CS4487 - Machine Learning

Lecture 3a - Linear Classifiers

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Outline

1. Discriminative linear classifiers
2. Logistic regression
3. Support vector machines (SVM)

Classification with Generative Model

- Steps to build a classifier
  1. Collect training data (features $\mathbf{x}$ and class labels y)
  2. Learn class-conditional distribution (CCD), $p(\mathbf{x}|y)$.
  3. Use Bayes' rule to calculate class probability, $p(y|\mathbf{x})$.
- **Note:** the data is used to learn the CCD -- the classifier is secondary.
  - Density estimation is an "ill-posed" problem -- which density to use? how much data is needed?

- Advice from Vladimir Vapnik (inventor of SVM):

> When solving a problem, try to avoid solving a more general problem as an intermediate step.

- **Discriminative solution**
  - Solve for the classifier $p(y|\mathbf{x})$ directly!

- Terminology
  - **"Discriminative"** - learn to directly discriminate the classes apart using the features.
  - **"Generative"** - learn model of how the features are generated from different classes.

Linear Classifier

- **Setup**
  - Observation (feature vectors) $\mathbf{x} \in \mathbb{R}^d$
  - Class $y \in \{-1, +1\}$
- **Goal**: given a feature vector $\mathbf{x}$, predict its class y.
  - Calculate a *linear function* of the feature vector $\mathbf{x}$.
    - $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b = \sum_{j=1}^{d} w_j x_j + b$
      - $\mathbf{w} \in \mathbb{R}^d$ are the weights of the linear function.
      - multiply each feature value with a weight, and then add together.
  - Predict from the value:
    - if $f(\mathbf{x}) > 0$ then predict Class $y = 1$
    - if $f(\mathbf{x}) < 0$ then predict Class $y = -1$
    - Equivalently, $y = \mathrm{sign}(f(\mathbf{x}))$

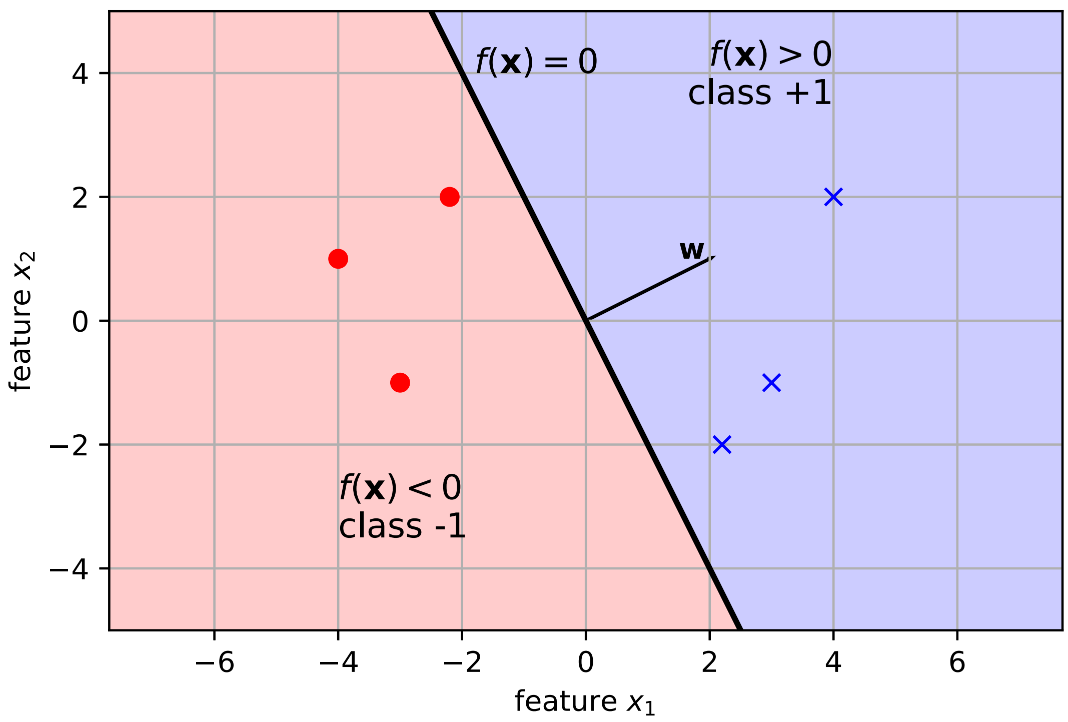
Geometric Interpretation

- The linear classifier separates the features space into 2 *half-spaces*
  - corresponding to feature values belonging to Class +1 and Class -1
  - the class boundary is normal to $\mathbf{w}$.
    - also called the *separating hyperplane*.

- Example: $\mathbf{w} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$, $b = 0$

In [4]:
```
linclass
```

Out[4]:



Separating Hyperplane

- In a d-dimensional feature space, the parameters are $\mathbf{w} \in \mathbb{R}^d$.
- The equation $\mathbf{w}^T\mathbf{x} + b = 0$ defines a $(d-1)$-dim. linear surface:
  - for $d = 2$, $\mathbf{w}$ defines a 1-D line.
  - for $d = 3$, $\mathbf{w}$ defines a 2-D plane.
  - ...
  - in general, we call it a hyperplane.

Learning the classifier

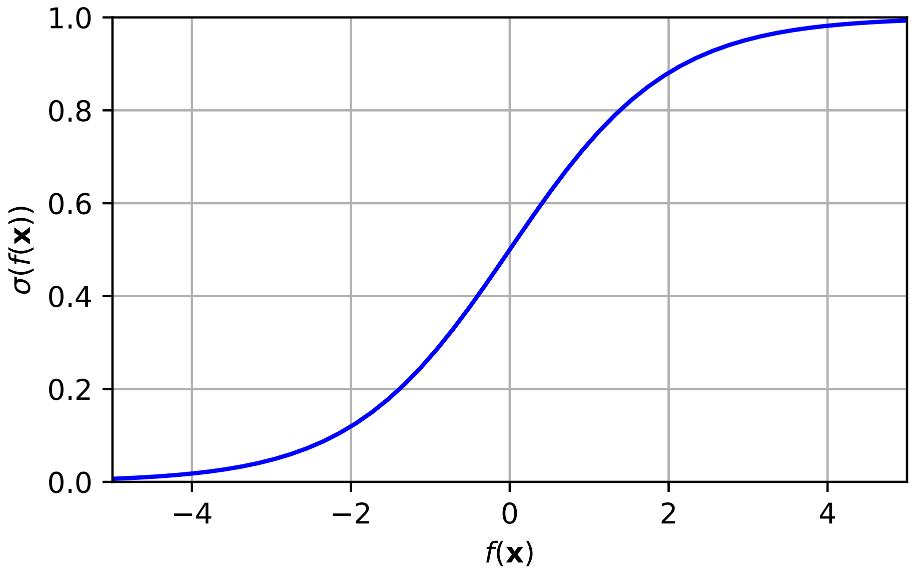
- How to set the classifier parameters $(\mathbf{w}, b)$?
  - Learn them from training data!
- Classifiers differ in the objectives used to learn the parameters $(\mathbf{w}, b)$.
  - We will look at two examples:
    - *logistic regression*
    - *support vector machine (SVM)*

Logistic regression

- Use a probabilistic approach
- Need to map the function values $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$ to probability values between 0 and 1.
  - *sigmoid* function maps from real number to interval [0,1]
  - $\sigma(z) = \frac{1}{1+e^{-z}}$

In [6]:
```
sigmoidplot
```

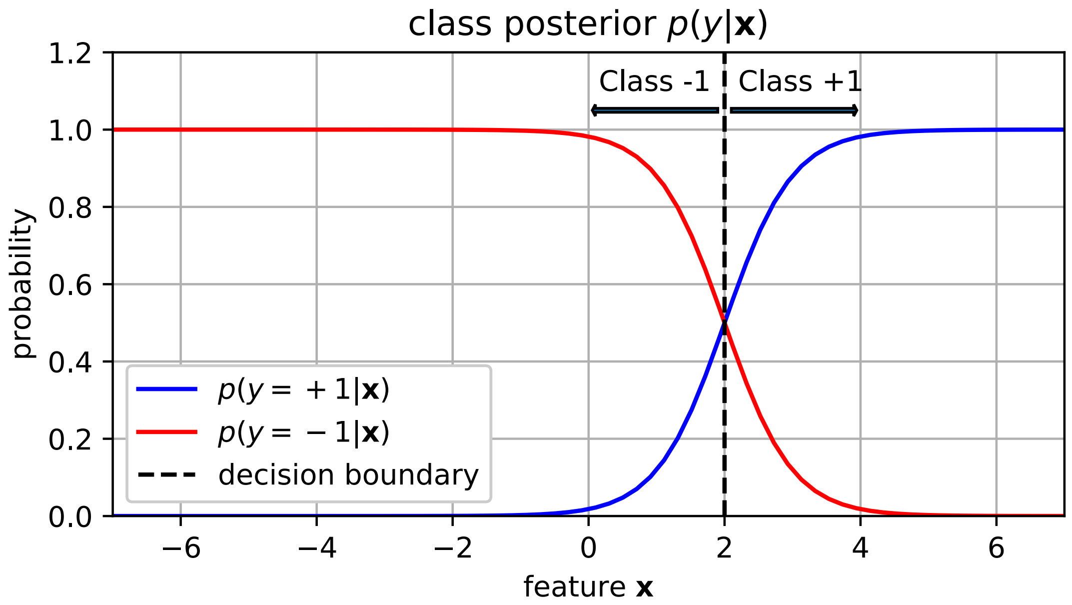
Out[6]:



- Given a feature vector x, the probability of a class is:
  - $p(y = +1|\mathbf{x}) = \sigma(f(\mathbf{x}))$
  - $p(y = -1|\mathbf{x}) = 1 - \sigma(f(\mathbf{x}))$
- Note: here we are directly modeling the class posterior probability!
  - not the class-conditional $p(\mathbf{x}|y)$

In [8]:
```
lrexample
```

Out[8]:



Learning the parameters

- Given training data $\{\mathbf{x}_i, y_i\}_{i=1}^N$, learn the function parameters $(\mathbf{w}, b)$ using maximum likelihood estimation.
- maximize the likelihood of the data $\{\mathbf{x}_i, y_i\}$:

$$(\mathbf{w}^*, b^*) = \operatorname*{argmax}_{\mathbf{w},b} \sum_{i=1}^{N} \log p(y_i|\mathbf{x}_i)$$

- to prevent *overfitting*, add a prior distribution on $\mathbf{w}$.
  - assume Gaussian distribution on $\mathbf{w}$ with variance $1/C$

$$(\mathbf{w}^*, b^*) = \operatorname*{argmax}_{\mathbf{w},b} \log p(\mathbf{w}) + \sum_{i=1}^{N} \log p(y_i|\mathbf{x}_i)$$

- Equivalently,

$$(\mathbf{w}^*, b^*) = \underset{\mathbf{w},b}{\operatorname{argmin}} \frac{1}{C}\mathbf{w}^T\mathbf{w} + \sum_{i=1}^{N} \log(1 + \exp(-y_i(\mathbf{w}^T\mathbf{x}_i + b)))$$

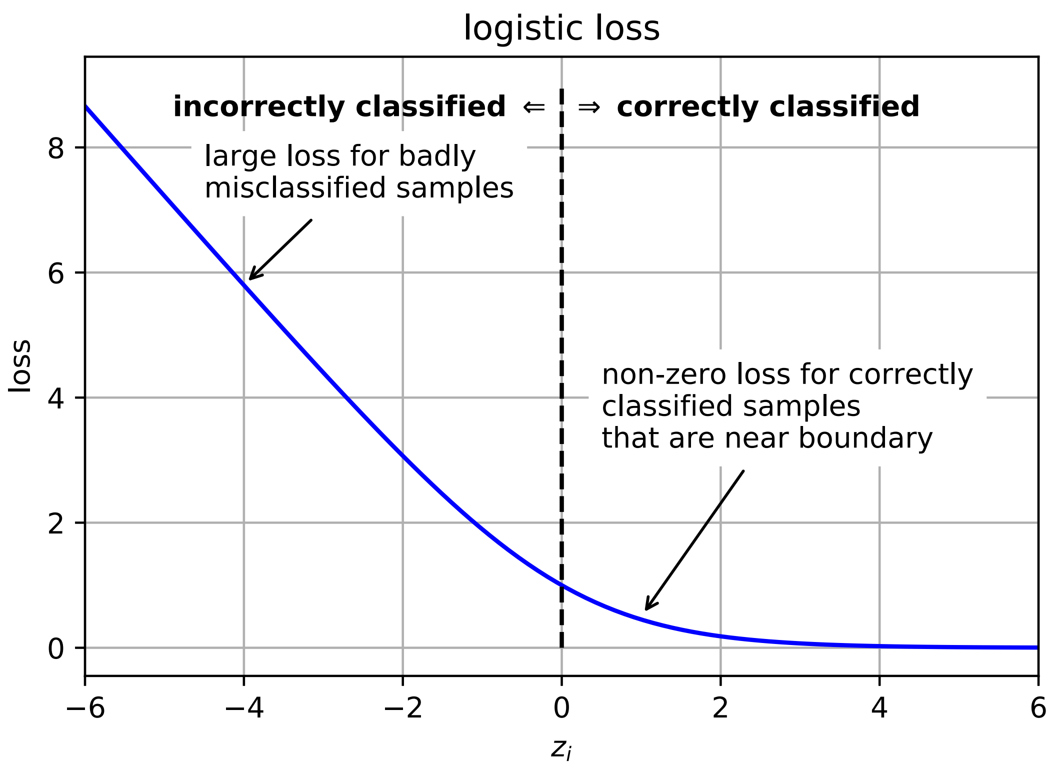
- the first term is the *regularization term*
  - Note: $\mathbf{w}^T\mathbf{w} = \sum_{j=1}^{d} w_j^2$
  - penalty term that keeps entries in $\mathbf{w}$ from getting too large.
  - C is the regularization *hyperparameter*
    - larger C value allow large values in $\mathbf{w}$.
    - smaller C value discourage large values in $\mathbf{w}$.

$$(\mathbf{w}^*, b^*) = \underset{\mathbf{w},b}{\operatorname{argmin}} \frac{1}{C}\mathbf{w}^T\mathbf{w} + \sum_{i=1}^{N} \log(1 + \exp(-y_i(\mathbf{w}^T\mathbf{x}_i + b)))$$

- the second term is the *data-fit term*
  - wants to make the parameters $(\mathbf{w}, b)$ to well fit the data.
  - Define $z_i = y_i f(\mathbf{x}_i)$
    - Interesing observation:
      - $z_i > 0$ when sample $\mathbf{x}_i$ is classified correctly
      - $z_i < 0$ when sample $\mathbf{x}_i$ is classified incorrectly
      - $z_i = 0$ when sample is on classifier boundary
  - logistic loss function: $L(z_i) = \log(1 + \exp(-z_i))$

In [10]:
```
lossfig
```

Out[10]:



- **no closed-form solution**
  - use an iterative optimization algorithm to find the optimal solution
  - e.g. *gradient descent* - step downhill in each iteration.
    - $\mathbf{w} \leftarrow \mathbf{w} - \eta \frac{dE}{d\mathbf{w}}$
    - where E is the objective function
    - η is the *learning rate* (how far to step in each iteration).

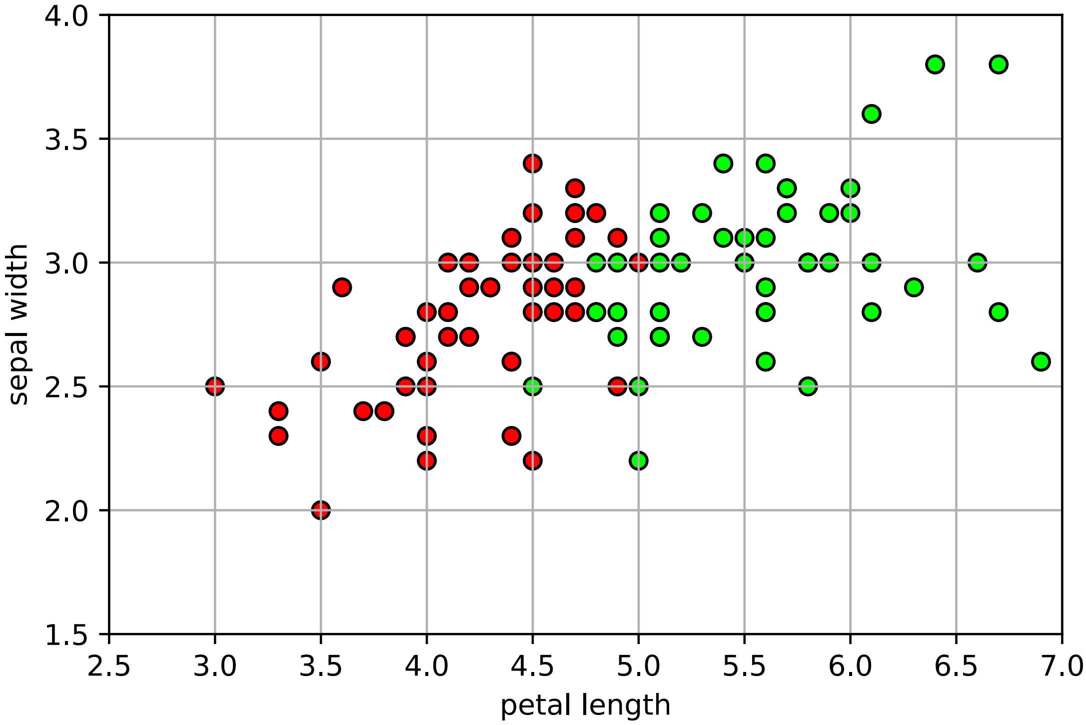
Example: Iris Data

In [11]:
```
# load iris data each row is (petal length, sepal width, class)
irisdata = loadtxt('iris2.csv', delimiter=',', skiprows=1)

X = irisdata[:,0:2]  # the first two columns are features (petal length, sepal w
idth)
Y = irisdata[:,2]    # the third column is the class label (versicolor=1, virgin
ica=2)
                     #  --> automaticaly mapped to (-1, +1) when training classi
fier

print(X.shape)
```

```
(100, 2)
```

In [12]:
```
# a colormap for making the scatter plot: class -1 will be red, class +1 will be
green
mycmap = matplotlib.colors.LinearSegmentedColormap.from_list('mycmap', ["#FF0000
", "#FFFFFF", "#00FF00"])

axbox = [2.5, 7, 1.5, 4] # common axis range

# a function for setting a common plot
def irisaxis(axbox):
    plt.xlabel('petal length'); plt.ylabel('sepal width')
    plt.axis(axbox); plt.grid(True)
```

In [13]:
```
# show the data
plt.figure()
plt.scatter(X[:,0], X[:,1], c=Y, cmap=mycmap, edgecolors='k')
irisaxis(axbox)
```



In [14]:
```
# randomly split data into 50% train and 50% test set
trainX, testX, trainY, testY = \
  model_selection.train_test_split(X, Y,
  train_size=0.5, test_size=0.5, random_state=4487)

print(trainX.shape)
print(testX.shape)
```

```
(50, 2)
(50, 2)
```

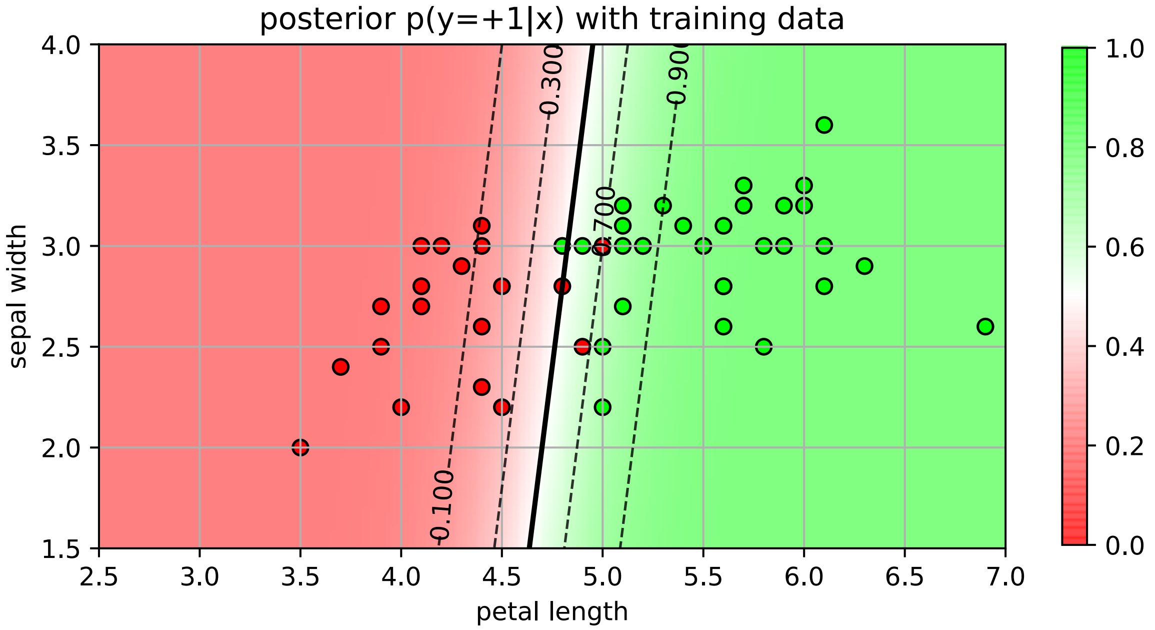
In [15]:
```
# learn logistic regression classifier
# (C is a regularization hyperparameter)
logreg = linear_model.LogisticRegression(C=100)
logreg.fit(trainX, trainY)

print("w =", logreg.coef_)
print("b =", logreg.intercept_)
```

```
w = [[ 4.87521863 -0.61512848]]
b = [-21.67874573]
```

- Equation:
  - $f(x) = (4.87 * petal\_length) - (0.62 * sepal\_width) - 21.68$
- Interpretation:
  - large petal length makes f(x) positive, so large petal length is associated with class +1.

In [19]:

```
# show the posterior and training data
plt.figure(figsize=(8,6))
plot_posterior(logreg, axbox, mycmap)
plt.scatter(trainX[:,0], trainX[:,1], c=trainY, cmap=mycmap, edgecolors='k')
plt.title('posterior p(y=+1|x) with training data');
```



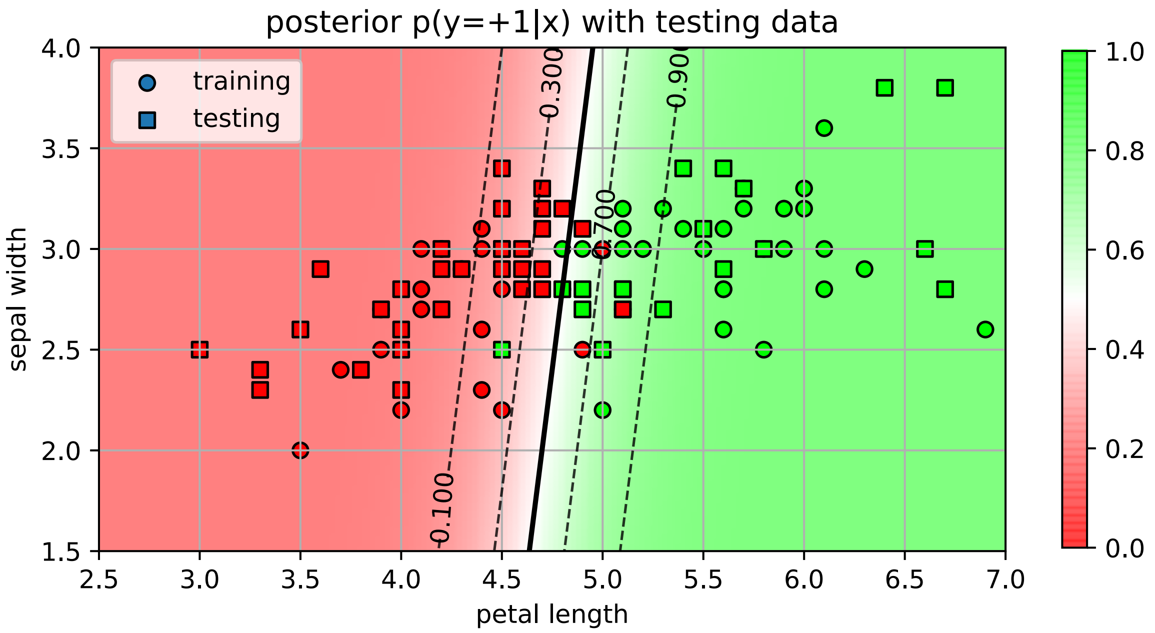
In [20]:

```
# predict from the model
predY = logreg.predict(testX)

# calculate accuracy
acc = metrics.accuracy_score(testY, predY)
print("test accuracy =", acc)
```

```
test accuracy = 0.92
```

In [21]:

```
# show the posterior and training data
plt.figure(figsize=(8,6))
plot_posterior(logreg, axbox, mycmap)
plt.scatter(trainX[:,0], trainX[:,1], c=trainY, cmap=mycmap, marker="o", label="
training", edgecolors='k')
plt.scatter(testX[:,0], testX[:,1], c=testY, cmap=mycmap, marker="s", label="tes
ting", edgecolors='k')
plt.title('posterior p(y=+1|x) with testing data');
plt.legend(loc=0);
```

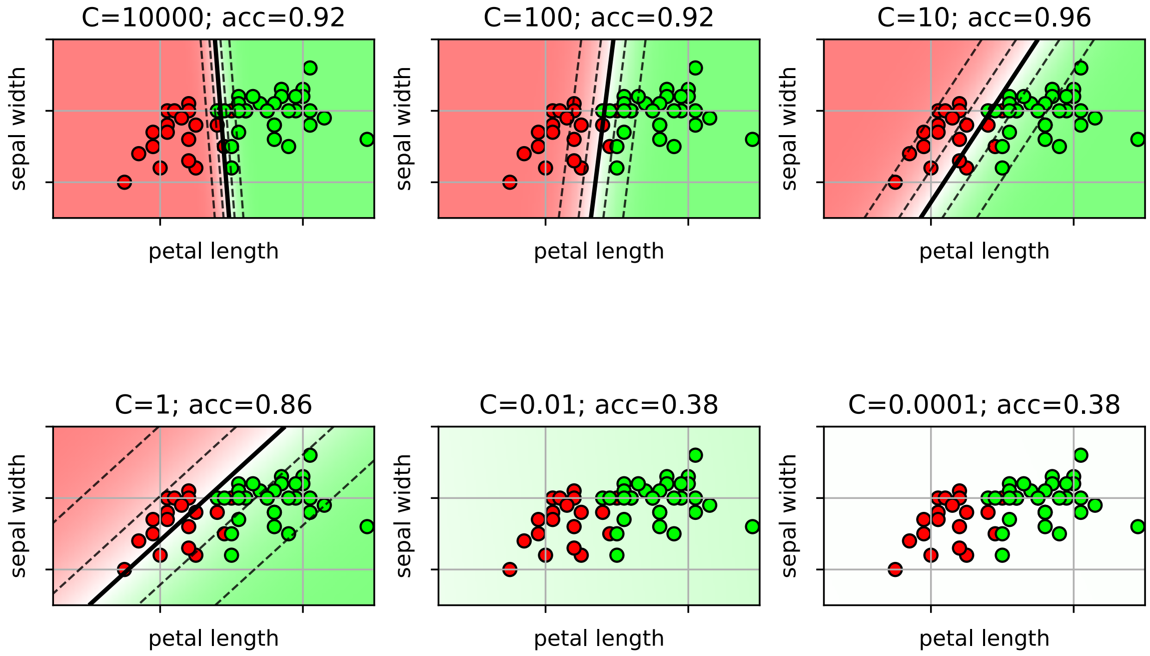


Selecting the regularization hyperparameter

- the regularization hyperparameter C has a big effect on the decision boundary and the accuracy.
- How to set the value of C?

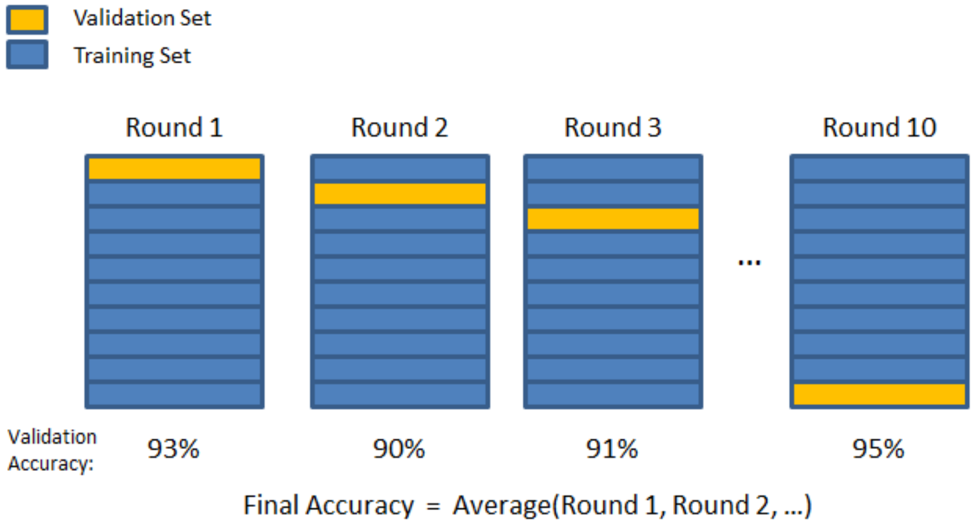
In [23]:
```
lrC
```

Out[23]:



Cross-validation

- Use *cross-validation* on the training set to select the best value of C.
- Run many experiments on the training set to see which parameters work on different versions of the data.
  - Split the data into batches of training and validation data.
  - Try a range of C values on each split.
  - Pick the value that works best over all splits.



- **Procedure**
  1. select a range of C values to try
  2. Repeat K times
     A. Split the training set into training data and validation data
     B. Learn a classifier for each value of C
     C. Record the accuracy on the validation data for each C
  3. Select the value of C that has the highest average accuracy over all K folds.
  4. Retrain the classifier using all data and the selected C.

- scikit-learn already has built-in `cross_validation` module (more later).
- for logistic regression, use *LogisticRegressionCV* class

In [24]:

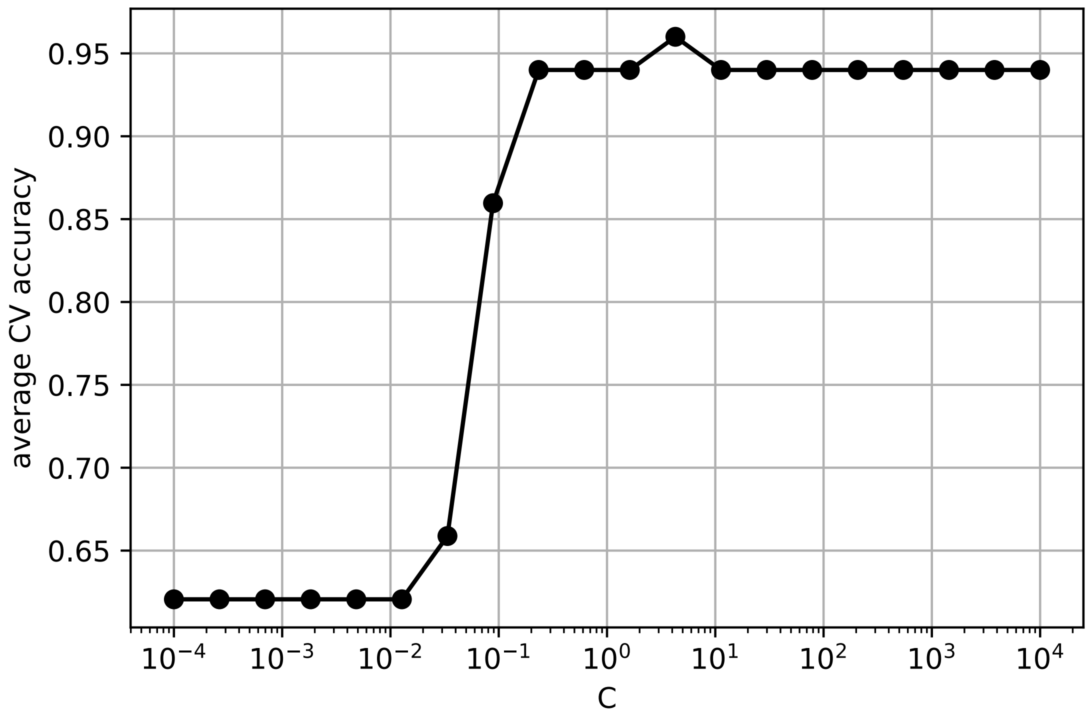
```
# learn logistic regression classifier usinc CV
#  Cs is an array of possible C values
#  cv is the number of folds
#  n_jobs is the number of parallel jobs to run (makes it faster)
#    -1 means use all cores
logreg = linear_model.LogisticRegressionCV(Cs=logspace(-4,4,20), cv=5, n_jobs=-1
)
logreg.fit(trainX, trainY)

print("w=", logreg.coef_)
print("b=", logreg.intercept_)

# predict from the model
predY = logreg.predict(testX)

# calculate accuracy
acc = metrics.accuracy_score(testY, predY)
print("test accuracy=", acc)
```

```
w= [[4.61911642 0.72396452]]
b= [-24.24716674]
test accuracy= 0.9
```

Which C was selected?

In [25]:
```
print("C =", logreg.C_)

# calculate the average score for each C
avgscores = mean(logreg.scores_[2],0)  # 2 is the class label
plt.figure()
plt.semilogx(logreg.Cs_, avgscores, 'ko-')
plt.xlabel('C'); plt.ylabel('average CV accuracy')
plt.grid(True);
```

```
C = [4.2813324]
```



Multi-class classification

- So far, we have only learned a classifier for 2 classes (+1, -1)
  - called a **binary classifier**
- For more than 2 classes, split the problem up into several binary classifier problems.
  - **1-vs-rest**
    - *Training:* for each class, train a classifier for that class versus the other classes.
      - For example, if there are 3 classes, then train 3 binary classifiers: 1 vs {2,3}; 2 vs {1,3}; 3 vs {1,2}
    - *Prediction:* calculate probability for each binary classifier. Select the class with highest probability.

Example on 3-class Iris data

In [26]:

```
# load iris data each row is (petal length, sepal width, class)
irisdata = loadtxt('iris3.csv', delimiter=',', skiprows=1)

X = irisdata[:,0:2]  # the first two columns are features (petal length, sepal w
idth)
Y = irisdata[:,2]    # the third column is the class label (setosa=0, versicolor
=1, virginica=2)

print(X.shape)
```

```
(150, 2)
```

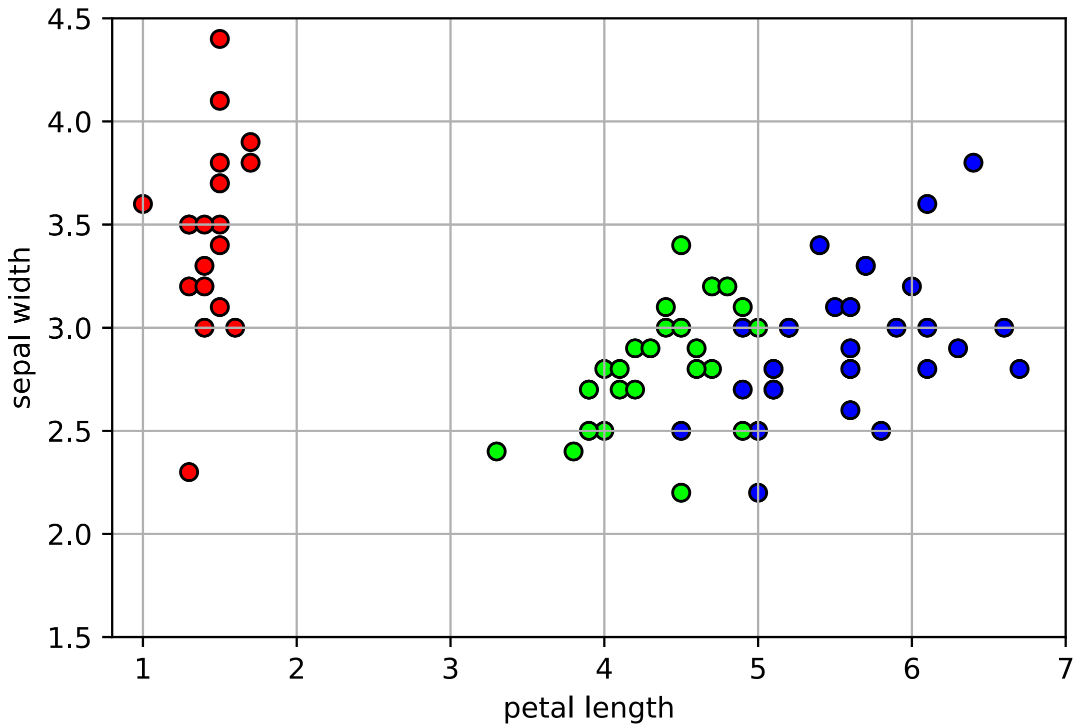
In [27]:

```
# randomly split data into 50% train and 50% test set
trainX, testX, trainY, testY = \
  model_selection.train_test_split(X, Y,
  train_size=0.5, test_size=0.5, random_state=4487)

print(trainX.shape)
print(testX.shape)
```

```
(75, 2)
(75, 2)
```

In [28]:

```
# look at training data

axbox3 = [0.8, 7, 1.5, 4.5]
# make a colormap for viewing 3 classes
mycmap3 = matplotlib.colors.LinearSegmentedColormap.from_list('mycmap', ["#FF000
0", "#00FF00", "#0000FF"])

plt.scatter(trainX[:,0], trainX[:,1], c=trainY, cmap=mycmap3, edgecolors='k')
plt.axis(axbox3); plt.grid(True);
plt.xlabel('petal length'); plt.ylabel('sepal width');
```



In [29]:

```
# learn logistic regression classifier (one-vs-all)
mlogreg = linear_model.LogisticRegression(C=10)
mlogreg.fit(trainX, trainY)

# now contains 3 hyperplanes and 3 bias terms (one for each class)
print("w=", mlogreg.coef_)
print("b=", mlogreg.intercept_)

# predict from the model
predY = mlogreg.predict(testX)

# calculate accuracy
acc = metrics.accuracy_score(testY, predY)
print("test accuracy=", acc)
```

```
w= [[-3.09131694  2.52132269]
 [ 0.06064355 -1.58022283]
 [ 3.35076433 -3.48981157]]
b= [ 0.73591801  3.79651516 -6.36532274]
test accuracy= 0.9733333333333334
```

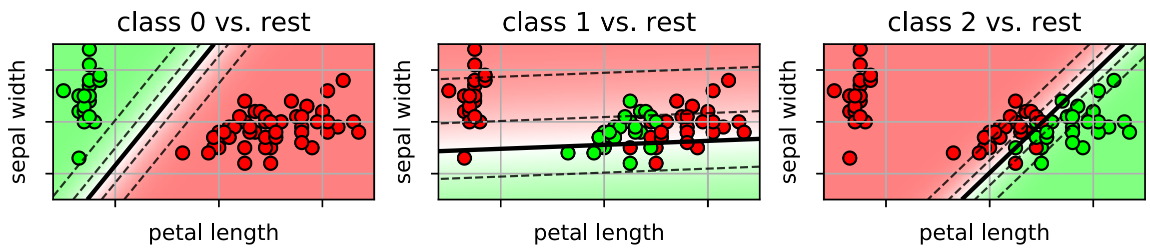
- the individual 1-vs-rest binary classifiers

In [31]:

```
print("w=", mlogreg.coef_)
print("b=", mlogreg.intercept_)

mlrfig
```

```
w= [[-3.09131694  2.52132269]
 [ 0.06064355 -1.58022283]
 [ 3.35076433 -3.48981157]]
b= [ 0.73591801  3.79651516 -6.36532274]
```

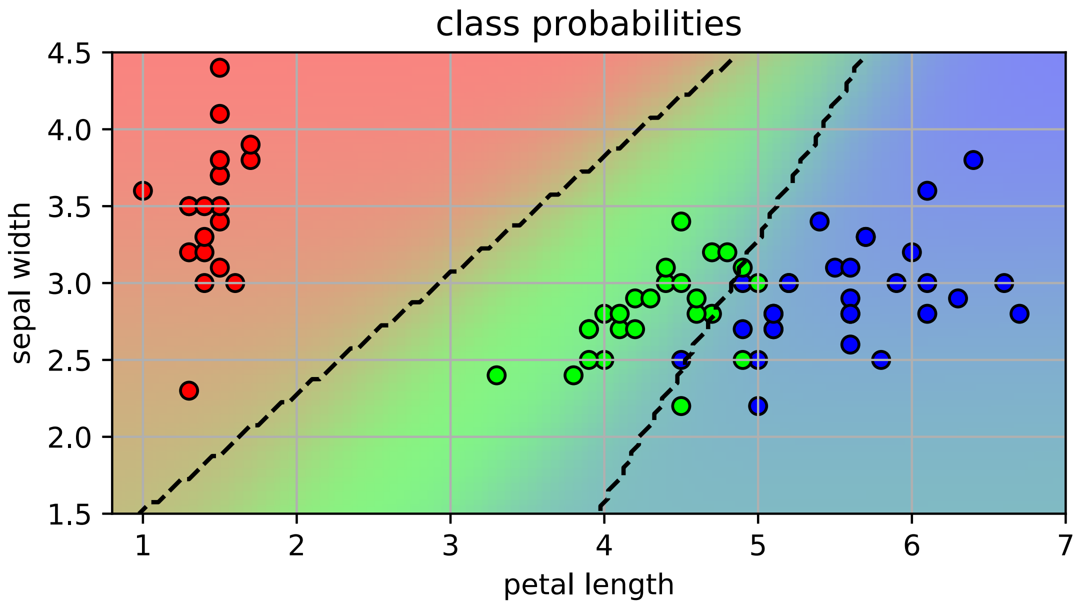
Out[31]:



- the final classifier, combining all 1 vs rest classifiers

In [33]:
```
lr3class
```

Out[33]:



Multiclass logistic regression

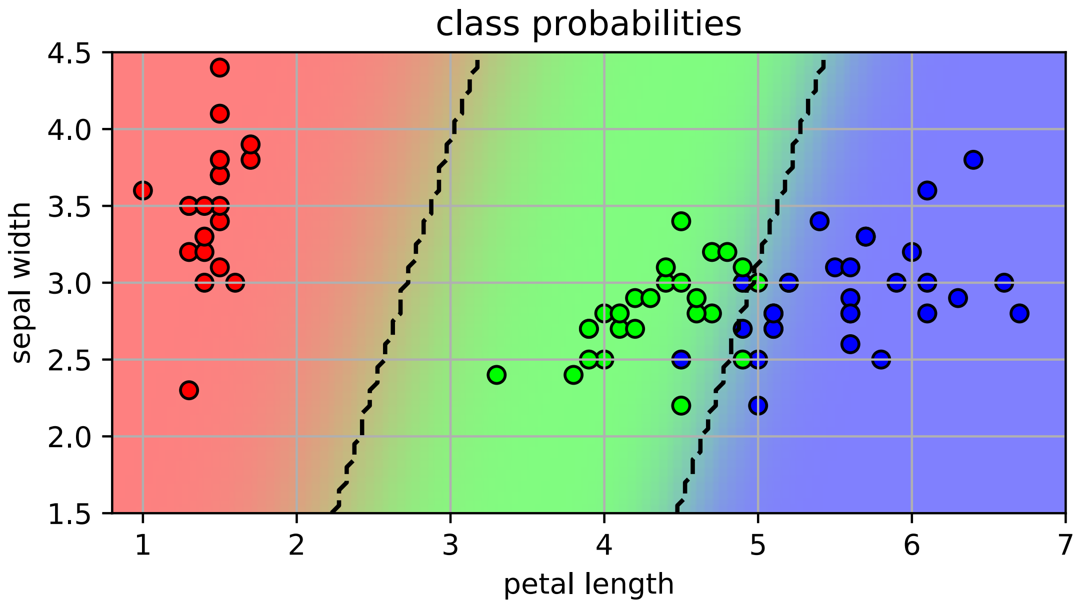
- Another way to get a multi-class classifier is to define a multi-class objective.
  - One weight vector $\mathbf{w}_c$ for each class c.
- Define probabilities with **softmax** function
  - analogous to sigmoid function for binary logistic regression.
  - $p(y=c|\mathbf{x}) = \frac{\exp(\mathbf{w}_c^T\mathbf{x})}{\exp(\mathbf{w}_1^T\mathbf{x})+\cdots+\exp(\mathbf{w}_K^T\mathbf{x})}$
  - The class with largest reponse of $\mathbf{w}_c^T\mathbf{x}$ will have the highest probability.
- Estimate the $\{\mathbf{w}_j\}$ parameters using MLE as before.

In [34]:
```
# learn logistic regression classifier
mlogreg = linear_model.LogisticRegression(C=10,
            multi_class='multinomial', solver='lbfgs')
            # use multi-class and corresponding solver
mlogreg.fit(trainX, trainY)

# now contains 3 hyperplanes and 3 bias terms (one for each class)
print("w=", mlogreg.coef_)
print("b=", mlogreg.intercept_)

# predict from the model
predY = mlogreg.predict(testX)

# calculate accuracy
acc = metrics.accuracy_score(testY, predY)
print("test accuracy=", acc)
```

```
w= [[-4.13092437  1.30718735]
 [-0.71717021  0.23609022]
 [ 4.84809458 -1.54327757]]
b= [ 11.46078594   5.40723484 -16.86802078]
test accuracy= 0.9733333333333334
```

In [36]:
```
lr3classm
```

Out[36]:

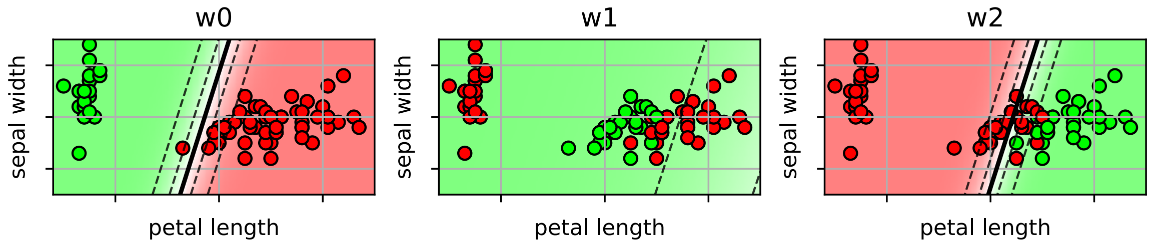


- individual weight vectors work together to partition the space

In [38]:
```
print("w=", mlogreg.coef_)
print("b=", mlogreg.intercept_)

lr3lvr
```

```
w= [[-4.13092437  1.30718735]
 [-0.71717021  0.23609022]
 [ 4.84809458 -1.54327757]]
b= [ 11.46078594   5.40723484 -16.86802078]
```

Out[38]:



Logistic Regression Summary

- **Classifier:**
  - linear function $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$
  - Given a feature vector $\mathbf{x}$, the probability of a class is:
    - $p(y = +1|\mathbf{x}) = \sigma(f(\mathbf{x}))$
    - $p(y = -1|\mathbf{x}) = 1 - \sigma(f(\mathbf{x}))$
    - *sigmoid* function: $\sigma(z) = \frac{1}{1+e^{-z}}$
  - logistic loss function: $L(z) = \log(1 + \exp(-z))$
- **Training:**
  - Maximize the likelihood of the training data.
  - Use regularization to prevent overfitting.
    - Use cross-validation to pick the regularization hyperparameter C.

- **Classification:**
  - Given a new sample $\mathbf{x}^*$:
    - pick class with highest probability $p(y|\mathbf{x}^*)$:
      - $y^* = \begin{cases} +1, p(y = +1|\mathbf{x}^*) > p(y = -1|\mathbf{x}^*) \\ -1, \text{otherwise} \end{cases}$
    - alternatively, just use $f(\mathbf{x}^*)$
      - $y^* = \begin{cases} +1, f(\mathbf{x}^*) > 0 \\ -1, \text{otherwise} \end{cases} = \text{sign}(f(\mathbf{x}_*))$