1.4. Support Vector Machines

Support vector machines (SVMs) are a set of supervised learning methods used for classification, regression and outliers detection.

The advantages of support vector machines are:

- Effective in high dimensional spaces.
- Still effective in cases where number of dimensions is greater than the number of samples.
- Uses a subset of training points in the decision function (called support vectors), so it is also memory efficient.
- Versatile: different Kernel functions can be specified for the decision function. Common kernels are provided, but it is also possible to specify custom kernels.

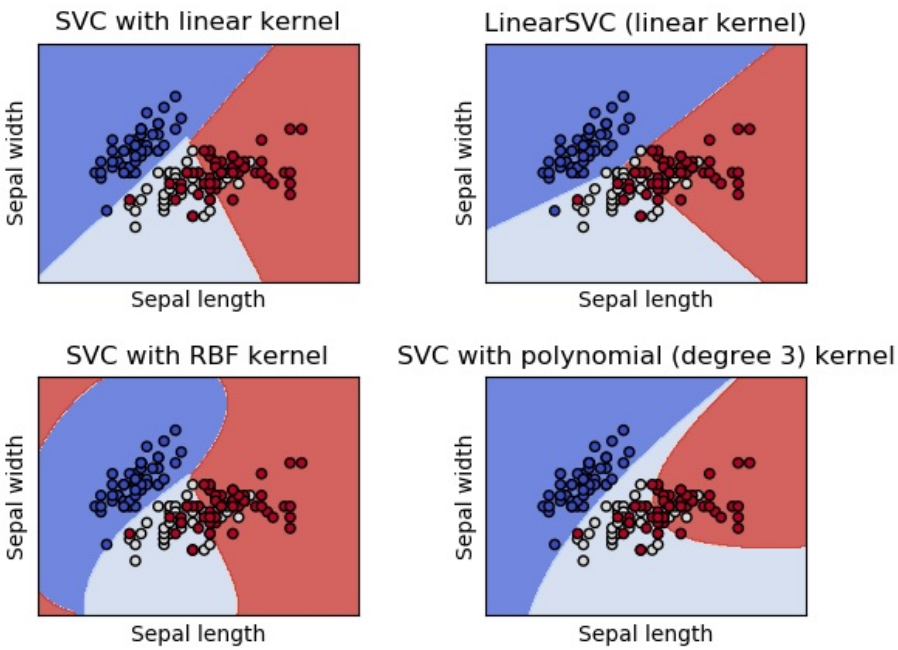
The disadvantages of support vector machines include:

- If the number of features is much greater than the number of samples, avoid over-fitting in choosing Kernel functions and regularization term is crucial.
- SVMs do not directly provide probability estimates, these are calculated using an expensive five-fold cross-validation (see Scores and probabilities, below).

The support vector machines in scikit-learn support both dense (`numpy.ndarray` and convertible to that by `numpy.asarray`) and sparse (any `scipy.sparse`) sample vectors as input. However, to use an SVM to make predictions for sparse data, it must have been fit on such data. For optimal performance, use C-ordered `numpy.ndarray` (dense) or `scipy.sparse.csr_matrix` (sparse) with `dtype=float64`.

1.4.1. Classification

`SVC`, **`NuSVC`** and **`LinearSVC`** are classes capable of performing multi-class classification on a dataset.



`SVC` and **`NuSVC`** are similar methods, but accept slightly different sets of parameters and have different mathematical formulations (see section Mathematical formulation). On the other hand, **`LinearSVC`** is another implementation of Support Vector Classification for the case of a linear kernel. Note that **`LinearSVC`** does not accept keyword `kernel`, as this is assumed to be linear. It also lacks some of the members of **`SVC`** and **`NuSVC`**, like `support_`.

As other classifiers, **`SVC`**, **`NuSVC`** and **`LinearSVC`** take as input two arrays: an array X of size `[n_samples, n_features]` holding the training samples, and an array y of class labels (strings or integers), size `[n_samples]`:

```
>>> from sklearn import svm
>>> X = [[0, 0], [1, 1]]
>>> y = [0, 1]
>>> clf = svm.SVC()
>>> clf.fit(X, y)
SVC()
```

After being fitted, the model can then be used to predict new values:

```
>>> clf.predict([[2., 2.]])
array([1])
```

SVMs decision function depends on some subset of the training data, called the support vectors. Some properties of these support vectors can be found in members `support_vectors_`, `support_` and `n_support`:

```
>>> # get support vectors
>>> clf.support_vectors_
array([[0., 0.],
       [1., 1.]])
>>> # get indices of support vectors
>>> clf.support_
array([0, 1]...)
>>> # get number of support vectors for each class
>>> clf.n_support_
array([1, 1]...)
```

1.4.1.1. Multi-class classification

SVC and **NuSVC** implement the "one-against-one" approach (Knerr et al., 1990) for multi- class classification. If `n_class` is the number of classes, then `n_class * (n_class - 1) / 2` classifiers are constructed and each one trains data from two classes. To provide a consistent interface with other classifiers, the `decision_function_shape` option allows to monotically transform the results of the "one-against-one" classifiers to a decision function of shape `(n_samples, n_classes)`.

```
>>> X = [[0], [1], [2], [3]]
>>> Y = [0, 1, 2, 3]
>>> clf = svm.SVC(decision_function_shape='ovo')
>>> clf.fit(X, Y)
SVC(decision_function_shape='ovo')
>>> dec = clf.decision_function([[1]])
>>> dec.shape[1] # 4 classes: 4*3/2 = 6
6
>>> clf.decision_function_shape = "ovr"
>>> dec = clf.decision_function([[1]])
>>> dec.shape[1] # 4 classes
4
```

On the other hand, **LinearSVC** implements "one-vs-the-rest" multi-class strategy, thus training n_class models. If there are only two classes, only one model is trained:

```
>>> lin_clf = svm.LinearSVC()
>>> lin_clf.fit(X, Y)
LinearSVC()
>>> dec = lin_clf.decision_function([[1]])
>>> dec.shape[1]
4
```

See Mathematical formulation for a complete description of the decision function.

Note that the **LinearSVC** also implements an alternative multi-class strategy, the so-called multi-class SVM formulated by Crammer and Singer, by using the option `multi_class='crammer_singer'`. This method is consistent, which is not true for one-vs-rest classification. In practice, one-vs-rest classification is usually preferred, since the results are mostly similar, but the runtime is significantly less.

For "one-vs-rest" **LinearSVC** the attributes `coef_` and `intercept_` have the shape `[n_class, n_features]` and `[n_class]` respectively. Each row of the coefficients corresponds to one of the `n_class` many "one-vs-rest" classifiers and similar for the intercepts, in the order of the "one" class.

In the case of "one-vs-one" **SVC**, the layout of the attributes is a little more involved. In the case of having a linear kernel, the attributes `coef_` and `intercept_` have the shape `[n_class * (n_class - 1) / 2, n_features]` and `[n_class * (n_class - 1) / 2]` respectively. This is similar to the layout for **LinearSVC** described above, with each row now corresponding to a binary classifier. The order for classes 0 to n is "0 vs 1", "0 vs 2" , ... "0 vs n", "1 vs 2", "1 vs 3", "1 vs n", . . . "n-1 vs n".

The shape of `dual_coef_` is `[n_class-1, n_SV]` with a somewhat hard to grasp layout. The columns correspond to the support vectors involved in any of the `n_class * (n_class - 1) / 2` "one-vs-one" classifiers. Each of the support vectors is used in `n_class - 1` classifiers. The `n_class - 1` entries in each row correspond to the dual coefficients for these classifiers.

This might be made more clear by an example:

Consider a three class problem with class 0 having three support vectors v_0^0, v_0^1, v_0^2 and class 1 and 2 having two support vectors v_1^0, v_1^1 and v_2^0, v_2^1 respectively. For each support vector v_i^j, there are two dual coefficients. Let's call the coefficient of support vector v_i^j in the classifier between classes i and k $\alpha_{i,k}^j$. Then `dual_coef_` looks like this:

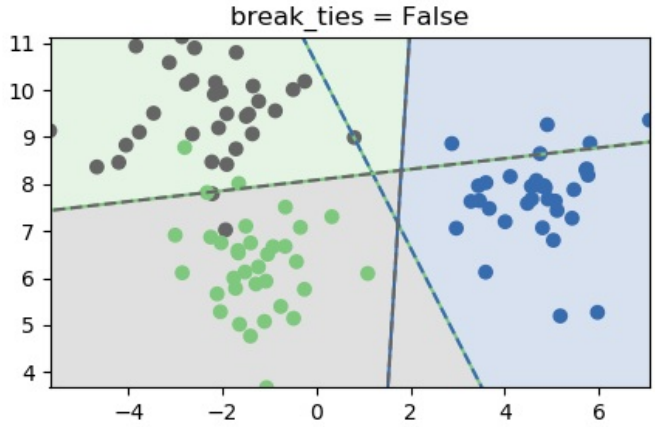
$\alpha_{0,1}^0$	$\alpha_{0,2}^0$	Coefficients for SVs of class 0
$\alpha_{0,1}^1$	$\alpha_{0,2}^1$	
$\alpha_{0,1}^2$	$\alpha_{0,2}^2$	
$\alpha_{1,0}^0$	$\alpha_{1,2}^0$	Coefficients for SVs of class 1
$\alpha_{1,0}^1$	$\alpha_{1,2}^1$	
$\alpha_{2,0}^0$	$\alpha_{2,1}^0$	Coefficients for SVs of class 2
$\alpha_{2,0}^1$	$\alpha_{2,1}^1$	

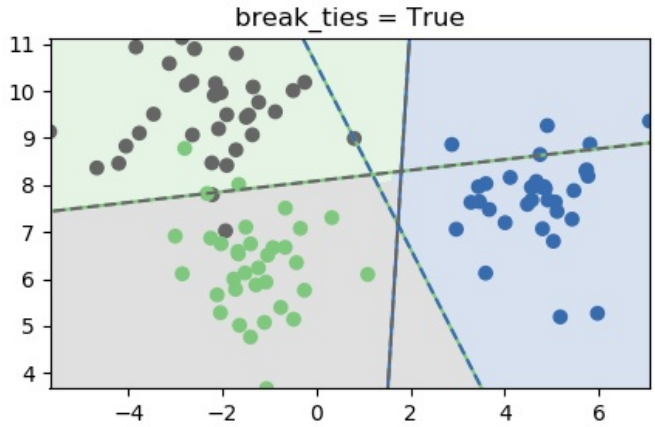
1.4.1.2. Scores and probabilities

The `decision_function` method of **`SVC`** and **`NuSVC`** gives per-class scores for each sample (or a single score per sample in the binary case). When the constructor option `probability` is set to `True`, class membership probability estimates (from the methods `predict_proba` and `predict_log_proba`) are enabled. In the binary case, the probabilities are calibrated using Platt scaling: logistic regression on the SVM's scores, fit by an additional cross-validation on the training data. In the multiclass case, this is extended as per Wu et al. (2004).

Needless to say, the cross-validation involved in Platt scaling is an expensive operation for large datasets. In addition, the probability estimates may be inconsistent with the scores, in the sense that the "argmax" of the scores may not be the argmax of the probabilities. (E.g., in binary classification, a sample may be labeled by `predict` as belonging to a class that has probability <½ according to `predict_proba`.) Platt's method is also known to have theoretical issues. If confidence scores are required, but these do not have to be probabilities, then it is advisable to set `probability=False` and use `decision_function` instead of `predict_proba`.

Please note that when `decision_function_shape='ovr'` and `n_classes > 2`, unlike `decision_function`, the `predict` method does not try to break ties by default. You can set `break_ties=True` for the output of `predict` to be the same as `np.argmax(clf.decision_function(...), axis=1)`, otherwise the first class among the tied classes will always be returned; but have in mind that it comes with a computational cost.





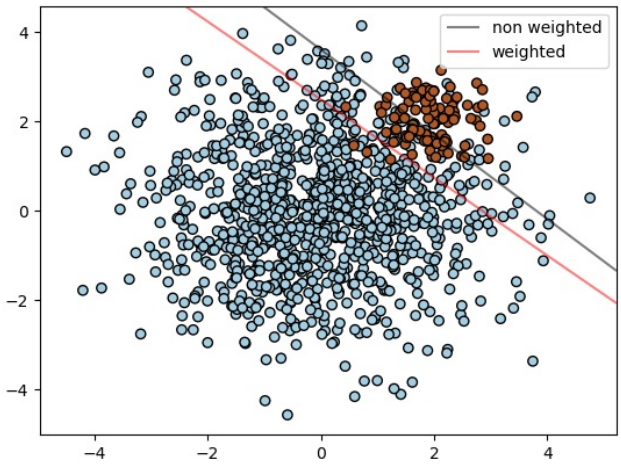
References:

- Wu, Lin and Weng, "Probability estimates for multi-class classification by pairwise coupling", JMLR 5:975-1005, 2004.
- Platt "Probabilistic outputs for SVMs and comparisons to regularized likelihood methods".

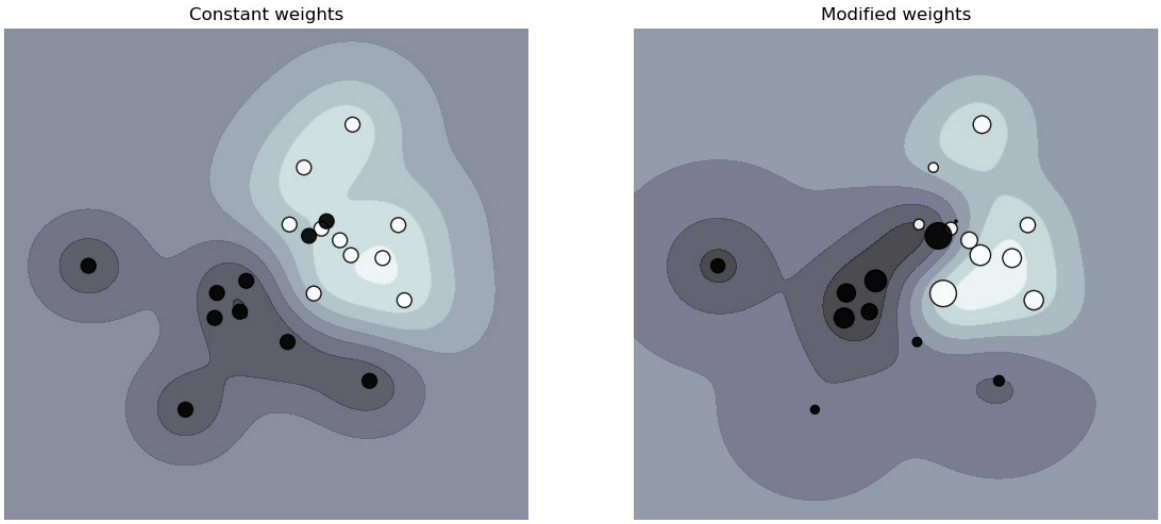
1.4.1.3. Unbalanced problems

In problems where it is desired to give more importance to certain classes or certain individual samples keywords `class_weight` and `sample_weight` can be used.

SVC (but not **NuSVC**) implement a keyword `class_weight` in the `fit` method. It's a dictionary of the form `{class_label : value}`, where value is a floating point number > 0 that sets the parameter `C` of class `class_label` to `C * value`.



SVC, **NuSVC**, **SVR**, **NuSVR**, **LinearSVC**, **LinearSVR** and **OneClassSVM** implement also weights for individual samples in method `fit` through keyword `sample_weight`. Similar to `class_weight`, these set the parameter `C` for the i-th example to `C * sample_weight[i]`.



Examples:

- Plot different SVM classifiers in the iris dataset,
- SVM: Maximum margin separating hyperplane,
- SVM: Separating hyperplane for unbalanced classes
- SVM-Anova: SVM with univariate feature selection,
- Non-linear SVM
- SVM: Weighted samples,

1.4.2. Regression

The method of Support Vector Classification can be extended to solve regression problems. This method is called Support Vector Regression.

The model produced by support vector classification (as described above) depends only on a subset of the training data, because the cost function for building the model does not care about training points that lie beyond the margin. Analogously, the model produced by Support Vector Regression depends only on a subset of the training data, because the cost function for building the model ignores any training data close to the model prediction.

There are three different implementations of Support Vector Regression: **SVR**, **NuSVR** and **LinearSVR**. **LinearSVR** provides a faster implementation than **SVR** but only considers linear kernels, while **NuSVR** implements a slightly different formulation than **SVR** and **LinearSVR**. See Implementation details for further details.

As with classification classes, the fit method will take as argument vectors X, y, only that in this case y is expected to have floating point values instead of integer values:

```
>>> from sklearn import svm
>>> X = [[0, 0], [2, 2]]
>>> y = [0.5, 2.5]
>>> clf = svm.SVR()
>>> clf.fit(X, y)
SVR()
>>> clf.predict([[1, 1]])
array([1.5])
```

Examples:

- Support Vector Regression (SVR) using linear and non-linear kernels

1.4.3. Density estimation, novelty detection

The class **OneClassSVM** implements a One-Class SVM which is used in outlier detection.

See Novelty and Outlier Detection for the description and usage of OneClassSVM.

1.4.4. Complexity

Support Vector Machines are powerful tools, but their compute and storage requirements increase rapidly with the number of training vectors. The core of an SVM is a quadratic programming problem (QP), separating support vectors from the rest of the training data. The QP solver used by this libsvm-based implementation scales between $O(n_{features} \times n_{samples}^2)$ and $O(n_{features} \times n_{samples}^3)$ depending on how efficiently the libsvm cache is used in practice (dataset dependent). If the data is very sparse $n_{features}$ should be replaced by the average number of non-zero features in a sample vector.

Also note that for the linear case, the algorithm used in **LinearSVC** by the liblinear implementation is much more efficient than its libsvm-based **SVC** counterpart and can scale almost linearly to millions of samples and/or features.

1.4.5. Tips on Practical Use

- **Avoiding data copy**: For `SVC`, `SVR`, `NuSVC` and `NuSVR`, if the data passed to certain methods is not C-ordered contiguous, and double precision, it will be copied before calling the underlying C implementation. You can check whether a given numpy array is C-contiguous by inspecting its `flags` attribute.

  For `LinearSVC` (and `LogisticRegression`) any input passed as a numpy array will be copied and converted to the liblinear internal sparse data representation (double precision floats and int32 indices of non-zero components). If you want to fit a large-scale linear classifier without copying a dense numpy C-contiguous double precision array as input we suggest to use the `SGDClassifier` class instead. The objective function can be configured to be almost the same as the `LinearSVC` model.

- **Kernel cache size**: For `SVC`, `SVR`, `NuSVC` and `NuSVR`, the size of the kernel cache has a strong impact on run times for larger problems. If you have enough RAM available, it is recommended to set `cache_size` to a higher value than the default of 200(MB), such as 500(MB) or 1000(MB).

- **Setting C**: `C` is `1` by default and it's a reasonable default choice. If you have a lot of noisy observations you should decrease it. It corresponds to regularize more the estimation.

  `LinearSVC` and `LinearSVR` are less sensitive to `C` when it becomes large, and prediction results stop improving after a certain threshold. Meanwhile, larger `C` values will take more time to train, sometimes up to 10 times longer, as shown by Fan et al. (2008)

- Support Vector Machine algorithms are not scale invariant, so **it is highly recommended to scale your data**. For example, scale each attribute on the input vector X to [0,1] or [-1,+1], or standardize it to have mean 0 and variance 1. Note that the *same* scaling must be applied to the test vector to obtain meaningful results. See section Preprocessing data for more details on scaling and normalization.

- Parameter `nu` in `NuSVC`/`OneClassSVM`/`NuSVR` approximates the fraction of training errors and support vectors.

- In `SVC`, if data for classification are unbalanced (e.g. many positive and few negative), set `class_weight='balanced'` and/or try different penalty parameters `C`.

- **Randomness of the underlying implementations**: The underlying implementations of `SVC` and `NuSVC` use a random number generator only to shuffle the data for probability estimation (when `probability` is set to `True`). This randomness can be controlled with the `random_state` parameter. If `probability` is set to `False` these estimators are not random and `random_state` has no effect on the results. The underlying `OneClassSVM` implementation is similar to the ones of `SVC` and `NuSVC`. As no probability estimation is provided for `OneClassSVM`, it is not random.

  The underlying `LinearSVC` implementation uses a random number generator to select features when fitting the model with a dual coordinate descent (i.e when `dual` is set to `True`). It is thus not uncommon, to have slightly different results for the same input data. If that happens, try with a smaller tol parameter. This randomness can also be controlled with the `random_state` parameter. When `dual` is set to `False` the underlying implementation of `LinearSVC` is not random and `random_state` has no effect on the results.

- Using L1 penalization as provided by `LinearSVC(loss='l2', penalty='l1', dual=False)` yields a sparse solution, i.e. only a subset of feature weights is different from zero and contribute to the decision function. Increasing `C` yields a more complex model (more feature are selected). The `C` value that yields a "null" model (all weights equal to zero) can be calculated using `l1_min_c`.

References:

- Fan, Rong-En, et al., "LIBLINEAR: A library for large linear classification.", Journal of machine learning research 9.Aug (2008): 1871-1874.

1.4.6. Kernel functions

The *kernel function* can be any of the following:

- linear: $\langle x, x' \rangle$.
- polynomial: $(\gamma \langle x, x' \rangle + r)^d$. d is specified by keyword `degree`, r by `coef0`.
- rbf: $\exp(-\gamma \|x - x'\|^2)$. γ is specified by keyword `gamma`, must be greater than 0.
- sigmoid $(\tanh(\gamma \langle x, x' \rangle + r))$, where r is specified by `coef0`.

Different kernels are specified by keyword kernel at initialization:

```
>>> linear_svc = svm.SVC(kernel='linear')
>>> linear_svc.kernel
'linear'
>>> rbf_svc = svm.SVC(kernel='rbf')
>>> rbf_svc.kernel
'rbf'
```

1.4.6.1. Custom Kernels

You can define your own kernels by either giving the kernel as a python function or by precomputing the Gram matrix.

Classifiers with custom kernels behave the same way as any other classifiers, except that:

- Field `support_vectors_` is now empty, only indices of support vectors are stored in `support_`
- A reference (and not a copy) of the first argument in the `fit()` method is stored for future reference. If that array changes between the use of `fit()` and `predict()` you will have unexpected results.

1.4.6.1.1. Using Python functions as kernels

You can also use your own defined kernels by passing a function to the keyword `kernel` in the constructor.

Your kernel must take as arguments two matrices of shape `(n_samples_1, n_features)`, `(n_samples_2, n_features)` and return a kernel matrix of shape `(n_samples_1, n_samples_2)`.

The following code defines a linear kernel and creates a classifier instance that will use that kernel:

```
>>> import numpy as np
>>> from sklearn import svm
>>> def my_kernel(X, Y):
...     return np.dot(X, Y.T)
...
>>> clf = svm.SVC(kernel=my_kernel)
```

Examples:

- SVM with custom kernel.

1.4.6.1.2. Using the Gram matrix

Set `kernel='precomputed'` and pass the Gram matrix instead of X in the fit method. At the moment, the kernel values between *all* training vectors and the test vectors must be provided.

```
>>> import numpy as np
>>> from sklearn import svm
>>> X = np.array([[0, 0], [1, 1]])
>>> y = [0, 1]
>>> clf = svm.SVC(kernel='precomputed')
>>> # linear kernel computation
>>> gram = np.dot(X, X.T)
>>> clf.fit(gram, y)
SVC(kernel='precomputed')
>>> # predict on training examples
>>> clf.predict(gram)
array([0, 1])
```

1.4.6.1.3. Parameters of the RBF Kernel

When training an SVM with the *Radial Basis Function* (RBF) kernel, two parameters must be considered: `C` and `gamma`. The parameter `C`, common to all SVM kernels, trades off misclassification of training examples against simplicity of the decision surface. A low `C` makes the decision surface smooth, while a high `C` aims at classifying all training examples correctly. `gamma` defines how much influence a single training example has. The larger `gamma` is, the closer other examples must be to be affected.

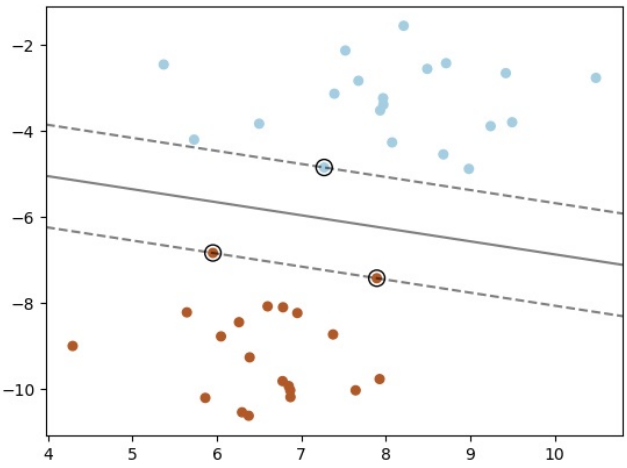
Proper choice of `C` and `gamma` is critical to the SVM's performance. One is advised to use `sklearn.model_selection.GridSearchCV` with `C` and `gamma` spaced exponentially far apart to choose good values.

Examples:

- RBF SVM parameters

1.4.7. Mathematical formulation

A support vector machine constructs a hyper-plane or set of hyper-planes in a high or infinite dimensional space, which can be used for classification, regression or other tasks. Intuitively, a good separation is achieved by the hyper-plane that has the largest distance to the nearest training data points of any class (so-called functional margin), since in general the larger the margin the lower the generalization error of the classifier.



1.4.7.1. SVC

Given training vectors $x_i \in \mathbb{R}^p$, i=1,..., n, in two classes, and a vector $y \in \{1, -1\}^n$, SVC solves the following primal problem:

$$\begin{aligned} \min_{w,b,\zeta} \frac{1}{2} w^T w + C \sum_{i=1}^{n} \zeta_i \\ \text{subject to } y_i(w^T \phi(x_i) + b) \geq 1 - \zeta_i, \\ \zeta_i \geq 0, i = 1, \ldots, n \end{aligned}$$

Its dual is

$$\begin{aligned} \min_{\alpha} \frac{1}{2} \alpha^T Q \alpha - e^T \alpha \\ \text{subject to } y^T \alpha = 0 \\ 0 \leq \alpha_i \leq C, i = 1, \ldots, n \end{aligned}$$

where e is the vector of all ones, $C > 0$ is the upper bound, Q is an n by n positive semidefinite matrix, $Q_{ij} \equiv y_i y_j K(x_i, x_j)$, where $K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$ is the kernel. Here training vectors are implicitly mapped into a higher (maybe infinite) dimensional space by the function ϕ.

The decision function is:

$$\operatorname{sgn}(\sum_{i=1}^{n} y_i \alpha_i K(x_i, x) + \rho)$$

Note: While SVM models derived from libsvm and liblinear use `C` as regularization parameter, most other estimators use `alpha`. The exact equivalence between the amount of regularization of two models depends on the exact objective function optimized by the model. For example, when the estimator used is `sklearn.linear_model.Ridge` regression, the relation between them is given as $C = \frac{1}{alpha}$.

This parameters can be accessed through the members `dual_coef_` which holds the product $y_i \alpha_i$, `support_vectors_` which holds the support vectors, and `intercept_` which holds the independent term ρ :

References:

- "Automatic Capacity Tuning of Very Large VC-dimension Classifiers", I. Guyon, B. Boser, V. Vapnik - Advances in neural information processing 1993.
- "Support-vector networks", C. Cortes, V. Vapnik - Machine Learning, 20, 273-297 (1995).

1.4.7.2. NuSVC

We introduce a new parameter ν which controls the number of support vectors and training errors. The parameter $\nu \in (0, 1]$ is an upper bound on the fraction of training errors and a lower bound of the fraction of support vectors.

It can be shown that the ν-SVC formulation is a reparameterization of the C-SVC and therefore mathematically equivalent.

1.4.7.3. SVR

Given training vectors $x_i \in \mathbb{R}^p$, i=1,..., n, and a vector $y \in \mathbb{R}^n$ ε-SVR solves the following primal problem:

$$\begin{aligned} \min_{w,b,\zeta,\zeta^*} \frac{1}{2} w^T w + C \sum_{i=1}^{n} (\zeta_i + \zeta_i^*) \\ \text{subject to } y_i - w^T \phi(x_i) - b \leq \varepsilon + \zeta_i, \\ w^T \phi(x_i) + b - y_i \leq \varepsilon + \zeta_i^*, \\ \zeta_i, \zeta_i^* \geq 0, i = 1, \ldots, n \end{aligned}$$

Its dual is

$$\begin{aligned} \min_{\alpha,\alpha^*} \frac{1}{2} (\alpha - \alpha^*)^T Q (\alpha - \alpha^*) + \varepsilon e^T (\alpha + \alpha^*) - y^T (\alpha - \alpha^*) \\ \text{subject to } e^T (\alpha - \alpha^*) = 0 \\ 0 \leq \alpha_i, \alpha_i^* \leq C, i = 1, \ldots, n \end{aligned}$$

where e is the vector of all ones, $C > 0$ is the upper bound, Q is an n by n positive semidefinite matrix, $Q_{ij} \equiv K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$ is the kernel. Here training vectors are implicitly mapped into a higher (maybe infinite) dimensional space by the function ϕ.

The decision function is:

$$\sum_{i=1}^{n} (\alpha_i - \alpha_i^*) K(x_i, x) + \rho$$

These parameters can be accessed through the members `dual_coef_` which holds the difference $\alpha_i - \alpha_i^*$, `support_vectors_` which holds the support vectors, and `intercept_` which holds the independent term ρ

References:

- "A Tutorial on Support Vector Regression", Alex J. Smola, Bernhard Schölkopf - Statistics and Computing archive Volume 14 Issue 3, August 2004, p. 199-222.

1.4.8. Implementation details

Internally, we use libsvm and liblinear to handle all computations. These libraries are wrapped using C and Cython.

References:

For a description of the implementation and details of the algorithms used, please refer to

- LIBSVM: A Library for Support Vector Machines.
- LIBLINEAR – A Library for Large Linear Classification.

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