Computer Science

CSC380: Principles of Data Science

Basic machine learning 2

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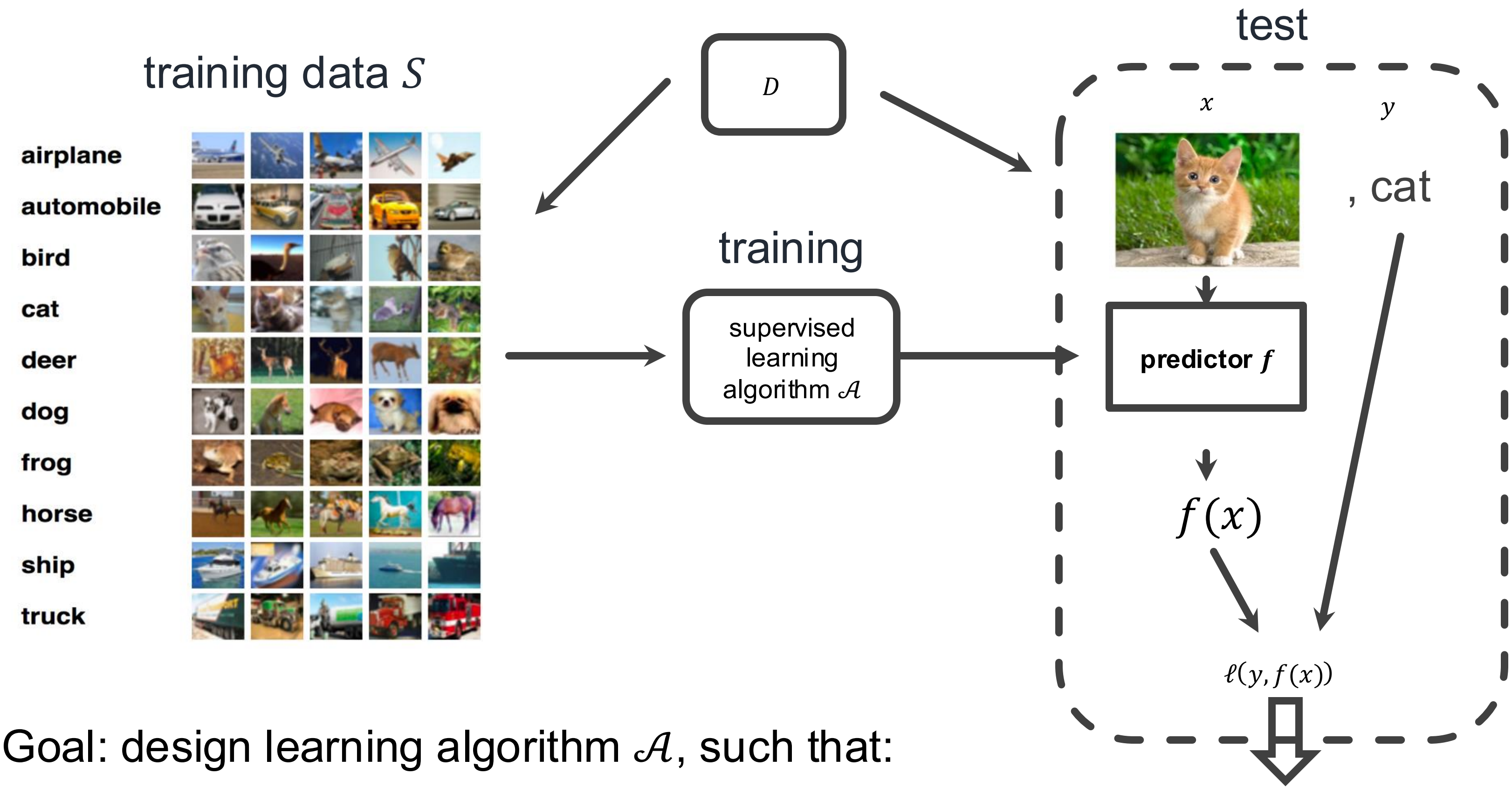
Outline

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

Classification recap

Supervised learning setup in one figure



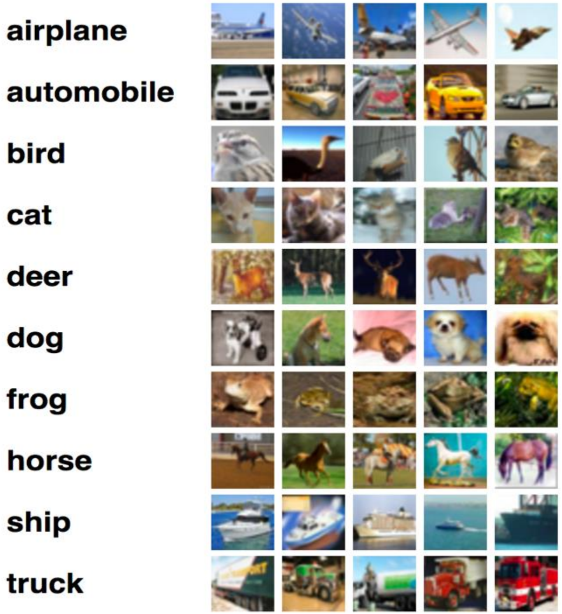
- Goal: design learning algorithm $\mathcal{A}$, such that:
- after training, its output predictor f has low test error

Test error: average of $\ell(y, f(x))$ in test set

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

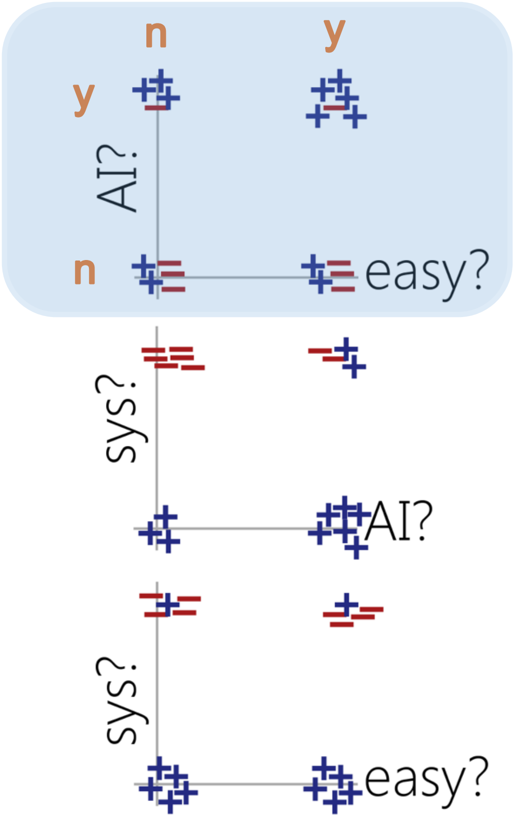
Example: Course Recommendation

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: +

Label: -

Features



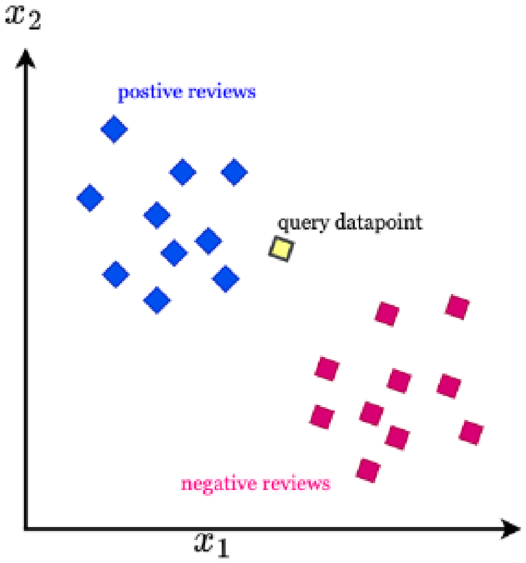
Each course's feature is Represented as points in 5-dimensional space

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

Observation: examples with same labels tend to be closer!

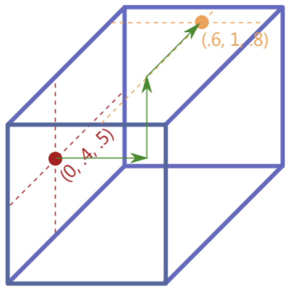
Nearest neighbor classification

- 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



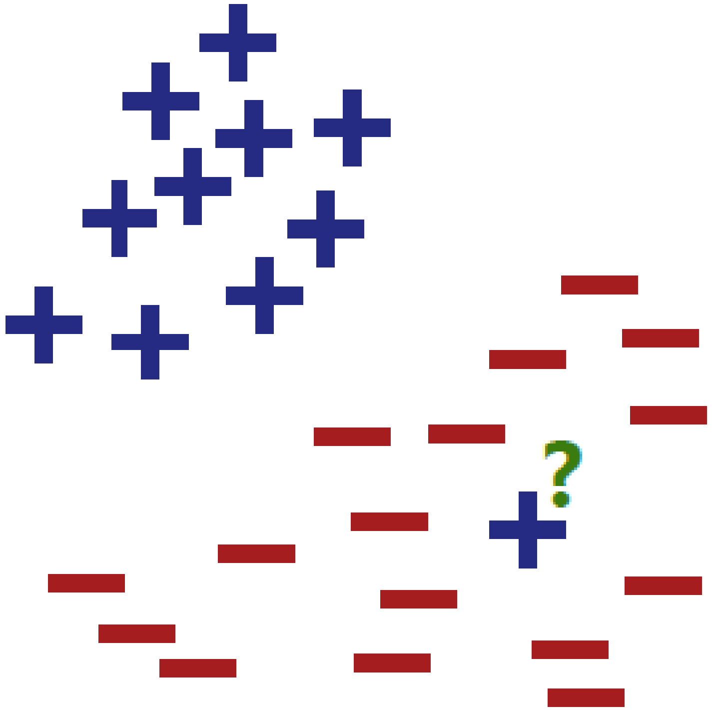
Measuring nearest neighbors

- 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 **<u>real values</u>**?
  - 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 -

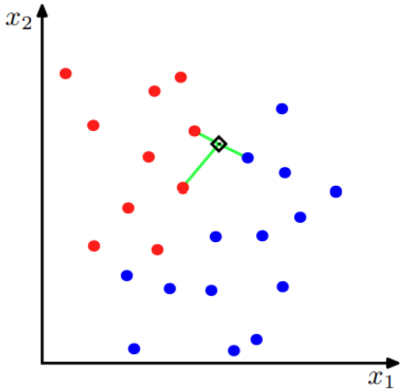
Problem: predicting using 1 nearest neighbor's label can be sensitive to noisy data

How to mitigate this?

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

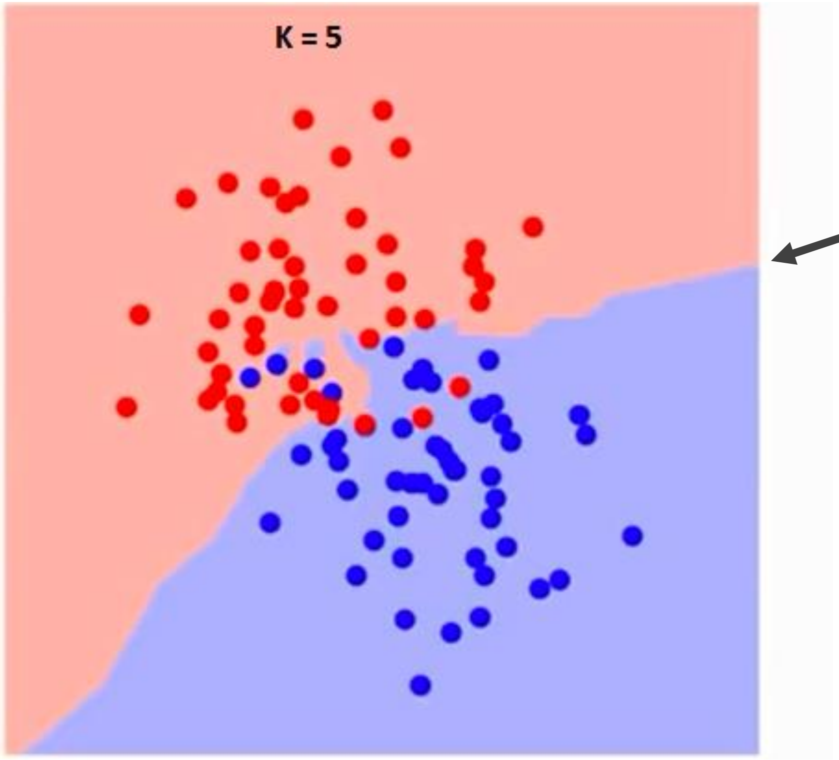
- Training set: $S = \{ (x_1, y_1), \ldots, (x_m, y_m) \}$

- **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



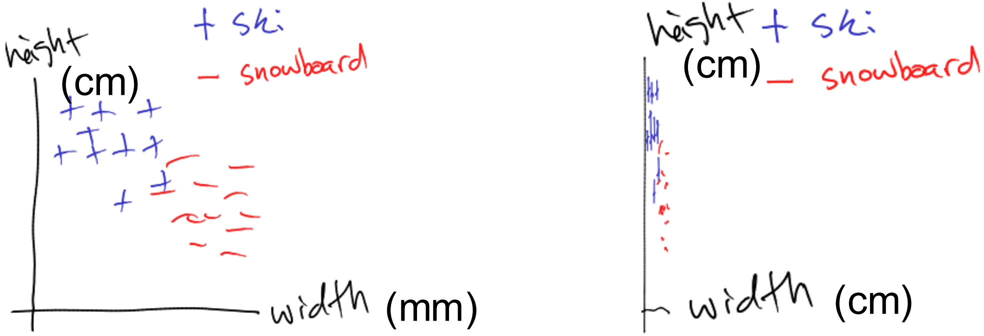
decision boundary

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

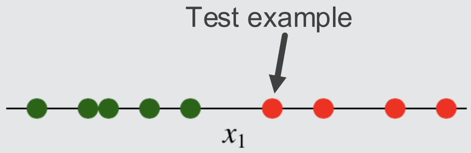
- Features having different scale can be problematic
- [Definition] **Standardization**
  - For each feature f, compute $\mu_f = \frac{1}{m}\sum_{i=1}^{m} x_f^{(i)}$, $\sigma_f = \sqrt{\frac{1}{m}\sum_{i=1}^{m}\left(x_f^{(i)} - \mu_f\right)^2}$
  - Then, transform the data by $\forall f \in \{1,\dots,d\},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

after transformation, each feature has mean 0 and variance 1

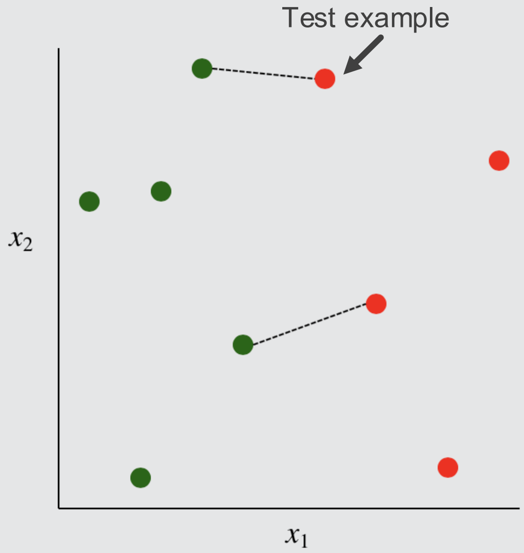
- Be sure to keep the “standardize” function and apply it to the test points.
  - Save $\{(\mu_f, \sigma_f)\}_{f=1}^{d}$
  - For test point x^*, apply $x_f^* \leftarrow \frac{x_f^* - \mu_f}{\sigma_f}, \forall f$

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

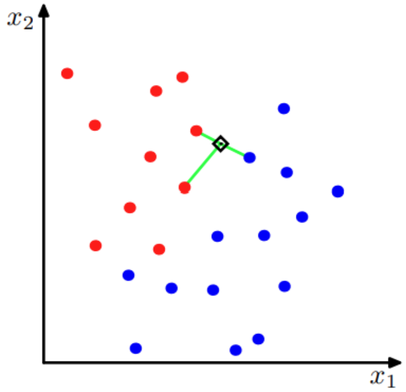


- Mitigation: feature selection

Issue 3: choosing k

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

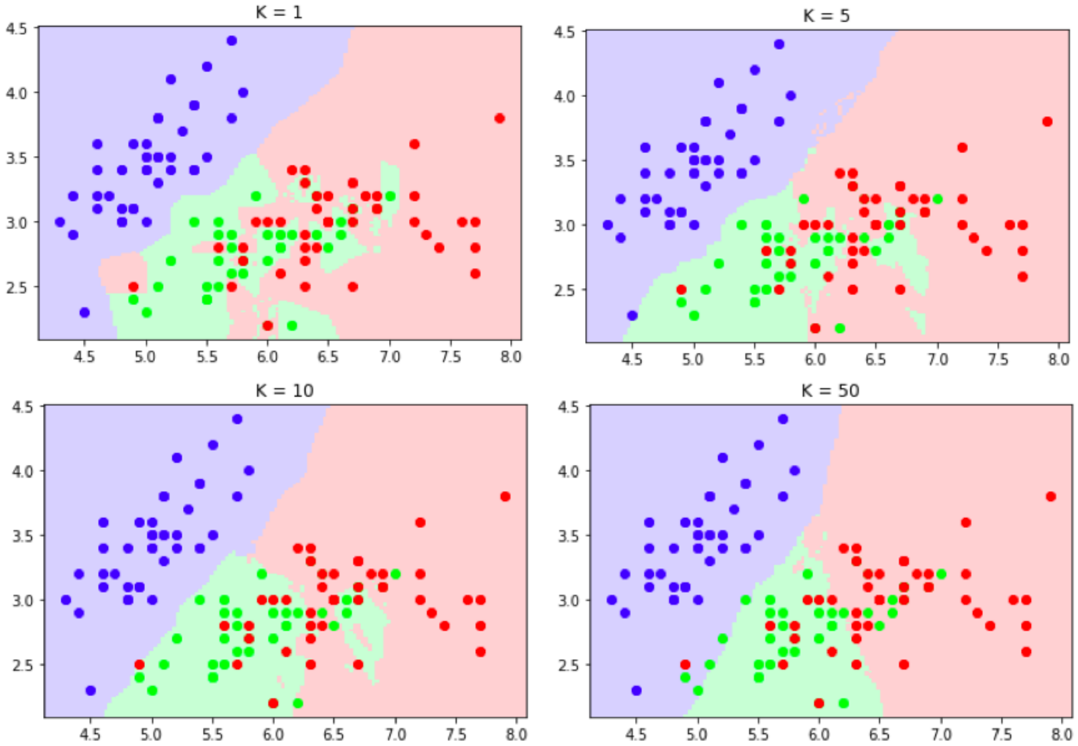
- Q: What is the training error of a 1-NN classifier?
  - 0
  - Overfitting



Issue 3: choosing k

k can be viewed as a model complexity measure

Smaller k results in a more complex model

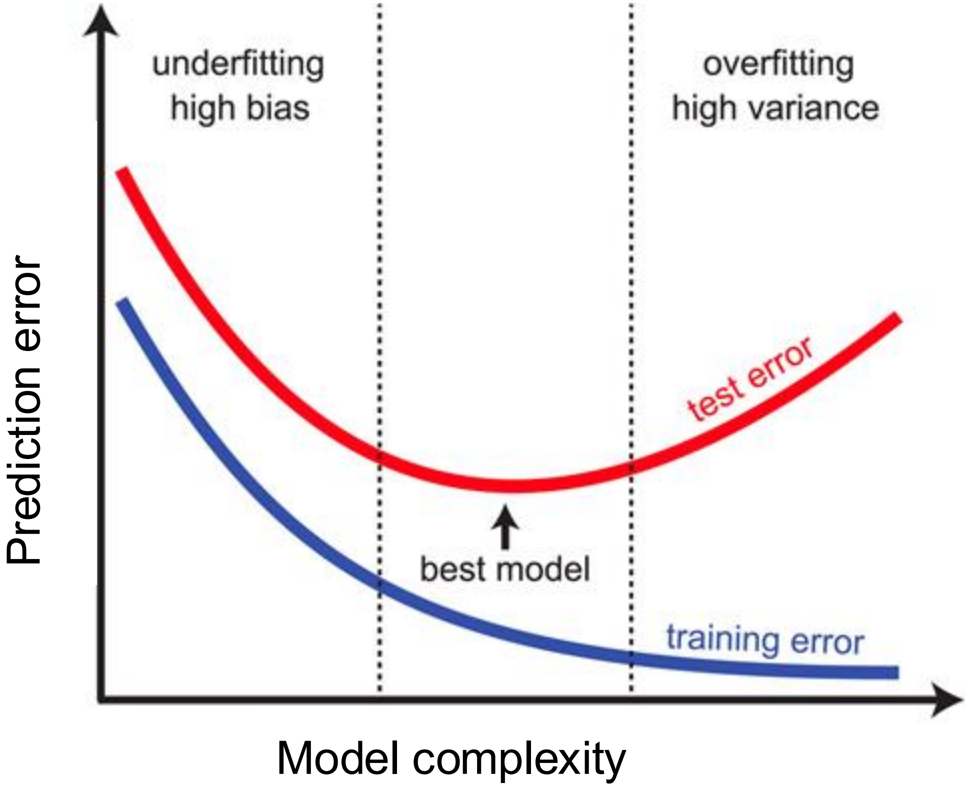


Issue 3: choosing k

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

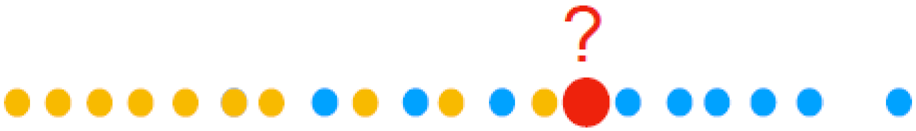
Classification with logistic regression

Training data: number of hours studied for the course.

Labels: Pass (1) or Fail (0)

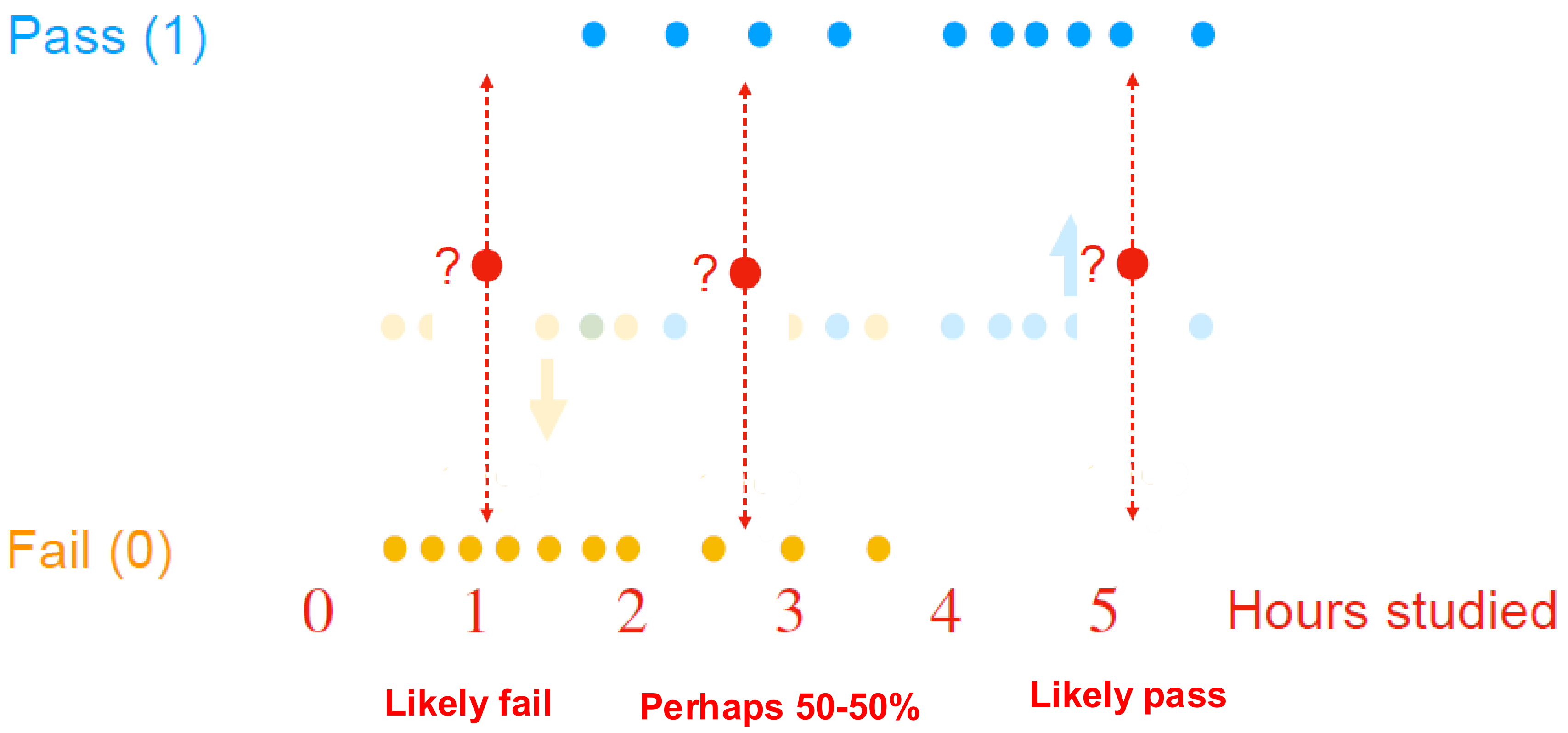
Classification with logistic regression

- 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

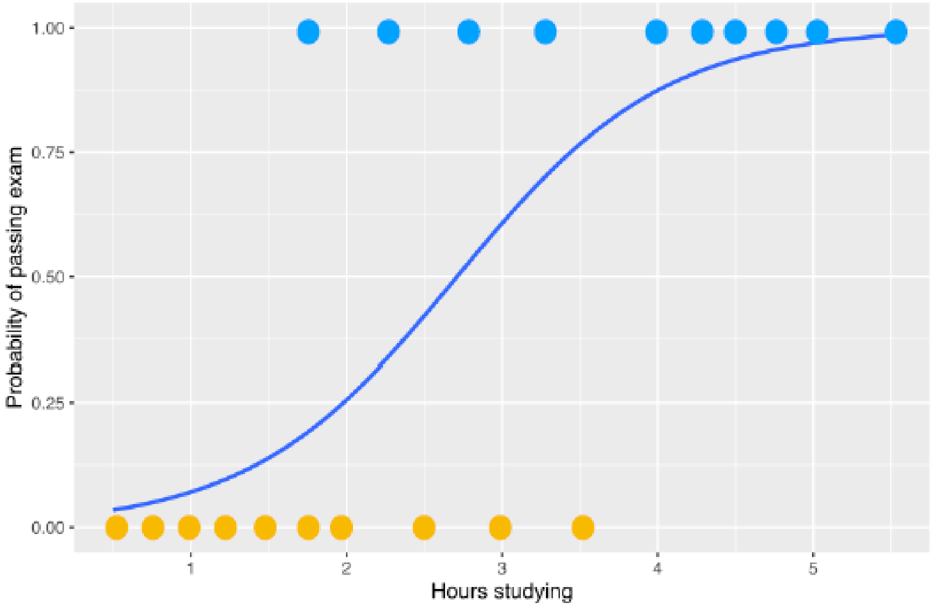
Classification with logistic regression



Classification with logistic regression

$Y = 1$

$Y = 0$

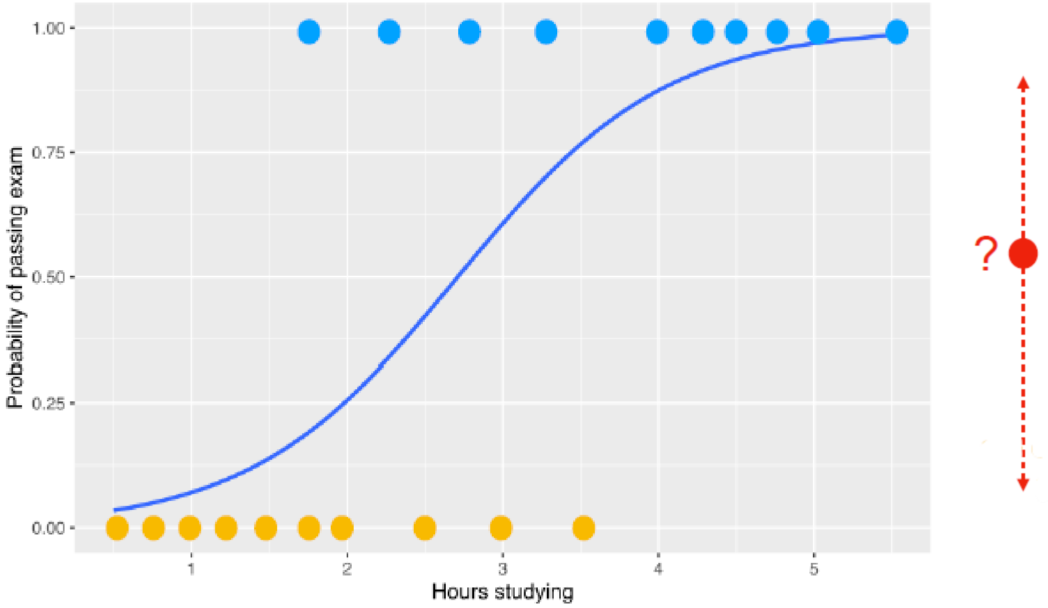


X: feature

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

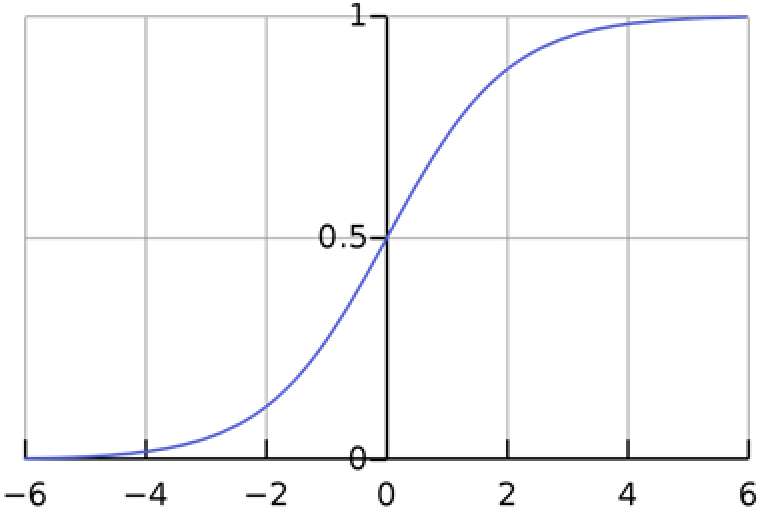
We will assume that:

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

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*



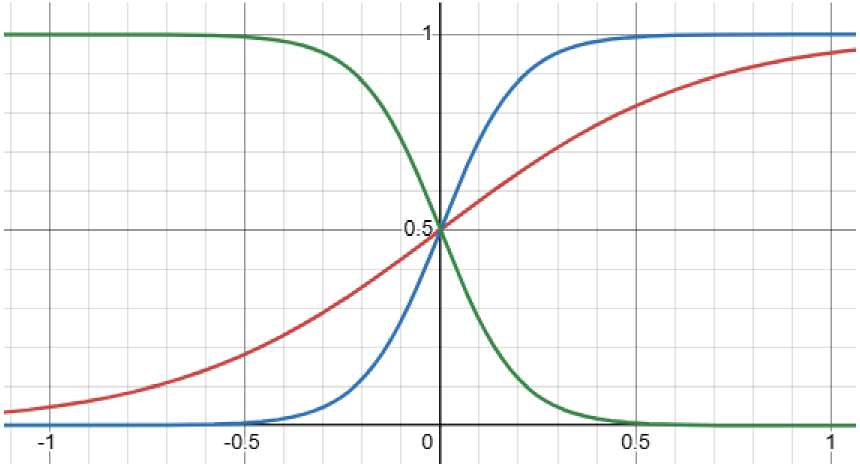
Logistic regression model

w controls the shape of the probability curve

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

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

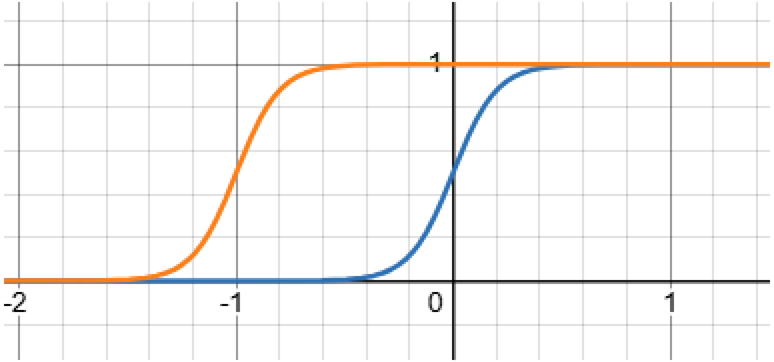
$$p = \frac{1}{1+e^{10\,x}}$$



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 = $\frac{1}{1+e^{-1}} = 0.73$

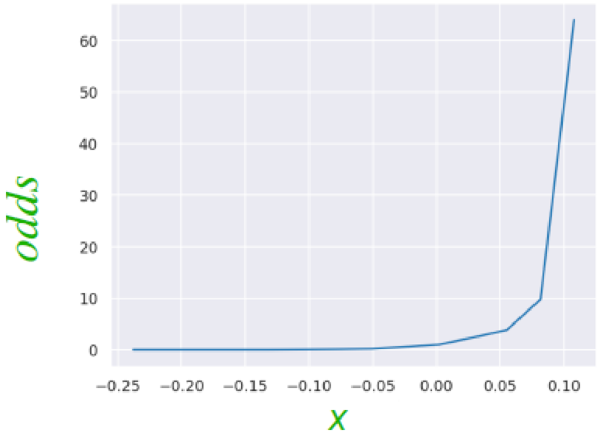
Classification with logistic regression

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

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

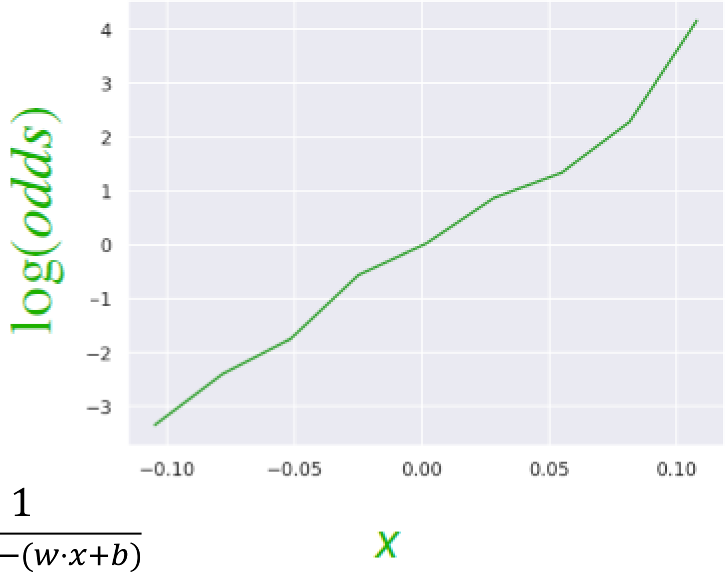
- Still not ideal: odd bounded from below



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

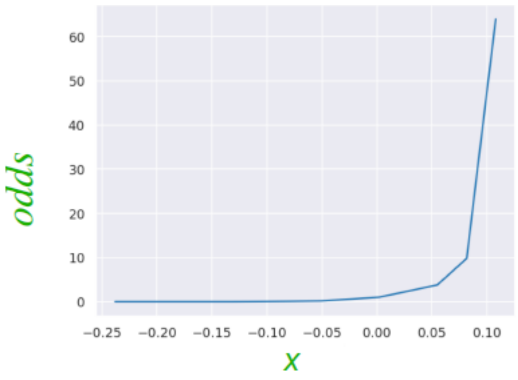


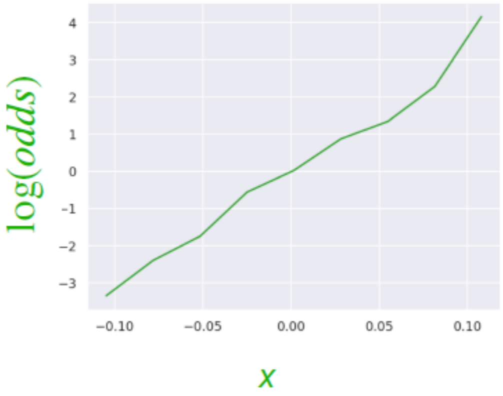
$$\ln \frac{p}{1-p} = w \cdot x + b \quad \Rightarrow \quad \frac{p}{1-p} = e^{w\,x+b} \quad \Rightarrow \quad p = \frac{1}{1 + e^{-(w \cdot x + b)}}$$

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, +∞]   [-∞, +∞]



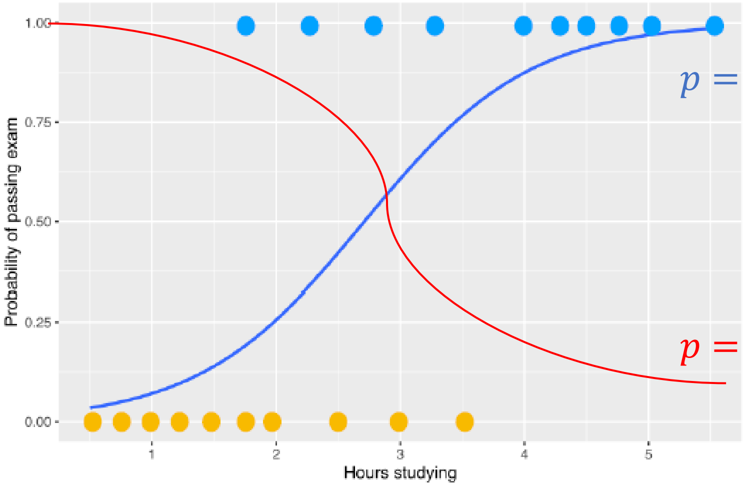


Fitting a logistic regression model

- 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

$Y = 1$



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

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

$Y = 0$

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

Fitting a logistic regression model

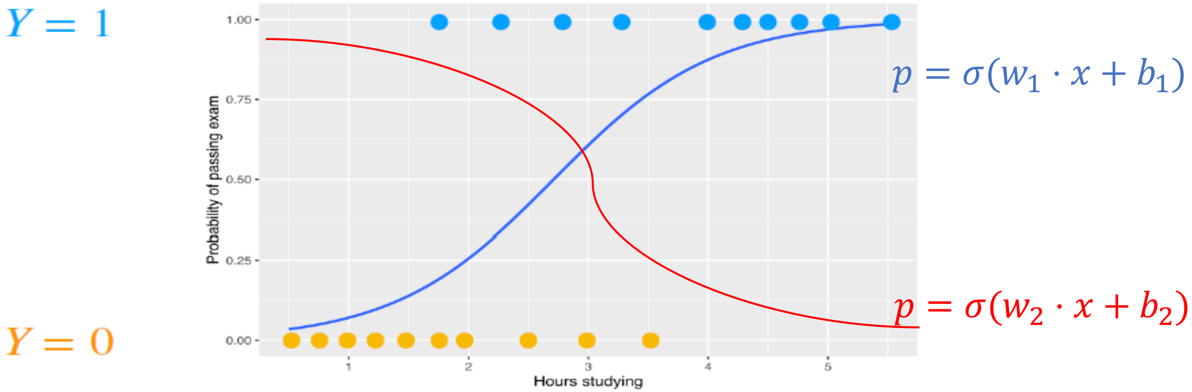
We'd like to choose w and b such that:

for x whose label is more likely to be 1

=> p is large

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

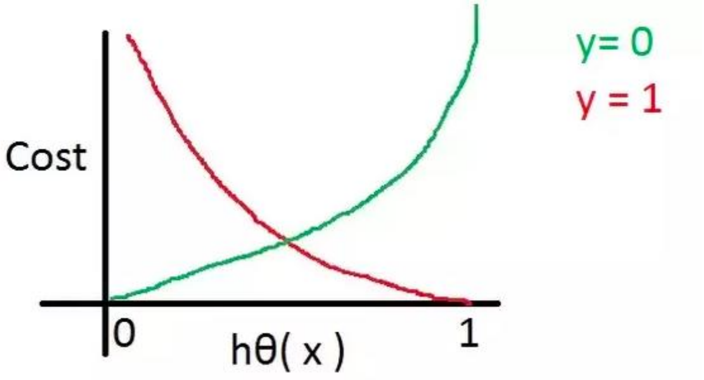
=> penalize more if p is small



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

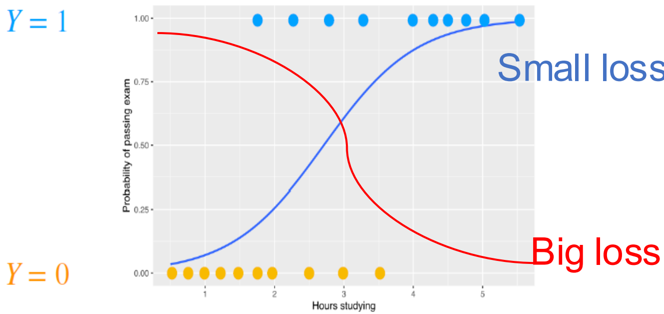
- We find w and b to minimize:

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

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

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

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.

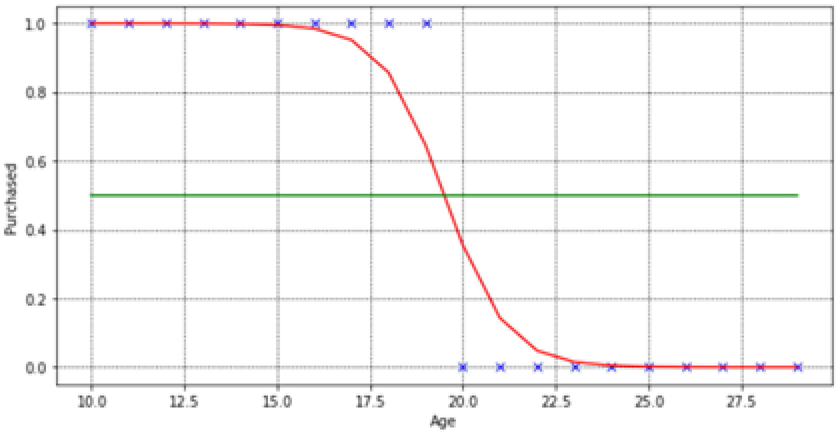
Scikit-Learn Logistic Regression

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')
```

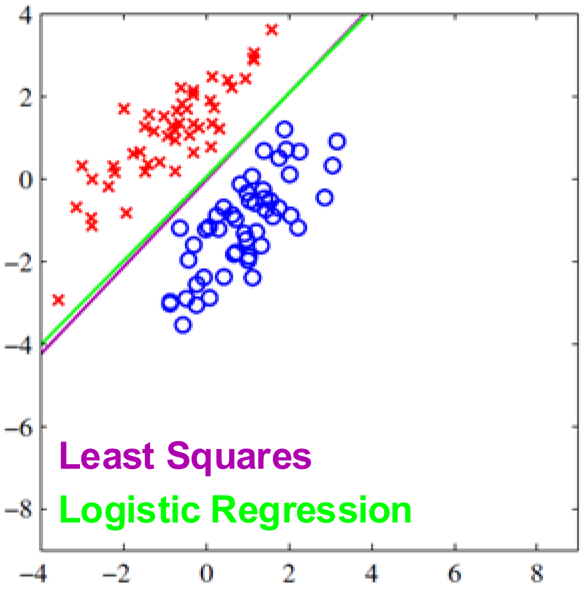


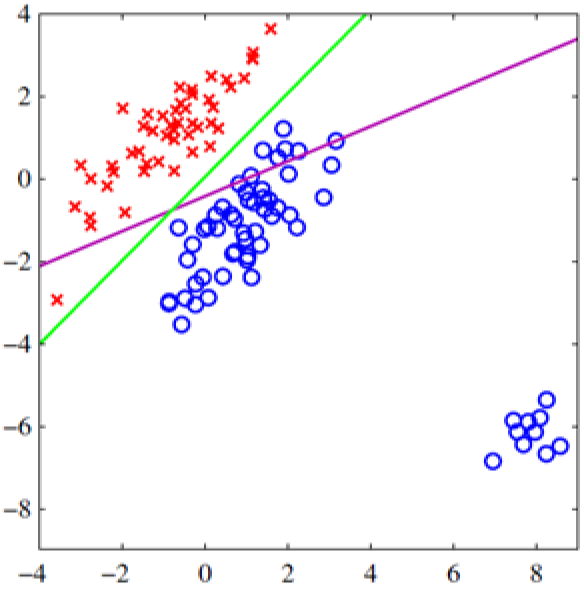
Function `predict_proba(X)` returns prediction of class assignment probabilities for each class. It returns n by C matrix if n data points were provided as argument.

(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**