lecture2 - intro to ML

September 12, 2022

#

DATA1030: Hands-on Data Science

##

Intro to ML

0.1 Mudcard

- **"I was curious if we could go a little more in depth with what constitutes a""good"" dataset to run an ML algorithm on, such as how large of a dataset would be sufficient to ensure that the dataset size itself does not contribute to lower accuracy.**
  - the dataset should have at least a couple of 100 rows (data points) and at least 5-10 features
  - if your dataset is smaller than that, reach out to me
  - the dataset size is very rarely in your control, you just need to work with what you have because it can be very costly to collect more data
  - so focus mostly on the topic of the dataset and find something that interests you
- **I am also curious about resources for webscraping for building a new dataset.**
  - python has a couple of excellent packages for webscraping like Beautiful Soup, Seleneum, the requests package, etc
  - feel free to use any of those
- **Connecting different companies with the machine learning techniques they use.**
  - companies don't usually publicize the techniques they use, it is often considered proprietary information
- **"I just want to know how to use GitHub, because When I was in undergraduate grade, I haven't used it too often.**
  - you can look for online tutorials on how to use github, you can also check out the CCV website, they also offer workshops on git
- **You mentioned how machine learning models have an advantage because traditional code have lots of if statements for the spam filter example. Why are decision trees used? Decision trees can grow to be very messy as well.**
  - yes, they can but that's OK. you don't need to decide on which features to split on, you don't need to code and maintain the if statements yourself
  - clever computer scientists wrote functions for you to take care of it
- **Will all quizzes be group work? Or will some quizzes be individual?**
  - some will be individual

  - there will usually be a group quiz half way through the lecture because students regain some energy and concentration if they move around a bit
  - sitting still for 1.5 hours is not conducive of learning
- **It was a little unclear what it means for ML to not have a "target variable"**
- **If unsupervised learning has no labels, no one variable that you try to predict - then what,Äôs the point of them?**
  - unsupervised learning is usually used for clustering or customer segmentation
- **In the quiz you mentioned that the multiple outcome prediction is classification and continuous would be regression. However, isn't logistic regression a binary predictor?**
- **Muddiest part was the categorical variable versus continuous, given that there are regression analyses of categorical variables.**
  - binary prediction is classification
  - logistic regression is a bit confusing. logistic regression is an ML algorithm to solve classification problems
  - we will cover this but the logic function is applied to the linear regression model to create an output which is between 0 and 1 - a probability that a certain point belongs to class 0
- **How is a neural network defined as "shallow", "medium", and "deep"? I'm assuming this has something to do with the number of layers, but some high-level view on the same would be helpful.**
  - yes, for a fully connected neural network, shallow, medium, and deep refers to the number of layers
  - if it's another type of architecture (like LSTM, CNN), it's usually defined by the number of neurons
- **what is matrix means for X?**
  - matrix is a mathematical term, it is a rectangular array of numbers arranged in rows and columns

0.2 Learning objectives

By the end of the lecture, you will be able to - describe the main goals of the ML pipeline - list the main steps of the ML pipeline - explain the bias-variance trade off

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0.3.1 An ML example

- let's assume you just moved to an island and you never had papayas before but it is common on the island
- what do you do?
- sample some papayas and collect some info
  - for each papaya you try, you collect color, firmness, and whether it tasted good or not
  - classification problem with two features
- once you have enough data, you can train a machine learning model to predict if a new previously unseen papaya is tasty or not based on its color and firmness

0.3.2 Let's define this problem!

- **the learner's input**
  - Domain set $\mathcal{X}$ - a set of objects we wish to label. In the papaya example: the set of all papayas. $\mathcal{X}$ can be in infinite set or a set that's too large to handle on any computer (e.g., all possible 640x480 images with 3 color channels and 256 possible pixel values)
    - domain points are represented by a vector of features e.g., (color, firmness)
    - domain points are also called instances, and $\mathcal{X}$ is also called the instance space
  - Label set $\mathcal{Y}$ - a set of possible labels. In the papaya example: we restrict our label set to {0,1}, 0 meaning the papaya tastes bad, 1 meaning the papaya tastes good.
    - such a label set is categorical, i.e., we have a classification problem at hand
    - the label set can be continuous too, e.g., the real number between 0 and 1, meaning that 0.5 is an OK tasting papaya.
    - the label set can also be probabilistic
      - i.e., two papayas with the same color and firmness can sometimes be tasty and sometimes bad
      - this is quite normal, the features you collect usually do not uniquely determine the label
  - Training data $S = ((x_1, y_1), ..., (x_m, y_m))$ - a finite sequence of pairs from $\mathcal{X}$, $\mathcal{Y}$. This is what the learner has access to.
    - S is also called the training set, and examples in S are also called training examples
    - $X = (x_1, ..., x_m)$ is the feature matrix which is usually a 2D matrix, and $Y = (y_1, ..., y_m)$ is the target variable which is a vector.
- **the learner's output**
  - a prediction rule $h : \mathcal{X} \to \mathcal{Y}$ - this is also called the predictor, a hypothesis, or in the papaya example a classifier. It would be a regressor if $\mathcal{Y}$ was continuous. In the papaya example, the predictor is the rule that our learner will employ to predict if a papaya will be tasty based on color and firmness as he examines them e.g., in the farmer's market or before picking the fruit from the tree.
  - this prediction rule is generated based on S so $h : X \to Y$ is more appropriate
  - once the prediction rule is determined, we can use it to predict the label to previously unseen data

0.4 How is S used?

- in ML, you only use part of S to train the model
- you hold out some fraction of S to calculate what's called the **generalization error**
- it measures how well the model is expected to perform on previously unseen data
- it helps to avoid models that overfit or underfit
  - overfit: model is too complex, it performs very well on the training set but it doesn't generalize to previously unseen data
  - underfit: the model is too simple, it performs poorly on te training set and on previously unseen data as well

0.5 Recap the goals:

- use the training data (X and y) to develop a model which can accurately predict the target variable (y_new') for previously unseen data (X_new)

  - model performance or 'accuracy' is a metric you need to choose to measure model performance and objectively compare various models
- measure the generalization error: measure how well the model is expected to perform on previously unseen data

0.6 Learning objectives

By the end of the lecture, you will be able to - describe the main goals of the ML pipeline - **list the main steps of the ML pipeline** - explain the bias-variance trade off

0.7 The steps

1. Exploratory Data Analysis (EDA): you need to understand your data and verify that it doesn't contain errors - do as much EDA as you can!

2. Split the data into different sets: most often the sets are train, validation, and test (or holdout) - practitioners often make errors in this step! - you can split the data randomly, based on groups, based on time, or any other non-standard way if necessary to answer your ML question

3. Preprocess the data: ML models only work if X and Y are numbers! Some ML models additionally require each feature to have 0 mean and 1 standard deviation (standardized features) - often the original features you get contain strings (for example a gender feature would contain 'male', 'female', 'non-binary', 'unknown') which needs to be transformed into numbers - often the features are not standardized (e.g., age is between 0 and 100) but it needs to be standardized

4. Choose an evaluation metric: depends on the priorities of the stakeholders - often requires quite a bit of thinking and ethical considerations

5. Choose one or more ML techniques: it is highly recommended that you try multiple models - start with simple models like linear or logistic regression - try also more complex models like nearest neighbors, support vector machines, random forest, etc.

6. Tune the hyperparameters of your ML models (aka cross-validation) - ML techniques have hyperparameters that you need to optimize to achieve best performance - for each ML model, decide which parameters to tune and what values to try - loop through each parameter combination - train one model for each parameter combination - evaluate how well the model performs on the validation set - take the parameter combo that gives the best validation score - evaluate that model on the test set to report how well the model is expected to perform on previously unseen data

7. Interpret your model: black boxes are often not useful - check if your model uses features that make sense (excellent tool for debugging) - often model predictions are not enough, you need to be able to explain how the model arrived to a particular prediction (e.g., in health care)

0.8 Quiz

0.9 Learning objectives

By the end of the lecture, you will be able to - describe the main goals of the ML pipeline - list the main steps of the ML pipeline - **explain the bias-variance trade off**

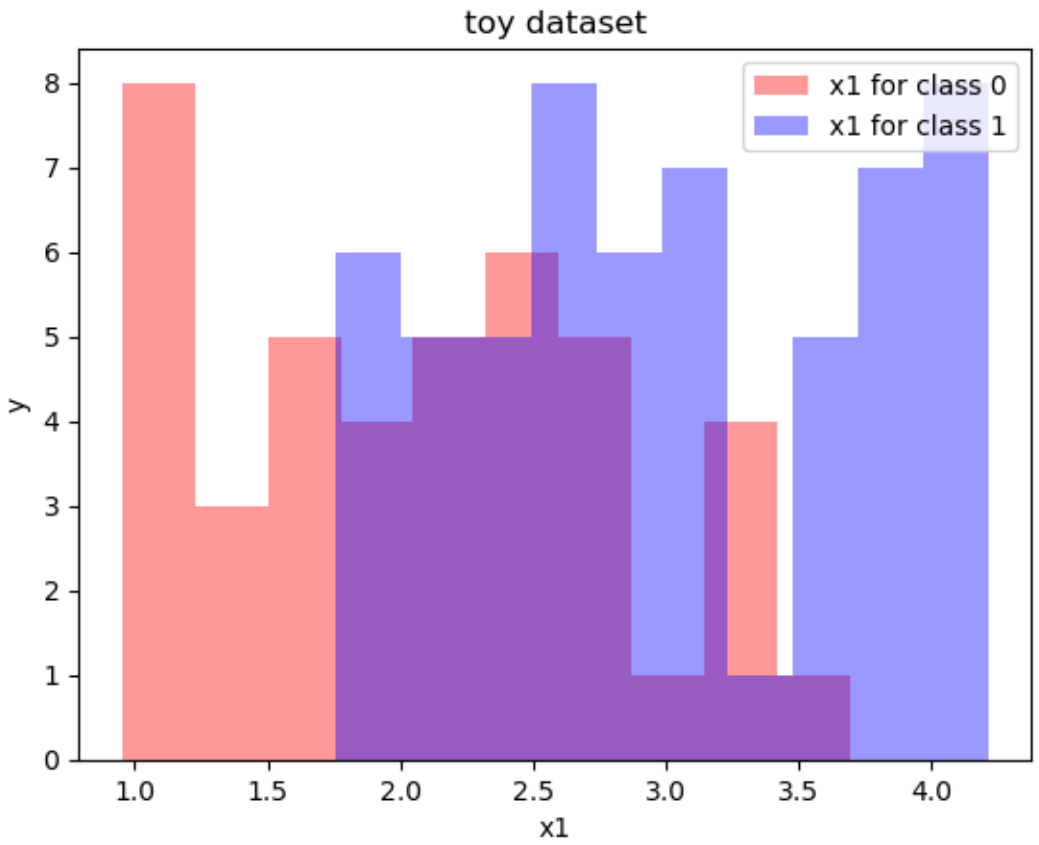
0.10 Bias-variance tradeoff illustrated through a simple ML pipeline

[1]:
```
# import packages

import pandas as pd
import numpy as np
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.metrics import accuracy_score
from sklearn.svm import SVC
from matplotlib import pylab as plt
import matplotlib
from matplotlib.colors import ListedColormap
%matplotlib inline

# scikit-learn code is reproducable is the random seed is fixed.
np.random.seed(2)

# read in the data
# our toy dataset, we don't know how it was generated.
df = pd.read_csv('data/toy_data.csv')

X = df[['x1','x2']].values
y = df['y'].values

print(np.shape(X))
print(np.shape(y))
print(np.unique(y,return_counts=True))
```

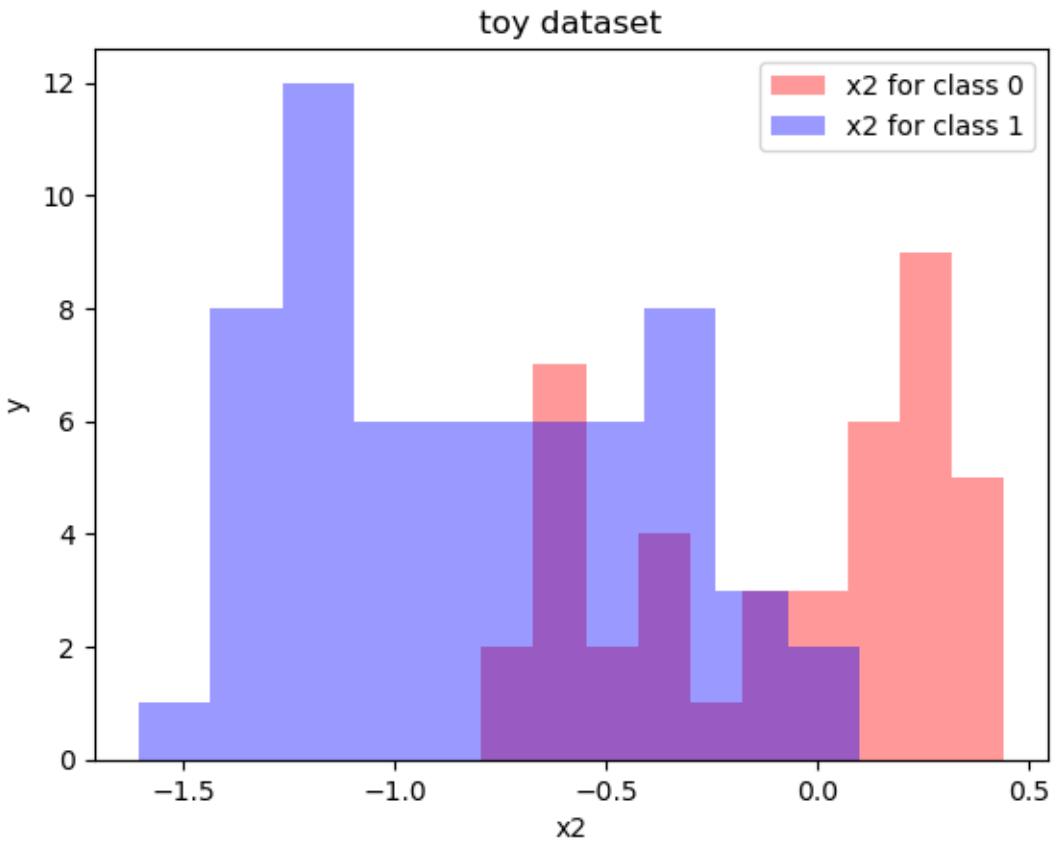
```
(100, 2)
(100,)
(array([0, 1]), array([42, 58]))
```

1. Exploratory Data Analysis (EDA)

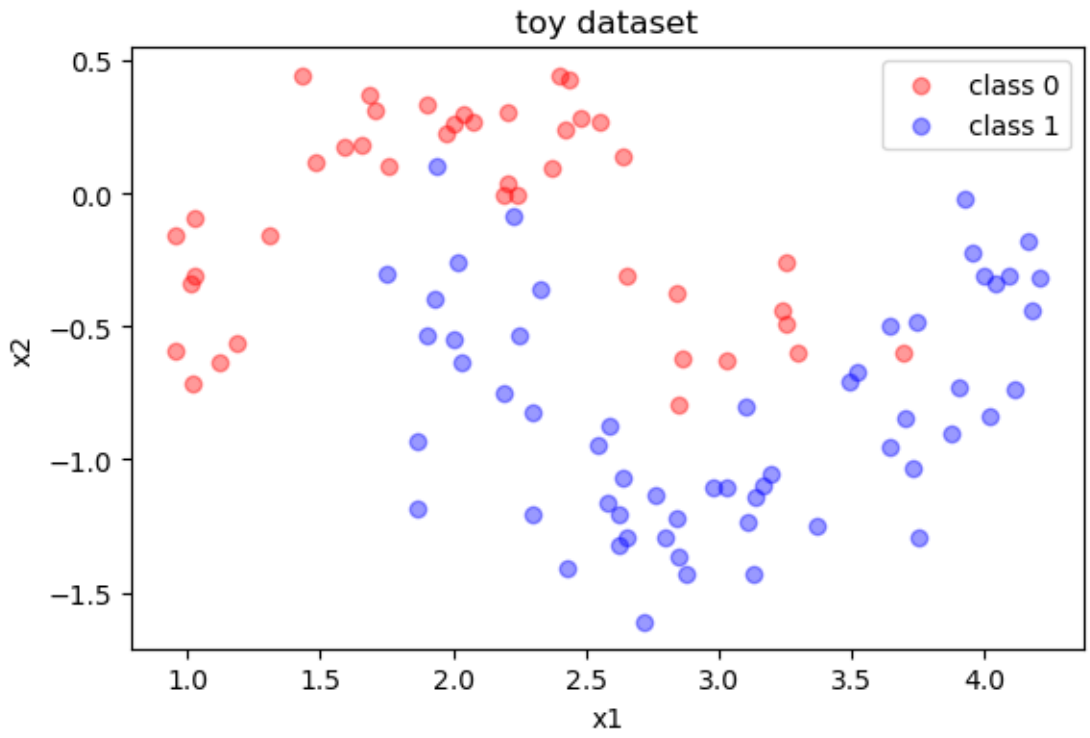
[2]:
```
plt.hist(X[y==0,0],alpha=0.4,color='r',label='x1 for class 0')
plt.hist(X[y==1,0],alpha=0.4,color='b',label='x1 for class 1')
plt.xlabel('x1')
plt.ylabel('y')
plt.title('toy dataset')
plt.legend()
plt.show()
```



[3]:
```
plt.hist(X[y==0,1],alpha=0.4,color='r',label='x2 for class 0')
plt.hist(X[y==1,1],alpha=0.4,color='b',label='x2 for class 1')
plt.xlabel('x2')
plt.ylabel('y')
plt.title('toy dataset')
plt.legend()
plt.show()
```



[4]:
```
plt.scatter(X[y==0,0],X[y==0,1],color='r',label='class 0',alpha=0.4)
plt.scatter(X[y==1,0],X[y==1,1],color='b',label='class 1',alpha=0.4)
plt.xlabel('x1')
plt.ylabel('x2')
plt.title('toy dataset')
plt.gca().set_aspect('equal')
plt.legend()
plt.show()
```



2. Split the data into different sets

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

```
Help on function train_test_split in module sklearn.model_selection._split:

train_test_split(*arrays, test_size=None, train_size=None, random_state=None,
shuffle=True, stratify=None)
    Split arrays or matrices into random train and test subsets.

    Quick utility that wraps input validation and
    ``next(ShuffleSplit().split(X, y))`` and application to input data
    into a single call for splitting (and optionally subsampling) data in a
    oneliner.

    Read more in the :ref:`User Guide <cross_validation>`.

    Parameters
    ----------
    *arrays : sequence of indexables with same length / shape[0]
        Allowed inputs are lists, numpy arrays, scipy-sparse
        matrices or pandas dataframes.

    test_size : float or int, default=None
```

```
    If float, should be between 0.0 and 1.0 and represent the proportion
    of the dataset to include in the test split. If int, represents the
    absolute number of test samples. If None, the value is set to the
    complement of the train size. If ``train_size`` is also None, it will
    be set to 0.25.

train_size : float or int, default=None
    If float, should be between 0.0 and 1.0 and represent the
    proportion of the dataset to include in the train split. If
    int, represents the absolute number of train samples. If None,
    the value is automatically set to the complement of the test size.

random_state : int, RandomState instance or None, default=None
    Controls the shuffling applied to the data before applying the split.
    Pass an int for reproducible output across multiple function calls.
    See :term:`Glossary <random_state>`.

shuffle : bool, default=True
    Whether or not to shuffle the data before splitting. If shuffle=False
    then stratify must be None.

stratify : array-like, default=None
    If not None, data is split in a stratified fashion, using this as
    the class labels.
    Read more in the :ref:`User Guide <stratification>`.

Returns
-------
splitting : list, length=2 * len(arrays)
    List containing train-test split of inputs.

    .. versionadded:: 0.16
        If the input is sparse, the output will be a
        ``scipy.sparse.csr_matrix``. Else, output type is the same as the
        input type.

Examples
--------
>>> import numpy as np
>>> from sklearn.model_selection import train_test_split
>>> X, y = np.arange(10).reshape((5, 2)), range(5)
>>> X
array([[0, 1],
       [2, 3],
       [4, 5],
       [6, 7],
       [8, 9]])
>>> list(y)
```

```
[0, 1, 2, 3, 4]

>>> X_train, X_test, y_train, y_test = train_test_split(
…     X, y, test_size=0.33, random_state=42)
…
>>> X_train
array([[4, 5],
       [0, 1],
       [6, 7]])
>>> y_train
[2, 0, 3]
>>> X_test
array([[2, 3],
       [8, 9]])
>>> y_test
[1, 4]

>>> train_test_split(y, shuffle=False)
[[0, 1, 2], [3, 4]]
```

[6]:
```
X_train, X_other, y_train, y_other = train_test_split(X,y,test_size=0.4)
print(np.shape(X_other),np.shape(y_other))
print('train:',np.shape(X_train),np.shape(y_train))

X_val, X_test, y_val, y_test = train_test_split(X_other,y_other,test_size=0.5)
print('val:',np.shape(X_val),np.shape(y_val))
print('test:',np.shape(X_test),np.shape(y_test))
```

```
(40, 2) (40,)
train: (60, 2) (60,)
val: (20, 2) (20,)
test: (20, 2) (20,)
```

3. Preprocess the data

[7]:
```
help(StandardScaler)
```

```
Help on class StandardScaler in module sklearn.preprocessing._data:

class StandardScaler(sklearn.base._OneToOneFeatureMixin,
sklearn.base.TransformerMixin, sklearn.base.BaseEstimator)
 |  StandardScaler(*, copy=True, with_mean=True, with_std=True)
 |
 |  Standardize features by removing the mean and scaling to unit variance.
 |
 |  The standard score of a sample `x` is calculated as:
 |
 |      z = (x - u) / s
```

```
|
|  where `u` is the mean of the training samples or zero if `with_mean=False`,
|  and `s` is the standard deviation of the training samples or one if
|  `with_std=False`.
|
|  Centering and scaling happen independently on each feature by computing
|  the relevant statistics on the samples in the training set. Mean and
|  standard deviation are then stored to be used on later data using
|  :meth:`transform`.
|
|  Standardization of a dataset is a common requirement for many
|  machine learning estimators: they might behave badly if the
|  individual features do not more or less look like standard normally
|  distributed data (e.g. Gaussian with 0 mean and unit variance).
|
|  For instance many elements used in the objective function of
|  a learning algorithm (such as the RBF kernel of Support Vector
|  Machines or the L1 and L2 regularizers of linear models) assume that
|  all features are centered around 0 and have variance in the same
|  order. If a feature has a variance that is orders of magnitude larger
|  than others, it might dominate the objective function and make the
|  estimator unable to learn from other features correctly as expected.
|
|  This scaler can also be applied to sparse CSR or CSC matrices by passing
|  `with_mean=False` to avoid breaking the sparsity structure of the data.
|
|  Read more in the :ref:`User Guide <preprocessing_scaler>`.
|
|  Parameters
|  ----------
|  copy : bool, default=True
|      If False, try to avoid a copy and do inplace scaling instead.
|      This is not guaranteed to always work inplace; e.g. if the data is
|      not a NumPy array or scipy.sparse CSR matrix, a copy may still be
|      returned.
|
|  with_mean : bool, default=True
|      If True, center the data before scaling.
|      This does not work (and will raise an exception) when attempted on
|      sparse matrices, because centering them entails building a dense
|      matrix which in common use cases is likely to be too large to fit in
|      memory.
|
|  with_std : bool, default=True
|      If True, scale the data to unit variance (or equivalently,
|      unit standard deviation).
|
|  Attributes
```

```
|  ----------
|  scale_ : ndarray of shape (n_features,) or None
|      Per feature relative scaling of the data to achieve zero mean and unit
|      variance. Generally this is calculated using `np.sqrt(var_)`. If a
|      variance is zero, we can't achieve unit variance, and the data is left
|      as-is, giving a scaling factor of 1. `scale_` is equal to `None`
|      when `with_std=False`.
|
|      .. versionadded:: 0.17
|         *scale_*
|
|  mean_ : ndarray of shape (n_features,) or None
|      The mean value for each feature in the training set.
|      Equal to ``None`` when ``with_mean=False``.
|
|  var_ : ndarray of shape (n_features,) or None
|      The variance for each feature in the training set. Used to compute
|      `scale_`. Equal to ``None`` when ``with_std=False``.
|
|  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_samples_seen_ : int or ndarray of shape (n_features,)
|      The number of samples processed by the estimator for each feature.
|      If there are no missing samples, the ``n_samples_seen`` will be an
|      integer, otherwise it will be an array of dtype int. If
|      `sample_weights` are used it will be a float (if no missing data)
|      or an array of dtype float that sums the weights seen so far.
|      Will be reset on new calls to fit, but increments across
|      ``partial_fit`` calls.
|
|  See Also
|  --------
|  scale : Equivalent function without the estimator API.
|
|  :class:`~sklearn.decomposition.PCA` : Further removes the linear
|      correlation across features with 'whiten=True'.
|
|  Notes
|  -----
```

```
|  NaNs are treated as missing values: disregarded in fit, and maintained in
|  transform.
|
|  We use a biased estimator for the standard deviation, equivalent to
|  `numpy.std(x, ddof=0)`. Note that the choice of `ddof` is unlikely to
|  affect model performance.
|
|  For a comparison of the different scalers, transformers, and normalizers,
|  see :ref:`examples/preprocessing/plot_all_scaling.py
|  <sphx_glr_auto_examples_preprocessing_plot_all_scaling.py>`.
|
|  Examples
|  --------
|  >>> from sklearn.preprocessing import StandardScaler
|  >>> data = [[0, 0], [0, 0], [1, 1], [1, 1]]
|  >>> scaler = StandardScaler()
|  >>> print(scaler.fit(data))
|  StandardScaler()
|  >>> print(scaler.mean_)
|  [0.5 0.5]
|  >>> print(scaler.transform(data))
|  [[-1. -1.]
|   [-1. -1.]
|   [ 1.  1.]
|   [ 1.  1.]]
|  >>> print(scaler.transform([[2, 2]]))
|  [[3. 3.]]
|
|  Method resolution order:
|      StandardScaler
|      sklearn.base._OneToOneFeatureMixin
|      sklearn.base.TransformerMixin
|      sklearn.base.BaseEstimator
|      builtins.object
|
|  Methods defined here:
|
|  __init__(self, *, copy=True, with_mean=True, with_std=True)
|      Initialize self.  See help(type(self)) for accurate signature.
|
|  fit(self, X, y=None, sample_weight=None)
|      Compute the mean and std to be used for later scaling.
|
|      Parameters
|      ----------
|      X : {array-like, sparse matrix} of shape (n_samples, n_features)
|          The data used to compute the mean and standard deviation
|          used for later scaling along the features axis.
```

```
|
|      y : None
|          Ignored.
|
|      sample_weight : array-like of shape (n_samples,), default=None
|          Individual weights for each sample.
|
|          .. versionadded:: 0.24
|             parameter *sample_weight* support to StandardScaler.
|
|      Returns
|      -------
|      self : object
|          Fitted scaler.
|
|  inverse_transform(self, X, copy=None)
|      Scale back the data to the original representation.
|
|      Parameters
|      ----------
|      X : {array-like, sparse matrix} of shape (n_samples, n_features)
|          The data used to scale along the features axis.
|      copy : bool, default=None
|          Copy the input X or not.
|
|      Returns
|      -------
|      X_tr : {ndarray, sparse matrix} of shape (n_samples, n_features)
|          Transformed array.
|
|  partial_fit(self, X, y=None, sample_weight=None)
|      Online computation of mean and std on X for later scaling.
|
|      All of X is processed as a single batch. This is intended for cases
|      when :meth:`fit` is not feasible due to very large number of
|      `n_samples` or because X is read from a continuous stream.
|
|      The algorithm for incremental mean and std is given in Equation 1.5a,b
|      in Chan, Tony F., Gene H. Golub, and Randall J. LeVeque. "Algorithms
|      for computing the sample variance: Analysis and recommendations."
|      The American Statistician 37.3 (1983): 242-247:
|
|      Parameters
|      ----------
|      X : {array-like, sparse matrix} of shape (n_samples, n_features)
|          The data used to compute the mean and standard deviation
|          used for later scaling along the features axis.
|
```

```
|      y : None
|          Ignored.
|
|      sample_weight : array-like of shape (n_samples,), default=None
|          Individual weights for each sample.
|
|          .. versionadded:: 0.24
|             parameter *sample_weight* support to StandardScaler.
|
|      Returns
|      -------
|      self : object
|          Fitted scaler.
|
|  transform(self, X, copy=None)
|      Perform standardization by centering and scaling.
|
|      Parameters
|      ----------
|      X : {array-like, sparse matrix of shape (n_samples, n_features)
|          The data used to scale along the features axis.
|      copy : bool, default=None
|          Copy the input X or not.
|
|      Returns
|      -------
|      X_tr : {ndarray, sparse matrix} of shape (n_samples, n_features)
|          Transformed array.
|
|  ----------------------------------------------------------------------
|  Methods inherited from sklearn.base._OneToOneFeatureMixin:
|
|  get_feature_names_out(self, input_features=None)
|      Get output feature names for transformation.
|
|      Parameters
|      ----------
|      input_features : array-like of str or None, default=None
|          Input features.
|
|          - If `input_features` is `None`, then `feature_names_in_` is
|            used as feature names in. If `feature_names_in_` is not defined,
|            then the following input feature names are generated:
|            `["x0", "x1", …, "x(n_features_in_ - 1)"]`.
|          - If `input_features` is an array-like, then `input_features` must
|            match `feature_names_in_` if `feature_names_in_` is defined.
|
|      Returns
```

```
 |      -------
 |      feature_names_out : ndarray of str objects
 |          Same as input features.
 |
 |  ----------------------------------------------------------------------
 |  Data descriptors inherited from sklearn.base._OneToOneFeatureMixin:
 |
 |  __dict__
 |      dictionary for instance variables (if defined)
 |
 |  __weakref__
 |      list of weak references to the object (if defined)
 |
 |  ----------------------------------------------------------------------
 |  Methods inherited from sklearn.base.TransformerMixin:
 |
 |  fit_transform(self, X, y=None, **fit_params)
 |      Fit to data, then transform it.
 |
 |      Fits transformer to `X` and `y` with optional parameters `fit_params`
 |      and returns a transformed version of `X`.
 |
 |      Parameters
 |      ----------
 |      X : array-like of shape (n_samples, n_features)
 |          Input samples.
 |
 |      y :  array-like of shape (n_samples,) or (n_samples, n_outputs),
default=None
 |          Target values (None for unsupervised transformations).
 |
 |      **fit_params : dict
 |          Additional fit parameters.
 |
 |      Returns
 |      -------
 |      X_new : ndarray array of shape (n_samples, n_features_new)
 |          Transformed array.
 |
 |  ----------------------------------------------------------------------
 |  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.
```

[8]:
```
scaler = StandardScaler().fit(X_train)
# the scaler object contains the feature means and variations in the training␣
 ↪set
print(scaler.mean_)
print(scaler.var_)

# the scaler is used to transform the sets
X_train_prep = scaler.transform(X_train)
X_val_prep = scaler.transform(X_val)
X_test_prep = scaler.transform(X_test)
```

```
[ 2.61729782 -0.55283401]
[0.74350517 0.32379089]
```

4. Choose an evaluation metric

[9]:
```
help(accuracy_score)
```

```
Help on function accuracy_score in module sklearn.metrics._classification:

accuracy_score(y_true, y_pred, *, normalize=True, sample_weight=None)
    Accuracy classification score.

    In multilabel classification, this function computes subset accuracy:
    the set of labels predicted for a sample must *exactly* match the
    corresponding set of labels in y_true.

    Read more in the :ref:`User Guide <accuracy_score>`.

    Parameters
    ----------
    y_true : 1d array-like, or label indicator array / sparse matrix
        Ground truth (correct) labels.

    y_pred : 1d array-like, or label indicator array / sparse matrix
        Predicted labels, as returned by a classifier.

    normalize : bool, default=True
        If ``False``, return the number of correctly classified samples.
        Otherwise, return the fraction of correctly classified samples.

    sample_weight : array-like of shape (n_samples,), default=None
        Sample weights.

    Returns
    -------
    score : float
        If ``normalize == True``, return the fraction of correctly
        classified samples (float), else returns the number of correctly
        classified samples (int).

        The best performance is 1 with ``normalize == True`` and the number
        of samples with ``normalize == False``.

    See Also
    --------
    balanced_accuracy_score : Compute the balanced accuracy to deal with
        imbalanced datasets.
    jaccard_score : Compute the Jaccard similarity coefficient score.
    hamming_loss : Compute the average Hamming loss or Hamming distance between
        two sets of samples.
    zero_one_loss : Compute the Zero-one classification loss. By default, the
```

```
    function will return the percentage of imperfectly predicted subsets.

    Notes
    -----
    In binary classification, this function is equal to the `jaccard_score`
    function.

    Examples
    --------
    >>> from sklearn.metrics import accuracy_score
    >>> y_pred = [0, 2, 1, 3]
    >>> y_true = [0, 1, 2, 3]
    >>> accuracy_score(y_true, y_pred)
    0.5
    >>> accuracy_score(y_true, y_pred, normalize=False)
    2

    In the multilabel case with binary label indicators:

    >>> import numpy as np
    >>> accuracy_score(np.array([[0, 1], [1, 1]]), np.ones((2, 2)))
    0.5
```

0.11 Quiz

5. Choose one or more ML techniques

[10]:
```
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()
 |
 |  ----------------------------------------------------------------------
 |  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.
```

6. Tune the hyperparameters of your ML models (aka cross-validation)

[11]:
```
Cs = np.logspace(-1,3,13)
print(Cs)
train_scores = []
```

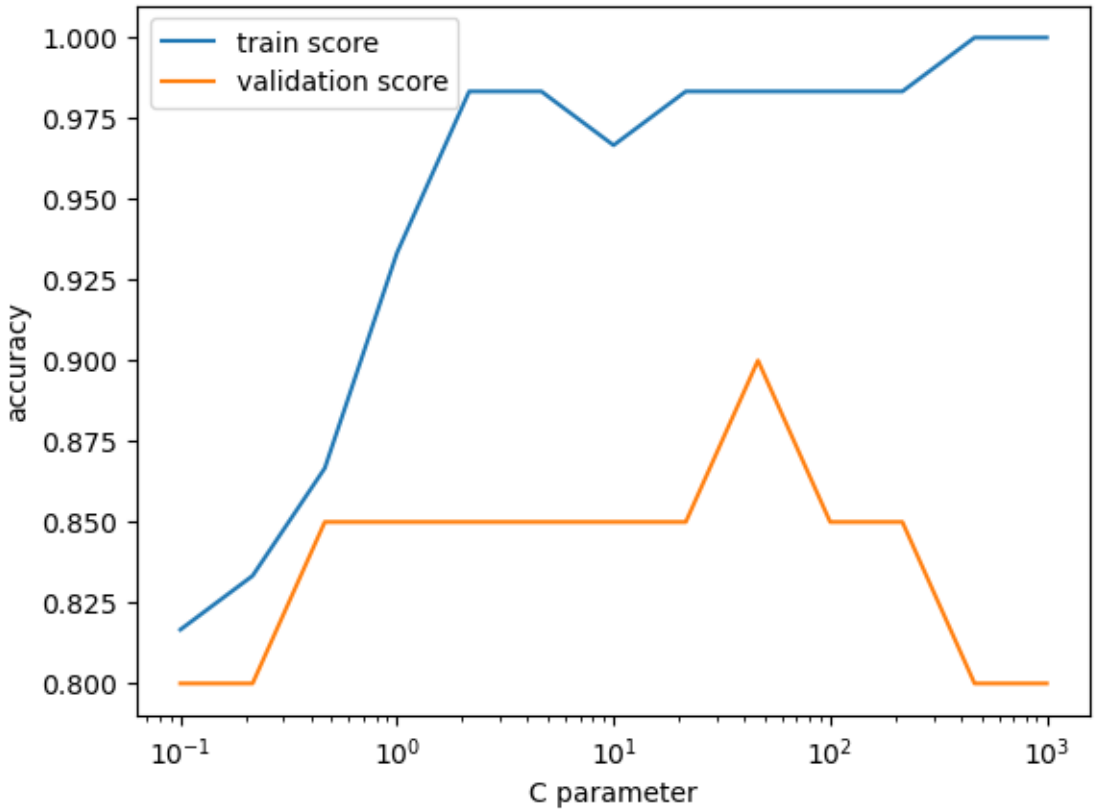
```
validation_scores = []
models = []
for C in Cs:
    classifier = SVC(kernel='rbf',C = C, probability=True) # this is our␣
 ↪classifier
    classifier.fit(X_train_prep,y_train) # the model is fitted to the training␣
 ↪data

    y_train_pred = classifier.predict(X_train_prep)
    train_accuracy = accuracy_score(y_train,y_train_pred) # calculate the␣
 ↪validation accuracy
    train_scores.append(train_accuracy)

    y_val_pred = classifier.predict(X_val_prep) # predict the validation set
    validation_accuracy = accuracy_score(y_val,y_val_pred) # calculate the␣
 ↪validation accuracy
    validation_scores.append(validation_accuracy)

    models.append(classifier)
    print(C, train_accuracy, validation_accuracy)
```

```
[1.00000000e-01 2.15443469e-01 4.64158883e-01 1.00000000e+00
 2.15443469e+00 4.64158883e+00 1.00000000e+01 2.15443469e+01
 4.64158883e+01 1.00000000e+02 2.15443469e+02 4.64158883e+02
 1.00000000e+03]
0.1 0.8166666666666667 0.8
0.21544346900318834 0.8333333333333334 0.8
0.46415888336127786 0.8666666666666667 0.85
1.0 0.9333333333333333 0.85
2.1544346900318834 0.9833333333333333 0.85
4.6415888336127775 0.9833333333333333 0.85
10.0 0.9666666666666667 0.85
21.54434690031882 0.9833333333333333 0.85
46.41588833612777 0.9833333333333333 0.9
100.0 0.9833333333333333 0.85
215.44346900318823 0.9833333333333333 0.85
464.15888336127773 1.0 0.8
1000.0 1.0 0.8
```

0.12 The bias - variance tradeoff

[12]:
```
plt.plot(Cs,train_scores,label='train score')
plt.plot(Cs,validation_scores,label='validation score')
plt.semilogx()
plt.legend()
plt.xlabel('C parameter')
plt.ylabel('accuracy')
```

```
plt.show()
```



- **high bias model** (aka underfitting)
  - it performs poorly on the train and validation sets
  - small C values in the example above
- **high variance model** (aka overfitting)
  - it performs very well on the training set but it performs poorly on the validation set
  - high C
- the goal of the parameter tuning is to find the balance between bias and variance
  - usually the best model is the one with the best validation score
  - C = 46 in our case

1 Quiz

1.0.1 How does the best model perform on the test set?

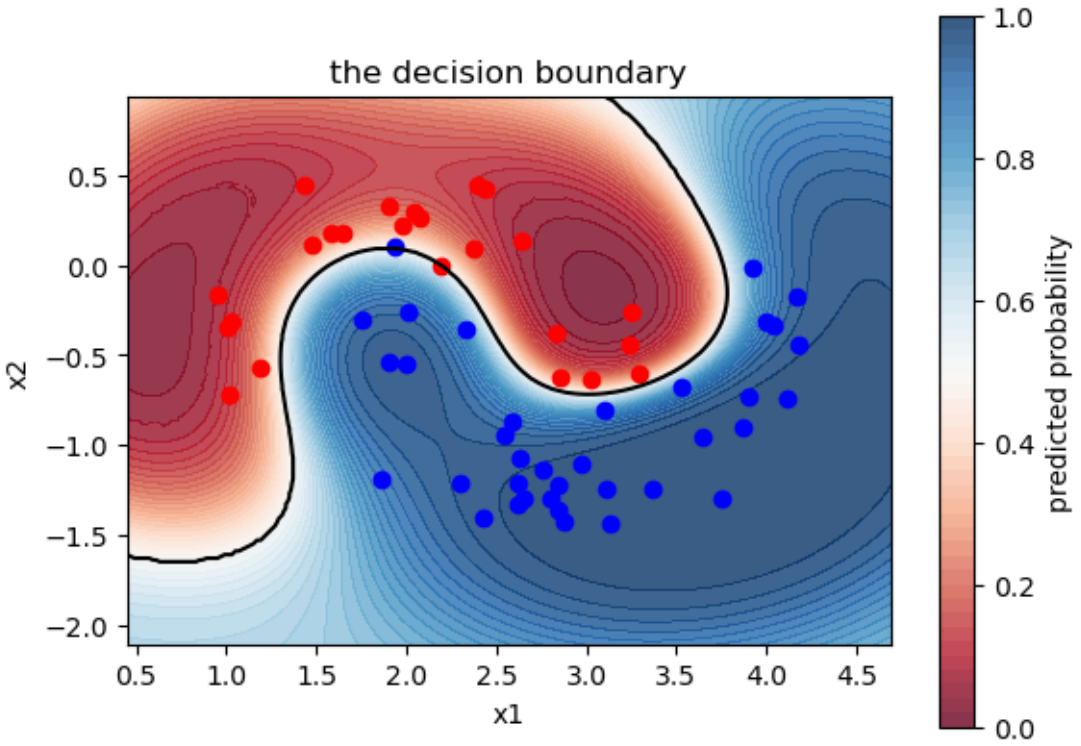
- this score tells us how well the model generalizes to previously unseen data because the test set was not touched before
- usually it is close to the best validation score

[13]:
```
y_test_pred = models[-5].predict(X_test_prep)
print(accuracy_score(y_test, y_test_pred))
```

```
0.95
```

7. Interpret your model - with two features, this is easy - plot the decision boundary and probabilities

[14]:
```
# Plot the decision boundary. For that, we will assign a color to each
# point in the mesh [x_min, m_max]x[y_min, y_max].

cm = plt.cm.RdBu
cm_bright = ListedColormap(['#FF0000', '#0000FF'])
h = .02  # step size in the mesh
x_min, x_max = X[:, 0].min() - .5, X[:, 0].max() + .5
y_min, y_max = X[:, 1].min() - .5, X[:, 1].max() + .5
xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                     np.arange(y_min, y_max, h))

# use the best model with C = 46
classifier = models[-5]
# scale the data before predicting! this is very important!
Z = classifier.predict_proba(scaler.transform(np.c_[xx.ravel(), yy.ravel()]))[:
 ↪, 1]

# Put the result into a color plot
Z = Z.reshape(xx.shape)
plt.contour(xx, yy, Z,vmin=0,vmax=1,levels=[0.5],colors=['k'])
plt.contourf(xx, yy, Z, cmap=cm, alpha=.8,vmin=0,vmax=1,levels=np.arange(0,1.
 ↪02,0.02))
plt.colorbar(ticks=[0,0.2,0.4,0.6,0.8,1],label='predicted probability')
plt.scatter(X_train[y_train==0,0],X_train[y_train==0,1],color='r',label='class␣
 ↪0')
plt.scatter(X_train[y_train==1,0],X_train[y_train==1,1],color='b',label='class␣
 ↪1')
plt.xlabel('x1')
plt.ylabel('x2')
plt.title('the decision boundary')
plt.gca().set_aspect('equal')
plt.savefig('figures/decision_boundary.jpg',dpi=150)
plt.show()
```


the decision boundary
x2
x1
predicted probability
0.5
0.0
−0.5
−1.0
−1.5
−2.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
1.0
0.8
0.6
0.4
0.2
0.0

2 Mud card

[ ]: