Computer Science

CSC380: Principles of Data Science

Basic machine learning 2

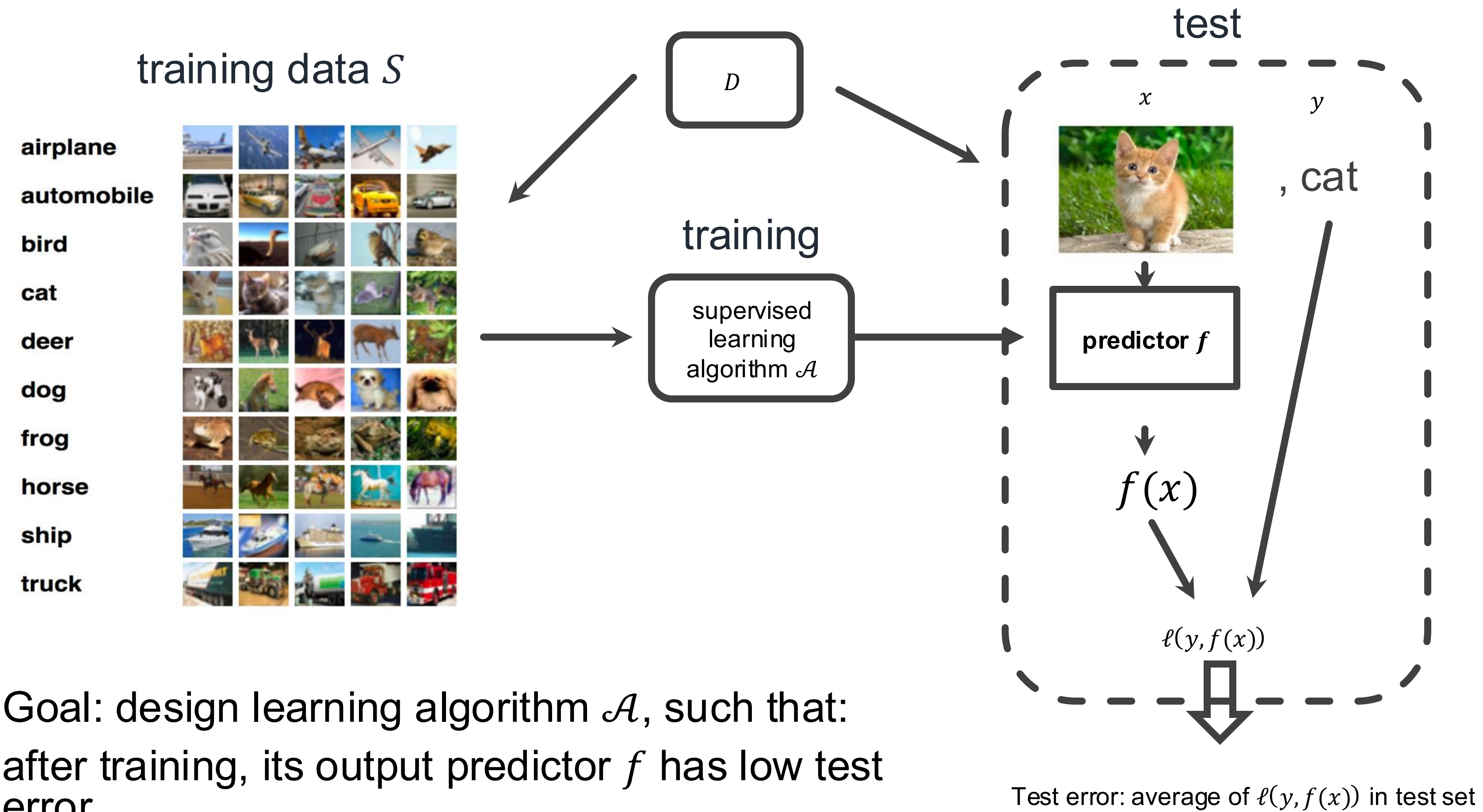
Xinchen Yu

Outline

- Classification basics
- Nearest neighbor Classification
- Logistic regression
- Classification: other considerations
  - Binary classification beyond accuracy
  - Multiclass classification

Classification recap

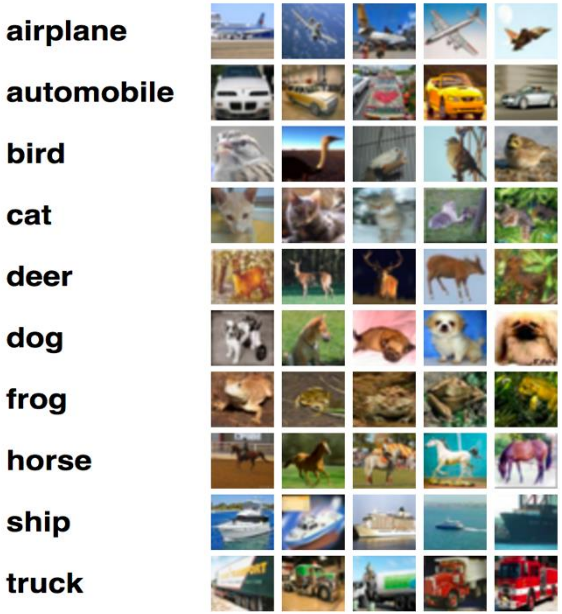
Supervised learning setup in one figure



- Goal: design learning algorithm $\mathcal{A}$, such that:
- after training, its output predictor f has low test error

Classification

- The labels are categorical
- Loss function ℓ: measures the quality of prediction $\hat{y}$ respect to true label y
  - $\ell(y, \hat{y}) = I(y \neq \hat{y})$
  - I: indicator of predicate; 1 if true; 0 if false
- A classifier f's error on a dataset S is the fraction of examples in S that it predicts incorrectly.
  - f's training / test error is its error on training / test set
  - Accuracy = 1 – error



In-class activity: finding test error

A company develops a simple **spam classifier** f that predicts whether an email is **spam (1)** or **not spam (0)** based on the number of capital letters in the subject line.

f outputs **Spam** if the number of capital letters ≥ 5, and **Not Spam** otherwise.

Suppose the test dataset is as follows. Find f's test error.

Subject	True label	Predicted label
"WIN A FREE VACATION NOW!!!"	1	1
Meeting rescheduled to 3 PM	0	0
"HUGE DISCOUNT ON ALL ITEMS!!!"	1	1
URGENT: Please submit your report	0	1
Can you review this document?	0	0

f's test error = 1/5 = 20%

Nearest Neighbor Classification

Example: Course Recommendation

Rating	Easy?	AI?	Sys?	Thy?	Morning?
+2	y	y	n	y	n
+2	y	y	n	y	n
+2	n	y	n	n	n
+2	n	n	n	y	n
+2	n	y	y	n	y
+1	y	y	n	n	n
+1	y	y	n	y	n
+1	n	y	n	y	n
0	n	n	n	n	y
0	y	n	n	y	y
0	n	y	n	y	n
0	y	y	y	y	y
-1	y	y	y	n	y
-1	n	n	y	y	n
-1	n	n	y	n	y
-1	y	n	y	n	y
-2	n	n	y	y	n
-2	n	y	y	n	y
-2	y	n	y	n	n
-2	y	n	y	n	y

Label: "like"

Label: "dislike"

Features

Suppose we'd like to build a recommendation system for classes

We've collected information about many past classes

We can frame this as a classification problem:

Predict like/dislike from class features

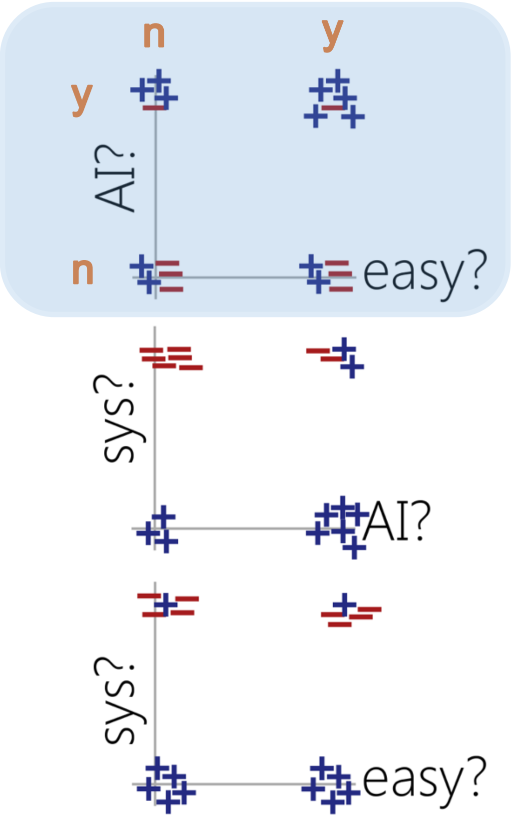
Example: Course Recommendation

Label: +

Label: -

Rating	Easy?	AI?	Sys?	Thy?	Morning?
+2	y	y	n	y	n
+2	y	y	n	y	n
+2	n	y	n	n	n
+2	n	n	n	y	n
+2	n	y	y	n	y
+1	y	y	n	n	n
+1	y	y	n	y	n
+1	n	y	n	y	n
0	n	n	n	n	y
0	y	n	n	y	y
0	n	y	n	y	n
0	y	y	y	y	y
-1	y	y	y	n	y
-1	n	n	y	y	n
-1	n	n	y	n	y
-1	y	n	y	n	y
-2	n	n	y	y	n
-2	n	y	y	n	y
-2	y	n	y	n	n
-2	y	n	y	n	y

Features



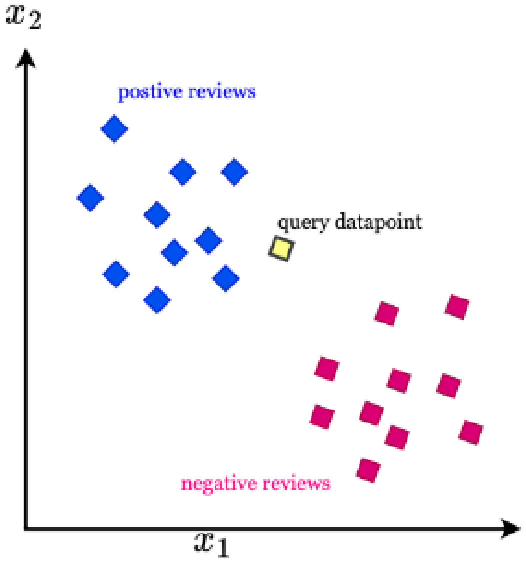
Each course's feature is Represented as points in 5-dimensional space

That's too many dimensions to plot…so we look at 2D projections…

Observation: examples with same labels tend to be closer!

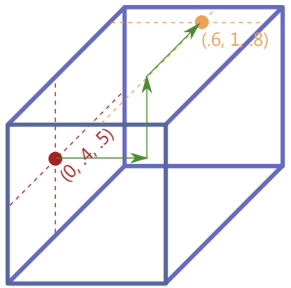
Nearest neighbor classification

- Given a new course, would like to predict its label (+/-)
- Idea: Find its most similar course in the training set, and use that course's label to predict



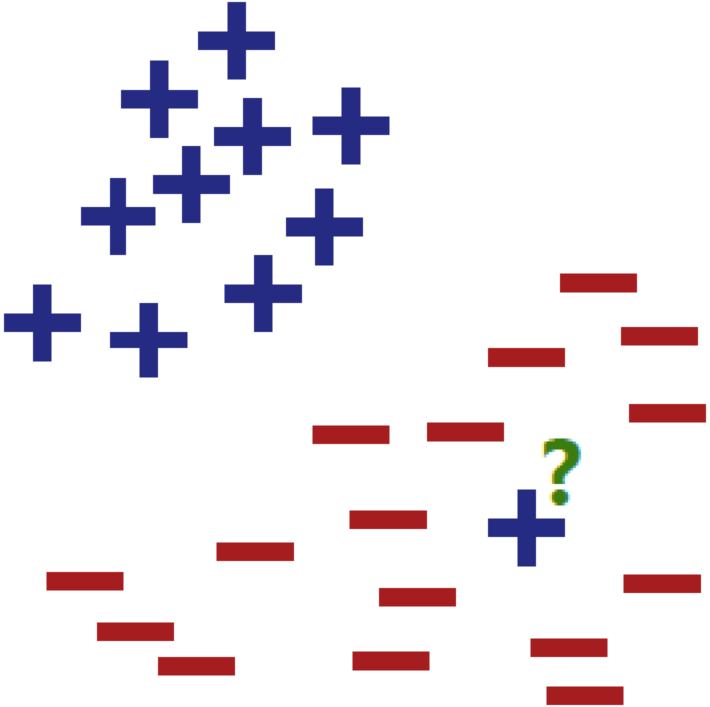
Measuring nearest neighbors

- Oftentimes convenient to work with feature $x \in \mathrm{R}^d$
- Distances in R^d: notation $x(f)$: $x = (x(1), \dots, x(d))$
  - (popular) Euclidean distance $d_2(x, x') = \sqrt{\sum_{f=1}^{d} \left(x(f) - x'(f)\right)^2}$
  - Manhattan distance $d_1(x, x') = \sum_{f=1}^{d} |x(f) - x'(f)|$



- How to extract features as **real values**?
  - Boolean features: {Y, N} -> {0,1}
  - Categorical features: {Red, Blue, Green, Black}
    - Convert to {1, 2, 3, 4}?
    - Better one-hot encoding: (1,0,0,0), .., (0,0,0,1) (IsRed?/isGreen?/isBlue?/IsBlack?)

Robustify Nearest Neighbor Classification



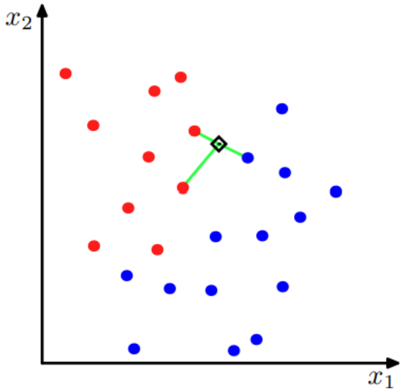
Q: Can we predict using 1 nearest neighbor's?

Query point ? Will be classified as + but should be -

Problem: predicting using 1 nearest neighbor's label can be sensitive to noisy data

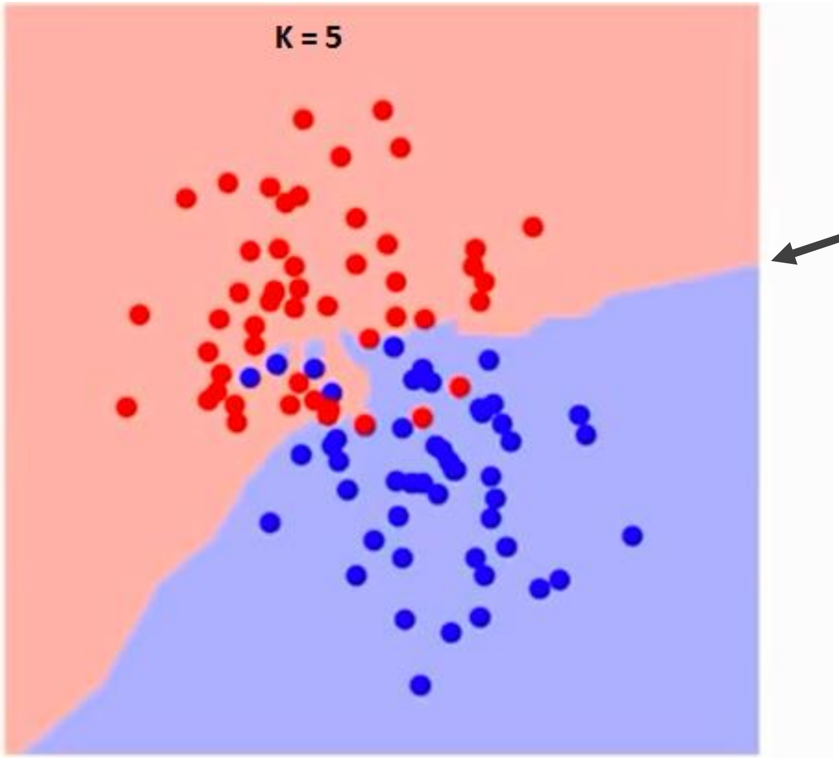
How to mitigate this?

k-nearest neighbors (k-NN): main concept



- Training set: $S = \{ (x_1, y_1), \ldots, (x_m, y_m) \}$
- **Key insight**: given test example x, its label should resemble the labels of *nearby points*
- Function
  - input: x
  - find the k nearest points to x from S; call their indices $N(x)$
  - output:
    - (classification) the majority vote of $\{y_i : i \in N(x)\}$
    - (regression) the average of $\{y_i : i \in N(x)\}$

k-NN classification example



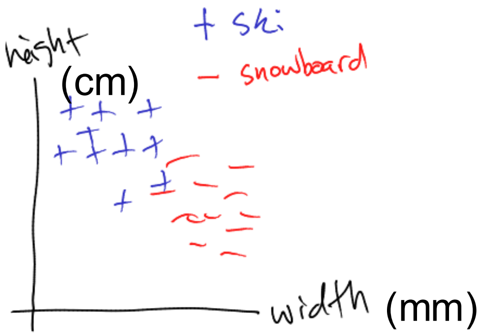
decision boundary

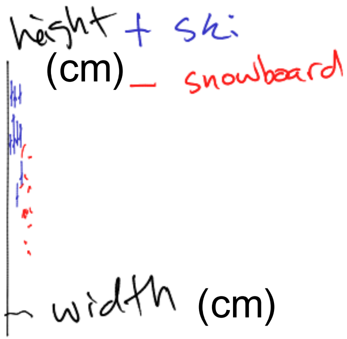
Issue 1: scaling

- Features having different scales can be problematic.

- Ex: ski vs. snowboard classification

$$d = \sqrt{(height_1 - height_2)^2 + (weight_1 - weight_2)^2}$$





- One solution: feature standardization

Make sure features are scaled fairly

- Features having different scale can be problematic
- [Definition] **Standardization**
  - For each feature f, compute $\mu_f = \frac{1}{m}\sum_{i=1}^{m} x_f^{(i)}$, $\sigma_f = \sqrt{\frac{1}{m}\sum_{i=1}^{m}\left(x_f^{(i)} - \mu_f\right)^2}$
  - Then, transform the data by $\forall f \in \{1,\ldots,d\}, \forall i \in \{1,\ldots,m\}$, $x_f^{(i)} \leftarrow \frac{x_f^{(i)} - \mu_f}{\sigma_f}$

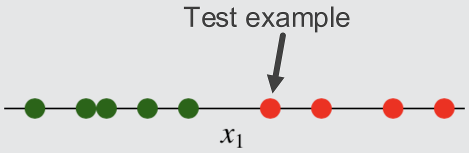
after transformation, each feature has mean 0 and variance 1

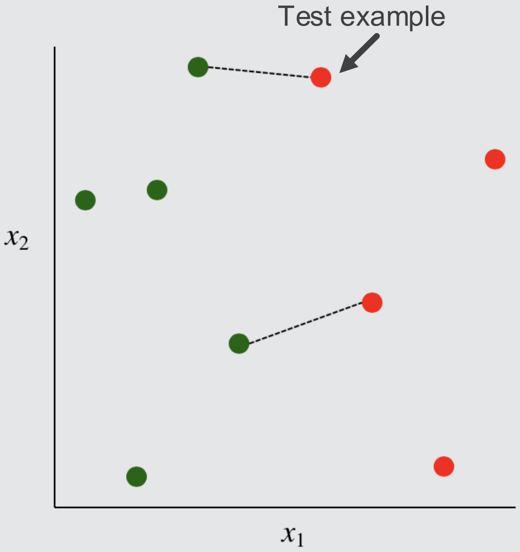
- Be sure to keep the “standardize” function and apply it to the test points.
  - Save $\{(\mu_f, \sigma_f)\}_{f=1}^{d}$
  - For test point x^*, apply $x_f^* \leftarrow \frac{x_f^* - \mu_f}{\sigma_f}, \forall f$

Issue 2: irrelevant features

here's a case in which there is one relevant feature x_1 and a 1-NN rule classifies each instance correctly

consider the effect of an irrelevant feature x_2 on distances and nearest neighbors



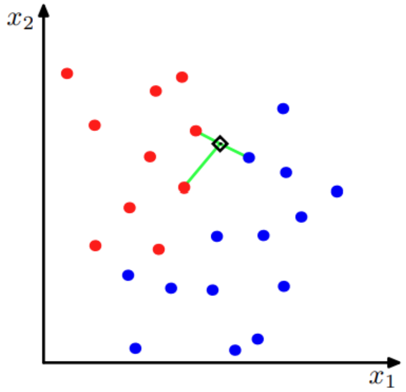


- Mitigation: feature selection

Issue 3: choosing k

- Q: How would a k-NN classifier predict when k=training set size?
  - Predict majority label everywhere
  - Underfitting

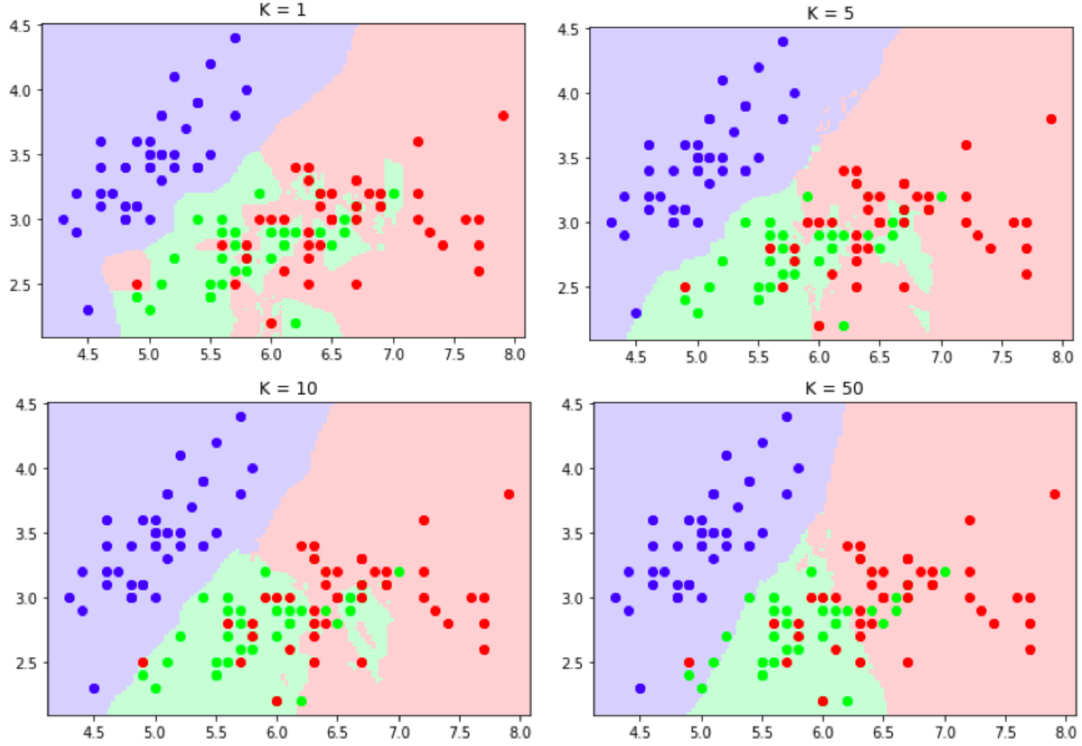
- Q: What is the training error of a 1-NN classifier?
  - 0
  - Overfitting



Issue 3: choosing k

k can be viewed as a model complexity measure

Smaller k results in a more complex model

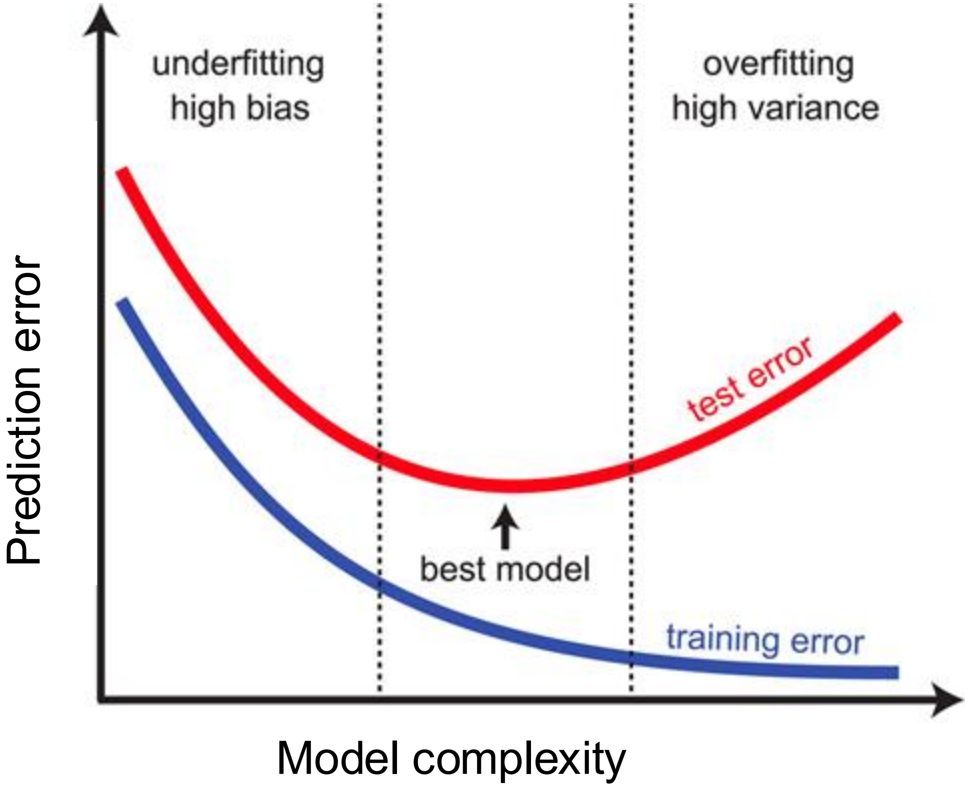


Issue 3: choosing k

We'd like to choose appropriate k to balance model bias and complexity

We can choose k in the same way we chose λ in ridge regression

- Cross validation



Scikit-learn nearest neighbors

class **sklearn.neighbors.NearestNeighbors**(**, **n_neighbors**=5, **radius**=1.0, **algorithm**='auto', **leaf_size**=30, **metric**='minkowski', **p**=2, **metric_params**=None, **n_jobs**=None*) [source]

Unsupervised learner for implementing neighbor searches.

```
# 1. Load the Iris dataset
iris = load_iris()
X = iris.data  # Features
y = iris.target  # Target labels (species)

# 2. Split the dataset into training and testing sets (80% train, 20% test)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)

# 3. Create the KNN classifier model
knn = KNeighborsClassifier(n_neighbors=3)  # Use 3 nearest neighbors

# 4. Train the model on the training data
knn.fit(X_train, y_train)
```

Scikit-learn nearest neighbors

```
# 5. Make predictions on the test set
y_pred = knn.predict(X_test)

# 6. Evaluate the model using accuracy
accuracy = accuracy_score(y_test, y_pred)
print(f'Accuracy of the KNN model: {accuracy * 100:.2f}%')

# Optionally, display the predictions vs. actual values
print(f'Predictions: {y_pred}')
print(f'Actual: {y_test}')
```

```
Accuracy of the KNN model: 100.00%
Predictions: [1 0 2 1 1 0 1 2 1 1 2 0 0 0 0 1 2 1 1 2 0 2 0 2 2 2 2 2 0 0]
Actual: [1 0 2 1 1 0 1 2 1 1 2 0 0 0 0 1 2 1 1 2 0 2 0 2 2 2 2 2 0 0]
```

Logistic regression

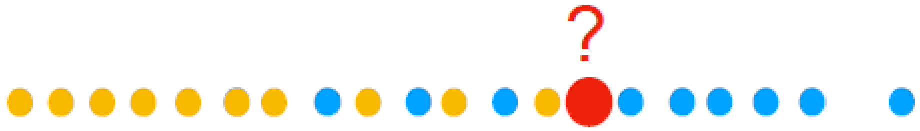
Classification with logistic regression

Training data: number of hours studied for the course.

Labels: Pass (1) or Fail (0)

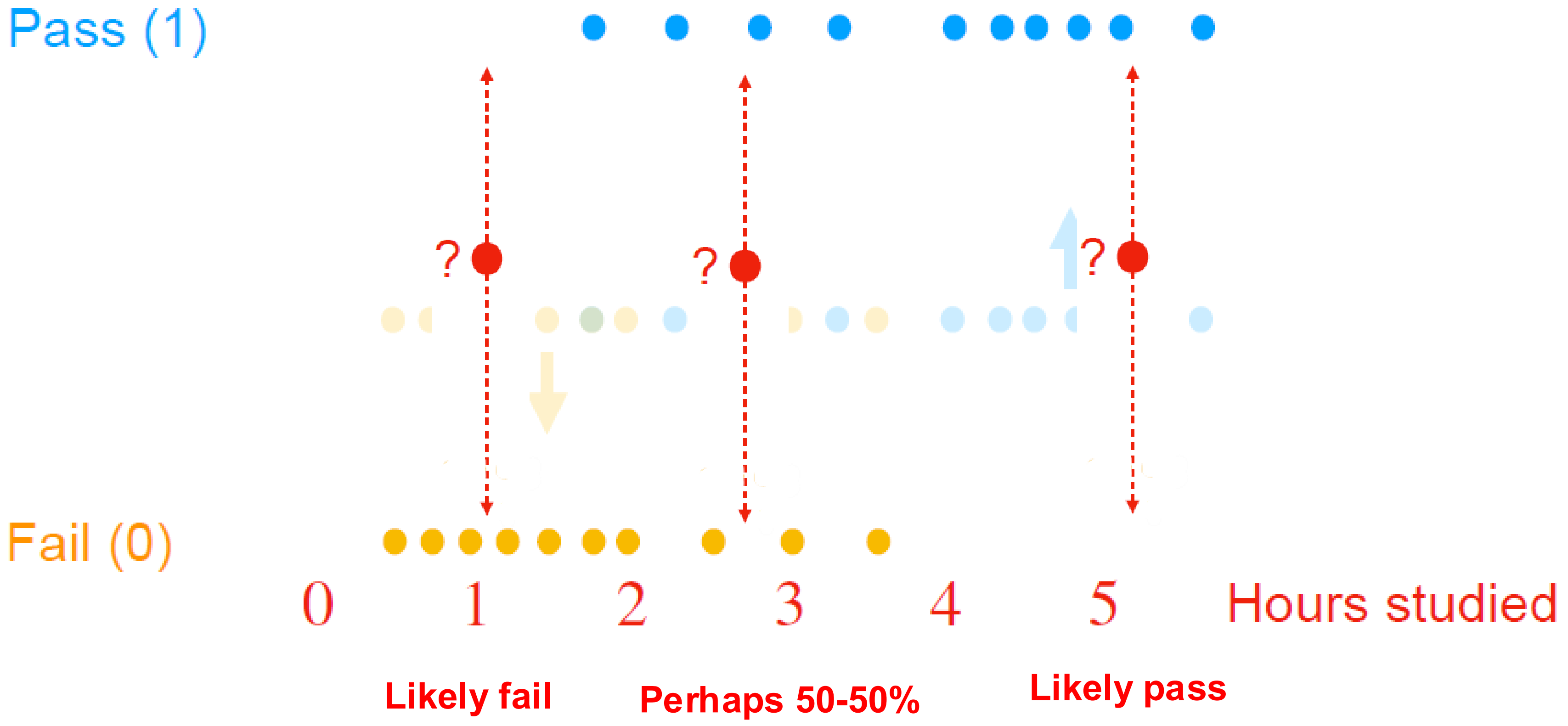
Classification with logistic regression

- Can we train a model so that given a new data point, we can predict whether that student passes or fails?



- Nearest neighbor: a geometric approach for this problem
- We will now approach this using an alternative probabilistic view

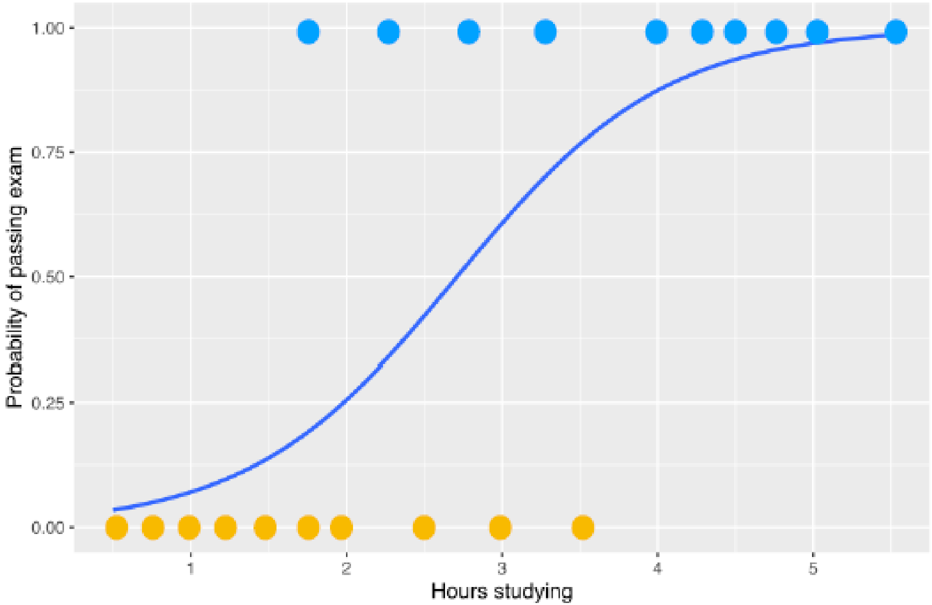
Classification with logistic regression



Classification with logistic regression

$Y = 1$

$Y = 0$

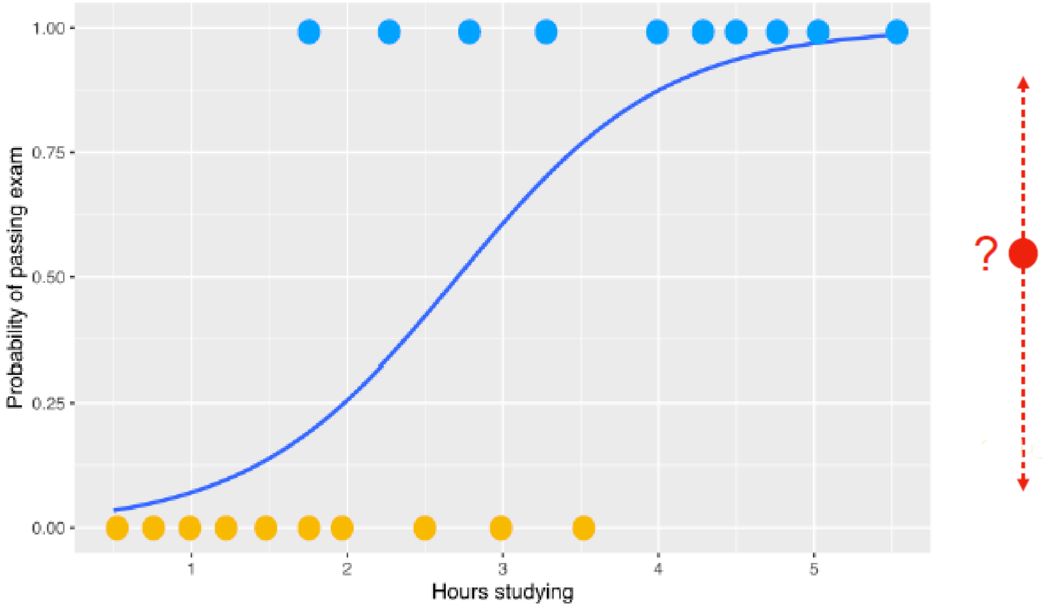


X: feature

Y: label

$$P(Y = 1 \mid X = x)$$

Classification with logistic regression



Blue curve plots:

$P(Y = 1 \mid X = x)$

We can predict the class of test point using blue curve:

If prob < 0.5

predict fail

Else

predict pass

What is a reasonable form of $P(Y = 1 \mid X = x)$?

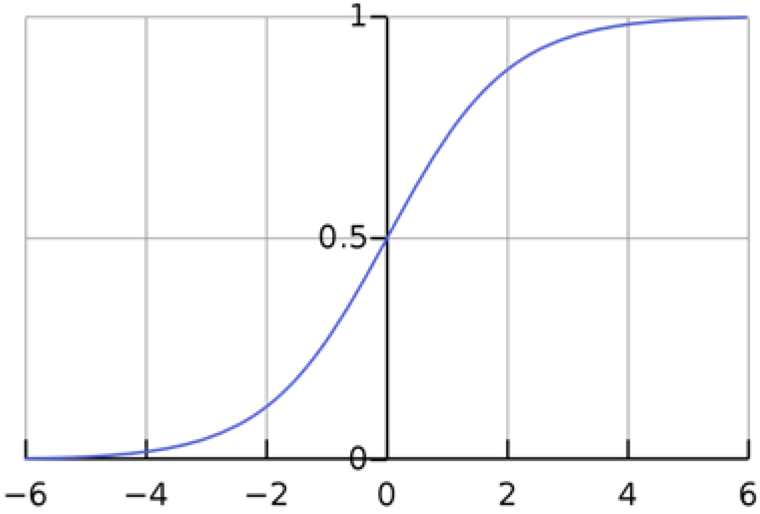
Classification with logistic regression

We will assume that:

$$P(Y = 1 \mid X = x) = \sigma(w \cdot x + b) = \frac{1}{1 + e^{-(w \cdot x + b)}}$$

i.e., $\sigma(w \cdot x + b)$, for some w, b

For d-dim x, this is dot product



$\sigma(z) := \frac{1}{1+e^{-z}}$ is the *logistic function*

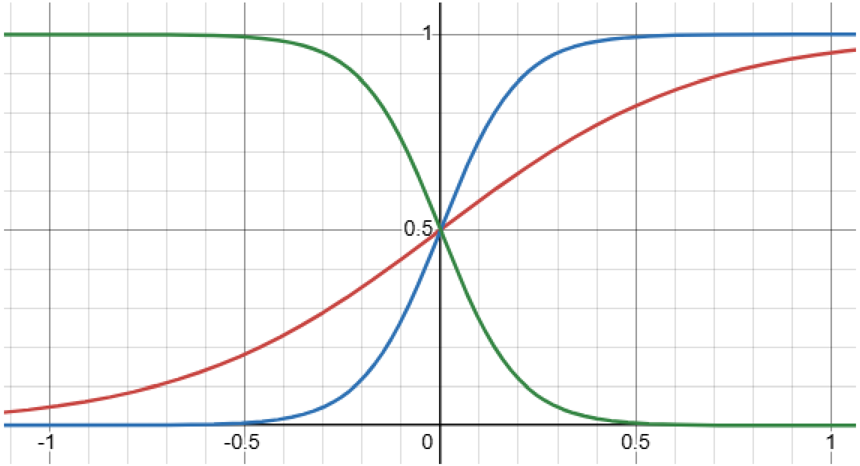
Logistic regression model

w controls the shape of the probability curve

$$p = \frac{1}{1 + e^{-10\,x}}$$

$$p = \frac{1}{1 + e^{-3\,x}}$$

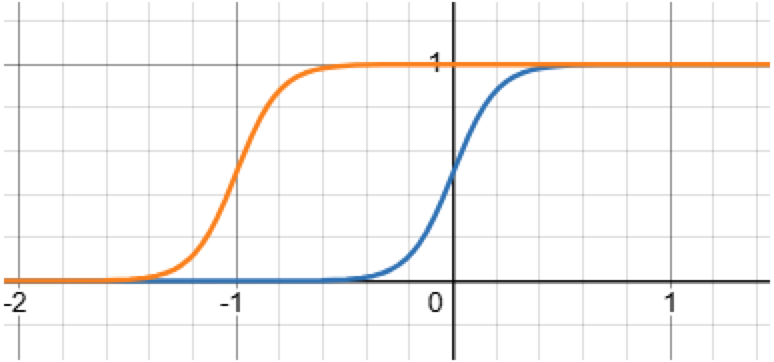
$$p = \frac{1}{1 + e^{10\,x}}$$



b controls the location of the probability curve

$$p = \frac{1}{1 + e^{-10\,x}}$$

$$p = \frac{1}{1 + e^{-10\,(x+1)}}$$



Classification with logistic regression

Example Suppose we fit logistic regression model with b = 0.15 and w = 0.575. What is the model's predicted probability that a student who have studied for x = 2 hours passes?

$P(Y = 1 \mid X = x) = \frac{1}{1+e^{-z}}$, where $z = w \cdot x + b = 1$

Thus, the predicted pass prob = $\frac{1}{1+e^{-1}} = 0.73$

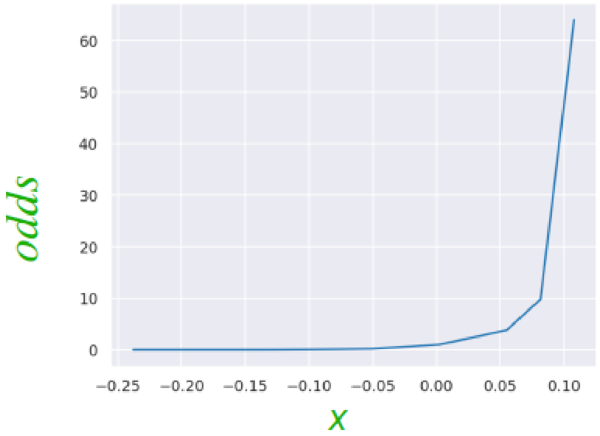
Classification with logistic regression

Where does the logistic function come from?

- Linear regression $w \cdot x + b$ is good at predicting unbounded outputs y
- Idea: transform p to a good unbounded function

$$\text{odd} = \frac{P(Y=1|x)}{P(Y=0|x)} = \frac{p}{1-p}$$

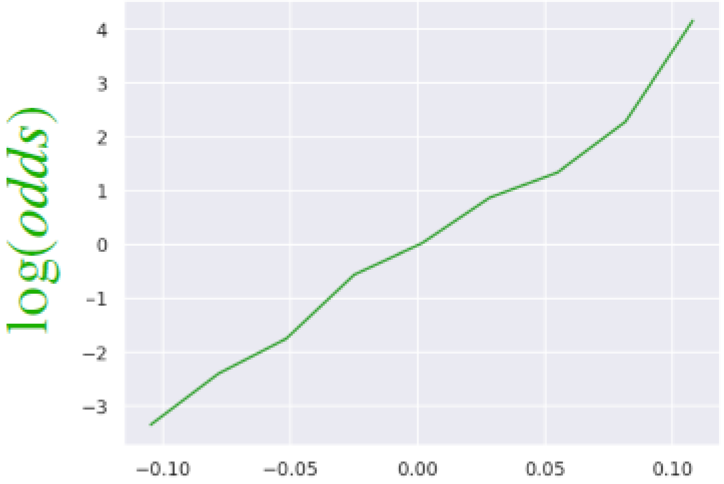
- Still not ideal: odd bounded from below



Classification with logistic regression

Where does the logistic function come from?

- Linear regression $w \cdot x + b$ is good at predicting unbounded outputs



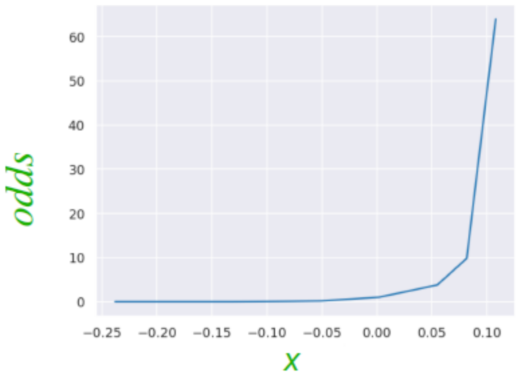
- $\log \text{odd} = \ln \frac{p}{1-p}$
- This now can take +/- values

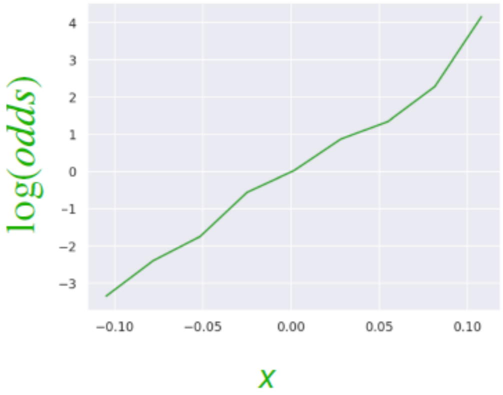
$$\ln \frac{p}{1-p} = w \cdot x + b \quad \Rightarrow \quad \frac{p}{1-p} = e^{w\,x+b} \quad \Rightarrow \quad p = \frac{1}{1 + e^{-(w \cdot x + b)}}$$

Where logistic function come from?

- $w \cdot x + b$ is unbounded
- We want to transform p into a form that produce unbounded outputs
  - $p \rightarrow \frac{p}{1-p} \rightarrow \ln \frac{p}{1-p}$

[0, 1] [0, +∞] [-∞, +∞]





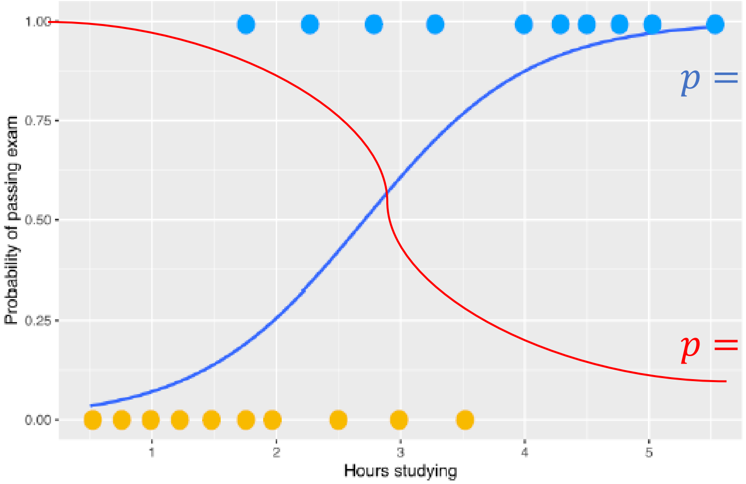
Fitting a logistic regression model

- Recall: loss for linear regression was MSE $\frac{1}{n}\sum_i (y_i - w \cdot x_i)^2$

- How about logistic regression?
  - y_i's are in 0, 1

$Y = 1$

$Y = 0$



$p = \sigma(w_1 \cdot x + b_1)$

$p = \sigma(w_2 \cdot x + b_2)$

Which logistic regression model fits data better, red or blue?

Fitting a logistic regression model

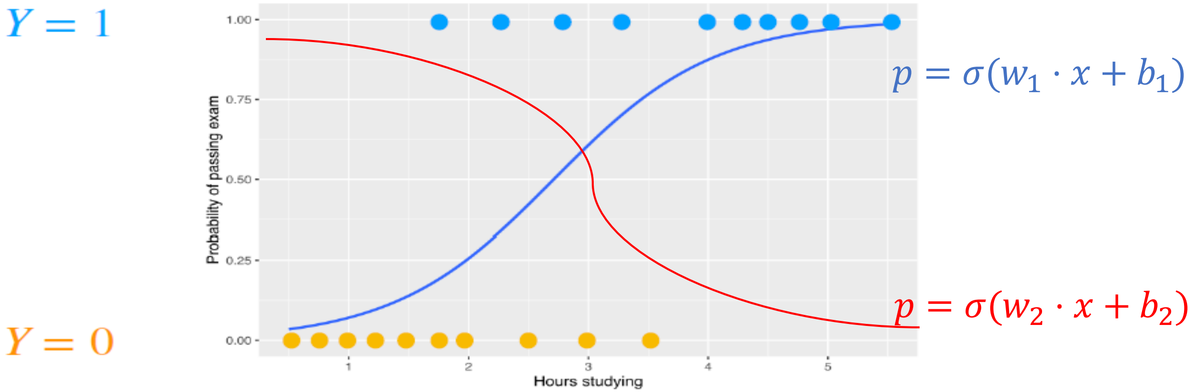
We'd like to choose w and b such that:

for x whose label is more likely to be 1

=> p is large

=> $w \cdot x + b$ is large

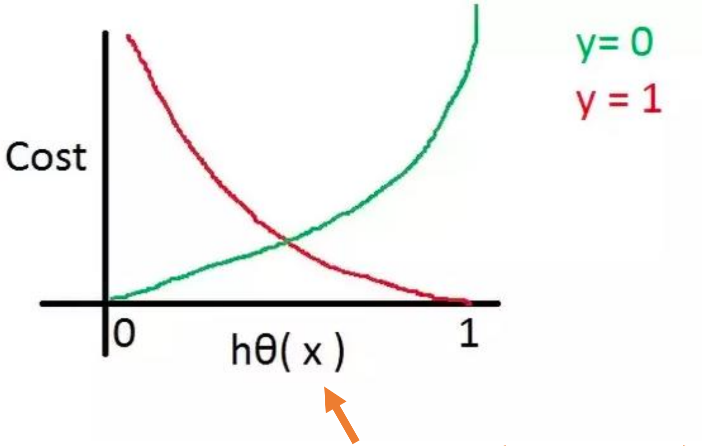
=> penalize more if p is small



Cross entropy loss

$$\ell(y,p) = y \ln\frac{1}{p} + (1-y)\ln\frac{1}{1-p}$$

$$= \begin{cases} \ln\frac{1}{p}, \ y = 1 \\ \ln\frac{1}{1-p}, y = 0 \end{cases}$$



$p_i = \sigma(w \cdot x_i + b)$

Minimizing CE loss incentivizes the model's predictive probability to align with labels

Fitting a logistic regression model

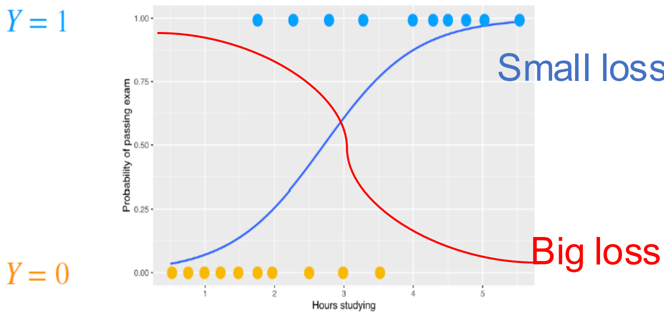
- We find w and b to minimize:

$$\sum_i \left(y_i \ln \frac{1}{p_i} + (1 - y_i) \ln \frac{1}{1-p_i} \right),$$

Logistic loss, aka Cross-entropy (CE) loss

where $p_i = P(Y = 1 \mid x_i) = \frac{1}{1+e^{-(w \cdot x_i + b)}}$

- What is the i-th example's loss when:
  - $y_i = 1$ and $p_i \approx 1$? ≈ 0
  - $y_i = 1$ and $p_i \approx 0$? Large
  - $y_i = 0$ and $p_i \approx 1$? Large
  - $y_i = 0$ and $p_i \approx 0$? ≈ 0



sklearn.linear_model.LogisticRegression

class sklearn.linear_model.LogisticRegression(*penalty='l2', *, dual=False, tol=0.0001, C=1.0, fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None, solver='lbfgs', max_iter=100, multi_class='auto', verbose=0, warm_start=False, n_jobs=None, l1_ratio=None*) [source]

penalty : *{'l1', 'l2', 'elasticnet', 'none'}, default='l2'*

Specify the norm of the penalty:

- `'none'`: no penalty is added;
- `'l2'`: add a L2 penalty term and it is the default choice;
- `'l1'`: add a L1 penalty term;
- `'elasticnet'`: both L1 and L2 penalty terms are added.

Similar to linear regression, add regularization to combat overfitting

$$\text{argmin}_w \text{ Logistic} - \text{Loss}(w) + \lambda|w|$$

tol : *float, default=1e-4*

Tolerance for stopping criteria.

C : *float, default=1.0*

$C = 1/\lambda$

Inverse of regularization strength; must be a positive float. Like in support vector machines, smaller values specify stronger regularization.

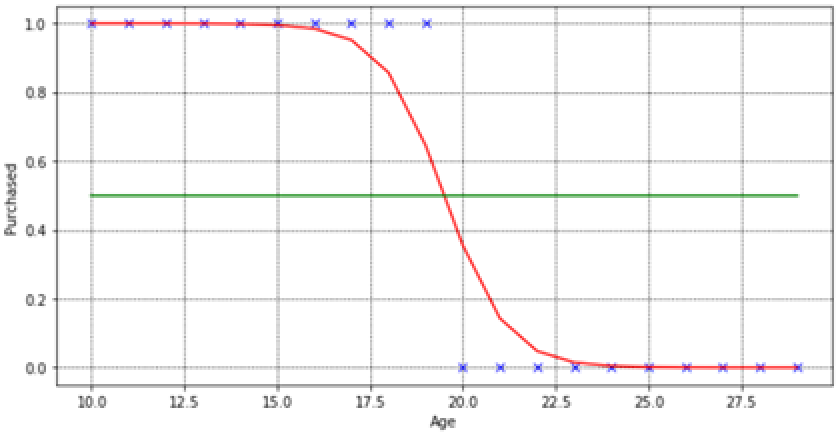
Scikit-Learn Logistic Regression

log_regression = sklearn.linear_model.LogisticRegression()

```
_ = log_regression.fit(pd.DataFrame(x), y)

y_pred = log_regression.predict_proba(pd.DataFrame(x))
log_y_pred_1 = [item[1] for item in y_pred]

fig = plt.figure(figsize=(10,5))
xlabel = 'Age'
ylabel = 'Purchased'
plt.xlabel(xlabel)
plt.ylabel(ylabel)
plt.grid(color='k', linestyle=':', linewidth=1)
plt.plot(x, y, 'xb')
plt.plot(x, log_y_pred_1, '-r')
_ = plt.plot(x, line_point_5,'-g')
```

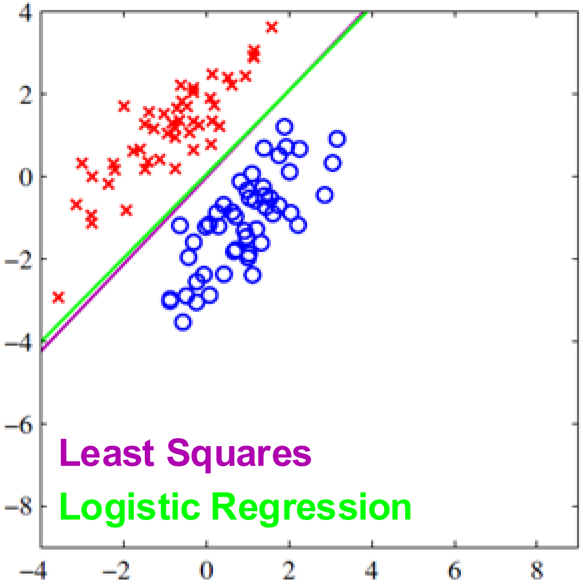


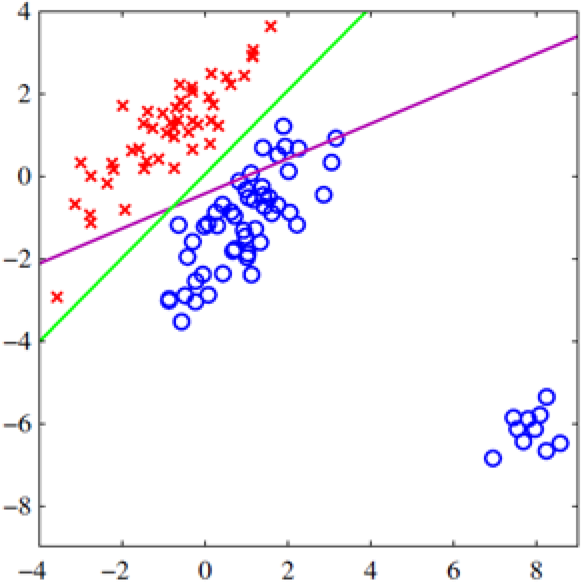
Function `predict_proba(X)` returns prediction of class assignment probabilities for each class. It returns n by C matrix if n data points were provided as argument.

(C=number classes)

https://towardsdatascience.com/why-linear-regression-is-not-suitable-for-binary-classification-c64457be8e28

Least Squares vs. Logistic Regression





Least squares regression may also be (ab)used for classification

- To predict a class, threshold $w \cdot x + b$ against 0.5
- Not designed for classification though -- sensitive to outliers

[Source: Bishop "PRML"]

Using Logistic Regression

Logistic Regression have two main usages

- building **predictive** classification models
- **understanding** how features relate to data classes / categories

Example South African Heart Disease (Hastie et al. 2001)
Data result from Coronary Risk-Factor Study in 3 rural areas of South Africa. Data are from white men 15-64yrs. Label is presence/absence of *myocardial infarction (MI).*

Example: African Heart Disease

	sbp	tobacco	ldl	famhist	obesity	alcohol	age	chd
0	160	12.00	5.73	1	25.30	97.20	52	1
1	144	0.01	4.41	0	28.87	2.06	63	1
2	118	0.08	3.48	1	29.14	3.81	46	0
3	170	7.50	6.41	1	31.99	24.26	58	1
4	134	13.60	3.50	1	25.99	57.34	49	1

Features

- Systolic blood pressure
- Tobacco use
- Low density lipoprotein (ldl)
- Family history (discrete)
- Obesity
- Alcohol use
- Age

Q: How predictive is each of the features to myocardial infarction?

Looking at Data

Each scatterplot shows pair of risk factors.

Cases **with** MI (**red**) and **without** (**cyan**)

Features

- Systolic blood pressure
- Tobacco use
- Low density lipoprotein (ldl)
- Family history (discrete)
- Obesity
- Alcohol use
- Age

[Source: Hastie et al. (2001)]

Example: African Heart Disease

	Coefficient	Std. Error	Z Score
(Intercept)	−4.130	0.964	−4.285
sbp	0.006	0.006	1.023
tobacco	0.080	0.026	3.034
ldl	0.185	0.057	3.219
famhist	0.939	0.225	4.178
obesity	-0.035	0.029	−1.187
alcohol	0.001	0.004	0.136
age	0.043	0.010	4.184

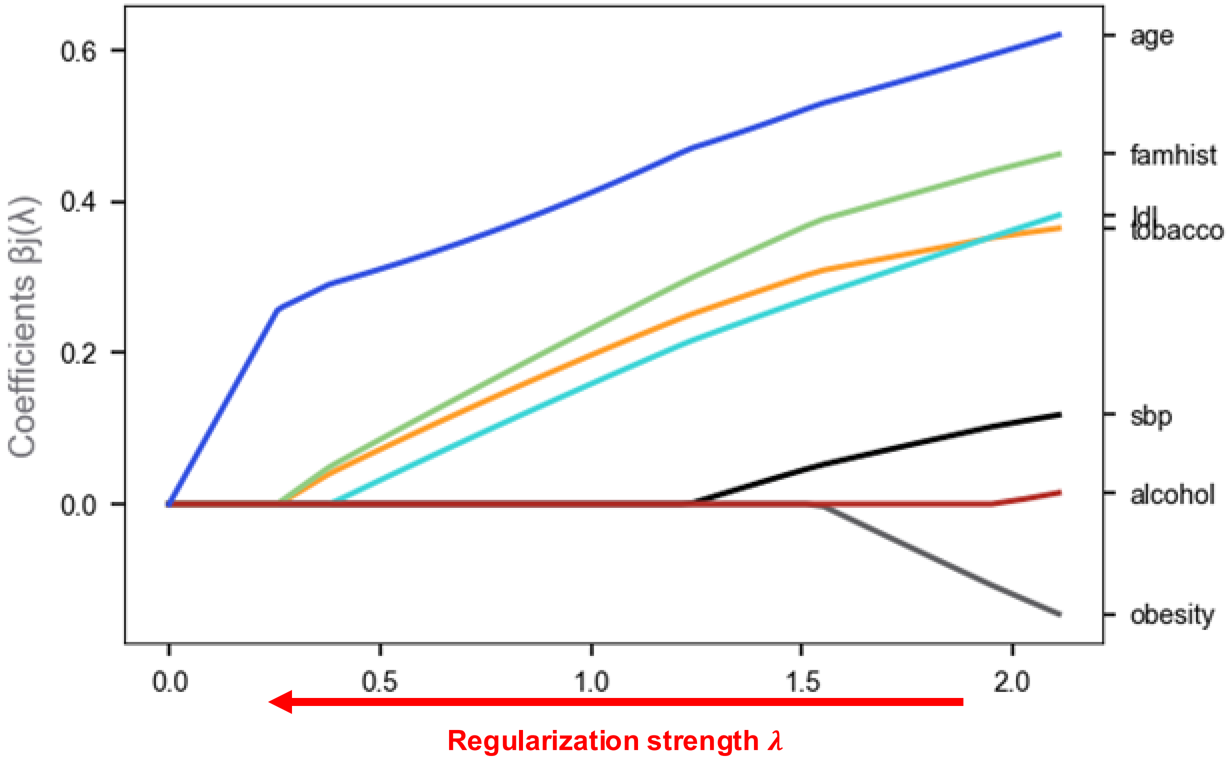
Z-score: score indicating the significance of each feature

|Z-score| > 2: feature is significant (we will learn more in *statistics*)

Finding Systolic blood pressure (sbp), obesity, and alcohol are **not significant predictors**

L1 regularized logistic regression coefficients

$$\text{argmin}_w \ \text{Logistic\_Loss}(w) + \lambda |w|_1$$



https://github.com/empathy87/The-Elements-of-Statistical-Learning-Python-Notebooks/blob/master/examples/South%20African%20Heart%20Disease.ipynb

Evaluation measures for classification

Pipeline for machine learning & data analysis

1. Choose a model	How should we represent the world?
2. Choose a loss function	How do we quantify prediction error?
3. Fit the model	How do we choose the best parameters of our model given our data?
4. Evaluate model performance	How do we evaluate whether this process gave rise to a good model?

Model evaluation: baseline models

Baseline models: simplest reasonable models to compare against

- Uniform classifier: predict with one label consistently (i.e., Most common label classifier, Least common label classifier)
- Blind classifier: predict random labels

	Features				Label	Most common Prediction	Least common Prediction	Random Prediction
Training data	x_{11}	x_{12}	$\cdots$	x_{1p}	Yes	Yes	No	Yes
	x_{21}	x_{22}	$\cdots$	x_{2p}	No	Yes	No	No
	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$			
Test data	x_{n1}	x_{n2}	$\cdots$	x_{np}	Yes	Yes	No	Yes

Classification: model evaluation

Confusion matrix

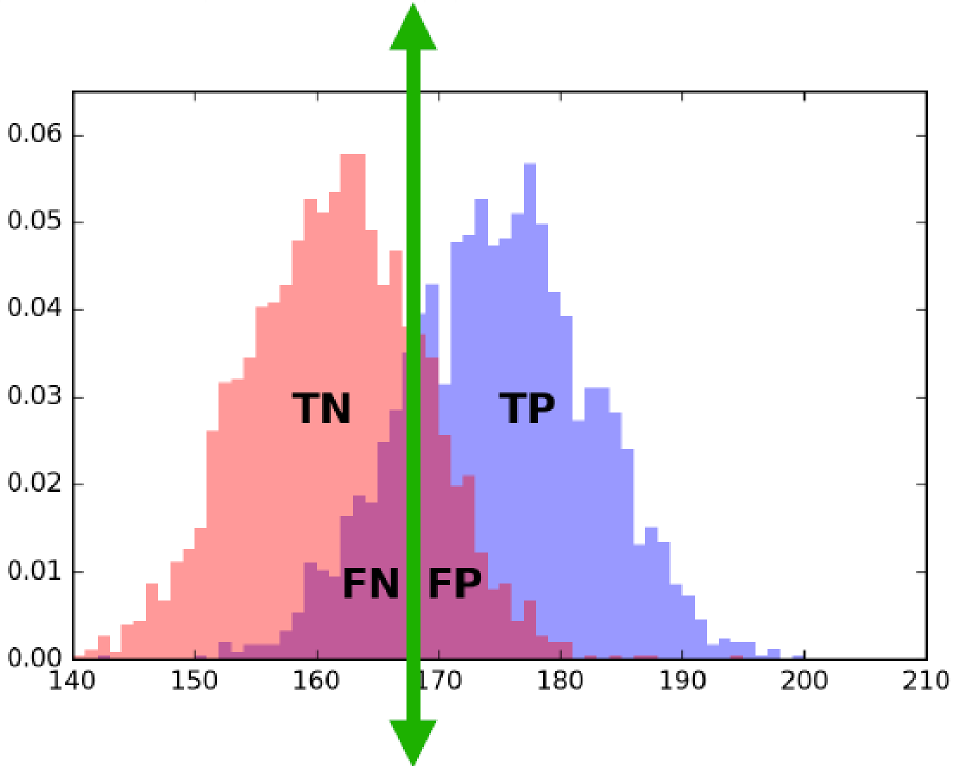
Confusion Matrix

	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	True Positives (TPs)	False Positives (FPs)
Predicted Negative (0)	False Negatives (FNs)	True Negatives (TNs)

- True positives (TP): + labeled as +
- True negatives (TN): - labeled as –
- False positives (FP): - labeled as +
- False negatives (FN): + labeled as -

Classification: model evaluation

- Example: classify everyone of height ≥168cm as male (1)



Fill out the tables: TP, TN, FP, FN

Cancer diagnosis. Positive class 5%, consider 100 data points.

- Left: Blind classifier (random label)
- Middle: Most common label classifier (always negative)
- Right: Least common label classifier (always)

Confusion Matrix

	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	2.5	47.5
Predicted Negative (0)	2.5	47.5

Confusion Matrix

	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	0	0
Predicted Negative (0)	5	95

Confusion Matrix

	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	5	95
Predicted Negative (0)	0	0

Accuracy

Accuracy ratio of correct predictions over all predictions

$$\text{Accuracy} = \frac{TP + TN}{TP + FP + TN + FN} = P(f(x) = y)$$

Case 1: classes balanced, Positive class 50%

- Blind classifier accuracy = 50%
  - Predict random label
- Most common label classifier accuracy = 50%
  - Predict majority class (doesn't matter 1 or 0)

Confusion Matrix

	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	True Positives (TPs)	False Positives (FPs)
Predicted Negative (0)	False Negatives (FNs)	True Negatives (TNs)

Fill out the tables: TP, TN, FP, FN

Cancer diagnosis. Positive class 50%, consider 100 data points.

- Left: Blind classifier (random label)
- Middle: Most common label classifier (always negative)

Confusion Matrix

	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	25	25
Predicted Negative (0)	25	25

Confusion Matrix

	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	0	0
Predicted Negative (0)	50	50

Accuracy

Accuracy ratio of correct predictions over all predictions

$$\text{Accuracy} = \frac{TP + TN}{TP + FP + TN + FN} = P(f(x) = y)$$

Case 2: classes are imbalanced, Positive class 5%

- Blind classifier accuracy = 50%
- Most common label classifier accuracy = 95%
  - Always predict 0

Accuracy can be misleading in the presence of class imbalance!

Confusion Matrix

	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	True Positives (TPs)	False Positives (FPs)
Predicted Negative (0)	False Negatives (FNs)	True Negatives (TNs)

Fill out the tables: TP, TN, FP, FN

Cancer diagnosis. Positive class 5%, consider 100 data points.

- Left: Blind classifier (random label)
- Middle: Most common label classifier (always negative)

Confusion Matrix

	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	2.5	47.5
Predicted Negative (0)	2.5	47.5

Confusion Matrix

	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	0	0
Predicted Negative (0)	5	95

Precision

Precision ratio of correct positive predictions over positive predictions

$$\text{Precision} = \frac{TP}{TP + FP} = P(y = 1 \mid f(x) = 1)$$

Example cancer diagnosis. Positive class 5%

Blind classifier precision $= P(y = 1) = 5\%$

Most common label classifier precision

$= P(y = 1 \mid f(x) = 1) =$ undefined

Least common label classifier precision

$= P(y = 1) = 5\%$

Confusion Matrix

	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	True Positives (TPs)	False Positives (FPs)
Predicted Negative (0)	False Negatives (FNs)	True Negatives (TNs)

Precision

Cancer diagnosis. Positive class 5%

- Left: Blind classifier
- Middle: Most common label classifier
- Right: Least common label classifier

Confusion Matrix

	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	2.5	47.5
Predicted Negative (0)	2.5	47.5

Confusion Matrix

	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	0	0
Predicted Negative (0)	5	95

Confusion Matrix

	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	5	95
Predicted Negative (0)	0	0

Recall

Recall ratio of correct positive predictions over all positive instances

$$\text{Recall} = \frac{TP}{P} = \frac{TP}{TP + FN} = P(f(x) = 1 \mid y = 1)$$

Example cancer diagnosis. Positive class 5%

Blind classifier recall $= P(f(x) = 1) =$ 50%

f(x) and y are independent

Most common label classifier recall

$= P(f(x) = 1 \mid y = 1) = 0$

Least common label classifier recall

$= P(f(x) = 1 \mid y = 1) =$ 100%

Confusion Matrix

	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	True Positives (TPs)	False Positives (FPs)
Predicted Negative (0)	False Negatives (FNs)	True Negatives (TNs)

Precision vs Recall

$$\text{Precision} = \frac{TP}{TP+FP} \qquad \text{Recall} = \frac{TP}{TP+FN}$$

Are false positives more important than false negatives?

Diagnostic screening for cancer:

Recall is more important

Might be OK to have FPs but not OK to have FNs

Spam filtering:

Precision is more important

Might be OK to have FNs but not OK to have FPs

F1-score

F1-score Harmonic mean of precision and recall

$$\mathrm{F1} = \frac{2\ \mathrm{precision} \times \mathrm{recall}}{\mathrm{precision} + \mathrm{recall}}$$

F1 score high => need both precision and recall to be high

	0.0	0.2	0.4	0.6	0.8	1.0
0.0	0.00	0.00	0.00	0.00	0.00	0.00
0.2	0.00	0.20	0.26	0.30	0.32	0.33
0.4	0.00	0.26	0.40	0.48	0.53	0.57
0.6	0.00	0.30	0.48	0.60	0.68	0.74
0.8	0.00	0.32	0.53	0.68	0.80	0.88
1.0	0.00	0.33	0.57	0.74	0.88	1.00

Table 5.2: Table of f-measures when varying precision and recall values.

Summary of recall & precision

- Class imbalanced ⇒ accuracy is misleading.
- High recall is easy to achieve
  - just predict + always
- High precision is hard to achieve in imbalanced classification
- F-score does the best job of any single statistic, but all four work together to describe the performance of a classifier.

Receiver Operating Characteristic (ROC) curve

Class prediction often done by thresholding some 'score'

- Changing the threshold results in a family of classifiers
- How to measure the performance of them altogether?

Example Use height to classify female vs male:

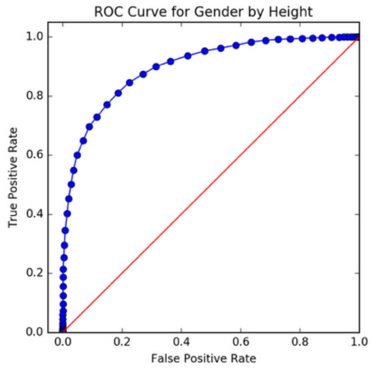
F, M, M, F, F, M, M

Increasing height

For each threshold, calculate

True positive rate $TPR = \frac{TP}{P}$ $\frac{4}{4}$

False positive rate $FPR = \frac{FP}{N}$ $\frac{2}{3}$

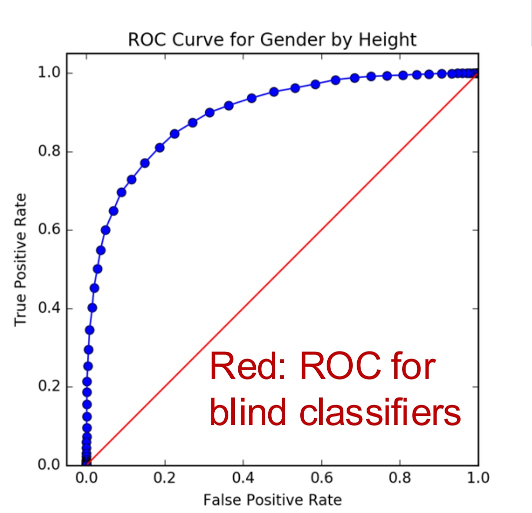


ROC Curve

For each threshold, calculate

True positive rate $TPR = \frac{TP}{P}$

False positive rate $FPR = \frac{FP}{N}$



The higher the curve, the better the classifiers & scores are

Area under ROC curve (AUROC): how good is the score when used for classification

Multiclass classification

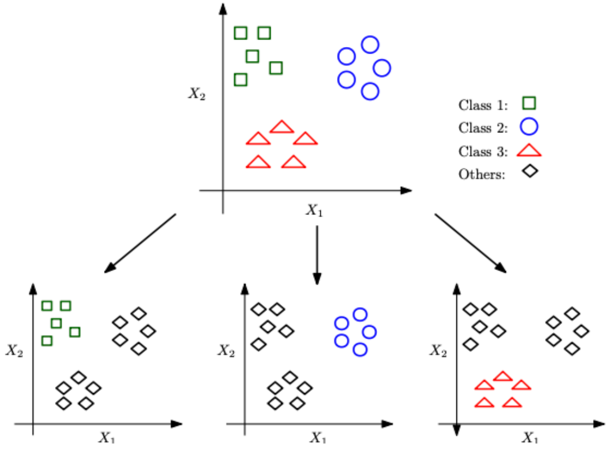
Multiclass classification

- Multiclass classification naturally happens in many real-world applications
  - E.g. movies: “drama”, “action”, “documentary”
  - E.g. objects: “automobile”, “airplanes”, “trees”

- Some of our methods are designed for binary classification, e.g. logistic regression
  - How to extend them to multiclass prediction?

Approach 1: reducing multiclass to binary

The "One-vs-rest" approach:



Training

For each class i:

Train f_i that classifies class i against the rest

Test

For test example x:

Use each f_i to predict its probability of belonging class i

Pick class i that has the highest probability

Alternative: "all pairs" approach

Approach 2: modifying the learning algorithm

Case study How to extend logistic regression to multiclass?

The multinomial logistic regression model:

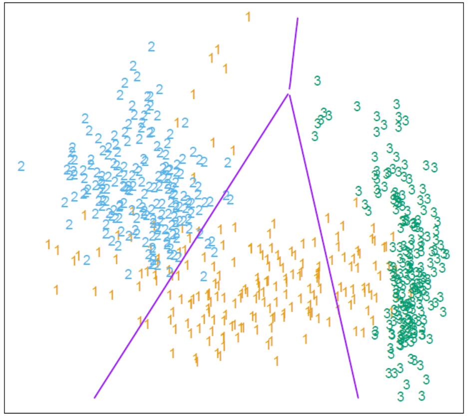
$$\log \frac{p(C=1 \mid x)}{p(C=K \mid x)} = w_1^T x$$

$p(C=i \mid x)$'s sum to 1

$$\log \frac{p(C=2 \mid x)}{p(C=K \mid x)} = w_2^T x$$

$$\vdots$$

$$\log \frac{p(C=K-1 \mid x)}{p(C=K \mid x)} = w_{K-1}^T x$$



Can define multiclass cross entropy loss accordingly, and minimize it

Comparison

- Reducing multiclass to binary
  - Pros: simple & general – binary classification algorithm as ‘black box’
- Modifying the learning algorithm
  - Pros: can exploit the structure of the problem more

sklearn.linear_model.LogisticRegression

class sklearn.linear_model.LogisticRegression(*penalty='l2', *, dual=False, tol=0.0001, C=1.0, fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None, solver='lbfgs', max_iter=100, multi_class='auto', verbose=0, warm_start=False, n_jobs=None, l1_ratio=None*) [source]

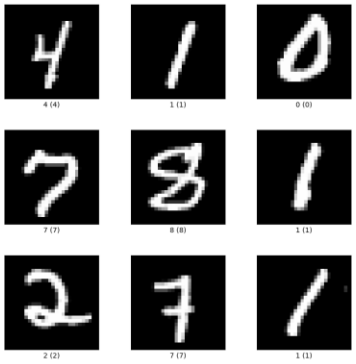
multi_class=‘ovr’ implements one-vs-rest

multi_class=‘multinomial’ implements multinomial

Multiclass classification: performance metrics

Multiclass confusion matrix

Example Optical Character Recognition



Predicted label $f(x)$

Actual label y

Digits	0	1	2	3	4	5	6	7	8	9
0	351	0	5	4	2	7	2	1	6	0
1	0	254	0	0	2	0	0	1	1	2
2	1	1	166	4	5	1	3	2	2	1
3	1	2	4	142	0	5	0	1	4	0
4	3	3	8	1	180	3	2	5	4	4
5	0	0	3	11	0	140	3	0	7	1
6	0	2	2	0	4	0	158	0	1	0
7	0	0	2	2	1	0	0	132	2	1
8	2	1	8	0	0	0	2	1	137	1
9	1	1	0	2	6	4	0	4	2	167

Multiclass classification: performance metrics

We can precision & recall separately for each class i

$$\text{Precision}_i = P(\, y = i \mid f(x) = i \,) = \frac{C[i,i]}{\sum_j C[j,i]}$$

$$\text{Recall}_i = P(\, f(x) = i \mid y = i \,) = \frac{C[i,i]}{\sum_j C[i,j]}$$

Example

$$\text{Precision}_0 = \frac{351}{359}$$

$$\text{Recall}_0 = \frac{351}{378}$$

Predicted label $f(x)$

Actual label y

Digits	0	1	2	3	4	5	6	7	8	9
0	351	0	5	4	2	7	2	1	6	0
1	0	254	0	0	2	0	0	1	1	2
2	1	1	166	4	5	1	3	2	2	1
3	1	2	4	142	0	5	0	1	4	0
4	3	3	8	1	180	3	2	5	4	4
5	0	0	3	11	0	140	3	0	7	1
6	0	2	2	0	4	0	158	0	1	0
7	0	0	2	2	1	0	0	132	2	1
8	2	1	8	0	0	0	2	1	137	1
9	1	1	0	2	6	4	0	4	2	167