```
[2]: # Global imports and settings
     %matplotlib inline
     from preamble import *
     plt.rcParams['savefig.dpi'] = 100 # Use 300 for PDF, 100 for slides
     HTML('''<style>html, body{overflow-y: visible !important} .CodeMirror{min-w
```

```
<IPython.core.display.HTML object>
```

Linear models

Linear models make a prediction using a linear function of the input features. Can be very powerful for or datasets with many features.

If you have more features than training data points, any target y can be perfectly modeled (on the training set) as a linear function.

Linear models for regression

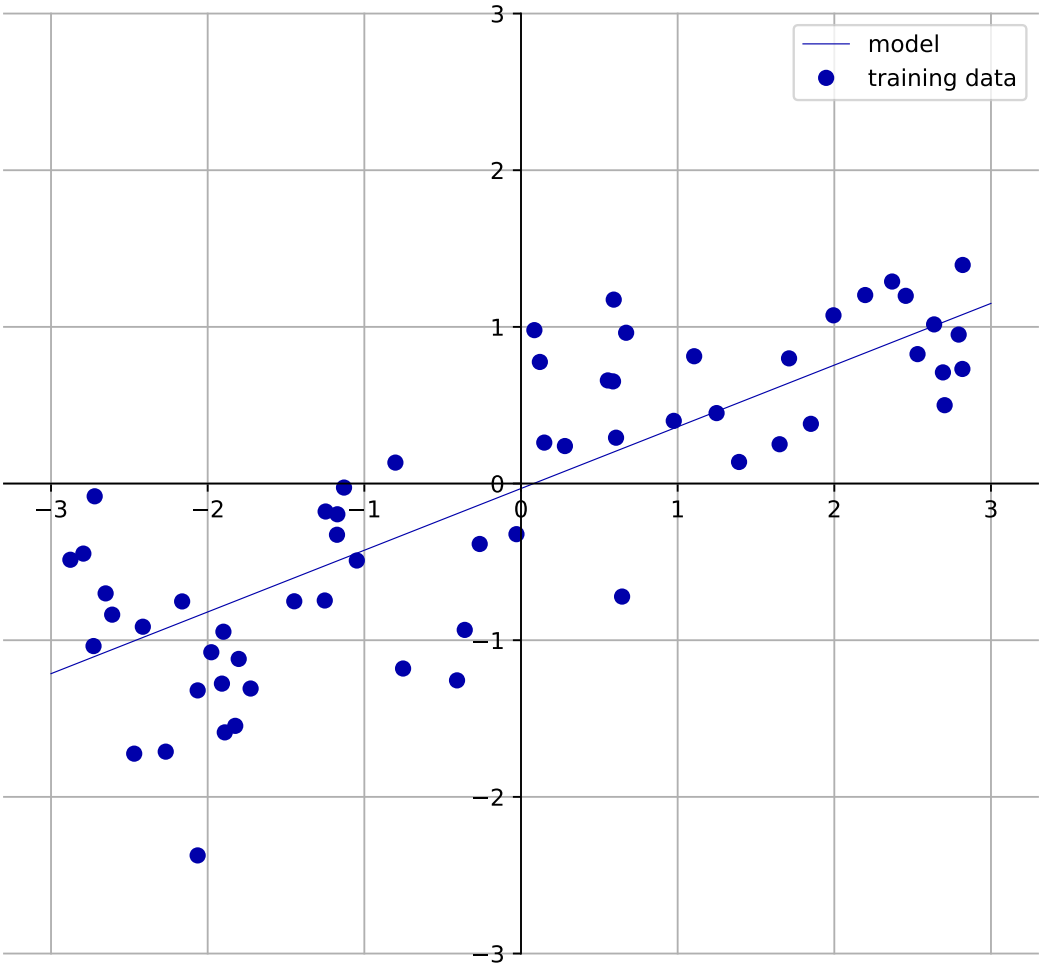
Prediction formula for input features x. w_i and b are the *model parameters* that need to be learned.

$\hat{y} = w_0 * x_0 + w_1 * x_1 + ... + w_p * x_p + b$

There are many different algorithms, differing in how w and b are learned from the training data.

```
[363]: mglearn.plots.plot_linear_regression_wave()
```

```
w[0]: 0.393906  b: -0.031804
```

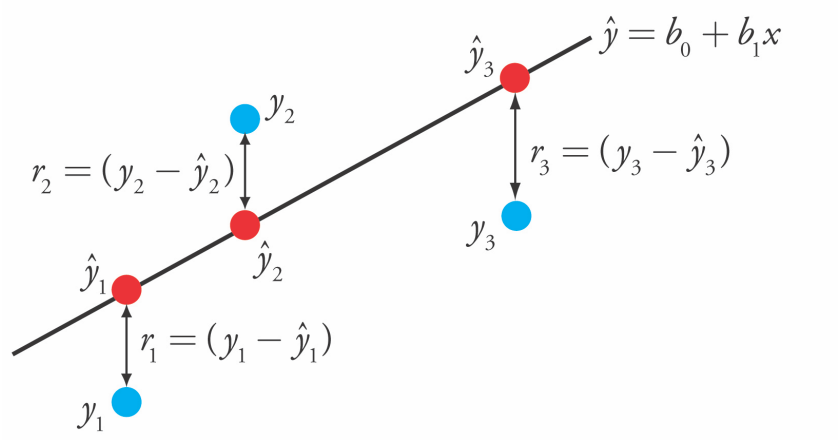


Linear Regression aka Ordinary Least Squares

- Finds the parameters w and b that minimize the *mean squared error* between predictions and the true regression targets, y, on the training set.
  - MSE: Sum of the squared differences between the predictions and the true values.
- Convex optimization problem with unique closed-form solution (if you have more data points than model parameters w)
- It has no hyperparameters, thus model complexity cannot be controlled.

Linear regression can be found in `sklearn.linear_model`. We'll evaluate it on the Boston Housing dataset.

```
[364]: from sklearn.model_selection import train_test_split
       from sklearn.linear_model import LinearRegression
       X, y = mglearn.datasets.load_extended_boston()

       X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
       lr = LinearRegression().fit(X_train, y_train)
```



least squares

```
[365]: print("Weights (coefficients): {}".format(lr.coef_))
       print("Bias (intercept): {}".format(lr.intercept_))
```

```
Weights (coefficients): [ -402.752   -50.071  -133.317   -12.002   -12.711    28
   -51.734    25.26     36.499   -10.104   -19.629   -21.368    14.647
  2895.054  1510.269   117.995   -26.566    31.249   -31.446    45.254
  1283.496 -2246.003   222.199    -0.466    40.766   -13.436   -19.096
    -2.776   -80.971     9.731     5.133    -0.788    -7.603    33.672
   -11.505    66.267   -17.563    42.983     1.277     0.61     57.187
    14.082    55.34    -30.348    18.812   -13.777    60.979   -12.579
   -12.002   -17.698   -34.028     7.15     -8.41     16.986   -12.941
   -11.806    57.133   -17.581     1.696    27.218   -16.745    75.03
   -30.272    47.78    -40.541     5.504    21.531    25.366   -49.485
    28.109    10.469   -71.559   -23.74      9.574    -3.788     1.214
    -4.72     41.238   -37.702    -2.156   -26.296   -33.202    45.932
   -23.014   -17.515   -14.085   -20.49     36.525   -94.897   143.234
   -15.674   -14.973   -28.613   -31.252    24.565   -17.805     4.035
     1.711    34.474    11.219     1.143     3.737    31.385]
Bias (intercept): 31.64517410082798
```

```
[366]: print("Training set score (R^2): {:.2f}".format(lr.score(X_train, y_train
       print("Test set score (R^2): {:.2f}".format(lr.score(X_test, y_test)))
```

```
Training set score (R^2): 0.95
Test set score (R^2): 0.61
```

Ridge regression

- Same formula as linear regression
- Adds a penalty term to the least squares sum : $\lambda \sum_i w_i^2$
- Requires that the coefficients (w) are close to zero.
  - Each feature should have as little effect on the outcome as possible
- Regularization: explicitly restrict a model to avoid overfitting.
- Type of L2 regularization: prefers many small weights

– L1 regularization prefers sparsity: many weights to be 0, others large

`Ridge` can also be found in `sklearn.linear_model`.

```
[367]: from sklearn.linear_model import Ridge

       ridge = Ridge().fit(X_train, y_train)
       print("Training set score: {:.2f}".format(ridge.score(X_train, y_train)))
       print("Test set score: {:.2f}".format(ridge.score(X_test, y_test)))
```

```
Training set score: 0.89
Test set score: 0.75
```

Test set score is higher and training set score lower: less overfitting!

The strength of the regularization can be controlled with the `alpha` parameter. Default is 1.0. * Increasing alpha forces coefficients to move more toward zero (more regularization) * Decreasing alpha allows the coefficients to be less restricted (less regularization)

```
[368]: ridge10 = Ridge(alpha=10).fit(X_train, y_train)
       print("Training set score: {:.2f}".format(ridge10.score(X_train, y_train)))
       print("Test set score: {:.2f}".format(ridge10.score(X_test, y_test)))
```

```
Training set score: 0.79
Test set score: 0.64
```

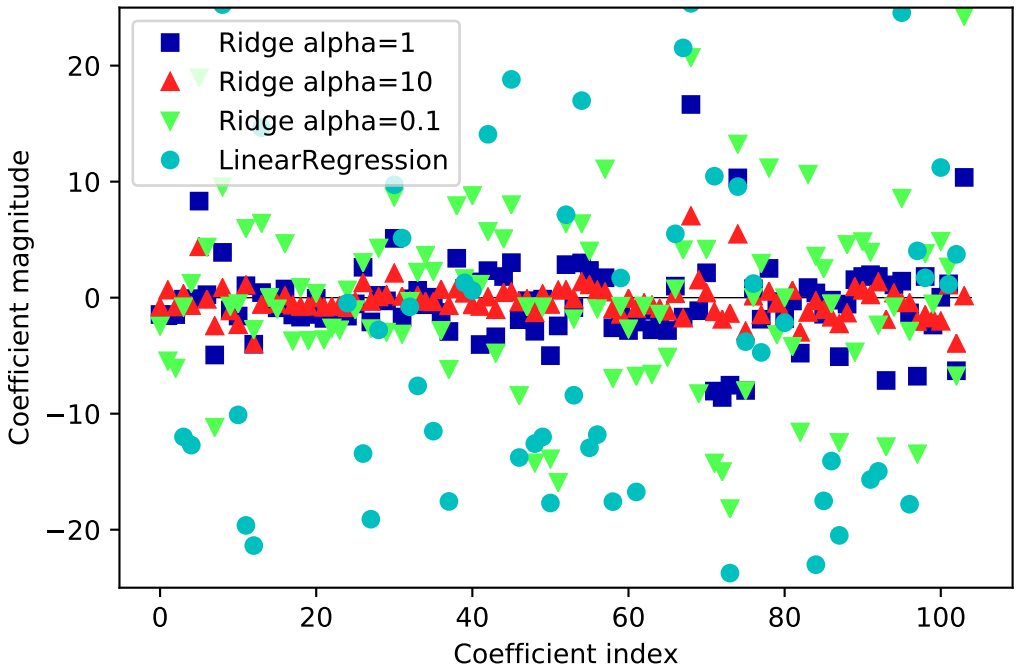
```
[369]: ridge01 = Ridge(alpha=0.1).fit(X_train, y_train)
       print("Training set score: {:.2f}".format(ridge01.score(X_train, y_train)))
       print("Test set score: {:.2f}".format(ridge01.score(X_test, y_test)))
```

```
Training set score: 0.93
Test set score: 0.77
```

We can plot the weight values for differents levels of regularization.

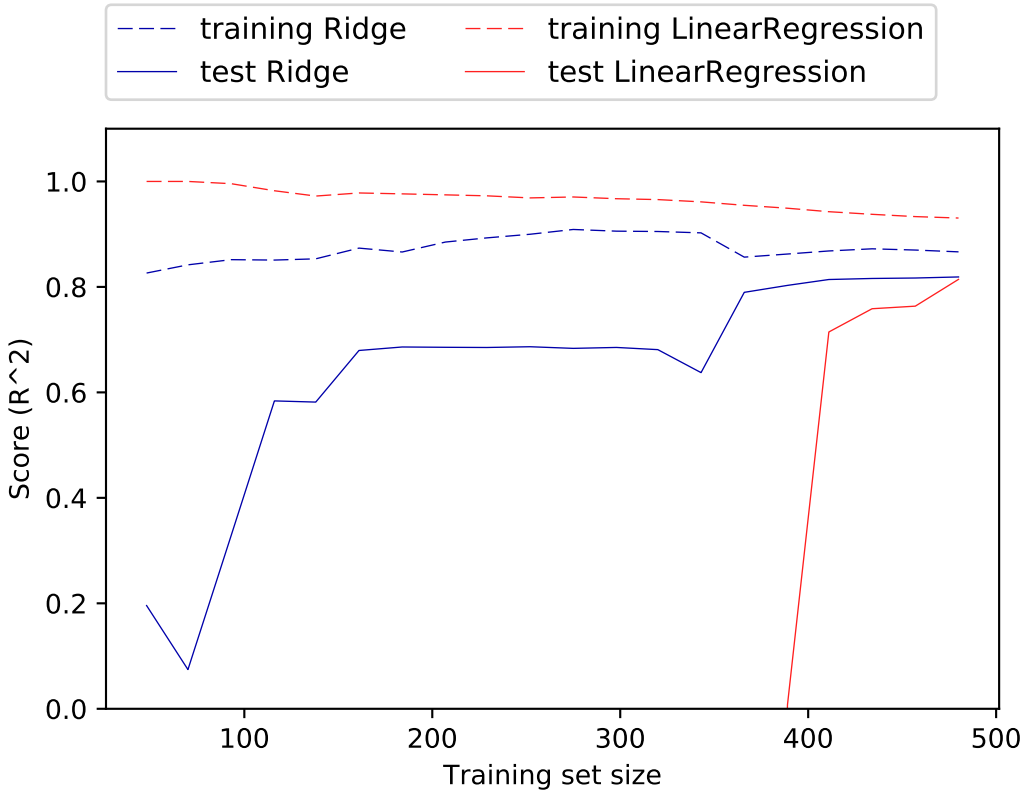
```
[370]: plt.plot(ridge.coef_, 's', label="Ridge alpha=1")
       plt.plot(ridge10.coef_, '^', label="Ridge alpha=10")
       plt.plot(ridge01.coef_, 'v', label="Ridge alpha=0.1")

       plt.plot(lr.coef_, 'o', label="LinearRegression")
       plt.xlabel("Coefficient index")
       plt.ylabel("Coefficient magnitude")
       plt.hlines(0, 0, len(lr.coef_))
       plt.ylim(-25, 25)
       plt.legend()
```

```
<matplotlib.legend.Legend at 0x11e95c898>
```



Another way to understand the influence of regularization is to fix a value of alpha but vary the amount of training data available. With enough training data, regularization becomes less important: ridge and linear regression will have the same performance.

```
[371]: mglearn.plots.plot_ridge_n_samples()
```



Lasso

- Another form of regularization
- Adds a penalty term to the least squares sum : $\lambda \sum_i |w_i|$
- Prefers coefficients to be exactly zero (L1 regularization).
- Some features are entirely ignored by the model: automatic feature selection.
- Same parameter `alpha` to control the strength of regularization.
- New parameter `max_iter`: the maximum number of iterations
  - Should be higher for small values of `alpha`

[372]:
```
from sklearn.linear_model import Lasso

lasso = Lasso().fit(X_train, y_train)
print("Training set score: {:.2f}".format(lasso.score(X_train, y_train)))
print("Test set score: {:.2f}".format(lasso.score(X_test, y_test)))
print("Number of features used: {}".format(np.sum(lasso.coef_ != 0)))
```

```
Training set score: 0.29
Test set score: 0.21
Number of features used: 4
```

[373]:
```
# we increase the default setting of "max_iter",
# otherwise the model would warn us that we should increase max_iter.
lasso001 = Lasso(alpha=0.01, max_iter=100000).fit(X_train, y_train)
print("Training set score: {:.2f}".format(lasso001.score(X_train, y_train
print("Test set score: {:.2f}".format(lasso001.score(X_test, y_test)))
print("Number of features used: {}".format(np.sum(lasso001.coef_ != 0)))
```

```
Training set score: 0.90
Test set score: 0.77
Number of features used: 33
```

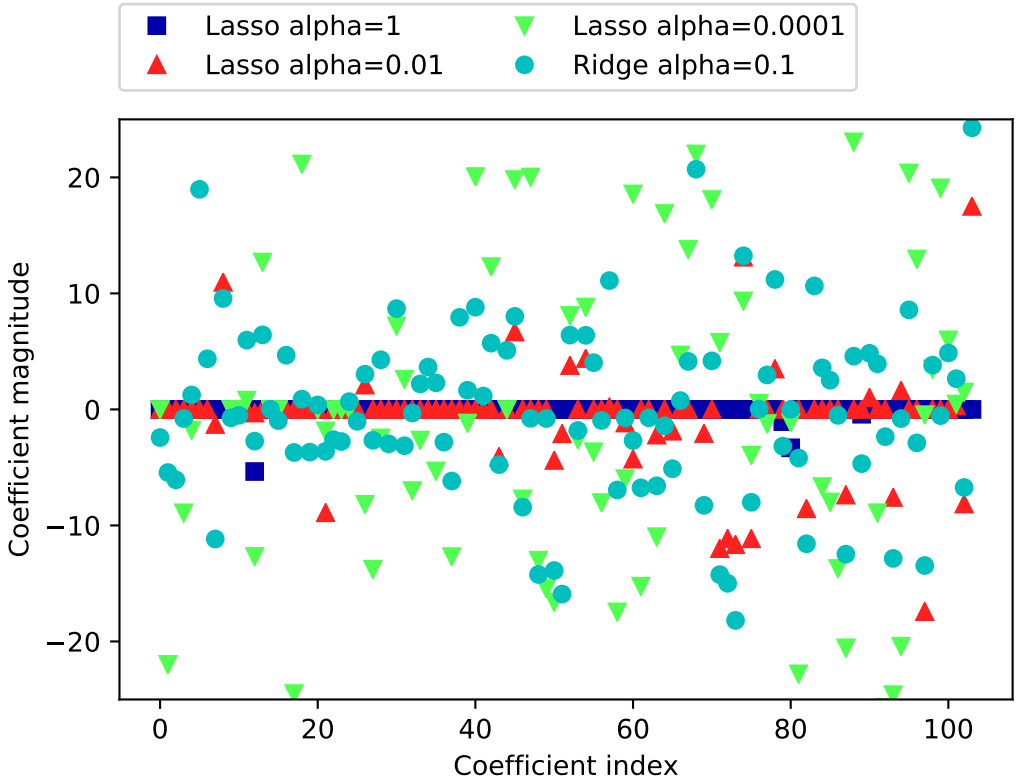
[374]:
```
lasso00001 = Lasso(alpha=0.0001, max_iter=100000).fit(X_train, y_train)
print("Training set score: {:.2f}".format(lasso00001.score(X_train, y_tra
print("Test set score: {:.2f}".format(lasso00001.score(X_test, y_test)))
print("Number of features used: {}".format(np.sum(lasso00001.coef_ != 0))
```

```
Training set score: 0.95
Test set score: 0.64
Number of features used: 94
```

We can again analyse what happens to the weigths:

[375]:
```
plt.plot(lasso.coef_, 's', label="Lasso alpha=1")
plt.plot(lasso001.coef_, '^', label="Lasso alpha=0.01")
plt.plot(lasso00001.coef_, 'v', label="Lasso alpha=0.0001")
```

```
plt.plot(ridge01.coef_, 'o', label="Ridge alpha=0.1")

plt.legend(ncol=2, loc=(0, 1.05))
plt.ylim(-25, 25)
plt.xlabel("Coefficient index")
plt.ylabel("Coefficient magnitude");
```



Interpreting L1 and L2 loss

- Red ellipses are the contours of the least squares error function
- In blue are the constraints imposed by the L1 (left) and L2 (right) loss functions
- For L1, the likelihood of hitting the objective with the corners is higher
  - Weights of other coefficients are 0, hence sparse representations
- For L2, it could intersect at any point, hence non-zero weights
- From *Elements of Statistical Learning*:

Linear models for Classification Aims to find a (hyper)plane that separates the examples of each class.
For binary classification (2 classes), we aim to fit the following function:
$\hat{y} = w_0 * x_0 + w_1 * x_1 + ... + w_p * x_p + b > 0$
When $\hat{y} < 0$, predict class -1, otherwise predict class +1
There are many algorithms for learning linear classification models, differing in:

- Loss function: evaluate how well the linear model fits the training data

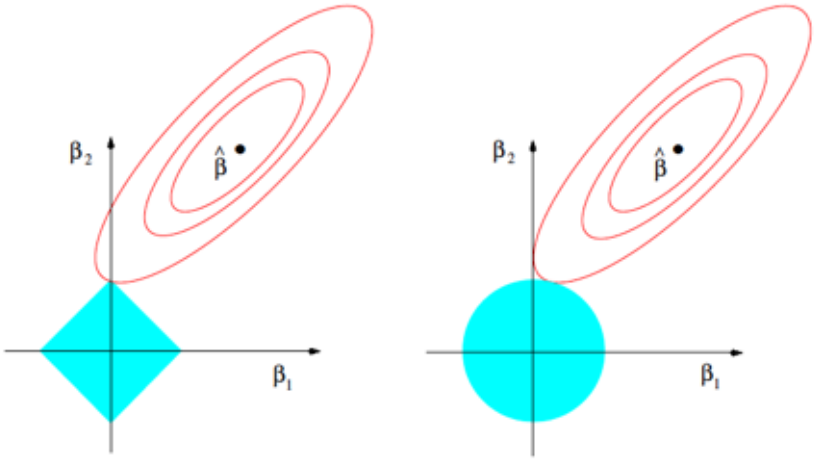


FIGURE 3.11. *Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions* $|\beta_1| + |\beta_2| \leq t$ *and* $\beta_1^2 + \beta_2^2 \leq t^2$*, respectively, while the red ellipses are the contours of the least squares error function.*

L1 and L2 loss

- Regularization techniques

Most common techniques:

- Logistic regression:
  - `sklearn.linear_model.LogisticRegression`
- Linear Support Vector Machine:
  - `sklearn.svm.LinearSVC`

Logistic regression Fits a logistic regression curve/surface to the data

Source

- Logistic regression predicts the target using the logarithm of the class probability:

$$Pr[1|x_1, ..., x_k] \rightarrow log(\frac{Pr[1|x_1, ..., x_k]}{1 - Pr[1|x_1, ..., x_k]})$$

- *Logit transformation* maps [0,1] to (-Inf,Inf)
- Resulting class probability (the green curve in the figure above):

$$Pr[1|x_1, ..., x_k] = \frac{1}{1 + exp(-(w_0 * x_0 + w_1 * x_1 + ... + w_p * x_p))})$$

- Parameters w are found from training data using *maximum likelihood*

Maximum likelihood

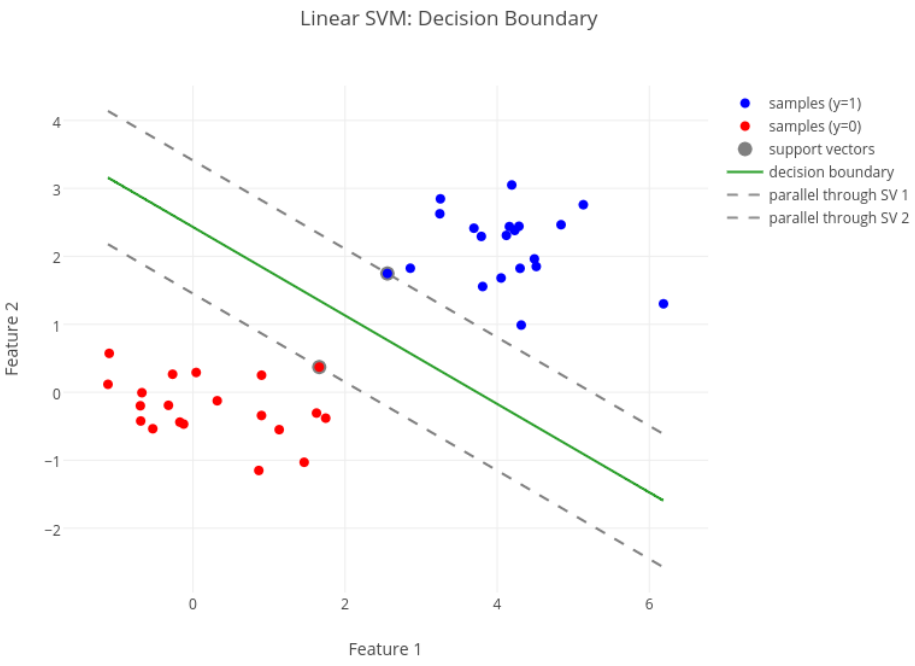
- Aim: maximize the probability of the observed training data with respect to the final model parameters
- We can use logaritms of probabilities and maximize conditional *log-likelihood* instead of the product of probabilities

$$\sum_{i=1}^{n}(1 - y^{(i)})log(1 - Pr[1|x_1^{(i)}, ..., x_k^{(i)}]) + y^{(i)}Pr[1|x_1^{(i)}, ..., x_k^{(i)}]$$

  - Class values $y^{(i)}$ are either 0 or 1

- Weights w_i need to be chosen to maximize log-likelihood
  - This can be done using *iterative re-weighted least squares*
  - Other optimization methods can be used as well

Linear Support Vector Machine Find hyperplane maximizing the *margin* between the classes

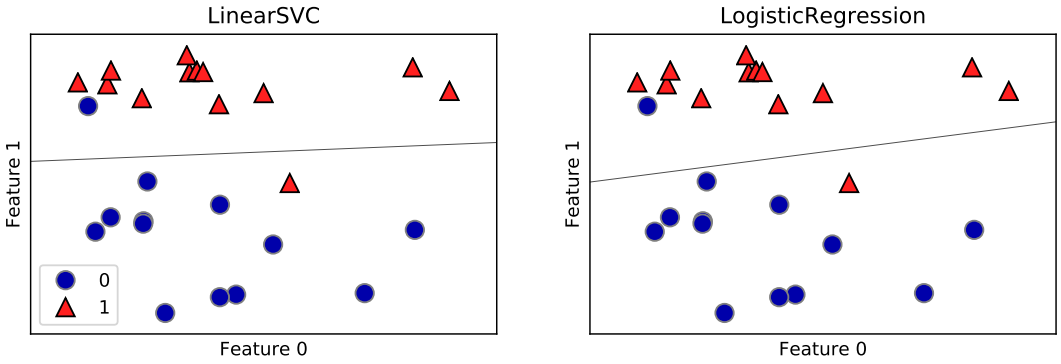


Prediction is identical to weighted kNN: find the support vector that is nearest, according to a distance measure (kernel) and a weight for each support vector.

We will discuss SVMs in a lot more detail in the coming lectures.

Comparison

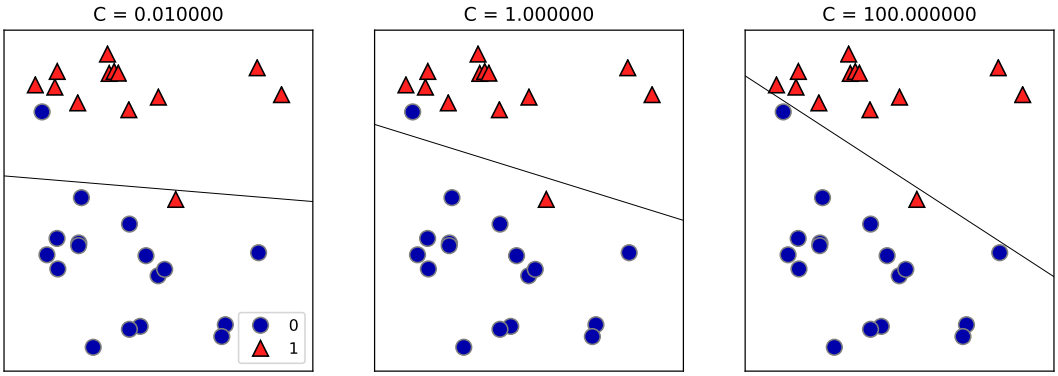
```
[376]: from sklearn.linear_model import LogisticRegression
       from sklearn.svm import LinearSVC

       X, y = mglearn.datasets.make_forge()

       fig, axes = plt.subplots(1, 2, figsize=(10, 3))

       for model, ax in zip([LinearSVC(), LogisticRegression()], axes):
           clf = model.fit(X, y)
           mglearn.plots.plot_2d_separator(clf, X, fill=False, eps=0.5,
                                           ax=ax, alpha=.7)
           mglearn.discrete_scatter(X[:, 0], X[:, 1], y, ax=ax)
           ax.set_title("{}".format(clf.__class__.__name__))
           ax.set_xlabel("Feature 0")
           ax.set_ylabel("Feature 1")
       axes[0].legend();
```



Both methods can be regularized: * L2 regularization by default, L1 also possible * C parameter: inverse of strength of regularization * higher C: less regularization * penalty for misclassifying points while keeping w_i close to 0

High C values (less regularization): fewer misclassifications but smaller margins.

```
[377]: mglearn.plots.plot_linear_svc_regularization()
```

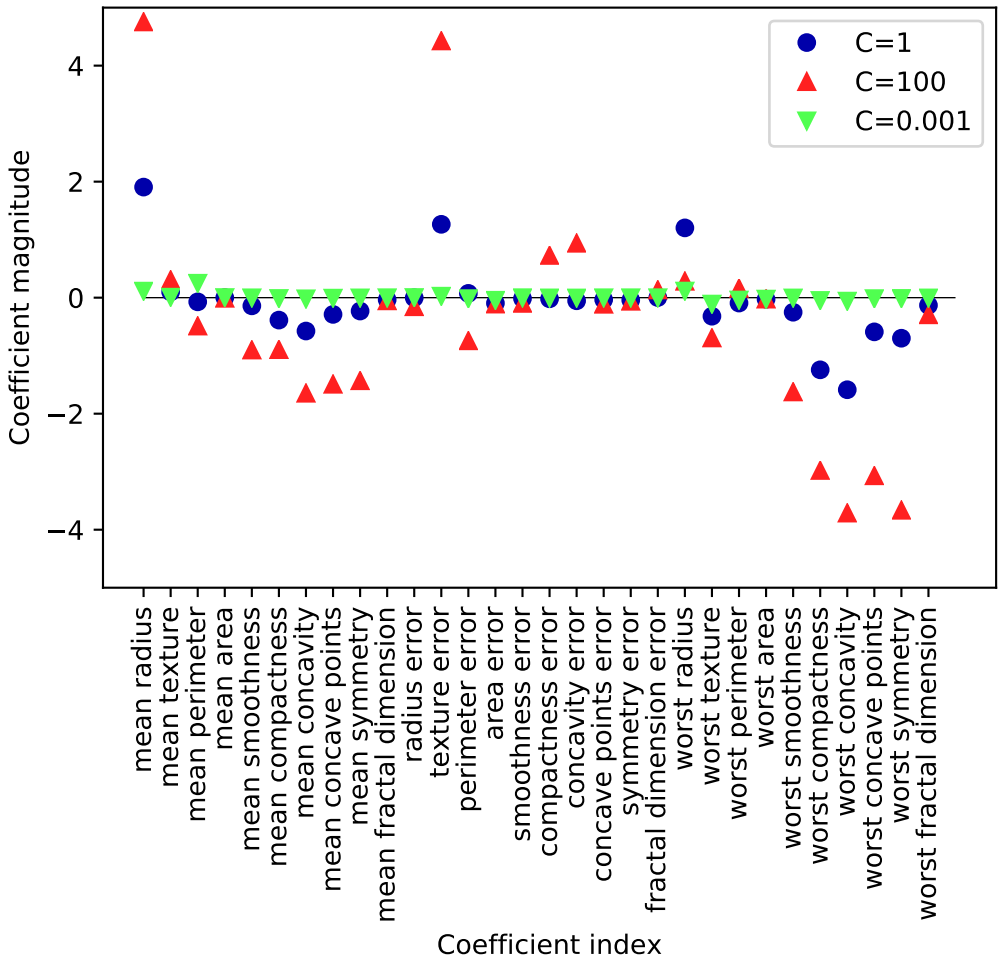


Model selection: Logistic regression

```
[378]: from sklearn.datasets import load_breast_cancer
       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)
       logreg = LogisticRegression().fit(X_train, y_train)
       print("Training set score: {:.3f}".format(logreg.score(X_train, y_train)))
       print("Test set score: {:.3f}".format(logreg.score(X_test, y_test)))

Training set score: 0.953
Test set score: 0.958


[379]: logreg100 = LogisticRegression(C=100).fit(X_train, y_train)
       print("Training set score: {:.3f}".format(logreg100.score(X_train, y_trai
       print("Test set score: {:.3f}".format(logreg100.score(X_test, y_test)))

Training set score: 0.972
Test set score: 0.965


[380]: logreg001 = LogisticRegression(C=0.01).fit(X_train, y_train)
       print("Training set score: {:.3f}".format(logreg001.score(X_train, y_trai
       print("Test set score: {:.3f}".format(logreg001.score(X_test, y_test)))

Training set score: 0.934
Test set score: 0.930
```

Effect of C on model parameters:

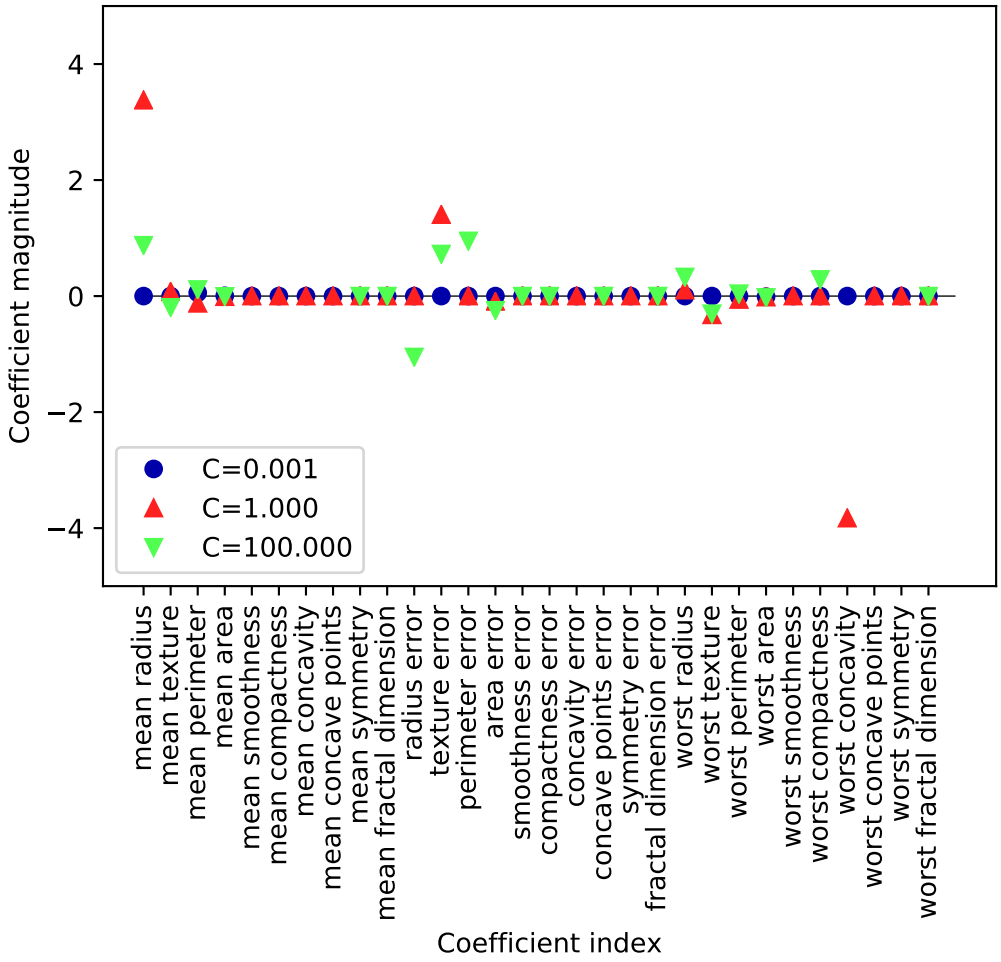
```
[381]: plt.plot(logreg.coef_.T, 'o', label="C=1")
       plt.plot(logreg100.coef_.T, '^', label="C=100")
       plt.plot(logreg001.coef_.T, 'v', label="C=0.001")
       plt.xticks(range(cancer.data.shape[1]), cancer.feature_names, rotation=90
       plt.hlines(0, 0, cancer.data.shape[1])
       plt.ylim(-5, 5)
       plt.xlabel("Coefficient index")
       plt.ylabel("Coefficient magnitude")
       plt.legend()

<matplotlib.legend.Legend at 0x120220d68>
```



Idem with L1 regularization (`penalty='l1'`):

```
[382]: for C, marker in zip([0.001, 1, 100], ['o', '^', 'v']):
           lr_l1 = LogisticRegression(C=C, penalty="l1").fit(X_train, y_train)
           print("Training accuracy of l1 logreg with C={:.3f}: {:.2f}".format(
                 C, lr_l1.score(X_train, y_train)))
           print("Test accuracy of l1 logreg with C={:.3f}: {:.2f}".format(
                 C, lr_l1.score(X_test, y_test)))
           plt.plot(lr_l1.coef_.T, marker, label="C={:.3f}".format(C))

       plt.xticks(range(cancer.data.shape[1]), cancer.feature_names, rotation=90
       plt.hlines(0, 0, cancer.data.shape[1])
       plt.xlabel("Coefficient index")
       plt.ylabel("Coefficient magnitude")

       plt.ylim(-5, 5)
       plt.legend(loc=3)

Training accuracy of l1 logreg with C=0.001: 0.91
Test accuracy of l1 logreg with C=0.001: 0.92
Training accuracy of l1 logreg with C=1.000: 0.96
```

```
Test accuracy of l1 logreg with C=1.000: 0.96
Training accuracy of l1 logreg with C=100.000: 0.99
Test accuracy of l1 logreg with C=100.000: 0.98


<matplotlib.legend.Legend at 0x121352cf8>
```



Linear Models for multiclass classification Common technique: one-vs.-rest approach:

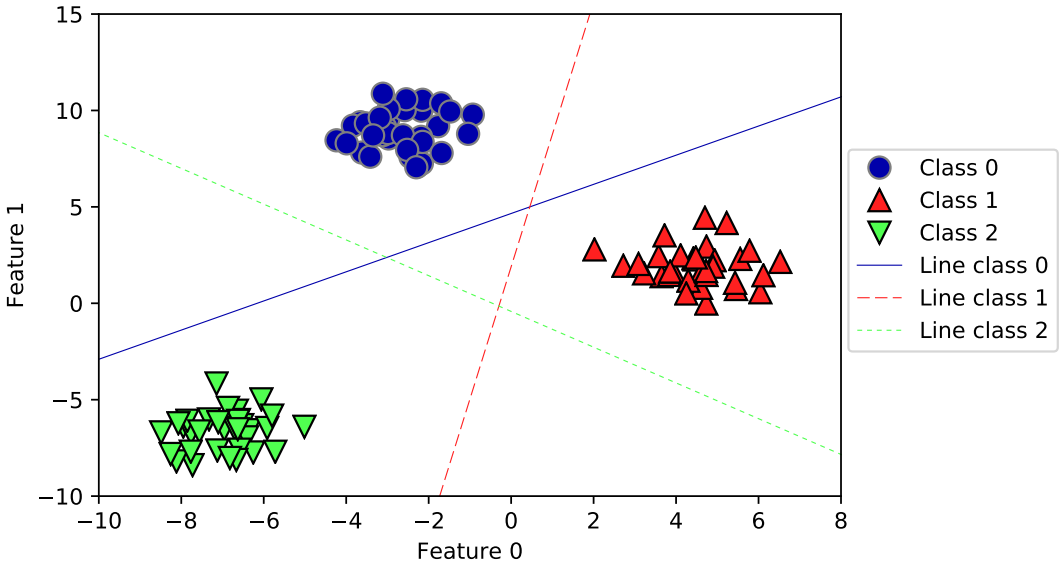
- A binary model is learned for each class vs. all other classes
- Creates as many binary models as there are classes
- Every binary classifiers makes a prediction, the one with the highest score (>0) wins

Build binary linear models:

```
[383]: from sklearn.datasets import make_blobs

       X, y = make_blobs(random_state=42)
       linear_svm = LinearSVC().fit(X, y)
```

```
        mglearn.discrete_scatter(X[:, 0], X[:, 1], y)
        line = np.linspace(-15, 15)
        for coef, intercept, color in zip(linear_svm.coef_, linear_svm.intercept_
                                          mglearn.cm3.colors):
            plt.plot(line, -(line * coef[0] + intercept) / coef[1], c=color)
        plt.ylim(-10, 15)
        plt.xlim(-10, 8)
        plt.xlabel("Feature 0")
        plt.ylabel("Feature 1")
        plt.legend(['Class 0', 'Class 1', 'Class 2', 'Line class 0', 'Line class
                    'Line class 2'], loc=(1.01, 0.3))
```

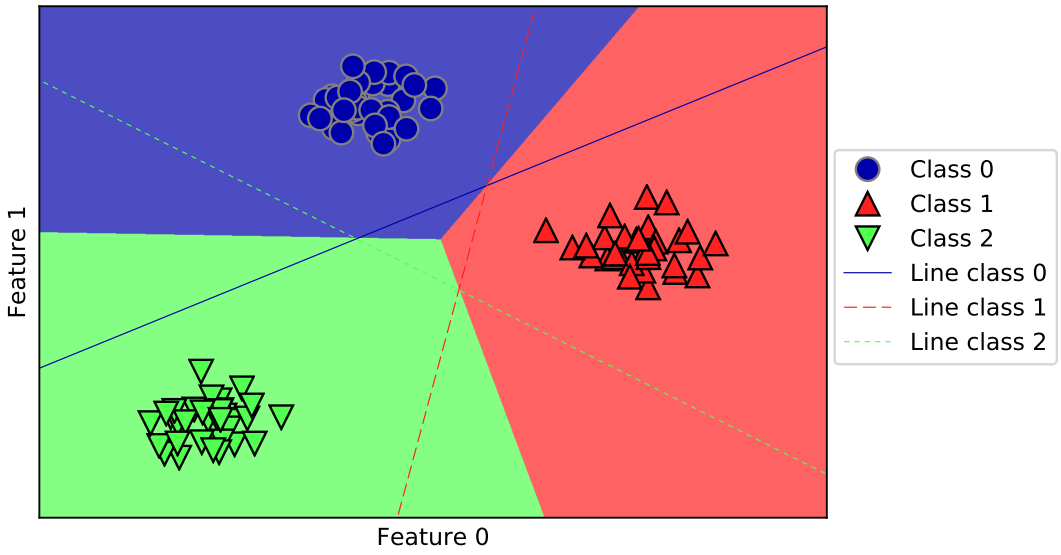
```
<matplotlib.legend.Legend at 0x11cc41470>
```



Actual predictions (decision boundaries):

```
[384]: mglearn.plots.plot_2d_classification(linear_svm, X, fill=True, alpha=.7)
        mglearn.discrete_scatter(X[:, 0], X[:, 1], y)
        line = np.linspace(-15, 15)
        for coef, intercept, color in zip(linear_svm.coef_, linear_svm.intercept_
                                          mglearn.cm3.colors):
            plt.plot(line, -(line * coef[0] + intercept) / coef[1], c=color)
        plt.legend(['Class 0', 'Class 1', 'Class 2', 'Line class 0', 'Line class
                    'Line class 2'], loc=(1.01, 0.3))
        plt.xlabel("Feature 0")
        plt.ylabel("Feature 1")
```

```
<matplotlib.text.Text at 0x11ec91358>
```



Strengths, weaknesses and parameters

Regularization parameters:

- Regression: alpha (higher values, simpler models)
  - Ridge (L2), Lasso (L1), LinearRegression (None)
- Classification: C (smaller values, simpler models)
  - LogisticRegression or SVC (both have L1/L2 option)

L1 vs L2:

- L2 is default
- Use L1 if you assume that few features are important
  - Or, if model interpretability is important

Other options:

- ElasticNet regression: allows L1 vs L2 trade-off
- SGDClassifier/SGDRegressor: optimize w_i,b with stochastic gradient descent (more scalable)

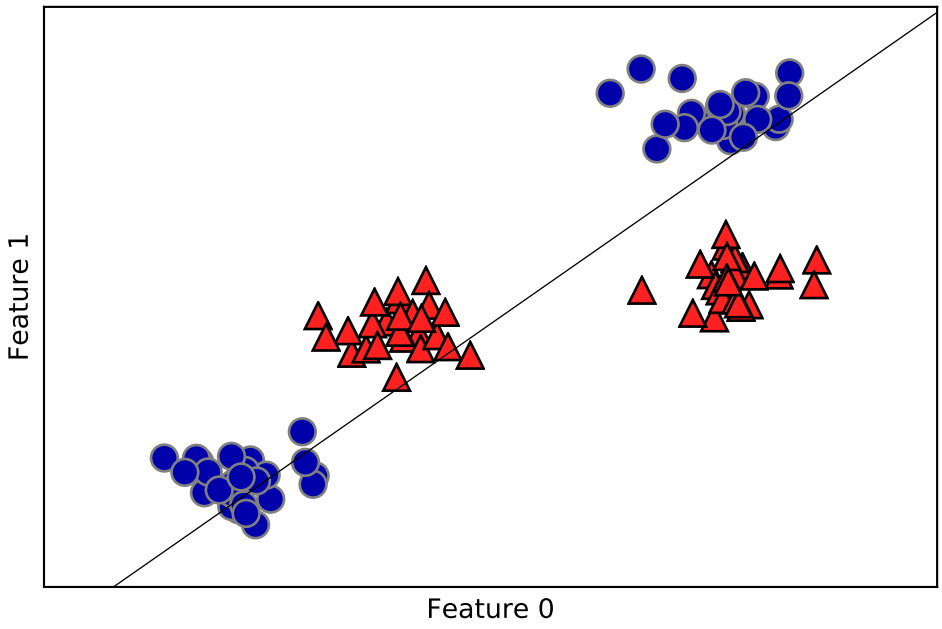
Consider linear models when:

- number of features is large compared to the number of samples
  - other algorithms perform better in low-dimensional spaces
- very large datasets (fast to train and predict)
  - other algorithms become (too) slow

Intuition: why linear models are powerful in high dimension

While linear models are limited on low-dimensional data, they can often fit high dimensional data very well.

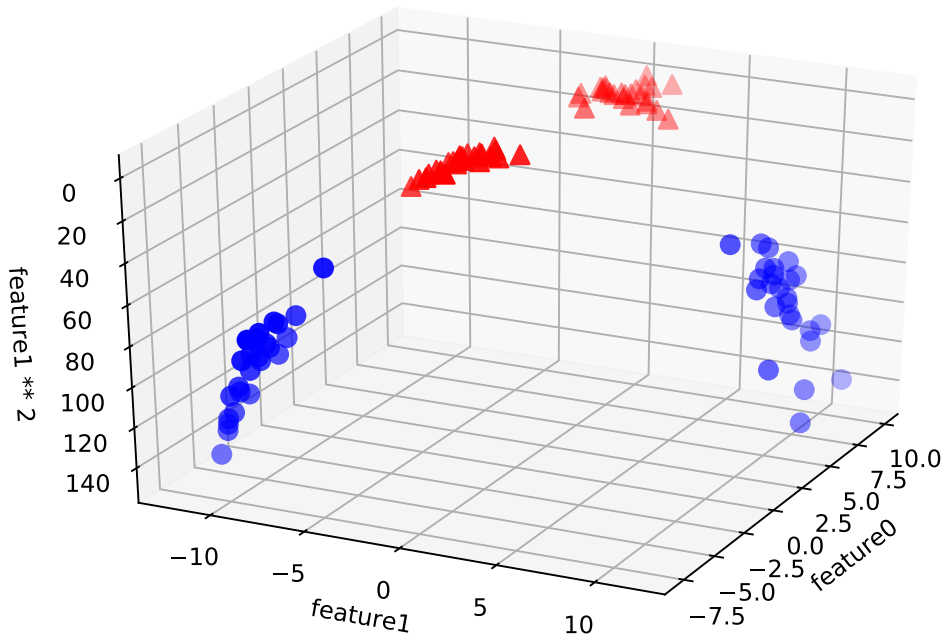
```
[385]: from sklearn.svm import LinearSVC
       X, y = make_blobs(centers=4, random_state=8)
       y = y % 2 # Reduces 4 classes to 2
       linear_svm = LinearSVC().fit(X, y)

       mglearn.plots.plot_2d_separator(linear_svm, X)
       mglearn.discrete_scatter(X[:, 0], X[:, 1], y)
       plt.xlabel("Feature 0")
       plt.ylabel("Feature 1");
```



While in the previous picture the classes (blue and red) cannot be linearly separated, imagine that we have another dimension that tells us more about each class.

```
[386]: # add the square of the first feature (this is just one way to add new fe
       X_new = np.hstack([X, X[:, 1:] ** 2])


       from mpl_toolkits.mplot3d import Axes3D, axes3d
       figure = plt.figure()
       # visualize in 3D
       ax = Axes3D(figure, elev=-152, azim=-26)
       # plot first all the points with y==0, then all with y == 1
       mask = y == 0
       ax.scatter(X_new[mask, 0], X_new[mask, 1], X_new[mask, 2], c='b',
                  cmap=mglearn.cm2, s=60)
       ax.scatter(X_new[~mask, 0], X_new[~mask, 1], X_new[~mask, 2], c='r', mark
```

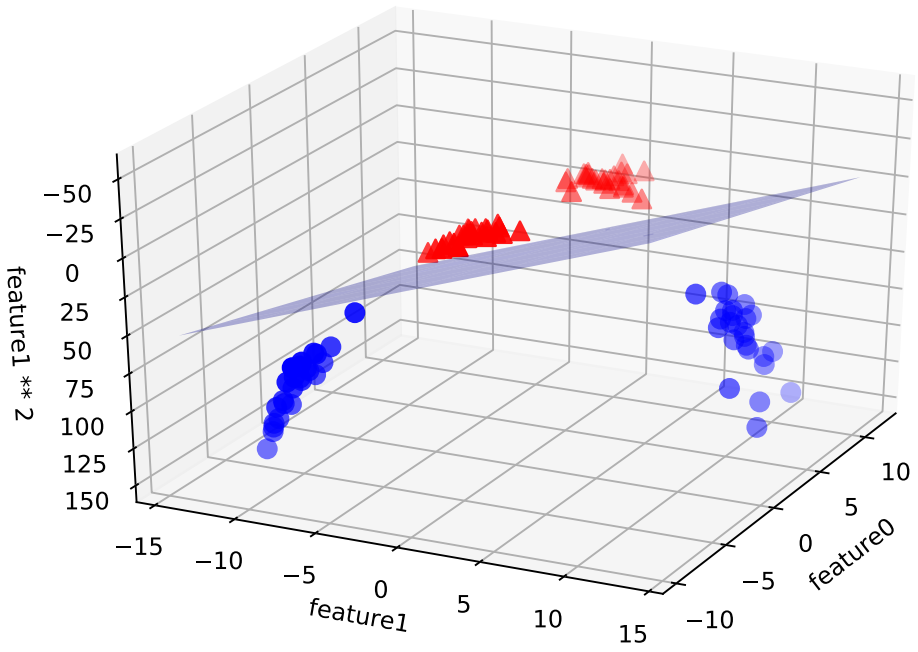
```
            cmap=mglearn.cm2, s=60)
ax.set_xlabel("feature0")
ax.set_ylabel("feature1")
ax.set_zlabel("feature1 ** 2");
```



Now we can fit a linear model
Note: We will come back to this when discussing *kernelization*, in which we construct new dimensions on purpose.

[387]:
```
linear_svm_3d = LinearSVC().fit(X_new, y)
coef, intercept = linear_svm_3d.coef_.ravel(), linear_svm_3d.intercept_

# show linear decision boundary
figure = plt.figure()
ax = Axes3D(figure, elev=-152, azim=-26)
xx = np.linspace(X_new[:, 0].min() - 2, X_new[:, 0].max() + 2, 50)
yy = np.linspace(X_new[:, 1].min() - 2, X_new[:, 1].max() + 2, 50)

XX, YY = np.meshgrid(xx, yy)
ZZ = (coef[0] * XX + coef[1] * YY + intercept) / -coef[2]
ax.plot_surface(XX, YY, ZZ, rstride=8, cstride=8, alpha=0.3)
ax.scatter(X_new[mask, 0], X_new[mask, 1], X_new[mask, 2], c='b',
           cmap=mglearn.cm2, s=60)
ax.scatter(X_new[~mask, 0], X_new[~mask, 1], X_new[~mask, 2], c='r', mark
           cmap=mglearn.cm2, s=60)

ax.set_xlabel("feature0")
ax.set_ylabel("feature1")
ax.set_zlabel("feature1 ** 2")
```

```
<matplotlib.text.Text at 0x121bba6d8>
```



Uncertainty estimates from classifiers

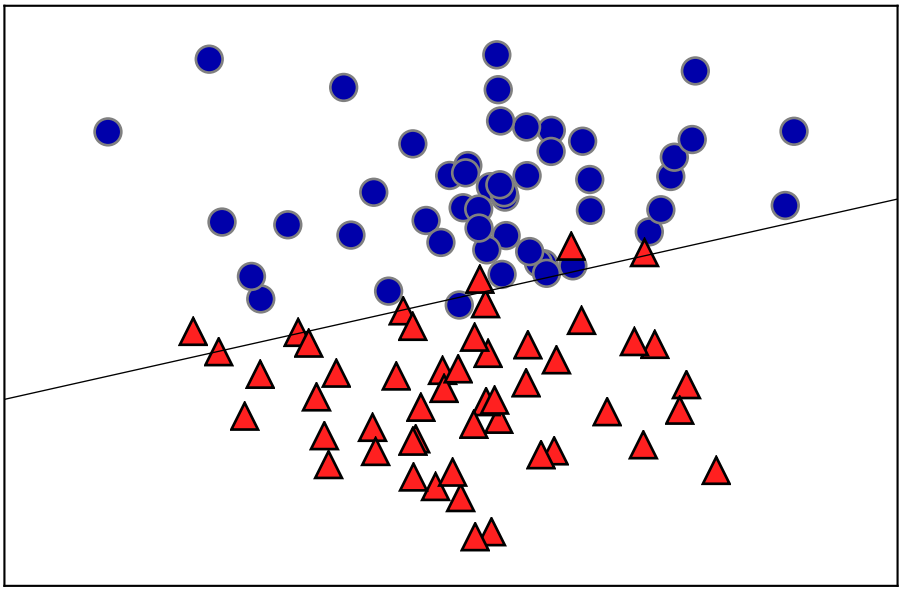
Classifiers can often provide uncertainty estimates of predictions.
In practice, you are often interested in how certain a classifier is about each class prediction (e.g. cancer treatments).

Scikit-learn offers 2 functions. Often, both are available for every learner, but not always.

- decision_function: returns floating point value for each sample
- predict_proba: return probability for each class

[388]:
```
# create and split a synthetic dataset
from sklearn.linear_model import LogisticRegression
from sklearn.datasets import make_blobs
X, y = make_blobs(centers=2, cluster_std=2.5, random_state=8)

# we rename the classes "blue" and "red"
y_named = np.array(["blue", "red"])[y]

# we can call train test split with arbitrary many arrays
# all will be split in a consistent manner
X_train, X_test, y_train_named, y_test_named, y_train, y_test = \
    train_test_split(X, y_named, y, random_state=0)

# build the logistic regression model
lr = LogisticRegression()
```

```
lr.fit(X_train, y_train_named)

mglearn.plots.plot_2d_separator(lr, X)
mglearn.discrete_scatter(X[:, 0], X[:, 1], y);
```



The Decision Function

In the binary classification case, the return value of decision_function is of shape (n_samples,), and it returns one floating-point number for each sample. The first class (class 0) is considered negative, the other (class 1) positive.

This value encodes how strongly the model believes a data point to belong to the "positive" class.

- Positive values indicate a preference for the "positive" class
- Negative values indicate a preference for the "negative" (other) class

```
[389]: # show the first few entries of decision_function
       print("Decision function:\n{}".format(lr.decision_function(X_test)[:6]))
```

```
Decision function:
[ 0.527  4.314  5.92   2.899  4.751 -7.035]
```

```
[390]: # Recover the predictions by looking at the sign
       print("Thresholded decision function:\n{}".format(
             lr.decision_function(X_test)[:6] > 0))
       print("Predictions:\n{}".format(lr.predict(X_test)[:6]))
```

```
Thresholded decision function:
[ True  True  True  True  True False]
Predictions:
['red' 'red' 'red' 'red' 'red' 'blue']
```

The range of decision_function can be arbitrary, and depends on the data and the model parameters. This makes it sometimes hard to interpret.

```
[391]: decision_function = lr.decision_function(X_test)
       print("Decision function minimum: {:.2f} maximum: {:.2f}".format(
             np.min(decision_function), np.max(decision_function)))
```

```
Decision function minimum: -10.48 maximum: 8.61
```

We can visualize the decision function as follows, with the actual decision boundary left and the values of the decision boudaries color-coded on the right.
Note how the test examples are labeled depending on the decision function.

```
[1]: fig, axes = plt.subplots(1, 2, figsize=(13, 5))

     mglearn.tools.plot_2d_separator(lr, X, ax=axes[0], alpha=.4,
                                     fill=True, cm=mglearn.cm2)
     scores_image = mglearn.tools.plot_2d_scores(lr, X, ax=axes[1],
                                                 alpha=.4, cm=mglearn.ReBl)

     for ax in axes:
         # plot training and test points
         mglearn.discrete_scatter(X_test[:, 0], X_test[:, 1], y_test,
                                  markers='^', ax=ax)
         mglearn.discrete_scatter(X_train[:, 0], X_train[:, 1], y_train,
                                  markers='o', ax=ax)
         ax.set_xlabel("Feature 0")
         ax.set_ylabel("Feature 1")
     cbar = plt.colorbar(scores_image, ax=axes.tolist())
     cbar.set_alpha(1)
     cbar.draw_all()
     axes[0].legend(["Test class 0", "Test class 1", "Train class 0",
                     "Train class 1"], ncol=4, loc=(.1, 1.1));
```

```
     ---------------------------------------------------------------------------

     NameError                                 Traceback (most recent call la

     <ipython-input-1-21291bf6fdaf> in <module>()
----> 1 fig, axes = plt.figure()
       2
       3 mglearn.tools.plot_2d_separator(lr, X, ax=axes[0], alpha=.4,
       4                                 fill=True, cm=mglearn.cm2)
       5 scores_image = mglearn.tools.plot_2d_scores(lr, X, ax=axes[1],


     NameError: name 'plt' is not defined
```

Predicting probabilities

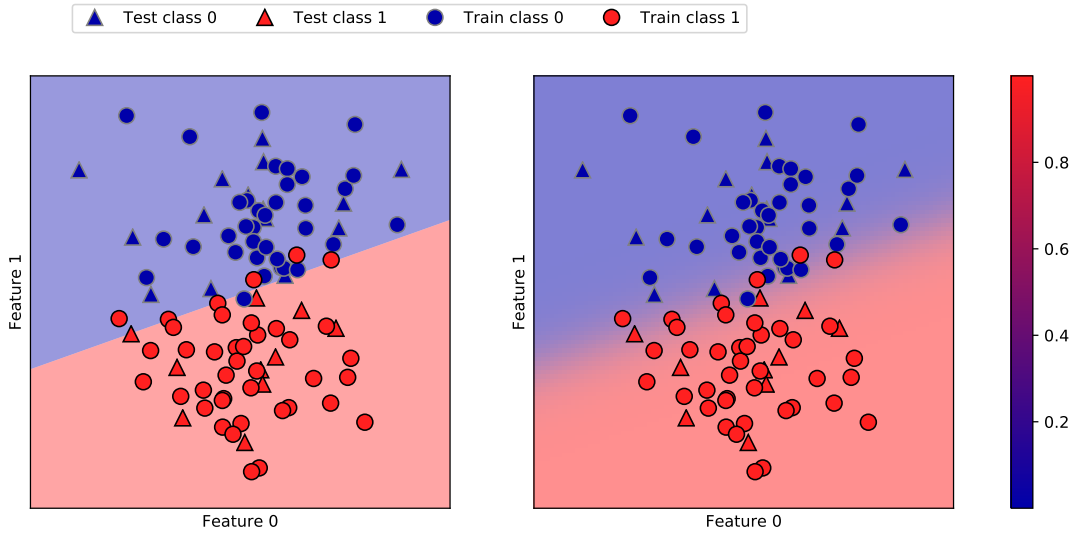
The output of predict_proba is a *probability* for each class, with one column per class. They sum up to 1.

```
[393]: print("Shape of probabilities: {}".format(lr.predict_proba(X_test).shape)
       # show the first few entries of predict_proba
       print("Predicted probabilities:\n{}".format(
             lr.predict_proba(X_test[:6])))
```

```
Shape of probabilities: (25, 2)
Predicted probabilities:
[[ 0.371  0.629]
 [ 0.013  0.987]
 [ 0.003  0.997]
 [ 0.052  0.948]
 [ 0.009  0.991]
 [ 0.999  0.001]]
```

We can visualize them again. Note that the gradient looks different now.

```
[394]: fig, axes = plt.subplots(1, 2, figsize=(13, 5))

       mglearn.tools.plot_2d_separator(
           lr, X, ax=axes[0], alpha=.4, fill=True, cm=mglearn.cm2)
       scores_image = mglearn.tools.plot_2d_scores(
           lr, X, ax=axes[1], alpha=.5, cm=mglearn.ReBl, function='predict_proba

       for ax in axes:
           # plot training and test points
           mglearn.discrete_scatter(X_test[:, 0], X_test[:, 1], y_test,
                                    markers='^', ax=ax)
           mglearn.discrete_scatter(X_train[:, 0], X_train[:, 1], y_train,
                                    markers='o', ax=ax)
           ax.set_xlabel("Feature 0")
           ax.set_ylabel("Feature 1")
       # don't want a transparent colorbar
       cbar = plt.colorbar(scores_image, ax=axes.tolist())
       cbar.set_alpha(1)
       cbar.draw_all()
       axes[0].legend(["Test class 0", "Test class 1", "Train class 0",
                       "Train class 1"], ncol=4, loc=(.1, 1.1));
```



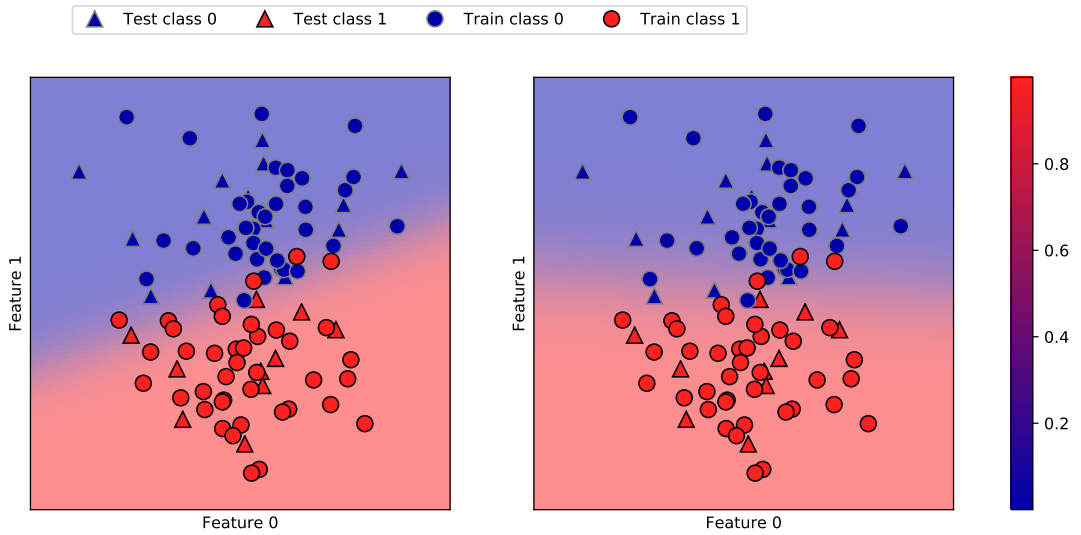
Interpreting probabilities

- The class with the highest probability is predicted.
- How well the uncertainty actually reflects uncertainty in the data depends on the model and the parameters.
  - An overfitted model tends to make more certain predictions, even if they might be wrong.
  - A model with less complexity usually has more uncertainty in its predictions.
- A model is called *calibrated* if the reported uncertainty actually matches how correct it is — A prediction made with 70% certainty would be correct 70% of the time.
  - LogisticRegression returns well calibrated predictions by default as it directly optimizes log-loss
  - Linear SVM are not well calibrated. They are *biased* towards points close to the decision boundary.
- Techniques exist to calibrate models in post-processing. More in the next lecture.

Compare logistic regression and linear SVM

```
[395]: from sklearn.svm import SVC
       svc = SVC(kernel="linear",C=0.1,probability=True).fit(X_train, y_train_na

       fig, axes = plt.subplots(1, 2, figsize=(13, 5))

       lr_image = mglearn.tools.plot_2d_scores(
           lr, X, ax=axes[0], alpha=.5, cm=mglearn.ReBl, function='predict_proba
       svc_image = mglearn.tools.plot_2d_scores(
           svc, X, ax=axes[1], alpha=.5, cm=mglearn.ReBl, function='predict_prob

       for ax in axes:
           # plot training and test points
           mglearn.discrete_scatter(X_test[:, 0], X_test[:, 1], y_test,
```

```
                                markers='^', ax=ax)
    mglearn.discrete_scatter(X_train[:, 0], X_train[:, 1], y_train,
                                markers='o', ax=ax)
    ax.set_xlabel("Feature 0")
    ax.set_ylabel("Feature 1")
# don't want a transparent colorbar
cbar = plt.colorbar(lr_image, ax=axes.tolist())
cbar.set_alpha(1)
cbar.draw_all()
axes[0].legend(["Test class 0", "Test class 1", "Train class 0",
                "Train class 1"], ncol=4, loc=(.1, 1.1));
```



Uncertainty in multi-class classification

- decision_function and predict_proba methods also work in the multiclass setting
- always have shape (n_samples, n_classes), except for decision_function in the binary case (which only returns the values for the positive class)

Example on the Iris dataset, which has 3 classes

[396]:
```
from sklearn.datasets import load_iris

iris = load_iris()
X_train, X_test, y_train, y_test = train_test_split(
    iris.data, iris.target, random_state=42)

lr2 = LogisticRegression()
lr2 = lr2.fit(X_train, y_train)

print("Decision function:\n{}".format(lr2.decision_function(X_test)[:6, :
# show the first few entries of predict_proba
print("Predicted probabilities:\n{}".format(lr2.predict_proba(X_test)[:6]
```

```
Decision function:
[[ -4.744   0.102  -1.084]
 [  3.699  -1.937 -10.976]
 [-10.128   0.898   4.262]
 [ -4.504  -0.5    -0.92 ]
 [ -4.881   0.249  -1.512]
 [  3.369  -1.644 -10.167]]
Predicted probabilities:
[[ 0.011  0.668  0.321]
 [ 0.886  0.114  0.   ]
 [ 0.     0.419  0.581]
 [ 0.016  0.561  0.423]
 [ 0.01   0.749  0.241]
 [ 0.857  0.143  0.   ]]
```

Summary

- Nearest neighbors
  - For small datasets, excellent baseline, easy to explain.
- Linear models
  - Go-to as a first algorithm to try, good for very large datasets, good for very high-dimensional data.
- Many more models to come
- We first need to learn how to select between them (and their hyperparameters): model selection