Support Vector Machines

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.. currentmodule:: sklearn.svm

Support vector machines (SVMs) are a set of supervised learning methods used for ref. classification <svm_classification>', ref.'regression <svm_regression>' and ref.'outliers detection <svm_outlier_detection>'.

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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 <a href="ref": svm_kernels" can be specified for the decision function. Common kernels are provided, but it is also possible to specify custom kernels.

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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 ref.'svm kernels' and regularization term is crucial.

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• SVMs do not directly provide probability estimates, these are calculated using an expensive five-fold cross-validation (see ref Scores and probabilities scores probabilities>`, below).

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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.

Classification

:class:'SVC', :class:'NuSVC' and :class:'LinearSVC' are classes capable of performing binary and multi-class classification on a dataset.

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<code>:class:`SVC`</code> and <code>:class:`NuSVC</code> are similar methods, but accept slightly different sets of parameters and have different mathematical formulations (see section <code>ref.`svm_mathematical_formulation</code>). On the other hand, <code>:class:`LinearSVC`</code> is another (faster) implementation of Support Vector Classification for the case of a linear kernel. Note that <code>:class:`LinearSVC</code> does not accept parameter <code>kernel</code>, as this is assumed to be linear. It also lacks some of the attributes of <code>:class:`SVC'</code> and <code>:class:`NuSVC'</code>, like <code>support_.</code>

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As other classifiers, "class: 'NuSVC' and "class: 'LinearSVC' take as input two arrays: an array X of shape $(n_samples, n features)$ holding the training samples, and an array y of class labels (strings or integers), of shape $(n_samples)$:

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```
>>> 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 (detailed in the ref.'svm_mathematical_formulation) depends on some subset of the training data, called the support vectors. Some properties of these support vectors can be found in attributes support_vectors_, support_ and
n support :

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Examples:

ref. sphx_glr_auto_examples_svm_plot_separating_hyperplane.py`,

```
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```

ref. sphx_glr_auto_examples_svm_plot_svm_nonlinear.py

```
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ref. sphx_glr_auto_examples_svm_plot_svm_anova.py`,

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Multi-class classification

class: SVC' and class: 'NuSVC' implement the "one-versus-one" approach for multi-class classification. In total, n_classes * (n_classes - 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 monotonically transform the results of the "one-versus-one" classifiers to a "one-vs-rest" decision function of shape (n_samples, n_classes).

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```
>>> 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, :class: LinearSVC' implements "one-vs-the-rest" multi-class strategy, thus training n_c lasses models.

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

See ref. sym mathematical formulation for a complete description of the decision function.

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Note that the <code>:class:'LinearSVC'</code> also implements an alternative multi-class strategy, the so-called multi-class SVM formulated by Crammer and Singer [16], by using the option <code>multi_class='crammer_singer'</code>. In practice, one-vs-rest classification is usually preferred, since the results are mostly similar, but the runtime is significantly less.

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For "one-vs-rest" :class: LinearSVC the attributes <code>coef_</code> and <code>intercept_</code> have the shape (<code>n_classes, n_features)</code> and (<code>n_classes,)</code> respectively. Each row of the coefficients corresponds to one of the <code>n_classes</code> "one-vs-rest" classifiers and similar

for the intercepts, in the order of the "one" class.

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In the case of "one-vs-one" <code>class:`SVC</code> and <code>class:`NuSVC</code>, the layout of the attributes is a little more involved. In the case of a linear kernel, the attributes <code>coef_</code> and <code>intercept_</code> have the shape <code>(n_classes * (n_classes - 1) / 2, n_features)</code> and <code>(n_classes * (n_classes - 1) / 2)</code> respectively. This is similar to the layout for <code>class:`LinearSVC</code> 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 n", ... "n-1 vs n".

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The shape of dual_coef_ is (n_classes-1, n_SV) with a somewhat hard to grasp layout. The columns correspond to the support vectors involved in any of the n_classes * (n_classes - 1) / 2 "one-vs-one" classifiers. Each support vector v has a dual coefficient in each of the n_classes - 1 classifiers comparing the class of v against another class. Note that some, but not all, of these dual coefficients, may be zero. The n_classes - 1 entries in each column are these dual coefficients, ordered by the opposing class.

This might be clearer with an example: consider a three class problem with class 0 having three support vectors v_0^0 , v_1^0 , v_2^0 and class 1 and 2 having two support vectors v_0^1 , v_1^1 and v_0^2 , v_1^2 respectively. For each support vector v_j^i , there are two dual coefficients. Let's call the coefficient of support vector v_j^i in the classifier between classes i and k $\alpha_j^{i,k}$. Then dual_coef_ looks like this:

$a_0^{0, 1}$	$\alpha_1^{0, 1}$	$\alpha_2^{0, 1}$	$a_0^{1,0}$	$a_1^{1,0}$	$\alpha_0^{2,0}$	$\alpha_1^{2,0}$
$a_0^{0,2}$	$\alpha_1^{0,2}$	$\alpha_2^{0,2}$	$\alpha_0^{1,2}$	$\alpha_1^{1,2}$	$\alpha_0^{2, 1}$	$\alpha_1^{2, 1}$
Coefficients for SVs of class 0			Coefficients for SVs of class 1		Coefficients for SVs of class 2	

Examples:

• ref. sphx glr_auto_examples_svm_plot_iris_svc.py,

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Scores and probabilities

The decision_function method of :class:`SVC` and :class:`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 [9]: 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 [10].

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Note

The same probability calibration procedure is available for all estimators via the class: "sklearn.calibration.CalibratedClassifierCV" (see :ref. calibration"). In the case of :class: "SVC" and :class: "NuSVC", this procedure is builtin in libsym which is used under the hood, so it does not rely on scikit-learn's :class: "sklearn.calibration.CalibratedClassifierCV".

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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:

- the "argmax" of the scores may not be the argmax of the probabilities
- in binary classification, a sample may be labeled by predict as belonging to the positive class even if the output of *predict_proba* is less than 0.5; and similarly, it could be labeled as negative even if the output of *predict_proba* is more than 0.5.

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 $decision_function$ for the output of $decision_function$ (...), $decision_function$ (...), $decision_function$ function function (...), $decision_function$ function fun

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Unbalanced problems

In problems where it is desired to give more importance to certain classes or certain individual samples, the parameters class weight and sample weight can be used.

class: SVC' (but not :class: NuSVC') implements the parameter 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. The figure below illustrates the decision boundary of an unbalanced problem, with and without weight correction.

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<code>:class:`SVC`</code>, <code>:class:`NuSVC'</code>, <code>:class:`NuSVC'</code>, <code>:class:`NuSVC'</code>, <code>:class:`LinearSVC'</code>, <code>:class:`LinearSVC'</code> and <code>:class:`OneClassSVM'</code> implement also weights for individual samples in the <code>fit</code> method through the <code>sample_weight</code> parameter. Similar to <code>class_weight</code>, this sets the parameter <code>c</code> for the i-th example to <code>c</code> * <code>sample_weight[i]</code>, which will encourage the classifier to get these samples right. The figure below illustrates the effect of sample weighting on the decision boundary. The size of the circles is proportional to the sample weights:

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• ref. sphx glr auto examples svm plot separating hyperplane unbalanced.py

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• ref. sphx glr auto examples svm plot weighted samples.py,

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```

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 ignores samples whose prediction is close to their target.

There are three different implementations of Support Vector Regression: :class: 'SVR', :class: 'NuSVR' and :class: 'LinearSVR' provides a faster implementation than :class: 'SVR' but only considers the linear kernel, while :class: 'NuSVR' implements a slightly different formulation than :class: 'SVR' and :class: 'LinearSVR'. See :ref.' svm_implementation_details' for further details.

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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]
>>> regr = svm.SVR()
>>> regr.fit(X, y)
SVR()
>>> regr.predict([[1, 1]])
array([1.5])
```

Examples:

ref. sphx_glr_auto_examples_svm_plot_svm_regression.py

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main) (doc) (modules) svm.rst, line 332); backlink

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```

Density estimation, novelty detection

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

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```

See ref outlier_detection for the description and usage of OneClassSVM.

```
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```

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 the libsym-based implementation scales between O(n_{features} \times n^2_{samples}) and O(n_{features} \times n^3_{samples})
```

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.

For the linear case, the algorithm used in :class: LinearSVC` by the liblinear implementation is much more efficient than its libsymbased :class: SVC` counterpart and can scale almost linearly to millions of samples and/or features.

```
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Tips on Practical Use

Avoiding data copy: For :class: 'SVC', :class: 'SVR', :class: 'NuSVC' and :class: '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.

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main) (doc) (modules) svm.rst, line 368); backlink

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```

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main\) (doc) (modules) svm.rst, line 368); backlink
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```

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\doc\(modules\) svm.rst, line 368); backlink
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```

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\) (doc) (modules) svm.rst, line 368); backlink
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```

For :class: LinearSVC' (and :class: LogisticRegression <skleam.linear_model.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 :class:'SGDClassifier <skleam.linear_model.SGDClassifier>' class instead. The objective function can be configured to be almost the same as the :class:'LinearSVC' model.

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main) (doc) (modules) svm.rst, line 374); backlink
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```

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main) (doc) (modules) svm.rst, line 374); backlink

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```

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\(doc\) (modules) svm.rst, line 374); backlink

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```

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main\) (doc) (modules) svm.rst, line 374); backlink
```

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• Kernel cache size: For :class: 'SVC', :class: 'SVR', :class: 'NuSVC' and :class: '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).

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\) (doc) (modules) sym.rst, line 385); backlink
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```

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\) (doc) (modules) svm.rst, line 385); backlink

Unknown interpreted text role "class".
```

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\(doc\) (modules) svm.rst, line 385); backlink
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```

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\) (doc) (modules) svm.rst, line 385); backlink
Unknown interpreted text role "class".
```

• 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: decreasing C corresponds to more regularization.

class: LinearSVC and class: 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 in [11].

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\(doc\) (modules) svm.rst, line 396); backlink

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```

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main) (doc) (modules) svm.rst, line 396); backlink

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```

• 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. This can be done easily by using a :class:`~sklearn.pipeline.Pipeline`:

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\(doc\) (modules) sym.rst, line 401); backlink

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```

```
>>> from sklearn.pipeline import make_pipeline
>>> from sklearn.preprocessing import StandardScaler
>>> from sklearn.svm import SVC
>>> clf = make pipeline(StandardScaler(), SVC())
```

See section ref preprocessing for more details on scaling and normalization.

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main) (doc)
```

```
(modules) svm. rst, line 414); backlink
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```

- Regarding the *shrinking* parameter, quoting [12]: We found that if the number of iterations is large, then shrinking can shorten the training time. However, if we loosely solve the optimization problem (e.g., by using a large stopping tolerance), the code without using shrinking may be much faster
- Parameter nu in :class: NuSVC'/:class: OneClassSVM'/:class: NuSVR' approximates the fraction of training errors and support vectors.

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main\) (doc) (modules) svm.rst, line 425); backlink
```

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```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main) (doc) (modules) svm.rst, line 425); backlink

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```

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(modules) svm. rst, line 425); backlink
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• In :class: SVC', if the data is unbalanced (e.g. many positive and few negative), set class_weight='balanced' and/or try different penalty parameters c.

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main) (doc) (modules) svm.rst, line 428); backlink

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```

• Randomness of the underlying implementations: The underlying implementations of :class: `SVC` and :class: `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 :class: `OneClassSVM` implementation is similar to the ones of :class: `SVC` and :class: `NuSVC`. As no probability estimation is provided for :class: `OneClassSVM`, it is not random.

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main\) (doc) (modules) svm.rst, line 432); backlink
```

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```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main) (doc) (modules) svm.rst, line 432); backlink
```

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```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\) (doc) (modules) sym.rst, line 432); backlink
```

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```
(modules) svm.rst, line 432); backlink
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```

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main\) (doc) (modules) svm.rst, line 432); backlink

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```

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\(doc\) (modules) sym.rst, line 432); backlink
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```

The underlying <code>class:'LinearSVC'</code> implementation uses a random number generator to select features when fitting the model with a dual coordinate descent (i.e when <code>dual</code> is set to <code>True</code>). 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 <code>random_state</code> parameter. When <code>dual</code> is set to <code>False</code> the underlying implementation of <code>class:'LinearSVC'</code> is not random and <code>random_state</code> has no effect on the results.

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\) (doc) (modules) sym.rst, line 442); backlink
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```

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\) (doc) (modules) sym.rst, line 442); backlink

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```

• Using L1 penalization as provided by LinearSVC (penalty='ll', 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 features are selected). The c value that yields a "null" model (all weights equal to zero) can be calculated using :func:'ll_min_c'.

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\(doc\) (modules) sym.rst, line 451); backlink

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```

Kernel functions

The kernel function can be any of the following:

- linear: □x x'□
- polynomial: $(y \square x, x' \square + r)^d$, where d is specified by parameter degree, r by coef0.
- rbf. $\exp(-\gamma //(x-x^2))$, where y is specified by parameter gamma, must be greater than 0.
- sigmoid $tanh(y \square x, x' \square + r)$, where r is specified by coef0.

Different kernels are specified by the kernel parameter:

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

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 :class: ~sklearn.model selection.GridSearchCV with c and gamma spaced exponentially far apart to choose good values.

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\(doc\) (modules) svm.rst, line 497); backlink
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```

Examples:

• ref. sphx glr auto examples svm plot rbf parameters.py

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\(doc\) (modules) svm.rst, line 503); backlink

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```

ref. sphx glr auto examples svm plot svm nonlinear.py

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\(doc\) (modules) sym.rst, line 504); backlink

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```

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.

Using Python functions as kernels

You can use your own defined kernels by passing a function to the kernel parameter.

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:

ref. sphx_glr_auto_examples_svm_plot_custom_kernel.py.

```
System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main)\) (doc) (modules) sym.rst, line 546); backlink
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```

Using the Gram matrix

You can pass pre-computed kernels by using the kernel='precomputed' option. You should then pass Gram matrix instead of X to the fit and predict methods. The kernel values between all training vectors and the test vectors must be provided:

```
>>> import numpy as np
>>> from sklearn.datasets import make_classification
>>> from sklearn.model_selection import train_test_split
```

```
>>> from sklearn import svm
>>> X, y = make_classification(n_samples=10, random_state=0)
>>> X_train , X_test , y_train, y_test = train_test_split(X, y, random_state=0)
>>> clf = svm.SVC(kernel='precomputed')
>>> # linear kernel computation
>>> gram_train = np.dot(X_train, X_train.T)
>>> clf.fit(gram_train, y_train)
SVC(kernel='precomputed')
>>> # predict on training examples
>>> gram_test = np.dot(X_test, X_train.T)
>>> clf.predict(gram_test)
array([0, 1, 0])
```

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. The figure below shows the decision function for a linearly separable problem, with three samples on the margin boundaries, called "support vectors":

In general, when the problem isn't linearly separable, the support vectors are the samples within the margin boundaries.

We recommend [13] and [14] as good references for the theory and practicalities of SVMs.

SVC

Given training vectors $x_i \in \mathbb{R}^p$, $\models 1,...$, n, in two classes, and a vector $y \in \{1, -1\}^n$, our goal is to find $w \in \mathbb{R}^p$ and $b \in \mathbb{R}$ such that the prediction given by $sign(w^T\varphi(x) + b)$ is correct for most samples.

SVC solves the following primal problem:

$$\min_{w, b, \zeta} \frac{1}{2} w^T w + C \bigcap_{i=1}^n \zeta_i$$

$$= 1$$
subject
$$toy_i(w^T \varphi(x_i) + b) \ge 1 - \zeta_i$$

$$\zeta_i \ge 0, i = 1, ..., n$$

Intuitively, we're trying to maximize the margin (by minimizing $||w||^2 = w^{Tw}$), while incurring a penalty when a sample is misclassified or within the margin boundary. Ideally, the value $y_i(w^T\varphi(x_i) + b)$ would be ≥ 1 for all samples, which indicates a perfect prediction. But problems are usually not always perfectly separable with a hyperplane, so we allow some samples to be at a distance ζ_i from their correct margin boundary. The penalty term C controls the strength of this penalty, and as a result, acts as an inverse regularization parameter (see note below).

The dual problem to the primal is

$$\min_{\alpha} \frac{1}{2} \alpha^{T} Q \alpha - e^{T} \alpha$$
subject toy^T $\alpha = 0$

$$0 \le \alpha_{i} \le C, i = 1, ..., n$$

where e is the vector of all ones, and Q is an n by n positive semidefinite matrix, $Q_{ij} \equiv y_i y_j K(x_i, x_j)$, where $K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j)$ is the kernel. The terms α_i are called the dual coefficients, and they are upper-bounded by C. This dual representation highlights the fact that training vectors are implicitly mapped into a higher (maybe infinite) dimensional space by the function φ : see kernel trick.

Once the optimization problem is solved, the output of term decision function for a given sample x becomes:

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and the predicted class correspond to its sign. We only need to sum over the support vectors (i.e. the samples that lie within the margin) because the dual coefficients a_i are zero for the other samples.

These parameters can be accessed through the attributes $dual_coef_which holds$ the product $y_i\alpha_i$, $support_vectors_which holds$ the support vectors, and $intercept_which holds$ the independent term b

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 'class:'~sklearn.linear_model.Ridge' regression, the relation between them is given as $C = \frac{1}{alnha}$.

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LinearSVC

The primal problem can be equivalently formulated as

$$\min_{w, b} \frac{1}{2} w^T w + C \underset{i=1}{\square} \max(0, 1 - y_i (w^T \varphi(x_i) + b)),$$

where we make use of the hinge loss. This is the form that is directly optimized by class: LinearSVC', but unlike the dual form, this one does not involve inner products between samples, so the famous kernel trick cannot be applied. This is why only the linear kernel is supported by class: LinearSVC' (φ is the identity function).

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NuSVC

The v-SVC formulation [15] is a reparameterization of the C-SVC and therefore mathematically equivalent.

We introduce a new parameter v (instead of C) which controls the number of support vectors and margin errors: $v \in (0, 1]$ is an upper bound on the fraction of margin errors and a lower bound of the fraction of support vectors. A margin error corresponds to a sample that lies on the wrong side of its margin boundary: it is either misclassified, or it is correctly classified but does not lie beyond the margin.

SVR

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

$$\min_{w, b, \zeta, \zeta^*} \frac{1}{2} w^T w + C \bigcap_{i=1}^n (\zeta_i + \zeta_i^*)$$

subject to
$$y_i - w^T \varphi(x_i) - b \le \varepsilon + \zeta_i$$
,
$$w^T \varphi(x_i) + b - y_i \le \varepsilon + \zeta_i^*,$$

$$\zeta_i, \zeta_i^* \ge 0, i = 1, ..., n$$

Here, we are penalizing samples whose prediction is at least ε away from their true target. These samples penalize the objective by ζ_i or ζ_i^* , depending on whether their predictions lie above or below the ε tube.

The dual problem is

$$\min_{\alpha, \alpha} \frac{1}{2} (\alpha - \alpha^*)^T \mathcal{Q}(\alpha - \alpha^*) + \varepsilon e^T (\alpha + \alpha^*) - y^T (\alpha - \alpha^*)$$

$$\text{subject to} e^T (\alpha - \alpha^*) = 0$$

$$0 \le \alpha_i, \alpha_i^* \le C, i = 1, ..., n$$

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

The prediction is:

$$\Box_{\alpha_i - \alpha_i^*) K(x_i, x) + b$$

$$i \in SV$$

These parameters can be accessed through the attributes $dual_coef_which holds$ the difference $a_i - a_i^*$, $support_vectors_which holds$ the support vectors, and $intercept_which holds$ the independent term b

LinearSVR

The primal problem can be equivalently formulated as

$$\min_{w, b} \frac{1}{2} w^T w + C \underset{i=1}{\square} \max(0, |y_i - (w^T \varphi(x_i) + b)| - \varepsilon),$$

where we make use of the epsilon-insensitive loss, i.e. errors of less than ε are ignored. This is the form that is directly optimized by :class: LinearSVR'.

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Implementation details

Internally, we use libsvm [12] and liblinear [11] to handle all computations. These libraries are wrapped using C and Cython. For a description of the implementation and details of the algorithms used, please refer to their respective papers.

References:

- [9] Platt "Probabilistic outputs for SVMs and comparisons to regularized likelihood methods".
- [10] Wu, Lin and Weng, "Probability estimates for multi-class classification by pairwise coupling", JMLR 5:975-1005, 2004.
- [11] (1,2) Fan, Rong-En, et al., "LIBLINEAR: A library for large linear classification.", Journal of machine learning research 9. Aug (2008): 1871-1874.
- [12] (1,2) Chang and Lin, LIBSVM: A Library for Support Vector Machines.
- [13] Bishop, Pattern recognition and machine learning, chapter 7 Sparse Kernel Machines
- [14] :doi: "A Tutorial on Support Vector Regression" <10.1023/B:STCO.0000035301.49549.88> Alex J. Smola,

 $Bernhard\ Sch\tilde{A}\P lkopf\ -\ Statistics\ and\ Computing\ archive\ Volume\ 14\ Issue\ 3,\ August\ 2004,\ p.\ 199-222.$

System Message: ERROR/3 (D:\onboarding-resources\sample-onboarding-resources\scikit-learn-main\doc\modules\(scikit-learn-main) (doc) (modules) svm.rst, line 798); backlink

Unknown interpreted text role "doi".

- [15] Schökopf et. al New Support Vector Algorithms
- [16] Crammer and Singer On the Algorithmic Implementation of Multiclass Kernel-based Vector Machines, JMLR 2001.