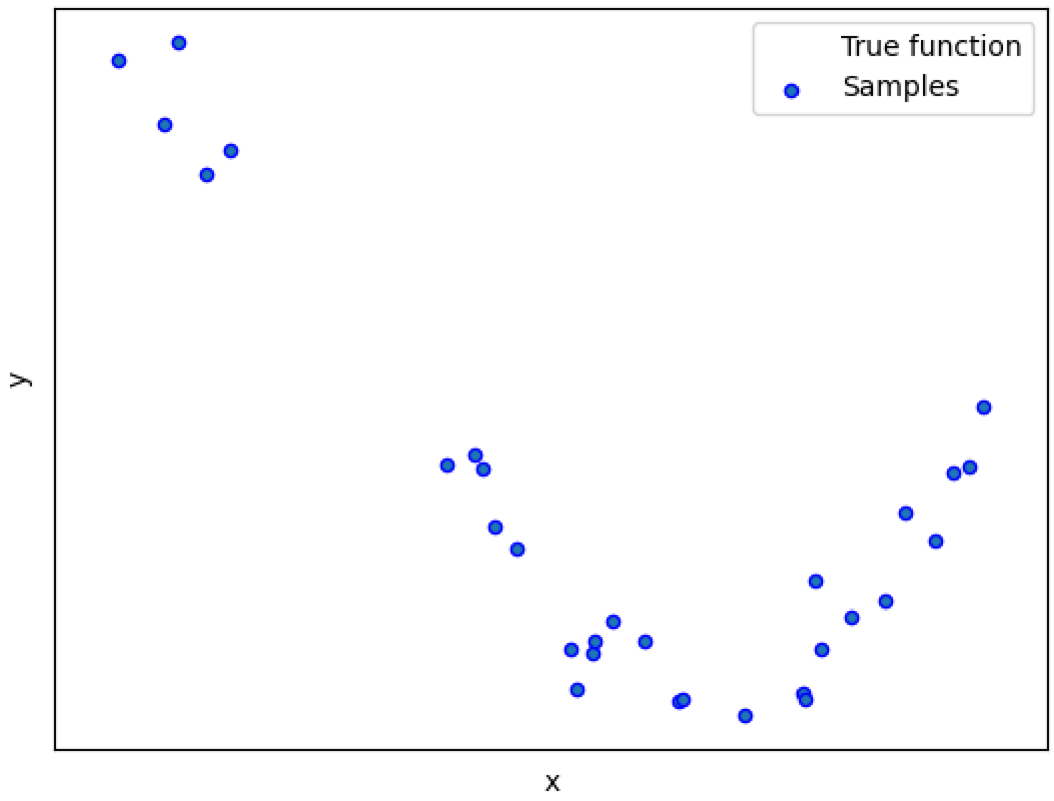
ML1 Practical 6: Model Selection & Evaluation

Example: Logistic Regression with Polynomial Features

In the following plot, we see a function $f(x) = cos(\frac{3}{2}\pi x)$ and some noisy samples from that function. We use three different estimators to fit the function: linear regression with polynomial features of degree 1, 4 and 15. We see that the first estimator can at best provide only a poor fit to the samples and the true function because it is too simple (high bias), the second estimator approximates it almost perfectly and the last estimator approximates the training data perfectly but does not fit the true function very well, i.e. it is very sensitive to varying training data (high variance).

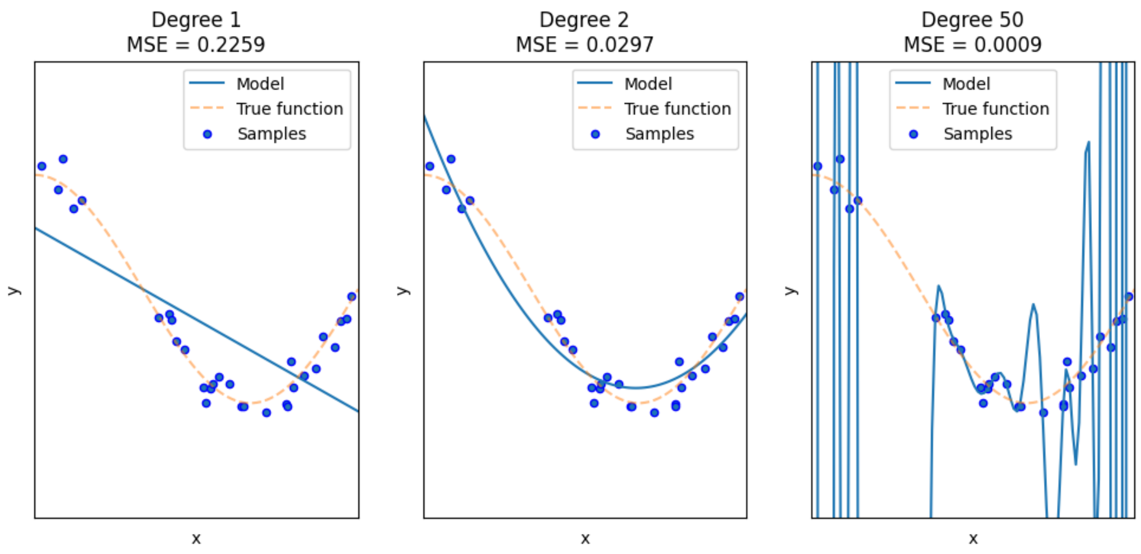
In [2]:
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import cross_val_score


def true_fun(X):
    return np.cos(1.5 * np.pi * X)


def generate_dataset(n_samples=30):
    np.random.seed(0)
    X = np.sort(np.random.rand(n_samples))
    y = true_fun(X) + np.random.randn(n_samples) * 0.1
    return X, y

X, y = generate_dataset()
```

In [3]:
```
xs = np.linspace(0., 1., 100)
ax = plt.gca()
plt.setp(ax, xticks=(), yticks=())
plt.plot(xs, true_fun(xs), c='C1', label='True function', alpha=0.0, ls='
plt.scatter(X, y,edgecolor="b", s=20, label="Samples")
plt.xlabel('x')
plt.ylabel('y')
plt.legend()
plt.show()
```



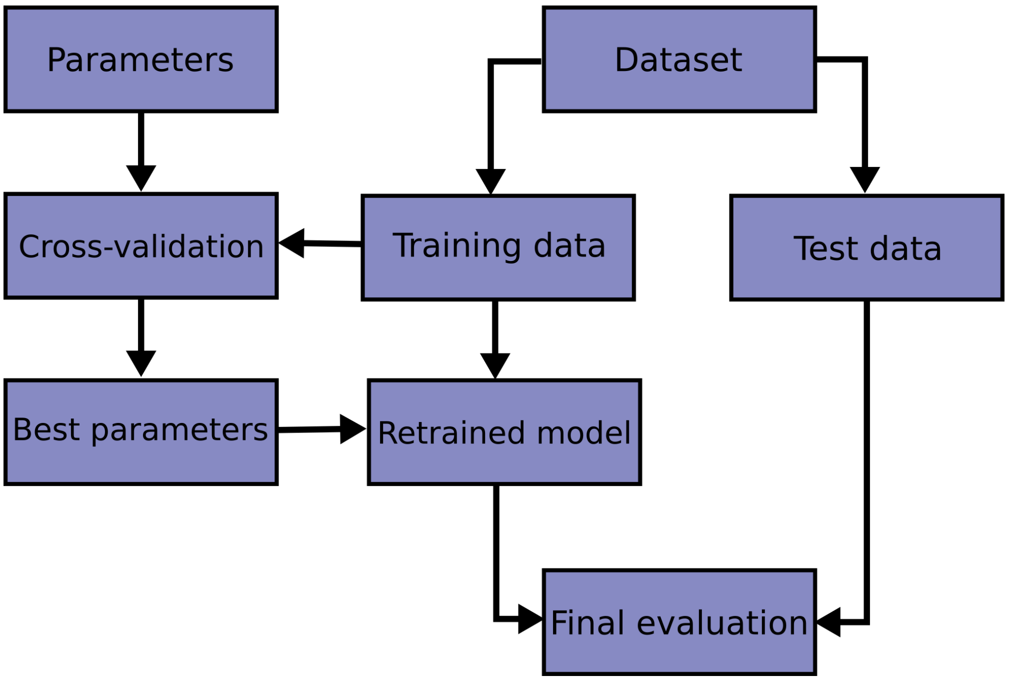
This example demonstrates the problems of underfitting and overfitting and how we can use linear regression with polynomial features to approximate nonlinear functions. The plot shows the function that we want to approximate, which is a part of the cosine function. In addition, the samples from the real function and the approximations of different models are displayed. The models have polynomial features of different degrees. We can see that a linear function (polynomial with degree 1) is not sufficient to fit the training samples. This is called **underfitting**. A polynomial of degree 4 approximates the true function almost perfectly. However, for higher degrees the model will **overfit** the training data, i.e. it learns the noise of the training data. We evaluate quantitatively **overfitting / underfitting** by using cross-validation. We calculate the mean squared error (MSE) on the validation set, the higher, the less likely the model generalizes correctly from the training data.

In [4]:
```
from sklearn.metrics import mean_squared_error
degrees = [1, 2, 50]
plt.figure(figsize=(4 * len(degrees), 5))
for i in range(len(degrees)):
    ax = plt.subplot(1, len(degrees), i + 1)
    plt.setp(ax, xticks=(), yticks=())

    polynomial_features = PolynomialFeatures(degree=degrees[i], include_b
    linear_regression = LinearRegression()
    pipeline = Pipeline(
        [
            ("polynomial_features", polynomial_features),
            ("linear_regression", linear_regression),
        ]
    )
    pipeline.fit(X[:, np.newaxis], y)
    y_pred = pipeline.predict(X[:, np.newaxis])
    scores = mean_squared_error(y, y_pred)
    X_test = np.linspace(0, 1, 100)
    plt.plot(X_test, pipeline.predict(X_test[:, np.newaxis]), label="Mode
    plt.plot(X_test, true_fun(X_test), label="True function", alpha=0.5,
    plt.scatter(X, y, edgecolor="b", s=20, label="Samples")
    plt.xlabel("x")
    plt.ylabel("y")
    plt.xlim((0, 1))
    plt.ylim((-2, 2))
    plt.legend(loc="best")
    plt.title(
        "Degree {}\nMSE = {:.4f}".format(
            degrees[i], scores
        )
    )
plt.show()
```



Cross Validation

Learning the parameters of a prediction function and testing it on the same data is a methodological mistake: a model that would just repeat the labels of the samples that it has just seen would have a perfect score but would fail to predict anything useful on yet-unseen data. This situation is called overfitting. To avoid it, it is common practice when performing a (supervised) machine learning experiment to hold out part of the available data as a test set `X_test, y_test`. Note that the word “experiment” is not intended to denote academic use only, because even in commercial settings machine learning usually starts out experimentally. Here is a flowchart of typical cross validation workflow in model training. The best parameters can be determined by grid search techniques.



Every estimator has its advantages and drawbacks. Its generalization error can be decomposed in terms of bias, variance and noise. The bias of an estimator is its average error for different training sets. The variance of an estimator indicates how sensitive it is to varying training sets. Noise is a property of the data.

Getting Started

The famous Iris dataset, first used by Sir R.A. Fisher. The dataset is taken from Fisher's paper. This is perhaps the best known dataset to be found in the pattern recognition literature. Fisher's paper is a classic in the field and is referenced frequently to this day. The data set contains 3 classes of 50 instances each, where each class refers to a type of iris plant. One class is linearly separable from the other 2; the latter are NOT linearly separable from each other.The dataset contains a set of 150 records under five attributes - sepal length, sepal width, petal length, petal width and species.

In [5]:
```
import numpy as np
from sklearn.model_selection import train_test_split
from sklearn import datasets
X, y = datasets.load_iris(return_X_y=True)
```

We can now quickly sample a training set while holding out 20% of the data for testing (evaluating) our classifier:

```
In [6]: X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
```

```
In [7]: print(f"X_train.shape: {X_train.shape}")
        print(f"X_test.shape:  {X_test.shape}")
        print(f"y_train.shape: {y_train.shape}")
        print(f"y_test.shape:  {y_test.shape}")
```

```
X_train.shape: (120, 4)
X_test.shape:  (30, 4)
y_train.shape: (120,)
y_test.shape:  (30,)
```

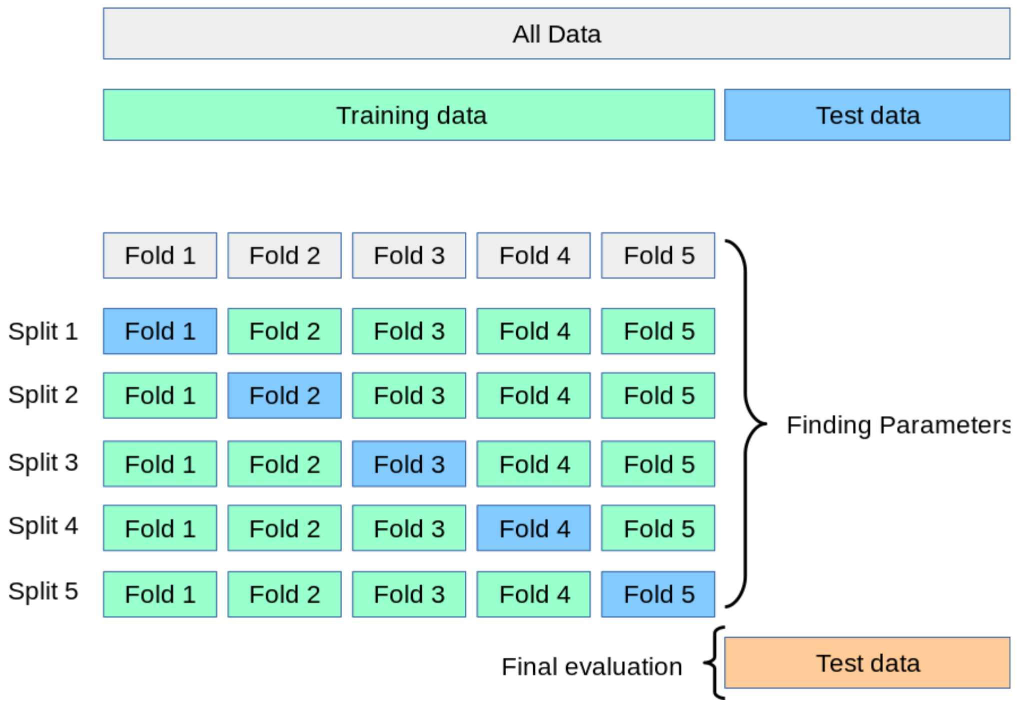
When evaluating different settings (“hyperparameters”) for estimators, such as the C setting that must be manually set for an SVM, there is still a risk of overfitting on the test set because the parameters can be tweaked until the estimator performs optimally. This way, knowledge about the test set can “leak” into the model and evaluation metrics no longer report on generalization performance. To solve this problem, yet another part of the dataset can be held out as a so-called “validation set”: training proceeds on the training set, after which evaluation is done on the validation set, and when the experiment seems to be successful, final evaluation can be done on the test set.

However, by partitioning the available data into three sets, we drastically reduce the number of samples which can be used for learning the model, and the results can depend on a particular random choice for the pair of (train, validation) sets.

A solution to this problem is a procedure called cross-validation (CV for short). A test set should still be held out for final evaluation, but the validation set is no longer needed when doing CV. In the basic approach, called k-fold CV, the training set is split into k smaller sets (other approaches are described below, but generally follow the same principles). The following procedure is followed for each of the k “folds”:

- A model is trained using $k - 1$ of the folds as training data;
- the resulting model is validated on the remaining part of the data (i.e., it is used as a test set to compute a performance measure such as accuracy).

The performance measure reported by k-fold cross-validation is then the average of the values computed in the loop. This approach can be computationally expensive, but does not waste too much data (as is the case when fixing an arbitrary validation set), which is a major advantage in problems such as inverse inference where the number of samples is very small.



Example: Linear Regression with Polynomial Features cont'

The simplest way to use cross-validation is to call the `cross_val_score` helper function on the estimator and the dataset.

The following example demonstrates how to estimate the accuracy of logistic regression on our dataset by splitting the data, fitting a model and computing the score 5 consecutive times (with different splits each time):

In [8]:
```
X, y = generate_dataset()
clf = LinearRegression()
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
scores = cross_val_score(clf, X_train[:, None], y_train, cv=5)
scores.mean()
```

Out[8]:
```
-0.372135740557323
```

Bias and variance are inherent properties of estimators and we usually have to select learning algorithms and hyperparameters so that both bias and variance are as low as possible. Another way to reduce the variance of a model is to use more training data. However, you should only collect more training data if the true function is too complex to be approximated by an estimator with a lower variance.

In the simple one-dimensional problem that we have seen in the example it is easy to see whether the estimator suffers from bias or variance. However, in high-dimensional spaces, models can become very difficult to visualize.

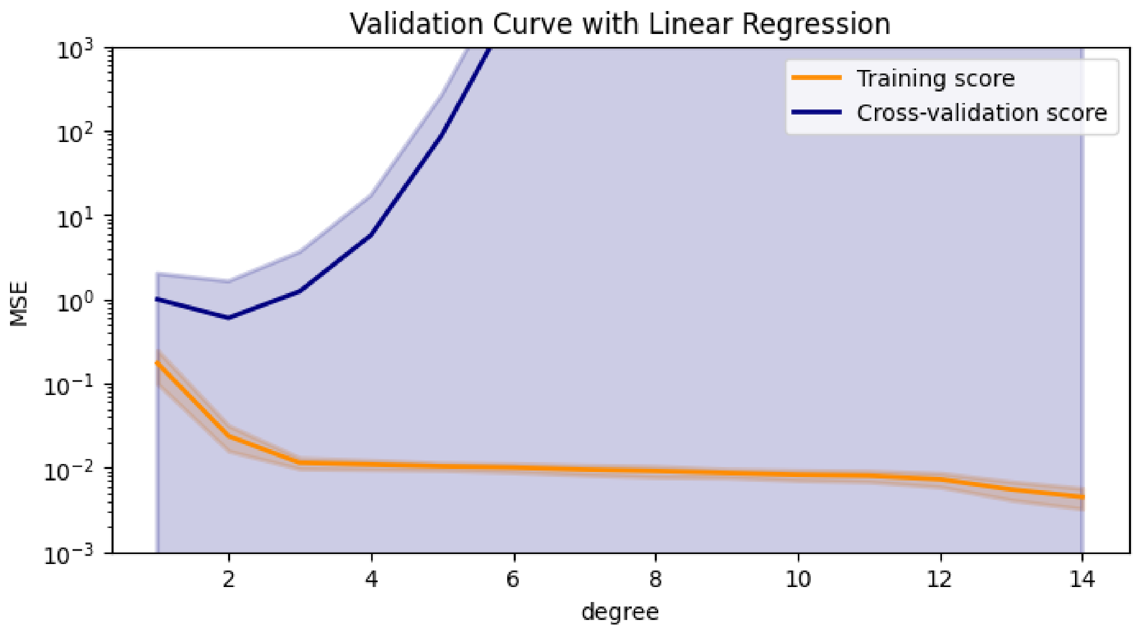
Validation curve

To validate a model we need a scoring function, for example accuracy for classifiers. The proper way of choosing multiple hyperparameters of an estimator is of course grid search or similar methods that select the hyperparameter with the maximum score on a validation set or multiple validation sets. Note that if we optimize the hyperparameters based on a validation score the validation score is biased and not a good estimate of the generalization any longer. To get a proper estimate of the generalization we have to compute the score on another test set.

However, it is sometimes helpful to plot the influence of a single hyperparameter on the training score and the validation score to find out whether the estimator is overfitting or underfitting for some hyperparameter values.

In [9]:
```
import matplotlib.pyplot as plt
import numpy as np

from sklearn.model_selection import cross_validate

param_range = np.arange(1, 15)

train_scores = []
test_scores = []
for degree in param_range:
    polynomial_features = PolynomialFeatures(degree=degree, include_bias=
    linear_regression = LinearRegression()
    pipeline = Pipeline(
        [
            ("polynomial_features", polynomial_features),
            ("linear_regression", linear_regression),
        ]
    )
    result = cross_validate(pipeline, X[:, np.newaxis], y, return_train_s
    train_scores.append(result['train_score'])
    test_scores.append(result['test_score'])
train_scores = np.asarray(train_scores)
test_scores = np.asarray(test_scores)

train_scores_mean = np.mean(-train_scores, axis=1)
train_scores_std = np.std(-train_scores, axis=1)
test_scores_mean = np.mean(-test_scores, axis=1)
test_scores_std = np.std(-test_scores, axis=1)

plt.figure(figsize=(8, 4))
plt.title("Validation Curve with Linear Regression")
plt.xlabel(r"degree")
plt.ylabel("MSE")
plt.ylim(10.**-3, 10.**3)
plt.yscale('log')
lw = 2
plt.plot(param_range, train_scores_mean, label="Training score", color="d
plt.fill_between(
    param_range,
    train_scores_mean - train_scores_std,
    train_scores_mean + train_scores_std,
    alpha=0.2,
    color="darkorange",
    lw=lw,
)
```

```
plt.plot(
    param_range, test_scores_mean, label="Cross-validation score", color=
)
plt.fill_between(
    param_range,
    test_scores_mean - test_scores_std,
    test_scores_mean + test_scores_std,
    alpha=0.2,
    color="navy",
    lw=lw,
)
plt.legend(loc="best")
plt.show()
```



Metrics

Classification Metrics

The `sklearn.metrics` module implements several loss, score, and utility functions to measure classification performance. Some metrics might require probability estimates of the positive class, confidence values, or binary decisions values. Most implementations allow each sample to provide a weighted contribution to the overall score, through the `sample_weight` parameter.

Accuracy score

The `accuracy_score` function computes the accuracy, either the fraction (default) or the count (normalize=False) of correct predictions.

If $\hat{y}_i$ is the predicted value of the i-th sample and y_i is the corresponding true value, then the fraction of correct predictions over n_samples is defined as

$$\frac{1}{n_\text{samples}} \sum_{i=0}^{n_\text{samples}-1} 1(\hat{y}_i = y_i)$$

where $1(\cdot)$ is the indicator function.

```
In [10]: import numpy as np
         from sklearn.metrics import accuracy_score
         y_pred = [0, 2, 1, 3]
         y_true = [0, 1, 2, 3]
         accuracy_score(y_true, y_pred)
```

```
Out[10]: 0.5
```

Top-k accuracy score

The `top_k_accuracy_score` function is a generalization of accuracy_score. The difference is that a prediction is considered correct as long as the true label is associated with one of the `k` highest predicted scores. `accuracy_score` is the special case of `k = 1`.

```
In [11]: from sklearn.metrics import top_k_accuracy_score
         y_true = np.array([0, 1, 2, 2])
         y_score = np.array([[0.5, 0.2, 0.2],
                             [0.3, 0.4, 0.2],
                             [0.2, 0.4, 0.3],
                             [0.7, 0.2, 0.1]])
         top_k_accuracy_score(y_true, y_score, k=2)
```

```
Out[11]: 0.75
```

Confusion Matrix

The `confusion_matrix` function evaluates classification accuracy by computing the confusion matrix with each row corresponding to the true class (Wikipedia and other references may use different convention for axes).

By definition, entry i, j in a confusion matrix is the number of observations actually in group i, but predicted to be in group j. Here is an example:

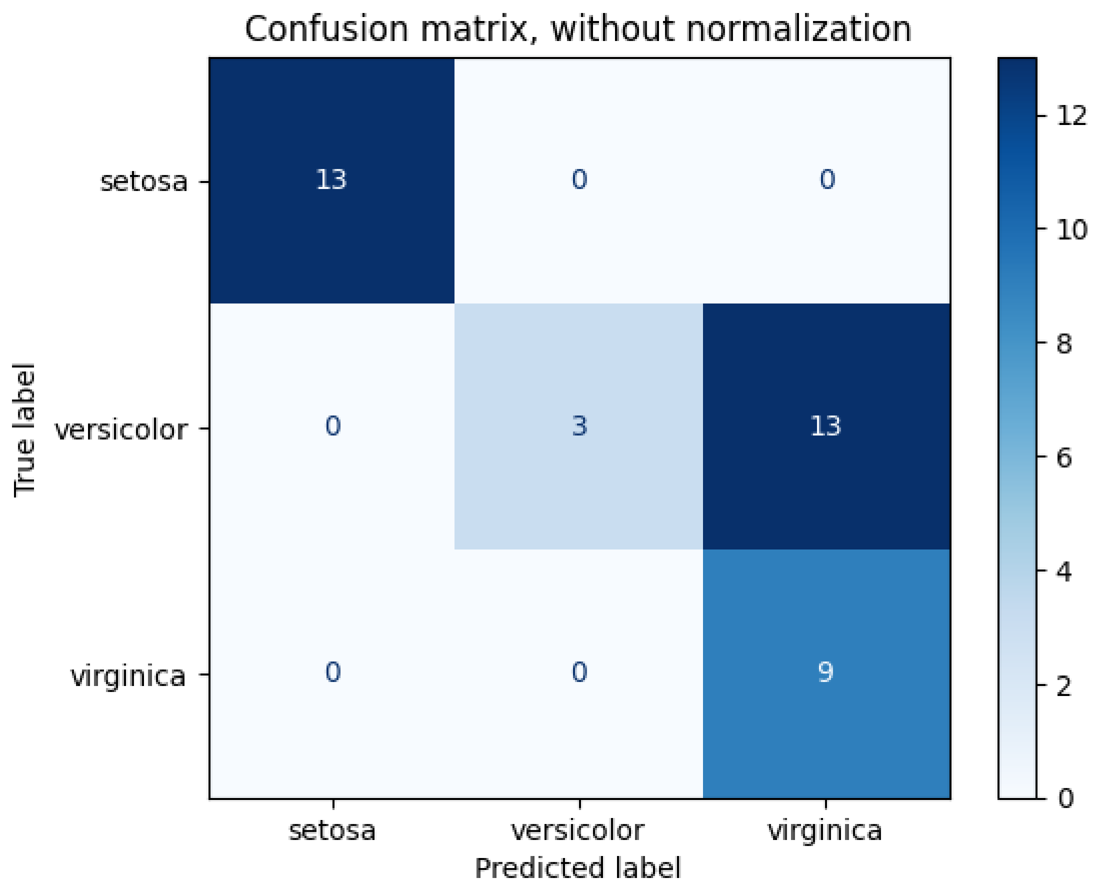
```
In [12]: from sklearn.metrics import confusion_matrix
         y_true = [2, 0, 2, 2, 0, 1]
         y_pred = [0, 0, 2, 2, 0, 2]
         confusion_matrix(y_true, y_pred)
```

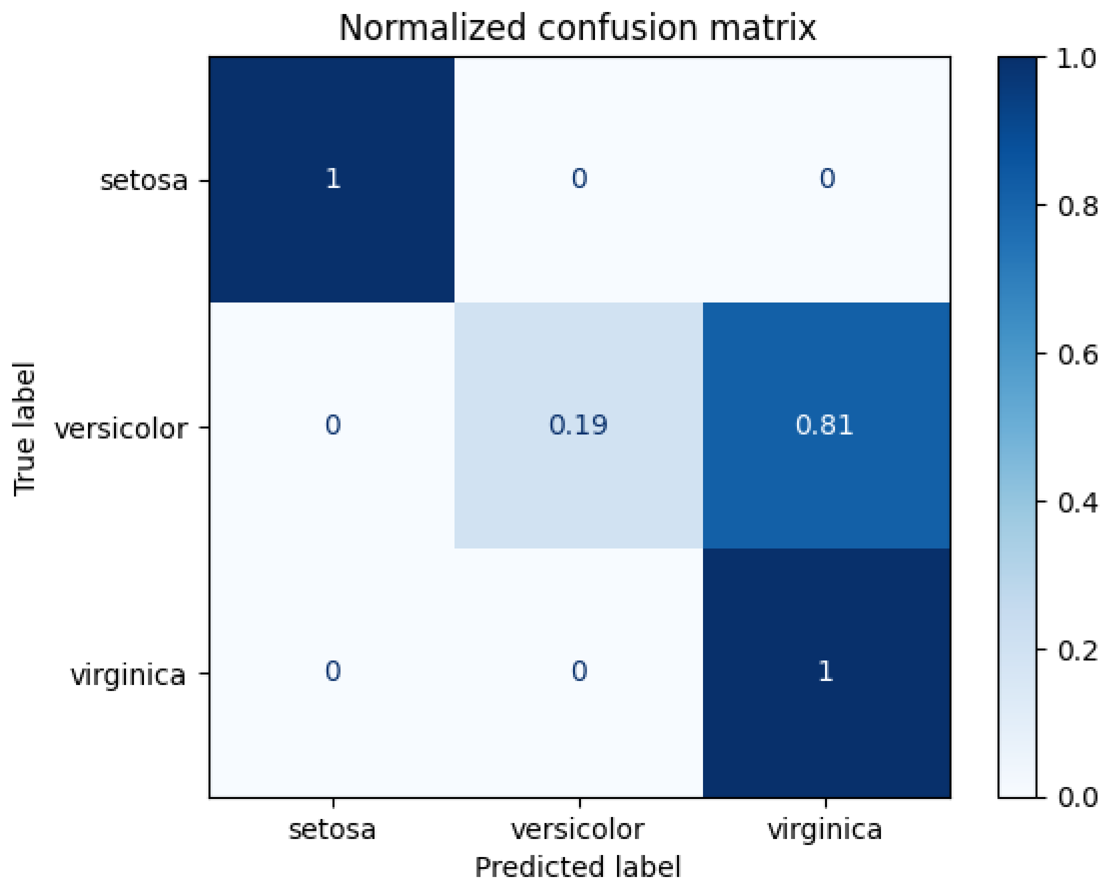
```
Out[12]: array([[2, 0, 0],
                [0, 0, 1],
                [1, 0, 2]])
```

```
In [13]: import numpy as np
         import matplotlib.pyplot as plt

         from sklearn import linear_model, datasets
         from sklearn.model_selection import train_test_split
```

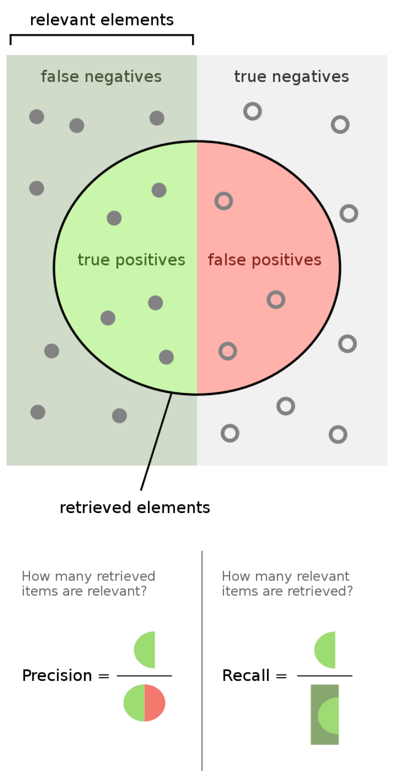
```python
from sklearn.metrics import ConfusionMatrixDisplay

# import some data to play with
iris = datasets.load_iris()
X = iris.data
y = iris.target
class_names = iris.target_names

# Split the data into a training set and a test set
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)

# Run classifier, using a model that is too regularized (C too low) to se
# the impact on the results
classifier = linear_model.LogisticRegression(C=0.01).fit(X_train, y_train

np.set_printoptions(precision=2)

# Plot non-normalized confusion matrix
titles_options = [
    ("Confusion matrix, without normalization", None),
    ("Normalized confusion matrix", "true"),
]
for title, normalize in titles_options:
    disp = ConfusionMatrixDisplay.from_estimator(
        classifier,
        X_test,
        y_test,
        display_labels=class_names,
        cmap=plt.cm.Blues,
        normalize=normalize,
    )
    disp.ax_.set_title(title)

    print(title)
    print(disp.confusion_matrix)

plt.show()
```

```
Confusion matrix, without normalization
[[13  0  0]
 [ 0  3 13]
 [ 0  0  9]]
Normalized confusion matrix
[[1.   0.   0.  ]
 [0.   0.19 0.81]
 [0.   0.   1.  ]]
```





Precision-Recall



Example of Precision-Recall metric to evaluate classifier output quality.

Precision-Recall is a useful measure of success of prediction when the classes are very imbalanced. In information retrieval, precision is a measure of result relevancy, while recall is a measure of how many truly relevant results are returned.

The precision-recall curve shows the tradeoff between precision and recall for different threshold. A high area under the curve represents both high recall and high precision, where high precision relates to a low false positive rate, and high recall relates to a low false negative rate. High scores for both show that the classifier is returning accurate results (high precision), as well as returning a majority of all positive results (high recall).

A system with high recall but low precision returns many results, but most of its predicted labels are incorrect when compared to the training labels. A system with high precision but low recall is just the opposite, returning very few results, but most of its predicted labels are correct when compared to the training labels. An ideal system with high precision and high recall will return many results, with all results labeled correctly.

Precision (P) is defined as the number of true positives (T_p) over the number of true positives plus the number of false positives (F_p).

$$P = \frac{T_p}{T_p+F_p}$$

Recall (R) is defined as the number of true positives (T_p) over the number of true positives plus the number of false negatives (F_n).

$$R = \frac{T_p}{T_p+F_n}$$

These quantities are also related to the (F_1) score, which is defined as the harmonic mean of precision and recall.

$$F1 = 2\frac{P \times R}{P+R}$$

Note that the precision may not decrease with recall. The definition of precision ($\frac{T_p}{T_p+F_p}$) shows that lowering the threshold of a classifier may increase the denominator, by increasing the number of results returned. If the threshold was previously set too high, the new results may all be true positives, which will increase precision. If the previous threshold was about right or too low, further lowering the threshold will introduce false positives, decreasing precision.

Recall is defined as $\frac{T_p}{T_p+F_n}$, where T_p+F_n does not depend on the classifier threshold. This means that lowering the classifier threshold may increase recall, by increasing the number of true positive results. It is also possible that lowering the threshold may leave recall unchanged, while the precision fluctuates.

The relationship between recall and precision can be observed in the stairstep area of the plot - at the edges of these steps a small change in the threshold considerably reduces precision, with only a minor gain in recall.

Average precision (AP) summarizes such a plot as the weighted mean of precisions achieved at each threshold, with the increase in recall from the previous threshold used as the weight:

$$\text{AP} = \sum_n (R_n - R_{n-1}) P_n$$

where P_n and R_n are the precision and recall at the nth threshold. A pair (R_k, P_k) is referred to as an *operating point*.

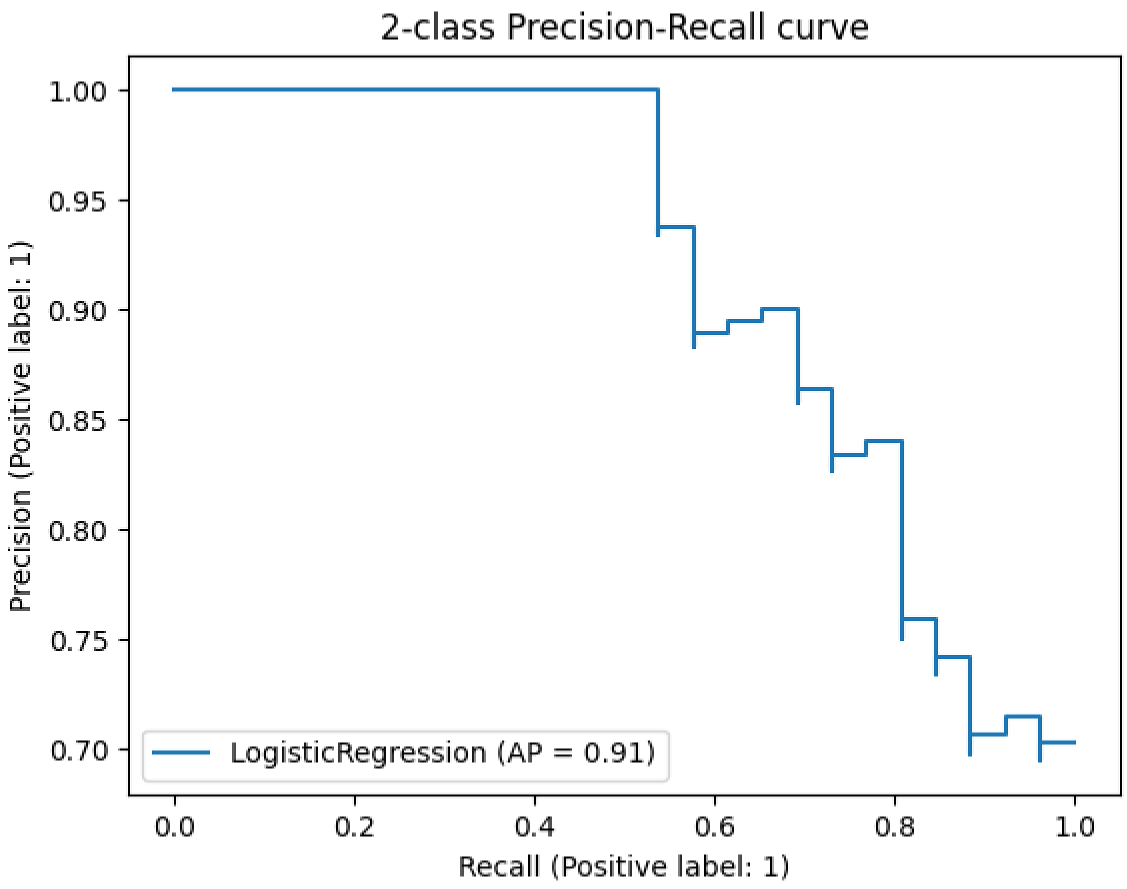
Precision-recall curves are typically used in binary classification to study the output of a classifier. In order to extend the precision-recall curve and average precision to multi-class or multi-label classification, it is necessary to binarize the output. One curve can be drawn per label, but one can also draw a precision-recall curve by considering each element of the label indicator matrix as a binary prediction (micro-averaging).

In [14]:
```
import numpy as np
from sklearn.datasets import load_iris
from sklearn.model_selection import train_test_split

X, y = load_iris(return_X_y=True)

# Add noisy features
random_state = np.random.RandomState(0)
n_samples, n_features = X.shape
X = np.concatenate([X, random_state.randn(n_samples, 200 * n_features)],

# Limit to the two first classes, and split into training and test
X_train, X_test, y_train, y_test = train_test_split(
    X[y < 2], y[y < 2], test_size=0.5, random_state=random_state
)
```

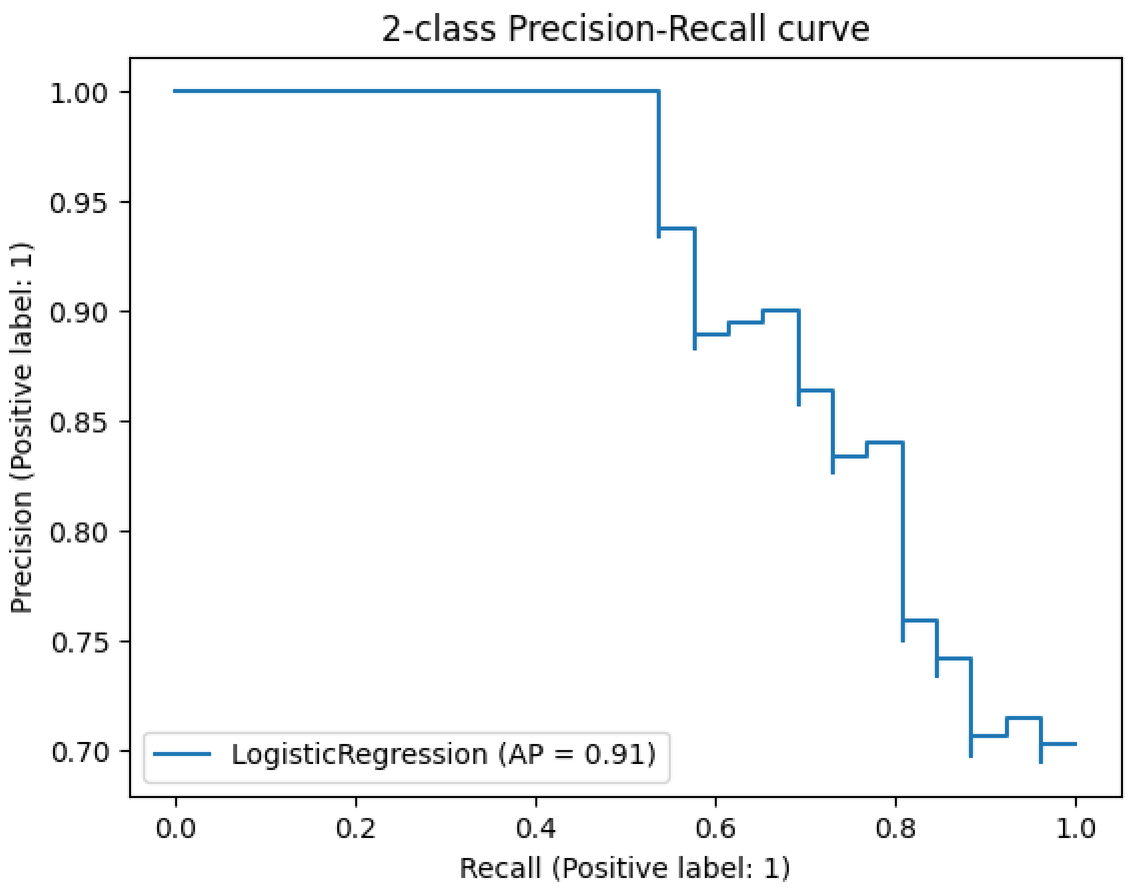
In [15]:
```
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.linear_model import LogisticRegression

classifier = make_pipeline(StandardScaler(), LogisticRegression(random_st
classifier.fit(X_train, y_train)
```

Out[15]:
```
Pipeline(steps=[('standardscaler', StandardScaler()),
                ('logisticregression',
                 LogisticRegression(random_state=RandomState(MT19937) at
0x7F3542EA65A0))])
```

In [16]:
```
from sklearn.metrics import PrecisionRecallDisplay

display = PrecisionRecallDisplay.from_estimator(
    classifier, X_test, y_test, name="LogisticRegression"
)
_ = display.ax_.set_title("2-class Precision-Recall curve")
```



In [17]:
```
y_score = classifier.decision_function(X_test)

display = PrecisionRecallDisplay.from_predictions(y_test, y_score, name="
_ = display.ax_.set_title("2-class Precision-Recall curve")
```



Regression Metrics

Mean squared error

The `mean_squared_error` function computes mean square error, a risk metric corresponding to the expected value of the squared (quadratic) error or loss.

If $\hat{y}_i$ is the predicted value of the i-th sample, and y_i is the corresponding true value, then the mean squared error (MSE) estimated over n_{samples} is defined as

$$\frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}}-1} (y_i - \hat{y}_i)^2$$

```
In [18]: from sklearn.metrics import mean_squared_error
         y_true = [3, -0.5, 2, 7]
         y_pred = [2.5, 0.0, 2, 8]
         mean_squared_error(y_true, y_pred)
```

```
Out[18]: 0.375
```

Hyperparameter Optimization

Hyper-parameters are parameters that are not directly learnt within estimators. In scikit-learn they are passed as arguments to the constructor of the estimator classes. Typical examples include `C`, `kernel` and `gamma` for Support Vector Classifier, `alpha` for Lasso, etc.

It is possible and recommended to search the hyper-parameter space for the best cross validation score.

Any parameter provided when constructing an estimator may be optimized in this manner.

A search consists of:

- an estimator (regressor or classifier such as sklearn.svm.SVC());
- a parameter space;
- a method for searching or sampling candidates;
- a cross-validation scheme; and
- a score function.

Two generic approaches to parameter search are provided in scikit-learn: for given values, `GridSearchCV` exhaustively considers all parameter combinations, while `RandomizedSearchCV` can sample a given number of candidates from a parameter space with a specified distribution.

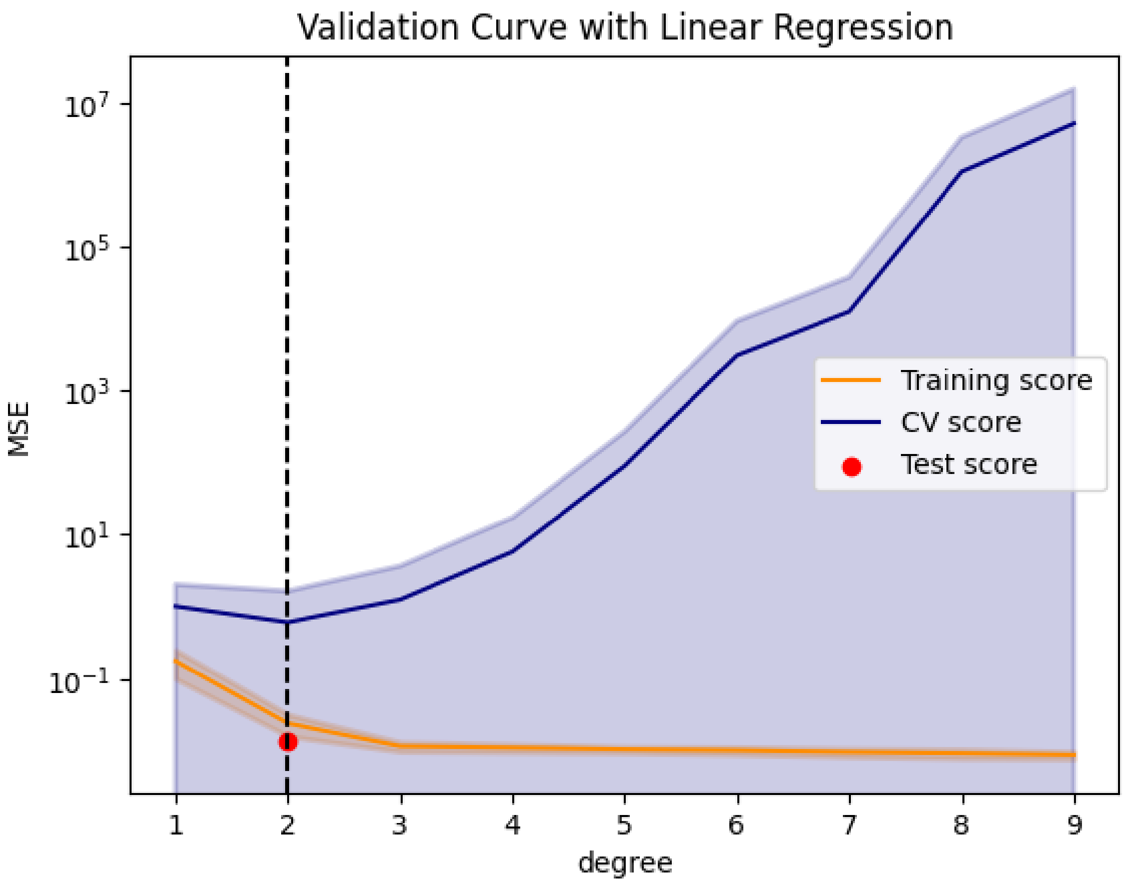
GridSearchCV

The grid search provided by `GridSearchCV` exhaustively generates candidates from a grid of parameter values specified with the `param_grid` parameter. For instance, the following `param_grid`:

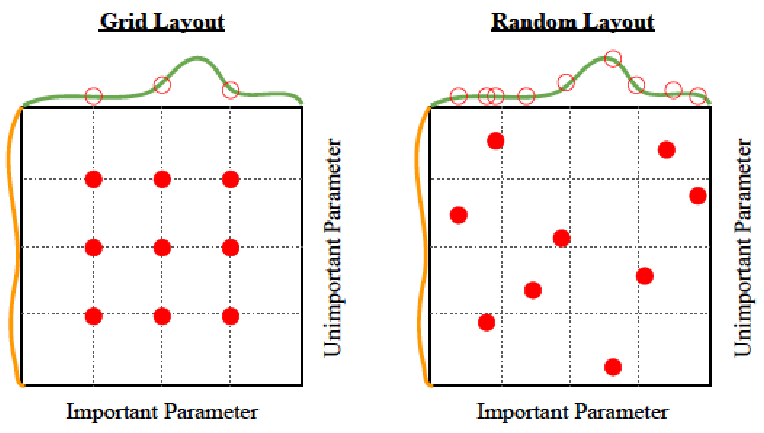
In [19]:
```
X, y = generate_dataset()
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
```

In [20]:
```
from sklearn.model_selection import GridSearchCV

polynomial_features = PolynomialFeatures(include_bias=False)
linear_regression = LinearRegression()
pipeline = Pipeline(
    [
        ("polynomial_features", polynomial_features),
        ("linear_regression", linear_regression),
    ]
)
degrees = np.arange(1, 10)
param_grid = [
    {'polynomial_features__degree': degrees}
]

clf = GridSearchCV(pipeline, param_grid, cv=5, return_train_score=True, s
clf.fit(X[:, None], y)

mean_train_score = -clf.cv_results_['mean_train_score']
mean_test_score = -clf.cv_results_['mean_test_score']
std_train_score = clf.cv_results_['std_train_score']
std_test_score = clf.cv_results_['std_test_score']
```

```
plt.plot(degrees, mean_train_score, color='darkorange', label='Training s
plt.fill_between(
    degrees,
    mean_train_score - std_train_score,
    mean_train_score + std_train_score,
    alpha=0.2,
    color="darkorange",
    lw=2,
)
plt.plot(degrees, mean_test_score, color='navy', label='CV score')
plt.fill_between(
    degrees,
    mean_test_score - std_test_score,
    mean_test_score + std_test_score,
    alpha=0.2,
    color="navy",
    lw=2,
)

best_degree = clf.best_params_['polynomial_features__degree']
test_score = -clf.score(X_test[:, None], y_test)
plt.axvline(best_degree, c='k', ls='--')
plt.scatter(best_degree, test_score, c='r', label='Test score')

plt.xlabel('degree')
plt.ylabel('MSE')
plt.yscale('log')
plt.legend()
plt.title("Validation Curve with Linear Regression")
plt.show()
```



Random Search

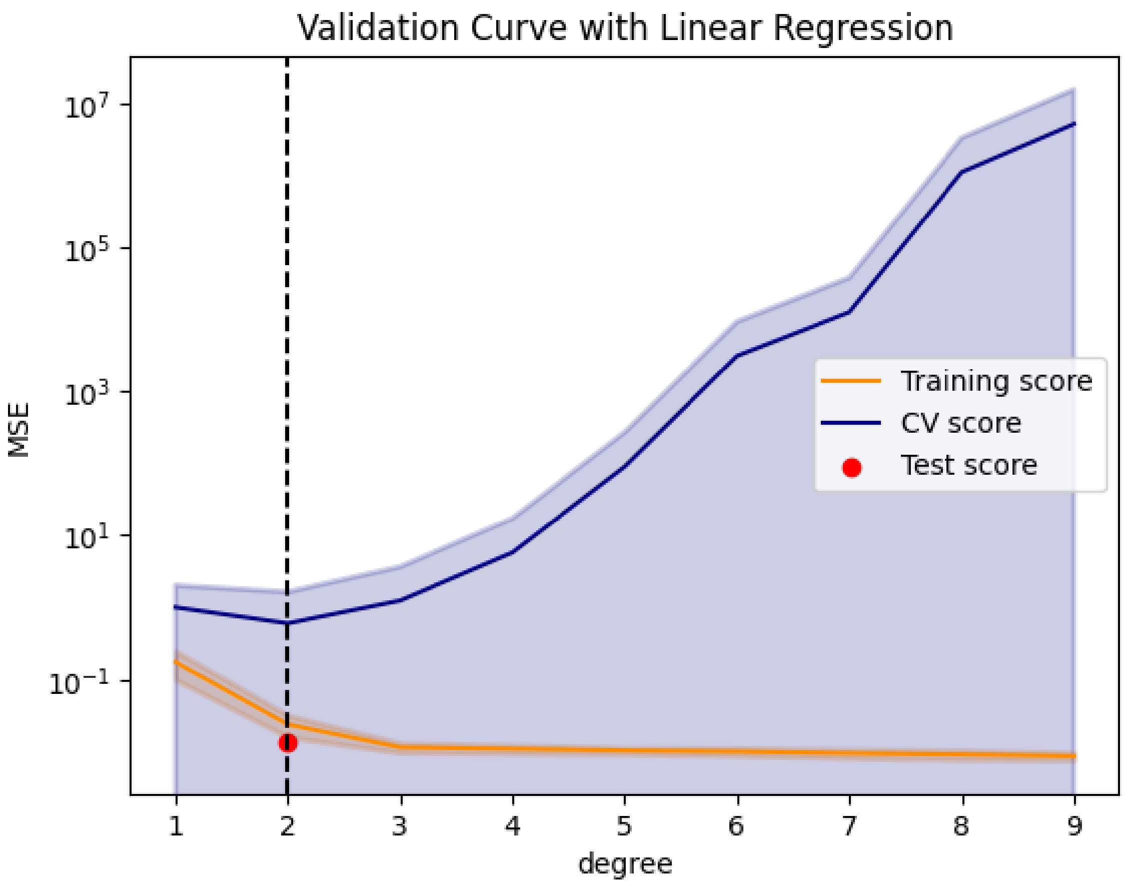


In [21]:

```
from sklearn.model_selection import RandomizedSearchCV

polynomial_features = PolynomialFeatures(include_bias=False)
linear_regression = LinearRegression()
pipeline = Pipeline(
    [
        ("polynomial_features", polynomial_features),
        ("linear_regression", linear_regression),
    ]
)
degrees = np.arange(1, 10)
param_grid = [
    {'polynomial_features__degree': degrees}
]

clf = RandomizedSearchCV(pipeline, param_grid, cv=5, return_train_score=T
clf.fit(X[:, None], y)

mean_train_score = -clf.cv_results_['mean_train_score']
mean_test_score = -clf.cv_results_['mean_test_score']
std_train_score = clf.cv_results_['std_train_score']
std_test_score = clf.cv_results_['std_test_score']

plt.plot(degrees, mean_train_score, color='darkorange', label='Training s
plt.fill_between(
    degrees,
    mean_train_score - std_train_score,
    mean_train_score + std_train_score,
    alpha=0.2,
    color="darkorange",
    lw=2,
)
plt.plot(degrees, mean_test_score, color='navy', label='CV score')
plt.fill_between(
    degrees,
    mean_test_score - std_test_score,
    mean_test_score + std_test_score,
    alpha=0.2,
    color="navy",
    lw=2,
)
```

```
best_degree = clf.best_params_['polynomial_features__degree']
test_score = -clf.score(X_test[:, None], y_test)
plt.axvline(best_degree, c='k', ls='--')
plt.scatter(best_degree, test_score, c='r', label='Test score')

plt.xlabel('degree')
plt.ylabel('MSE')
plt.yscale('log')
plt.legend()
plt.title("Validation Curve with Linear Regression")
plt.show()
```

```
/home/horst2204/miniconda3/envs/synch_dynapse/lib/python3.7/site-package
s/sklearn/model_selection/_search.py:296: UserWarning: The total space o
f parameters 9 is smaller than n_iter=10. Running 9 iterations. For exha
ustive searches, use GridSearchCV.
  UserWarning,
```



Further Reading

- https://github.com/FacebookResearch/Nevergrad

```
In [ ]:
```