Lecture 4:
Logistic Regression

Shuai Li

John Hopcroft Center, Shanghai Jiao Tong University

shuaili8.github.io

https://shuaili8.github.io/Teaching/VE445/index.html

Last lecture

- Linear regression
  - Normal equation
  - Gradient methods
  - Examples
  - Probabilistic view
  - Applications
  - Regularization

Today’s lecture

- Discriminative / Generative Models
- Logistic regression (binary classification)
  - Cross entropy
  - Formulation, sigmoid function
  - Training—gradient descent
- More measures for binary classification (AUC, AUPR)
- Class imbalance
- Multi-class logistic regression

Discriminative / Generative Models

Discriminative / Generative Models

- Discriminative models
  - Modeling the dependence of unobserved variables on observed ones
  - also called conditional models.
  - Deterministic: $y = f_\theta(x)$
  - Probabilistic: $p_\theta(y|x)$
- Generative models
  - Modeling the joint probabilistic distribution of data
  - Given some hidden parameters or variables

$$p_\theta(x, y)$$

  - Then do the conditional inference

$$p_\theta(y|x) = \frac{p_\theta(x, y)}{p_\theta(x)} = \frac{p_\theta(x, y)}{\sum_{y'} p_\theta(x, y')}$$

Discriminative Models

- Discriminative models
  - Modeling the dependence of unobserved variables on observed ones
  - also called conditional models.
  - Deterministic: $y = f_\theta(x)$
  - Probabilistic: $p_\theta(y|x)$

  - Directly model the dependence for label prediction
  - Easy to define dependence on specific features and models
  - Practically yielding higher prediction performance
  - E.g. linear regression, logistic regression, k nearest neighbor, SVMs, (multi-layer) perceptrons, decision trees, random forest

Generative Models

- Generative models
  - Modeling the joint probabilistic distribution of data
  - Given some hidden parameters or variables

$$p_\theta(x, y)$$

  - Then do the conditional inference

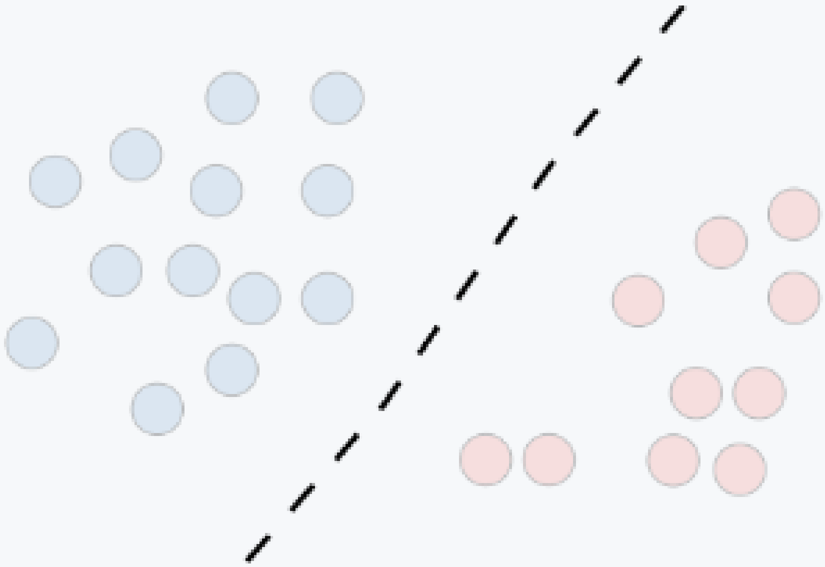
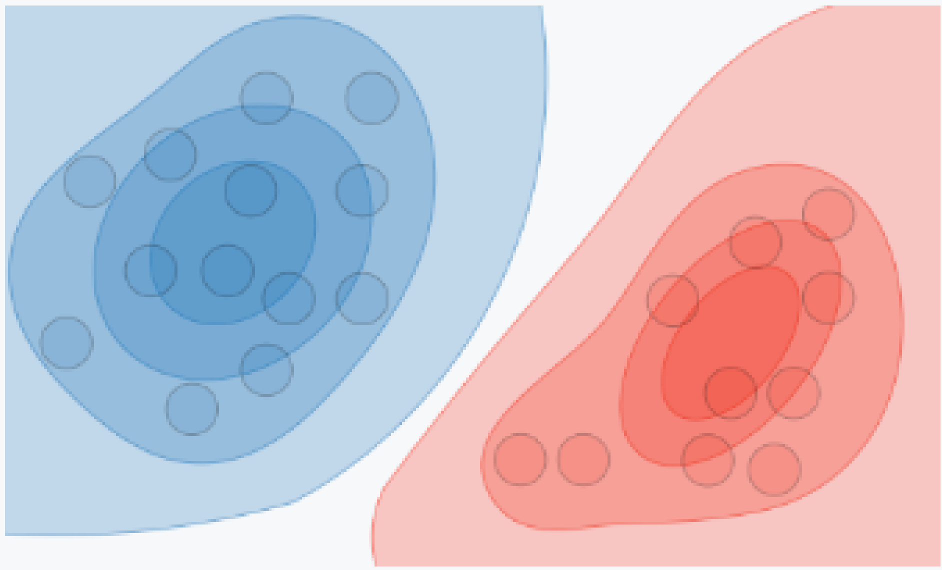
$$p_\theta(y|x) = \frac{p_\theta(x, y)}{p_\theta(x)} = \frac{p_\theta(x, y)}{\sum_{y'} p_\theta(x, y')}$$

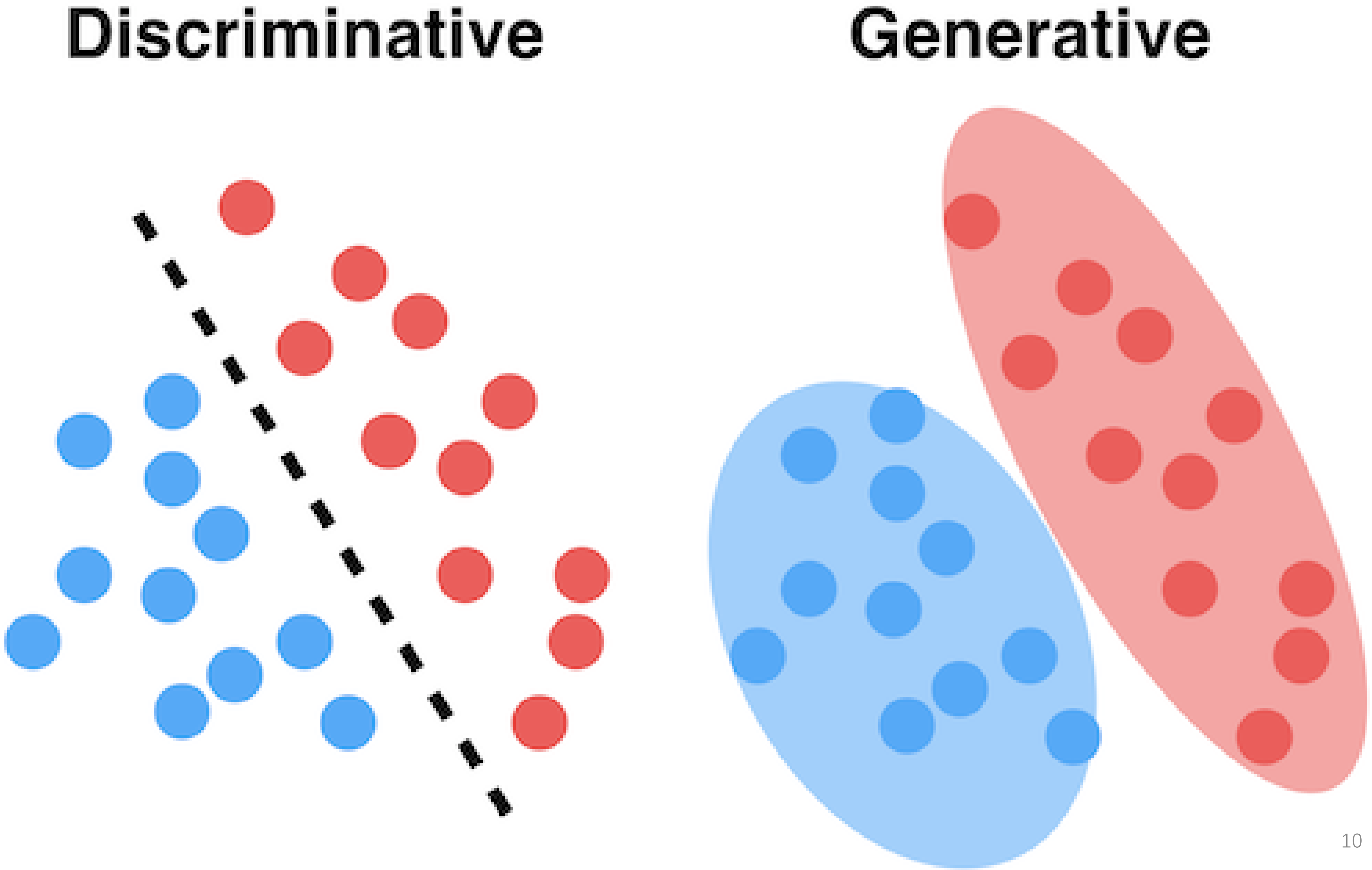
- Recover the data distribution [essence of data science]
- Benefit from hidden variables modeling
- E.g. Naive Bayes, Hidden Markov Model, Mixture Gaussian, Markov Random Fields, Latent Dirichlet Allocation

Discriminative Models vs Generative Models

- In General
  - A Discriminative model models the **decision boundary between the classes**
  - A Generative Model explicitly models the **actual distribution of each class**

- Example: Our training set is a bag of fruits. Only apples and oranges Each labeled. Imagine a post-it note stuck to the fruit
  - A generative model will model various attributes of fruits such as color, weight, shape, etc
  - A discriminative model might model color alone, **should that suffice** to distinguish apples from oranges

	Discriminative model	Generative model
Goal	Directly estimate $P(y\|x)$	Estimate $P(x\|y)$ to then deduce $P(y\|x)$
What's learned	Decision boundary	Probability distributions of the data
Illustration		
Examples	Regressions, SVMs	GDA, Naive Bayes


Discriminative
Generative

Linear Discriminative Models

- Discriminative model
  - modeling the dependence of unobserved variables on observed ones
  - also called conditional models
  - **Deterministic**: $y = f_\theta(x)$
  - Probabilistic: $p_\theta(y|x)$

- Linear regression model

$$y = f_\theta(x) = \theta_0 + \sum_{j=1}^{d} \theta_j x_j = \theta^\top x$$

$$x = (1, x_1, x_2, \ldots, x_d)$$

Logistic Regression

From linear regression to logistic regression

- Logistic regression
  - Similar to linear regression
    - Given the numerical features of a sample, predict the numerical label value
    - E.g. given the size, weight, and thickness of the cell wall, predict the age of the cell
  - The values y we now want to predict take on only a small number of discrete values
    - E.g. to predict the cell is benign or malignant

Example

- Given the data of cancer cells below, how to predict they are benign or malignant?

Id	Cl.thickness	Cell.size	Cell.shape	Marg.adhesion	Epith.c.size	Bare.nuclei	Bl.cromatin	Normal.nucleoli	Mitoses	Class
1000025	5	1	1	1	2	1	3	1	1	benign
1002945	5	4	4	5	7	10	3	2	1	benign
1015425	3	1	1	1	2	2	3	1	1	benign
1016277	6	8	8	1	3	4	3	7	1	benign
1017023	4	1	1	3	2	1	3	1	1	benign
1017122	8	10	10	8	7	10	9	7	1	malignant
1018099	1	1	1	1	2	10	3	1	1	benign
1018561	2	1	2	1	2	1	3	1	1	benign
1033078	2	1	1	1	2	1	1	1	5	benign
1033078	4	2	1	1	2	1	2	1	1	benign
1035283	1	1	1	1	1	1	3	1	1	benign
1036172	2	1	1	1	2	1	2	1	1	benign
1041801	5	3	3	3	2	3	4	4	1	malignant

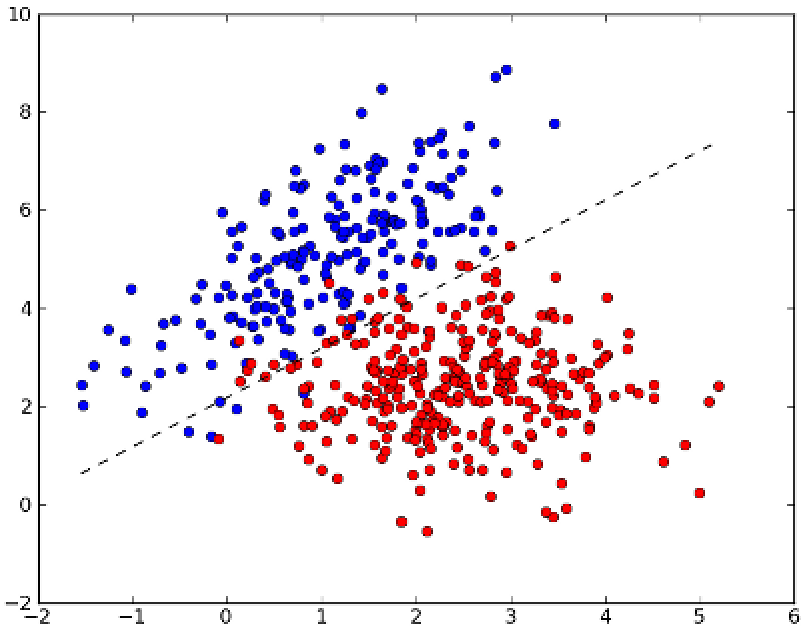
Logistics regression

- It is a Classification problem
  - Compared to regression problem, which predicts the labels from many numerical features
- Many applications
  - Spam Detection: Predicting if an email is Spam or not based on word frequencies
  - Credit Card Fraud: Predicting if a given credit card transaction is fraud or not based on their previous usage
  - Health: Predicting if a given mass of tissue is benign or malignant
  - Marketing: Predicting if a given user will buy an insurance product or not

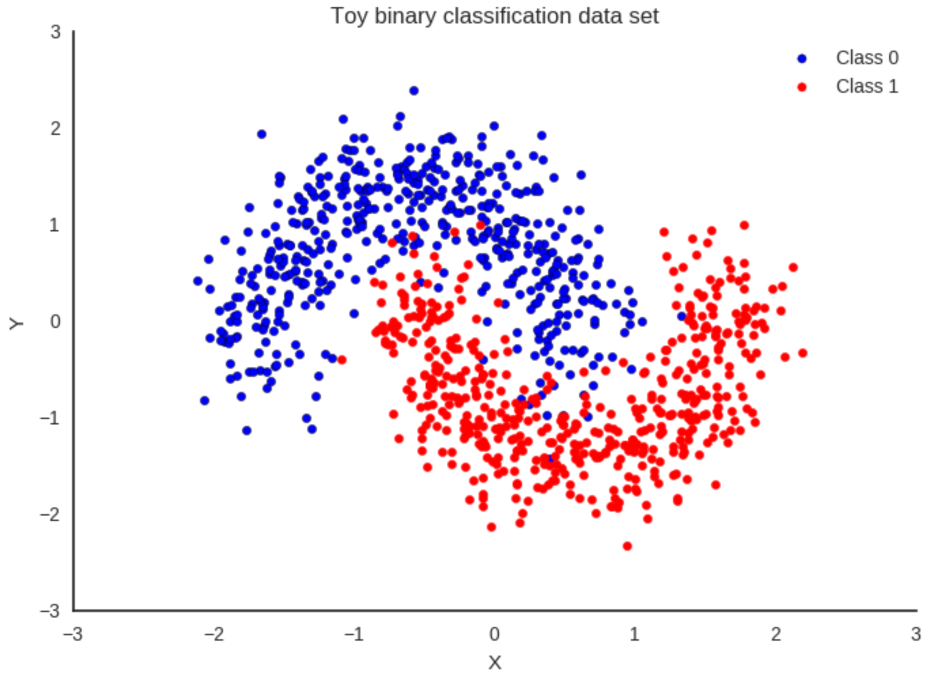
Classification problem

- Given:
  - A description of an instance $x \in X$
  - A fixed set of categories: $C = \{c_1, c_2, \ldots, c_m\}$
- Determine:
  - The category of $x : f(x) \in C$ where $f(x)$ is a categorization function whose domain is $\mathbb{X}$ and whose range is C
  - If the category set binary, i.e. $C = \{0, 1\}$ ({false, true}, {negative, positive}) then it is called binary classification

Binary classification



Linearly separable



Nonlinearly separable

Linear discriminative model

- Discriminative model
  - modeling the dependence of unobserved variables on observed ones
  - also called conditional models.
  - Deterministic: $y = f_\theta(x)$
  - **Probabilistic**: $p_\theta(y|x)$

- For binary classification
  - $p_\theta(y = 1 \mid x)$
  - $p_\theta(y = 0 \mid x) = 1 - p_\theta(y = 1 \mid x)$

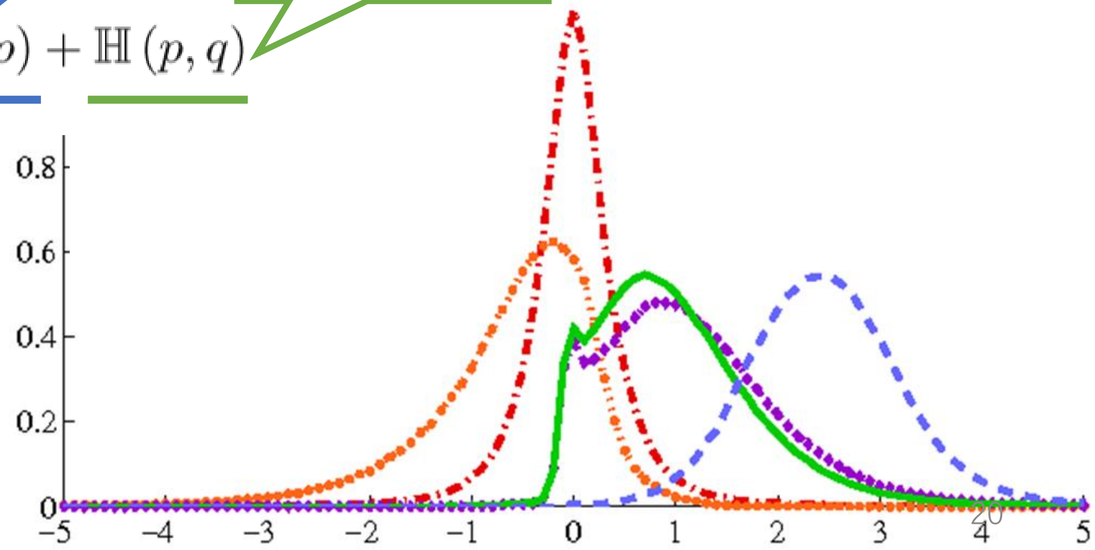
Loss Functions

KL divergence

- Regression: mean squared error (MSE)
- Kullback-Leibler divergence (KL divergence)
  - Measure the dissimilarity of two probability distributions

$$\mathbb{KL}\left(p\|q\right) \triangleq \sum_{k=1}^{K} p_k \log \frac{p_k}{q_k}$$

$$\mathbb{KL}\left(p\|q\right) = \underbrace{\sum_k p_k \log p_k}_{} - \underbrace{\sum_k p_k \log q_k}_{} = \underbrace{-\mathbb{H}\left(p\right)}_{\text{Entropy}} + \underbrace{\mathbb{H}\left(p, q\right)}_{\text{Cross entropy}}$$



Question:
Which one is more similar to norm distribution?

KL divergence (cont.)

- Information inequality

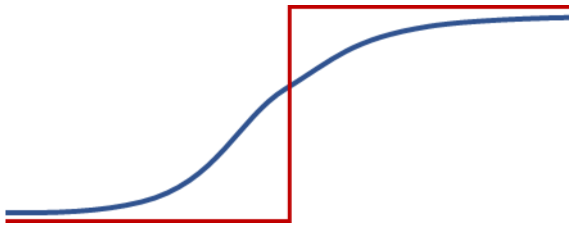
$$\mathbb{KL}(p||q) \geq 0 \textit{ with equality iff } p = q.$$

- Entropy
  - $\mathbb{H}(X) \triangleq -\sum_{k=1}^{K} p(X = k) \log_2 p(X = k)$
  - Is a measure of the uncertainty
  - Discrete distribution with the maximum entropy is the uniform distribution

- Cross entropy
  - $\mathbb{H}(p, q) \triangleq -\sum_{k} p_k \log q_k$
  - Is the average number of bits needed to encode data coming from a source with distribution p when we use model q to define our codebook

Cross entropy loss

- Cross entropy
  - Discrete case: $H(p,q) = -\sum_x p(x) \log q(x)$
  - Continuous case: $H(p,q) = -\int_x \; p(x) \log q(x)$
- Cross entropy loss in classification:
  - Red line p: the ground truth label distribution.
  - Blue line q: the predicted label distribution.



Example for binary classification

- Cross entropy: $H(p, q) = -\sum_x p(x) \log q(x)$

- Given a data point $(x, 0)$ with prediction probability
$$q_\theta(y = 1|x) = 0.4$$
the cross entropy loss on this point is
$$L = -p(y = 0|x) \log q_\theta(y = 0|x) - p(y = 1|x) \log q_\theta(y = 1|x)$$
$$= -\log(1 - 0.4) = \log \frac{5}{3}$$

- What is the cross entropy loss for data point $(x, 1)$ with prediction probability
$$q_\theta(y = 1|x) = 0.3$$

Cross entropy loss for binary classification

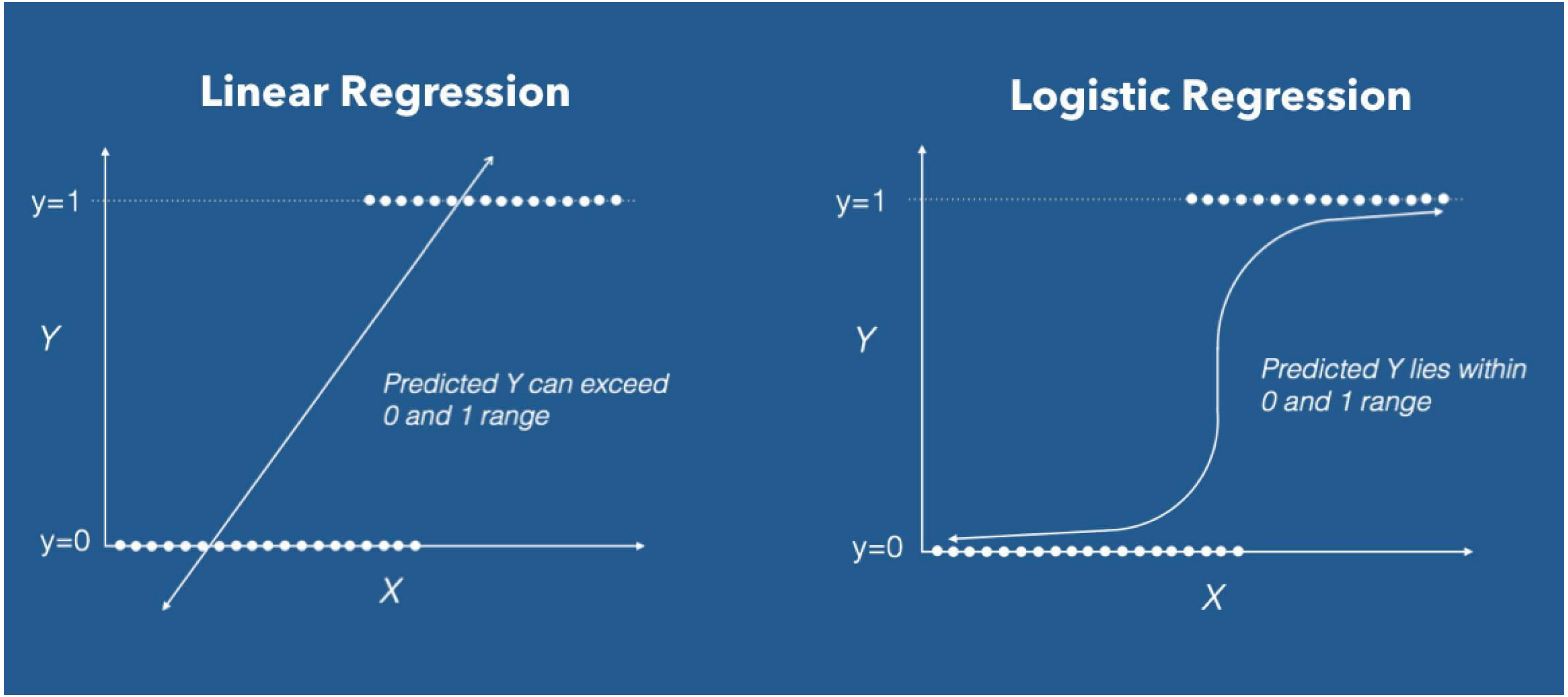
- Loss function for data point (x, y) with prediction model
$$p_\theta(\cdot\,|x)$$
is
$$L(y, x, p_\theta)$$
$$= -1_{y=1} \log p_\theta(1|x) - 1_{y=0} \log p_\theta(0|x)$$
$$= -y \log p_\theta(1|x) - (1 - \mathrm{y}) \log (1 - p_\theta(1|x))$$

Cross entropy loss for multiple classification

- Loss function for data point (x, y) with prediction model
$$p_\theta(\cdot\,|x)$$
is
$$L(y, x, p_\theta) = -\sum_{i=1}^{m} 1_{y=C_k} \log p_\theta(C_k|x)$$

Binary Classification

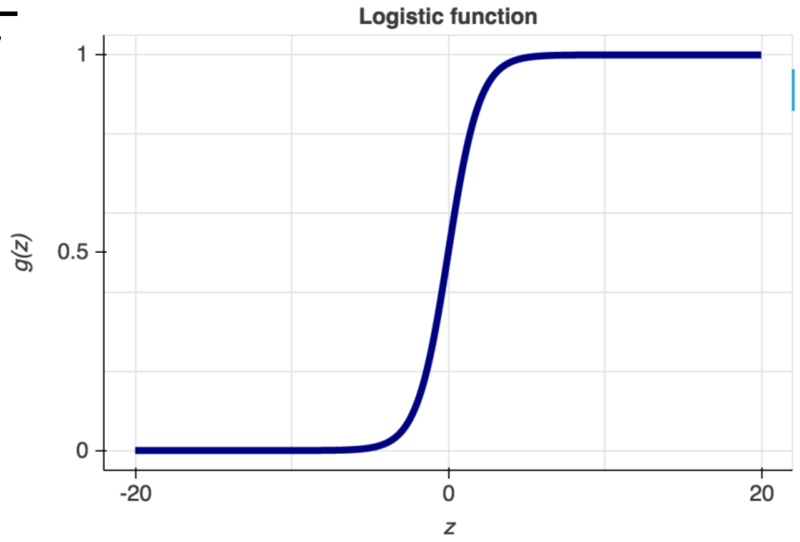
Binary classification: linear and logistic



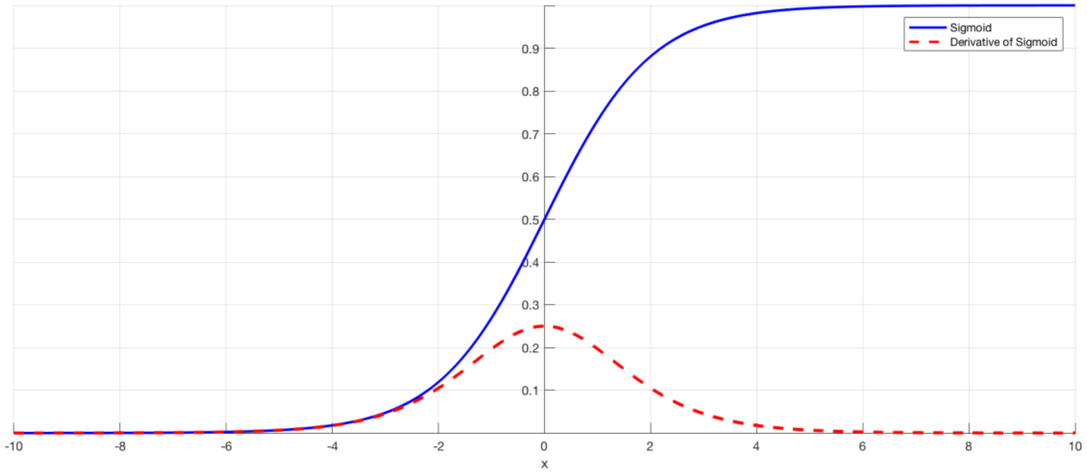
Binary classification: linear and logistic

- Linear regression:
  - Target is predicted by $h_\theta(x) = \theta^\top x$

- Logistic regression
  - Target is predicted by $h_\theta(x) = \sigma(\theta^\top x) = \dfrac{1}{1+ e^{-\theta^\top x}}$
    where
    $$\sigma(z) = \frac{1}{1 + e^{-z}}$$
    is the logistic function or the sigmoid function



Properties for the sigmoid function



- $\sigma(z) = \frac{1}{1+e^{-z}}$
  - Bounded in $(0,1)$
  - $\sigma(z) \to 1$ when $z \to \infty$
  - $\sigma(z) \to 0$ when $z \to -\infty$
- $\underline{\sigma'(z)} = \frac{d}{dz}\frac{1}{1+e^{-z}} = -(1+e^{-z})^{-2} \cdot (-e^{-z})$

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

$$= \frac{1}{1+e^{-z}}\left(1 - \frac{1}{1+e^{-z}}\right)$$

$$\underline{= \sigma(z)\big(1 - \sigma(z)\big)}$$

Logistic regression

- Binary classification

$$p_\theta(y=1|x) = \sigma(\theta^\top x) = \frac{1}{1+e^{-\theta^\top x}}$$

$$p_\theta(y=0|x) = \frac{e^{-\theta^\top x}}{1+e^{-\theta^\top x}}$$

- Cross entropy loss function

is also convex in θ

$$\mathcal{L}(y, x, p_\theta) = -y \log \sigma(\theta^\top x) - (1-y)\log(1-\sigma(\theta^\top x))$$

- Gradient

$$\frac{\partial \mathcal{L}(y, x, p_\theta)}{\partial \theta} = -y\frac{1}{\sigma(\theta^\top x)}\sigma(z)(1-\sigma(z))x - (1-y)\frac{-1}{1-\sigma(\theta^\top x)}\sigma(z)(1-\sigma(z))x$$

$$= (\sigma(\theta^\top x) - y)x$$

$$\theta \leftarrow \theta + \eta(y - \sigma(\theta^\top x))x$$

$$\boxed{\frac{\partial \sigma(z)}{\partial z} = \sigma(z)(1-\sigma(z))}$$

$$\theta_{\text{new}} \leftarrow \theta_{\text{old}} - \eta\frac{\partial \mathcal{L}(\theta)}{\partial \theta}$$

Label decision

- Logistic regression provides the probability

$$p_\theta(y=1|x) = \sigma(\theta^\top x) = \frac{1}{1+e^{-\theta^\top x}}$$

$$p_\theta(y=0|x) = \frac{e^{-\theta^\top x}}{1+e^{-\theta^\top x}}$$

- The final label of an instance is decided by setting a threshold h

$$\hat{y} = \begin{cases} 1, & p_\theta(y=1|x) > h \\ 0, & \text{otherwise} \end{cases}$$

How to choose the threshold

- Precision-recall trade-off
  - $\text{Precision} = \frac{\text{TP}}{\text{TP+FP}}$
  - $\text{Recall} = \frac{\text{TP}}{\text{TP+FN}}$

  - Higher threshold
    - More FN and less FP
    - Higher precision
    - Lower recall
  - Lower threshold
    - More FP and less FN
    - Lower precision
    - Higher recall

$$\hat{y} = \begin{cases} 1, & p_\theta(y = 1|x) > h \\ 0, & \text{otherwise} \end{cases}$$

Example

- We have the heights and weights of a group of students
  - Height: in inches,
  - Weight: in pounds
  - Male: 1, female, 0

- Please build a Logistic regression model to predict their genders

```
"Height","Weight","Male"
73.847017017515,241.893563180437,1
68.7819040458903,162.3104725213,1
74.1101053917849,212.7408555565,1
71.7309784033377,220.042470303077,1
69.8817958611153,206.349800623871,1
67.2530156878065,152.212155757083,1
68.7850812516616,183.927888604031,1
68.3485155115879,167.971110489509,1
67.018949662883,175.92944039571,1
63.4564939783664,156.399676387112,1
...
63.1794982498071,141.266099582434,0
62.6366749337994,102.85356321483,0
62.0778316936514,138.691680275738,0
60.0304337715611,97.6874322554917,0
59.0982500313486,110.529685683049,0
66.1726521477708,136.777454183235,0
67.067154649054,170.867905890713,0
63.8679922137577,128.475318784122,0
69.0342431307346,163.852461346571,0
61.9442458795172,113.649102675312,0
```

Example (cont.)

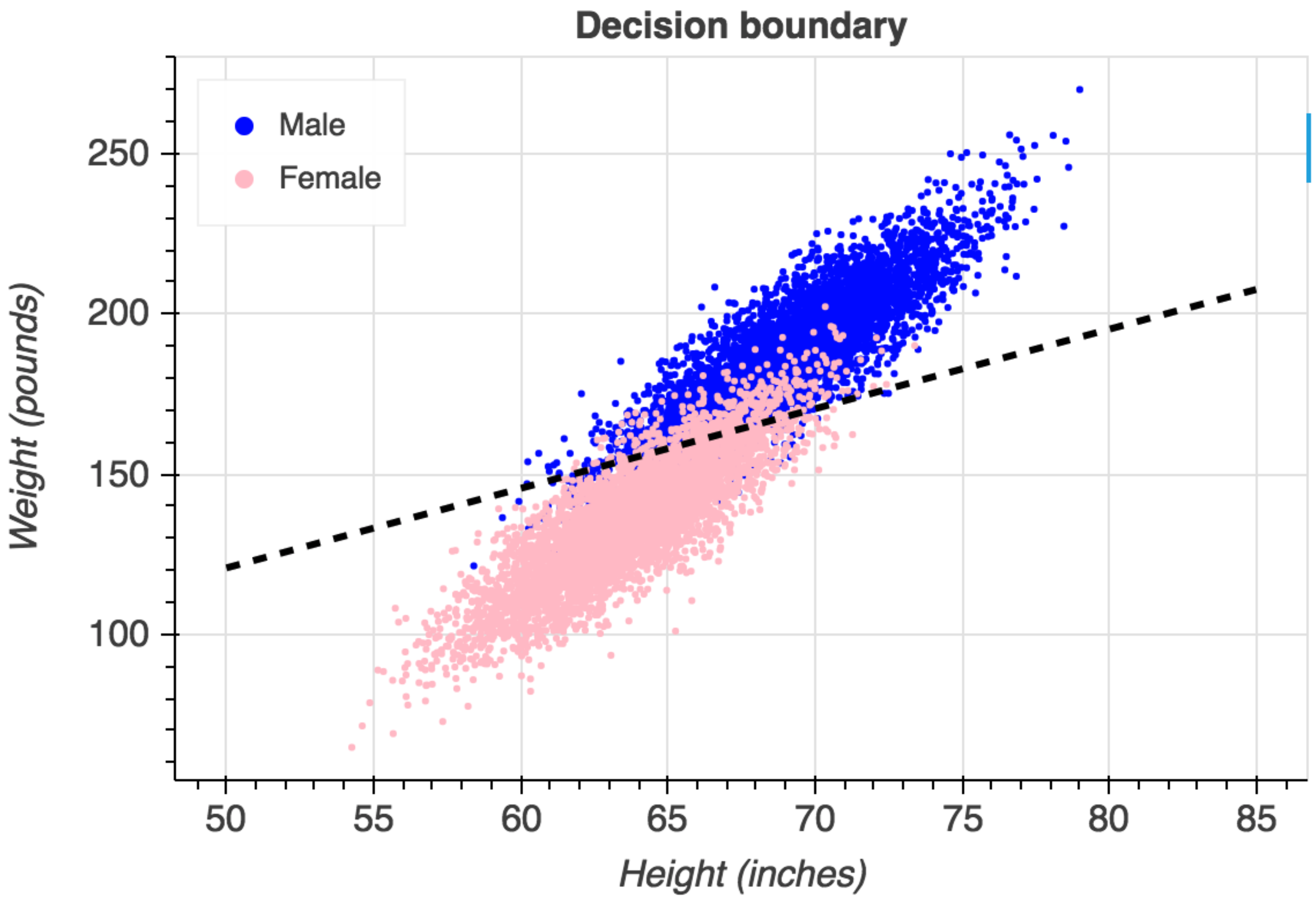
- As there are only two features, height and weight, the logistic regression equation is: $h_\theta(x) = \frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}$

- Solve it by gradient descent

There will be a lab hw on logistic regression

- The solution is $\theta = \begin{bmatrix} 0.69254 \\ -0.49269 \\ 0.19834 \end{bmatrix}$

Example (cont.)



- Threshold $h = 0.5$
- Decision boundary is
$$\theta_0 + \theta_1 x_1 + \theta_2 x_2 = 0$$

- Above the decision boundary lie most of the blue points that correspond to the Male class, and below it all the pink points that correspond to the Female class.

- The predictions won't be perfect and can be improved by including more features (beyond weight and height), and by potentially using a different decision boundary (e.g. nonlinear)

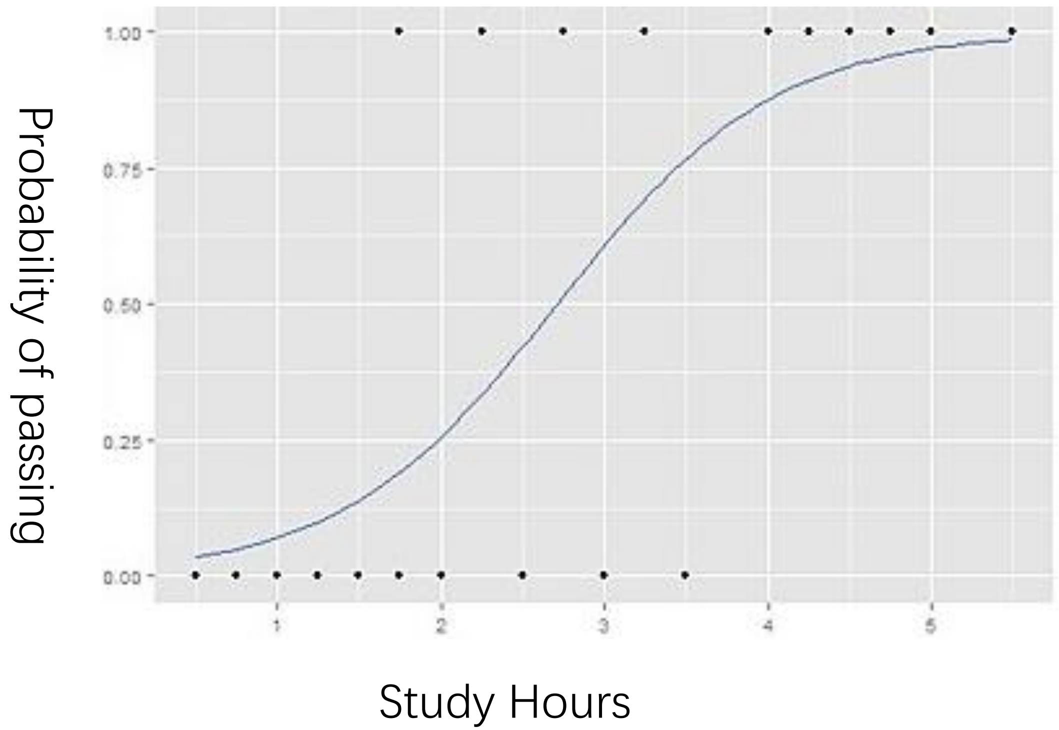
Example 2

- A group of 20 students spends between 0 and 6 hours studying for an exam. How does the number of hours spent studying affect the probability of the student passing the exam?

Hours	Pass		Hours	Pass
0.50	0		2.75	1
0.75	0		3.00	0
1.00	0		3.25	1
1.25	0		3.50	0
1.50	0		4.00	1
1.75	0		4.25	1
1.75	1		4.50	1
2.00	0		4.75	1
2.25	1		5.00	1
2.50	0		5.50	1

Example 2 (cont.)

- $h_\theta(x) = \dfrac{1}{1+e^{-(1.5046*hours-4.0777)}}$



Interpretation of logistic regression

- Given a probability p, the odds of p is defined as $odds = \frac{p}{1-p}$
- The logit is defined as the log of the odds: $\ln(odds) = \ln(\frac{p}{1-p})$
- Let $\ln(odds) = \theta^T x$, we will have $\ln(\frac{p}{1-p}) = \theta^T x$, and

$$p = \frac{1}{1 + e^{-\theta^T x}}$$

- So in logistic regression, the logit of an event(predicted positive)'s probability is defined as a result of linear regression

More Measures for Classification

Confusion matrix

- Remember what we have learned about the confusion matrix

		Prediction	
		1	0
Label	1	True Positive	False Negative
	0	False Positive	True Negative

- **Precision**: the ratio of true class 1 cases in those with prediction 1

$$\text{Prec} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

		Prediction	
		1	0
Label	1	True Positive	False Negative
	0	False Positive	True Negative

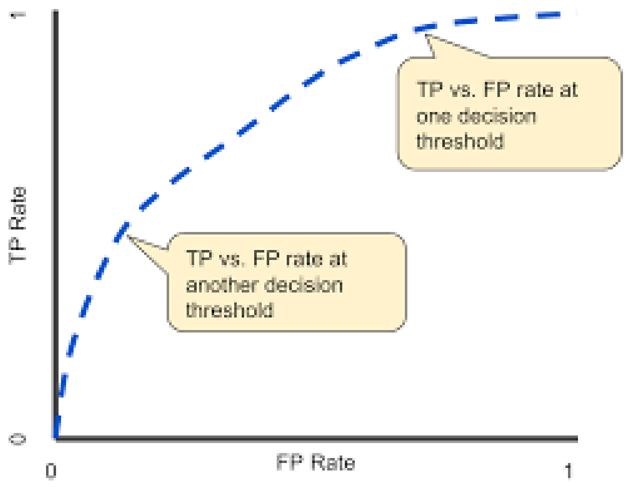
- **Recall**: the ratio of cases with prediction 1 in all true class 1 cases

$$\text{Rec} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{F1} = \frac{2 \times \text{Prec} \times \text{Recall}}{\text{Prec} + \text{Rec}}$$

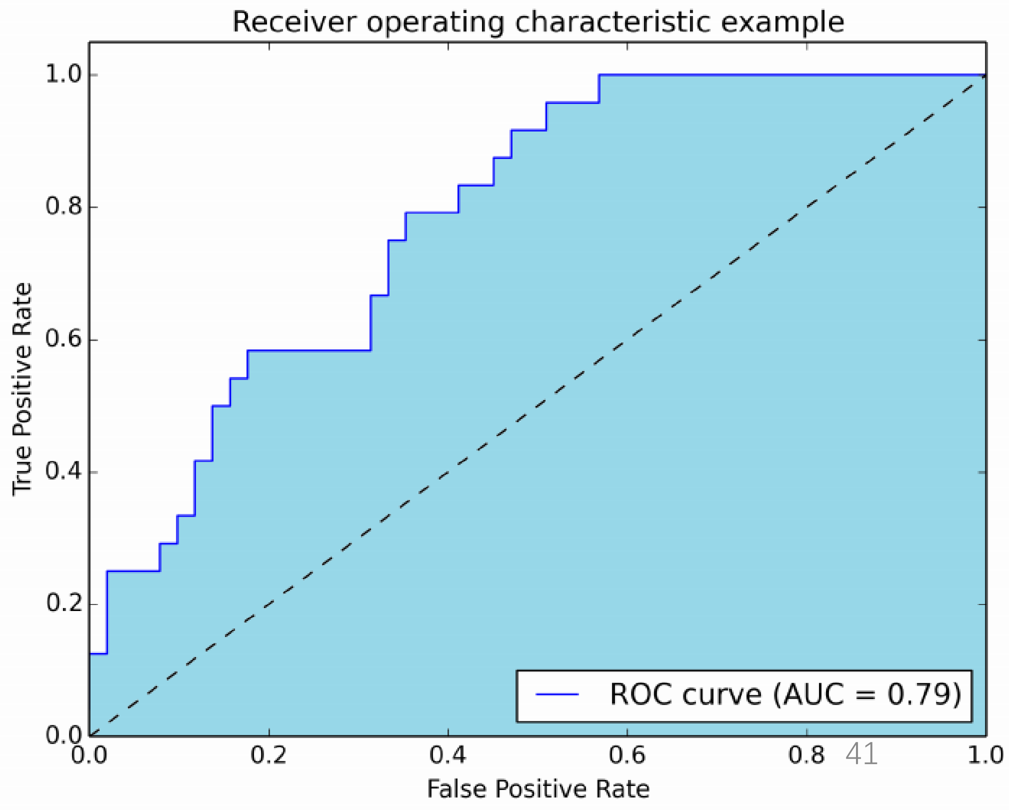
- These are the basic matrices to measure the classifier

Area Under ROC Curve (AUC)

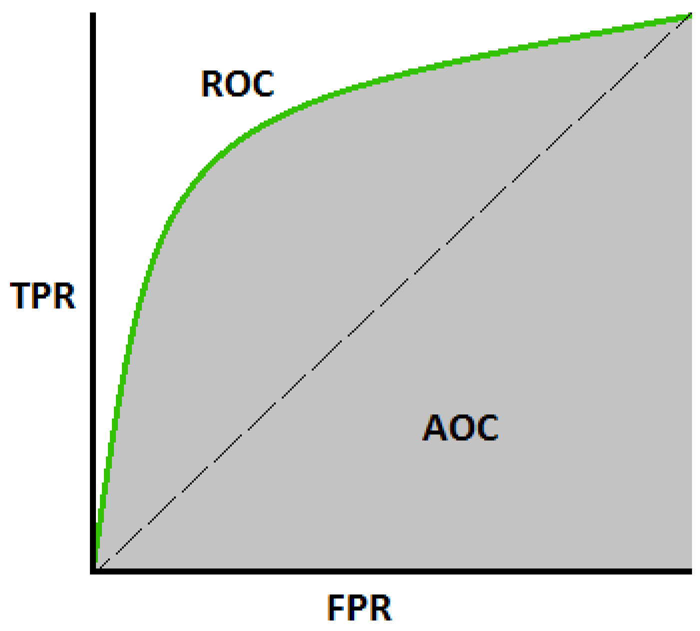


- A performance measurement for classification problem at various thresholds settings
- Tells how much the model is capable of distinguishing between classes
- Receiver Operating Characteristic (ROC) Curve
  - TPR against FPR
  - TPR/Recall/Sensitivity $= \frac{TP}{TP+FN}$

    FPR=1-Specificity= $\frac{FP}{TN+FP}$



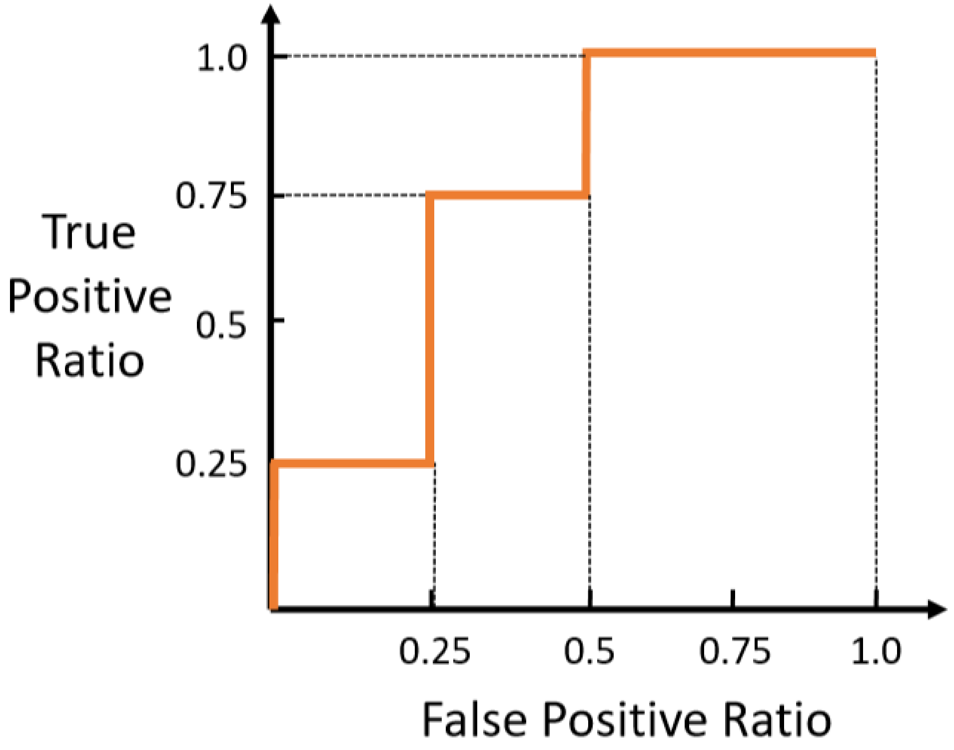
AUC (cont.)



TPR: true positive rate
FPR: false positive rate

- It’s the relationship between TPR and FPR when the threshold is changed from 0 to 1
- In the top right corner, threshold is 0, and every thing is predicted to be positive, so both TPR and FPR is 1
- In the bottom left corner, threshold is 1, and every thing is predicted to be negative, so both TPR and FPR is 0
- The size of the area under this curve (AUC) is an important matric to binary classifier
- Perfect classifier get AUC=1 and random classifier get AUC = 0.5

AUC example

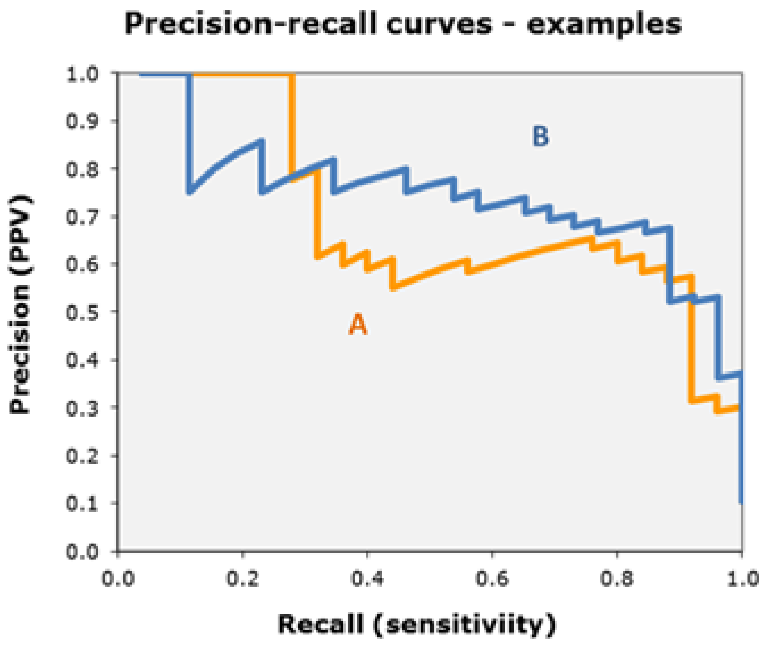


AUC = 0.75

Prediction	Label
0.91	1
0.85	0
0.77	1
0.72	1
0.61	0
0.48	1
0.42	0
0.33	0

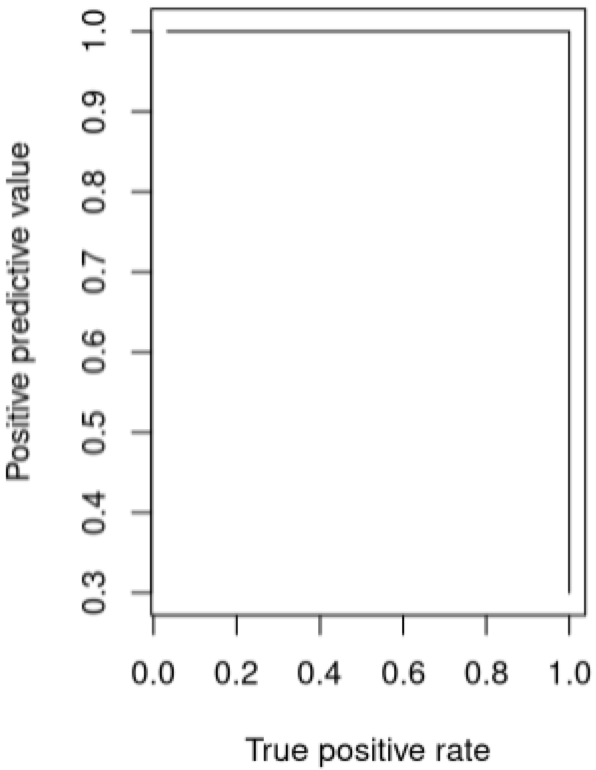
Precision recall curve

- The precision recall curve, or pr curve, is another plot to measure the performance of binary classifier.

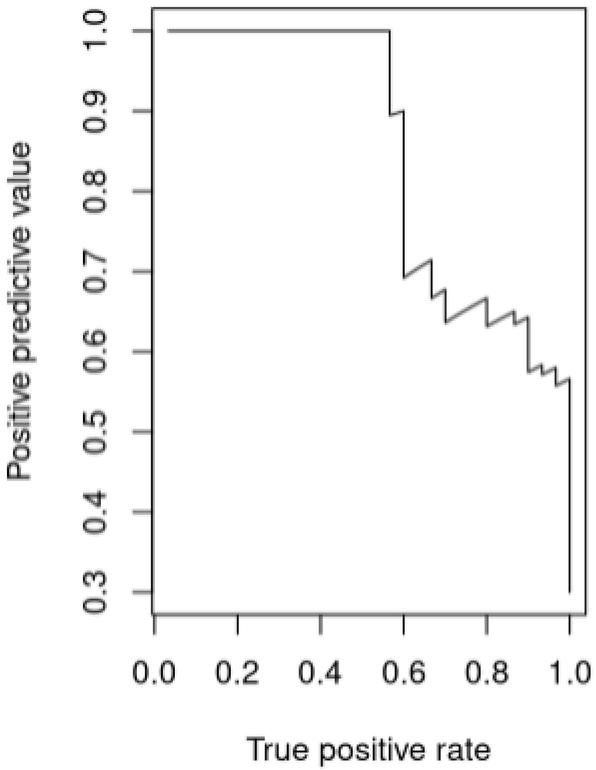


- It’s the relationship between Precision and Recall when the threshold is changed from 0 to 1
- It’s more complex than the ROC curve
- The size of the area under this curve is an important matric to binary classifier
- It can handle imbalanced dataset
- Usually, the classifiers gets lower AUPR value than AUC value

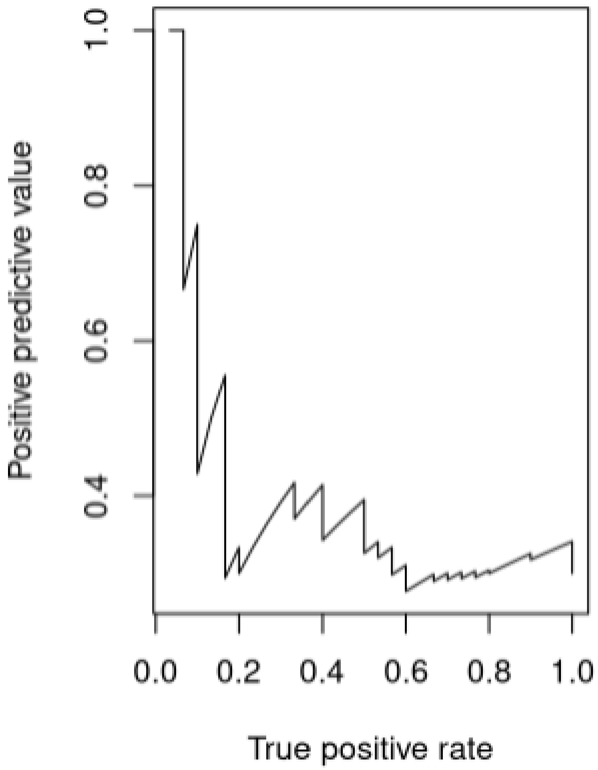
AUPR examples



Perfect: 1



Good: 0.92



Random: 0.56

Class Imbalance

Class imbalance

- Down sampling
  - Sample less on frequent class
- Up sampling
  - Sample more on infrequent class
- Hybrid Sampling
  - Combine them two

Weighted loss functions

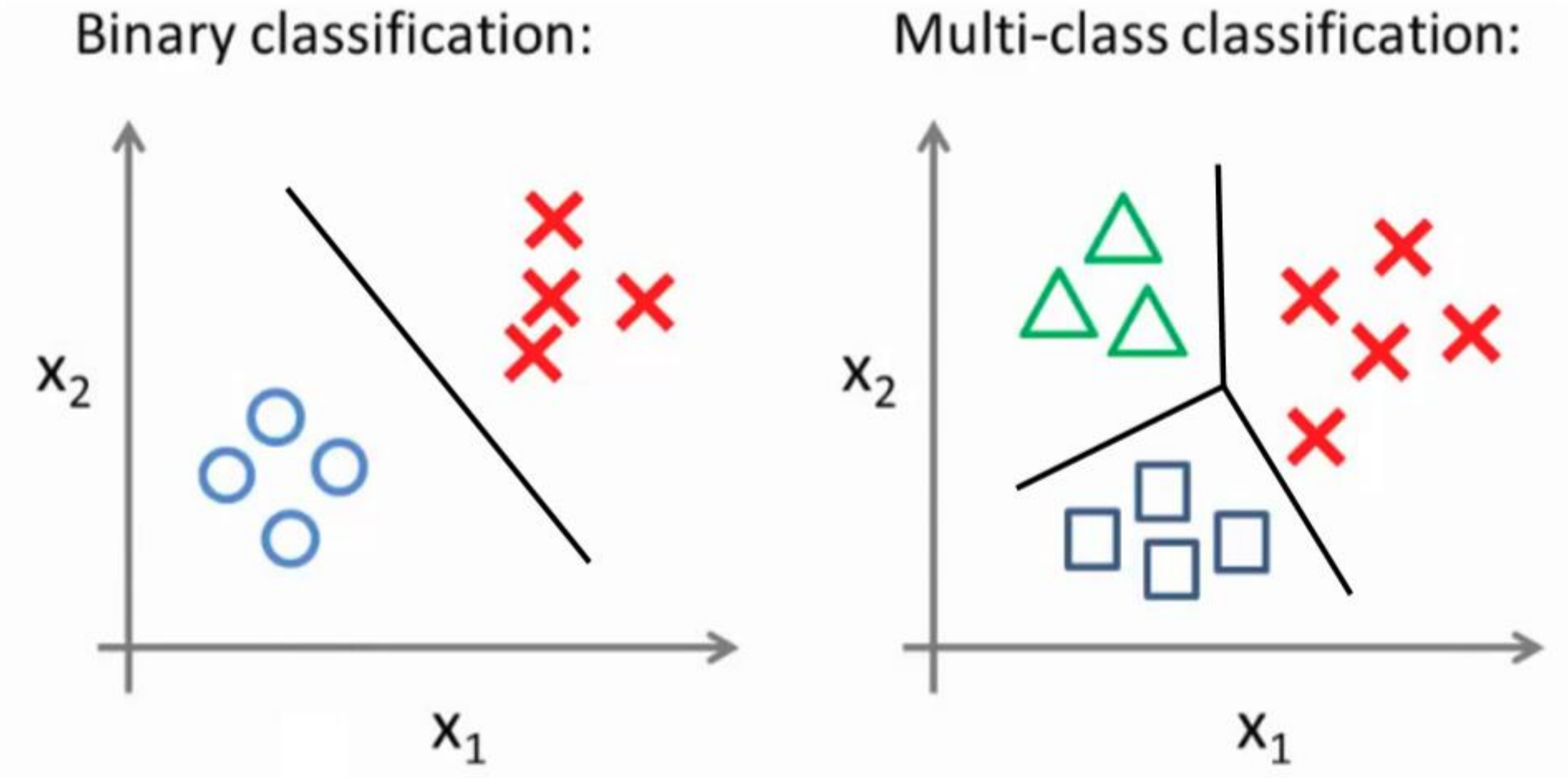
$$L(y, x, p_\theta) = -y \log p_\theta(1|x) - (1 - \mathrm{y})\log(1 - p_\theta(1|x))$$

$$L(y, x, p_\theta) = -w_1 y \log p_\theta(1|x) - w_0(1 - \mathrm{y})\log(1 - p_\theta(1|x))$$

Multi-Class Logistic Regression

Multi-class classification

- $L(y, x, p_\theta) = -\sum_{i=1}^{m} 1_{y=C_k} \log p_\theta(C_k|x)$



Multi-Class Logistic Regression

- Class set $C = \{c_1, c_2, \ldots, c_m\}$

- Predicting the probability of $p_\theta(y = c_j|x)$

$$p_\theta(y = c_j|x) = \frac{e^{\theta_j^\top x}}{\sum_{k=1}^m e^{\theta_k^\top x}} \quad \text{for } j = 1, \ldots, m$$

- Softmax
  - Parameters $\theta = \{\theta_1, \theta_2, \ldots, \theta_m\}$
  - Can be normalized with m-1 groups of parameters

Multi-Class Logistic Regression

- Learning on one instance $(x, y = c_j)$
  - Maximize log-likelihood

$$\max_{\theta} \log p_\theta(y = c_j|x)$$

  - Gradient

$$\begin{aligned}
\frac{\partial \log p_\theta(y = c_j|x)}{\partial \theta_j} &= \frac{\partial}{\partial \theta_j} \log \frac{e^{\theta_j^\top x}}{\sum_{k=1}^m e^{\theta_k^\top x}} \\
&= x - \frac{\partial}{\partial \theta_j} \log \sum_{k=1}^m e^{\theta_k^\top x} \\
&= x - \frac{e^{\theta_j^\top x} x}{\sum_{k=1}^m e^{\theta_k^\top x}}
\end{aligned}$$

Summary

- Discriminative / Generative Models
- Logistic regression (binary classification)
  - Cross entropy
  - Formulation, sigmoid function
  - Training—gradient descent
- More measures for binary classification (AUC, AUPR)
- Class imbalance
- Multi-class logistic regression

Next Lecture

SVM

Shuai Li

https://shuaili8.github.io

Questions?

https://shuaili8.github.io/Teaching/VE445/index.html