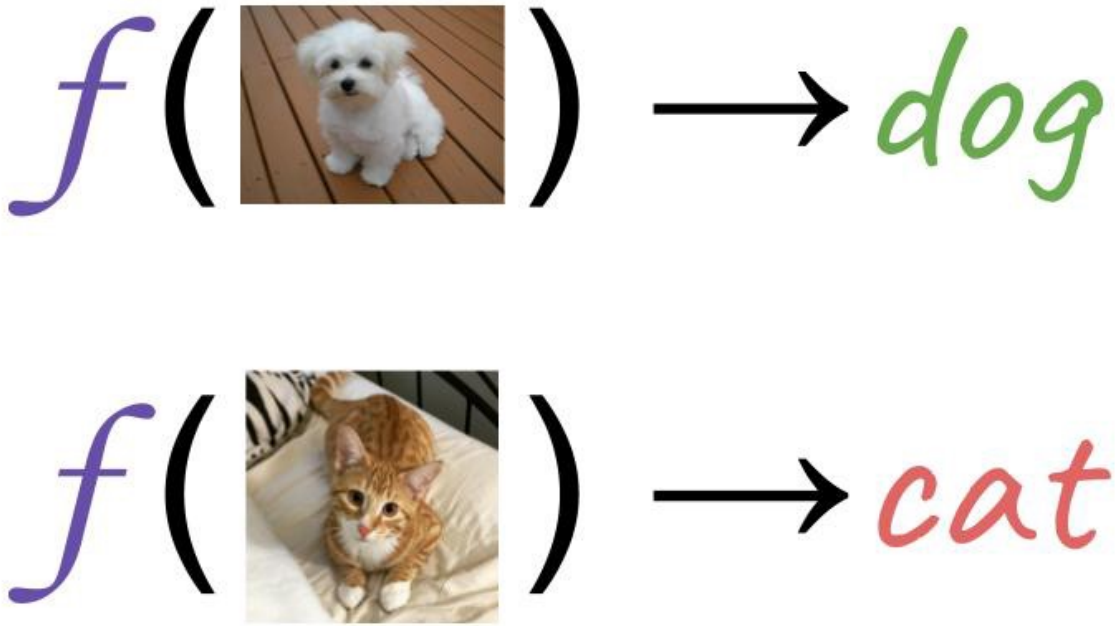
Logistic Regression and Classifications

Shaobo Li

University of Kansas

From Continuous to Categorical Outcome



- Response Y: discrete value
  - e.g., $Y = \{\text{dog, cat}\}$
  - or $Y = \{0, 1\}$, 1 - dog; 0 - not dog

Classification Methods

- K-Nearest Neighbor
- Logistic regression
- Classification tree
- Random forest
- Boosted tree
- Support vector machine
- Neural networks
- Deep learning
- ...
- Is clustering a classification model?

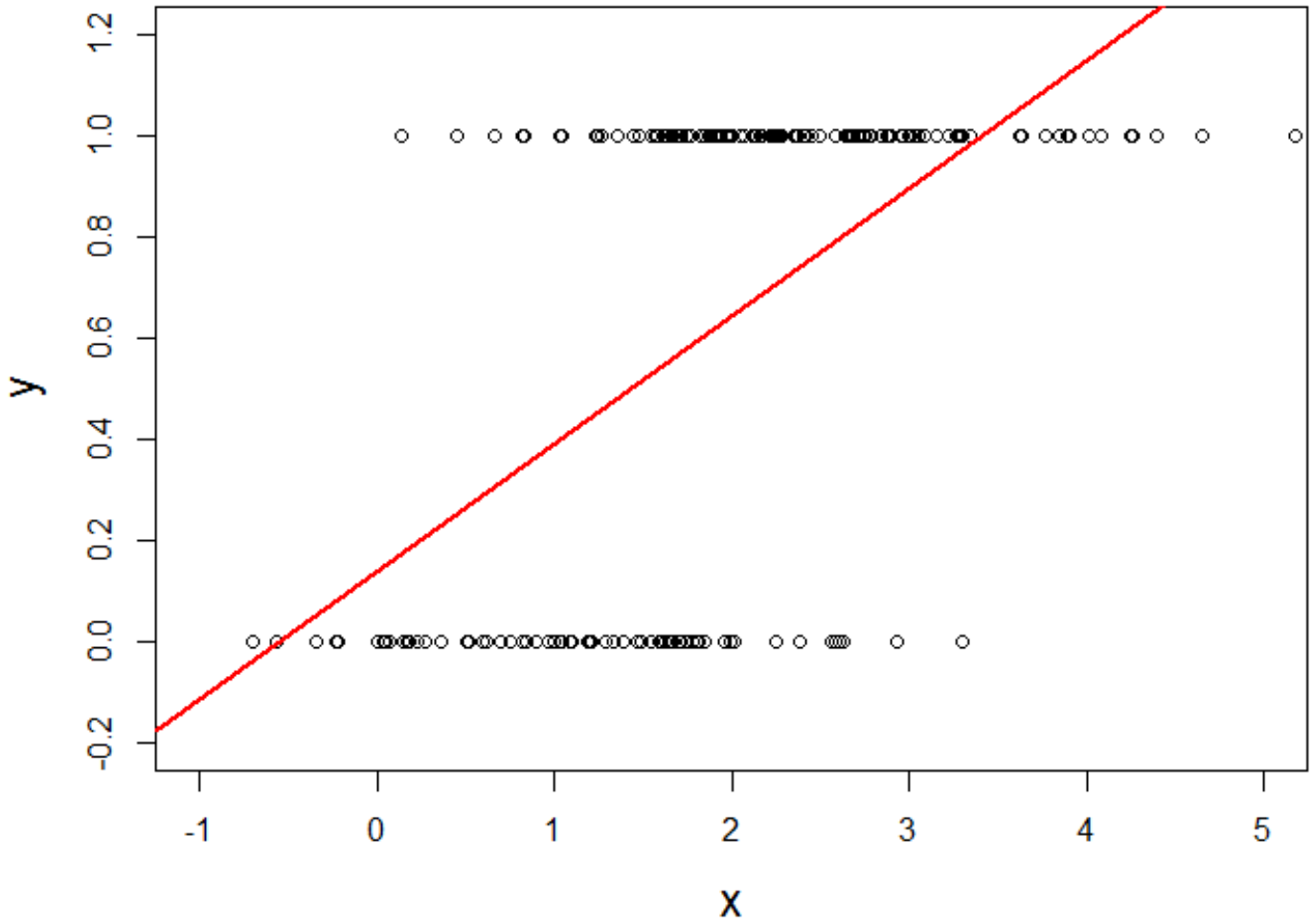
Why Not Linear Regression

- Example: default prediction
  - Default ($Y = 1$) vs. Nondefault ($Y = 0$)
  - X_1: credit card balance level, X_2: income level
- Suppose the estimated linear regression is

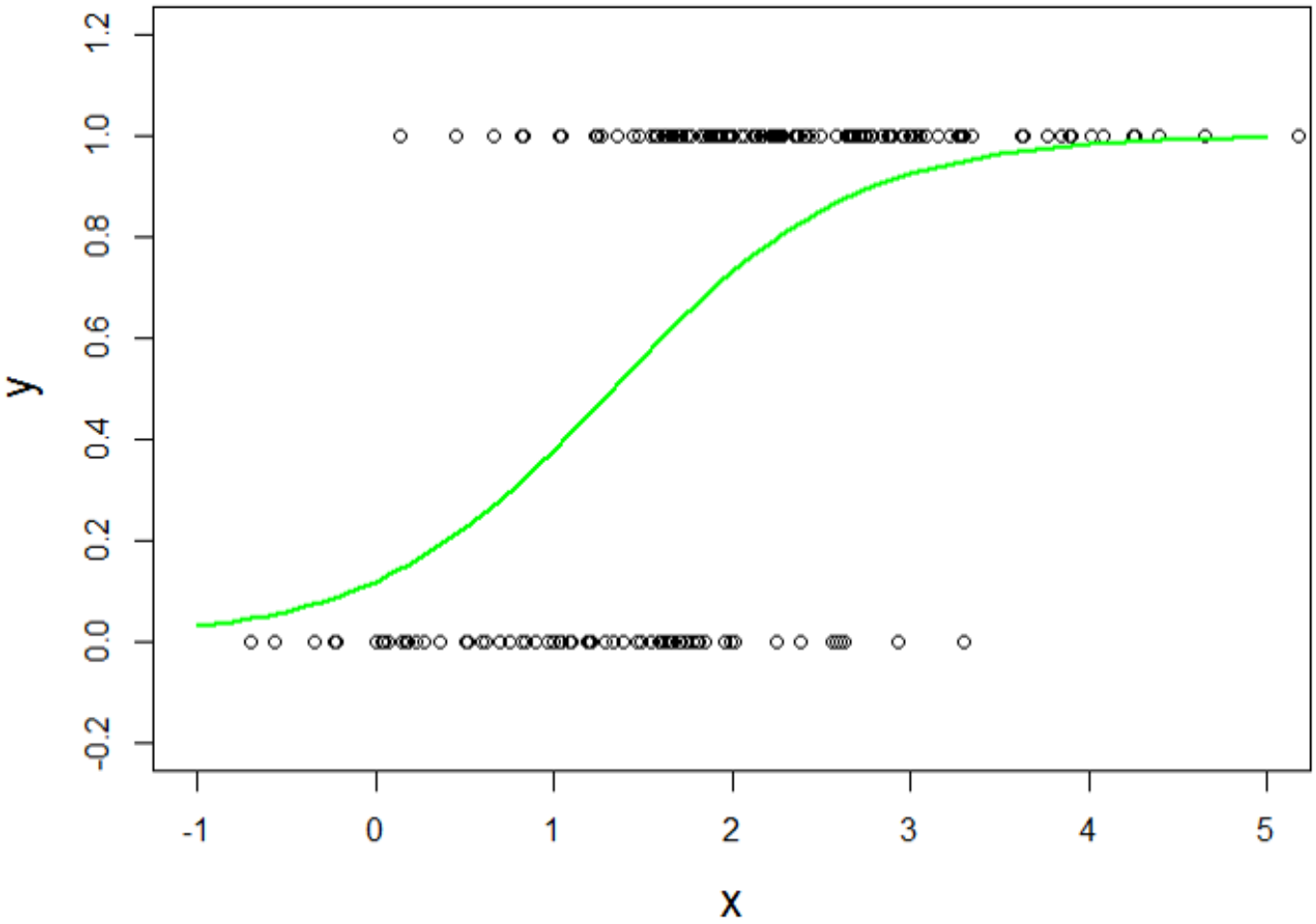
$$\hat{Y} = -1.5 + 2X_1 - X_2$$

- What is the predicted value if a person's balance level is 1 and income level is 3?
- How to interpret this value?

An Illustration



An Illustration



Classification

- Denote $\mathcal{C}(X)$ as a classifier
- Most DM algorithms produce probabilistic outcome
  - e.g. probability that X belongs to each class
- Classification is based on certain decision rules
- Example: The model prediction tells that the probability of default is 0.2, then

Threshold	<0.1	>0.1
Class	Nondefault	Default

Logistic Regression

- For binary response:

$$\mathbb{P}(y_i = 1|\mathbf{x}_i) = \frac{1}{1 + \exp(-\beta^T \mathbf{x}_i)}$$

  - Sigmoid function: $s(u) = \frac{1}{1+e^{-u}}$
  - Interpretation: **probability** of event conditional on X
- More than two classes: *multinomial logistic model*
- Can you re-write the model such that the right-hand side is the linear predictor?

Odds and Interpretation of β

- Let $P = \mathbb{P}(Y = 1|\mathbf{X})$, then

$$\text{logit}(P) = \log\left(\frac{P}{1-P}\right) = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p$$

  - The probability ratio $\frac{P}{1-P}$ is called odds, a function of X
  - Logistic model is also called log-odds model

- Interpretation of β_1
  - with 1 unit increase on X_1, the log odds changes by β_1
  - Can we say the odds changes by e^{β_1}?

- By simple algebra, given all X's are fixed except for X_j

$$\beta_j = \log\left(\frac{\text{Odds}(X_j + 1)}{\text{Odds}(X_j)}\right)$$

this is *log of odds ratio*.

Odds and Interpretation of β

Exercise: Suppose we are interested in predicting corporate bankruptcy using the logistic model. The parameter estimate for Earning is -1.29. This number means:
Holding all other predictors fixed, for every one-unit increase in earning,

a) the probability of bankruptcy decreases 1.29%.

b) the odds of bankruptcy decreases 1.29%.

c) the odds of bankruptcy changes by $(e^{\beta_1} - 1) * 100\%$.

d) the odds of bankruptcy decreases 1.29.

e) the log of odds of bankruptcy decreases by 1.29.

f) the odds of bankruptcy is 1.29 times lower.

g) the odds of bankruptcy is $e^{1.29}$ times lower.

Multinomial Logit Model

- Response $Y = 1, 2, ..., K$, K classes
- Given predictors $\mathbf{x}_i$

$$\log\left(\frac{\mathbb{P}(y_i = 2)}{\mathbb{P}(Y_i = 1)}\right) = \beta_2^T \mathbf{x}_i$$
$$\log\left(\frac{\mathbb{P}(y_i = 3)}{\mathbb{P}(Y_i = 1)}\right) = \beta_3^T \mathbf{x}_i$$
$$\vdots$$
$$\log\left(\frac{\mathbb{P}(y_i = K)}{\mathbb{P}(Y_i = 1)}\right) = \beta_K^T \mathbf{x}_i$$

- The first class "1" is the reference
- There are $(K-1) \times (p+1)$ coefficients need to be estimated.

Loss Function (in machine learning)

- Recall OLS

$$L_{OLS}(\beta) = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2$$

- For logistic regression, we have a different loss

$$L_{logit}(\beta) = \sum_{i=1}^{n} -2 \left[y_i \log p_i + (1 - y_i) \log(1 - p_i) \right]$$

where $p_i = \frac{1}{1+\exp(-\beta_0 - \sum_{j=1}^{p} \beta_j x_{ij})}$

Maximum Likelihood Estimation (in statistics)

- $y_i = \begin{cases} 1 & \text{with Prob. } p_i \\ 0 & \text{with Prob. } 1-p_i \end{cases}$, $p_i = \frac{1}{1+\exp(-\beta_0 - \sum_{j=1}^{p} \beta_j x_{ij})}$
- Likelihood function of ith observation $y_i|\mathbf{x}_i$:

$$Likelihood_i = p_i^{y_i} \times (1-p_i)^{1-y_i}$$

- Likelihood function of all observations, $i = 1, ..., n$:

$$Likelihood = \prod_{i=1}^{n} p_i^{y_i} \times (1-p_i)^{1-y_i}$$

- log-likelihood for all observations:

$$logLik(\beta) = \sum_{i=1}^{n} [y_i \log p_i + (1-y_i) \log(1-p_i)]$$

How to solve for β?

- Unlike OLS, there is no analytical solution for logit model
- Numeric solution (below is a univariate example)
  - Gradient descent

$$\hat{\beta}^{(n+1)} = \hat{\beta}^{(n)} - \alpha * L'(\hat{\beta}^{(n)})$$

where α is called learning rate.

  - Newton's method (a very good tutorial)

$$\hat{\beta}^{(n+1)} = \hat{\beta}^{(n)} - \frac{L'(\hat{\beta}^{(n)})}{L''(\hat{\beta}^{(n)})}$$

- We call derivative for univariate: $f'(x)$, $f''(x)$
- We call gradient for multivariate: $\nabla f(x)$, $\nabla^2 f(x)$

Prediction — From Probability to Class

- Direct outcome of model: probability
- Next step: classification
- Need decision rule (cut-off probability – p-cut)
- Not unique

Confusion Matrix

- Classification table based on a specific cut-off probability
- Used for model assessment

	Pred=1	**Pred=0**
True=1	True Positive (TP)	False Negative (FN)
True=0	False Positive (FP)	True Negative (TN)

- FP: type I error; FN: type II error
- Different p-cut results in different confusion matrix
- Try to understand this table instead of memorizing!

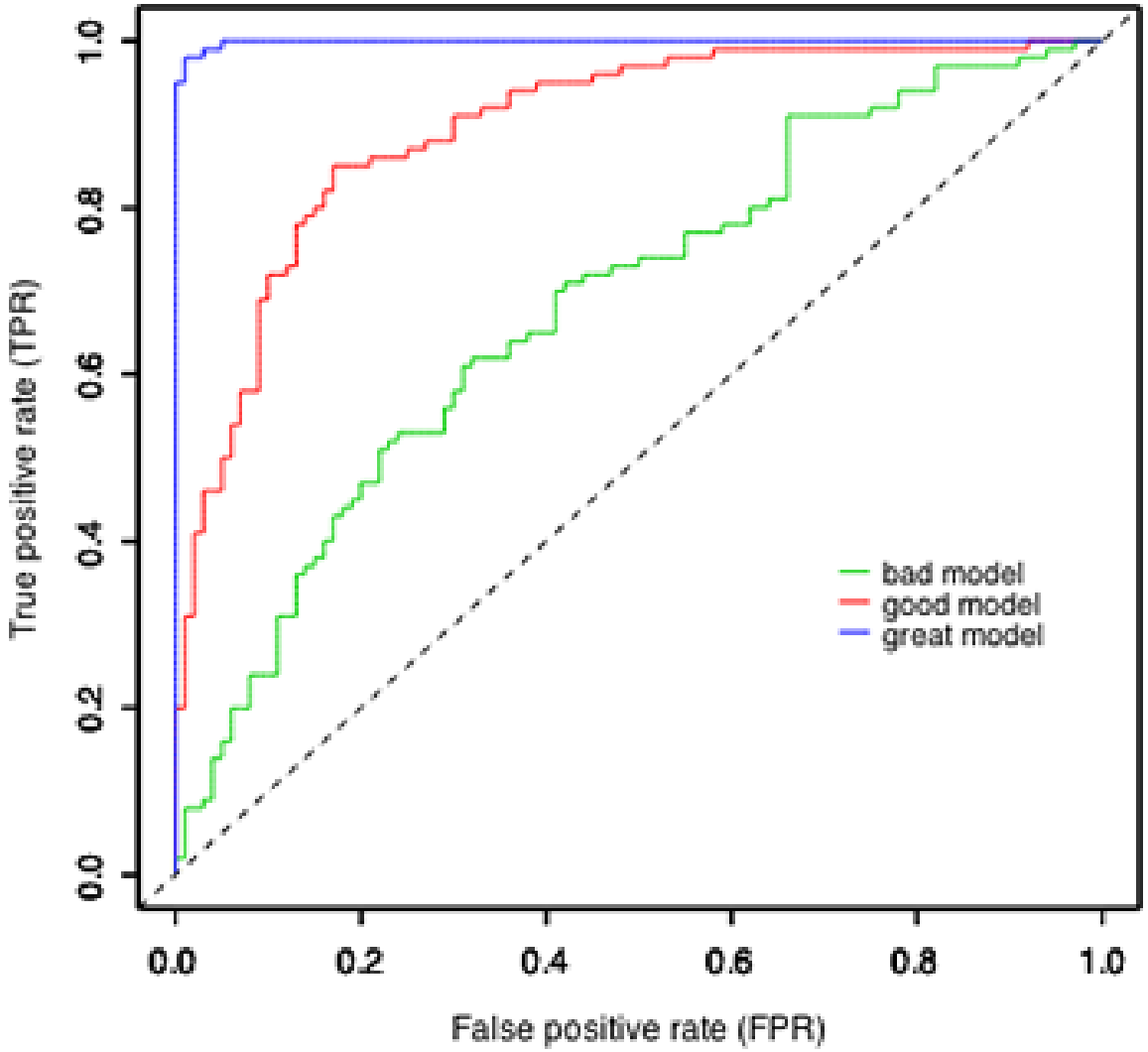
Some Useful Measures

- Misclassification rate (MR) $= \frac{\text{FP}+\text{FN}}{\text{Total}}$
- True positive rate (TPR) $= \frac{\text{TP}}{\text{TP}+\text{FN}}$: Sensitivity or Recall
- True negative rate (TNR) $= \frac{\text{TN}}{\text{FP}+\text{TN}}$: Specificity
- False positive rate (FPR) $= \frac{\text{FP}}{\text{FP}+\text{TN}}$: 1 – Specificity
- True negative rate (FNR) $= \frac{\text{FN}}{\text{TP}+\text{FN}}$: 1 – Sensitivity

ROC Curve

- Receiver Operating Characteristic
- Plot of FPR (X) against TPR (Y) at various p-cut values
- Overall model assessment (not for a particular decision rule)
- Unique for a given model
- Area under the curve (AUC): a measure of goodness-of-fit

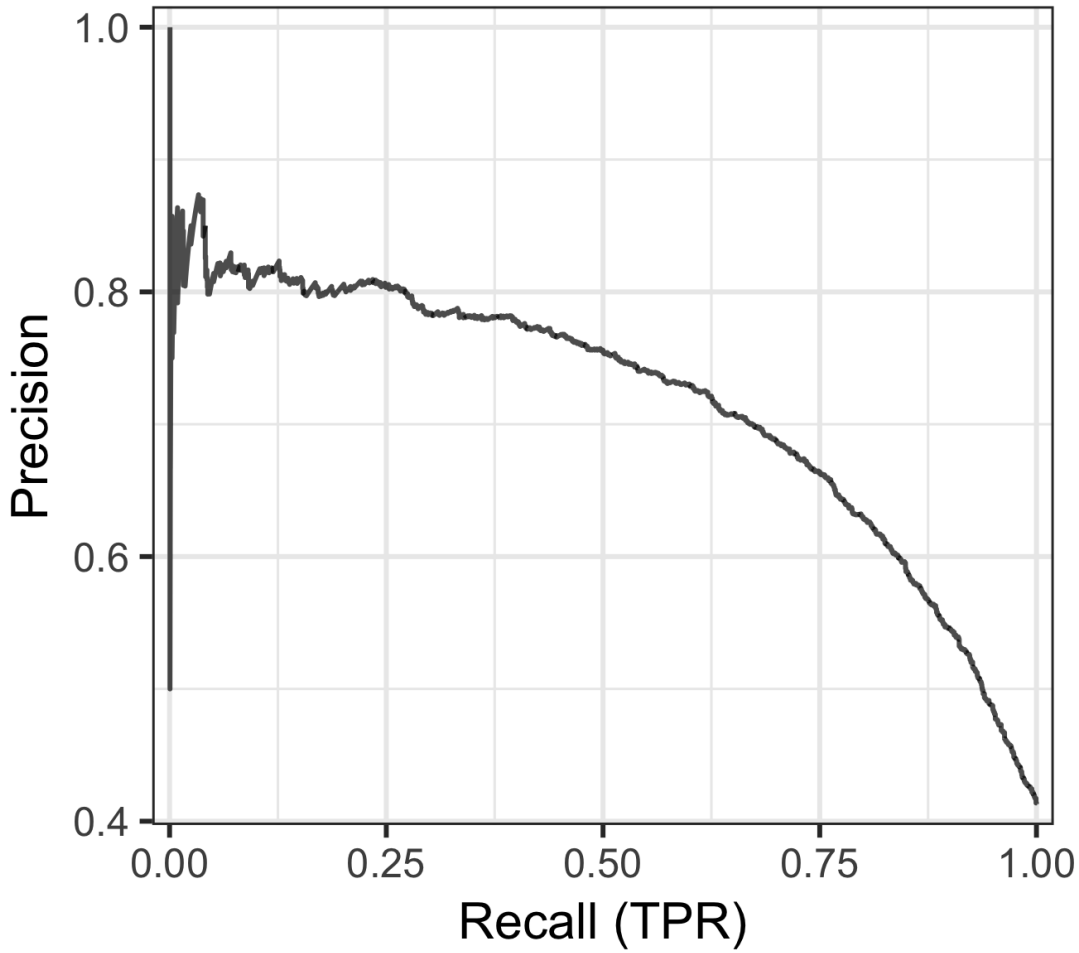
ROC Curve


True positive rate (TPR)
False positive rate (FPR)
0.0
0.2
0.4
0.6
0.8
1.0
bad model
good model
great model

Precision and Recall

- More accurate measure for imbalanced data
- Widely used in document retrieval (e.g., spam classification)
- Precision $= \frac{\text{TP}}{\text{TP}+\text{FP}}$
  - fraction of retrieved instances that are relevant
- Recall $= \frac{\text{TP}}{\text{TP}+\text{FN}}$, which is the same as TPR
  - fraction of relevant instances that are retrieved
- This pair of measures emphasizes the positive cases
- There is a trade-off between precision and recall
- $F1$-score: $F1 = 2 \times \frac{\text{precision} \times \text{recall}}{\text{precision}+\text{recall}}$. (harmonic mean)
  - a popular measure to balance the tradeoff.

Precision-Recall Curve



Exercise

The following R code demonstrate the idea of measuring the overall discriminant power of a model (predicted probability). Complete the code and draw ROC and PR curve. In addition, find the the optimal cut-off with respect to accuracy rate and F1-score.

Source on Save

```r
set.seed(750)
n <- 200
p <- runif(n)
y <- rbinom(n,1,p)
head(cbind(y,p))

pcut <- seq(0.1,0.9,0.05)
v1<- NULL
for(i in 1:length(pcut)){
  yhat <- (p>pcut[i])*1
  confMat <- table(y,yhat,dnn = c("True", "Pred"))
  TPR <- sum(y==1 & yhat==1)/sum(y==1)
  TNR <-
  FPR <-
  FNR <-
  Precis <-
  v1 <- rbind(v1, c(TPR=TPR, TNR=TNR, FPR=FPR, FNR=FNR, Precis=Precis))
  cat("pcut:", pcut[i], "TPR:", TPR, "TNR:", TNR, "FPR:", FPR, "FNR:", FNR, "Precision", Precis, '\n')
  print(confMat)
}

```

Download the code here.

Asymmetric Cost

- Example: compare following two confusion matrices based on two p-cut values

	Pred=1	**Pred=0**
True=1	10	40
True=0	10	440

	Pred=1	**Pred=0**
True=1	40	10
True=0	130	320

- Which one is better? In terms of what?
- What if this is about loan application
  - $Y = 1$: default customer
  - Default will cost much more than reject a loan application

Choice of Decision Threshold (p-cut)

- Do NOT simply use 0.5!
- In general, we use grid search method to optimize a measure of classification accuracy/loss
  - Cost function (symmetric or asymmetric) based on FP and FN
  - F1-score based on precision and recall

Discriminant Analysis

- Based on Bayes theorem:

$$\mathbb{P}(Y = k|X = x) = \frac{\mathbb{P}(X = x|Y = k) \times \mathbb{P}(Y = k)}{\mathbb{P}(X = x)}$$

- Discriminant analysis

$$\mathbb{P}(Y = k|X = x) = \frac{f_k(x) \times \pi_k}{\sum_{l=1}^{K} f_l(x) \times \pi_l}$$

- $f_k(x)$ is the assumed density function of X in class k
- π_k can be simply calculated as the fraction of $Y = k$

Linear Discriminant Function

- Given x, find the k such that $f_k(x) \times \pi_k$ is largest
- Therefore, only $f_k(x) \times \pi_k$ is of interest
- We assume $f_k(x)$ to be Gaussian density

$$f_k(x) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{(x-\mu_k)^2}{2\sigma_k^2}\right)$$

- By taking log and discard terms without k, we have

$$\delta_k(x) = x \cdot \frac{\mu_k}{\sigma_k^2} - \frac{\mu_k^2}{2\sigma_k^2} + \log(\pi_k)$$

- This is called *linear discriminant score function*

Comparison Between Logistic Model and LDA

- Logistic regression is a very popular classifier especially for binary classification problem
- LDA is often used when n is small and classes are well separated, and Gaussian assumption is reasonable. Also when $K > 2$.
- Both are linear methods