sklearn.gaussian_process.GaussianProcessRegressor

« *class* sklearn.gaussian_process.**GaussianProcessRegressor**(*kernel=None*, *alpha=1e-10*, *optimizer='fmin_l_bfgs_b'*, *n_restarts_optimizer=0*, *normalize_y=False*, *copy_X_train=True*, *random_state=None*) [source]

Gaussian process regression (GPR).

The implementation is based on Algorithm 2.1 of Gaussian Processes for Machine Learning (GPML) by Rasmussen and Williams.

In addition to standard scikit-learn estimator API, GaussianProcessRegressor:

- allows prediction without prior fitting (based on the GP prior)
- provides an additional method sample_y(X), which evaluates samples drawn from the GPR (prior or posterior) at given inputs
- exposes a method log_marginal_likelihood(theta), which can be used externally for other ways of selecting hyperparameters, e.g., via Markov chain Monte Carlo.

Read more in the User Guide.

New in version 0.18.

Parameters: **kernel** : *kernel object*

The kernel specifying the covariance function of the GP. If None is passed, the kernel "1.0 * RBF(1.0)" is used as default. Note that the kernel's hyperparameters are optimized during fitting.

alpha : *float or array-like, optional (default: 1e-10)*

Value added to the diagonal of the kernel matrix during fitting. Larger values correspond to increased noise level in the observations. This can also prevent a potential numerical issue during

fitting, by ensuring that the calculated values form a positive definite matrix. If an array is passed, it must have the same number of entries as the data used for fitting and is used as datapoint-dependent noise level. Note that this is equivalent to adding a WhiteKernel with c=alpha. Allowing to specify the noise level directly as a parameter is mainly for convenience and for consistency with Ridge.

optimizer : *string or callable, optional (default: “fmin_l_bfgs_b”)*

Can either be one of the internally supported optimizers for optimizing the kernel’s parameters, specified by a string, or an externally defined optimizer passed as a callable. If a callable is passed, it must have the signature:

```
def optimizer(obj_func, initial_theta, bounds):
    # * 'obj_func' is the objective function to be minimized, which
    #   takes the hyperparameters theta as parameter and an
    #   optional flag eval_gradient, which determines if the
    #   gradient is returned additionally to the function value
    # * 'initial_theta': the initial value for theta, which can be
    #   used by local optimizers
    # * 'bounds': the bounds on the values of theta
    ....
    # Returned are the best found hyperparameters theta and
    # the corresponding value of the target function.
    return theta_opt, func_min
```

Per default, the ‘fmin_l_bfgs_b’ algorithm from scipy.optimize is used. If None is passed, the kernel’s parameters are kept fixed. Available internal optimizers are:

```
'fmin_l_bfgs_b'
```

n_restarts_optimizer : *int, optional (default: 0)*

The number of restarts of the optimizer for finding the kernel’s parameters which maximize the log-marginal likelihood. The first run of the optimizer is performed from the kernel’s initial parameters, the remaining ones (if any) from thetas sampled log-uniform randomly from the space of allowed theta-values. If greater than 0, all bounds must be finite. Note that n_restarts_optimizer == 0 implies that one run is performed.

normalize_y : *boolean, optional (default: False)*

Whether the target values y are normalized, i.e., the mean of the observed target values become zero. This parameter should be set to True if the target values’ mean is expected to differ consid-

erable from zero. When enabled, the normalization effectively modifies the GP's prior based on the data, which contradicts the likelihood principle; normalization is thus disabled per default.

copy_X_train : *bool, optional (default: True)*

If True, a persistent copy of the training data is stored in the object. Otherwise, just a reference to the training data is stored, which might cause predictions to change if the data is modified externally.

random_state : *int, RandomState instance or None, optional (default: None)*

The generator used to initialize the centers. If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If None, the random number generator is the RandomState instance used by `np.random`.

Attributes:

X_train_ : *array-like, shape = (n_samples, n_features)*

Feature values in training data (also required for prediction)

y_train_ : *array-like, shape = (n_samples, [n_output_dims])*

Target values in training data (also required for prediction)

kernel_ : *kernel object*

The kernel used for prediction. The structure of the kernel is the same as the one passed as parameter but with optimized hyperparameters

L_ : *array-like, shape = (n_samples, n_samples)*

Lower-triangular Cholesky decomposition of the kernel in `X_train_`

alpha_ : *array-like, shape = (n_samples,)*

Dual coefficients of training data points in kernel space

log_marginal_likelihood_value_ : *float*

The log-marginal-likelihood of `self.kernel_.theta`

Examples

```
>>> from sklearn.datasets import make_friedman2
>>> from sklearn.gaussian_process import GaussianProcessRegressor
>>> from sklearn.gaussian_process.kernels import DotProduct, WhiteKernel
>>> X, y = make_friedman2(n_samples=500, noise=0, random_state=0)
```

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Previous

```
>>> kernel = DotProduct() + WhiteKernel()
>>> gpr = GaussianProcessRegressor(kernel=kernel,
...         random_state=0).fit(X, y)
>>> gpr.score(X, y)
0.3680...
>>> gpr.predict(X[:2,:], return_std=True)
(array([653.0..., 592.1...]), array([316.6..., 316.6...]))
```

Methods

fit(self, X, y)	Fit Gaussian process regression model.
get_params(self[, deep])	Get parameters for this estimator.
log_marginal_likelihood(self[, theta, …])	Returns log-marginal likelihood of theta for training data.
predict(self, X[, return_std, return_cov])	Predict using the Gaussian process regression model
sample_y(self, X[, n_samples, random_state])	Draw samples from Gaussian process and evaluate at X.
score(self, X, y[, sample_weight])	Returns the coefficient of determination R^2 of the prediction.
set_params(self, **params)	Set the parameters of this estimator.

__init__(*self*, *kernel=None*, *alpha=1e-10*, *optimizer='fmin_l_bfgs_b'*, *n_restarts_optimizer=0*, *normalize_y=False*, *copy_X_train=True*, *random_state=None*) [source]

fit(*self*, *X*, *y*) [source]

Fit Gaussian process regression model.

Parameters: **X** : *array-like, shape = (n_samples, n_features)*
Training data

y : *array-like, shape = (n_samples, [n_output_dims])*
Target values

Returns: **self** : *returns an instance of self.*

get_params(*self*, *deep=True*) [source]

Get parameters for this estimator.

Parameters: **deep** : *boolean, optional*

If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns: **params** : *mapping of string to any*

Parameter names mapped to their values.

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log_marginal_likelihood(*self*, *theta=None*, *eval_gradient=False*) [source]

Returns log-marginal likelihood of theta for training data.

Parameters: **theta** : *array-like, shape = (n_kernel_params,) or None*

Kernel hyperparameters for which the log-marginal likelihood is evaluated. If None, the pre-computed log_marginal_likelihood of `self.kernel_.theta` is returned.

eval_gradient : *bool, default: False*

If True, the gradient of the log-marginal likelihood with respect to the kernel hyperparameters at position theta is returned additionally. If True, theta must not be None.

Returns: **log_likelihood** : *float*

Log-marginal likelihood of theta for training data.

log_likelihood_gradient : *array, shape = (n_kernel_params,), optional*

Gradient of the log-marginal likelihood with respect to the kernel hyperparameters at position theta. Only returned when eval_gradient is True.

predict(*self*, *X*, *return_std=False*, *return_cov=False*) [source]

Predict using the Gaussian process regression model

We can also predict based on an unfitted model by using the GP prior. In addition to the mean of the predictive distribution, also its standard deviation (return_std=True) or covariance (return_cov=True). Note that at most one of the two can be requested.

Parameters:

X : *array-like, shape = (n_samples, n_features)*

Query points where the GP is evaluated

return_std : *bool, default: False*

If True, the standard-deviation of the predictive distribution at the query points is returned along with the mean.

return_cov : *bool, default: False*

If True, the covariance of the joint predictive distribution at the query points is returned along with the mean

Returns:

y_mean : *array, shape = (n_samples, [n_output_dims])*

Mean of predictive distribution a query points

y_std : *array, shape = (n_samples,), optional*

Standard deviation of predictive distribution at query points. Only returned when return_std is True.

y_cov : *array, shape = (n_samples, n_samples), optional*

Covariance of joint predictive distribution a query points. Only returned when return_cov is True.

sample_y(*self*, *X*, *n_samples=1*, *random_state=0*) [source]

Draw samples from Gaussian process and evaluate at X.

Parameters:

X : *array-like, shape = (n_samples_X, n_features)*

Query points where the GP samples are evaluated

n_samples : *int, default: 1*

The number of samples drawn from the Gaussian process

random_state : *int, RandomState instance or None, optional (default=0)*

If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If None, the random number generator is the RandomState instance used by `np.random`.

Returns: **y_samples** : *array, shape = (n_samples_X, [n_output_dims], n_samples)*

Values of n_samples samples drawn from Gaussian process and evaluated at query points.

« **score**(*self*, *X*, *y*, *sample_weight=None*) [source]

Returns the coefficient of determination R^2 of the prediction.

The coefficient R^2 is defined as (1 - u/v), where u is the residual sum of squares ((y_true - y_pred) ** 2).sum() and v is the total sum of squares ((y_true - y_true.mean()) ** 2).sum(). The best possible score is 1.0 and it can be negative (because the model can be arbitrarily worse). A constant model that always predicts the expected value of y, disregarding the input features, would get a R^2 score of 0.0.

Parameters: **X** : *array-like, shape = (n_samples, n_features)*

Test samples. For some estimators this may be a precomputed kernel matrix instead, shape = (n_samples, n_samples_fitted], where n_samples_fitted is the number of samples used in the fitting for the estimator.

y : *array-like, shape = (n_samples) or (n_samples, n_outputs)*

True values for X.

sample_weight : *array-like, shape = [n_samples], optional*

Sample weights.

Returns: **score** : *float*

R^2 of self.predict(X) wrt. y.

Notes

The R2 score used when calling `score` on a regressor will use `multioutput='uniform_average'` from version 0.23 to keep consistent with **`metrics.r2_score`**. This will influence the `score` method of all the multioutput regressors (except for **`multioutput.MultiOutputRegressor`**). To specify the default value manually and avoid the warning, please either call **`metrics.r2_score`** directly or make a custom scorer with **`metrics.make_scorer`** (the built-in scorer `'r2'` uses `multioutput='uniform_average'`).

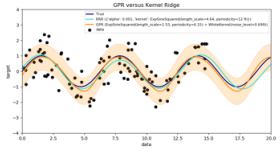
`set_params`(*self*, ***params*) [source]

Set the parameters of this estimator.

The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

Returns: self

Examples using `sklearn.gaussian_process.GaussianProcessRegressor`



Comparison of kernel ridge and Gaussian process regression

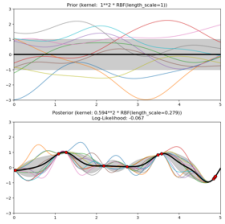
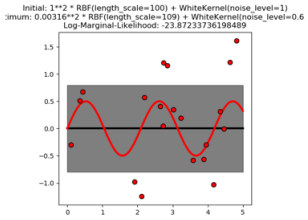
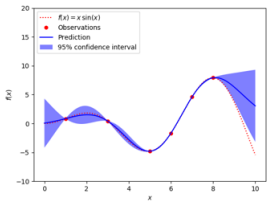


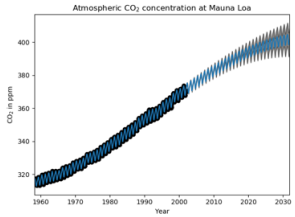
Illustration of prior and posterior Gaussian process for different kernels



Gaussian process regression (GPR) with noise-level estimation



Gaussian Processes regression: basic introductory example



Gaussian process regression (GPR) on Mauna Loa CO2 data.

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