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:
 - $\begin{array}{l} \bullet \ p(\mathbf{x}|y=1) = \prod_{i=1}^D \mathcal{N}(x_i|\mu_i,\sigma^2) \\ \bullet \ p(\mathbf{x}|y=2) = \prod_{i=1}^D \mathcal{N}(x_i|\nu_i,\sigma^2) \end{array}$
- - $p(y=1)=\pi_1$, $p(y=2)=\pi_2$.
- look at the log-ratio of CCDs,

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

Thus

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

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

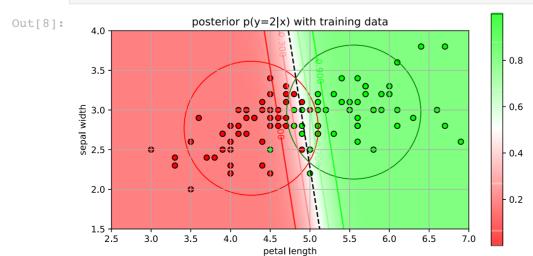
$$egin{aligned} \log p(y=1|\mathbf{x}) > \log p(y=2|\mathbf{x}) \ \log p(\mathbf{x}|y=1) + \log p(y=1) > \log p(\mathbf{x}|y=2) + \log p(y=2) \ \log rac{p(\mathbf{x}|y=1)}{p(\mathbf{x}|y=2)} + \log rac{p(y=1)}{p(y=2)} > 0 \end{aligned}$$

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

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

Example

In [8]: pfig



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

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

- $\circ w_i$ is a per-feature weight
- \circ b is a bias term
- the BDR in this case is a linear classifier:
 - select class y=1 when
 - $\circ \sum_{i=1}^D w_i x_i + b > 0$
 - \circ equivalently, $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b > 0$
- Here we obtain the weights 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
 - ullet Observation (feature vectors) $\mathbf{x} \in \mathbb{R}^d$
 - Class $y \in \{-1, +1\}$
- **Goal**: given a feature vector **x**, predict its class *y*.
 - Calculate a *linear function* of the feature vector **x**.

$$egin{aligned} \circ \ f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b = \sum_{j=1}^d w_j x_j + b \end{aligned}$$

- $\mathbf{w} \in \mathbb{R}^d$ are the weights of the linear function.
- o multiply each feature value with a weight, and then add together.
- Predict from the value:
 - $\circ~$ if $f(\mathbf{x})>0$ then predict Class y=1
 - \circ if $f(\mathbf{x}) < 0$ then predict Class y = -1
 - \circ Equivalently, $y = \operatorname{sign}(f(\mathbf{x}))$

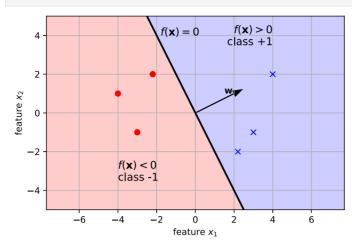
Geometric Interpretation

- 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 w.
 - also called the separating hyperplane.
- Example:

$$\mathbf{w} = \left[egin{array}{c} 2 \ 1 \end{array}
ight], b = 0$$

In [11]: linclass

Out[11]:



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, w defines a 1-D line.
 - for d=3, 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)

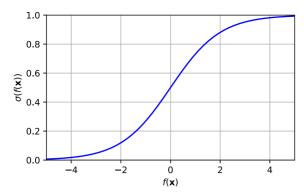
Logistic regression

- Use a probabilistic approach
 - ullet 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 [13]:

sigmoidplot

Out[13]:

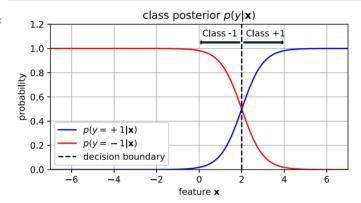


- Given a feature vector x, the probability of a class is:
 - $p(y = +1|\mathbf{x}) = \sigma(f(\mathbf{x}))$
 - $p(y = -1|\mathbf{x}) = 1 \sigma(f(\mathbf{x}))$
- Note: here we are directly modeling the class posterior probability!
 - not the class-conditional $p(\mathbf{x}|y)$

In [15]: 1

lrexample

Out[15]:



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:

$$(\mathbf{w}^*, b^*) = rgmax \sum_{\mathbf{w}, b}^N \log p(y_i | \mathbf{x}_i)$$

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

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

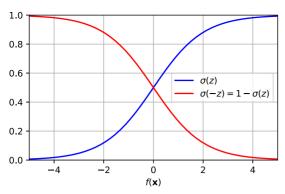
• Note the following property:

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

In [17]:

sigmoidplot

Out[17]:



· Thus,

$$p(y|\mathbf{x}) = \left\{ egin{aligned} \sigma(f(\mathbf{x})), & y = 1 \\ \sigma(-f(\mathbf{x})), & y = -1 \end{aligned}
ight.$$

· Simplifying the 2 cases into one equation,

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

· Taking the log,

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

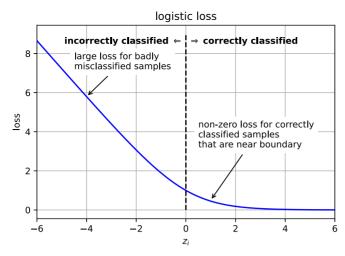
• Substituting into the MLE formulation:

$$egin{aligned} (\mathbf{w}^*, b^*) &= rgmax \sum_{\mathbf{w}, b}^N \log p(y_i | \mathbf{x}_i) \ &= rgmin \sum_{\mathbf{w}, b}^N \log (1 + e^{-y_i f(\mathbf{x}_i)}) \end{aligned}$$

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

In [19]: lossfig

Out[19]:

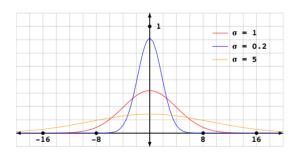


Regularization

- to prevent overfitting, add a prior distribution on w.
 - prefer solutions that are likely under the prior.

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

- assume Gaussian distribution on ${f w}$ with variance C/2
 - $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|0, \frac{C}{2}\mathbf{I})$
 - \circ small values of C keep ${f w}$ close to 0.
 - \circ 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,

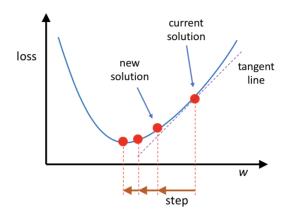
$$\mathbf{w}^*, b^*) = \operatorname*{argmin}_{\mathbf{w}, b} rac{1}{C} \mathbf{w}^T \mathbf{w} + \sum_{i=1}^N \log(1 + \exp(-y_i f(\mathbf{x}_i)))$$

- the first term is the regularization term
 - \bullet Note: $\mathbf{w}^T\mathbf{w} = \sum_{j=1}^d w_j^2$
 - penalty term that keeps entries in w from getting too large.
 - lacktriangledown C is the regularization *hyperparameter*
 - ∘ larger C values apply less penalty on large \mathbf{w} → allow large values in \mathbf{w} .
 - \circ smaller C values apply more penalty on large $\mathbf{w} \to \text{discourage large values in } \mathbf{w}$.
- 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.
 - $\circ \mathbf{w} \leftarrow \mathbf{w} \eta \frac{dE}{d\mathbf{w}}$
 - \circ where E is the objective function
 - \circ η is the *learning rate* (how far to step in each iteration).



Example: Iris Data

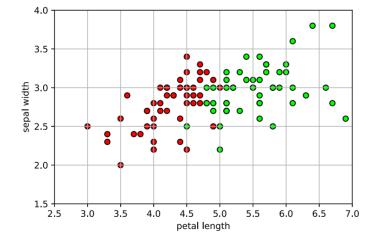
```
In [20]: # load iris data each row is (petal length, sepal width, class)
irisdata = loadtxt('iris2.csv', delimiter=',', skiprows=1)

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



```
In [23]: # 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 [24]:
             # 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}) = (4.87 * \text{petal\_length}) - (0.62 * \text{sepal\_width}) - 21.68
                   • large petal length makes f(\mathbf{x}) positive, so large petal length is associated with class +1.
In [26]:
             # 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');
                             posterior p(y=+1|x) with training data
               4.0
                                                                                  1.0
               3.5
                                                                                  0.8
             sepal width
                                                                                  0.6
                                                                                  0.4
               2.0
                                                                                  0.2
                                                                                  0.0
               1.5
                        3.0
                                           4.5
                                                        5.5
                                                              6.0
                                                                    6.5
                                                                           7.0
                                           petal length
In [27]:
             # 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 [29]:
             postfig
                             posterior p(y=+1|x) with testing data
Out[29]:
               4.0
                                                                                  1.0
                         training
                         testing
               3.5
                                                                                  0.8
             sepal width
               3.0
                                                                                  0.6
               2.5
                                                                                  0.4
                                                                                  0.2
               2.0
```

Selecting the regularization hyperparameter

5.5

6.0

6.5

7.0

0.0

3.5

4.0

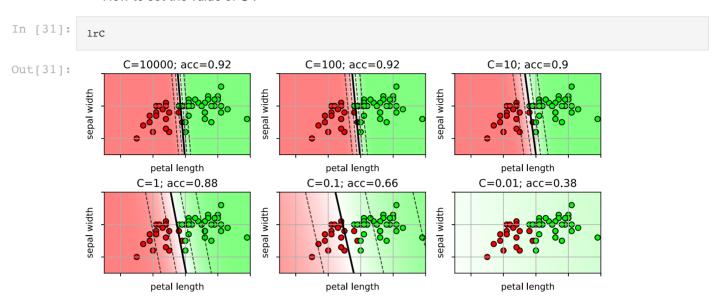
4.5

petal length

5.0

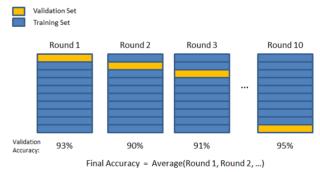
3.0

- ullet the regularization hyperparameter C has a large effect on the decision boundary and the accuracy.
 - ullet larger C makes the classifier more confident (posterior probabilities saturate to 0 and 1)
 - o 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?



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.
 - \circ Try a range of C values on each split.
 - Pick the value that works best over all splits.



Procedure

- 1. select a range of ${\cal C}$ 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 ${\cal C}$
- 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 [32]:
           # 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 [33]:
    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]

0.95
0.90
0.85
0.70
0.65
0.70
0.65
```

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.
 - $\circ~$ 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 [34]:
            # 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, virginica=2)
            print(X.shape)
            (150, 2)
In [35]:
            # 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 [36]:
           # 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", "#000FF
            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');
              4.5
              4.0
              3.5
            sepal width
              3.0
              2.5
              2.0
                                     petal length
In [37]:
            # 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= 0.97333333333333334

    the individual 1-vs-rest binary classifiers

In [39]:
```

print("w=", mlogreg.coef_)

```
print("b=", mlogreg.intercept_)
mlrfig
```

```
w= [[-3.54884501 1.11513222]

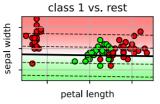
[-0.03185278 -2.23119433]

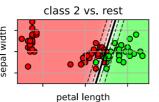
[ 5.41926127 -1.69411622]]

b= [ 6.26247277 6.1229662 -21.79941354]
```

Out[39]: class 0 vs. rest

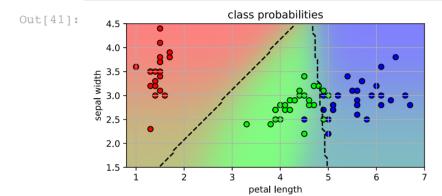
petal length





• the final classifier, combining all 1 vs rest classifiers

In [41]: lr3class



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.

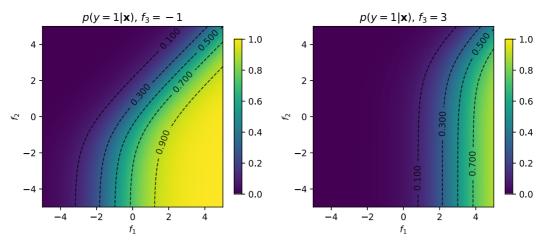
$$p(y=c|\mathbf{x}) = rac{e^{f_c(\mathbf{x})}}{e^{f_1(\mathbf{x})} + \cdots + e^{f_K(\mathbf{x})}}$$

- The class with largest response of $f_c(\mathbf{x})$ will have the highest probability.
- Example with K=3.

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

In [43]: sfmfig

Out[43]:



Parameter estimation

- Estimate the $\{\mathbf w_j\}$ parameters using MLE.
- Let (\mathbf{x}, \mathbf{y}) be a data sample pair:
 - 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}) .

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

- 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

```
[-0.71717021 0.23609022]

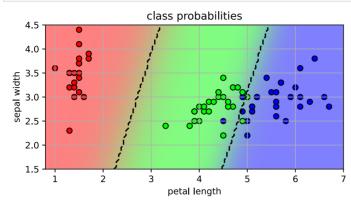
[ 4.84809458 -1.54327757]]

b= [ 11.46078594 5.40723484 -16.86802078]

test accuracy= 0.9733333333333333
```

In [46]: lr3classm

Out[46]:



• individual weight vectors work together to partition the space

Logistic Regression Summary

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

Lecture3a slides
$$y^* = egin{cases} +1, p(y=+1|\mathbf{x}^*) > p(y=-1|\mathbf{x}^*) \ -1, ext{otherwise} \end{cases}$$

 \circ alternatively, just use $f(\mathbf{x}^*)$

$$y^* = \left\{ egin{aligned} +1, f(\mathbf{x}^*) > 0 \ -1, ext{otherwise} \end{aligned}
ight. = ext{sign}(f(\mathbf{x}_*))$$

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

In []: