PATTERN RECOGNITION AND MACHINE LEARNING

Slide Set 4: Machine Learning

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Classification

- Many machine learning problems can be posed as **classification** tasks.
- Most classification tasks can be posed as a problem of partitioning a vector space into disjoint regions.
- These problems consist of following components:

$$\text{Samples: } \mathbf{x}[0], \mathbf{x}[1], \ldots, \mathbf{x}[N-1] \in \mathbb{R}^P$$
$$\text{Class labels: } y[0], y[1], \ldots, y[N-1] \in \{1, 2, \ldots, C\}$$
$$\text{Classifier: } F(\mathbf{x}) : \mathbb{R}^P \mapsto \{1, 2, \ldots, C\}$$

- Now, the task is to find the function F that maps the samples most accurately to their corresponding labels.
- For example: Find the function F that minimizes the number of erroneous predictions, *i.e.*, the cases $F(\mathbf{x}[k]) \neq y[k]$.

Regression

- The second large class of machine learning problems consists of **regression** tasks.
- For regression, the output is real-valued instead of categorical.
- These problems consist of following components:

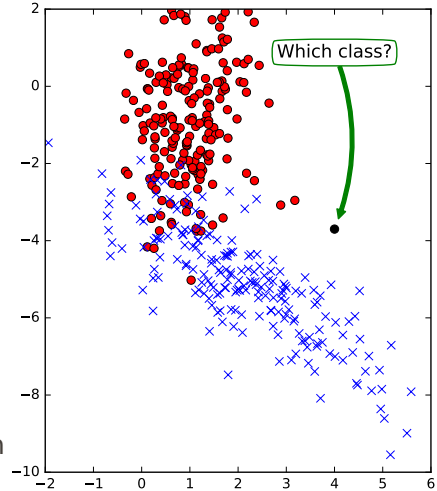
$$\begin{aligned} \text{Inputs: } & \mathbf{x}[0], \mathbf{x}[1], \ldots, \mathbf{x}[N-1] \in \mathbb{R}^P \\ \text{Targets: } & y[0], y[1], \ldots, y[N-1] \in \mathbb{R} \\ \text{Predictor: } & F(\mathbf{x}) : \mathbb{R}^P \mapsto \mathbb{R} \end{aligned}$$

- This time the task is to find the function F that maps the samples most accurately to their corresponding targets.
- For example: Find the function F that minimizes the squared sum of distances between predictions and targets:

$$\mathcal{E} = \sum_{k=0}^{N-1} \left(y[k] - F(\mathbf{x}[k]) \right)^2 .$$

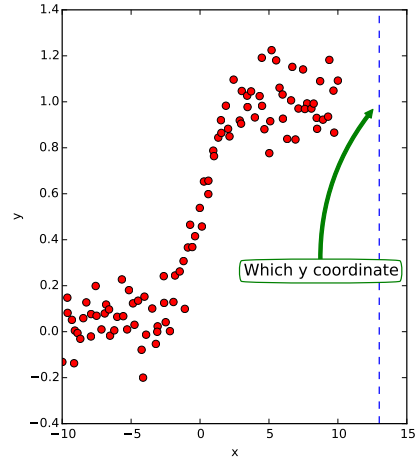
Classification Example

- For example, consider the 2-dimensional dataset on the right.
- The data consists of 200 blue crosses and 200 red circles.
- Based on these data, what would be a good partition of the 2D space into "red" and "blue" regions?
- What kind of boundaries are allowed between the regions?
  - Straight lines?
  - Continuous curved boundaries?
  - Boundary without any restriction?
- Note: In 2-D this can be solved manually, but not in 4000-D.



Regression Example

- For example, consider the 1-dimensional data on the right.
- The data consists of 100 data points, where y coordinate is a function of x.
- Based on these data, what would be a good prediction of the target value at $x = 1.3$ (the dashed line)?
- An obvious solution is to fit a curve into the data points. What kind of forms may the curve have?
  - Straight lines?
  - Continuous curves?

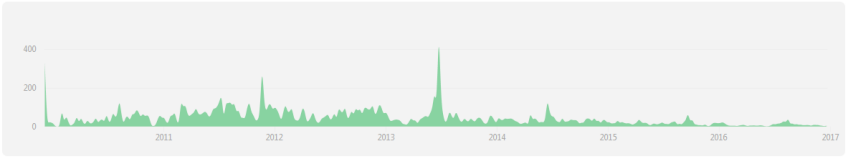


Different Classifiers

- We will study the following widely used classifiers.
  - Nearest Neighbor classifier
  - Linear classifiers (with linear boundary)
  - The support vector machine (with nonlinear boundary)
  - Ensemble classifiers: Random Forest
  - Black boxes: Neural networks and deep neural networks
- For the first four, we will refer to the *Scikit-Learn* module: **http://scikit-learn.org/**.
- The neural network part will be studied with the *Keras* package: **http://keras.io/**.

Scikit-Learn

- Scikit-Learn started as a Google Summer of Code project.
- The project became a success: There was a clear need for free elegant platform bringing together widely used methods.
- Instead of each contributor providing their own package, scikit-learn has a unified API for each method.
- For details: Pedregosa, *et al.* ”Scikit-learn: Machine learning in Python,” *The Journal of Machine Learning Research*,2011.



Scikit-Learn Methods

Sklearn API is straightforward:

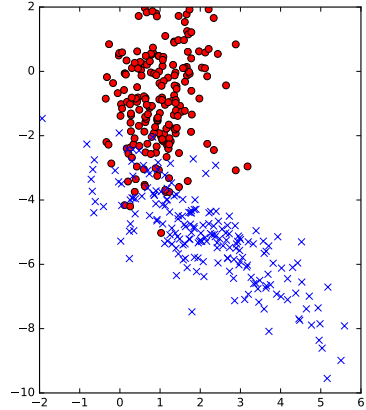
- **Initialization:** Each model has its own constructor, *e.g.*, `model = LogisticRegression(penalty = "l1", C = 0.1)`.
- **Training:** Every model implements a `.fit()` method that trains the model; *e.g.*, `model.fit(X_train, y_train)`
- **Prediction:** Every model implements a `.predict()` method that predicts the target output for new inputs; *e.g.*, `y_hat = model.predict(X_test)`
- **Probabilities:** Many models also implement a `.predict_proba()` method that predicts the class probabilities for new inputs; *e.g.*, `p = model.predict_proba(X_test)`

Sample Scikit-learn Session

```
# Training code:
from sklearn.linear_model import LogisticRegression

model = LogisticRegression()
model.fit(X, y)
```

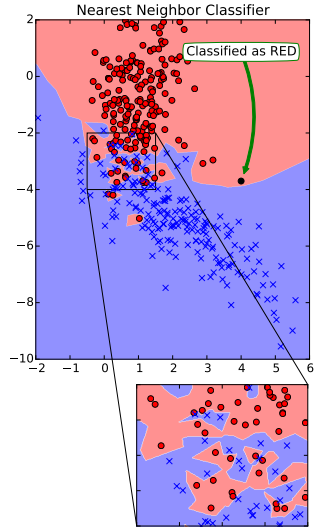
```
# Testing code:
>>> model.predict([1,2])
array([ 1.])

>>> model.predict([-10,-2])
array([ 0.]

>>> model.predict_proba([[1,2], [-10,-2]])
Out[35]:
array([[ 0.0044881 ,  0.9955119 ],
       [ 0.56097861,  0.43902139]])

# [1,2] is class 1 with 99.5 % confidence.
# [-10,-2] is class 0 with 56.1 % confidence.
```

- In the example code, X consists of 400 two-dimensional samples from two classes.



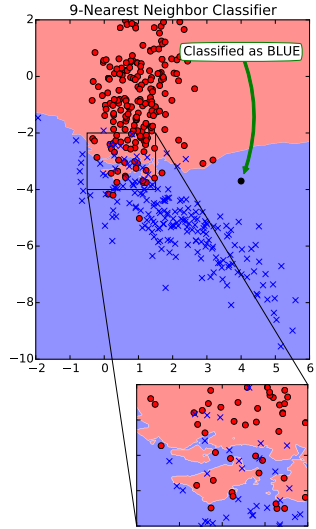
Nearest Neighbor Classifier

- Probably the most natural approach for deciding the class is simply to see what kind of samples are nearby.
- This is the idea behind the **Nearest neighbor** classifier: Just copy the class label of the most similar training sample to the unknown test sample.



K-Nearest Neighbor Classifier

- The problem with Nearest Neighbor is its fragility to changes in the training data.
- The classification boundary may change a lot by moving only one training sample.
- The robustness can be increased by taking a majority vote of more nearby samples.
- The **K-Nearest neighbor** classifier selects the most frequent class label among the *K* nearest training samples.



Nearest Neighbor in Scikit-learn

```
# Training code:
from sklearn.neighbors import KNeighborsClassifier

model = KNeighborsClassifier(n_neighbors = 5, metric = "euclidean")
model.fit(X, y)
```

```
# Testing code:
>>> model.predict([-10,-2])
array([ 0.])

>>> model.predict([1,2])
array([ 1.])

>>> model.predict_proba([0,-3])
array([[ 0.6,  0.4]])

# Ask what are the 5 nearest neighbors.
# Returns the distances and indices (rows) in X
>>> distances, indices = model.kneighbors([0,-3])
[0.144,  0.254,  0.362,  0.414,  0.422]
[379,  11, 215, 370, 198]

# What are the classes for these five:
>>> y[indices]
array([[ 0.,  1.,  0.,  0.,  1.]])
```

- Parameters of constructor include:
  - `n_neighbors`: Number of neighbors *K*
  - `metric`: How distance is calculated
  - `algorithm`: Which algorithm finds the nearest samples; *e.g.,* methods like *K-D Tree* or *brute force*
- Probability prediction counts how many of the nearest *K* samples belong to each group.
- Thus, the probabilities are very quantized and often either 0 or 1.

Benefits of Nearest Neighbor

- Training time is minimal: Either just store the data as is; or reorganize it into a tree structure for efficient search.
- Accuracy is often relatively good.
- Allows complicated definitions of distance, *e.g.*,
  - Find the 5 nearest samples holding attributes A and B but not C.
- New data can be added/deleted without retraining.

Problems with the Nearest Neighbor

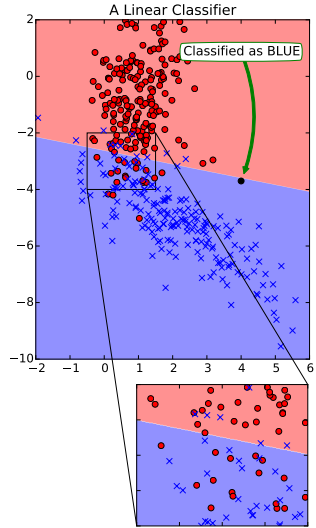
- Nearest neighbor is prone to overlearning: Especially the 1-NN forms local regions around every isolated data point.
- It is highly unlikely that these represent the general trend of the whole population.
- Moreover, the training step extremely fast while the classification step becomes extremely slow (consider training data with billion high-dimensional samples).
- Therefore, more compact representations are preferred: Training time is usually not critical while execution time is.

Linear Classifiers

- A linear classifier learns a linear decision boundary between classes.
- In mathematical terms, the classification rule can be written as

$$F(\mathbf{x}) = \begin{cases} \text{Class 1}, & \text{if } \mathbf{w}^T\mathbf{x} < b \\ \text{Class 2}, & \text{if } \mathbf{w}^T\mathbf{x} \geq b \end{cases}$$

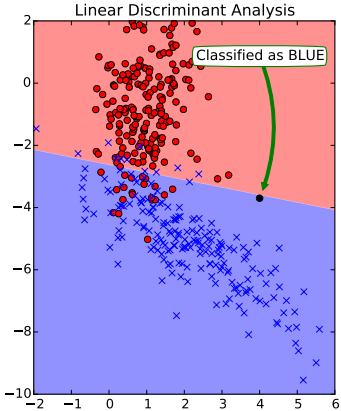
  where the weights $\mathbf{w}$ are learned from the data.
- The expression $\mathbf{w}^T\mathbf{x} = \sum_k w_k x_k$ essentially transforms the multidimensional data $\mathbf{x}$ to a real number, which is then compared to a threshold b.

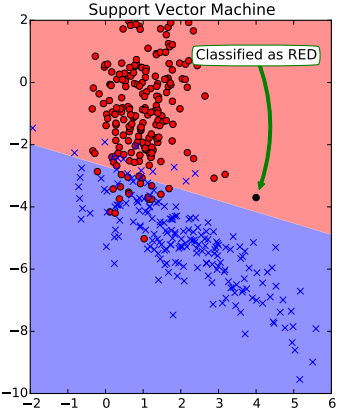


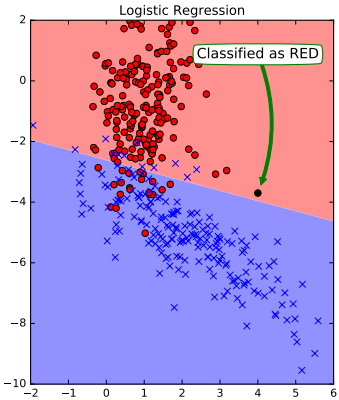
Flavors of Linear Classifiers

There exists many algorithms for learning the weights **w**, including:

- *Linear Discriminant Analysis (LDA)*
- *Support Vector Machine (SVM)*
- *Logistic Regression (LR)*







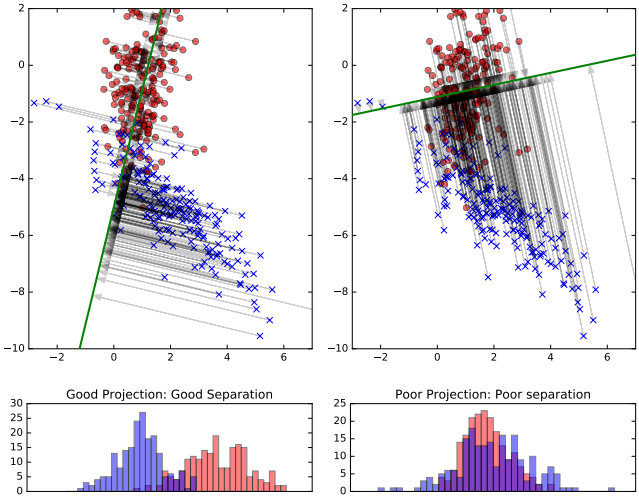
Flavors of Linear Classifiers

- The LDA:
  - The oldest of the three: Fisher, 1935.
  - "Find the projection that maximizes class separation", *i.e.*, pull the classes as far from each other as possible.
  - Closed form solution, fast to train.
- The SVM:
  - Vapnik and Chervonenkis, 1963.
  - "Maximize the margin between classes".
  - Slowest of the three[1], performs well with sparse high-dimensional data.
- Logistic Regression (*a.k.a. Generalized Linear Model*):
  - History traces back to 1700's, but proper formulation and efficient training algorithm by Nelder and Wedderburn in 1972.
  - Statistical algorithm: "Maximize the likelihood of the data".
  - Outputs also class probability. Has been extended to automatic feature selection.

[1] Slowest in *training*; testing time is the same for all

Linear Discriminant Analysis

- The LDA maps high dimensional data into a single scalar simultaneously pulling individual classes apart.
- Thus, the task is essentially finding a good linear projection $\mathbb{R}^N \mapsto \mathbb{R}$.



Linear Discriminant Analysis

- A good measure of class separation could be, *e.g.*, the distance between their projected means.
- However, this quantity depends on the scale, and increases simply by multiplying by a large number.
- Thus, we want to pull class means apart while keeping the variance of each class small.
- As a result, we look into the following separability score:

$$J(\mathbf{w}) = \frac{\text{Distance of Class Means}}{\text{Variance of Classes}} = \frac{(\mathbf{w}^T\boldsymbol{\mu}_1 - \mathbf{w}^T\boldsymbol{\mu}_0)^2}{\mathbf{w}^T\boldsymbol{\Sigma}_1\mathbf{w} + \mathbf{w}^T\boldsymbol{\Sigma}_0\mathbf{w}},$$

where $\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_0$ are the class means and $\boldsymbol{\Sigma}_1$ and $\boldsymbol{\Sigma}_0$ covariance matrices of the two classes.

Maximization of $J(\mathbf{w})$

- The Fisher separation score can be maximized analytically.
- First simplify $J(\mathbf{w})$ a bit:

$$J(\mathbf{w}) = \frac{(\mathbf{w}^T\boldsymbol{\mu}_1 - \mathbf{w}^T\boldsymbol{\mu}_0)^2}{\mathbf{w}^T\boldsymbol{\Sigma}_1\mathbf{w} + \mathbf{w}^T\boldsymbol{\Sigma}_0\mathbf{w}} = \frac{\mathbf{w}^T\mathbf{S}_B\mathbf{w}}{\mathbf{w}^T\mathbf{S}_W\mathbf{w}}$$

  with $\mathbf{S}_B = (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^T$ and $\mathbf{S}_W = \boldsymbol{\Sigma}_1 + \boldsymbol{\Sigma}_0$.
- This form is known as *Generalized Rayleigh Quotient*, which appears in many contexts.
- Using Lagrange multipliers, one can show that the maximum must satisfy

$$\mathbf{S}_B\mathbf{w} = \lambda\mathbf{S}_W\mathbf{w}$$

  with $\lambda \in \mathbb{R}$ a constant.

Maximization of $J(\mathbf{w})$

- The above condition is a *generalized eigenvalue problem*.
- In other words, there are many solutions: one for each eigenvalue.
- Thus, it is straightforward to conclude that the quantity

$$J(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

  is maximized when

$$\mathbf{S}_B \mathbf{w} = \lambda \mathbf{S}_W \mathbf{w}$$

  or equivalently

$$\mathbf{w}^T \mathbf{S}_B \mathbf{w} = \lambda \mathbf{w}^T \mathbf{S}_W \mathbf{w}$$

- Finally, the ratio $\mathbf{w}^T \mathbf{S}_B \mathbf{w} / \mathbf{w}^T \mathbf{S}_W \mathbf{w}$ is maximized by choosing λ as the largest eigenvalue (and $\mathbf{w}$ as the corresponding eigenvector).

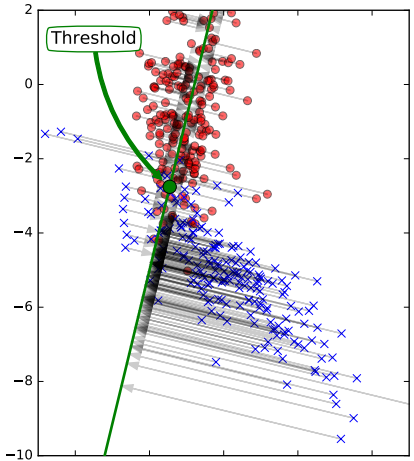
Solution 1 using Eigenvalues

```
# Training code:
import numpy as np
from scipy.linalg import eig

# X0 and X1 contain data of the 2 classes
m0 = np.mean(X0.T, axis = 0)
m1 = np.mean(X1.T, axis = 0)
C0 = np.cov(X0.T - np.tile(m0, (X0.shape[1], 1)), rowvar = False)
C1 = np.cov(X1.T - np.tile(m1, (X1.shape[1], 1)), rowvar = False)

SB = np.multiply.outer(m1 - m0, m1 - m0)
SW = C0 + C1

D, V = eig(SB, SW)
w = V[:, -1]

T = np.mean([np.dot(m1, w), np.dot(m2, w)])
```

```
# Testing code:
>>> w
array([ 0.23535937,  0.97190842])

>>> np.dot(w, [0,-2]) - T
0.606
# Positive -> in class "red circles"

>>> np.dot(w, [0,-3]) - T
-0.3657
# Negative -> in class "blue crosses"
```

- We need to solve the generalized eigenvalue problem $\mathbf{S}_B\mathbf{w} = \lambda\mathbf{S}_W\mathbf{w}$.
- `scipy` has a solver for that.
- `scipy.linalg.eig` returns
  - Array of eigenvalues `D` in increasing order.
  - Matrix of eigenvectors `V` (in columns).
- Thus, we want the rightmost (”−1$^{\text{th}}$”) column `V[:, -1]` (corresponding to largest eigenvalue).
- The decision is done by comparing the projected vector to threshold `T`; the center of projected class means.

LDA Projection with Threshold



Solution 2 without Eigenvalues

- It turns out that solving the generalized eigenvalue problem $\mathbf{S}_B\mathbf{w} = \lambda\mathbf{S}_W\mathbf{w}$ is not necessary.
- The maximum of $J(\mathbf{w})$ has to satisfy $\mathbf{S}_B\mathbf{w} = \lambda\mathbf{S}_W\mathbf{w}$, or equivalently, $\mathbf{S}_W^{-1}\mathbf{S}_B\mathbf{w} = \lambda\mathbf{w}$.
- Insert the definition of $\mathbf{S}_B$ to get:

$$\mathbf{S}_W^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)\underbrace{(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^T\mathbf{w}}_{\text{scalar } C} = \lambda\mathbf{w}$$

or,

$$\mathbf{S}_W^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)\frac{C}{\lambda} = \mathbf{w}$$

Solution 2 without Eigenvalues

- Thus, the maximum of $J(\mathbf{w})$ has to satisfy this condition as well (regardless of λ).
- We are looking for a direction vector $\mathbf{w}$, so the multiplier C/λ is not relevant either ($\frac{C}{\lambda}\mathbf{w}$ has the same direction as $\mathbf{w}$).
- Thus, $\mathbf{w}$ is given by

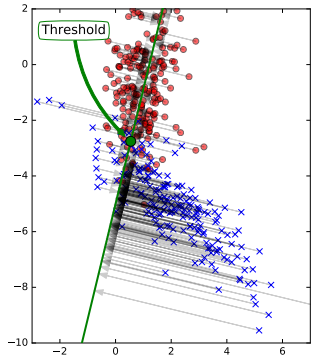
$$\mathbf{w} = \mathbf{S}_W^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) = (\boldsymbol{\Sigma}_0 + \boldsymbol{\Sigma}_1)^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0).$$

Solution 2 without Eigenvalues

```
# Training code:
import numpy as np
from scipy.linalg import eig

# X0 and X1 contain data of the 2 classes
m0 = np.mean(X0.T, axis = 0)
m1 = np.mean(X1.T, axis = 0)

C0 = np.cov(X0.T - np.tile(m0, (X0.shape[1], 1)), rowvar = False)
C1 = np.cov(X1.T - np.tile(m1, (X1.shape[1], 1)), rowvar = False)

w = np.dot(np.linalg.inv(C0 + C1), (m1 - m0))

T = np.mean([np.dot(m1, w), np.dot(m2, w)])
```

```
# Testing code:
>>> w
array([ 0.25237576,  1.04217702])

>>> np.dot(w, [0,-2]) - T
0.65004
# Positive -> in class "red circles"

>>> np.dot(w, [0,-3]) - T
-0.3921
# Negative -> in class "blue crosses"
```

- The Python code is very similar to the eigenvalue based solution.
- Note that the resulting w is not exactly the same: The lengths are different, but directions are the same.



Solution 3: Scikit-Learn

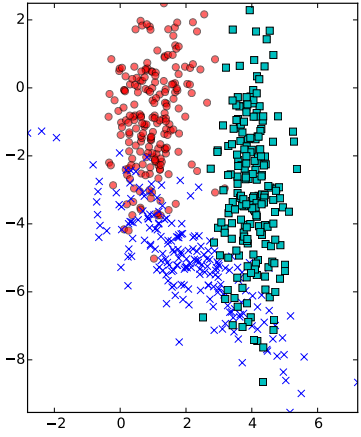
```
# Training code:
from sklearn.discriminant_analysis import
      LinearDiscriminantAnalysis

clf = LinearDiscriminantAnalysis()

# X contains all samples, and y their class
# labels: y = [0,1,1,0,...]
clf.fit(X, y)
```

```
# Testing code:
>>> clf.coef_      # This is our w vector
array([[ 0.50475151,  2.08435403]])

>>> clf.intercept_ # This is the threshold
array([ 5.46879769])

>>>  clf.predict([0, -2])
array([ 1.])

>>>  clf.predict([0, -3])
array([ 0.])

>>> clf.predict_proba([0, -3])
array([[ 0.68659846,  0.31340154]])
```

- Scikit-Learn implements LDA in a straightforward manner.
- First construct your classifier using `LinearDiscriminantAnalysis()`
- Then train the model using `fit()`
- Then predict classes using `predict()`
- Or class probabilities using `predict_proba()`

Multiclass LDA

- The LDA can be generalized to handle more than 2 classes.
- *Multiclass LDA* can be understood in two contexts:
  - As *dimensionality reduction:* We seek for a set of projections, that lower the dimensionality of the data while retaining its original separability.
  - As *classification:* We seek for a set of discriminant functions that give a probability score for each class.
- We are more interested in the latter interpretation.



Multiclass LDA

- In this case, the classifier is defined by a set of linear functions

$$g_1(\mathbf{x}) = \mathbf{w}_1^T\mathbf{x} + w_1$$
$$\vdots$$
$$g_K(\mathbf{x}) = \mathbf{w}_K^T\mathbf{x} + w_K$$

- Then the vector $\mathbf{x}$ is assigned class $k = 1, 2, \ldots, K$ if

$$g_k(\mathbf{x}) > g_j(\mathbf{x})$$

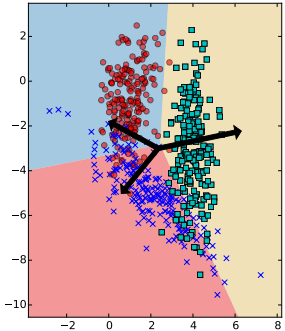
for all $j \neq k$.

Multiclass LDA

```
# Training code:
import numpy as np
from sklearn.discriminant_analysis import
       LinearDiscriminantAnalysis

clf = LinearDiscriminantAnalysis()

# X contains all samples, and y their class
# labels: y = [1,3,1,2,...]
clf.fit(X, y)
```

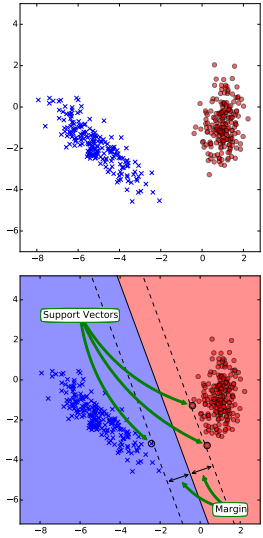
```
# Testing code:

# Show the three discriminants (rows):
>>> clf.coef_
array([[-1.00629245,  0.51513354],
       [-0.74957209, -0.8613368 ],
       [ 1.75586454,  0.34620326]])

# Compute discriminants for [0,-2]
>>> scores = np.dot(clf.coef_, [0,-2]) + clf.intercept_
array([ 0.56090889, -1.20225066, -6.31434368])
# First class (red) has largest score

# Predict class more easily using predict()
>>> clf.predict([[0, -2], [0, -4]])
array([ 1.,  2.])
```

- `LinearDiscriminantAnalysis()` model applies to multiclass case as well.
- The `fit()` method finds the three discriminants also shown in the plot below.



The Support Vector Machine

- The Support Vector Machine (SVM) is characterized by its *maximum margin property.*
- In other words, it attempts to maximize the margin between classes.
- In the attached example, the binary data is perfectly separable, and the SVM sets the boundary in the middle of the two classes.
- Thus, the boundary location is defined by three samples only; called *support vectors*.



The Support Vector Machine

- Maximizing the margin M for the SVM can be characterized as an optimization problem

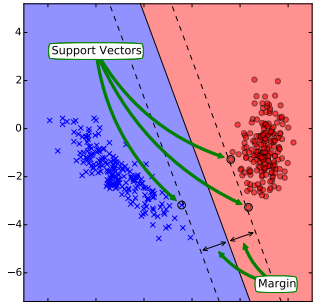
$$\underset{\mathbf{w},b,\|\mathbf{w}\|=1}{\text{maximize}} \quad M,$$

$$\textit{subject to}$$

$$y_i(\mathbf{x}_i^T\mathbf{w} + b) \geq M, \text{ for } i = 1, 2, \ldots, N$$

- Here, y_i encodes the class as $y_i \in \{-1, 1\}$, so the last condition can also be written as

$$\begin{cases} \mathbf{x}_i^T\mathbf{w} + b \geq M, & \text{if } y_i = 1 \\ \mathbf{x}_i^T\mathbf{w} + b \leq -M, & \text{if } y_i = -1 \end{cases}$$



The Support Vector Machine

- Alternatively, the SVM criterion can be simplified into an equivalent form

$$\begin{aligned} &\underset{\mathbf{w},b}{\text{minimize}} \quad \|\mathbf{w}\|, \\ &\textit{subject to} \\ &y_i(\mathbf{x}_i^T\mathbf{w} + b) \geq 1, \text{ for } i = 1, 2, \ldots, N \end{aligned}$$

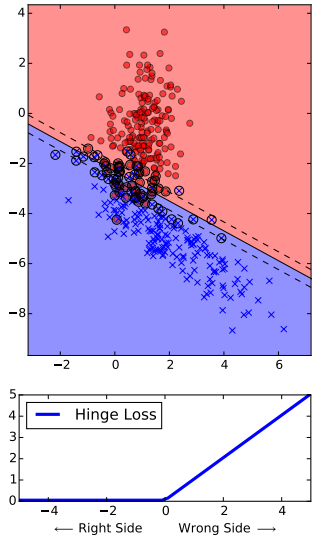
- This is a convex optimization problem with constraints. Efficient tailored algorithms exist.
- The implementation of Scikit-learn is based on the widely used LibSVM library.

The Support Vector Machine

- The earlier definition of SVM assumes that the classes are separate (and there exists a margin between classes).
- In reality we have to allow some samples to reside on the wrong side of the margin.
- The solution is to penalize for samples on the wrong side.
- The resulting function to be minimized is:

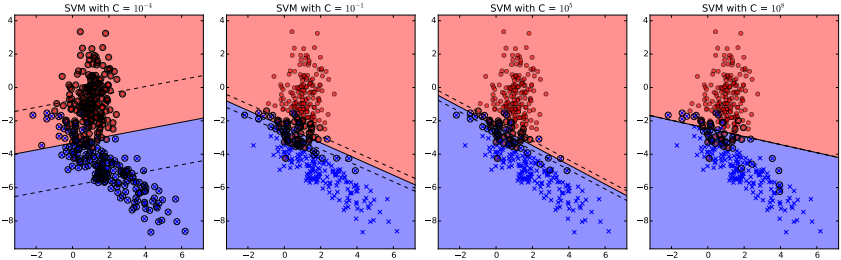
$$\underset{\mathbf{w},b}{\text{minimize}} \sum_{i=1}^{N} [\max(0, 1 - y_i(\mathbf{w}^T\mathbf{x}_i + b))] + C\|\mathbf{w}\|^2.$$

- For each sample on the wrong side, we add a penalty (called *hinge loss*) defined as $\max(0, x)$
- Note, that this increases the number of SV's.



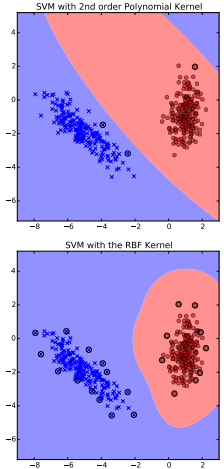
SVM in Scikit-Learn

- The parameter *C* determines the balance between margin width and penalty for being on the wrong side.
- Left to right: Linear SVM's with decreasing penalty.



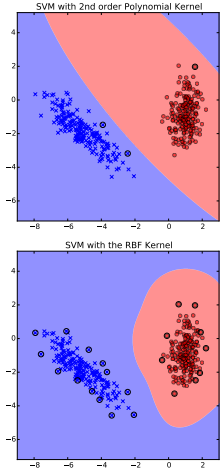
Kernel Trick

- The SVM can be extended to nonlinear boundaries using the *kernel trick*.
- The kernel trick essentially maps the data into a higher dimension and designs the linear SVM there.
- For example, the top plot can be generated as follows:
  - Map the 2D samples into 3D: $(x, y) \mapsto (x^2, y^2, \sqrt{2}xy)$
  - Train the SVM with the new 3D samples.
  - The decision boundary is linear in 3D but nonlinear in 2D.
- However, this explicit transformation is slow; the kernel trick does the same thing implicitly.



Kernel Trick

- It can be shown that substitution of the dot product by some nonlinear function is equivalent to the explicit mapping.
- More specifically, an algorithm can be kernelized by inserting a kernel function $\kappa(\mathbf{x}, \mathbf{y})$ in place of all dot products $\mathbf{x} \cdot \mathbf{y}$.
- It can be shown that under certain conditions on the kernel (*e.g.*, positive semidefiniteness), this is equivalent to an explicit mapping.
- A lot of research has been done on the relation of kernel and the corresponding mapping.
- However, we take a more practical approach and only consider an example.



Kernel Trick

- As an example, consider what happens when the inner product of 2D vectors $\mathbf{x} = (x_1, x_2)$ and $\mathbf{y} = (y_1, y_2)$ is substituted by its second power:

$$\kappa(\mathbf{x}, \mathbf{y}) = (\mathbf{x} \cdot \mathbf{y})^2$$

- We can expand the kernel as follows

$$\begin{aligned} \kappa(\mathbf{x}, \mathbf{y}) &= (\mathbf{x} \cdot \mathbf{y})^2 \\ &= (x_1 y_1 + x_2 y_2)^2 \\ &= (x_1 y_1)^2 + (x_2 y_2)^2 + 2 x_1 y_1 x_2 y_2 \end{aligned}$$

Kernel Trick

- The result can be cleverly rearranged to make it look like a dot product in 3D:

$$\begin{aligned}\kappa(\mathbf{x}, \mathbf{y}) &= (x_1 y_1)^2 + (x_2 y_2)^2 + 2 x_1 y_1 x_2 y_2 \\ &= (x_1 y_1)^2 + (x_2 y_2)^2 + (\sqrt{2} x_1 x_2)(\sqrt{2} y_1 y_2) \\ &= \left(x_1^2, x_2^2, \sqrt{2} x_1 x_2\right) \cdot \left(y_1^2, y_2^2, \sqrt{2} y_1 y_2\right)\end{aligned}$$

Kernel Trick

- Thus, the following two things are equivalent:
  - **Explicit Mapping**: Transform 2D data into 3D explicitly and fit the SVM with transformed data:

$$\begin{pmatrix} u \\ v \end{pmatrix} \mapsto \begin{pmatrix} u^2 \\ v^2 \\ \sqrt{2}uv \end{pmatrix}$$

  - **Implicit Mapping**: Substitute each dot product in the SVM algorithm by the kernel $\kappa(\mathbf{x}, \mathbf{y}) = (\mathbf{x} \cdot \mathbf{y})^2$ and fit with original 2D data.

Popular Kernels

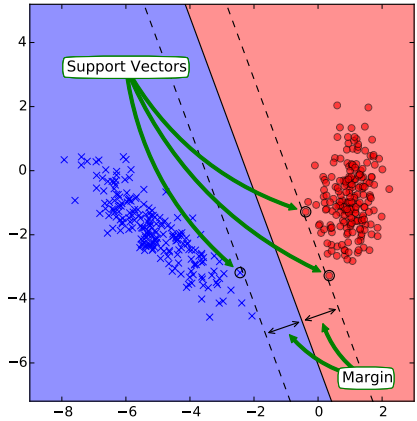
- As mentioned, there is lot of literature on kernels. Popular ones include
  - **Linear Kernel:** $\kappa(\mathbf{x}, \mathbf{y}) = \mathbf{x} \cdot \mathbf{y}$. This is the basic SVM with no mapping.
  - **Polynomial Kernel:** $\kappa(\mathbf{x}, \mathbf{y}) = (\mathbf{x} \cdot \mathbf{y})^d$. Raises dot product to d'th power.
  - **Inhomogeneous Polynomial Kernel:** $\kappa(\mathbf{x}, \mathbf{y}) = (\mathbf{x} \cdot \mathbf{y} + 1)^d$. Similar to polynomial kernel, but produces a bit more dimensions.
  - **Sigmoid Kernel:** $\kappa(\mathbf{x}, \mathbf{y}) = \tanh(a\mathbf{x} \cdot \mathbf{y} + b)$, with $a > 0$ and $b < 0$.
  - **Gaussian Kernel:** $\kappa(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{2\sigma^2}\right)$. Probably the most widely used kernel. Also known as **Radial Basis Function (RBF)** kernel.
- The RBF kernel is special in the sense that it corresponds to a mapping into an **infinite dimensional** vector space.
- In addition to the mathematical excitement, the RBF kernel is often the best performing one, as well.

SVM in Scikit-Learn

```
# Training code:
from sklearn.svm import SVC
# Alternatively: from sklearn.svm import LinearSVC

# Kernels include: "linear", "rbf", "poly", "sigmoid"
# C is the penalty term (default = 1)
clf = SVC(kernel = 'linear', C = 1)

# X contains all samples, and y their class
# labels: y = [0,1,1,0,...]
clf.fit(X, y)
```

```
# Testing code:
>>> clf.coef_ # This is our w vector (linear case)
array([[ 0.72817808,  0.26866005]])

>>> clf.intercept_ # This is the threshold
array([ 3.31965658])

>>> clf.predict([[-4,-2], [-2,0]])
array([ 0.,  1.])

>>> clf.support_vectors_
array([[-2.43263229, -3.18119051],
       [ 0.34905559, -3.27417889],
       [-0.38544996, -1.28336992]])
```

- Scikit-Learn wraps the LibSVM and LibLinear libraries (latter is linear kernel optimized).



Multiclass SVM

- SVM is inherently two-class.
- Generalization to many classes is done by comparing pairs of classes.
- For each class, we train a SVM that classifies this class vs. all others.
- Scikit-Learn provides a few *meta-classifiers* for this purpose.
  - `multiclass.OneVsRestClassifier` compares each class vs. all others (requires K classifiers)
  - `multiclass.OneVsOneClassifier` compares all class pairs (requires $K(K-1)/2$ classifiers)

Multiclass SVM

- A further extension is *multilabel* classification, where several classes can be present simultaneously.
- Targets are presented as binary indicators:

```
>>> from sklearn.preprocessing import MultiLabelBinarizer
>>> y = [[2, 3, 4], [2], [0, 1, 3], [0, 1, 2, 3, 4], [0, 1, 2]]
>>> MultiLabelBinarizer().fit_transform(y)
array([[0, 0, 1, 1, 1], # Classes 2,3,4 are "on"
       [0, 0, 1, 0, 0], # Class 3 is "on"
       [1, 1, 0, 1, 0], # ...
       [1, 1, 1, 1, 1],
       [1, 1, 1, 0, 0]])
```

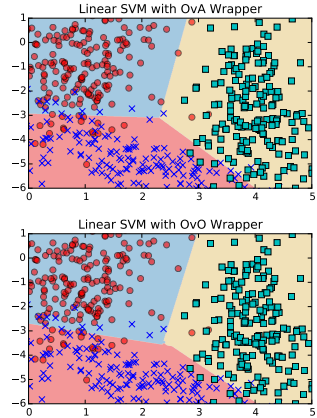
- Occurs often in, *e.g.,* image recognition problems: "What is shown in this picture."
- For example, the following attributes are "on" in the attached picture: {"**fly**", "**flower**", "**summer**"}

Multiclass SVM

```
# Training code:
from sklearn.svm import LinearSVC
from sklearn.multiclass import OneVsRestClassifier
from sklearn.multiclass import OneVsOneClassifier

clf_ova = OneVsRestClassifier(LinearSVC())
clf_ova.fit(X, y)

clf_ovo = OneVsOneClassifier(LinearSVC())
clf_ovo.fit(X, y)
```

```
# Testing code:
>>> clf_ova.predict(np.array([[2,-3.2], [4,-2]]))
array([ 2.,  3.])

>>> clf_ovo.predict(np.array([[2,-3.2], [4,-2]]))
array([ 1.,  3.])

>>> len(clf_ova.estimators_)
3
```

- SVC() in fact implements OvO heuristic inherently.
- LinearSVC() does not, so let's use that as our example.

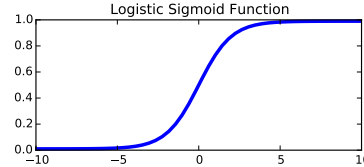


Logistic Regression

- The third member of linear classifier family is *Logistic Regression* (LR).
- Unlike the other two, LR is *probabilistic*, *i.e.*, it models the class probabilities instead of plain class memberships.
- For two-class case ($c \in \{0, 1\}$), the model is:

$$p(c = 1 \mid \mathbf{x}) = \frac{1}{1 + \exp[-(\mathbf{w}^T\mathbf{x} + b)]}.$$

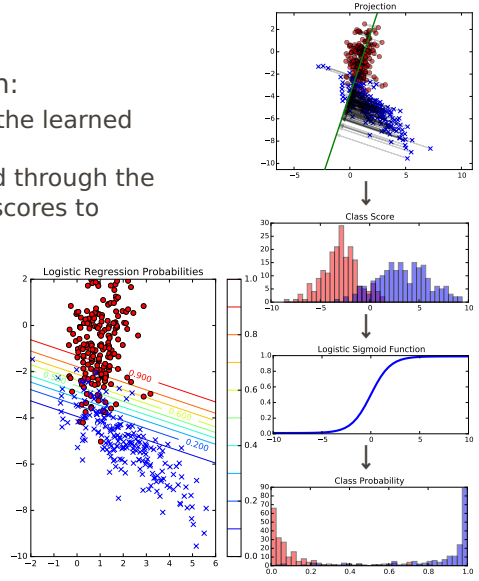
- Also: $p(c = 0 \mid \mathbf{x}) = 1 - p(c = 1 \mid \mathbf{x})$.
- In essence, the model maps the projection $\mathbf{w}^T\mathbf{x} + b$ through the sigmoid function (thus limiting the range to $[0, 1]$).



Logistic Regression

- The model is illustrated in the flowgraph:
  - The samples are projected to 1D using the learned weights **w** and b.
  - The resulting "class scores" are mapped through the logistic function, which transforms the scores to probabilities $p(c = 1 \mid \mathbf{x}) \in [0, 1]$.

- The probability estimates can also be mapped back to 2D, as shown in the figure on the right.



Training Logistic Regression Models

- Logistic regression is trained by *maximum likelihood*.
- In other words, we maximize the likelihood of observing these data points with respect to model parameters.
- The likelihood of samples $\mathbf{X} = [\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_{N-1}]$ with class labels $y_0, y_1, \ldots, y_{N-1} \in \{1, 2, \ldots, K\}$ to have occurred from the model with parameters $\boldsymbol{\theta}$ is

$$p(\mathbf{X} \mid \boldsymbol{\theta}) = \prod_{n=0}^{N-1} p_{y_n}(\mathbf{x}_n; \boldsymbol{\theta}).$$

- As usual, we consider the log-likelihood instead:

$$\ln p(\mathbf{X} \mid \boldsymbol{\theta}) = \sum_{n=0}^{N-1} \ln p_{y_n}(\mathbf{x}_n; \boldsymbol{\theta}).$$

Training Logistic Regression Models

- Due to simplicity, we will continue with the two-class case only.
- Let's label the classes as $y_k \in \{-1, 1\}$, because this will simplify the notation later.
- Also: let's hide the constant term b by catenating it at the end of $\mathbf{w}$:

$$\mathbf{w} \leftarrow [\mathbf{w}, b] \quad \text{and} \quad \mathbf{x} \leftarrow [\mathbf{x}, 1]$$

Training Logistic Regression Models

- The likelihood for classes -1 and 1 are now

$$
\begin{aligned}
p(\mathbf{x}_n \mid y_n = 1) &= \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x}_n)} \\
p(\mathbf{x}_n \mid y_n = -1) &= 1 - \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x}_n)} \\
&= \frac{(1 + \exp(-\mathbf{w}^T \mathbf{x}_n)) - 1}{1 + \exp(-\mathbf{w}^T \mathbf{x}_n)} \\
&= \frac{\exp(-\mathbf{w}^T \mathbf{x}_n)}{1 + \exp(-\mathbf{w}^T \mathbf{x}_n)} \\
&= \frac{1}{\exp(\mathbf{w}^T \mathbf{x}_n) + 1} = \frac{1}{1 + \exp(\mathbf{w}^T \mathbf{x}_n)}
\end{aligned}
$$

Training Logistic Regression Models

- Now $p(\mathbf{x}_n \mid y_n = 1)$ and $p(\mathbf{x}_n \mid y_n = -1)$ are almost the same form and can be conveniently combined into one formula:

$$p(\mathbf{x}_n \mid y_n) = \frac{1}{1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)}$$

- The likelihood for all samples $\mathbf{X} = [\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_{N-1}]$ is now

$$p(\mathbf{X} \mid \mathbf{w}, \mathbf{y}) = \prod_{n=0}^{N-1} \frac{1}{1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)}$$

Training Logistic Regression Models

- The log-likelihood becomes

$$\ln p(\mathbf{X} \mid \mathbf{w}, \mathbf{y}) = \sum_{n=0}^{N-1} \ln 1 - \ln(1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n))$$
$$= -\sum_{n=0}^{N-1} \ln(1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)).$$

Training Logistic Regression Models

- In order to maximize the likelihood, we can equivalently minimize the *logistic loss function*:

$$\text{log-loss} = \sum_{n=0}^{N-1} \ln(1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)).$$

- There exists several algorithms for minimization of logistic loss, *e.g.,*
  - Iterative Reweighted Least Squares **(IRLS)** is an algorithm specifically tailored for this kind of problems. Used by `statsmodels.api.Logit` and `statsmodels.api.MNLogit`.
  - Optimization theory based approaches. Since $\ln p(\mathbf{X} \mid \boldsymbol{\theta})$ is convex, in principle any optimization approach can be used. `scikit-learn` uses something called *Trust Region Newton Algorithm*.

Training Logistic Regression Models

- The optimization theory approach has become dominant, for two reasons:
  1. The SVM training can also be posed in the same framework: minimize the *hinge loss*:
  $$\text{hinge-loss} = \max(0, 1 - y_n \mathbf{w}^T \mathbf{x}_n).$$
  2. A general purpose optimizer can minimize modified losses, as well. Most importantly, one can add a penalty term into the loss function; *e.g.,*
  $$\text{penalized log-loss} = \sum_{n=0}^{N-1} \ln(1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)) + C\mathbf{w}^T\mathbf{w}$$
  where the latter term favors small coefficients in $\mathbf{w}$. We will return to this technique called *regularization* later.

Example: Effect of Regularization Parameter *C*

```
from sklearn.cross_validation import train_test_split

# Split data to training and testing
X_train, X_test, y_train, y_test = \
      train_test_split(X, y, test_size = 0.2)

# Test C values -4, -3, ..., 2
C_range = 10.0 ** np.arange(-4, 3)
clf = LogisticRegression()

for C in C_range:

   clf.C = C
   clf.fit(X_train, y_train)
   y_hat = clf.predict(X_test)
   accuracy = 100.0 * np.mean(y_hat == y_test)

   print ("Accuracy for C = %.2e is %.1f %% (||w|| = %.4f)" % \
         (C, accuracy, np.linalg.norm(clf.coef_)))
```

```
# Code output for the 3-class example data:

Accuracy for C = 1.00e-04 is 50.8 % (||w|| = 0.0660)
Accuracy for C = 1.00e-03 is 59.2 % (||w|| = 0.3332)
Accuracy for C = 1.00e-02 is 73.3 % (||w|| = 1.0372)
Accuracy for C = 1.00e-01 is 88.3 % (||w|| = 2.0715)
Accuracy for C = 1.00e+00 is 90.8 % (||w|| = 3.2153)
Accuracy for C = 1.00e+01 is 91.7 % (||w|| = 3.7732)
Accuracy for C = 1.00e+02 is 91.7 % (||w|| = 3.8704)
```

- In this example, we train the LR classifier with a range of values for parameter C.
- Each C value can be set inside a for loop as `clf.C = <new value>`
- We test the accuracy on a separate test data extracted from the complete data set.

Multiclass Logistic Regression

There are two ways to extend LR to multiclass.

1. A straightforward way would just normalize the exponential terms to sum up to 1:

$$p(c = k \mid \mathbf{x}) = \frac{\exp(\mathbf{w}_k^T \mathbf{x} + b_k)}{\sum_{j=1}^{K} \exp(\mathbf{w}_j^T \mathbf{x} + b_j)}$$

   However, one of the terms is unnecessary, because the probabilities add up to 1.

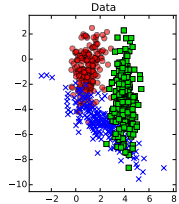
2. Thus, we get an alternative model with fewer parameters:

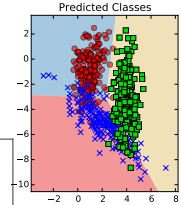
$$p(c = k \mid \mathbf{x}) = \frac{\exp(\mathbf{w}_k^T \mathbf{x} + b_k)}{1 + \sum_{j=1}^{K-1} \exp(\mathbf{w}_j^T \mathbf{x} + b_j)}, \quad k = 1, 2, \ldots, K-1$$

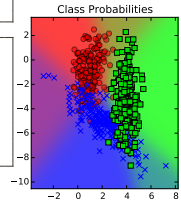
$$p(c = K \mid \mathbf{x}) = \frac{1}{1 + \sum_{j=1}^{K-1} \exp(\mathbf{w}_j^T \mathbf{x} + b_j)}.$$

Multiclass Version ❶

- The first approach designs one probability model $p(c = k \mid \mathbf{x})$ for each class.
- However, the model is ill-posed: there are infinitely many solutions (by scaling).
- Thus, the model needs to be regularized to create a unique solution.
- This is the model given by `scikit-learn`.







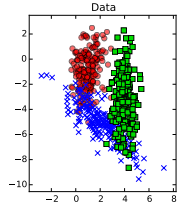

```python
# Training code:
from sklearn.linear_model import LogisticRegression

clf = LogisticRegression()
clf.fit(X, y)
```

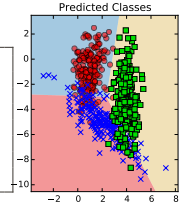
```python
# Test code:
>>> clf.predict([[1,-1], [4, -6]])
array([ 1.,  2.])

clf.predict_proba([[1,-1], [4, -6]])
array([[0.927, 0.038, 0.035],
       [0.001, 0.501, 0.498]]
```

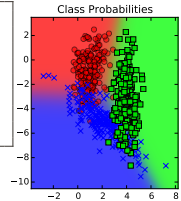
```python
# Model parameters:
>>> clf.coef_
array([[-1.23804226,  0.98973963],
       [-1.37272021, -1.53820378],
       [ 2.13288304,  0.54858162]])
>>> clf.intercept_
array([ 3.79924145, -3.50411623, -5.02047854])
```

Multiclass Version ❷

- The second version is historically older.
- Has a unique solution even without regularization.
- Is not implemented in `scikit-learn`, but can be found in `statsmodels` library.








```
# Training code:
from statsmodels.api import MNLogit

# statsmodel has a bit different API.
# In reality, X should zero-mean, but
# let's simplify the code a bit here.
clf = MNLogit(y, X)
clf = clf.fit()
```

```
# Test code:
>>> clf.predict([[1,-1], [4, -6]])
array([[0.972, 0.019, 0.009],
       [0.001, 0.471, 0.528]],

# clf.predict() gives probabilities.
# To get classes, we find the max:
>>>  clf.predict([[1,-1], [4, -6]]).argmax(axis = 1)
array([0, 2])
```

```
# Model parameters:

>> clf.params
array([[-0.06122776,  2.82418605],
       [-2.00590479, -0.4564178 ]])

# Note: only two sets of weights.
# Note2: no intercept; assumes zero mean
```