Supervised Learning – Part 3

ESM3081 Programming for Data Science

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Learning algorithms covered in this course

- **Supervised Learning** (Classification/Regression)
  - K-Nearest Neighbors
  - **Linear Models (Logistic/Linear Regression)**
  - Decision Trees
  - Random Forests
  - Gradient Boosting Machines
  - Support Vector Machines
  - Neural Networks

** Many algorithms have a classification and a regression variant, and we will describe both.*

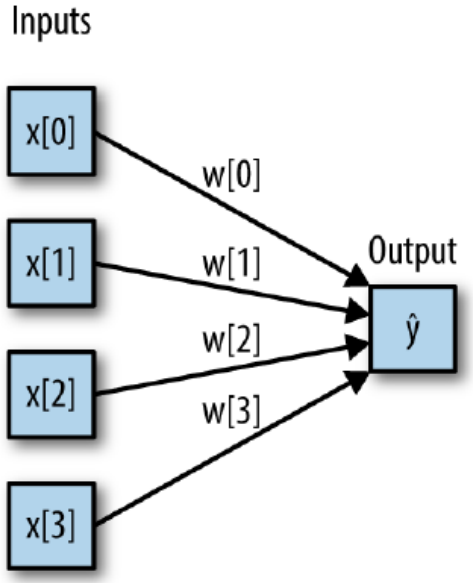
** We will review the most popular machine learning algorithms, explain how they learn from data and how they make predictions, and examine the strengths and weaknesses of each algorithm.*

Linear Models

Linear Models

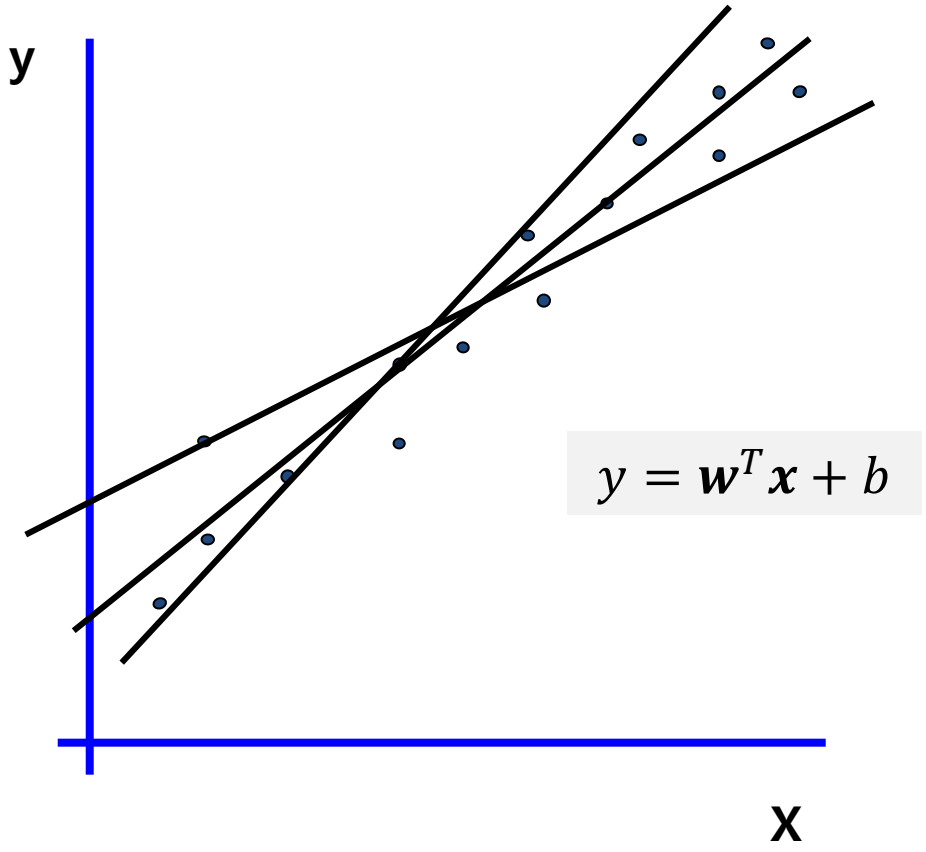
- **Linear models make a prediction using a *linear function* of the input features**

- **Learning algorithms for regression**
  - Linear Regression
  - Ridge Regression
  - Lasso Regression
  - Elastic Net Regression
  - Principal Component Regression
  - Partial Least Squares Regression
  - (Linear) Support Vector Regression
  - …
- **Learning algorithms for binary classification**
  - Logistic Regression
  - (Linear) Support Vector Machine
  - Linear Discriminant Analysis
  - …



Linear Regression

- For linear models for regression, the prediction $\hat{y}$ is a linear function of input features.

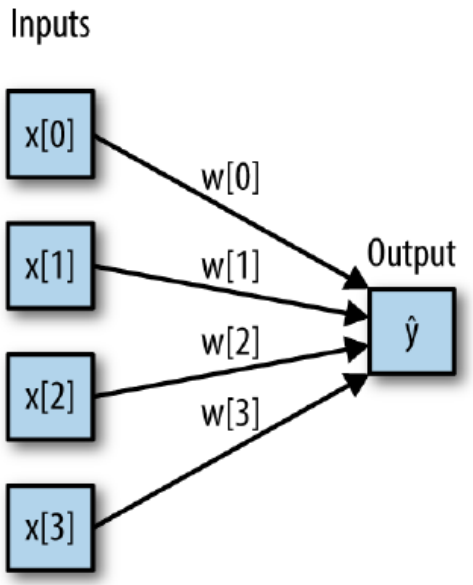


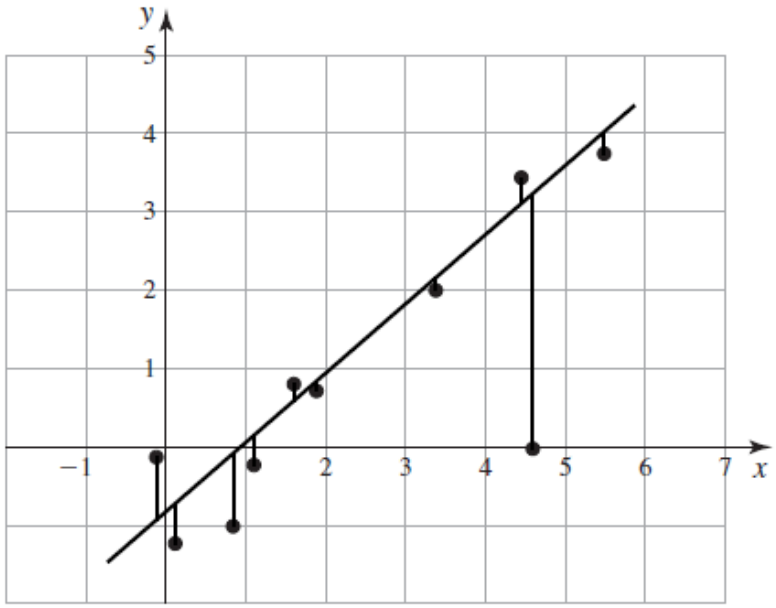
Linear Regression

- **Linear Regression (ordinary least squares (OLS))**
  - Linear regression finds the parameters $\mathbf{w}$ and b that minimize the *mean squared error* between predictions and the true regression targets on the training set.

$$\hat{y} = \mathbf{w}^T \boldsymbol{x} + b = w_1 x_1 + \cdots + w_d x_d + b$$
$$\boldsymbol{x} = (x_1, \ldots, x_d) \in \mathbb{R}^d, \qquad y, \hat{y} \in \mathbb{R}$$

  - Linear regression has no hyperparameters, thus has no way to control model complexity.





Linear Regression

- Given a (training) dataset $D = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \dots, (\boldsymbol{x}_n, y_n)\}$ such that $\boldsymbol{x}_i = (1, x_{i1}, \dots, x_{id}) \in \mathbb{R}^{d+1}$ is the *i*-th input vector of *d* features and $y_i \in \mathbb{R}$ is the corresponding target label.

  - the first entry is always set to "1"

- The output of model f (prediction of y)
  : $\hat{y} = f(\boldsymbol{x}) = \mathbf{w}^T \boldsymbol{x}$, where $\mathbf{w} = (w_0, w_1, \dots, w_d)$ is a vector of parameters.

  - $w_1, \dots, w_d$ are called "coefficients" or "weights"
  - w_0 is called "intercept" or "bias"

- **Training**: To find the optimal parameter $\mathbf{w}^*$ that minimizes the training error (cost function)

  Here we use "squared error" loss $L(y, \hat{y}) = (\hat{y} - y)^2$, then $J(\mathbf{w}) = \text{MSE}_{\text{train}}$

$$J(\mathbf{w}) = \frac{1}{n} \sum_{(\boldsymbol{x}_i, y_i) \in D} L(y_i, \hat{y}_i) = \frac{1}{n} \sum_{(\boldsymbol{x}_i, y_i) \in D} (\hat{y}_i - y_i)^2 = \frac{1}{n} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2$$

  - $\mathbf{X}$, $\mathbf{y}$ are matrix representation of D

Linear Regression

- **Training:** To find the optimal parameter $\mathbf{w}^*$ that minimizes the training error
  → **an optimization problem**

$$\mathrm{MSE}_{\mathrm{train}} = \frac{1}{n}\sum_{(\boldsymbol{x}_i, y_i)\in D}(\widehat{y}_i - y_i)^2 = \frac{1}{n}\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

▶ how? set the gradient to 0 → a closed-form solution (normal equation)

$$\nabla_{\mathbf{w}}\mathrm{MSE}_{\mathrm{train}} = \frac{1}{n}\nabla_{\mathbf{w}}\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 = 0$$

…

…

…

$$\mathbf{w}^* = \left(\mathbf{X}^{\mathrm{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y}$$

- The trained model $f(\boldsymbol{x}) = \mathbf{w}^{*\mathrm{T}}\boldsymbol{x}$

Probabilistic Interpretation of Linear Regression

- **Probabilistic Interpretation of Linear Regression**
  - Assume $y \sim \mathcal{N}(\hat{y}, \sigma^2), \hat{y} = \mathbf{w}^T \boldsymbol{x}$

$$p(y|\boldsymbol{x}; \mathbf{w}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y - \mathbf{w}^T \boldsymbol{x})^2}{2\sigma^2}\right)$$

p.d.f. of $N(\hat{y}, \sigma^2)$

- **Maximum Likelihood Estimation** (with respect to $\mathbf{w}$)

log-likelihood

$$\mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmax}} \prod_{(\boldsymbol{x}_i, y_i) \in D} p(y_i|\boldsymbol{x}_i; \mathbf{w}) = \underset{\mathbf{w}}{\operatorname{argmax}} \sum_{(\boldsymbol{x}_i, y_i) \in D} \log p(y_i|\boldsymbol{x}_i; \mathbf{w})$$

$$= \underset{\mathbf{w}}{\operatorname{argmax}} \left[-\frac{n}{2} \log 2\pi\sigma^2 - \frac{1}{2\sigma^2} \sum_{(\boldsymbol{x}_i, y_i) \in D} (y_i - \mathbf{w}^T \boldsymbol{x}_i)^2\right]$$

scikit-learn Practice: *LinearRegression*

https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LinearRegression.html

```
class sklearn.linear_model.LinearRegression(*, fit_intercept=True, copy_X=True,
n_jobs=None, positive=False)
```

Ordinary least squares Linear Regression.

LinearRegression fits a linear model with coefficients w = (w1, …, wp) to minimize the residual sum of squares between the observed targets in the dataset, and the targets predicted by the linear approximation.

Attributes	
coef_	*array of shape (n_features,) or (n_targets, n_features)* Estimated coefficients for the linear regression problem. If multiple targets are passed during the fit (y 2D), this is a 2D array of shape (n_targets, n_features), while if only one target is passed, this is a 1D array of length n_features.
intercept_	*float or array of shape (n_targets,)* Independent term in the linear model. Set to 0.0 if fit_intercept = False.

Methods	
fit(*X*, *y*)	Fit linear model.
predict(*X*)	Predict using the linear model.

scikit-learn Practice: *LinearRegression*

- **Example (*wave* dataset)**

[1]:
```
import mglearn
X, y = mglearn.datasets.make_wave(n_samples=60)

from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=42)
```

[2]:
```
from sklearn.linear_model import LinearRegression
reg = LinearRegression()
reg.fit(X_train, y_train)
```

```
LinearRegression()
```

[3]:
```
from sklearn.metrics import mean_absolute_error, mean_squared_error, r2_score

y_train_hat = reg.predict(X_train)
print('train MAE: %.5f'%mean_absolute_error(y_train,y_train_hat))
print('train RMSE: %.5f'%mean_squared_error(y_train,y_train_hat)**0.5)
print('train R_square: %.5f'%r2_score(y_train,y_train_hat))

y_test_hat = reg.predict(X_test)
print('test MAE: %.5f'%mean_absolute_error(y_test,y_test_hat))
print('test RMSE: %.5f'%mean_squared_error(y_test,y_test_hat)**0.5)
print('test R_square: %.5f'%r2_score(y_test,y_test_hat))
```

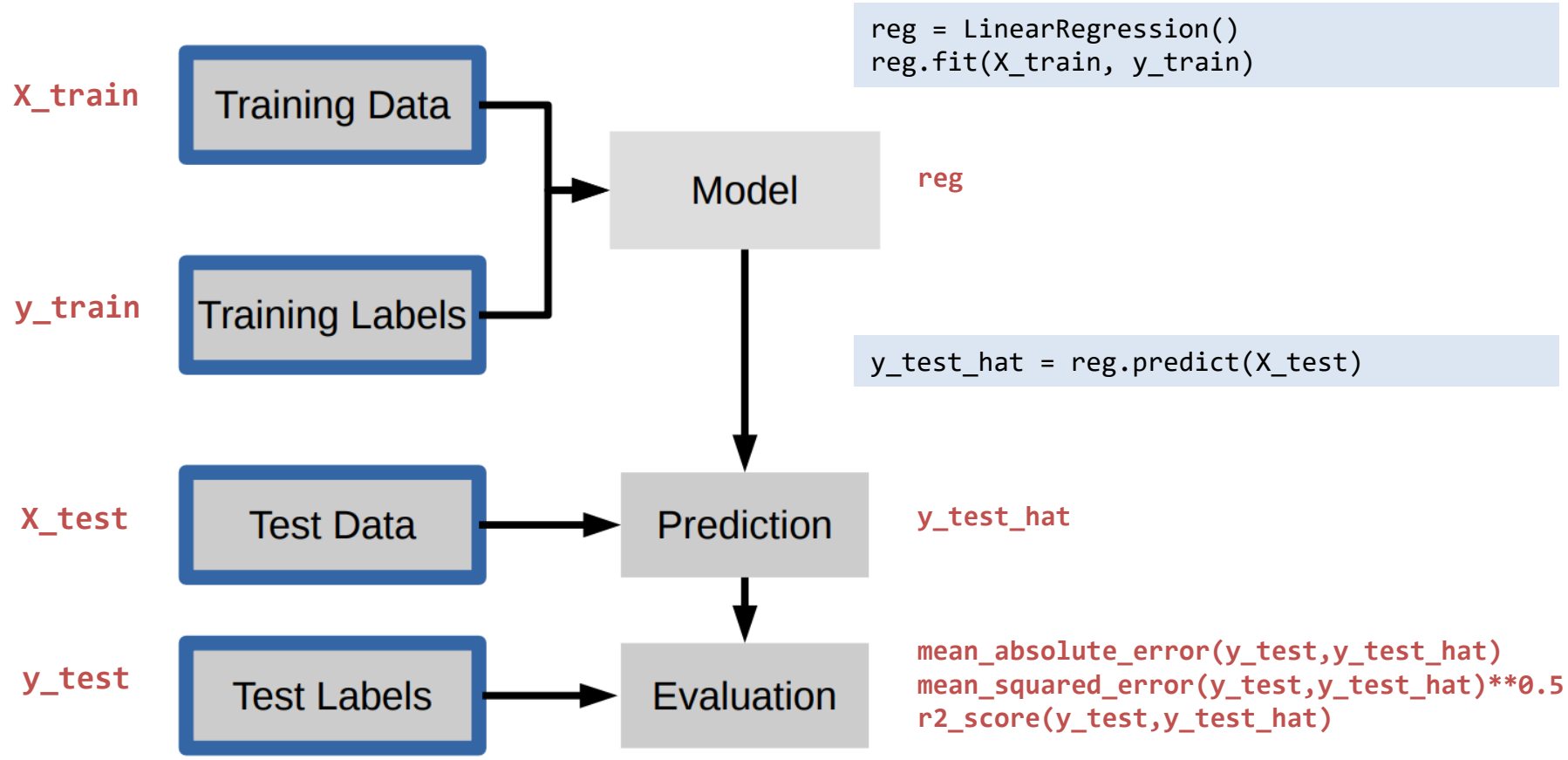
```
train MAE: 0.41817
train RMSE: 0.50589
train R_square: 0.67009
test MAE: 0.49453
test RMSE: 0.62826
test R_square: 0.65934
```

	X	Y
0	-0.75276	-1.18073
1	2.70429	0.50016
2	1.39196	0.13773
3	0.59195	1.17396
4	-2.06389	-1.32036
5	-2.06403	-2.37365
6	-2.65150	-0.70117
7	2.19706	1.20320
8	0.60669	0.29263
9	1.24844	0.44972
10	-2.87649	-0.48647
11	2.81946	1.39516
12	1.99466	1.07384
13	-1.72597	-1.30838
14	-1.90905	-1.27708
⋮	⋮	⋮

scikit-learn Practice: *LinearRegression*

- **Example (*wave* dataset)**

```
X, y = mglearn.datasets.make_wave(n_samples=60)
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=42)
```



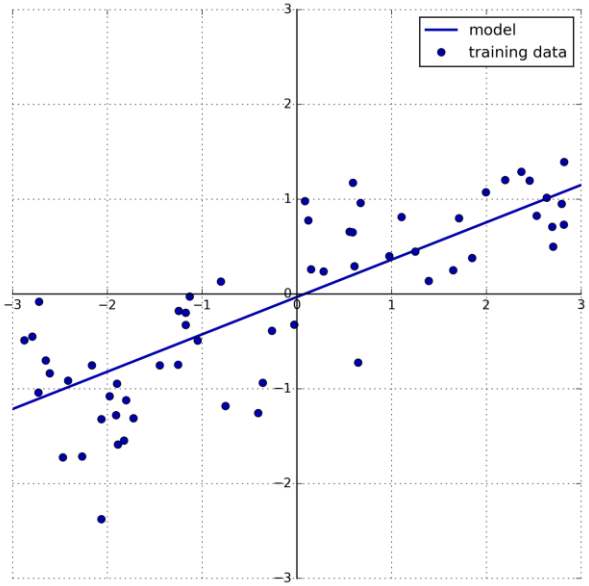
scikit-learn Practice: *LinearRegression*

- **Example (*wave* dataset)**

```
[4]: print('w0: %.5f'%reg.intercept_)
     print('w1: %.5f'%reg.coef_)
```

```
w0: -0.03180
w1: 0.39391
```

$$\hat{y} = -0.03180 + 0.39391x$$



scikit-learn Practice: *LinearRegression*

- **Example with the *extended_boston* dataset**
  - The dataset consists of 506 data points described by 104 features
  - The 104 features are the 13 original features together with the 91 possible combinations of two features within those 13 (all products between original features).
  - The regression task associated with this dataset is to predict the median value of homes in several Boston neighborhoods in the 1970s, using information such as crime rate, proximity to the Charles River, highway accessibility, and so on.

scikit-learn Practice: *LinearRegression*

- **Example (*extended_boston* dataset)**

[1]:
```
import mglearn
X, y = mglearn.datasets.load_extended_boston()
print(X.shape, y.shape)

from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
```

```
(506, 104) (506,)
```

[2]:
```
from sklearn.linear_model import LinearRegression
reg = LinearRegression()
reg.fit(X_train, y_train)
```

```
LinearRegression()
```

[3]:
```
from sklearn.metrics import mean_absolute_error, mean_squared_error, r2_score

y_train_hat = reg.predict(X_train)
print('train MAE: %.5f'%mean_absolute_error(y_train,y_train_hat))
print('train RMSE: %.5f'%mean_squared_error(y_train,y_train_hat)**0.5)
print('train R_square: %.5f'%r2_score(y_train,y_train_hat))

y_test_hat = reg.predict(X_test)
print('test MAE: %.5f'%mean_absolute_error(y_test,y_test_hat))
print('test RMSE: %.5f'%mean_squared_error(y_test,y_test_hat)**0.5)
print('test R_square: %.5f'%r2_score(y_test,y_test_hat))
```

```
train MAE: 1.56741
train RMSE: 2.02246
train R_square: 0.95205
test MAE: 3.22590
test RMSE: 5.66296
test R_square: 0.60747
```

When comparing training set and test set scores, we find that we predict very accurately on the training set, but the R^2 on the test set is much worse – ***overfitting***

Regularized Linear Regression

- **Linear Regression:** $\hat{y} = \mathbf{w}^T \boldsymbol{x}$

  Find the optimal parameter $\mathbf{w}^*$ that minimizes the training error (cost function)

$$J(\mathbf{w}) = \text{MSE}_{\text{train}} = \frac{1}{n} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

- **Ridge Regression:** $\hat{y} = \mathbf{w}^T \boldsymbol{x}$, **L2 regularization** for linear regression

  Add an L2 regularization term $\alpha \|\mathbf{w}\|_2^2$ *to the cost function*

$$\tilde{J}(\mathbf{w}) = \text{MSE}_{\text{train}} + \alpha \|\mathbf{w}\|_2^2 = \frac{1}{n} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \alpha \|\mathbf{w}\|_2^2$$

- **Lasso Regression:** $\hat{y} = \mathbf{w}^T \boldsymbol{x}$, **L1 regularization** for linear regression

  Add an L1 regularization term $\alpha \|\mathbf{w}\|_1$ *to the cost function*

$$\tilde{J}(\mathbf{w}) = \text{MSE}_{\text{train}} + \alpha \|\mathbf{w}\|_1 = \frac{1}{n} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \alpha \|\mathbf{w}\|_1$$

Regularized Linear Regression

- **Adding regularization (explicitly restricting a model to avoid *overfitting*) forces the learning algorithm to not only fit the data but also keep the magnitude of the model parameters as small as possible.**

- **The hyperparameter α controls how much you want to regularize the model.**
  - If $\alpha = 0$ then Regularized Linear Regression (Ridge and Lasso) is just Linear Regression.
  - If α is very large, then all parameters end up very close to zero and the result is a flat line.

scikit-learn Practice: *Ridge*

https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.Ridge.html

```
class sklearn.linear_model.Ridge(alpha=1.0, *, fit_intercept=True, copy_X=True,
max_iter=None, tol=0.0001, solver='auto', positive=False, random_state=None)
```

Linear least squares with l2 regularization.

Minimizes the objective function:

||y - Xw||^2_2 + alpha * ||w||^2_2

This model solves a regression model where the loss function is the linear least squares function and regularization is given by the l2-norm. Also known as Ridge Regression or Tikhonov regularization. This estimator has built-in support for multi-variate regression (i.e., when y is a 2d-array of shape (n_samples, n_targets)).

alpha	*{float, ndarray of shape (n_targets,)}, default=1.0* Constant that multiplies the L2 term, controlling regularization strength. alpha must be a non-negative float i.e. in [0, inf). When alpha = 0, the objective is equivalent to ordinary least squares, solved by the LinearRegression object. For numerical reasons, using alpha = 0 with the Ridge object is not advised. Instead, you should use the LinearRegression object. If an array is passed, penalties are assumed to be specific to the targets. Hence they must correspond in number.

scikit-learn Practice: *Ridge*

- **Example (*extended_boston* dataset)**

[1]:
```
import mglearn
X, y = mglearn.datasets.load_extended_boston()
print(X.shape, y.shape)

from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
```

```
(506, 104) (506,)
```

[2]:
```
from sklearn.linear_model import Ridge
reg = Ridge(alpha=1)
reg.fit(X_train, y_train)
```

```
Ridge(alpha=1)
```

[3]:
```
from sklearn.metrics import mean_absolute_error, mean_squared_error, r2_score

y_train_hat = reg.predict(X_train)
print('train MAE: %.5f'%mean_absolute_error(y_train,y_train_hat))
print('train RMSE: %.5f'%mean_squared_error(y_train,y_train_hat)**0.5)
print('train R_square: %.5f'%r2_score(y_train,y_train_hat))

y_test_hat = reg.predict(X_test)
print('test MAE: %.5f'%mean_absolute_error(y_test,y_test_hat))
print('test RMSE: %.5f'%mean_squared_error(y_test,y_test_hat)**0.5)
print('test R_square: %.5f'%r2_score(y_test,y_test_hat))
```

```
train MAE: 2.16564
train RMSE: 3.12130
train R_square: 0.88580
test MAE: 2.96269
test RMSE: 4.49428
test R_square: 0.75277
```

LinearRegression Results

```
train MAE: 1.56741
train RMSE: 2.02246
train R_square: 0.95205
test MAE: 3.22590
test RMSE: 5.66296
test R_square: 0.60747
```

scikit-learn Practice: *Ridge*

- **Example (*extended_boston* dataset): varying the hyperparameter α**

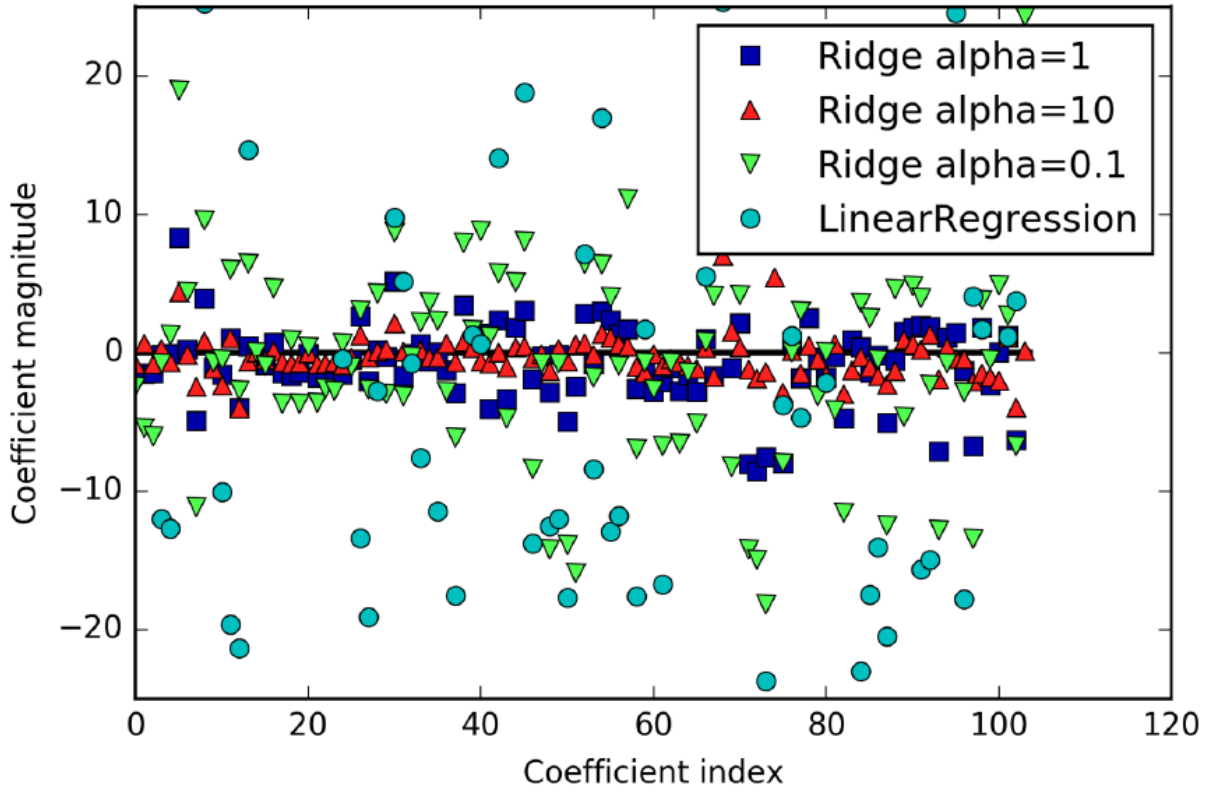
[1]:
```
import mglearn
from sklearn.model_selection import train_test_split
from sklearn.linear_model import Ridge
from sklearn.metrics import r2_score

X, y = mglearn.datasets.load_extended_boston()
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
```

[2]:
```
training_r2 = []
test_r2 = []

alpha_settings = [0, 0.1, 1, 10]
for alpha in alpha_settings:
    # build the model
    reg = Ridge(alpha=alpha)
    reg.fit(X_train, y_train)

    # r2 on the training set
    y_train_hat = reg.predict(X_train)
    training_r2.append(r2_score(y_train, y_train_hat))

    # r2 on the test set (generalization)
    y_test_hat = reg.predict(X_test)
    test_r2.append(r2_score(y_test, y_test_hat))
```

	alpha	training R_square	test R_square
0	0.0	0.95201	0.60296
1	0.1	0.92823	0.77221
2	1.0	0.88580	0.75277
3	10.0	0.78828	0.63594

scikit-learn Practice: *Ridge*

- **The effect of the hyperparameter α**
  - Comparing coefficient magnitudes for ridge regression
    - When α=10, the coefficients are mostly between around –3 and 3
    - When α=0 (Linear Regression), the coefficients have larger magnitude



scikit-learn Practice: *Lasso*

https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.Lasso.html

```
class sklearn.linear_model.Lasso(alpha=1.0, *, fit_intercept=True, precompute=False,
copy_X=True, max_iter=1000, tol=0.0001, warm_start=False, positive=False,
random_state=None, selection='cyclic')
```

Linear Model trained with L1 prior as regularizer (aka the Lasso).

The optimization objective for Lasso is:

(1 / (2 * n_samples)) * ||y - Xw||^2_2 + alpha * ||w||_1

Technically the Lasso model is optimizing the same objective function as the Elastic Net with l1_ratio=1.0 (no L2 penalty).

alpha	*float, default=1.0* Constant that multiplies the L1 term, controlling regularization strength. alpha must be a non-negative float i.e. in [0, inf). When alpha = 0, the objective is equivalent to ordinary least squares, solved by the LinearRegression object. For numerical reasons, using alpha = 0 with the Lasso object is not advised. Instead, you should use the LinearRegression object.

scikit-learn Practice: *Lasso*

- **Example (*extended_boston* dataset): varying the hyperparameter α**

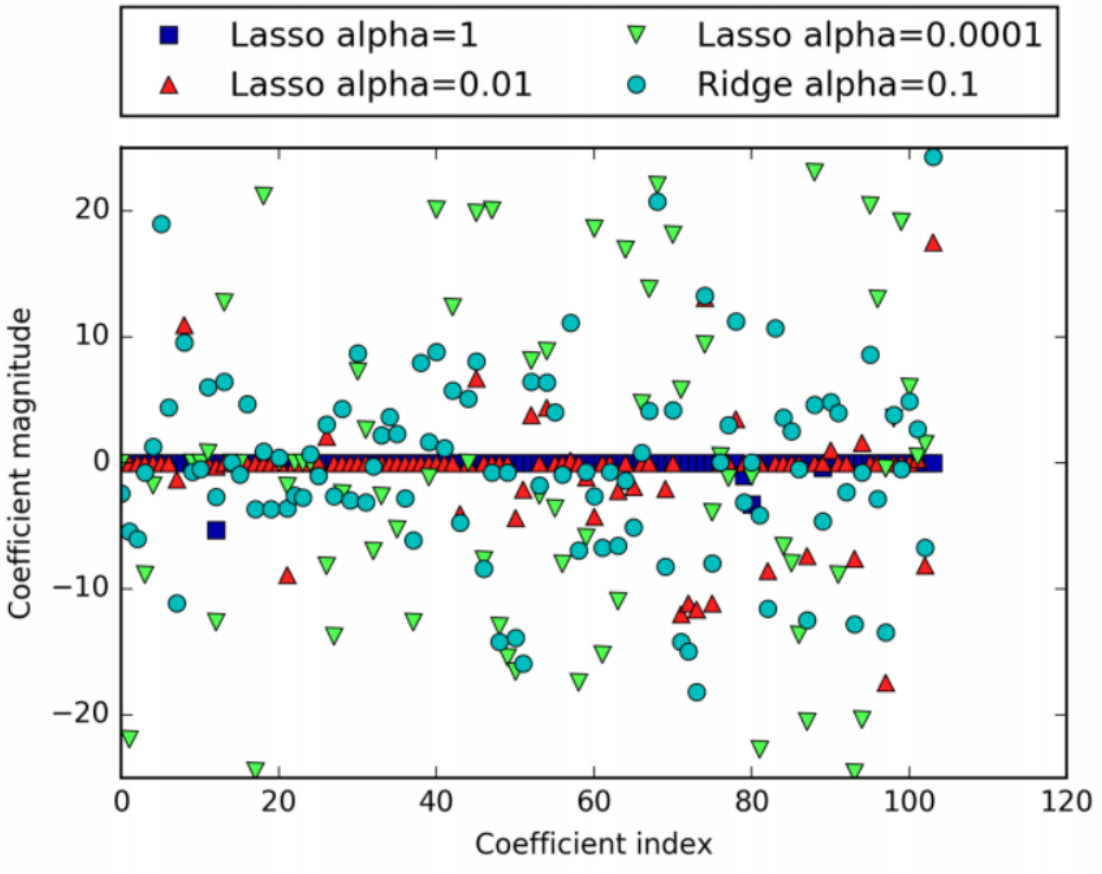
[1]:
```
import mglearn
from sklearn.model_selection import train_test_split
from sklearn.linear_model import Ridge
from sklearn.metrics import r2_score

X, y = mglearn.datasets.load_extended_boston()
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
```

[2]:
```
num_vars = []
training_r2 = []
test_r2 = []

alpha_settings = [0.0001, 0.001, 0.01, 0.1, 1]
for alpha in alpha_settings:
    # build the model
    reg = Lasso(alpha=alpha, max_iter=1000)
    reg.fit(X_train, y_train)

    # no. features used
    num_vars.append(sum(reg.coef_ != 0))

    # r2 on the training set
    y_train_hat = reg.predict(X_train)
    training_r2.append(r2_score(y_train, y_train_hat))

    # r2 on the test set (generalization)
    y_test_hat = reg.predict(X_test)
    test_r2.append(r2_score(y_test, y_test_hat))
```

	alpha	no. features used	training R_square	test R_square
0	0.0001	100	0.94209	0.69765
1	0.0010	76	0.93546	0.75480
2	0.0100	32	0.89611	0.76780
3	0.1000	8	0.77100	0.63020
4	1.0000	4	0.29324	0.20938

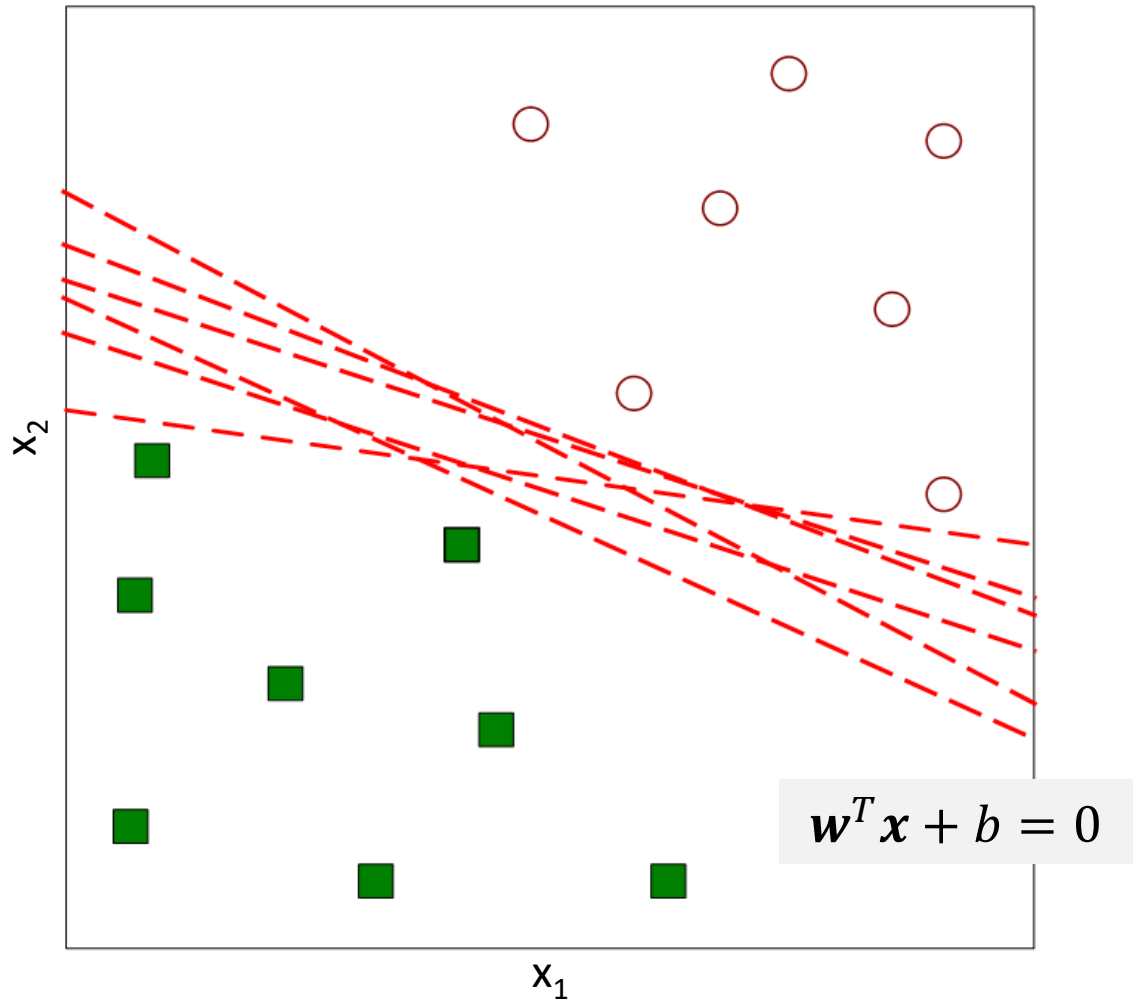
scikit-learn Practice: *Lasso*

- **The effect of the hyperparameter α**
  - Comparing coefficient magnitudes for lasso regression
    - Some coefficients are *exactly zero*, meaning that some features are entirely ignored by the model – feature selection



Logistic Regression

- For linear models for binary classification, the ***decision boundary (hyperplane)*** that separates two classes is a **linear function** of input features.



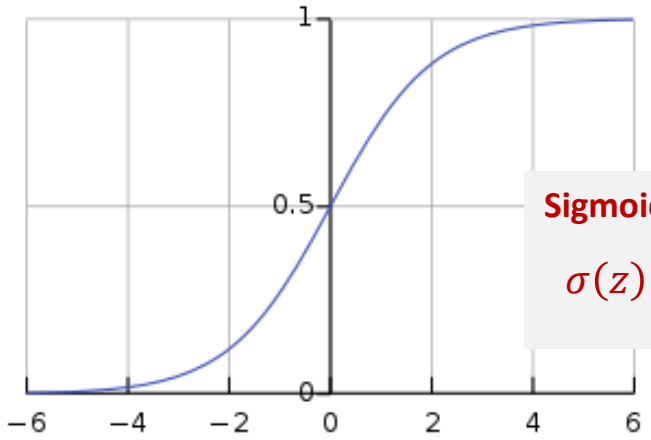
Logistic Regression

- **Logistic Regression**
  - Extends the idea of linear regression to situation where the target label is binary (y = 0 or 1)

$$\hat{y} = \sigma(\mathbf{w}^T \boldsymbol{x} + b) = \frac{1}{1 + \exp(-\mathbf{w}^T \boldsymbol{x} - b)}$$

$$\boldsymbol{x} = (x_1, \ldots, x_d) \in \mathbb{R}^d, \qquad y \in \{0,1\}, \qquad \hat{y} \in [0,1]$$

  - If $\hat{y} > 0.5$, classify as "1", If $\hat{y} < 0.5$, classify as "0"



Sigmoid function

$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$

Logistic Regression

- Given a (training) dataset $D = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \dots, (\boldsymbol{x}_n, y_n)\}$ such that $\boldsymbol{x}_i = (1, x_{i1}, \dots, x_{id}) \in \mathbb{R}^{d+1}$ is the *i*-th input vector of *d* features and $y_i \in \{0,1\}$ is the corresponding target label.

  - the first entry is always set to "1"

- The output of model f (prediction of y)

  : $\hat{y} = f(\boldsymbol{x}) = \sigma(\mathbf{w}^T \boldsymbol{x}) = \frac{1}{1+\exp(-\mathbf{w}^T \boldsymbol{x})}, \hat{y} \in [0,1]$

- **Training**: To find the optimal parameter $\mathbf{w}^*$ that minimizes the training error (cost function) → here we use "binary cross-entropy" loss

$$J(\mathbf{w}) = \frac{1}{n} \sum_{(\boldsymbol{x}_i, y_i) \in D} L(y_i, \hat{y}_i) = \frac{1}{n} \sum_{(\boldsymbol{x}_i, y_i) \in D} [-y_i \log \hat{y}_i - (1 - y_i) \log(1 - \hat{y}_i)]$$

Logistic Regression

- **Training**: To find the optimal parameter $\mathbf{w}^*$ that minimizes the training error (cost function)

$$J(\mathbf{w}) = \frac{1}{n} \sum_{(\boldsymbol{x}_i, y_i) \in D} L(y_i, \hat{y}_i) = \frac{1}{n} \sum_{(\boldsymbol{x}_i, y_i) \in D} [-y_i \log \hat{y}_i - (1 - y_i) \log(1 - \hat{y}_i)]$$

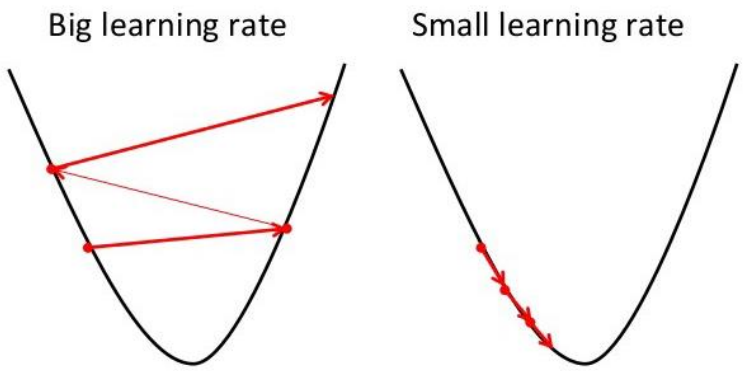
▶ how? gradient descent! (no closed-form solution)

Repeat the following until convergence

$$\mathbf{w} \coloneqq \mathbf{w} - \epsilon \nabla_{\mathbf{w}} J(\mathbf{w})$$

$$\rightarrow w_j \coloneqq w_j - \epsilon \frac{\partial}{\partial w_j} J(\boldsymbol{w}), \forall w_j \in \boldsymbol{w}$$

ϵ is the learning rate



- The trained model $f(\boldsymbol{x}) = \sigma(\mathbf{w}^{*\mathrm{T}} \boldsymbol{x})$

Logistic Regression

- $\boldsymbol{\theta} \coloneqq \boldsymbol{\theta} - \epsilon \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$? Where does it come from?

- **Let's recall "Taylor series" of calculus**
  - Taylor expansion of a function of $\boldsymbol{\theta}$

$$J(\boldsymbol{\theta}) = J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^T \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^T \nabla_{\boldsymbol{\theta}}^2 J(\boldsymbol{\theta}_0)(\boldsymbol{\theta} - \boldsymbol{\theta}_0) + \cdots$$

  - First-order approximation (assume that $\boldsymbol{\theta}$ is very close to $\boldsymbol{\theta}_0$)

$$J(\boldsymbol{\theta}) \simeq J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^T \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

  - We want to find a direction $\boldsymbol{\theta}_0 \to \boldsymbol{\theta}$ to make $J(\boldsymbol{\theta}) < J(\boldsymbol{\theta}_0)$

$$J(\boldsymbol{\theta}) - J(\boldsymbol{\theta}_0) \simeq (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^T \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0) < 0$$

linear function w.r.t. $\boldsymbol{\theta}$

  - The best direction

$$(\boldsymbol{\theta} - \boldsymbol{\theta}_0) \propto -\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

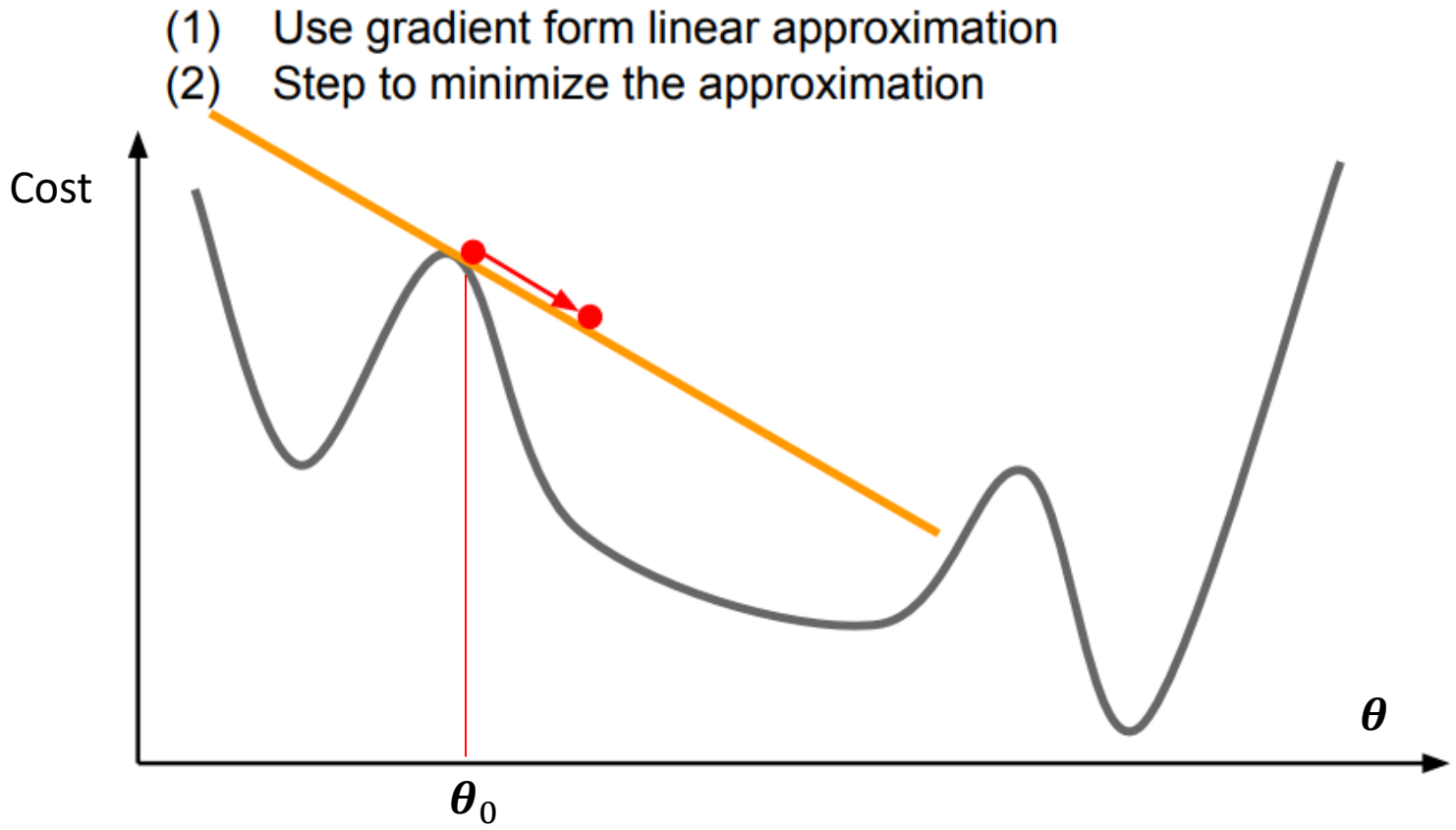
$$(\boldsymbol{\theta} - \boldsymbol{\theta}_0) = -\epsilon \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0), \epsilon > 0$$

$$\boldsymbol{\theta} = \boldsymbol{\theta}_0 - \epsilon \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0), \epsilon > 0$$

why?

Logistic Regression

- **Illustrative Example of Optimization based on First-Order Approximation**



Logistic Regression

$$L(y, \hat{y}) = -y \log \sigma(z) - (1 - y) \log\big(1 - \sigma(z)\big),$$

where $\hat{y} = \sigma(z), z = \mathbf{w}^T \boldsymbol{x} = w_0 + w_1 x_1 + \cdots + w_d x_d$

$$\frac{\partial L(\boldsymbol{w})}{\partial w_j} = \frac{\partial L(\boldsymbol{w})}{\partial z} \frac{\partial z}{\partial w_j} = (\hat{y} - y) x_j$$

$$\begin{aligned}
\frac{\partial L(\boldsymbol{w})}{\partial z} &= -y \frac{\partial \log \sigma(z)}{\partial z} - (1 - \mathrm{y}) \frac{\partial \log\big(1 - \sigma(z)\big)}{\partial z} \\
&= -y \frac{1}{\sigma(z)} \frac{\partial \sigma(z)}{\partial z} - (1 - \mathrm{y}) \frac{-1}{1 - \sigma(z)} \frac{\partial \sigma(z)}{\partial z} \\
&= -y \frac{1}{\sigma(z)} \sigma(z)\big(1 - \sigma(z)\big) - (1 - \mathrm{y}) \frac{-1}{1 - \sigma(z)} \sigma(z)\big(1 - \sigma(z)\big) \\
&= -y + \sigma(z) = \hat{y} - y
\end{aligned}$$

$$\frac{\partial z}{\partial w_j} = \frac{\partial (w_0 + w_1 x_1 + \cdots + w_d x_d)}{\partial w_j} = x_j$$

Probabilistic Interpretation of Logistic Regression

- **Probabilistic Interpretation of Logistic Regression**
  - Assume $y \sim \text{Bernoulli}(\hat{y})$, $\hat{y} = \sigma(\mathbf{w}^T \boldsymbol{x})$

$$p(y = 1|x; \mathbf{w}) = \sigma(\mathbf{w}^T \boldsymbol{x}) = \frac{1}{1 + \exp(-\mathbf{w}^T \boldsymbol{x})}$$

$$p(y = 0|x; \mathbf{w}) = 1 - \sigma(\mathbf{w}^T \boldsymbol{x}) = \frac{\exp(-\mathbf{w}^T \boldsymbol{x})}{1 + \exp(-\mathbf{w}^T \boldsymbol{x})}$$

$$\blacktriangledown$$

$$p(y|x; \mathbf{w}) = \big(\sigma(\mathbf{w}^T \boldsymbol{x})\big)^y \big(1 - \sigma(\mathbf{w}^T \boldsymbol{x})\big)^{1-y}$$

p.f. of Bernoulli($\hat{y}$)

- **Maximum Likelihood Estimation** (with respect to $\mathbf{w}$)

log-likelihood

$$\mathbf{w}^* = \underset{\mathbf{w}}{\text{argmax}} \prod_{(\boldsymbol{x}_i, y_i) \in D} p(y_i|\boldsymbol{x}_i; \mathbf{w}) = \underset{\mathbf{w}}{\text{argmax}} \sum_{(\boldsymbol{x}_i, y_i) \in D} \log p(y_i|\boldsymbol{x}_i; \mathbf{w})$$

$$= \underset{\mathbf{w}}{\text{argmax}} \sum_{(\boldsymbol{x}_i, y_i) \in D} [y_i \log \sigma(\mathbf{w}^T \boldsymbol{x}_i) + (1 - y_i) \log(1 - \sigma(\mathbf{w}^T \boldsymbol{x}_i))]$$

scikit-learn Practice: *LogisticRegression*

https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html

```
class sklearn.linear_model.LogisticRegression(penalty='l2', *, dual=False, tol=0.0001,
C=1.0, fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None,
solver='lbfgs', max_iter=100, multi_class='deprecated', verbose=0, warm_start=False,
n_jobs=None, l1_ratio=None)
```

Logistic Regression (aka logit, MaxEnt) classifier.

This class implements regularized logistic regression using the 'liblinear' library, 'newton-cg', 'sag', 'saga' and 'lbfgs' solvers. **Note that regularization is applied by default**. It can handle both dense and sparse input. Use C-ordered arrays or CSR matrices containing 64-bit floats for optimal performance; any other input format will be converted (and copied).

The 'newton-cg', 'sag', and 'lbfgs' solvers support only L2 regularization with primal formulation, or no regularization. The 'liblinear' solver supports both L1 and L2 regularization, with a dual formulation only for the L2 penalty. The Elastic-Net regularization is only supported by the 'saga' solver.

For multiclass problems, only 'newton-cg', 'sag', 'saga' and 'lbfgs' handle multinomial loss. 'liblinear' and 'newton-cholesky' only handle binary classification but can be extended to handle multiclass by using OneVsRestClassifier.

penalty	*{'l1', 'l2', 'elasticnet', None}, default='l2'* **** It applies an L2 regularization by default*** Specify the norm of the penalty: • None: no penalty is added; • 'l2': add a L2 penalty term and it is the default choice; • 'l1': add a L1 penalty term; • 'elasticnet': both L1 and L2 penalty terms are added.
C	*float, default=1.0* Inverse of regularization strength; must be a positive float. Like in support vector machines, smaller values specify stronger regularization.

scikit-learn Practice: *LogisticRegression*

- **Example (*forge* dataset)**

[1]:
```
import mglearn
X, y = mglearn.datasets.make_forge()

from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
```

[2]:
```
from sklearn.linear_model import LogisticRegression
clf = LogisticRegression()
clf.fit(X_train, y_train)
```

```
LogisticRegression()
```

[3]:
```
y_test_hat = clf.predict(X_test)
print(y_test)
print(y_test_hat)
```

```
[1 0 1 0 1 1 0]
[1 0 1 0 1 0 0]
```

[4]:
```
from sklearn.metrics import accuracy_score
y_train_hat = clf.predict(X_train)
print('train accuracy: %.5f'%accuracy_score(y_train, y_train_hat))
y_test_hat = clf.predict(X_test)
print('test accuracy: %.5f'%accuracy_score(y_test, y_test_hat))
```

```
train accuracy: 0.94737
test accuracy: 0.85714
```

scikit-learn Practice: *LogisticRegression*

- **Example (*breast_cancer* dataset): varying the hyperparameter *C***

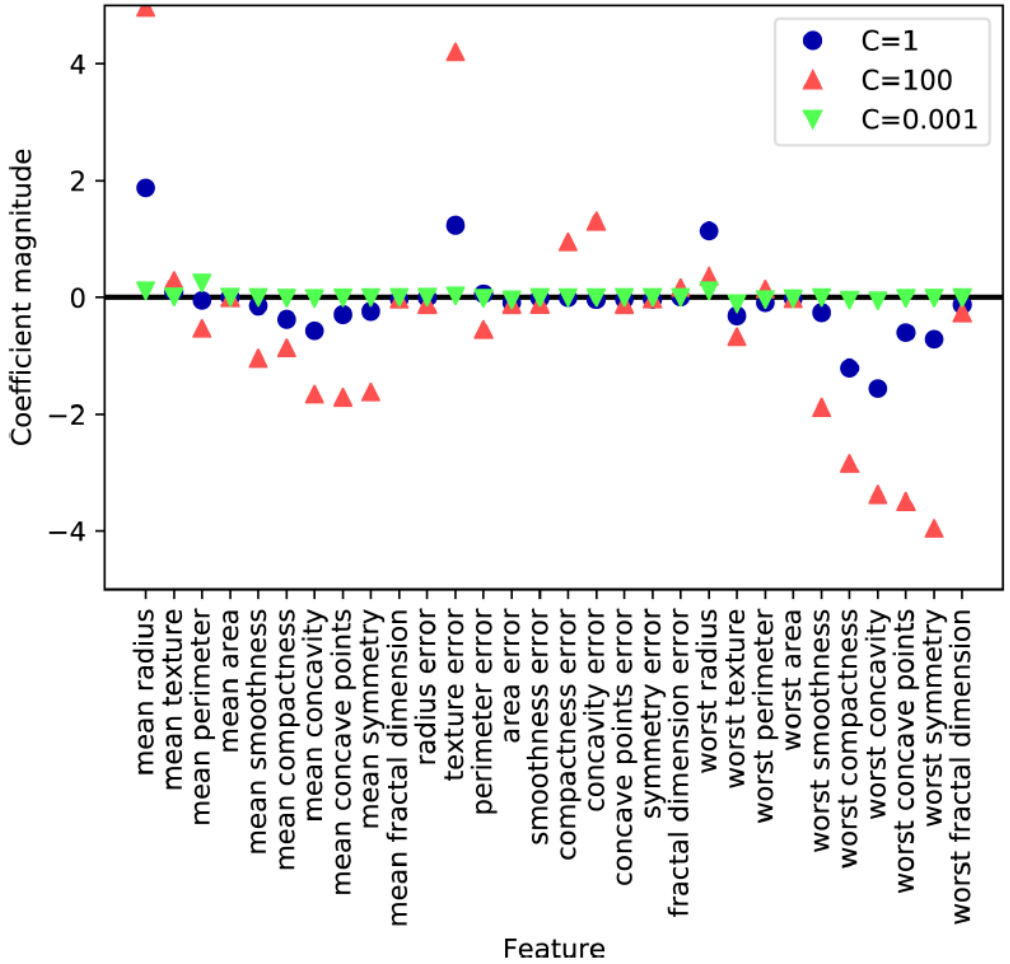
[1]:
```
from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import accuracy_score

cancer = load_breast_cancer()
X_train, X_test, y_train, y_test = train_test_split(
    cancer.data, cancer.target, stratify=cancer.target, random_state=42)
```

[2]:
```
training_accuracy = []
test_accuracy = []

C_settings = [0.01, 0.1, 1, 10, 100, 1000, 10000]
for C in C_settings:
    # build the model
    clf = LogisticRegression(C=C)
    clf.fit(X_train, y_train)

    # accuracy on the training set
    y_train_hat = clf.predict(X_train)
    training_accuracy.append(accuracy_score(y_train, y_train_hat))

    # accuracy on the test set (generalization)
    y_test_hat = clf.predict(X_test)
    test_accuracy.append(accuracy_score(y_test, y_test_hat))
```

	C	training accuracy	test accuracy
0	0.01	0.93427	0.93007
1	0.10	0.93662	0.94406
2	1.00	0.94836	0.94406
3	10.00	0.96009	0.95804
4	100.00	0.94366	0.96503
5	1000.00	0.94836	0.95804
6	10000.00	0.94601	0.95804

scikit-learn Practice: *LogisticRegression*

- **The effect of the hyperparameter C**
  - Coefficients learned by logistic regression for different values of C
    - Decreasing C results in more regularized model



Linear Models for Multi-class Classification

https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html

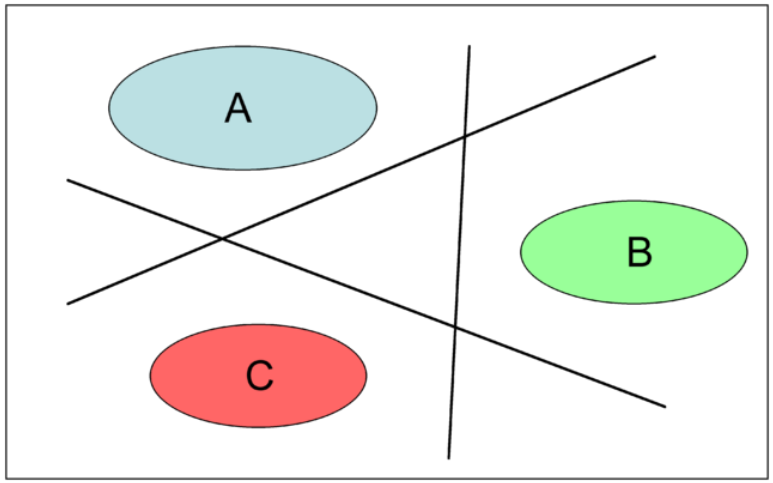
```
class sklearn.linear_model.LogisticRegression(penalty='l2', *, dual=False, tol=0.0001,
C=1.0, fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None,
solver='lbfgs', max_iter=100, multi_class='deprecated', verbose=0, warm_start=False,
n_jobs=None, l1_ratio=None)
```

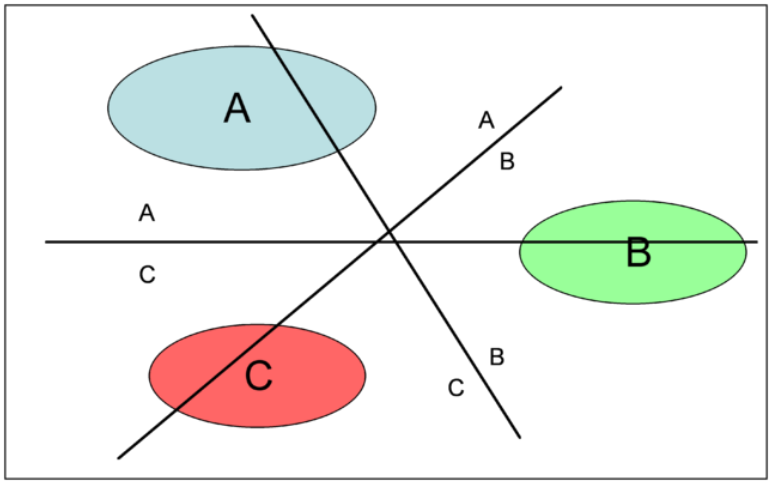
multi_class	*{'auto', 'ovr', 'multinomial'}, default='auto'* If the option chosen is 'ovr', then a binary problem is fit for each label. For 'multinomial' the loss minimised is the multinomial loss fit across the entire probability distribution, *even when the data is binary*. 'multinomial' is unavailable when solver='liblinear'. 'auto' selects 'ovr' if the data is binary, or if solver='liblinear', and otherwise selects 'multinomial'. ***Deprecated since version 1.5:*** multi_class was deprecated in version 1.5 and will be removed in 1.7. From then on, the recommended 'multinomial' will always be used for n_classes >= 3. Solvers that do not support 'multinomial' will raise an error. Use sklearn.multiclass.OneVsRestClassifier(LogisticRegression()) if you still want to use OvR.

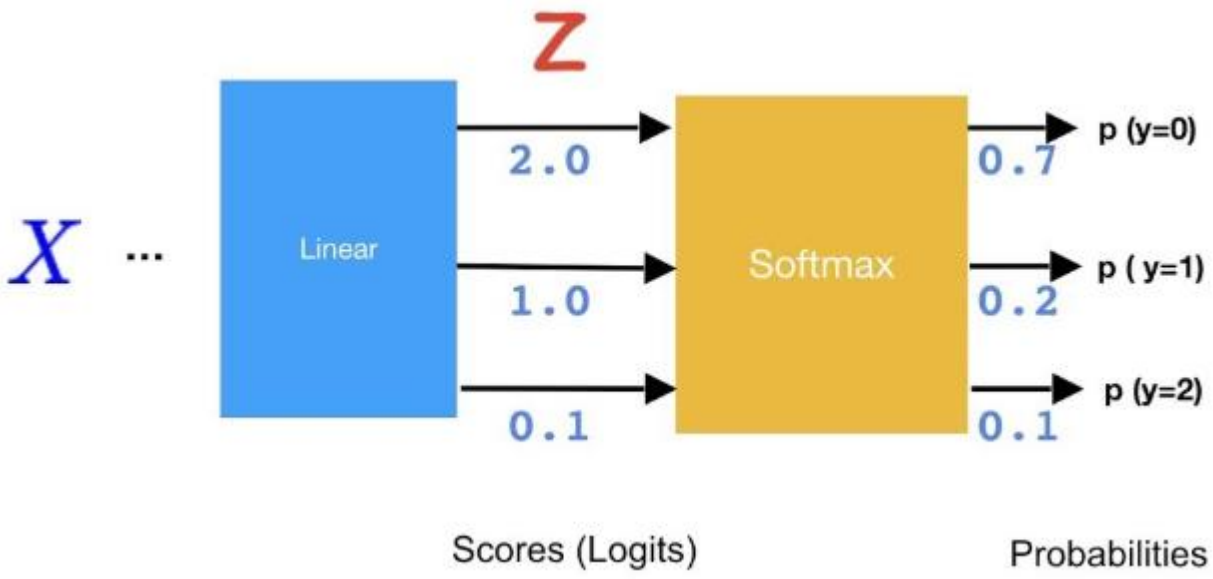
Linear Models for Multi-class Classification

- Naturally, linear models are for binary classification only. Common techniques to extend a binary classification algorithm to multi-class (*c* classes) classification are:
  - **One-vs.-Rest (OVR) Approach**
    - A model is trained for each class to separate that class from all other classes. → *c* models
    - To make a prediction, all models are run on a test point. The model that has the highest score on its single class "wins," and this class label is returned as the prediction.
  - **One-vs.-One (OVO) Approach**
    - A model is trained for each class pair → *c(c-1)/2* models
    - To make a prediction, the class label of a test data point is predicted based on majority voting by all models.
  - **Softmax Regression (a.k.a., Multinomial logistic regression)**
    - The model computes a score for each class
    - The softmax function converts these scores into probabilities that sum to 1.
    - The class with the highest probability is selected as the final prediction.

Linear Models for Multi-class Classification



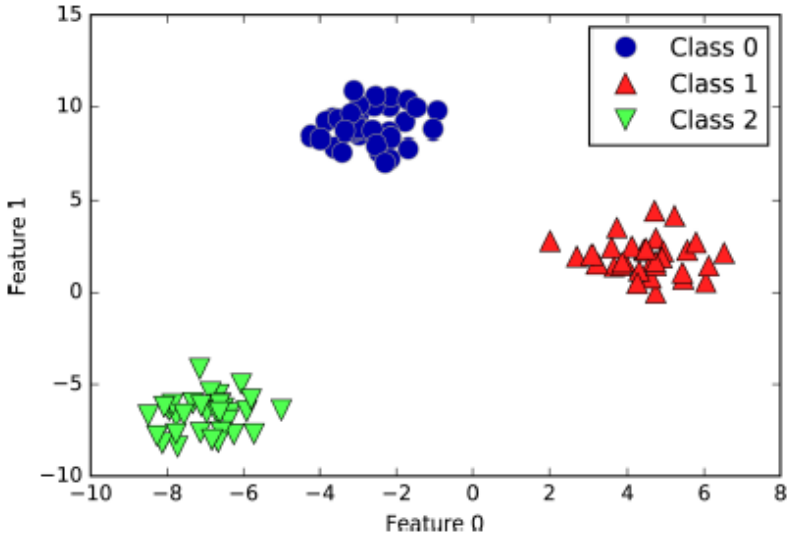




$$\sigma(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_k}} \quad \text{for } j = 1, \ldots, K.$$

scikit-learn Practice: *LogisticRegression*

- **Example (*blobs* dataset)**



[1]:
```
from sklearn.datasets import make_blobs
X, y = make_blobs(random_state=42)

from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
```

[2]:
```
from sklearn.multiclass import OneVsRestClassifier
from sklearn.linear_model import LogisticRegression
clf = OneVsRestClassifier(LogisticRegression())
clf.fit(X_train, y_train)
```

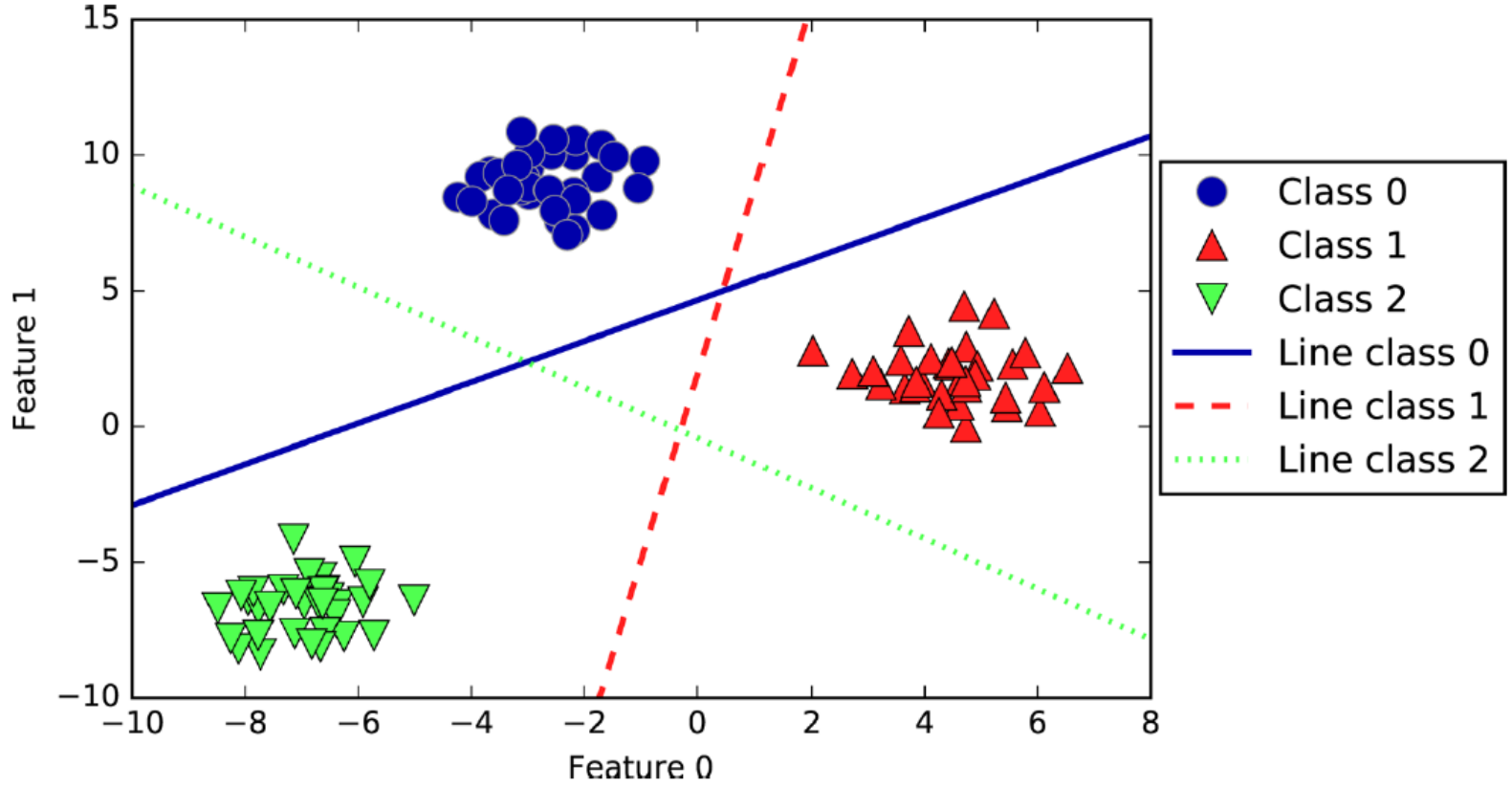
```
OneVsRestClassifier
estimator: LogisticRegression
```

[3]:
```
y_test_hat = clf.predict(X_test)
print(y_test)
print(y_test_hat)
```

```
[1 0 0 2 2 1 2 0 2 0 2 0 1 0 1 2 2 0 2 1 0 2 1 2 1]
[1 0 0 2 2 1 2 0 2 0 2 0 1 0 1 2 2 0 2 1 0 2 1 2 1]
```

scikit-learn Practice: *LogisticRegression*

- **Example (*blobs* dataset)**
  - Decision boundaries learned by the three models based on **the one-vs.-rest approach**



Discussion

- **The main hyperparameters of linear models**
  - The type of regularization (L1 vs L2)
  - The regularization strength hyperparameter α (or C)

  * Typically chosen to achieve the highest performance on validation data

  * It's important to preprocess your data (including *data scaling* and *one-hot encoding*)
- **Strengths**
  - Linear models are very fast to train, and also fast to predict.
  - They scale to very large datasets and work well with sparse data.
  - They make it relatively easy to understand how a prediction is made.
- **Weaknesses**
  - If your dataset has highly correlated features, it is often not entirely clear why coefficients are the way they are. (It is important to remove redundant features – feature selection)
  - They would perform worse if the relationship between features and target in your dataset is non-linear.

Discussion

- **Whether to use L1 regularization or L2 regularization**
  - Use L1 if
    - You have a large amount of features and assume that only a few of them are actually important.
    - You would like to have a model that is easy to interpret.
  - Use L2 otherwise
    - L2 regularization is usually the default choice