Unit 5
Linear Classification & Logistic Regression

Prof. Phil Schniter

THE OHIO STATE UNIVERSITY

ECE 4300: Introduction to Machine Learning, Sp20

Learning objectives

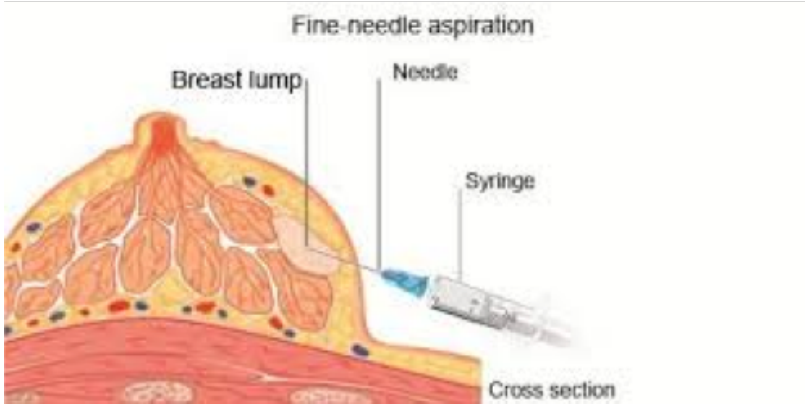
- Understand classification problems in machine learning:
  - Identify features, labels; binary vs multiclass; linear vs nonlinear
  - visualize scatterplots and decision regions
- For binary classification problems, understand ...
  - linear classifiers, separating hyperplanes, margin
  - why linear regression doesn't work
  - logistic regression: logistic function, cross-entropy loss, ML fitting, regularization
  - feature transformations
  - common error metrics: accuracy, precision, recall, F1
  - the effect of the decision threshold, ROC, AUC
- For multiclass classification problems, understand ...
  - solutions that use multiple binary classifiers
  - multinomial logistic regression: softmax function, cross-entropy, ML fitting
- How to implement and assess classification using sklearn

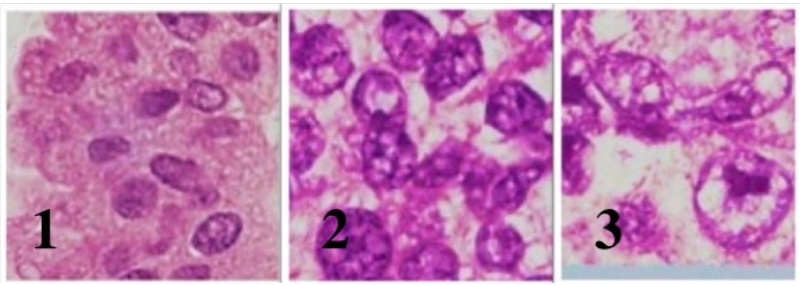
Outline

- Motivating Example: Diagnosing Breast Cancer
- Binary Classification
- Binary Logistic Regression
- Multiclass Classification
- Multinomial Logistic Regression
- Measuring Accuracy in Classification

Diagnosing Breast Cancer

- Fine-need aspiration of suspicious breast lumps:
  - Tissue is stained & viewed under microscope
  - Cytopathologist visually inspects cells
  - Tries to classify as benign or malignant
  - If malignant, also provides grading
- Would like to improve accuracy
- Can machine-learning help?





Grades of carcinoma cells
http://breast-cancer.ca/5a-types/

The Wisconsin Breast Cancer Data Set

Univ. of Wisconsin study:

- 683 samples
- 9 features (on right)
- target: malignant or benign
  - ground-truth was assessed using a biopsy

#	Attribute	Domain
1.	Sample code number	id number
2.	Clump Thickness	1 - 10
3.	Uniformity of Cell Size	1 - 10
4.	Uniformity of Cell Shape	1 - 10
5.	Marginal Adhesion	1 - 10
6.	Single Epithelial Cell Size	1 - 10
7.	Bare Nuclei	1 - 10
8.	Bland Chromatin	1 - 10
9.	Normal Nucleoli	1 - 10
10.	Mitoses	1 - 10
11.	Class:	(2 for benign, 4 for malignant)

Data:
https://archive.ics.uci.edu/ml/machine-learning-databases/breast-cancer-wisconsin/breast-cancer-wisconsin.data

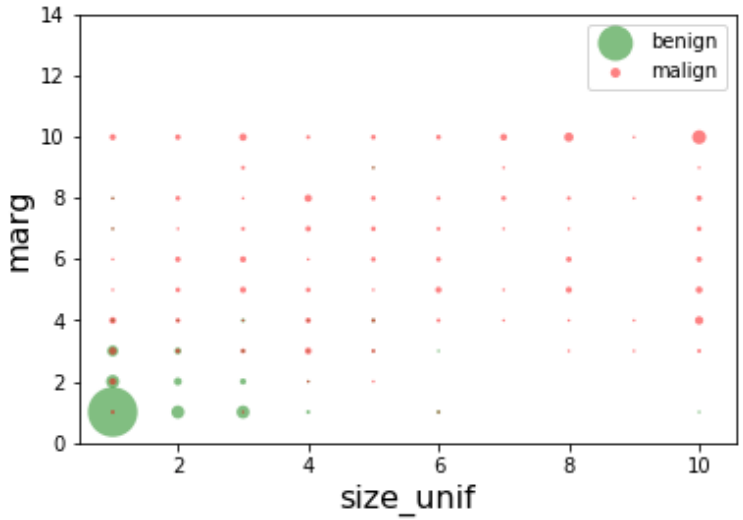
Explanation:
https://archive.ics.uci.edu/ml/machine-learning-databases/breast-cancer-wisconsin/breast-cancer-wisconsin.names

Original paper:

O.L. Mangasarian, W.N. Street, and W.H. Wolberg, "Breast cancer diagnosis and prognosis via linear programming," *Operations Research*, 1995.

Visualizing the data

- Choose two features
- Plot target count vs. features using variable-radius dots




```
# Compute the bin edges for the 2d histogram
x1val = np.array(list(set(X[:,0]))).astype(float)
x2val = np.array(list(set(X[:,1]))).astype(float)
x1, x2 = np.meshgrid(x1val,x2val)
x1e= np.hstack((x1val,np.max(x1val)+1))
x2e= np.hstack((x2val,np.max(x2val)+1))

# Make a plot for each class
yval = list(set(y))
color = ['g','r']
for i in range(len(yval)):
    I = np.where(y==yval[i])[0]
    cnt, x1e, x2e = np.histogram2d(X[I,0],X[I,1],[x1e,x2e])
    x1, x2 = np.meshgrid(x1val,x2val)
    plt.scatter(x1.ravel(), x2.ravel(), s=2*cnt.ravel(),alpha=0.5,
                c=color[i],edgecolors='none')
plt.ylim([0,14])
plt.legend(['benign','malign'], loc='upper right')
plt.xlabel(xnames[0], fontsize=16)
plt.ylabel(xnames[1], fontsize=16)
```

- How would we classify a test feature $\boldsymbol{x} = [x_1, x_2]$?

Outline

- Motivating Example: Diagnosing Breast Cancer
- Binary Classification
- Binary Logistic Regression
- Multiclass Classification
- Multinomial Logistic Regression
- Measuring Accuracy in Classification

Binary classification

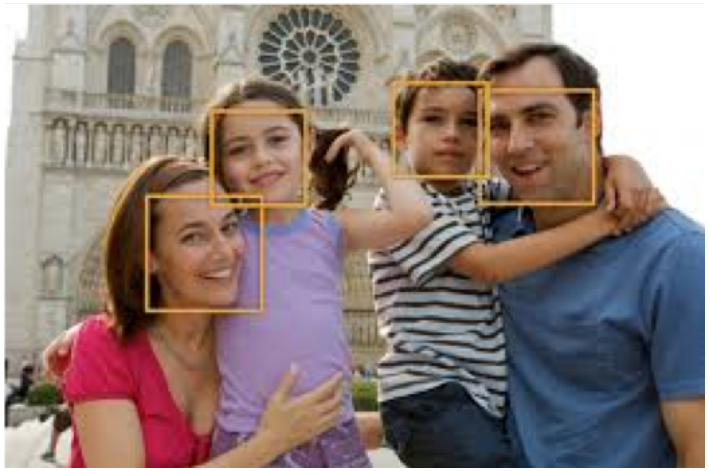
- Given training data $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$ with $\boldsymbol{x}_i \in \mathbb{R}^d$ and $y_i \in \{-1, 1\}$, our goal is to classify a test vector $\boldsymbol{x}$ as $y \in \{-1, 1\}$ (one of two "classes")
  - Unlike regression, the target y is now binary
  - Using $\{-1, 1\}$ leads to cleaner notation later
- Many applications:
  - Face detection: is a face present here or not?
  - Are these cells cancerous or not?
- Mathematically, want to design a classifier

$$f(\boldsymbol{x}) = \widehat{y} \in \{-1, 1\}$$

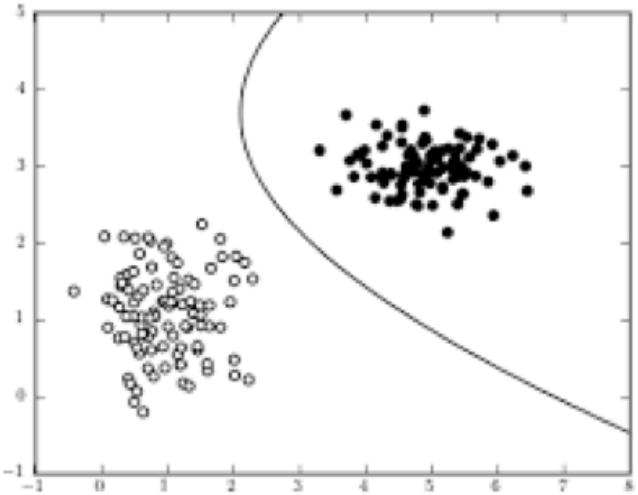
such that $\widehat{y} = y$ with high probability

- Note: $f(\cdot)$ is defined by its decision regions:

$\mathcal{R}_{-1} \triangleq \{\boldsymbol{x} : f(\boldsymbol{x}) = -1\}$ and $\mathcal{R}_1 \triangleq \{\boldsymbol{x} : f(\boldsymbol{x}) = 1\}$

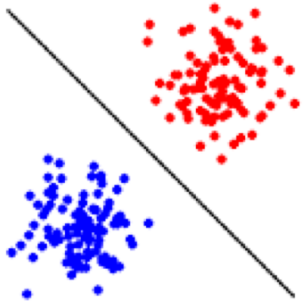


Example with $d = 2$:



Binary linear classification

- One option is binary *linear* classification:
  1) define the "score" or "discriminant", $z = b + \sum_{j=1}^{d} x_j w_j$, which is linear in the parameters b and w_j
  2) given $\boldsymbol{x}$, threshold the score to obtain $\widehat{y} = \begin{cases} 1 & \text{if } z \geq 0 \\ -1 & \text{if } z < 0 \end{cases}$
  3) learn weights $\boldsymbol{w} \triangleq [w_1, \ldots, w_d]^{\mathsf{T}}$ and intercept b from the training data $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n}$



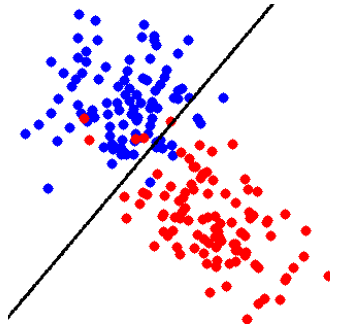
- Note that, at the decision boundary, we have

$$0 = z = b + \boldsymbol{x}^{\mathsf{T}} \boldsymbol{w}$$

Thus, the hyperplane

$$\{\boldsymbol{x} : b + \boldsymbol{x}^{\mathsf{T}} \boldsymbol{w} = 0\}$$

separates the decision regions



- This decision boundary is linear in $\boldsymbol{x}$ (see figures). When does this perform well?

Linear separability

- Linear classification performs well when the data $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$ is "linearly separable"
- Linearly separable means that there exists a hyperplane

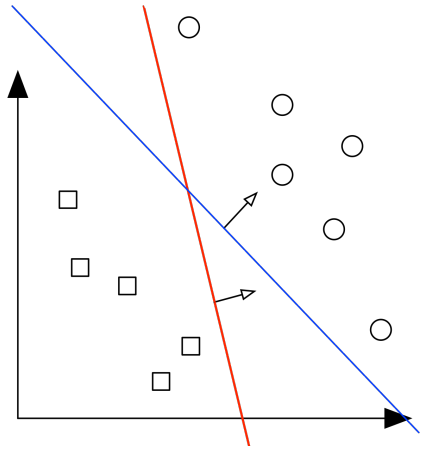
$$\{\boldsymbol{x} : b + \boldsymbol{x}^\mathsf{T}\boldsymbol{w} = 0\}$$

(for some b and $\boldsymbol{w}$) that separates the samples $\boldsymbol{x}_i$ according to their class $y_i \in \{-1, 1\}$

  - On one side of hyperplane lies all $\boldsymbol{x}_i$ for which $y_i = 1$, while on other other side lies all $\boldsymbol{x}_i$ for which $y_i = -1$

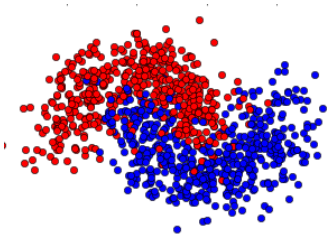
- Note: When such a separating hyperplane exists, it is usually not unique.

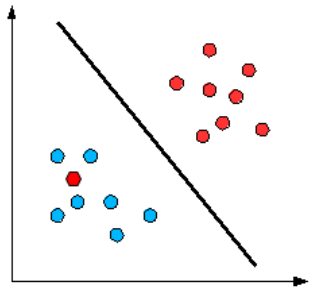
linear separability:

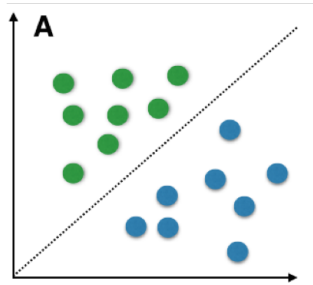


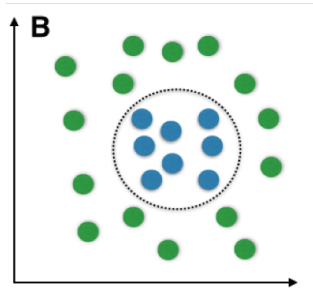
Linear versus nonlinear classification

- Most datasets are *not* linearly separable!
  - There are many possible reasons why
  - See examples on right (except Fig. A)
- Still, linear classification is worth considering
  - It is relatively easy to understand
  - It facilitates feature selection (i.e., shows which features matter)
  - It can incorporate nonlinear feature transformations
    - Fig. A: boundary is linear in (x_1, x_2)
    - Fig. B: boundary is nonlinear in (x_1, x_2) but linear in $\sqrt{x_1^2 + x_2^2}$
  - It can be used as a building block (e.g., for neural networks, decision trees, etc.)









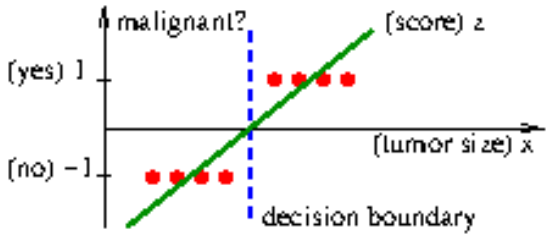
Linear classification vs. linear regression

- Suppose we want to do *linear* classification. How exactly do we fit $(b, \boldsymbol{w})$?
- Can we just use linear regression?
  - In other words, choose $(b, \boldsymbol{w})$ to minimize $\mathrm{RSS} = \left\| \boldsymbol{y} - \boldsymbol{A} \begin{bmatrix} b \\ \boldsymbol{w} \end{bmatrix} \right\|^2$ and then output

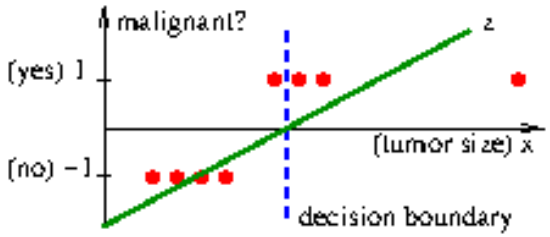
$$\widehat{y} = \begin{cases} 1 & \text{if } z \geq 0 \\ -1 & \text{if } z < 0 \end{cases}, \quad \text{where } z = [1 \ \boldsymbol{x}]^{\mathsf{T}} \begin{bmatrix} b_{\mathsf{ls}} \\ \boldsymbol{w}_{\mathsf{ls}} \end{bmatrix}$$

- No, this may not work well!
  - Consider simple case where $d = 1$
  - When $\{x_i\}$ is "balanced" (see figure), works okay
  - But when $\{x_i\}$ is "imbalanced," the least-squares regression line gets pulled to one side, and the threshold at $z = 0$ will make errors
- What's the problem?
  - RSS is not the right loss function for classification! (More details soon)

balanced $\{x_i\}$:



imbalanced $\{x_i\}$:



Linear regression fails on breast-cancer classification!

- Let's try the same linear-regression approach on the breast-cancer data (after converting targets to $y \in \pm 1$)
- Again, use decision boundary

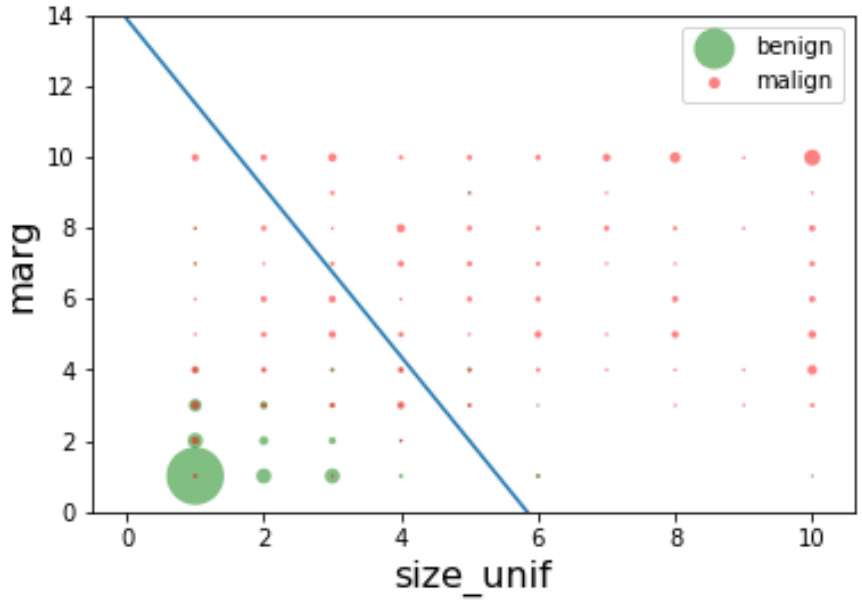
$$\{\boldsymbol{x} : b + \boldsymbol{x}^T \boldsymbol{w} = 0\}$$

which, in this $d = 2$ case, becomes

$$\{(x_1, x_2) : x_2 = -\frac{b}{w_2} - \frac{w_1}{w_2} x_1\}$$

- Because the $\{\boldsymbol{x}_i\}$ are imbalanced, the decision boundary is pulled north-east, and many red $\boldsymbol{x}_i$ are misclassified!
- Again we see that designing $(b, \boldsymbol{w})$ via linear regression does not work well for linear classification!

blue line shows decision boundary




```
yhat = regr.predict(X)
yhati = (yhat >=0.5).astype(int)
acc = np.mean(yhati == y)
print("Accuracy on training data using two features = %f" % acc)
```

```
Accuracy on training data using two features = 0.922401
```

Outline

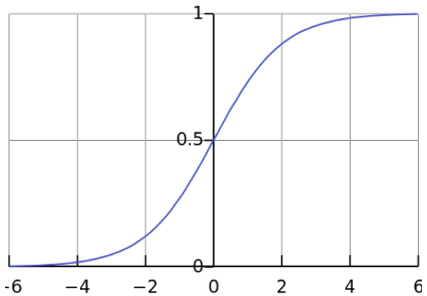
- Motivating Example: Diagnosing Breast Cancer
- Binary Classification
- Binary Logistic Regression
- Multiclass Classification
- Multinomial Logistic Regression
- Measuring Accuracy in Classification

Binary logistic regression

- Linear classification computes $z = b + \boldsymbol{x}^{\mathsf{T}}\boldsymbol{w}$ and sets $\widehat{y} = \begin{cases} 1 & z \geq 0 \\ -1 & z < 0 \end{cases}$
- How do we design the parameters $(b, \boldsymbol{w})$?
  - We saw that minimizing RSS is a bad idea!
- Idea: Given the score z, model the true label $y \in \pm 1$ as a random variable
- The most popular version of this uses

$$\Pr\{y=1 \,|\, z\} = \frac{e^z}{1+e^z}, \quad \Pr\{y=-1 \,|\, z\} = \frac{1}{1+e^z}.$$

  Note $\Pr\{y=0 \,|\, z\} + \Pr\{y=1 \,|\, z\} = 1 \; \forall z$, as required for a valid pmf.
  - The larger that z is, the more likely that $y = 1$
  - When $z = 0$, it's equally likely that $y = 1$ or $y = -1$
- $\dfrac{e^z}{1+e^z} = \dfrac{1}{1+e^{-z}}$ is known as the "logistic function" or "sigmoid function"



Understanding the logistic model

- Previously considered $\Pr\{y=1\,|\,z\}$. What about $\Pr\{y=1\,|\,\boldsymbol{x}\}$?
- Consider the simple case of a single scalar feature x and no intercept b:

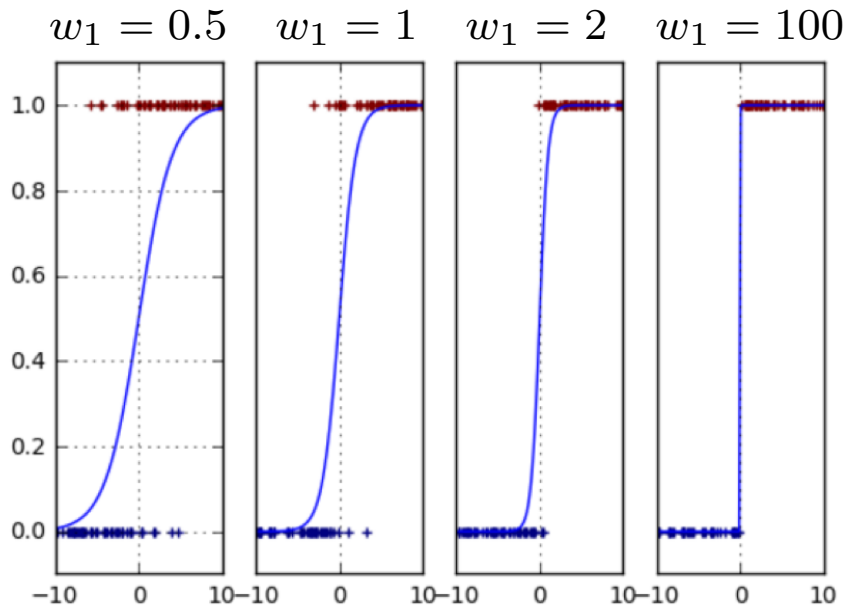
$$\Pr\{y=1\,|\,x\} = \frac{1}{1+e^{-z}} \text{ for } z = w_1 x$$

  - As the weight w_1 increases, the transition becomes sharper
  - Equivalently, as w_1 increases, there is less randomness in y

- Now add the intercept term b, giving

$$z = b + w_1 x = w_1\left(\frac{b}{w_1} + x\right)$$

So the transition occurs at $x = -\dfrac{b}{w_1}$



curve: $\Pr\{y=1\,|\,x\}$ versus x
markers: random $\{(y_i, x_i)\}_{i=1}^n$

Maximum likelihood estimation

- Given training data $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$, we can fit the model parameters $(b, \boldsymbol{w})$ using maximum likelihood (ML) estimation:

ML Estimation

1) Define a likelihood function $p(\boldsymbol{y}|\boldsymbol{X}; b, \boldsymbol{w})$ with model parameters $(b, \boldsymbol{w})$
   - As usual, $\boldsymbol{y} \triangleq [y_1, \ldots, y_n]^{\mathsf{T}}$ and $\boldsymbol{X} \triangleq [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n]^{\mathsf{T}}$

2) The ML model parameters are
$$\begin{aligned}(b_{\mathsf{ml}}, \boldsymbol{w}_{\mathsf{ml}}) &\triangleq \arg\max_{b,\boldsymbol{w}} p(\boldsymbol{y}|\boldsymbol{X}; b, \boldsymbol{w}) \\ &= \arg\max_{b,\boldsymbol{w}} \ln p(\boldsymbol{y}|\boldsymbol{X}; b, \boldsymbol{w}) \\ &= \arg\min_{b,\boldsymbol{w}} \big\{ -\ln p(\boldsymbol{y}|\boldsymbol{X}; b, \boldsymbol{w}) \big\}\end{aligned}$$

- In fact, we used the ML approach for linear regression:
  - There, the likelihood was $p(\boldsymbol{y}|\boldsymbol{X}; \boldsymbol{\beta}) = \mathcal{N}(\boldsymbol{y}; \boldsymbol{A}\boldsymbol{\beta}, \sigma_\epsilon^2 \boldsymbol{I})$ with $\boldsymbol{A} = [\boldsymbol{1}\ \boldsymbol{X}]$
  - thus $-\ln p(\boldsymbol{y}|\boldsymbol{X}; \boldsymbol{\beta}) = \frac{1}{2\sigma^2} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{\beta}\|^2 + \text{constant}$
  - and so $\boldsymbol{\beta}_{\mathsf{ml}} = \arg\min_{\boldsymbol{\beta}} \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{\beta}\|^2 = \arg\min_{\boldsymbol{\beta}} \mathrm{RSS}(\boldsymbol{\beta}) = \boldsymbol{\beta}_{\mathsf{ls}}$
- For logistic regression, we use the ML approach with a different likelihood!

ML estimation for logistic regression

- Logistic regression assumes that y_i depends only on $\boldsymbol{x}_i$ (not $\boldsymbol{x}_k|_{k\neq i}$), and that

$$\Pr\{y_i=1\,|\,\boldsymbol{x}_i;b,\boldsymbol{w}\}=\tfrac{e^{z_i}}{1+e^{z_i}},\quad \Pr\{y_i=-1\,|\,\boldsymbol{x}_i;b,\boldsymbol{w}\}=\tfrac{1}{1+e^{z_i}},\quad z_i=b+\boldsymbol{x}_i^{\mathsf{T}}\boldsymbol{w}$$

- Thus we have

$$p(\boldsymbol{y}|\boldsymbol{X};b,\boldsymbol{w})=\textstyle\prod_{i=1}^n p(y_i|\boldsymbol{x}_i;b,\boldsymbol{w}) \qquad \text{via independence assumption}$$

$$-\ln p(\boldsymbol{y}|\boldsymbol{X};b,\boldsymbol{w})=-\textstyle\sum_{i=1}^n \ln p(y_i|\boldsymbol{x}_i;b,\boldsymbol{w}) \qquad \text{since } \ln(ab)=\ln a+\ln b$$

$$=-\textstyle\sum_{i=1}^n \frac{y_i+1}{2}\ln\Pr\{y_i=1\,|\,\boldsymbol{x}_i;b,\boldsymbol{w}\}+(1-\frac{y_i+1}{2})\ln\Pr\{y_i=-1\,|\,\boldsymbol{x}_i;b,\boldsymbol{w}\}$$

$$\text{since } \tfrac{y_i+1}{2}=\begin{cases}1 & y_i=1\\ 0 & y_i=-1\end{cases}$$

$$=-\textstyle\sum_{i=1}^n \frac{y_i+1}{2}\big(z_i-\ln[1+e^{z_i}]\big)+(1-\frac{y_i+1}{2})\big(0-\ln[1+e^{z_i}]\big)$$

$$=-\textstyle\sum_{i=1}^n \Big(\frac{y_i+1}{2}z_i-\frac{y_i+1}{2}\ln[1+e^{z_i}]-\ln[1+e^{z_i}]+\frac{y_i+1}{2}\ln[1+e^{z_i}]\Big)$$

$$=-\textstyle\sum_{i=1}^n \big(\frac{y_i+1}{2}z_i-\ln[1+e^{z_i}]\big)$$

- The ML estimates of $(b,\boldsymbol{w})$ are the values that minimize this expression

Cross-entropy loss

In summary...

- When $y_i \in \{-1, 1\}$, the ML weights for binary logistic regression are

$$\boxed{(b_{\text{ml}}, \boldsymbol{w}_{\text{ml}}) \triangleq \arg\min_{b,\boldsymbol{w}} \sum_{i=1}^{n} \left(\ln[1 + e^{z_i}] - \tfrac{y_i+1}{2} z_i \right) \quad \text{for} \quad z_i = b + \boldsymbol{x}_i^{\mathsf{T}} \boldsymbol{w}}$$

  which must be solved numerically

- When $y_i \in \{0, 1\}$, the ML weights for binary logistic regression are

$$\boxed{(b_{\text{ml}}, \boldsymbol{w}_{\text{ml}}) \triangleq \arg\min_{b,\boldsymbol{w}} \sum_{i=1}^{n} \left(\ln[1 + e^{z_i}] - y_i z_i \right) \quad \text{for} \quad z_i = b + \boldsymbol{x}_i^{\mathsf{T}} \boldsymbol{w}}$$

  which is commonly occuring alternative

- The summation is known as the "logistic loss" or "binary cross-entropy loss"

Adding regularization

Assuming $y_i \in \{0, 1\}$ for the following expressions ...

- Usually, L2 regularization is used with the cross-entropy loss:

$$(b_{\text{lr}}, \boldsymbol{w}_{\text{lr}}) = \arg\min_{b,\boldsymbol{w}} \left\{ \sum_{i=1}^{n} \big(\ln[1 + e^{z_i}] - y_i z_i \big) + \alpha \|\boldsymbol{w}\|^2 \right\} \quad \text{for} \quad z_i = b + \boldsymbol{x}_i^{\mathsf{T}} \boldsymbol{w}$$

  - Why? When the training data is linearly separable, the cross-entropy loss decreases as $|w_j|$ increases, and so $\|\boldsymbol{w}_{\text{ml}}\| = \infty$. L2 regularization keeps $\boldsymbol{w}_{\text{lr}}$ finite

- Could instead use L1 regularization, and thus perform feature selection:

$$(b_{\text{lr}}, \boldsymbol{w}_{\text{lr}}) = \arg\min_{b,\boldsymbol{w}} \left\{ \sum_{i=1}^{n} \big(\ln[1 + e^{z_i}] - y_i z_i \big) + \alpha \|\boldsymbol{w}\|_1 \right\} \quad \text{for} \quad z_i = b + \boldsymbol{x}_i^{\mathsf{T}} \boldsymbol{w}$$

- With L2 regularization, could use small (but positive) α to avoid bias
- Or, with L1 or L2 regularization, could tune α using K-fold cross-validation

Logistic regression in sklearn

In sklearn, there is a nice LogisticRegression method:

- Note: L2 regularization is used by default
  - Don't forget to standardize $\boldsymbol{X}$!
- The *inverse* regularization strength is controlled by the parameter `C` > 0
  - So use *large* `C` to avoid regularization-induced bias

```
logreg = linear_model.LogisticRegression(C=1e5)
```

```
Xs = preprocessing.scale(X)
logreg.fit(Xs, y)
```

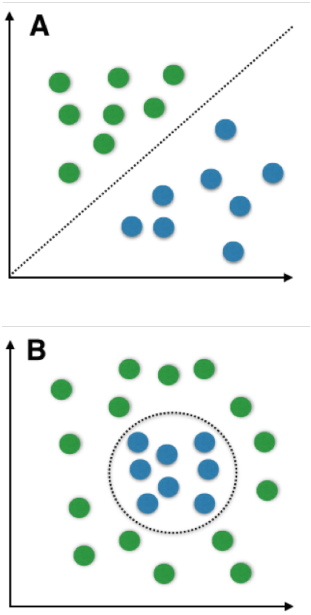
```
LogisticRegression(C=100000.0, class_weight=None, dual=False,
          fit_intercept=True, intercept_scaling=1, max_iter=100,
          multi_class='ovr', n_jobs=1, penalty='l2', random_state=None,
          solver='liblinear', tol=0.0001, verbose=0, warm_start=False)
```

```
yhat = logreg.predict(Xs)
acc = np.mean(yhat == y)
print("Accuracy on training data = %f" % acc)
```

```
Accuracy on training data = 0.969253
```

Feature transformations

- Can we implement *curved* boundaries with *linear* classification methods like logistic regression?
- Yes! Through feature transformation ...
  - Example: given raw features (x_1, x_2), we could transform to $\boldsymbol{x} \triangleq [x_1, x_2, x_1^2, x_2^2]^{\mathsf{T}}$
  - Then the "linear" score $z = b + \boldsymbol{x}^{\mathsf{T}}\boldsymbol{w}$ would be *quadratic* in the raw features (x_1, x_2)
- One-hot coding is another important feature transformation. We saw how it can be used for categorical features like $x_j \in \{\text{Ford}, \text{BMW}, \text{GM}\}$



Outline

- Motivating Example: Diagnosing Breast Cancer
- Binary Classification
- Binary Logistic Regression
- Multiclass Classification
- Multinomial Logistic Regression
- Measuring Accuracy in Classification

Multiclass classification

- What if there are $K \geq 2$ classes?
  - Binary classification is the special case $K = 2$
- Goal: Given training data $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$ with $\boldsymbol{x}_i \in \mathbb{R}^d$ and $y_i \in \{1, \ldots, K\}$, we want to classify a test vector $\boldsymbol{x}$ as $y \in \{1, \ldots, K\}$
  - Unlike regression, the target y is categorical
- Mathematically, we want to design a classifier

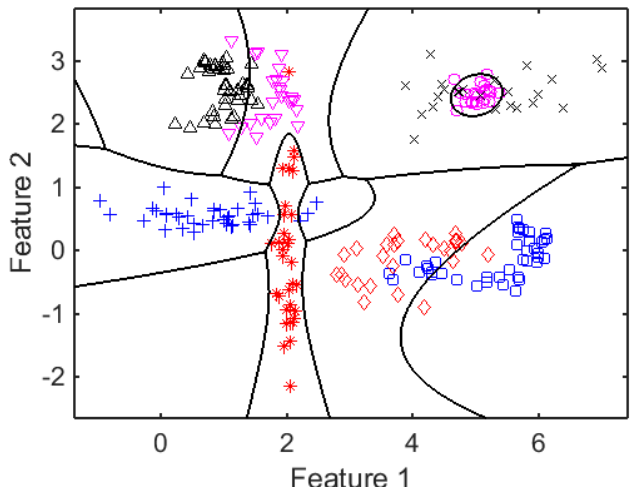
$$f(\boldsymbol{x}) = \widehat{y} \in \{1, \ldots, K\}$$

such that $\widehat{y} = y$ with high probability

- Again, $f(\cdot)$ is defined by its decision regions:

$$\mathcal{R}_k \triangleq \{\boldsymbol{x} : f(\boldsymbol{x}) = k\} \quad \text{for} \quad k = 1, \ldots, K$$

example where $K = 10$:



Multiclass classification using binary classifiers

Multiclass classification is difficult. Can we tackle it using *binary* methods? Yes!

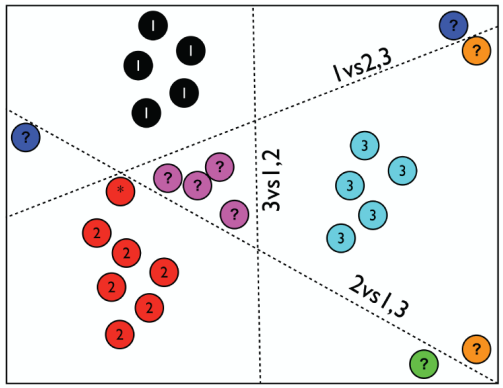
Two main approaches:

- Voting on binary outcomes
  - 1-vs-all: For each class k, decide if $\boldsymbol{x}$ is in-k vs not-in-k, then choose the k with most votes
  - 1-vs-1: For each pair (k, l), decide if $\boldsymbol{x}$ is in-k vs in-l, then choose k with most votes

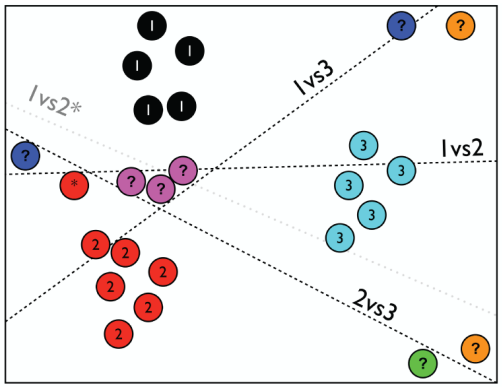
  Problem: Tied votes lead to ambiguities! (see right)

- Choosing the highest confidence value
  - 1-vs-all: For each class k, compute confidence that $\boldsymbol{x}$ is in-k vs not-in-k, then choose the k with highest confidence

  Ambiguities avoided by continuous-valued confidence!
  We'll study one example (MLR) in more detail . . .



(b) 1-vs-All



(a) 1-vs-1

Outline

- Motivating Example: Diagnosing Breast Cancer
- Binary Classification
- Binary Logistic Regression
- Multiclass Classification
- Multinomial Logistic Regression
- Measuring Accuracy in Classification

Multinomial logistic regression

Suppose we combine multiple binary classifiers using the "1-vs-all confidence-value" approach (p. 25). With binary *linear* classifiers, we would do:

- For each class $k = 1, \ldots, K$,
  - design b_k and $\boldsymbol{w}_k = [w_{k1}, \ldots, w_{kd}]^\mathsf{T}$ to classify in-k or not-in-k
  - compute a linear score from $\boldsymbol{x}$, i.e., $z_k = b_k + \sum_{j=1}^{d} x_j w_{kj}$

  then choose the winner via: $\widehat{y} = \arg\max_k \underbrace{\Pr\{y=k \,|\, \boldsymbol{z}\}}_{\text{confidence value}}$

- In multinomial logistic regression, we adopt the "softmax" likelihood function:

$$\Pr\{y=k \,|\, \boldsymbol{z}\} = \frac{e^{z_k}}{\sum_{l=1}^{K} e^{z_l}} \quad \text{(noting that } \sum_{k=1}^{K} \Pr\{y=k \,|\, \boldsymbol{z}\} = 1 \;\forall \boldsymbol{z})$$

- The softmax has the property that, if $z_{k_{\max}} \gg z_k$ for all $k \neq k_{\max}$, then

$$\frac{e^{z_k}}{\sum_{l=1}^{K} e^{z_l}} \approx \begin{cases} 1 & \text{if } k = k_{\max} \\ 0 & \text{if } k \neq k_{\max} \end{cases}$$

so it's a "soft" version of "$\delta_{k-k_{\max}}$"

One-hot label-coding for MLR

- We design $\boldsymbol{b} = [b_1, \ldots, b_K]^{\mathsf{T}}$ & $\boldsymbol{W} \triangleq [\boldsymbol{w}_1, \ldots, \boldsymbol{w}_K]$ using ML estimation, i.e.,

$$(\boldsymbol{b}_{\text{ml}}, \boldsymbol{W}_{\text{ml}}) \triangleq \arg\max_{\boldsymbol{b},\boldsymbol{W}} p(\boldsymbol{y}|\boldsymbol{X}; \boldsymbol{b}, \boldsymbol{W}) = \arg\min_{\boldsymbol{b},\boldsymbol{W}} \left\{ -\sum_{i=1}^{n} \ln p(y_i|\boldsymbol{x}_i; \boldsymbol{b}, \boldsymbol{W}) \right\}$$

- Suppose we turn the categorical label $y_i \in \{1, \ldots, K\}$ into a binary vector $\boldsymbol{y}_i \triangleq [y_{i1}, \ldots, y_{iK}]^{\mathsf{T}}$ using one-hot-coding, i.e.,

$$y_{ik} = \begin{cases} 1 & \text{if } y_i = k \\ 0 & \text{if } y_i \neq k \end{cases} \quad \text{for all } i = 1, \ldots, n$$

- Then, similar to the binary $y_i \in \{0, 1\}$ case, we can write

$$\begin{aligned} -\ln p(y_i|\boldsymbol{x}_i; \boldsymbol{b}, \boldsymbol{W}) &= -\textstyle\sum_{k=1}^{K} y_{ik} \ln \Pr\{y_i = k \,|\, \boldsymbol{x}_i; \boldsymbol{b}, \boldsymbol{W}\} \\ &= -\textstyle\sum_{k=1}^{K} y_{ik} \ln \frac{e^{z_{ik}}}{\sum_l e^{z_{il}}} \quad \text{with } z_{ik} = b_k + \boldsymbol{x}_i^{\mathsf{T}} \boldsymbol{w}_k \\ &= -\textstyle\sum_{k=1}^{K} y_{ik} \big(z_{ik} - \ln \big[\sum_{l=1}^{K} e^{z_{il}} \big] \big) \\ &= \ln \big[\textstyle\sum_{l=1}^{K} e^{z_{il}} \big] - \sum_{k=1}^{K} y_{ik} z_{ik}, \quad \text{since } \sum_{k=1}^{K} y_{ik} = 1 \ \forall i \end{aligned}$$

Multinomial cross-entropy loss

- Combining the results from the previous page, we get

$$(\boldsymbol{b}_{\text{ml}}, \boldsymbol{W}_{\text{ml}}) = \arg\min_{\boldsymbol{b},\boldsymbol{W}} \underbrace{\left\{ \sum_{i=1}^{n} \left(\ln \left[\sum_{k=1}^{K} e^{z_{ik}} \right] - \sum_{k=1}^{K} y_{ik} z_{ik} \right) \right\}}_{\triangleq J_{\text{lr}}(\boldsymbol{b}, \boldsymbol{W})}, \quad z_{ik} = b_k + \boldsymbol{x}_i^{\mathsf{T}} \boldsymbol{w}_k$$

  where $J_{\text{lr}}(\boldsymbol{W})$ is known as the cross-entropy loss

- Could also add $\alpha \|\boldsymbol{W}\|_F^2$ (L2 regularization) or $\alpha \|\boldsymbol{W}\|_1$ (L1 regularization), and tune α via cross-validation

- With or without regularization, there is no closed-form expression for optimal $(\boldsymbol{b}, \boldsymbol{W})$, but the optimization problems are convex and can be solved numerically

- For this, sklearn provides an excellent LogisticRegression implementation

Outline

- Motivating Example: Diagnosing Breast Cancer
- Binary Classification
- Binary Logistic Regression
- Multiclass Classification
- Multinomial Logistic Regression
- Measuring Accuracy in Classification

Performance metrics for binary classification

- In binary classification, there are 2 types of error:
  - False Positive (or false alarm)
  - False Negative (or missed detection)

contingency table or confusion matrix

	$y=1$	$y=0$
$\widehat{y}=1$	TP	FP
$\widehat{y}=0$	FN	TN

- The implications of these errors can be very different!
  - e.g., consider breast cancer diagnosis

- Common machine-learning performance metrics:
  - precision: $\Pr\{y=1 \,|\, \widehat{y}=1\} = \frac{\mathsf{TP}}{\mathsf{TP}+\mathsf{FP}}$ — given a positive test, how often is the patient cancerous?
  - recall: $\Pr\{\widehat{y}=1 \,|\, y=1\} = \frac{\mathsf{TP}}{\mathsf{TP}+\mathsf{FN}}$ — given that the patient has cancer, how often is it detected?
  - F1-score: $\left[\frac{1}{2}\left(\frac{1}{\mathsf{precision}} + \frac{1}{\mathsf{recall}}\right)\right]^{-1}$ — harmonic mean of precision & recall
  - accuracy: $\Pr\{\widehat{y}=y\} = \frac{\mathsf{TP}+\mathsf{TN}}{\mathsf{TP}+\mathsf{FN}+\mathsf{TN}+\mathsf{FP}}$ — how often is the test correct?

- Common metrics in medicine:
  - sensitivity: $\Pr\{\widehat{y}=1 \,|\, y=1\} = \frac{\mathsf{TP}}{\mathsf{TP}+\mathsf{FN}}$ — given that the patient has cancer, how often is it detected?
  - specificity: $\Pr\{\widehat{y}=0 \,|\, y=0\} = \frac{\mathsf{TN}}{\mathsf{TN}+\mathsf{FP}}$ — given a healthy patient, how often is diagnosis correct?

https://en.wikipedia.org/wiki/Evaluation_of_binary_classifiers

Breast cancer demo

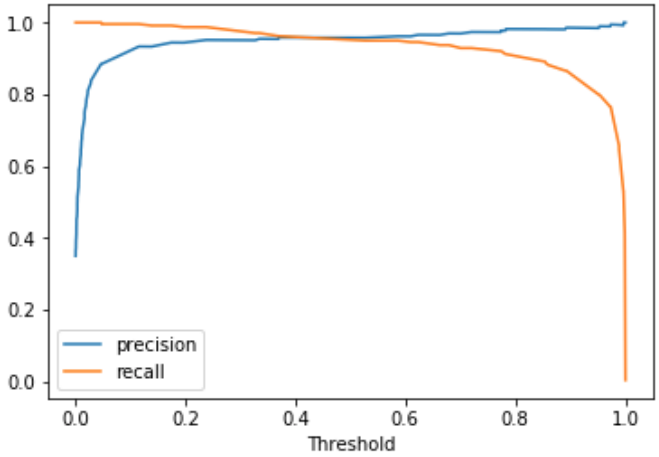
- We now assess classification performance on the breast cancer demo
- Use 10-fold cross-validation
- sklearn includes support for computing precision, recall, F1 score, and accuracy (as defined on previous page)

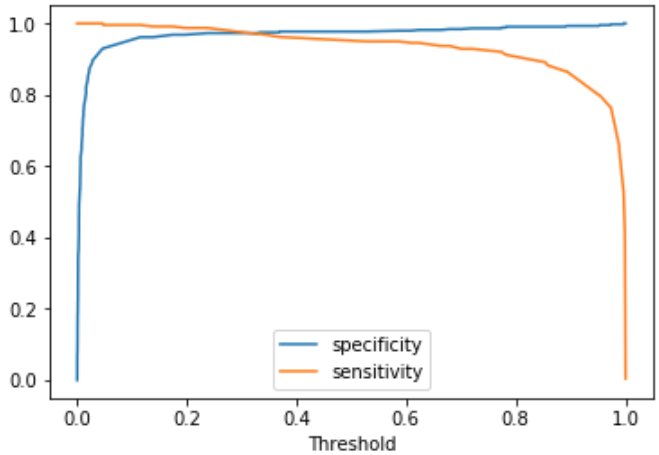
```
from sklearn.model_selection import KFold
from sklearn.metrics import precision_recall_fscore_support

nfold = 10
kf = KFold(n_splits=nfold,shuffle=True)
prec = []
rec = []
f1 = []
acc = []
for train, test in kf.split(Xs):
    # Get training and test data
    Xtr = Xs[train,:]
    ytr = y[train]
    Xts = Xs[test,:]
    yts = y[test]

    # Fit a model
    logreg.fit(Xtr, ytr)
    yhat = logreg.predict(Xts)

    # Measure performance
    preci,reci,f1i,_= precision_recall_fscore_support(yts,yhat,average='binary')
    prec.append(preci)
    rec.append(reci)
    f1.append(f1i)
    acci = np.mean(yhat == yts)
    acc.append(acci)

# Take average values of the metrics
precm = np.mean(prec)
recm = np.mean(rec)
f1m = np.mean(f1)
accm= np.mean(acc)

# Compute the standard errors
prec_se = np.std(prec)/np.sqrt(nfold-1)
rec_se = np.std(rec)/np.sqrt(nfold-1)
f1_se = np.std(f1)/np.sqrt(nfold-1)
acc_se = np.std(acc)/np.sqrt(nfold-1)
```

```
Precision = 0.9554, SE=0.0095
Recall =    0.9513, SE=0.0095
f1 =        0.9527, SE=0.0051
Accuracy =  0.9678, SE=0.0037
```

Making hard decisions

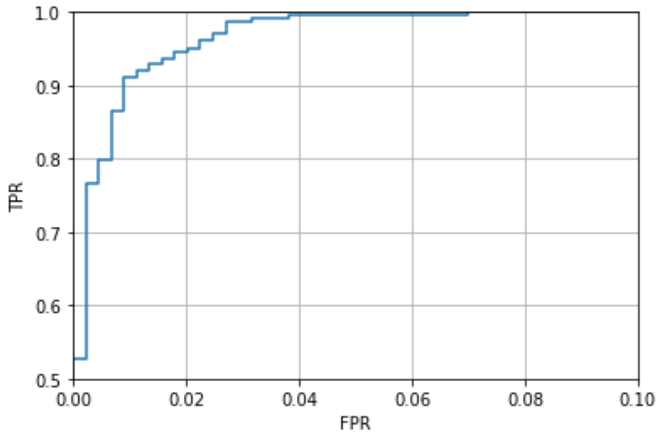
- Logistic regression outputs a confidence value, $\Pr\{y=1 \,|\, \boldsymbol{x}\} \in [0,1]$
- Can convert to a hard decision by thresholding:
  - Set $\widehat{y}=1$ when $\Pr\{y=1 \,|\, \boldsymbol{x}\} > t$ for threshold t
- $t = 1/2$ minimizes the error rate, $\Pr\{\widehat{y} \neq y\}$
  - i.e., maximizes accuracy
- $t \in [0,1]$ trades precision for recall
  - precision: $\Pr\{y=1 \,|\, \widehat{y}=1\}$
  - recall: $\Pr\{\widehat{y}=1 \,|\, y=1\}$
- $t \in [0,1]$ trades sensitivity for specificity
  - sensitivity: $\Pr\{\widehat{y}=1 \,|\, y=1\}$
  - specificity: $\Pr\{\widehat{y}=0 \,|\, y=0\}$

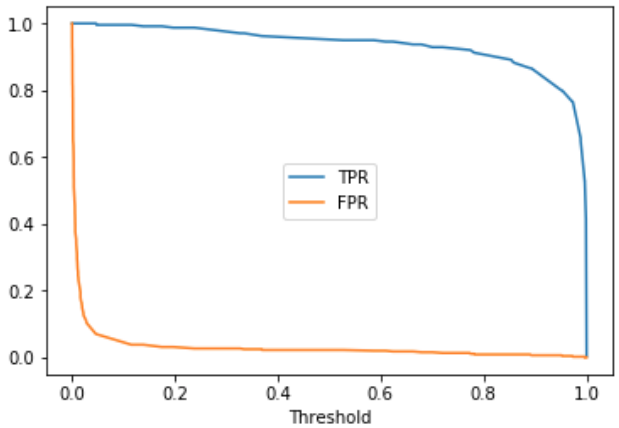




The ROC curve and the AUC

- The receiver operating characteristic (ROC) is the plot of TPR versus FPR
  - FPR: $\Pr\{\widehat{y}=1 \,|\, y=0\}$
  - TPR: $\Pr\{\widehat{y}=1 \,|\, y=1\}$
- The threshold t controls location on curve
- The area under the curve (AUC) is a threshold-independent performance metric






```
from sklearn import metrics
yprob = logreg.predict_proba(Xs)
fpr, tpr, thresholds = metrics.roc_curve(y,yprob[:,1])
```

```
auc=metrics.roc_auc_score(y,yprob[:,1])
print("AUC=%f" % auc)
```

```
AUC=0.996344
```

Performance metrics for multiclass classification

- In multiclass classification, there are many possible error types
- If columns of confusion matrix are normalized to sum-to-one . . .
  - (k,l)th entry becomes $\Pr\{\widehat{y}=k \,|\, y=l\}$
  - diagonal terms show per-class accuracy, $\Pr\{\widehat{y}=k \,|\, y=k\}$

contingency table or confusion matrix

	$y=1$	$y=2$	$\cdots$	$y=K$
$\widehat{y}=1$	10	3	$\cdots$	4
$\widehat{y}=2$	1	14	$\cdots$	3
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$\widehat{y}=K$	4	2	$\cdots$	7

- The overall accuracy can be computed as

$$\Pr\{\widehat{y}=y\} = \sum_{k=1}^{K} \Pr\{\widehat{y}=k \,|\, y=k\} \Pr\{y=k\}$$

Learning objectives

- Understand classification problems in machine learning:
  - Identify features, labels; binary vs multiclass; linear vs nonlinear
  - visualize scatterplots and decision regions
- For binary classification problems, understand ...
  - linear classifiers, separating hyperplanes, margin
  - why linear regression doesn't work
  - logistic regression: logistic function, cross-entropy loss, ML fitting, regularization
  - feature transformations
  - common error metrics: accuracy, precision, recall, F1
  - the effect of the decision threshold, ROC, AUC
- For multiclass classification problems, understand ...
  - solutions that use multiple binary classifiers
  - multinomial logistic regression: softmax function, cross-entropy, ML fitting
- How to implement and assess classification using sklearn