base.MultiOutputMixin
 |      sklearn.ensemble._base.BaseEnsemble
 |      sklearn.base.MetaEstimatorMixin
 |      sklearn.base.BaseEstimator
 |      builtins.object
 |
 |  Methods defined here:
 |
 |  __init__(self, n_estimators=100, *, criterion='squared_error',
max_depth=None, min_samples_split=2, min_samples_leaf=1,
min_weight_fraction_leaf=0.0, max_features=1.0, max_leaf_nodes=None,
min_impurity_decrease=0.0, bootstrap=True, oob_score=False, n_jobs=None,
random_state=None, verbose=0, warm_start=False, ccp_alpha=0.0, max_samples=None)
 |      Initialize self.  See help(type(self)) for accurate signature.
 |
 |  ----------------------------------------------------------------------
 |  Data and other attributes defined here:
 |
 |  __abstractmethods__ = frozenset()
 |
 |  __annotations__ = {}
 |
 |  ----------------------------------------------------------------------
```

```
|  Methods inherited from ForestRegressor:
|
|  predict(self, X)
|      Predict regression target for X.
|
|      The predicted regression target of an input sample is computed as the
|      mean predicted regression targets of the trees in the forest.
|
|      Parameters
|      ----------
|      X : {array-like, sparse matrix} of shape (n_samples, n_features)
|          The input samples. Internally, its dtype will be converted to
|          ``dtype=np.float32``. If a sparse matrix is provided, it will be
|          converted into a sparse ``csr_matrix``.
|
|      Returns
|      -------
|      y : ndarray of shape (n_samples,) or (n_samples, n_outputs)
|          The predicted values.
|
|  ----------------------------------------------------------------------
|  Methods inherited from sklearn.base.RegressorMixin:
|
|  score(self, X, y, sample_weight=None)
|      Return the coefficient of determination of the prediction.
|
|      The coefficient of determination :math:`R^2` is defined as
|      :math:`(1 - \frac{u}{v})`, where :math:`u` is the residual
|      sum of squares ``((y_true - y_pred)** 2).sum()`` and :math:`v`
|      is the total sum of squares ``((y_true - y_true.mean()) ** 2).sum()``.
|      The best possible score is 1.0 and it can be negative (because the
|      model can be arbitrarily worse). A constant model that always predicts
|      the expected value of `y`, disregarding the input features, would get
|      a :math:`R^2` score of 0.0.
|
|      Parameters
|      ----------
|      X : array-like of shape (n_samples, n_features)
|          Test samples. For some estimators this may be a precomputed
|          kernel matrix or a list of generic objects instead with shape
|          ``(n_samples, n_samples_fitted)``, where ``n_samples_fitted``
|          is the number of samples used in the fitting for the estimator.
|
|      y : array-like of shape (n_samples,) or (n_samples, n_outputs)
|          True values for `X`.
|
|      sample_weight : array-like of shape (n_samples,), default=None
|          Sample weights.
```

```
|
|      Returns
|      -------
|      score : float
|          :math:`R^2` of ``self.predict(X)`` wrt. `y`.
|
|      Notes
|      -----
|      The :math:`R^2` score used when calling ``score`` on a regressor uses
|      ``multioutput='uniform_average'`` from version 0.23 to keep consistent
|      with default value of :func:`~sklearn.metrics.r2_score`.
|      This influences the ``score`` method of all the multioutput
|      regressors (except for
|      :class:`~sklearn.multioutput.MultiOutputRegressor`).
|
|  ----------------------------------------------------------------------
|  Data descriptors inherited from sklearn.base.RegressorMixin:
|
|  __dict__
|      dictionary for instance variables (if defined)
|
|  __weakref__
|      list of weak references to the object (if defined)
|
|  ----------------------------------------------------------------------
|  Methods inherited from BaseForest:
|
|  apply(self, X)
|      Apply trees in the forest to X, return leaf indices.
|
|      Parameters
|      ----------
|      X : {array-like, sparse matrix} of shape (n_samples, n_features)
|          The input samples. Internally, its dtype will be converted to
|          ``dtype=np.float32``. If a sparse matrix is provided, it will be
|          converted into a sparse ``csr_matrix``.
|
|      Returns
|      -------
|      X_leaves : ndarray of shape (n_samples, n_estimators)
|          For each datapoint x in X and for each tree in the forest,
|          return the index of the leaf x ends up in.
|
|  decision_path(self, X)
|      Return the decision path in the forest.
|
|      .. versionadded:: 0.18
|
```

```
|      Parameters
|      ----------
|      X : {array-like, sparse matrix} of shape (n_samples, n_features)
|          The input samples. Internally, its dtype will be converted to
|          ``dtype=np.float32``. If a sparse matrix is provided, it will be
|          converted into a sparse ``csr_matrix``.
|
|      Returns
|      -------
|      indicator : sparse matrix of shape (n_samples, n_nodes)
|          Return a node indicator matrix where non zero elements indicates
|          that the samples goes through the nodes. The matrix is of CSR
|          format.
|
|      n_nodes_ptr : ndarray of shape (n_estimators + 1,)
|          The columns from indicator[n_nodes_ptr[i]:n_nodes_ptr[i+1]]
|          gives the indicator value for the i-th estimator.
|
|  fit(self, X, y, sample_weight=None)
|      Build a forest of trees from the training set (X, y).
|
|      Parameters
|      ----------
|      X : {array-like, sparse matrix} of shape (n_samples, n_features)
|          The training input samples. Internally, its dtype will be converted
|          to ``dtype=np.float32``. If a sparse matrix is provided, it will be
|          converted into a sparse ``csc_matrix``.
|
|      y : array-like of shape (n_samples,) or (n_samples, n_outputs)
|          The target values (class labels in classification, real numbers in
|          regression).
|
|      sample_weight : array-like of shape (n_samples,), default=None
|          Sample weights. If None, then samples are equally weighted. Splits
|          that would create child nodes with net zero or negative weight are
|          ignored while searching for a split in each node. In the case of
|          classification, splits are also ignored if they would result in any
|          single class carrying a negative weight in either child node.
|
|      Returns
|      -------
|      self : object
|          Fitted estimator.
|
|  ----------------------------------------------------------------------
|  Readonly properties inherited from BaseForest:
|
|  feature_importances_
```

```
 |      The impurity-based feature importances.
 |
 |      The higher, the more important the feature.
 |      The importance of a feature is computed as the (normalized)
 |      total reduction of the criterion brought by that feature.  It is also
 |      known as the Gini importance.
 |
 |      Warning: impurity-based feature importances can be misleading for
 |      high cardinality features (many unique values). See
 |      :func:`sklearn.inspection.permutation_importance` as an alternative.
 |
 |      Returns
 |      -------
 |      feature_importances_ : ndarray of shape (n_features,)
 |          The values of this array sum to 1, unless all trees are single node
 |          trees consisting of only the root node, in which case it will be an
 |          array of zeros.
 |
 |  n_features_
 |      DEPRECATED: Attribute `n_features_` was deprecated in version 1.0 and
will be removed in 1.2. Use `n_features_in_` instead.
 |
 |      Number of features when fitting the estimator.
 |
 |  ----------------------------------------------------------------------
 |  Methods inherited from sklearn.ensemble._base.BaseEnsemble:
 |
 |  __getitem__(self, index)
 |      Return the index'th estimator in the ensemble.
 |
 |  __iter__(self)
 |      Return iterator over estimators in the ensemble.
 |
 |  __len__(self)
 |      Return the number of estimators in the ensemble.
 |
 |  ----------------------------------------------------------------------
 |  Methods inherited from sklearn.base.BaseEstimator:
 |
 |  __getstate__(self)
 |
 |  __repr__(self, N_CHAR_MAX=700)
 |      Return repr(self).
 |
 |  __setstate__(self, state)
 |
 |  get_params(self, deep=True)
 |      Get parameters for this estimator.
```

```
|
|       Parameters
|       ----------
|       deep : bool, default=True
|           If True, will return the parameters for this estimator and
|           contained subobjects that are estimators.
|
|       Returns
|       -------
|       params : dict
|           Parameter names mapped to their values.
|
|   set_params(self, **params)
|       Set the parameters of this estimator.
|
|       The method works on simple estimators as well as on nested objects
|       (such as :class:`~sklearn.pipeline.Pipeline`). The latter have
|       parameters of the form ``<component>__<parameter>`` so that it's
|       possible to update each component of a nested object.
|
|       Parameters
|       ----------
|       **params : dict
|           Estimator parameters.
|
|       Returns
|       -------
|       self : estimator instance
|           Estimator instance.
```

[3]:
```
################################################################
# HUGE thanks to Drew Solomon and Yifei Song (DSI alumni)
# for preparing the visualizations in this course!
################################################################
# check out helper_functions.ipynb for more details
%run ./helper_functions.ipynb

hyperparameters = {
    'n_estimators': [1, 3, 10, 30],
    'max_depth': [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
}

vis(X, y, RandomForestRegressor, hyperparameters, X_new)
```

```
interactive(children=(SelectionSlider(description='n_estimators', options=(1, 3,␣
↪10, 30), value=1), SelectionS…
```

1.2 How to avoid overfitting with random forests?

- tune some (or all) of following hyperparameters:
  - max_depth
  - max_features
- With sklearn random forests, **do not tune n_estimators**!
  - the larger this value is, the better the forest will be
  - set n_estimators to maybe 100 while tuning hyperparameters
  - increase it if necessary once the best hyperparameters are found

ML algo	suitable for large datasets?	behaviour wrt outliers	non-linear?	params to tune	smooth predic-tions	easy to interpret?
linear regression	yes	linear ex-trapolation	no	l1 and/or l2 reg	yes	yes
logistic regression	yes	scales with distance from the decision boundary	no	l1 and/or l2 reg	yes	yes
random forest regression	so so	constant	yes	max_features, max_depth	no	so so
random forest classification	tbd	tbd	tbd	tbd	tbd	tbd
SVM rbf regression	tbd	tbd	tbd	tbd	tbd	tbd
SVM rbf classification	tbd	tbd	tbd	tbd	tbd	tbd

1.3 A random forest in classification

[4]:
```
from sklearn.datasets import make_moons
import numpy as np
from sklearn.ensemble import RandomForestClassifier
from sklearn.model_selection import ParameterGrid

# create the data
X,y = make_moons(noise=0.2, random_state=1,n_samples=200)
# set the hyperparameters
clf = RandomForestClassifier(n_estimators=1,max_depth=3,random_state=0)
# fit the model
clf.fit(X,y)
# predict new data
#y_new = clf.predict(X_new)
# predict probabilities
#y_new = clf.predict_proba(X_new)
```

[4]:
```
RandomForestClassifier(max_depth=3, n_estimators=1, random_state=0)
```

[5]:
```
help(RandomForestClassifier)
```

```
Help on class RandomForestClassifier in module sklearn.ensemble._forest:

class RandomForestClassifier(ForestClassifier)
 |  RandomForestClassifier(n_estimators=100, *, criterion='gini',
max_depth=None, min_samples_split=2, min_samples_leaf=1,
min_weight_fraction_leaf=0.0, max_features='sqrt', max_leaf_nodes=None,
min_impurity_decrease=0.0, bootstrap=True, oob_score=False, n_jobs=None,
random_state=None, verbose=0, warm_start=False, class_weight=None,
ccp_alpha=0.0, max_samples=None)
 |
 |  A random forest classifier.
 |
 |  A random forest is a meta estimator that fits a number of decision tree
 |  classifiers on various sub-samples of the dataset and uses averaging to
 |  improve the predictive accuracy and control over-fitting.
 |  The sub-sample size is controlled with the `max_samples` parameter if
 |  `bootstrap=True` (default), otherwise the whole dataset is used to build
 |  each tree.
 |
 |  Read more in the :ref:`User Guide <forest>`.
 |
 |  Parameters
 |  ----------
 |  n_estimators : int, default=100
 |      The number of trees in the forest.
 |
 |      .. versionchanged:: 0.22
 |         The default value of ``n_estimators`` changed from 10 to 100
 |         in 0.22.
 |
 |  criterion : {"gini", "entropy", "log_loss"}, default="gini"
 |      The function to measure the quality of a split. Supported criteria are
 |      "gini" for the Gini impurity and "log_loss" and "entropy" both for the
 |      Shannon information gain, see :ref:`tree_mathematical_formulation`.
 |      Note: This parameter is tree-specific.
 |
 |  max_depth : int, default=None
 |      The maximum depth of the tree. If None, then nodes are expanded until
 |      all leaves are pure or until all leaves contain less than
 |      min_samples_split samples.
 |
 |  min_samples_split : int or float, default=2
 |      The minimum number of samples required to split an internal node:
```

```
|
|      - If int, then consider `min_samples_split` as the minimum number.
|      - If float, then `min_samples_split` is a fraction and
|        `ceil(min_samples_split * n_samples)` are the minimum
|        number of samples for each split.
|
|      .. versionchanged:: 0.18
|         Added float values for fractions.
|
|  min_samples_leaf : int or float, default=1
|      The minimum number of samples required to be at a leaf node.
|      A split point at any depth will only be considered if it leaves at
|      least ``min_samples_leaf`` training samples in each of the left and
|      right branches.  This may have the effect of smoothing the model,
|      especially in regression.
|
|      - If int, then consider `min_samples_leaf` as the minimum number.
|      - If float, then `min_samples_leaf` is a fraction and
|        `ceil(min_samples_leaf * n_samples)` are the minimum
|        number of samples for each node.
|
|      .. versionchanged:: 0.18
|         Added float values for fractions.
|
|  min_weight_fraction_leaf : float, default=0.0
|      The minimum weighted fraction of the sum total of weights (of all
|      the input samples) required to be at a leaf node. Samples have
|      equal weight when sample_weight is not provided.
|
|  max_features : {"sqrt", "log2", None}, int or float, default="sqrt"
|      The number of features to consider when looking for the best split:
|
|      - If int, then consider `max_features` features at each split.
|      - If float, then `max_features` is a fraction and
|        `round(max_features * n_features)` features are considered at each
|        split.
|      - If "auto", then `max_features=sqrt(n_features)`.
|      - If "sqrt", then `max_features=sqrt(n_features)`.
|      - If "log2", then `max_features=log2(n_features)`.
|      - If None, then `max_features=n_features`.
|
|      .. versionchanged:: 1.1
|          The default of `max_features` changed from `"auto"` to `"sqrt"`.
|
|      .. deprecated:: 1.1
|          The `"auto"` option was deprecated in 1.1 and will be removed
|          in 1.3.
|
```

```
|      Note: the search for a split does not stop until at least one
|      valid partition of the node samples is found, even if it requires to
|      effectively inspect more than ``max_features`` features.
|
|  max_leaf_nodes : int, default=None
|      Grow trees with ``max_leaf_nodes`` in best-first fashion.
|      Best nodes are defined as relative reduction in impurity.
|      If None then unlimited number of leaf nodes.
|
|  min_impurity_decrease : float, default=0.0
|      A node will be split if this split induces a decrease of the impurity
|      greater than or equal to this value.
|
|      The weighted impurity decrease equation is the following::
|
|          N_t / N * (impurity - N_t_R / N_t * right_impurity
|                              - N_t_L / N_t * left_impurity)
|
|      where ``N`` is the total number of samples, ``N_t`` is the number of
|      samples at the current node, ``N_t_L`` is the number of samples in the
|      left child, and ``N_t_R`` is the number of samples in the right child.
|
|      ``N``, ``N_t``, ``N_t_R`` and ``N_t_L`` all refer to the weighted sum,
|      if ``sample_weight`` is passed.
|
|      .. versionadded:: 0.19
|
|  bootstrap : bool, default=True
|      Whether bootstrap samples are used when building trees. If False, the
|      whole dataset is used to build each tree.
|
|  oob_score : bool, default=False
|      Whether to use out-of-bag samples to estimate the generalization score.
|      Only available if bootstrap=True.
|
|  n_jobs : int, default=None
|      The number of jobs to run in parallel. :meth:`fit`, :meth:`predict`,
|      :meth:`decision_path` and :meth:`apply` are all parallelized over the
|      trees. ``None`` means 1 unless in a :obj:`joblib.parallel_backend`
|      context. ``-1`` means using all processors. See :term:`Glossary
|      <n_jobs>` for more details.
|
|  random_state : int, RandomState instance or None, default=None
|      Controls both the randomness of the bootstrapping of the samples used
|      when building trees (if ``bootstrap=True``) and the sampling of the
|      features to consider when looking for the best split at each node
|      (if ``max_features < n_features``).
|      See :term:`Glossary <random_state>` for details.
```

```
 |
 |  verbose : int, default=0
 |      Controls the verbosity when fitting and predicting.
 |
 |  warm_start : bool, default=False
 |      When set to ``True``, reuse the solution of the previous call to fit
 |      and add more estimators to the ensemble, otherwise, just fit a whole
 |      new forest. See :term:`the Glossary <warm_start>`.
 |
 |  class_weight : {"balanced", "balanced_subsample"}, dict or list of dicts,
default=None
 |      Weights associated with classes in the form ``{class_label: weight}``.
 |      If not given, all classes are supposed to have weight one. For
 |      multi-output problems, a list of dicts can be provided in the same
 |      order as the columns of y.
 |
 |      Note that for multioutput (including multilabel) weights should be
 |      defined for each class of every column in its own dict. For example,
 |      for four-class multilabel classification weights should be
 |      [{0: 1, 1: 1}, {0: 1, 1: 5}, {0: 1, 1: 1}, {0: 1, 1: 1}] instead of
 |      [{1:1}, {2:5}, {3:1}, {4:1}].
 |
 |      The "balanced" mode uses the values of y to automatically adjust
 |      weights inversely proportional to class frequencies in the input data
 |      as ``n_samples / (n_classes * np.bincount(y))``
 |
 |      The "balanced_subsample" mode is the same as "balanced" except that
 |      weights are computed based on the bootstrap sample for every tree
 |      grown.
 |
 |      For multi-output, the weights of each column of y will be multiplied.
 |
 |      Note that these weights will be multiplied with sample_weight (passed
 |      through the fit method) if sample_weight is specified.
 |
 |  ccp_alpha : non-negative float, default=0.0
 |      Complexity parameter used for Minimal Cost-Complexity Pruning. The
 |      subtree with the largest cost complexity that is smaller than
 |      ``ccp_alpha`` will be chosen. By default, no pruning is performed. See
 |      :ref:`minimal_cost_complexity_pruning` for details.
 |
 |      .. versionadded:: 0.22
 |
 |  max_samples : int or float, default=None
 |      If bootstrap is True, the number of samples to draw from X
 |      to train each base estimator.
 |
 |      - If None (default), then draw `X.shape[0]` samples.
```

```
|      - If int, then draw `max_samples` samples.
|      - If float, then draw `max_samples * X.shape[0]` samples. Thus,
|        `max_samples` should be in the interval `(0.0, 1.0]`.
|
|      .. versionadded:: 0.22
|
|  Attributes
|  ----------
|  base_estimator_ : DecisionTreeClassifier
|      The child estimator template used to create the collection of fitted
|      sub-estimators.
|
|  estimators_ : list of DecisionTreeClassifier
|      The collection of fitted sub-estimators.
|
|  classes_ : ndarray of shape (n_classes,) or a list of such arrays
|      The classes labels (single output problem), or a list of arrays of
|      class labels (multi-output problem).
|
|  n_classes_ : int or list
|      The number of classes (single output problem), or a list containing the
|      number of classes for each output (multi-output problem).
|
|  n_features_ : int
|      The number of features when ``fit`` is performed.
|
|      .. deprecated:: 1.0
|          Attribute `n_features_` was deprecated in version 1.0 and will be
|          removed in 1.2. Use `n_features_in_` instead.
|
|  n_features_in_ : int
|      Number of features seen during :term:`fit`.
|
|      .. versionadded:: 0.24
|
|  feature_names_in_ : ndarray of shape (`n_features_in_`,)
|      Names of features seen during :term:`fit`. Defined only when `X`
|      has feature names that are all strings.
|
|      .. versionadded:: 1.0
|
|  n_outputs_ : int
|      The number of outputs when ``fit`` is performed.
|
|  feature_importances_ : ndarray of shape (n_features,)
|      The impurity-based feature importances.
|      The higher, the more important the feature.
|      The importance of a feature is computed as the (normalized)
```

```
 |      total reduction of the criterion brought by that feature.  It is also
 |      known as the Gini importance.
 |
 |      Warning: impurity-based feature importances can be misleading for
 |      high cardinality features (many unique values). See
 |      :func:`sklearn.inspection.permutation_importance` as an alternative.
 |
 |  oob_score_ : float
 |      Score of the training dataset obtained using an out-of-bag estimate.
 |      This attribute exists only when ``oob_score`` is True.
 |
 |  oob_decision_function_ : ndarray of shape (n_samples, n_classes) or
(n_samples, n_classes, n_outputs)
 |      Decision function computed with out-of-bag estimate on the training
 |      set. If n_estimators is small it might be possible that a data point
 |      was never left out during the bootstrap. In this case,
 |      `oob_decision_function_` might contain NaN. This attribute exists
 |      only when ``oob_score`` is True.
 |
 |  See Also
 |  --------
 |  sklearn.tree.DecisionTreeClassifier : A decision tree classifier.
 |  sklearn.ensemble.ExtraTreesClassifier : Ensemble of extremely randomized
 |      tree classifiers.
 |
 |  Notes
 |  -----
 |  The default values for the parameters controlling the size of the trees
 |  (e.g. ``max_depth``, ``min_samples_leaf``, etc.) lead to fully grown and
 |  unpruned trees which can potentially be very large on some data sets. To
 |  reduce memory consumption, the complexity and size of the trees should be
 |  controlled by setting those parameter values.
 |
 |  The features are always randomly permuted at each split. Therefore,
 |  the best found split may vary, even with the same training data,
 |  ``max_features=n_features`` and ``bootstrap=False``, if the improvement
 |  of the criterion is identical for several splits enumerated during the
 |  search of the best split. To obtain a deterministic behaviour during
 |  fitting, ``random_state`` has to be fixed.
 |
 |  References
 |  ----------
 |  .. [1] L. Breiman, "Random Forests", Machine Learning, 45(1), 5-32, 2001.
 |
 |  Examples
 |  --------
 |  >>> from sklearn.ensemble import RandomForestClassifier
 |  >>> from sklearn.datasets import make_classification
```

```
 |  >>> X, y = make_classification(n_samples=1000, n_features=4,
 |  …                            n_informative=2, n_redundant=0,
 |  …                            random_state=0, shuffle=False)
 |  >>> clf = RandomForestClassifier(max_depth=2, random_state=0)
 |  >>> clf.fit(X, y)
 |  RandomForestClassifier(…)
 |  >>> print(clf.predict([[0, 0, 0, 0]]))
 |  [1]
 |
 |  Method resolution order:
 |      RandomForestClassifier
 |      ForestClassifier
 |      sklearn.base.ClassifierMixin
 |      BaseForest
 |      sklearn.base.MultiOutputMixin
 |      sklearn.ensemble._base.BaseEnsemble
 |      sklearn.base.MetaEstimatorMixin
 |      sklearn.base.BaseEstimator
 |      builtins.object
 |
 |  Methods defined here:
 |
 |  __init__(self, n_estimators=100, *, criterion='gini', max_depth=None,
min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0,
max_features='sqrt', max_leaf_nodes=None, min_impurity_decrease=0.0,
bootstrap=True, oob_score=False, n_jobs=None, random_state=None, verbose=0,
warm_start=False, class_weight=None, ccp_alpha=0.0, max_samples=None)
 |      Initialize self.  See help(type(self)) for accurate signature.
 |
 |  ----------------------------------------------------------------------
 |  Data and other attributes defined here:
 |
 |  __abstractmethods__ = frozenset()
 |
 |  __annotations__ = {}
 |
 |  ----------------------------------------------------------------------
 |  Methods inherited from ForestClassifier:
 |
 |  predict(self, X)
 |      Predict class for X.
 |
 |      The predicted class of an input sample is a vote by the trees in
 |      the forest, weighted by their probability estimates. That is,
 |      the predicted class is the one with highest mean probability
 |      estimate across the trees.
 |
 |      Parameters
```

```
|      ----------
|      X : {array-like, sparse matrix} of shape (n_samples, n_features)
|          The input samples. Internally, its dtype will be converted to
|          ``dtype=np.float32``. If a sparse matrix is provided, it will be
|          converted into a sparse ``csr_matrix``.
|
|      Returns
|      -------
|      y : ndarray of shape (n_samples,) or (n_samples, n_outputs)
|          The predicted classes.
|
|  predict_log_proba(self, X)
|      Predict class log-probabilities for X.
|
|      The predicted class log-probabilities of an input sample is computed as
|      the log of the mean predicted class probabilities of the trees in the
|      forest.
|
|      Parameters
|      ----------
|      X : {array-like, sparse matrix} of shape (n_samples, n_features)
|          The input samples. Internally, its dtype will be converted to
|          ``dtype=np.float32``. If a sparse matrix is provided, it will be
|          converted into a sparse ``csr_matrix``.
|
|      Returns
|      -------
|      p : ndarray of shape (n_samples, n_classes), or a list of such arrays
|          The class probabilities of the input samples. The order of the
|          classes corresponds to that in the attribute :term:`classes_`.
|
|  predict_proba(self, X)
|      Predict class probabilities for X.
|
|      The predicted class probabilities of an input sample are computed as
|      the mean predicted class probabilities of the trees in the forest.
|      The class probability of a single tree is the fraction of samples of
|      the same class in a leaf.
|
|      Parameters
|      ----------
|      X : {array-like, sparse matrix} of shape (n_samples, n_features)
|          The input samples. Internally, its dtype will be converted to
|          ``dtype=np.float32``. If a sparse matrix is provided, it will be
|          converted into a sparse ``csr_matrix``.
|
|      Returns
|      -------
```

```
|      p : ndarray of shape (n_samples, n_classes), or a list of such arrays
|          The class probabilities of the input samples. The order of the
|          classes corresponds to that in the attribute :term:`classes_`.
|
|  ----------------------------------------------------------------------
|  Methods inherited from sklearn.base.ClassifierMixin:
|
|  score(self, X, y, sample_weight=None)
|      Return the mean accuracy on the given test data and labels.
|
|      In multi-label classification, this is the subset accuracy
|      which is a harsh metric since you require for each sample that
|      each label set be correctly predicted.
|
|      Parameters
|      ----------
|      X : array-like of shape (n_samples, n_features)
|          Test samples.
|
|      y : array-like of shape (n_samples,) or (n_samples, n_outputs)
|          True labels for `X`.
|
|      sample_weight : array-like of shape (n_samples,), default=None
|          Sample weights.
|
|      Returns
|      -------
|      score : float
|          Mean accuracy of ``self.predict(X)`` wrt. `y`.
|
|  ----------------------------------------------------------------------
|  Data descriptors inherited from sklearn.base.ClassifierMixin:
|
|  __dict__
|      dictionary for instance variables (if defined)
|
|  __weakref__
|      list of weak references to the object (if defined)
|
|  ----------------------------------------------------------------------
|  Methods inherited from BaseForest:
|
|  apply(self, X)
|      Apply trees in the forest to X, return leaf indices.
|
|      Parameters
|      ----------
|      X : {array-like, sparse matrix} of shape (n_samples, n_features)
```

```
|          The input samples. Internally, its dtype will be converted to
|          ``dtype=np.float32``. If a sparse matrix is provided, it will be
|          converted into a sparse ``csr_matrix``.
|
|      Returns
|      -------
|      X_leaves : ndarray of shape (n_samples, n_estimators)
|          For each datapoint x in X and for each tree in the forest,
|          return the index of the leaf x ends up in.
|
|  decision_path(self, X)
|      Return the decision path in the forest.
|
|      .. versionadded:: 0.18
|
|      Parameters
|      ----------
|      X : {array-like, sparse matrix} of shape (n_samples, n_features)
|          The input samples. Internally, its dtype will be converted to
|          ``dtype=np.float32``. If a sparse matrix is provided, it will be
|          converted into a sparse ``csr_matrix``.
|
|      Returns
|      -------
|      indicator : sparse matrix of shape (n_samples, n_nodes)
|          Return a node indicator matrix where non zero elements indicates
|          that the samples goes through the nodes. The matrix is of CSR
|          format.
|
|      n_nodes_ptr : ndarray of shape (n_estimators + 1,)
|          The columns from indicator[n_nodes_ptr[i]:n_nodes_ptr[i+1]]
|          gives the indicator value for the i-th estimator.
|
|  fit(self, X, y, sample_weight=None)
|      Build a forest of trees from the training set (X, y).
|
|      Parameters
|      ----------
|      X : {array-like, sparse matrix} of shape (n_samples, n_features)
|          The training input samples. Internally, its dtype will be converted
|          to ``dtype=np.float32``. If a sparse matrix is provided, it will be
|          converted into a sparse ``csc_matrix``.
|
|      y : array-like of shape (n_samples,) or (n_samples, n_outputs)
|          The target values (class labels in classification, real numbers in
|          regression).
|
|      sample_weight : array-like of shape (n_samples,), default=None
```

```
 |          Sample weights. If None, then samples are equally weighted. Splits
 |          that would create child nodes with net zero or negative weight are
 |          ignored while searching for a split in each node. In the case of
 |          classification, splits are also ignored if they would result in any
 |          single class carrying a negative weight in either child node.
 |
 |      Returns
 |      -------
 |      self : object
 |          Fitted estimator.
 |
 |  ----------------------------------------------------------------------
 |  Readonly properties inherited from BaseForest:
 |
 |  feature_importances_
 |      The impurity-based feature importances.
 |
 |      The higher, the more important the feature.
 |      The importance of a feature is computed as the (normalized)
 |      total reduction of the criterion brought by that feature.  It is also
 |      known as the Gini importance.
 |
 |      Warning: impurity-based feature importances can be misleading for
 |      high cardinality features (many unique values). See
 |      :func:`sklearn.inspection.permutation_importance` as an alternative.
 |
 |      Returns
 |      -------
 |      feature_importances_ : ndarray of shape (n_features,)
 |          The values of this array sum to 1, unless all trees are single node
 |          trees consisting of only the root node, in which case it will be an
 |          array of zeros.
 |
 |  n_features_
 |      DEPRECATED: Attribute `n_features_` was deprecated in version 1.0 and
will be removed in 1.2. Use `n_features_in_` instead.
 |
 |      Number of features when fitting the estimator.
 |
 |  ----------------------------------------------------------------------
 |  Methods inherited from sklearn.ensemble._base.BaseEnsemble:
 |
 |  __getitem__(self, index)
 |      Return the index'th estimator in the ensemble.
 |
 |  __iter__(self)
 |      Return iterator over estimators in the ensemble.
 |
```

```
|  __len__(self)
|      Return the number of estimators in the ensemble.
|
|  ----------------------------------------------------------------------
|  Methods inherited from sklearn.base.BaseEstimator:
|
|  __getstate__(self)
|
|  __repr__(self, N_CHAR_MAX=700)
|      Return repr(self).
|
|  __setstate__(self, state)
|
|  get_params(self, deep=True)
|      Get parameters for this estimator.
|
|      Parameters
|      ----------
|      deep : bool, default=True
|          If True, will return the parameters for this estimator and
|          contained subobjects that are estimators.
|
|      Returns
|      -------
|      params : dict
|          Parameter names mapped to their values.
|
|  set_params(self, **params)
|      Set the parameters of this estimator.
|
|      The method works on simple estimators as well as on nested objects
|      (such as :class:`~sklearn.pipeline.Pipeline`). The latter have
|      parameters of the form ``<component>__<parameter>`` so that it's
|      possible to update each component of a nested object.
|
|      Parameters
|      ----------
|      **params : dict
|          Estimator parameters.
|
|      Returns
|      -------
|      self : estimator instance
|          Estimator instance.
```

[6]:
```
# initialize RandomForestClassifier
ML_algo = RandomForestClassifier(random_state=42)

# set RF parameter grid
hyperparameters = {
    'n_estimators': [1, 3, 10, 30],
    'max_depth': [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
}

plot_clf_contour(hyperparameters, X, y)
```

```
interactive(children=(SelectionSlider(description='n_estimators', options=(1, 3,␣
↪10, 30), value=1), SelectionS…
```

```
FigureWidget({
    'data': [{'colorbar': {'title': {'text': 'predicted probability'}},
              'colorsca…
```

ML algo	suitable for large datasets?	behaviour wrt outliers	non-linear?	params to tune	smooth predictions	easy to interpret?
linear regression	yes	linear extrapolation	no	l1 and/or l2 reg	yes	yes
logistic regression	yes	scales with distance from the decision boundary	no	l1 and/or l2 reg	yes	yes
random forest regression	so so	constant	yes	max_features, max_depth	no	so so
random forest classification	so so	step-like, difficult to tell	yes	max_features, max_depth	no	so so
SVM rbf regression	tbd	tbd	tbd	tbd	tbd	tbd
SVM rbf classification	tbd	tbd	tbd	tbd	tbd	tbd

2 Quiz 1

2.1 Support Vector Machine

- very versatile technique, it comes in lots of flavors/types, read more about it here
- SVM classifier motivation
  - points in n dimensional space with class 0 and 1
  - we want to find the (n-1) dimensional hyperplane that best separates the points
  - this hyperplane is our (linear) decision boundary

- we cover SVMs with radial basis functions (rbf)
  - we apply a kernel function (a non-linear transformation) to the data points
  - the kernel function basically "smears" the points
  - gaussian rbf kernel: $\exp(-\gamma(|x - x'|)^2)$ where $\gamma > 0$

2.2 SVR

[7]:
```
import numpy as np
from sklearn.svm import SVR
np.random.seed(10)
def true_fun(X):
    return np.cos(1.5 * np.pi * X)

n_samples = 30

X = np.random.rand(n_samples)
y = true_fun(X) + np.random.randn(n_samples) * 0.1

X_new = np.linspace(-0.5, 1.5, 2000)

reg = SVR(gamma = 1, C = 1)
reg.fit(X[:, np.newaxis],y)
y_new = reg.predict(X_new[:, np.newaxis])
```

[8]:
```
help(SVR)
```

```
Help on class SVR in module sklearn.svm._classes:

class SVR(sklearn.base.RegressorMixin, sklearn.svm._base.BaseLibSVM)
 |  SVR(*, kernel='rbf', degree=3, gamma='scale', coef0=0.0, tol=0.001, C=1.0,
epsilon=0.1, shrinking=True, cache_size=200, verbose=False, max_iter=-1)
 |
 |  Epsilon-Support Vector Regression.
 |
 |  The free parameters in the model are C and epsilon.
 |
 |  The implementation is based on libsvm. The fit time complexity
 |  is more than quadratic with the number of samples which makes it hard
 |  to scale to datasets with more than a couple of 10000 samples. For large
 |  datasets consider using :class:`~sklearn.svm.LinearSVR` or
 |  :class:`~sklearn.linear_model.SGDRegressor` instead, possibly after a
 |  :class:`~sklearn.kernel_approximation.Nystroem` transformer.
 |
 |  Read more in the :ref:`User Guide <svm_regression>`.
 |
 |  Parameters
 |  ----------
 |  kernel : {'linear', 'poly', 'rbf', 'sigmoid', 'precomputed'} or callable,
```

```
default='rbf'
 |       Specifies the kernel type to be used in the algorithm.
 |       If none is given, 'rbf' will be used. If a callable is given it is
 |       used to precompute the kernel matrix.
 |
 |  degree : int, default=3
 |      Degree of the polynomial kernel function ('poly').
 |      Ignored by all other kernels.
 |
 |  gamma : {'scale', 'auto'} or float, default='scale'
 |      Kernel coefficient for 'rbf', 'poly' and 'sigmoid'.
 |
 |      - if ``gamma='scale'`` (default) is passed then it uses
 |        1 / (n_features * X.var()) as value of gamma,
 |      - if 'auto', uses 1 / n_features.
 |
 |      .. versionchanged:: 0.22
 |         The default value of ``gamma`` changed from 'auto' to 'scale'.
 |
 |  coef0 : float, default=0.0
 |      Independent term in kernel function.
 |      It is only significant in 'poly' and 'sigmoid'.
 |
 |  tol : float, default=1e-3
 |      Tolerance for stopping criterion.
 |
 |  C : float, default=1.0
 |      Regularization parameter. The strength of the regularization is
 |      inversely proportional to C. Must be strictly positive.
 |      The penalty is a squared l2 penalty.
 |
 |  epsilon : float, default=0.1
 |       Epsilon in the epsilon-SVR model. It specifies the epsilon-tube
 |       within which no penalty is associated in the training loss function
 |       with points predicted within a distance epsilon from the actual
 |       value.
 |
 |  shrinking : bool, default=True
 |      Whether to use the shrinking heuristic.
 |      See the :ref:`User Guide <shrinking_svm>`.
 |
 |  cache_size : float, default=200
 |      Specify the size of the kernel cache (in MB).
 |
 |  verbose : bool, default=False
 |      Enable verbose output. Note that this setting takes advantage of a
 |      per-process runtime setting in libsvm that, if enabled, may not work
 |      properly in a multithreaded context.
```

```
|
|  max_iter : int, default=-1
|      Hard limit on iterations within solver, or -1 for no limit.
|
|  Attributes
|  ----------
|  class_weight_ : ndarray of shape (n_classes,)
|      Multipliers of parameter C for each class.
|      Computed based on the ``class_weight`` parameter.
|
|  coef_ : ndarray of shape (1, n_features)
|      Weights assigned to the features (coefficients in the primal
|      problem). This is only available in the case of a linear kernel.
|
|      `coef_` is readonly property derived from `dual_coef_` and
|      `support_vectors_`.
|
|  dual_coef_ : ndarray of shape (1, n_SV)
|      Coefficients of the support vector in the decision function.
|
|  fit_status_ : int
|      0 if correctly fitted, 1 otherwise (will raise warning)
|
|  intercept_ : ndarray of shape (1,)
|      Constants in decision function.
|
|  n_features_in_ : int
|      Number of features seen during :term:`fit`.
|
|      .. versionadded:: 0.24
|
|  feature_names_in_ : ndarray of shape (`n_features_in_`,)
|      Names of features seen during :term:`fit`. Defined only when `X`
|      has feature names that are all strings.
|
|      .. versionadded:: 1.0
|
|  n_iter_ : int
|      Number of iterations run by the optimization routine to fit the model.
|
|      .. versionadded:: 1.1
|
|  n_support_ : ndarray of shape (n_classes,), dtype=int32
|      Number of support vectors for each class.
|
|  shape_fit_ : tuple of int of shape (n_dimensions_of_X,)
|      Array dimensions of training vector ``X``.
|
```

```
|  support_ : ndarray of shape (n_SV,)
|      Indices of support vectors.
|
|  support_vectors_ : ndarray of shape (n_SV, n_features)
|      Support vectors.
|
|  See Also
|  --------
|  NuSVR : Support Vector Machine for regression implemented using libsvm
|      using a parameter to control the number of support vectors.
|
|  LinearSVR : Scalable Linear Support Vector Machine for regression
|      implemented using liblinear.
|
|  References
|  ----------
|  .. [1] `LIBSVM: A Library for Support Vector Machines
|      <http://www.csie.ntu.edu.tw/~cjlin/papers/libsvm.pdf>`_
|
|  .. [2] `Platt, John (1999). "Probabilistic outputs for support vector
|      machines and comparison to regularizedlikelihood methods."
|      <http://citeseer.ist.psu.edu/viewdoc/summary?doi=10.1.1.41.1639>`_
|
|  Examples
|  --------
|  >>> from sklearn.svm import SVR
|  >>> from sklearn.pipeline import make_pipeline
|  >>> from sklearn.preprocessing import StandardScaler
|  >>> import numpy as np
|  >>> n_samples, n_features = 10, 5
|  >>> rng = np.random.RandomState(0)
|  >>> y = rng.randn(n_samples)
|  >>> X = rng.randn(n_samples, n_features)
|  >>> regr = make_pipeline(StandardScaler(), SVR(C=1.0, epsilon=0.2))
|  >>> regr.fit(X, y)
|  Pipeline(steps=[('standardscaler', StandardScaler()),
|                  ('svr', SVR(epsilon=0.2))])
|
|  Method resolution order:
|      SVR
|      sklearn.base.RegressorMixin
|      sklearn.svm._base.BaseLibSVM
|      sklearn.base.BaseEstimator
|      builtins.object
|
|  Methods defined here:
|
|  __init__(self, *, kernel='rbf', degree=3, gamma='scale', coef0=0.0,
```

```
tol=0.001, C=1.0, epsilon=0.1, shrinking=True, cache_size=200, verbose=False,
max_iter=-1)
 |      Initialize self.  See help(type(self)) for accurate signature.
 |
 |  ----------------------------------------------------------------------
 |  Data and other attributes defined here:
 |
 |  __abstractmethods__ = frozenset()
 |
 |  __annotations__ = {}
 |
 |  ----------------------------------------------------------------------
 |  Methods inherited from sklearn.base.RegressorMixin:
 |
 |  score(self, X, y, sample_weight=None)
 |      Return the coefficient of determination of the prediction.
 |
 |      The coefficient of determination :math:`R^2` is defined as
 |      :math:`(1 - \frac{u}{v})`, where :math:`u` is the residual
 |      sum of squares ``((y_true - y_pred)** 2).sum()`` and :math:`v`
 |      is the total sum of squares ``((y_true - y_true.mean()) ** 2).sum()``.
 |      The best possible score is 1.0 and it can be negative (because the
 |      model can be arbitrarily worse). A constant model that always predicts
 |      the expected value of `y`, disregarding the input features, would get
 |      a :math:`R^2` score of 0.0.
 |
 |      Parameters
 |      ----------
 |      X : array-like of shape (n_samples, n_features)
 |          Test samples. For some estimators this may be a precomputed
 |          kernel matrix or a list of generic objects instead with shape
 |          ``(n_samples, n_samples_fitted)``, where ``n_samples_fitted``
 |          is the number of samples used in the fitting for the estimator.
 |
 |      y : array-like of shape (n_samples,) or (n_samples, n_outputs)
 |          True values for `X`.
 |
 |      sample_weight : array-like of shape (n_samples,), default=None
 |          Sample weights.
 |
 |      Returns
 |      -------
 |      score : float
 |          :math:`R^2` of ``self.predict(X)`` wrt. `y`.
 |
 |      Notes
 |      -----
 |      The :math:`R^2` score used when calling ``score`` on a regressor uses
```

```
 |      ``multioutput='uniform_average'`` from version 0.23 to keep consistent
 |      with default value of :func:`~sklearn.metrics.r2_score`.
 |      This influences the ``score`` method of all the multioutput
 |      regressors (except for
 |      :class:`~sklearn.multioutput.MultiOutputRegressor`).
 |
 |  ----------------------------------------------------------------------
 |  Data descriptors inherited from sklearn.base.RegressorMixin:
 |
 |  __dict__
 |      dictionary for instance variables (if defined)
 |
 |  __weakref__
 |      list of weak references to the object (if defined)
 |
 |  ----------------------------------------------------------------------
 |  Methods inherited from sklearn.svm._base.BaseLibSVM:
 |
 |  fit(self, X, y, sample_weight=None)
 |      Fit the SVM model according to the given training data.
 |
 |      Parameters
 |      ----------
 |      X : {array-like, sparse matrix} of shape (n_samples, n_features)
or (n_samples, n_samples)
 |          Training vectors, where `n_samples` is the number of samples
 |          and `n_features` is the number of features.
 |          For kernel="precomputed", the expected shape of X is
 |          (n_samples, n_samples).
 |
 |      y : array-like of shape (n_samples,)
 |          Target values (class labels in classification, real numbers in
 |          regression).
 |
 |      sample_weight : array-like of shape (n_samples,), default=None
 |          Per-sample weights. Rescale C per sample. Higher weights
 |          force the classifier to put more emphasis on these points.
 |
 |      Returns
 |      -------
 |      self : object
 |          Fitted estimator.
 |
 |      Notes
 |      -----
 |      If X and y are not C-ordered and contiguous arrays of np.float64 and
 |      X is not a scipy.sparse.csr_matrix, X and/or y may be copied.
 |
```

```
|      If X is a dense array, then the other methods will not support sparse
|      matrices as input.
|
|  predict(self, X)
|      Perform regression on samples in X.
|
|      For an one-class model, +1 (inlier) or -1 (outlier) is returned.
|
|      Parameters
|      ----------
|      X : {array-like, sparse matrix} of shape (n_samples, n_features)
|          For kernel="precomputed", the expected shape of X is
|          (n_samples_test, n_samples_train).
|
|      Returns
|      -------
|      y_pred : ndarray of shape (n_samples,)
|          The predicted values.
|
|  ----------------------------------------------------------------------
|  Readonly properties inherited from sklearn.svm._base.BaseLibSVM:
|
|  coef_
|      Weights assigned to the features when `kernel="linear"`.
|
|      Returns
|      -------
|      ndarray of shape (n_features, n_classes)
|
|  n_support_
|      Number of support vectors for each class.
|
|  ----------------------------------------------------------------------
|  Methods inherited from sklearn.base.BaseEstimator:
|
|  __getstate__(self)
|
|  __repr__(self, N_CHAR_MAX=700)
|      Return repr(self).
|
|  __setstate__(self, state)
|
|  get_params(self, deep=True)
|      Get parameters for this estimator.
|
|      Parameters
|      ----------
|      deep : bool, default=True
```

```
|          If True, will return the parameters for this estimator and
|          contained subobjects that are estimators.
|
|      Returns
|      -------
|      params : dict
|          Parameter names mapped to their values.
|
|  set_params(self, **params)
|      Set the parameters of this estimator.
|
|      The method works on simple estimators as well as on nested objects
|      (such as :class:`~sklearn.pipeline.Pipeline`). The latter have
|      parameters of the form ``<component>__<parameter>`` so that it's
|      possible to update each component of a nested object.
|
|      Parameters
|      ----------
|      **params : dict
|          Estimator parameters.
|
|      Returns
|      -------
|      self : estimator instance
|          Estimator instance.
```

[9]:
```
hyperparameters = {
    'gamma': [1e-3, 1e-1, 1e1, 1e3, 1e5],
    'C': [1e-1, 1e0, 1e1]
}

vis(X, y, SVR, hyperparameters, X_new)
```

```
interactive(children=(SelectionSlider(description='gamma', options=(0.001, 0.1,␣
 ↪10.0, 1000.0, 100000.0), value…
```

3 Quiz 2

Let's measure how long it takes to fit a linear regression, random forest regression, and SVR as a function of `n_samples` using our toy regression dataset.

Check this stackoverflow post to figure out how to measure the execution time of a couple of lines of code.

Set n_estimators to 10 and max_depth to 3 in the random forest.

Set the gamma and C parameters to 1 in SVR.

Fit models with n_samples = 1000, 2000, 3000, 4000, 5000. Measure how long it takes to fit each model.

Plot the run time as a function of n_samples for the three models. You might need to adjust the y axis range to check some of the statements.

Which of these statements are true?

- The random forest run-time scales linearly with n_samples.
- The linear regression model is the fastest to fit.
- The SVR run-time scales worse than linear. (I.e., if we double n_sample, the fit time more than doubles.)

[10]:
```
import time
from sklearn.linear_model import LinearRegression

n_samples = np.linspace(1000,5000,5,dtype=int)

timer_lin = []
timer_RF = []
timer_SVR = []

for n_sample in n_samples:
    X = np.random.rand(n_sample)
    y = true_fun(X) + np.random.randn(n_sample) * 0.1

    # add your code below

# prepare the plot below:
```

ML algo	suitable for large datasets?	behaviour wrt outliers	non-linear?	params to tune	smooth predic-tions	easy to interpret?
linear regression	yes	linear ex-trapolation	no	l1 and/or l2 reg	yes	yes
logistic regression	yes	scales with distance from the decision boundary	no	l1 and/or l2 reg	yes	yes
random forest regression	so so	constant	yes	max_features, max_depth	no	so so
random forest classification	so so	step-like, difficult to tell	yes	max_features, max_depth	no	so so
SVM rbf regression	no	non-linear extrapola-tion	yes	C, gamma	yes	so so

ML algo	suitable for large datasets?	behaviour wrt outliers	non-linear?	params to tune	smooth predic-tions	easy to interpret?
SVM rbf classification	tbd	tbd	tbd	tbd	tbd	tbd

3.1 SVC

[11]:
```
from sklearn.datasets import make_moons
import numpy as np
from sklearn.svm import SVC

# create the data
X,y = make_moons(noise=0.2, random_state=1,n_samples=200)
# set the hyperparameters
clf = SVC(gamma = 1, C = 1, probability=True)
# fit the model
clf.fit(X,y)
# predict new data
#y_new = clf.predict(X_new)
# predict probabilities
#y_new = clf.predict_proba(X_new)
```

[11]:
```
SVC(C=1, gamma=1, probability=True)
```

[12]:
```
help(SVC)
```

```
Help on class SVC in module sklearn.svm._classes:

class SVC(sklearn.svm._base.BaseSVC)
 |  SVC(*, C=1.0, kernel='rbf', degree=3, gamma='scale', coef0=0.0,
shrinking=True, probability=False, tol=0.001, cache_size=200, class_weight=None,
verbose=False, max_iter=-1, decision_function_shape='ovr', break_ties=False,
random_state=None)
 |
 |  C-Support Vector Classification.
 |
 |  The implementation is based on libsvm. The fit time scales at least
 |  quadratically with the number of samples and may be impractical
 |  beyond tens of thousands of samples. For large datasets
 |  consider using :class:`~sklearn.svm.LinearSVC` or
 |  :class:`~sklearn.linear_model.SGDClassifier` instead, possibly after a
 |  :class:`~sklearn.kernel_approximation.Nystroem` transformer.
 |
 |  The multiclass support is handled according to a one-vs-one scheme.
 |
 |  For details on the precise mathematical formulation of the provided
```

```
 |  kernel functions and how `gamma`, `coef0` and `degree` affect each
 |  other, see the corresponding section in the narrative documentation:
 |  :ref:`svm_kernels`.
 |
 |  Read more in the :ref:`User Guide <svm_classification>`.
 |
 |  Parameters
 |  ----------
 |  C : float, default=1.0
 |      Regularization parameter. The strength of the regularization is
 |      inversely proportional to C. Must be strictly positive. The penalty
 |      is a squared l2 penalty.
 |
 |  kernel : {'linear', 'poly', 'rbf', 'sigmoid', 'precomputed'} or callable,
default='rbf'
 |      Specifies the kernel type to be used in the algorithm.
 |      If none is given, 'rbf' will be used. If a callable is given it is
 |      used to pre-compute the kernel matrix from data matrices; that matrix
 |      should be an array of shape ``(n_samples, n_samples)``.
 |
 |  degree : int, default=3
 |      Degree of the polynomial kernel function ('poly').
 |      Ignored by all other kernels.
 |
 |  gamma : {'scale', 'auto'} or float, default='scale'
 |      Kernel coefficient for 'rbf', 'poly' and 'sigmoid'.
 |
 |      - if ``gamma='scale'`` (default) is passed then it uses
 |        1 / (n_features * X.var()) as value of gamma,
 |      - if 'auto', uses 1 / n_features.
 |
 |      .. versionchanged:: 0.22
 |         The default value of ``gamma`` changed from 'auto' to 'scale'.
 |
 |  coef0 : float, default=0.0
 |      Independent term in kernel function.
 |      It is only significant in 'poly' and 'sigmoid'.
 |
 |  shrinking : bool, default=True
 |      Whether to use the shrinking heuristic.
 |      See the :ref:`User Guide <shrinking_svm>`.
 |
 |  probability : bool, default=False
 |      Whether to enable probability estimates. This must be enabled prior
 |      to calling `fit`, will slow down that method as it internally uses
 |      5-fold cross-validation, and `predict_proba` may be inconsistent with
 |      `predict`. Read more in the :ref:`User Guide <scores_probabilities>`.
 |
```

```
|  tol : float, default=1e-3
|      Tolerance for stopping criterion.
|
|  cache_size : float, default=200
|      Specify the size of the kernel cache (in MB).
|
|  class_weight : dict or 'balanced', default=None
|      Set the parameter C of class i to class_weight[i]*C for
|      SVC. If not given, all classes are supposed to have
|      weight one.
|      The "balanced" mode uses the values of y to automatically adjust
|      weights inversely proportional to class frequencies in the input data
|      as ``n_samples / (n_classes * np.bincount(y))``.
|
|  verbose : bool, default=False
|      Enable verbose output. Note that this setting takes advantage of a
|      per-process runtime setting in libsvm that, if enabled, may not work
|      properly in a multithreaded context.
|
|  max_iter : int, default=-1
|      Hard limit on iterations within solver, or -1 for no limit.
|
|  decision_function_shape : {'ovo', 'ovr'}, default='ovr'
|      Whether to return a one-vs-rest ('ovr') decision function of shape
|      (n_samples, n_classes) as all other classifiers, or the original
|      one-vs-one ('ovo') decision function of libsvm which has shape
|      (n_samples, n_classes * (n_classes - 1) / 2). However, note that
|      internally, one-vs-one ('ovo') is always used as a multi-class strategy
|      to train models; an ovr matrix is only constructed from the ovo matrix.
|      The parameter is ignored for binary classification.
|
|      .. versionchanged:: 0.19
|          decision_function_shape is 'ovr' by default.
|
|      .. versionadded:: 0.17
|         *decision_function_shape='ovr'* is recommended.
|
|      .. versionchanged:: 0.17
|         Deprecated *decision_function_shape='ovo' and None*.
|
|  break_ties : bool, default=False
|      If true, ``decision_function_shape='ovr'``, and number of classes > 2,
|      :term:`predict` will break ties according to the confidence values of
|      :term:`decision_function`; otherwise the first class among the tied
|      classes is returned. Please note that breaking ties comes at a
|      relatively high computational cost compared to a simple predict.
|
|      .. versionadded:: 0.22
```

```
|
|  random_state : int, RandomState instance or None, default=None
|      Controls the pseudo random number generation for shuffling the data for
|      probability estimates. Ignored when `probability` is False.
|      Pass an int for reproducible output across multiple function calls.
|      See :term:`Glossary <random_state>`.
|
|  Attributes
|  ----------
|  class_weight_ : ndarray of shape (n_classes,)
|      Multipliers of parameter C for each class.
|      Computed based on the ``class_weight`` parameter.
|
|  classes_ : ndarray of shape (n_classes,)
|      The classes labels.
|
|  coef_ : ndarray of shape (n_classes * (n_classes - 1) / 2, n_features)
|      Weights assigned to the features (coefficients in the primal
|      problem). This is only available in the case of a linear kernel.
|
|      `coef_` is a readonly property derived from `dual_coef_` and
|      `support_vectors_`.
|
|  dual_coef_ : ndarray of shape (n_classes -1, n_SV)
|      Dual coefficients of the support vector in the decision
|      function (see :ref:`sgd_mathematical_formulation`), multiplied by
|      their targets.
|      For multiclass, coefficient for all 1-vs-1 classifiers.
|      The layout of the coefficients in the multiclass case is somewhat
|      non-trivial. See the :ref:`multi-class section of the User Guide
|      <svm_multi_class>` for details.
|
|  fit_status_ : int
|      0 if correctly fitted, 1 otherwise (will raise warning)
|
|  intercept_ : ndarray of shape (n_classes * (n_classes - 1) / 2,)
|      Constants in decision function.
|
|  n_features_in_ : int
|      Number of features seen during :term:`fit`.
|
|      .. versionadded:: 0.24
|
|  feature_names_in_ : ndarray of shape (`n_features_in_`,)
|      Names of features seen during :term:`fit`. Defined only when `X`
|      has feature names that are all strings.
|
|      .. versionadded:: 1.0
```

```
|
|  n_iter_ : ndarray of shape (n_classes * (n_classes - 1) // 2,)
|      Number of iterations run by the optimization routine to fit the model.
|      The shape of this attribute depends on the number of models optimized
|      which in turn depends on the number of classes.
|
|      .. versionadded:: 1.1
|
|  support_ : ndarray of shape (n_SV)
|      Indices of support vectors.
|
|  support_vectors_ : ndarray of shape (n_SV, n_features)
|      Support vectors.
|
|  n_support_ : ndarray of shape (n_classes,), dtype=int32
|      Number of support vectors for each class.
|
|  probA_ : ndarray of shape (n_classes * (n_classes - 1) / 2)
|  probB_ : ndarray of shape (n_classes * (n_classes - 1) / 2)
|      If `probability=True`, it corresponds to the parameters learned in
|      Platt scaling to produce probability estimates from decision values.
|      If `probability=False`, it's an empty array. Platt scaling uses the
|      logistic function
|      ``1 / (1 + exp(decision_value * probA_ + probB_))``
|      where ``probA_`` and ``probB_`` are learned from the dataset [2]_. For
|      more information on the multiclass case and training procedure see
|      section 8 of [1]_.
|
|  shape_fit_ : tuple of int of shape (n_dimensions_of_X,)
|      Array dimensions of training vector ``X``.
|
|  See Also
|  --------
|  SVR : Support Vector Machine for Regression implemented using libsvm.
|
|  LinearSVC : Scalable Linear Support Vector Machine for classification
|      implemented using liblinear. Check the See Also section of
|      LinearSVC for more comparison element.
|
|  References
|  ----------
|  .. [1] `LIBSVM: A Library for Support Vector Machines
|      <http://www.csie.ntu.edu.tw/~cjlin/papers/libsvm.pdf>`_
|
|  .. [2] `Platt, John (1999). "Probabilistic outputs for support vector
|      machines and comparison to regularizedlikelihood methods."
|      <http://citeseer.ist.psu.edu/viewdoc/summary?doi=10.1.1.41.1639>`_
|
```

```
 |  Examples
 |  --------
 |  >>> import numpy as np
 |  >>> from sklearn.pipeline import make_pipeline
 |  >>> from sklearn.preprocessing import StandardScaler
 |  >>> X = np.array([[-1, -1], [-2, -1], [1, 1], [2, 1]])
 |  >>> y = np.array([1, 1, 2, 2])
 |  >>> from sklearn.svm import SVC
 |  >>> clf = make_pipeline(StandardScaler(), SVC(gamma='auto'))
 |  >>> clf.fit(X, y)
 |  Pipeline(steps=[('standardscaler', StandardScaler()),
 |                  ('svc', SVC(gamma='auto'))])
 |
 |  >>> print(clf.predict([[-0.8, -1]]))
 |  [1]
 |
 |  Method resolution order:
 |      SVC
 |      sklearn.svm._base.BaseSVC
 |      sklearn.base.ClassifierMixin
 |      sklearn.svm._base.BaseLibSVM
 |      sklearn.base.BaseEstimator
 |      builtins.object
 |
 |  Methods defined here:
 |
 |  __init__(self, *, C=1.0, kernel='rbf', degree=3, gamma='scale', coef0=0.0,
shrinking=True, probability=False, tol=0.001, cache_size=200, class_weight=None,
verbose=False, max_iter=-1, decision_function_shape='ovr', break_ties=False,
random_state=None)
 |      Initialize self.  See help(type(self)) for accurate signature.
 |
 |  ----------------------------------------------------------------------
 |  Data and other attributes defined here:
 |
 |  __abstractmethods__ = frozenset()
 |
 |  __annotations__ = {}
 |
 |  ----------------------------------------------------------------------
 |  Methods inherited from sklearn.svm._base.BaseSVC:
 |
 |  decision_function(self, X)
 |      Evaluate the decision function for the samples in X.
 |
 |      Parameters
 |      ----------
 |      X : array-like of shape (n_samples, n_features)
```

```
 |          The input samples.
 |
 |      Returns
 |      -------
 |      X : ndarray of shape (n_samples, n_classes * (n_classes-1) / 2)
 |          Returns the decision function of the sample for each class
 |          in the model.
 |          If decision_function_shape='ovr', the shape is (n_samples,
 |          n_classes).
 |
 |      Notes
 |      -----
 |      If decision_function_shape='ovo', the function values are proportional
 |      to the distance of the samples X to the separating hyperplane. If the
 |      exact distances are required, divide the function values by the norm of
 |      the weight vector (``coef_``). See also `this question
 |      <https://stats.stackexchange.com/questions/14876/
 |      interpreting-distance-from-hyperplane-in-svm>`_ for further details.
 |      If decision_function_shape='ovr', the decision function is a monotonic
 |      transformation of ovo decision function.
 |
 |  predict(self, X)
 |      Perform classification on samples in X.
 |
 |      For an one-class model, +1 or -1 is returned.
 |
 |      Parameters
 |      ----------
 |      X : {array-like, sparse matrix} of shape (n_samples, n_features) or
(n_samples_test, n_samples_train)
 |          For kernel="precomputed", the expected shape of X is
 |          (n_samples_test, n_samples_train).
 |
 |      Returns
 |      -------
 |      y_pred : ndarray of shape (n_samples,)
 |          Class labels for samples in X.
 |
 |  predict_log_proba(self, X)
 |      Compute log probabilities of possible outcomes for samples in X.
 |
 |      The model need to have probability information computed at training
 |      time: fit with attribute `probability` set to True.
 |
 |      Parameters
 |      ----------
 |      X : array-like of shape (n_samples, n_features) or
(n_samples_test, n_samples_train)
```

```
|          For kernel="precomputed", the expected shape of X is
|          (n_samples_test, n_samples_train).
|
|      Returns
|      -------
|      T : ndarray of shape (n_samples, n_classes)
|          Returns the log-probabilities of the sample for each class in
|          the model. The columns correspond to the classes in sorted
|          order, as they appear in the attribute :term:`classes_`.
|
|      Notes
|      -----
|      The probability model is created using cross validation, so
|      the results can be slightly different than those obtained by
|      predict. Also, it will produce meaningless results on very small
|      datasets.
|
|  predict_proba(self, X)
|      Compute probabilities of possible outcomes for samples in X.
|
|      The model need to have probability information computed at training
|      time: fit with attribute `probability` set to True.
|
|      Parameters
|      ----------
|      X : array-like of shape (n_samples, n_features)
|          For kernel="precomputed", the expected shape of X is
|          (n_samples_test, n_samples_train).
|
|      Returns
|      -------
|      T : ndarray of shape (n_samples, n_classes)
|          Returns the probability of the sample for each class in
|          the model. The columns correspond to the classes in sorted
|          order, as they appear in the attribute :term:`classes_`.
|
|      Notes
|      -----
|      The probability model is created using cross validation, so
|      the results can be slightly different than those obtained by
|      predict. Also, it will produce meaningless results on very small
|      datasets.
|
|  ----------------------------------------------------------------------
|  Readonly properties inherited from sklearn.svm._base.BaseSVC:
|
|  probA_
|      Parameter learned in Platt scaling when `probability=True`.
```

```
|
|      Returns
|      -------
|      ndarray of shape  (n_classes * (n_classes - 1) / 2)
|
|  probB_
|      Parameter learned in Platt scaling when `probability=True`.
|
|      Returns
|      -------
|      ndarray of shape  (n_classes * (n_classes - 1) / 2)
|
|  ----------------------------------------------------------------------
|  Methods inherited from sklearn.base.ClassifierMixin:
|
|  score(self, X, y, sample_weight=None)
|      Return the mean accuracy on the given test data and labels.
|
|      In multi-label classification, this is the subset accuracy
|      which is a harsh metric since you require for each sample that
|      each label set be correctly predicted.
|
|      Parameters
|      ----------
|      X : array-like of shape (n_samples, n_features)
|          Test samples.
|
|      y : array-like of shape (n_samples,) or (n_samples, n_outputs)
|          True labels for `X`.
|
|      sample_weight : array-like of shape (n_samples,), default=None
|          Sample weights.
|
|      Returns
|      -------
|      score : float
|          Mean accuracy of ``self.predict(X)`` wrt. `y`.
|
|  ----------------------------------------------------------------------
|  Data descriptors inherited from sklearn.base.ClassifierMixin:
|
|  __dict__
|      dictionary for instance variables (if defined)
|
|  __weakref__
|      list of weak references to the object (if defined)
|
|  ----------------------------------------------------------------------
```

```
 |  Methods inherited from sklearn.svm._base.BaseLibSVM:
 |
 |  fit(self, X, y, sample_weight=None)
 |      Fit the SVM model according to the given training data.
 |
 |      Parameters
 |      ----------
 |      X : {array-like, sparse matrix} of shape (n_samples, n_features)
or (n_samples, n_samples)
 |          Training vectors, where `n_samples` is the number of samples
 |          and `n_features` is the number of features.
 |          For kernel="precomputed", the expected shape of X is
 |          (n_samples, n_samples).
 |
 |      y : array-like of shape (n_samples,)
 |          Target values (class labels in classification, real numbers in
 |          regression).
 |
 |      sample_weight : array-like of shape (n_samples,), default=None
 |          Per-sample weights. Rescale C per sample. Higher weights
 |          force the classifier to put more emphasis on these points.
 |
 |      Returns
 |      -------
 |      self : object
 |          Fitted estimator.
 |
 |      Notes
 |      -----
 |      If X and y are not C-ordered and contiguous arrays of np.float64 and
 |      X is not a scipy.sparse.csr_matrix, X and/or y may be copied.
 |
 |      If X is a dense array, then the other methods will not support sparse
 |      matrices as input.
 |
 |  ----------------------------------------------------------------------
 |  Readonly properties inherited from sklearn.svm._base.BaseLibSVM:
 |
 |  coef_
 |      Weights assigned to the features when `kernel="linear"`.
 |
 |      Returns
 |      -------
 |      ndarray of shape (n_features, n_classes)
 |
 |  n_support_
 |      Number of support vectors for each class.
 |
```

```
|  ----------------------------------------------------------------------
|  Methods inherited from sklearn.base.BaseEstimator:
|
|  __getstate__(self)
|
|  __repr__(self, N_CHAR_MAX=700)
|      Return repr(self).
|
|  __setstate__(self, state)
|
|  get_params(self, deep=True)
|      Get parameters for this estimator.
|
|      Parameters
|      ----------
|      deep : bool, default=True
|          If True, will return the parameters for this estimator and
|          contained subobjects that are estimators.
|
|      Returns
|      -------
|      params : dict
|          Parameter names mapped to their values.
|
|  set_params(self, **params)
|      Set the parameters of this estimator.
|
|      The method works on simple estimators as well as on nested objects
|      (such as :class:`~sklearn.pipeline.Pipeline`). The latter have
|      parameters of the form ``<component>__<parameter>`` so that it's
|      possible to update each component of a nested object.
|
|      Parameters
|      ----------
|      **params : dict
|          Estimator parameters.
|
|      Returns
|      -------
|      self : estimator instance
|          Estimator instance.
```

[13]:
```
# initialize RandomForestClassifier
ML_algo = SVC(probability=True)

# SVC parameter grid
```

```
hyperparameters = {
    'gamma': [1e-3, 1e-1, 1e1, 1e3, 1e5],
    'C': [1e-1, 1e0, 1e1]
}

plot_clf_contour(hyperparameters, X, y)
```

```
interactive(children=(SelectionSlider(description='gamma', options=(0.001, 0.1,␣
↪10.0, 1000.0, 100000.0), value…
```

```
FigureWidget({
    'data': [{'colorbar': {'title': {'text': 'predicted probability'}},
              'colorsca…
```

ML algo	suitable for large datasets?	behaviour wrt outliers	non-linear?	params to tune	smooth predictions	easy to interpret?
linear regression	yes	linear extrapolation	no	l1 and/or l2 reg	yes	yes
logistic regression	yes	scales with distance from the decision boundary	no	l1 and/or l2 reg	yes	yes
random forest regression	so so	constant	yes	max_features, max_depth	no	so so
random forest classification	so so	step-like, difficult to tell	yes	max_features, max_depth	no	so so
SVM rbf regression	no	non-linear extrapolation	yes	C, gamma	yes	so so
SVM rbf classification	no	50-50	yes	C, gamma	yes	so so

4 Quiz 3

Bias variance trade off

Which gamma value gives the best trade off between high bias and high variance? Work through the steps to answer the question.

- Use random_state = 42 where-ever necessary.
- Split X, y into X_train, X_val, y_train, y_val such that 70% of the points are in train.
- Fit SVC models with C = 1, and gamma = 1e-3, 1e-2, 1e-1, 1e0, 1e1, 1e2, 1e3 on the training set.
- Measure the validation accuracy for each gamma.
- Which gamma value gives the highest validation accuracy?

[ ]:

4.1 Mud card