CS5489 - 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.

Revisit the Naive Bayes Gaussian Classifier

- CCDs: assume the same variance for all Gaussians:
  - $p(\mathbf{x}|y=1) = \prod_{i=1}^{D} \mathcal{N}(x_i|\mu_i, \sigma^2)$
  - $p(\mathbf{x}|y=2) = \prod_{i=1}^{D} \mathcal{N}(x_i|\nu_i, \sigma^2)$
- prior:
  - $p(y=1) = \pi_1, p(y=2) = \pi_2$.

- look at the log-ratio of CCDs,

$$
\begin{aligned}
\log \frac{p(\mathbf{x}|y=1)}{p(\mathbf{x}|y=2)} &= \log \frac{\prod_{i=1}^{D} \mathcal{N}(x_i|\mu_i, \sigma^2)}{\prod_{i=1}^{D} \mathcal{N}(x_i|\nu_i, \sigma^2)} \\
&= \sum_{i=1}^{D} \log \mathcal{N}(x_i|\mu_i, \sigma^2) - \log \mathcal{N}(x_i|\nu_i, \sigma^2) \\
&= \sum_{i=1}^{D} -\frac{1}{2\sigma^2}(x_i - \mu_i)^2 + \frac{1}{2\sigma^2}(x_i - \nu_i)^2
\end{aligned}
$$

- Thus

$$
\log \frac{p(\mathbf{x}|y=1)}{p(\mathbf{x}|y=2)} = \frac{1}{\sigma^2} \sum_{i=1}^{D} (\mu_i - \nu_i) x_i + \frac{1}{2\sigma^2} \sum_{i=1}^{D} (\nu_i^2 - \mu_i^2)
$$

- **Bayes decision rule:** Compute the posterior probability of each class $p(y = j|\mathbf{x})$
  - select class 1 when:

$$
\begin{aligned}
\log p(y=1|\mathbf{x}) &> \log p(y=2|\mathbf{x}) \\
\log p(\mathbf{x}|y=1) + \log p(y=1) &> \log p(\mathbf{x}|y=2) + \log p(y=2) \\
\log \frac{p(\mathbf{x}|y=1)}{p(\mathbf{x}|y=2)} + \log \frac{p(y=1)}{p(y=2)} &> 0
\end{aligned}
$$

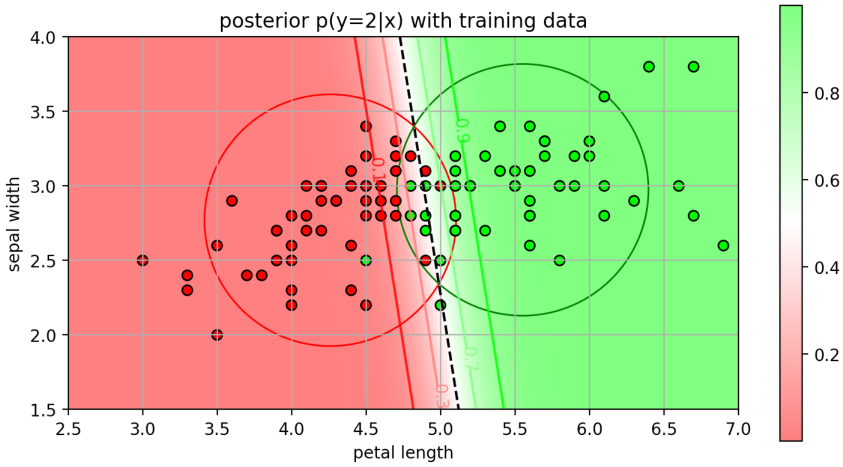
- substituting for the CCDs and priors, the BDR is:
  - select class $y = 1$ when:

$$
\sum_{i=1}^{D} \frac{1}{\sigma^2} (\mu_i - \nu_i) x_i + \frac{1}{2\sigma^2} \sum_{i=1}^{D} (\nu_i^2 - \mu_i^2) + \log \frac{\pi_1}{\pi_2} > 0
$$

- Example

In [11]:
```
pfig
```

Out[11]:



- BDR in this case is a **linear** function
  - select class $y = 1$ when:

$$
\sum_{i=1}^{D} \underbrace{\frac{1}{\sigma^2} (\mu_i - \nu_i)}_{w_i} x_i + \underbrace{\frac{1}{2\sigma^2} \sum_{i=1}^{D} (\nu_i^2 - \mu_i^2) + \log \frac{\pi_1}{\pi_2}}_{b} > 0
$$

```
- $w_i$ is a per-feature weight
- $b$ is a bias term
```

- the BDR in this case is a **linear** classifier:
  - select class $y = 1$ when
    - $\sum_{i=1}^{D} w_i x_i + b > 0$
    - equivalently, $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b > 0$
- Here we obtain the weights $\mathbf{w}$ by learning the CCDs
  - assuming Naive Bayes Gaussians with shared variance.
  - this is a generative model since we learn how the data is generated for each class (CCDs).

- How to learn the linear classifier in a discriminative way?
  - directly learn the posterior $p(y|\mathbf{x})$.
  - we will look at a generic linear classifier.

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

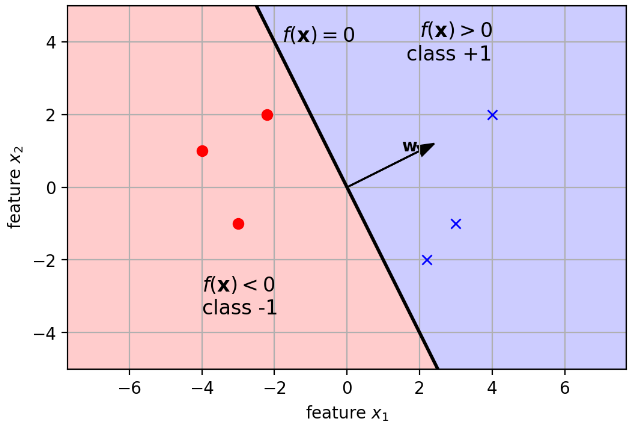
- The linear classifier separates the features space into 2 *half-spaces*
  - corresponding to feature values belonging to Class +1 and Class -1
  - the class boundary is normal to $\mathbf{w}$.
    - also called the *separating hyperplane*.

- Example:

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

In [14]:
```
linclass
```

Out [14]:



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

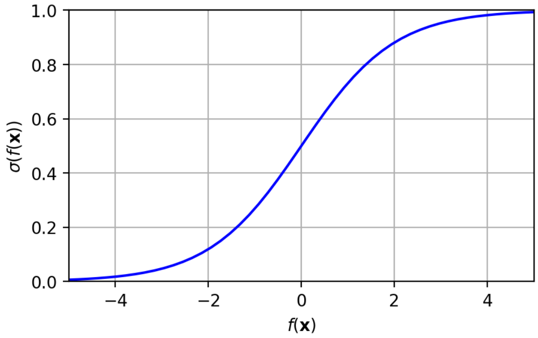
- How to set the classifier parameters $(\mathbf{w}, b)$?
  - Learn them from training data!
- Classifiers differ in the objectives used to learn the parameters $(\mathbf{w}, b)$.
  - We will look at two examples:
    - *logistic regression*
    - *support vector machine (SVM)*

Logistic regression

- Use a probabilistic approach
  - Map the linear function $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$ to probability values between 0 and 1 using a *sigmoid* function.
  - $\sigma(z) = \frac{1}{1+e^{-z}}$

In [16]:
```
sigmoidplot
```

Out [16]:

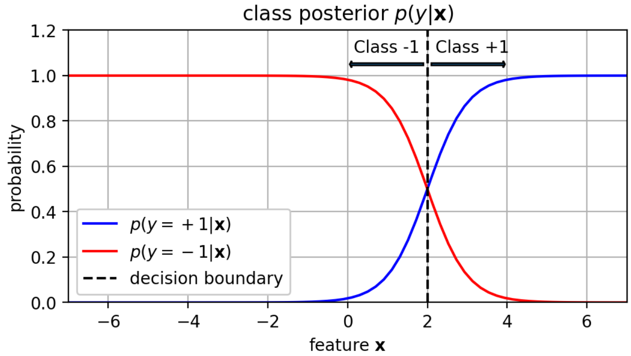


- Given a feature vector x, the probability of a class is:
  - $p(y = +1|\mathbf{x}) = \sigma(f(\mathbf{x}))$
  - $p(y = -1|\mathbf{x}) = 1 - \sigma(f(\mathbf{x}))$
- Note: here we are directly modeling the class posterior probability!

- not the class-conditional $p(\mathbf{x}|y)$

In [18]:
```
lrexample
```

Out[18]:



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 $\{\mathbf{x}_i, y_i\}$ according to the posterior:

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

- posterior is a Bernoulli distribution (given $\mathbf{x}$):

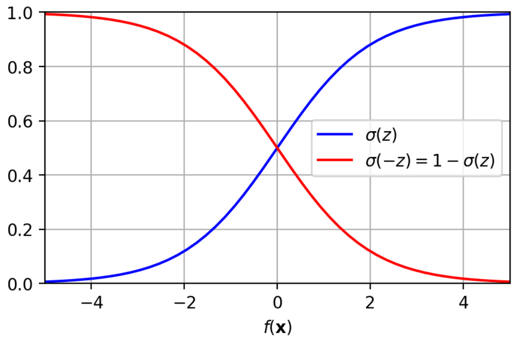
$$p(y|\mathbf{x}) = \begin{cases} \sigma(f(\mathbf{x})), & y = 1 \\ 1 - \sigma(f(\mathbf{x})), & y = -1 \end{cases}$$

- Note the following property:

$$1 - \sigma(z) = \sigma(-z)$$

In [20]:
```
sigmoidplot
```

Out[20]:



- Thus,

$$p(y|\mathbf{x}) = \begin{cases} \sigma(f(\mathbf{x})), & y = 1 \\ \sigma(-f(\mathbf{x})), & y = -1 \end{cases}$$

- Simplifying the 2 cases into one equation,

$$p(y|\mathbf{x}) = \sigma(yf(\mathbf{x}))$$

- Taking the log,

$$\log p(y|\mathbf{x}) = \log \sigma(yf(\mathbf{x}))$$
$$= \log \frac{1}{1+e^{-yf(\mathbf{x})}}$$

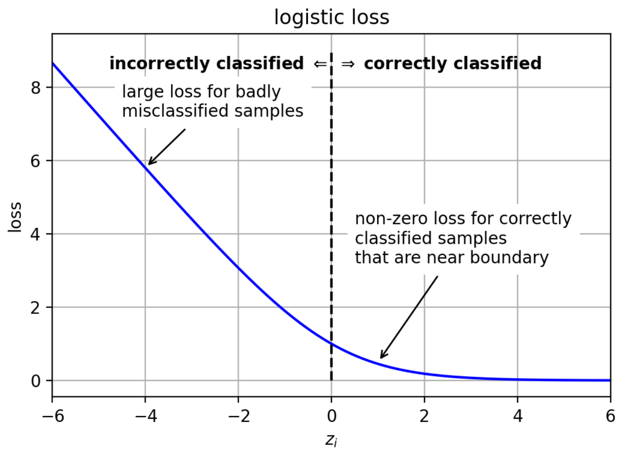
- Substituting into the MLE formulation:

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

- the term on the right is a *data-fit term*
  - wants to make the parameters $(\mathbf{w}, b)$ to well fit the data.
  - Define $z_i = y_i f(\mathbf{x}_i)$
    - Interesting 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 [22]:
```
lossfig
```

Out[22]:

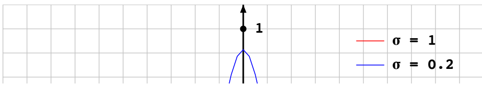


Regularization

- to prevent *overfitting*, add a prior distribution on $\mathbf{w}$.
  - prefer solutions that are likely under the prior.

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

- assume Gaussian distribution on $\mathbf{w}$ with variance $C/2$
  - $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|0, \frac{C}{2}\mathbf{I})$
    - small values of C keep $\mathbf{w}$ close to 0.
    - large values of C allow larger values of $\mathbf{w}$.
  - $\log p(\mathbf{w}) = -\frac{1}{C}\mathbf{w}^T\mathbf{w} + \text{constant}$



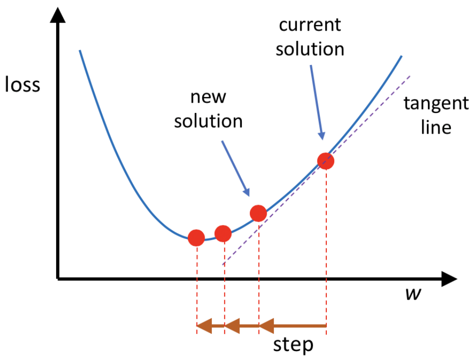
- Substituting,

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

- 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 values apply less penalty on large $\mathbf{w}$ → allow large values in $\mathbf{w}$.
    - smaller C values apply more penalty on large $\mathbf{w}$ → discourage large values in $\mathbf{w}$.
- the second term is the *data fit term* - same as before.

Optimization

- **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).

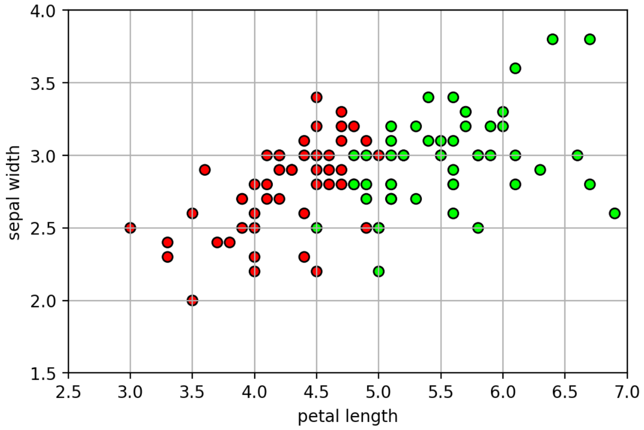


Example: Iris Data

In [23]:
```
# 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 width)
Y = irisdata[:,2]    # the third column is the class label (versicolor=1, virginica=2)
                     #  --> automaticaly mapped to (-1, +1) when training classifier

print(X.shape)
```

```
(100, 2)
```

In [25]:
```
# show the data
plt.figure()
plt.scatter(X[:,0], X[:,1], c=Y, cmap=mycmap, edgecolors='k')
irisaxis(axbox)
```



In [26]:
```
# 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)
```

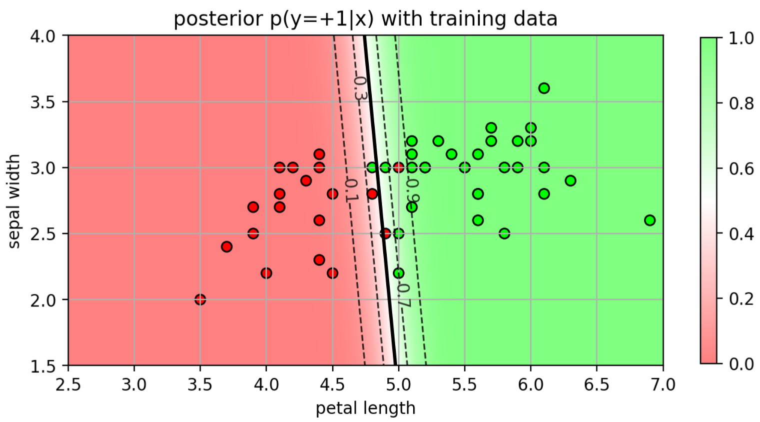
```
(50, 2)
(50, 2)
```

In [27]:
```
# 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 = [[9.51275841 0.89596567]]
b = [-48.68254369]
```

- Equation:
  - $f(\mathbf{x}) = (9.51 * \text{petal\_length}) + (0.895 * \text{sepal\_width}) - 48.68$
- Interpretation:
  - large petal length makes $f(\mathbf{x})$ positive, so large petal length is associated with class +1.

In [29]:
```
# 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');
```



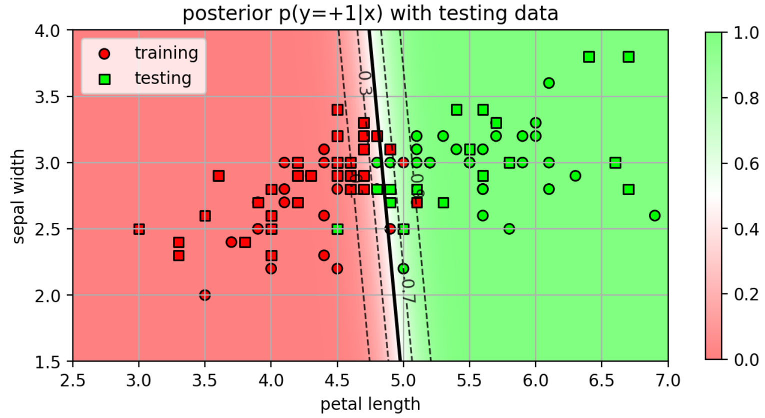
In [30]:
```
# predict from the model
predY = logreg.predict(testX)

# calculate accuracy
```

```
acc = metrics.accuracy_score(testY, predY)
```

```
test accuracy = 0.92
```

In [32]:
```
postfig
```

Out[32]:

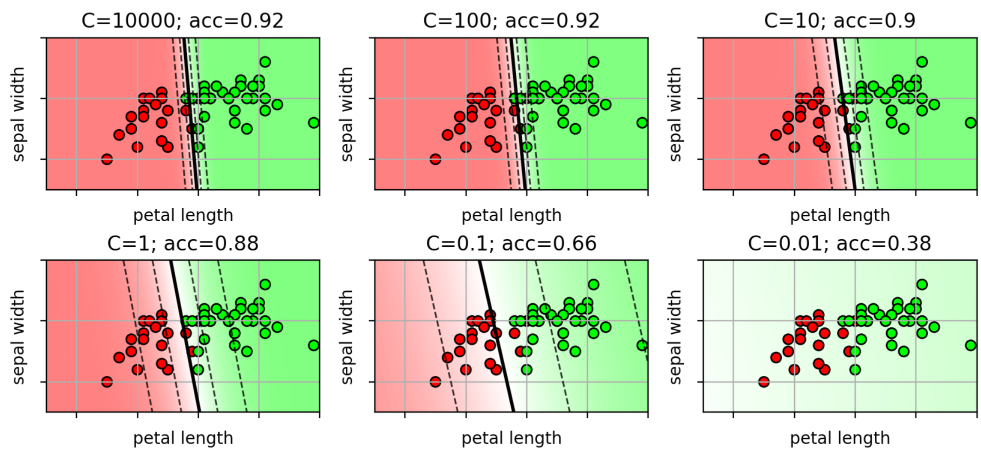


Selecting the regularization hyperparameter

- the regularization hyperparameter C has a large effect on the decision boundary and the accuracy.
  - larger C makes the classifier more confident (posterior probabilities saturate to 0 and 1)
    - more likely to overfit
  - smaller C makes the classifer less confident (wider range of posterior probabilities).
    - less likely to overfit
- How to set the value of C?

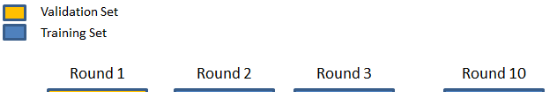
In [34]:
```
lrC
```

Out[34]:



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
  3. Split the training set into training data and validation data
  4. Learn a classifier for each value of C
  5. Record the accuracy on the validation data for each C
  6. Select the value of C that has the highest average accuracy over all K folds.
  7. 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

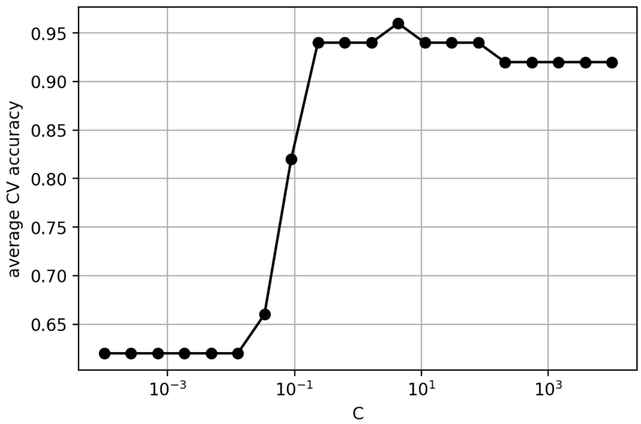
In [35]:
```
# learn logistic regression classifier using CV
#  Cs is an array of possible C values
#  cv is the number of folds
#  n_jobs=-1 means run in parallel with all cores
logreg = linear_model.LogisticRegressionCV(Cs=logspace(-4,4,20), cv=5, n_jobs=-1)
logreg.fit(trainX, trainY)

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= [[4.61911023 0.72397804]]
b= [-24.24716682]
test accuracy= 0.9
```

Which C was selected?

In [36]:
```
print("C =", logreg.C_)
# calculate the average score for each C
avgscores = mean(logreg.scores_[2],0)   # 2 is the class label
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

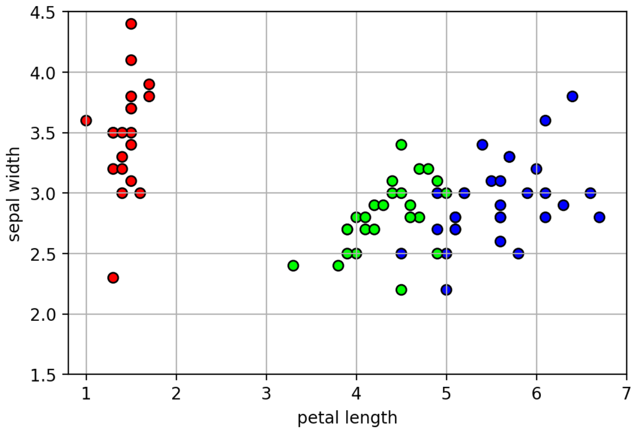
In [37]:
```
# load iris data each row is (petal length, sepal width, class)
irisdata = loadtxt('iris3.csv', delimiter=',', skiprows=1)

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

print(X.shape)
```

```
(150, 2)
```

In [38]:
```
# 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 [39]:
```
# 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', ["#FF0000", "#00FF00

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 [40]:
```
# learn logistic regression classifier (one-vs-all)
mlogreg = linear_model.LogisticRegression(C=10, multi_class='ovr')
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)
```

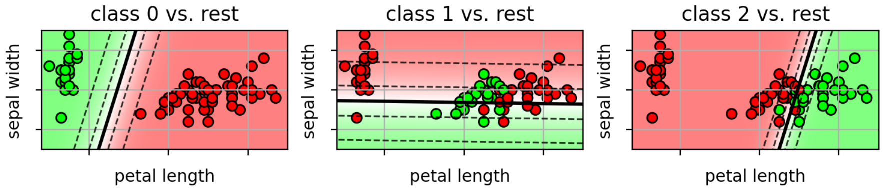
```
w= [[-3.54884501  1.11513222]
 [-0.03185278 -2.23119433]
 [ 5.41926127 -1.69411622]]
b= [  6.26247277   6.1229662  -21.79941354]
test accuracy= 0.9733333333333334
```

- the individual 1-vs-rest binary classifiers

In [42]:
```
print("w=", mlogreg.coef_)
print("b=", mlogreg.intercept_)

mlrfig
```

```
w= [[-3.54884501  1.11513222]
 [-0.03185278 -2.23119433]
 [ 5.41926127 -1.69411622]]
b= [  6.26247277   6.1229662  -21.79941354]
```

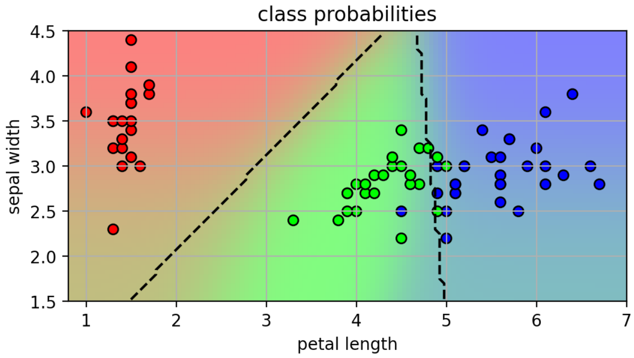
Out[42]:



- the final classifier, combining all 1 vs rest classifiers

In [44]:
```
lr3class
```

Out[44]:



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.
  - linear function for each class, $f_c(\mathbf{x}) = \mathbf{w}_c^T\mathbf{x}$.
- Define probabilities with **softmax** function
  - analogous to sigmoid function for binary logistic regression.

$$p(y=c|\mathbf{x}) = \frac{e^{f_c(\mathbf{x})}}{e^{f_1(\mathbf{x})} + \cdots + e^{f_K(\mathbf{x})}}$$

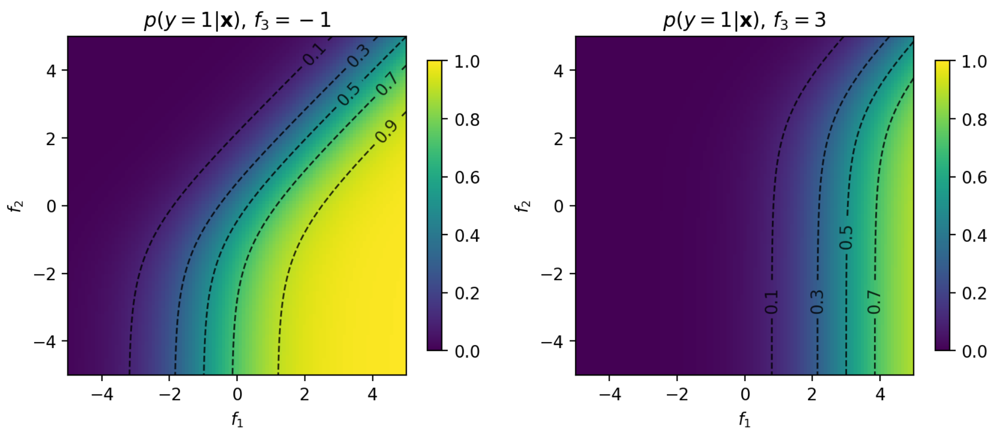
- The class with largest response of $f_c(\mathbf{x})$ will have the highest probability.

- Example with $K=3$.

$$p(y=1|\mathbf{x}) = \frac{e^{f_1(\mathbf{x})}}{e^{f_1(\mathbf{x})} + e^{f_2(\mathbf{x})} + e^{f_3(\mathbf{x})}}$$

In [46]:
```
sfmfig
```

Out[46]:



Parameter estimation

- Estimate the $\{\mathbf{w}_j\}$ parameters using MLE.
- Let $(\mathbf{x}, \mathbf{y})$ be a data sample pair:
  - $\mathbf{x}$ feature vector.
  - $\mathbf{y} = [y_1, \cdots, y_K]$ is a one-hot vector, where $y_c = 1$ when class c, and 0 otherwise.
- Data likelihood of $(\mathbf{x}, \mathbf{y})$.

$$\begin{aligned} \text{likelihood:} \quad & p(\mathbf{y}|\mathbf{x}) = \prod_{j=1}^{K} p(y = j|\mathbf{x})^{y_j} \\ \text{log-likelihood:} \quad & \log p(\mathbf{y}|\mathbf{x}) = \sum_{j=1}^{K} y_j \log p(y = j|\mathbf{x}) \\ \text{negative log-likelihood:} \quad & -\log p(\mathbf{y}|\mathbf{x}) = -\sum_{j=1}^{K} y_j \log p(y = j|\mathbf{x}) \end{aligned}$$

  - equivalent to the *cross-entropy loss*

- Given dataset $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^N$
  - maximize the data log-likelihood:

$$\max_{\{\mathbf{w}_j\}} \sum_{i=1}^{N} \log p(\mathbf{y}_i|\mathbf{x}_i) = \max_{\{\mathbf{w}_j\}} \sum_{i=1}^{N} \sum_{j=1}^{K} y_{ij} \log p(y = j|\mathbf{x}_i)$$

  - i.e., minimize the cross-entropy loss

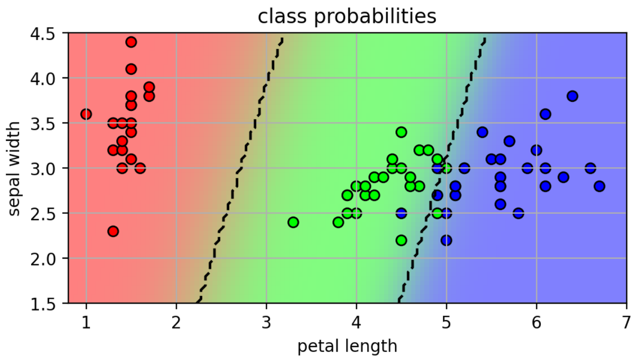
In [47]:
```
# learn logistic regression classifier
mlogreg = linear_model.LogisticRegression(C=10,
            multi_class='multinomial')
            # use multi-class and corresponding solver
mlogreg.fit(trainX, trainY)

# 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 [49]:
```
lr3classm
```

Out[49]:

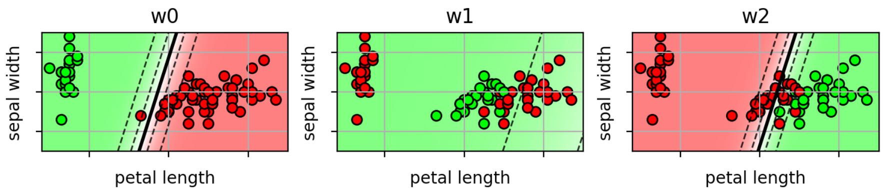


- individual weight vectors work together to partition the space

In [51]:
```
print("w=", mlogreg.coef_)
print("b=", mlogreg.intercept_)

lr31vr
```

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

Out[51]:



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 $f(\mathbf{x}^*)$

$$y^* = \begin{cases} +1, f(\mathbf{x}^*) > 0 \\ -1, \text{otherwise} \end{cases} = \text{sign}(f(\mathbf{x}_*))$$

- **Extend to multi-class:**
  - K linear functions, one for each class.
  - compute probability using softmax function