Machine learning in practice

Presentation of a simple ML task example

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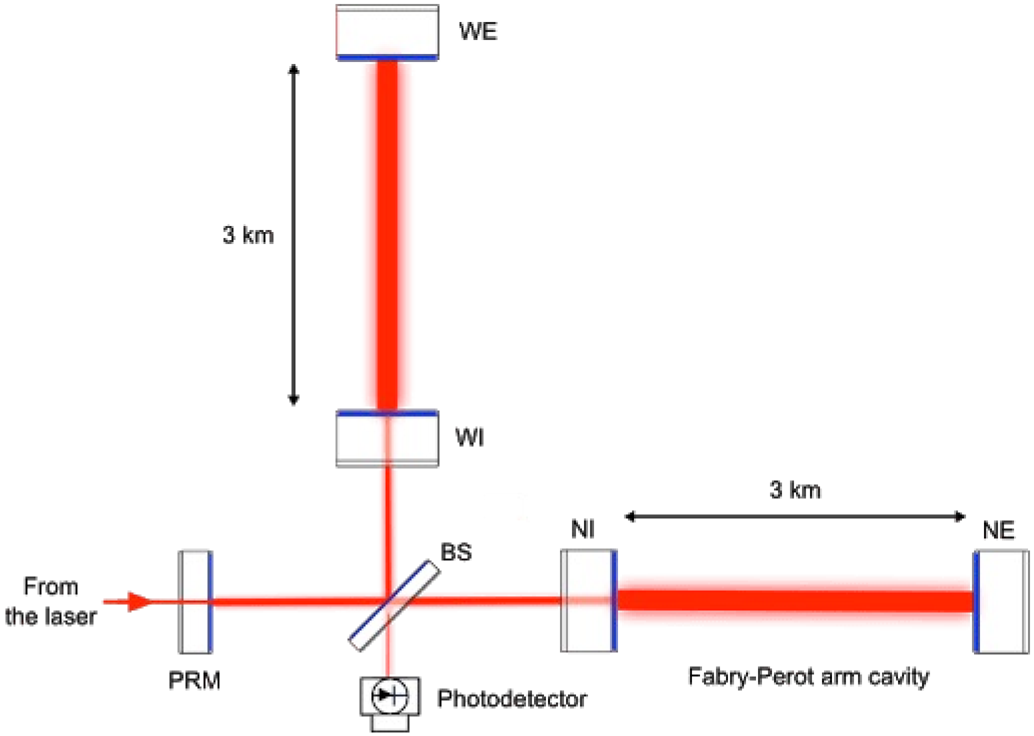
Context



Virgo interferometer

Gravitational waves

↓

Change of the relative length of the arms

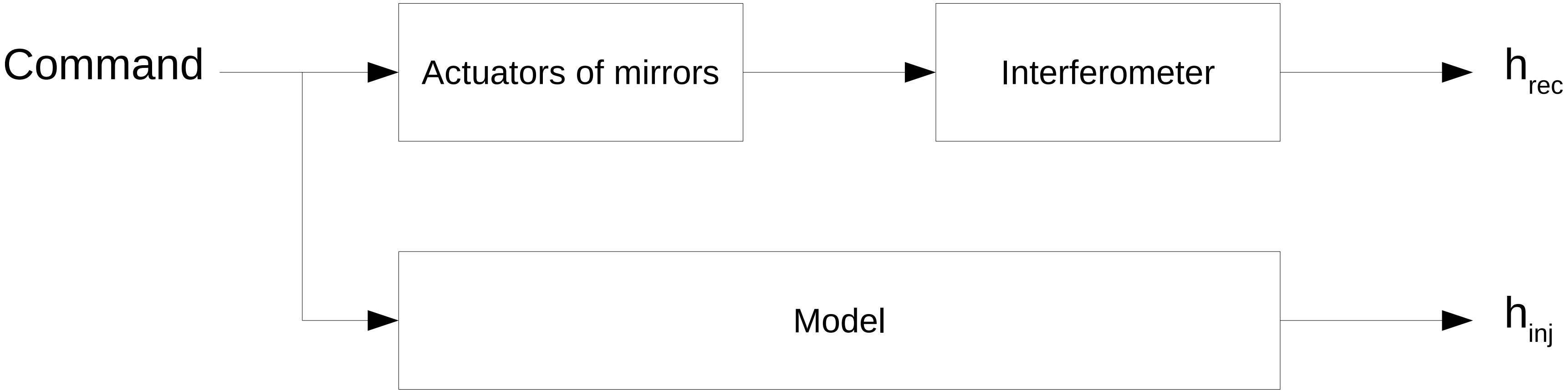
↓

Change of the interferences at the photodetector

↓

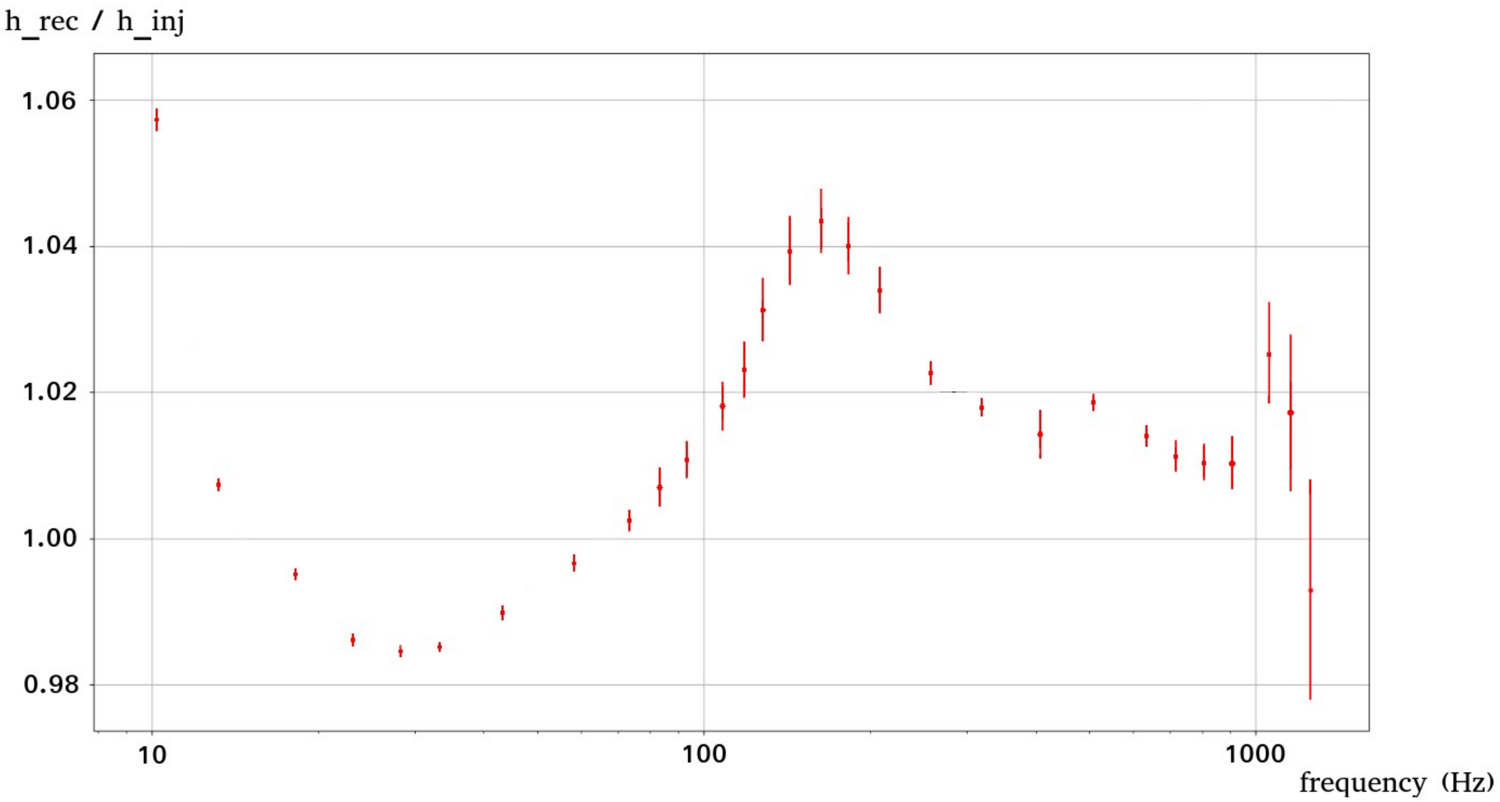
Reconstruction of gravitational waves signal

Context



We “inject” a sinusoid command at a precise frequency f, then we get the interferometer response at this frequency

Context



Context

We call:

$X = \log(f)$ the “feature”

$y = h_{rec} / h_{inj}$ the “label”

We search a function F such as:

$y = f(X)$

Tools

python™

scikit learn

Going further...

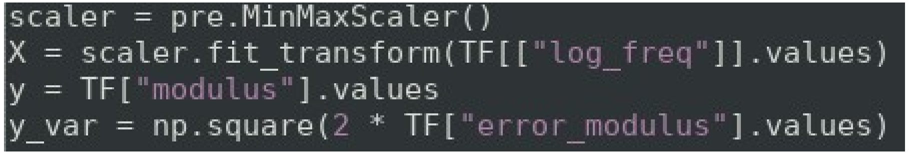
TensorFlow

PyTorch

Keras

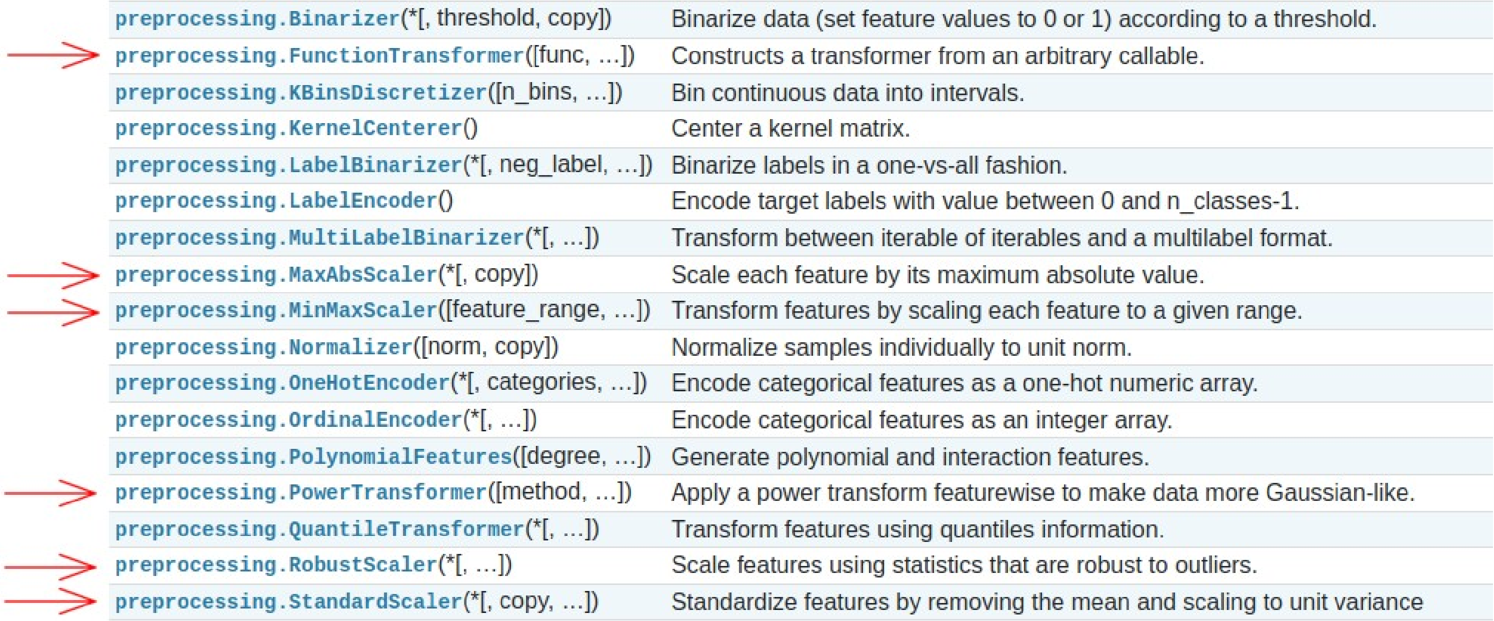
Preprocessing

Standardization :



```
scaler = pre.MinMaxScaler()
X = scaler.fit_transform(TF[["log_freq"]].values)
y = TF["modulus"].values
y_var = np.square(2 * TF["error_modulus"].values)
```

Rescale data, “MinMaxScaler” is a linear transformation which make data fit between 0 and 1



	`preprocessing.Binarizer`(*[, threshold, copy])	Binarize data (set feature values to 0 or 1) according to a threshold.
→	`preprocessing.FunctionTransformer`([func, …])	Constructs a transformer from an arbitrary callable.
	`preprocessing.KBinsDiscretizer`([n_bins, …])	Bin continuous data into intervals.
	`preprocessing.KernelCenterer`()	Center a kernel matrix.
	`preprocessing.LabelBinarizer`(*[, neg_label, …])	Binarize labels in a one-vs-all fashion.
	`preprocessing.LabelEncoder`()	Encode target labels with value between 0 and n_classes-1.
	`preprocessing.MultiLabelBinarizer`(*[, …])	Transform between iterable of iterables and a multilabel format.
→	`preprocessing.MaxAbsScaler`(*[, copy])	Scale each feature by its maximum absolute value.
→	`preprocessing.MinMaxScaler`([feature_range, …])	Transform features by scaling each feature to a given range.
	`preprocessing.Normalizer`([norm, copy])	Normalize samples individually to unit norm.
	`preprocessing.OneHotEncoder`(*[, categories, …])	Encode categorical features as a one-hot numeric array.
	`preprocessing.OrdinalEncoder`(*[, …])	Encode categorical features as an integer array.
	`preprocessing.PolynomialFeatures`([degree, …])	Generate polynomial and interaction features.
→	`preprocessing.PowerTransformer`([method, …])	Apply a power transform featurewise to make data more Gaussian-like.
	`preprocessing.QuantileTransformer`(*[, …])	Transform features using quantiles information.
→	`preprocessing.RobustScaler`(*[, …])	Scale features using statistics that are robust to outliers.
→	`preprocessing.StandardScaler`(*[, copy, …])	Standardize features by removing the mean and scaling to unit variance

Gaussian process regression

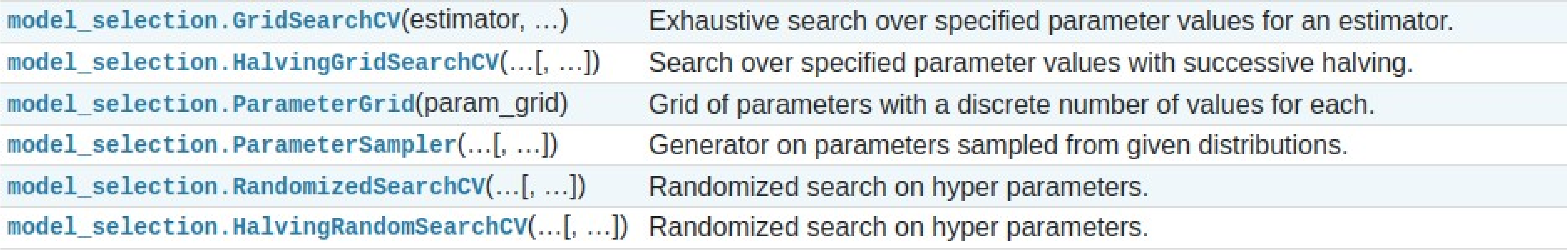
- A gaussian process is a set of gaussian random variables, indexed by a variable x,
- It is characterized by its mean “µ(x)”, and its covariance “cov(x_1,x_2)”

The covariance used in this example: $cov(x_1, x_2) = \gamma_1^2 + \gamma_2^2 \times \exp\left(\frac{(x_1 - x_2)^2}{2l^2}\right)$

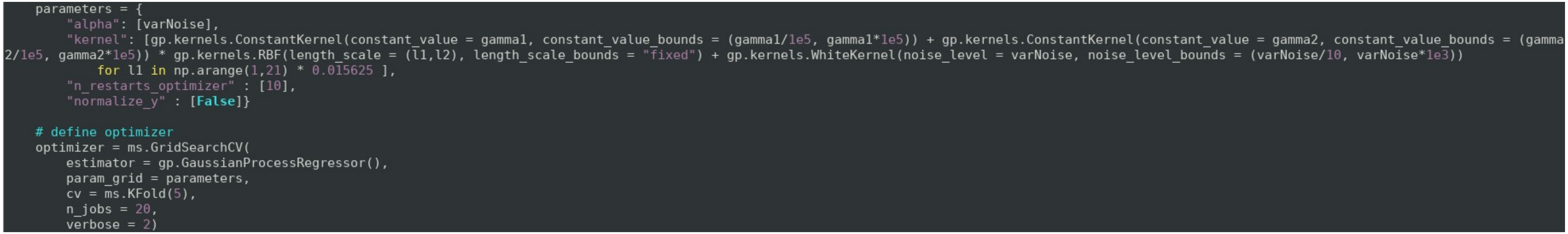
The regression is computed thanks to the input data, and the covariance matrix

Tuning hyperparameters

Make a set of hyperparameter values, and test the algorithm with each hyperparameter value.



`model_selection.GridSearchCV`(estimator, …)	Exhaustive search over specified parameter values for an estimator.
`model_selection.HalvingGridSearchCV`(…[, …])	Search over specified parameter values with successive halving.
`model_selection.ParameterGrid`(param_grid)	Grid of parameters with a discrete number of values for each.
`model_selection.ParameterSampler`(…[, …])	Generator on parameters sampled from given distributions.
`model_selection.RandomizedSearchCV`(…[, …])	Randomized search on hyper parameters.
`model_selection.HalvingRandomSearchCV`(…[, …])	Randomized search on hyper parameters.

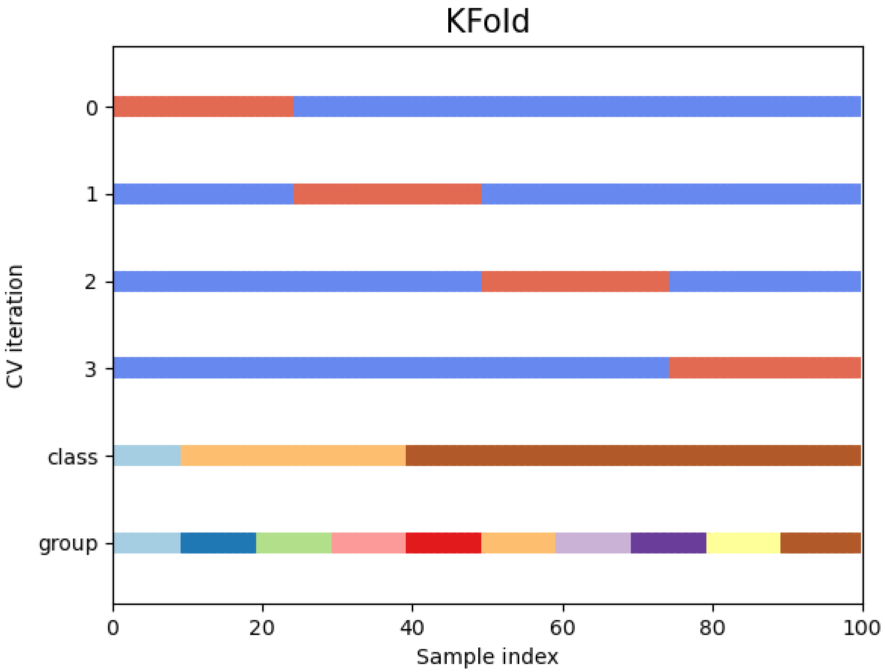


```
    parameters = {
        "alpha": [varNoise],
        "kernel": [gp.kernels.ConstantKernel(constant_value = gamma1, constant_value_bounds = (gamma1/1e5, gamma1*1e5)) + gp.kernels.ConstantKernel(constant_value = gamma2, constant_value_bounds = (gamma
2/1e5, gamma2*1e5)) * gp.kernels.RBF(length_scale = (l1,l2), length_scale_bounds = "fixed") + gp.kernels.WhiteKernel(noise_level = varNoise, noise_level_bounds = (varNoise/10, varNoise*1e3))
            for l1 in np.arange(1,21) * 0.015625 ],
        "n_restarts_optimizer" : [10],
        "normalize_y" : [False]}

    # define optimizer
    optimizer = ms.GridSearchCV(
        estimator = gp.GaussianProcessRegressor(),
        param_grid = parameters,
        cv = ms.KFold(5),
        n_jobs = 20,
        verbose = 2)
```

Evaluate an algorithm

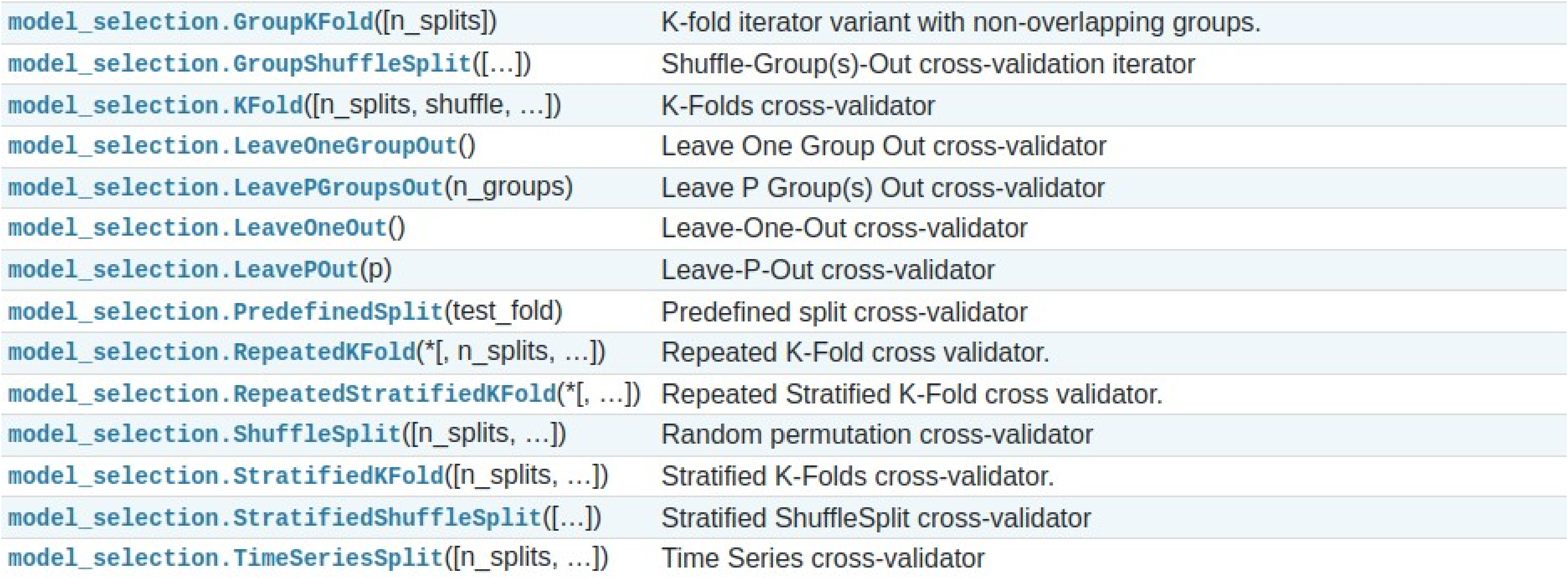
Cross validation



- Split the dataset into two: The trainng dataset and the testing dataset,
- Train the algorithm with the Training dataset
- Predict the labels of the testing dataset,
- Compare the predicted labels with the true value of the label

Evaluate an algorithm

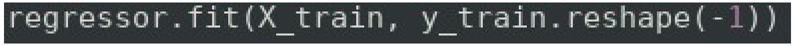
There are many algorithms to split the dataset,



model_selection.GroupKFold([n_splits])	K-fold iterator variant with non-overlapping groups.
model_selection.GroupShuffleSplit([…])	Shuffle-Group(s)-Out cross-validation iterator
model_selection.KFold([n_splits, shuffle, …])	K-Folds cross-validator
model_selection.LeaveOneGroupOut()	Leave One Group Out cross-validator
model_selection.LeavePGroupsOut(n_groups)	Leave P Group(s) Out cross-validator
model_selection.LeaveOneOut()	Leave-One-Out cross-validator
model_selection.LeavePOut(p)	Leave-P-Out cross-validator
model_selection.PredefinedSplit(test_fold)	Predefined split cross-validator
model_selection.RepeatedKFold(*[, n_splits, …])	Repeated K-Fold cross validator.
model_selection.RepeatedStratifiedKFold(*[, …])	Repeated Stratified K-Fold cross validator.
model_selection.ShuffleSplit([n_splits, …])	Random permutation cross-validator
model_selection.StratifiedKFold([n_splits, …])	Stratified K-Folds cross-validator.
model_selection.StratifiedShuffleSplit([…])	Stratified ShuffleSplit cross-validator
model_selection.TimeSeriesSplit([n_splits, …])	Time Series cross-validator

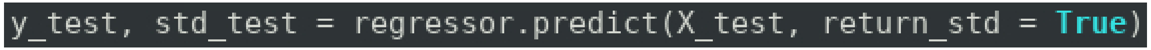
Make prediction

- Define a regressor with optimized hyperparameters and fit model with data



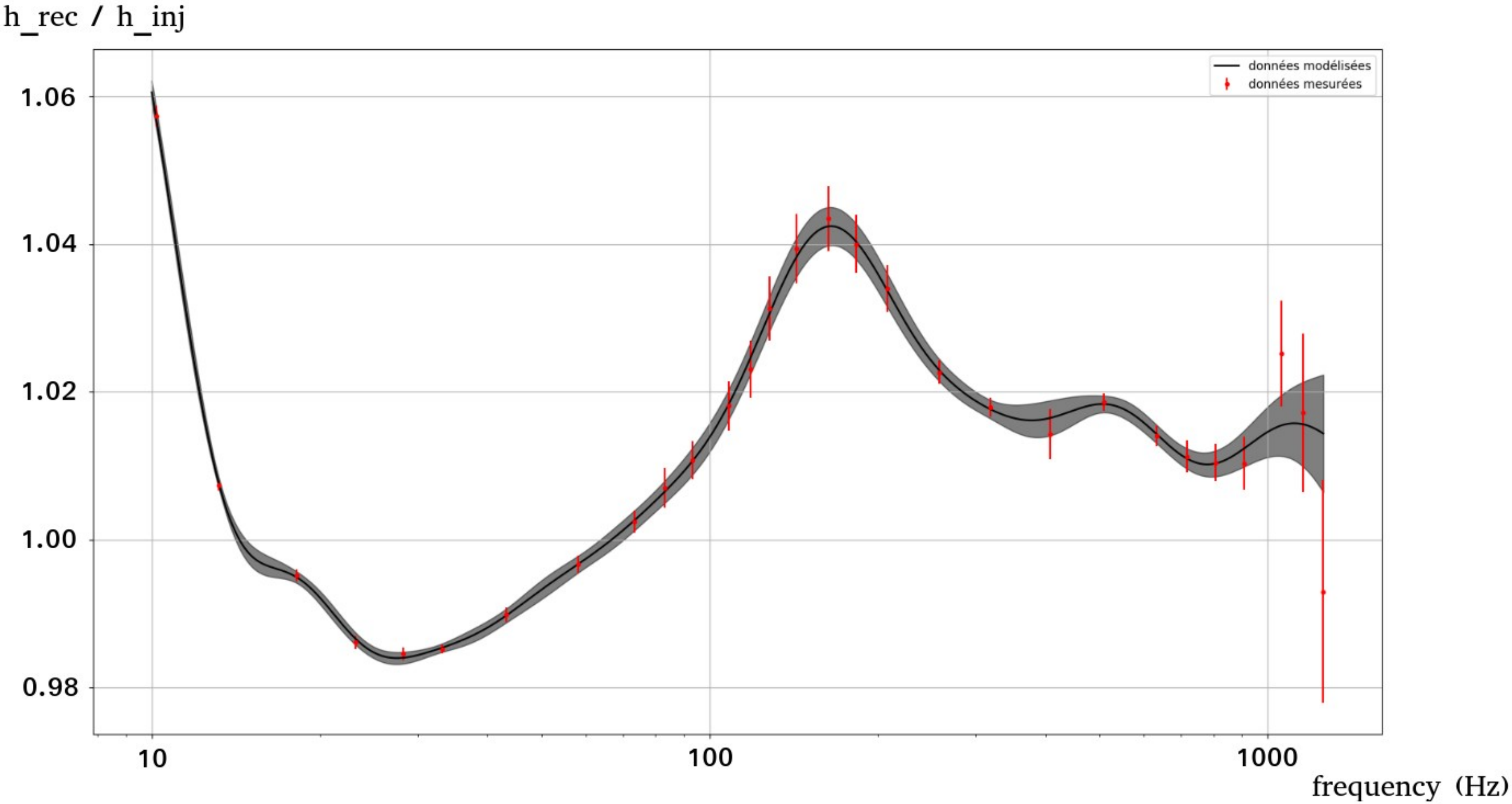
```
regressor.fit(X_train, y_train.reshape(-1))
```

- Predict values of label at the test dataset



```
y_test, std_test = regressor.predict(X_test, return_std = True)
```

Make prediction



Thank you for your attention