6.7. Kernel Approximation

This submodule contains functions that approximate the feature mappings that correspond to certain kernels, as they are used for example in support vector machines (see Support Vector Machines). The following feature functions perform non-linear transformations of the input, which can serve as a basis for linear classification or other algorithms.

The advantage of using approximate explicit feature maps compared to the kernel trick, which makes use of feature maps implicitly, is that explicit mappings can be better suited for online learning and can significantly reduce the cost of learning with very large datasets. Standard kernelized SVMs do not scale well to large datasets, but using an approximate kernel map it is possible to use much more efficient linear SVMs. In particular, the combination of kernel map approximations with `SGDClassifier` can make non-linear learning on large datasets possible.

Since there has not been much empirical work using approximate embeddings, it is advisable to compare results against exact kernel methods when possible.

See also: Polynomial regression: extending linear models with basis functions for an exact polynomial transformation.

6.7.1. Nystroem Method for Kernel Approximation

The Nystroem method, as implemented in `Nystroem` is a general method for low-rank approximations of kernels. It achieves this by essentially subsampling the data on which the kernel is evaluated. By default `Nystroem` uses the `rbf` kernel, but it can use any kernel function or a precomputed kernel matrix. The number of samples used - which is also the dimensionality of the features computed - is given by the parameter `n_components`.

6.7.2. Radial Basis Function Kernel

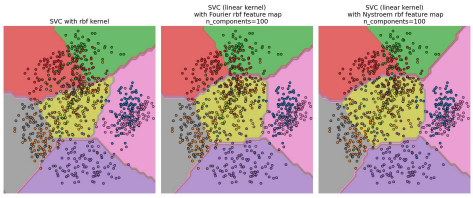
The `RBFSampler` constructs an approximate mapping for the radial basis function kernel, also known as *Random Kitchen Sinks* [RR2007]. This transformation can be used to explicitly model a kernel map, prior to applying a linear algorithm, for example a linear SVM:

```
>>> from sklearn.kernel_approximation import RBFSampler
>>> from sklearn.linear_model import SGDClassifier
>>> X = [[0, 0], [1, 1], [1, 0], [0, 1]]
>>> y = [0, 0, 1, 1]
>>> rbf_feature = RBFSampler(gamma=1, random_state=1)
>>> X_features = rbf_feature.fit_transform(X)
>>> clf = SGDClassifier(max_iter=5)
>>> clf.fit(X_features, y)
SGDClassifier(max_iter=5)
>>> clf.score(X_features, y)
1.0
```

The mapping relies on a Monte Carlo approximation to the kernel values. The `fit` function performs the Monte Carlo sampling, whereas the `transform` method performs the mapping of the data. Because of the inherent randomness of the process, results may vary between different calls to the `fit` function.

The `fit` function takes two arguments: `n_components`, which is the target dimensionality of the feature transform, and `gamma`, the parameter of the RBF-kernel. A higher `n_components` will result in a better approximation of the kernel and will yield results more similar to those produced by a kernel SVM. Note that "fitting" the feature function does not actually depend on the data given to the `fit` function. Only the dimensionality of the data is used. Details on the method can be found in [RR2007].

For a given value of `n_components` `RBFSampler` is often less accurate as `Nystroem`. `RBFSampler` is cheaper to compute, though, making use of larger feature spaces more efficient.



Comparing an exact RBF kernel (left) with the approximation (right)

Examples:

- Explicit feature map approximation for RBF kernels

6.7.3. Additive Chi Squared Kernel

The additive chi squared kernel is a kernel on histograms, often used in computer vision.

The additive chi squared kernel as used here is given by

$$k(x, y) = \sum_i \frac{2x_i y_i}{x_i + y_i}$$

This is not exactly the same as `sklearn.metrics.additive_chi2_kernel`. The authors of [VZ2010] prefer the version above as it is always positive definite. Since the kernel is additive, it is possible to treat all components x_i separately for embedding. This makes it possible to sample the Fourier transform in regular intervals, instead of approximating using Monte Carlo sampling.

The class `AdditiveChi2Sampler` implements this component wise deterministic sampling. Each component is sampled n times, yielding $2n+1$ dimensions per input dimension (the multiple of two stems from the real and complex part of the Fourier transform). In the literature, n is usually chosen to be 1 or 2, transforming the dataset to size `n_samples * 5 * n_features` (in the case of $n = 2$).

The approximate feature map provided by `AdditiveChi2Sampler` can be combined with the approximate feature map provided by `RBFSampler` to yield an approximate feature map for the exponentiated chi squared kernel. See the [VZ2010] for details and [VVZ2010] for combination with the `RBFSampler`.

6.7.4. Skewed Chi Squared Kernel

The skewed chi squared kernel is given by:

$$k(x, y) = \prod_i \frac{2\sqrt{x_i + c}\sqrt{y_i + c}}{x_i + y_i + 2c}$$

It has properties that are similar to the exponentiated chi squared kernel often used in computer vision, but allows for a simple Monte Carlo approximation of the feature map.

The usage of the `SkewedChi2Sampler` is the same as the usage described above for the `RBFSampler`. The only difference is in the free parameter, that is called c. For a motivation for this mapping and the mathematical details see [LS2010].

6.7.5. Polynomial Kernel Approximation via Tensor Sketch

The polynomial kernel is a popular type of kernel function given by:

$$k(x, y) = (\gamma x^\top y + c_0)^d$$

where:

- `x`, `y` are the input vectors
- `d` is the kernel degree

Intuitively, the feature space of the polynomial kernel of degree `d` consists of all possible degree-`d` products among input features, which enables learning algorithms using this kernel to account for interactions between features.

The TensorSketch [PP2013] method, as implemented in `PolynomialCountSketch`, is a scalable, input data independent method for polynomial kernel approximation. It is based on the concept of Count sketch [WIKICS] [CCF2002] , a dimensionality reduction technique similar to feature hashing, which instead uses several independent hash functions. TensorSketch obtains a Count Sketch of the outer product of two vectors (or a vector with itself), which can be used as an approximation of the polynomial kernel feature space. In particular, instead of explicitly computing the outer product, TensorSketch computes the Count Sketch of the vectors and then uses polynomial multiplication via the Fast Fourier Transform to compute the Count Sketch of their outer product.

Conveniently, the training phase of TensorSketch simply consists of initializing some random variables. It is thus independent of the input data, i.e. it only depends on the number of input features, but not the data values. In addition, this method can transform samples in $\mathcal{O}(n_{\text{samples}}(n_{\text{features}} + n_{\text{components}} \log(n_{\text{components}})))$ time, where $n_{\text{components}}$ is the desired output dimension, determined by `n_components`.

Examples:

- Scalable learning with polynomial kernel approximation

6.7.6. Mathematical Details

Kernel methods like support vector machines or kernelized PCA rely on a property of reproducing kernel Hilbert spaces. For any positive definite kernel function k (a so called Mercer kernel), it is guaranteed that there exists a mapping ϕ into a Hilbert space $\mathcal{H}$, such that

$$k(x, y) = \langle \phi(x), \phi(y) \rangle$$

Where $\langle \cdot, \cdot \rangle$ denotes the inner product in the Hilbert space.

If an algorithm, such as a linear support vector machine or PCA, relies only on the scalar product of data points x_i, one may use the value of $k(x_i, x_j)$, which corresponds to applying the algorithm to the mapped data points $\phi(x_i)$. The advantage of using k is that the mapping ϕ never has to be calculated explicitly, allowing for arbitrary large features (even infinite).

One drawback of kernel methods is, that it might be necessary to store many kernel values $k(x_i, x_j)$ during optimization. If a kernelized classifier is applied to new data y_j, $k(x_i, y_j)$ needs to be computed to make predictions, possibly for many different x_i in the training set.

The classes in this submodule allow to approximate the embedding ϕ, thereby working explicitly with the representations $\phi(x_i)$, which obviates the need to apply the kernel or store training examples.

References:

[RR2007] (1,2)
"Random features for large-scale kernel machines" Rahimi, A. and Recht, B. - Advances in neural information processing 2007,

[LS2010]
"Random Fourier approximations for skewed multiplicative histogram kernels" Li, F., Ionescu, C., and Sminchisescu, C. - Pattern Recognition, DAGM 2010, Lecture Notes in Computer Science.

[VZ2010] (1,2)
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[WIKICS]
"Wikipedia: Count sketch"