Machine learning lecture slides

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COMS 4771 Fall 2020

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Prediction theory

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Outline

- Statistical model for binary outcomes
- Plug-in principle and IID model
- Maximum likelihood estimation
- Statistical model for binary classification
- Analysis of nearest neighbor classifier
- Estimating the error rate of a classifier
- Beyond binary classificaiton and the IID model

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Statistical model for binary outcomes

- Example: coin toss
- Physical model: hard
- Statistical model: outcome is random
  - *Bernoulli distribution* with heads probability $\theta \in [0, 1]$
  - Encode heads as 1 and tails as 0
  - Written as $\mathrm{Bernoulli}(\theta)$
  - Notation: $Y \sim \mathrm{Bernoulli}(\theta)$ means Y is a random variable with distribution $\mathrm{Bernoulli}(\theta)$.
- Goal: correctly predict outcome

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Optimal prediction

- Suppose $Y \sim \text{Bernoulli}(\theta)$.
  - Suppose θ known.
  - Optimal prediction:

$$\mathbf{1}_{\{\theta > 1/2\}}$$

    - Indicator function notation:

$$\mathbf{1}_{\{Q\}} := \begin{cases} 1 & \text{if } Q \text{ is true} \\ 0 & \text{if } Q \text{ is false} \end{cases}$$

  - The optimal prediction is incorrect with probability

$$\min\{\theta, 1-\theta\}$$

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Learning to make predictions

- If θ unknown:
  - Assume we have data: outcomes of previous coin tosses
  - Data should be related to what we want to predict: same coin is being tossed

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Plug-in principle and IID model

- *Plug-in principle*:
  - Estimate unknown(s) based on data (e.g., θ)
  - Plug estimates into formula for optimal prediction

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- When can we estimate the unknowns?
  - Observed data should be related to the outcome we want to predict
  - *IID model*: Observations & (unseen) outcome are *iid* random variables
  - *iid*: independent and identically distributed
  - Crucial modeling assumption that makes learning possible

- When is the IID assumption not reasonable? ...

Statistical models

- *Parametric statistical model* $\{P_\theta : \theta \in \Theta\}$
  - collection of parameterized probability distributions for data
  - Θ is the *parameter space*
  - One distribution per parameter value $\theta \in \Theta$
- E.g., distributions on n binary outcomes treated as iid Bernoulli random variables
  - $\Theta = [0, 1]$
  - Overload notation: P_θ is the *probability mass function* (*pmf*) for the distribution.
  - What is formula for $P_\theta(y_1, \dots, y_n)$ for $(y_1, \dots, y_n) \in \{0, 1\}^n$?

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- *Likelihood* of parameter θ (given observed data)
  - $L(\theta) = P_\theta(y_1, \ldots, y_n)$
- *Maximum likelihood estimation*:
  - Choose θ with highest likelihood
- *Log-likelihood*
  - Sometimes more convenient
  - ln is increasing, so $\ln L(\theta)$ orders the parameters in the same way as $L(\theta)$

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Maximum likelihood estimation (2)

- Coin toss example
  - Log-likelihood

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$$\ln L(\theta) = \sum_{i=1}^{n} y_i \ln \theta + (1 - y_i) \ln(1 - \theta)$$

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  - Use calculus to determine formula for maximizer
  - This is a little annoying, but someone else has already done it for you:

$$\hat{\theta}_{\text{MLE}} := \frac{1}{n} \sum_{i=1}^{n} y_i.$$

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Back to plug-in principle

- We are given data $y_1, \dots, y_n \in \{0, 1\}^n$, which we model using the IID model from before
- Obtain estimate $\hat{\theta}_{\mathrm{MLE}}$ of known θ based on $y_1, \dots, y_n$
- Plug-in $\hat{\theta}_{\mathrm{MLE}}$ for θ in formula for optimal prediction:

$$\hat{Y} := \mathbf{1}_{\{\hat{\theta}_{\mathrm{MLE}} > 1/2\}}.$$

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Analysis of the plug-in prediction (1)

- How good is the plug-in prediction?
  - Study behavior under the IID model, where $Y_1, \ldots, Y_N, Y \sim_{\text{iid}} \text{Bernoulli}(\theta)$.
    - $Y_1, \ldots, Y_n$ are the data we collected
    - Y is the outcome to predict
    - θ is the unknown parameter
  - Recall: optimal prediction is incorrect with probability $\min\{\theta, 1 - \theta\}$
  - We cannot hope $\hat{Y}$ to beat this, but we can hope it is not much worse.

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Analysis of the plug-in prediction (2)

- **Theorem**:
  $\Pr(\hat{Y} \neq Y) \leq \min\{\theta, 1-\theta\} + \frac{1}{2} \cdot |\theta - 0.5| \cdot e^{-2n(\theta-0.5)^2}$.
  - The first term is the optimal error probability.
  - The second term comes from the probability that the $\hat{\theta}_{\mathrm{MLE}}$ is on the opposite side of $1/2$ as θ.
    - This probability is very small when n is large!
    - If S is number of heads in n independent tosses of coin with bias θ, then $S \sim \mathrm{Binomial}(n, \theta)$ (*Binomial distribution*)

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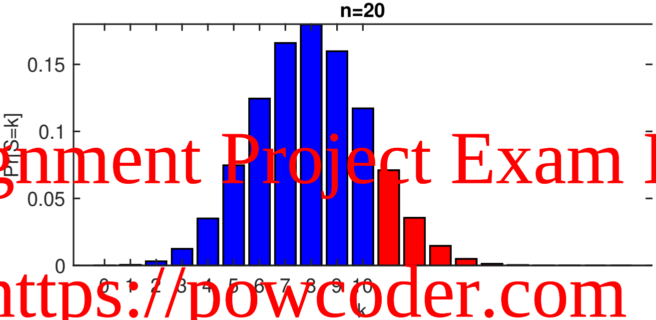

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Figure 1: $\Pr(S > n/2)$ for $S \sim \text{Binomial}(n, \theta)$, $n = 20$

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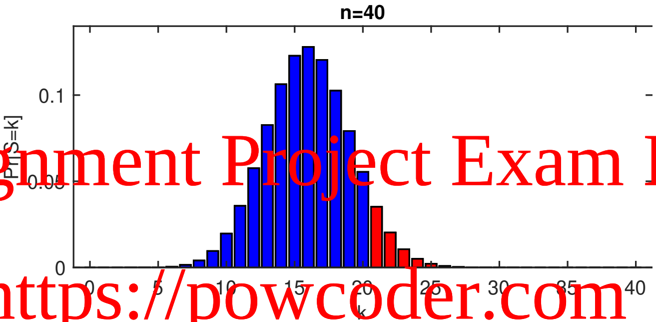

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Figure 2: $\Pr(S > n/2)$ for $S \sim \text{Binomial}(n, \theta)$, $n = 40$

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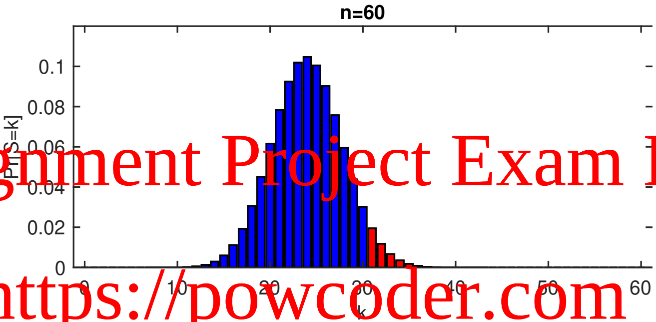

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Figure 3: $\Pr(S > n/2)$ for $S \sim \text{Binomial}(n, \theta)$, $n = 60$

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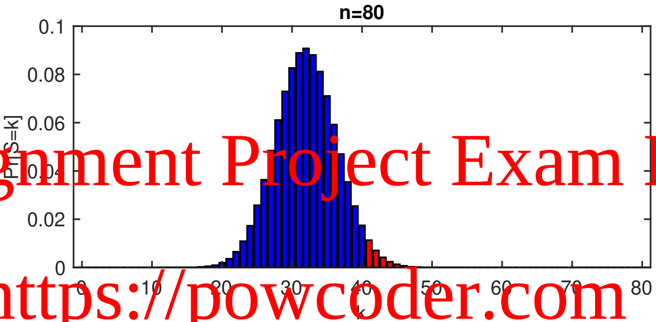

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Figure 4: $\Pr(S > n/2)$ for $S \sim \mathrm{Binomial}(n, \theta)$, $n = 80$

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Statistical model for labeled data in binary classification

- Example: spam filtering
- Labeled example: $(x, y) \in \mathcal{X} \times \{0, 1\}$
- $\mathcal{X}$ is input (feature) space; $\{0, 1\}$ is the output (label) space
  - $\mathcal{X}$ is not necessarily the space of inputs itself (e.g., space of all emails), but rather the space of what we measure about inputs
- We only see x (email), and then must make prediction of y (spam or not-spam)
- Statistical model: (X, Y) is random
  - X has some *marginal probability distribution*
  - *Conditional probability distribution* of Y given $X = x$ is Bernoulli with heads probability $\eta(x)$
  - $\eta \colon \mathcal{X} \to [0, 1]$ is a function, sometimes called the *regression function* or *conditional mean function* (since $\mathbb{E}[Y \mid X = x] = \eta(x)$).

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Error rate of a classifier

- For a classifier $f \colon \mathcal{X} \to \{0,1\}$, the *error rate* of f (with respect to the distribution of (X,Y)) is

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$$\operatorname{err}(f) := \Pr(f(X) \neq Y).$$

  Recall that we had previously used the notation

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$$\operatorname{err}(f, S) = \frac{1}{|S|} \sum_{(x,y) \in S} \mathbf{1}_{\{f(x) \neq y\}},$$

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  which is the same as $\Pr(f(X) \neq Y)$ when the distribution of (X,Y) is uniform over the labeled examples in S.
- Caution: This notation $\operatorname{err}(f)$ does not make explicit the dependence on (the distribution of) the random example (X,Y). You will need to determine this from context.

- Consider any random variables A and B.
- Conditional expectation of A given B:
  - Written $\mathbb{E}[A \mid B]$
  - A random variable! What is its expectation?
  - *Law of iterated expectations* (a.k.a. *tower property*):

$$\mathbb{E}[\mathbb{E}[A \mid B]] = \mathbb{E}[A]$$

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Conditional expectations (2)

- Example: roll a fair 6-sided die
  - $A =$ number shown facing up
  - $B =$ parity of number shown facing up
  - $C := \mathbb{E}[A \mid B]$ is random variable with

$$\Pr\left(C = \mathbb{E}[A \mid B = \text{odd}] = \frac{1}{3}(1+3+5) = 3\right) = \frac{1}{2}$$

$$\Pr\left(C = \mathbb{E}[A \mid B = \text{even}] = \frac{1}{3}(2+4+6) = 4\right) = \frac{1}{2}$$

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Bayes classifier

- *Optimal classifier* (*Bayes classifier*):

$$f^\star(x) = \mathbf{1}_{\{\eta(x) > 1/2\}}$$

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where η is the conditional mean function

  - Classifier with smallest probability of mistake
  - Depends on the function η, which is typically unknown!

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- *Optimal error rate* (*Bayes error rate*):
  - Write error rate as $\mathrm{err}(f^\star) = \Pr(f^\star(X) \neq Y) = \mathbb{E}[\mathbf{1}_{\{f^\star(X) \neq Y\}}]$
  - Conditional on X, probability of mistake is $\min\{\eta(X), 1 - \eta(X)\}$.
  - So, optimal error rate is

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$$\begin{aligned}\mathrm{err}(f^\star) &= \mathbb{E}[\mathbf{1}_{\{f^\star(X) \neq Y\}}] \\ &= \mathbb{E}[\mathbb{E}[\mathbf{1}_{\{f^\star(X) \neq Y\}} \mid X]] \\ &= \mathbb{E}[\min\{\eta(X), 1 - \eta(X)\}].\end{aligned}$$

Example: spam filtering

- Suppose input x is a single (binary) feature, "is email all-caps?"
- How to interpret "the probability that email is spam given $x = 1$?"
- What does it mean for the Bayes classifier $f^\star$ to be optimal?

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- What to do if η is unknown?
  - Training data: $(x_1, y_1), \ldots, (x_n, y_n)$
  - Assume data are related to what we want to predict
  - Let $Z := (X, Y)$, and $Z_i := (X_i, Y_i)$ for $i = 1, \ldots, n$.
  - IID model: $Z_1, \ldots, Z_n, Z$ are iid random variables
  - $Z = (X, Y)$ is the (unseen) "test" example
  - (Technically, each labeled example is a $(\mathcal{X} \times \{0, 1\})$-valued random variable. If $\mathcal{X} = \mathbb{R}^d$, can regard as vector of $d + 1$ random variables.)

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Performance of nearest neighbor classifier

- Study in context of IID model
- Assume $\eta(x) \approx \eta(x')$ whenever x and x' are close.
  - This is where the modeling assumption comes in (via choice of distance function)!

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- Let (X, Y) be the "test" example, and suppose $(X_{\hat{\imath}}, Y_{\hat{\imath}})$ is the nearest neighbor among training data $S = ((X_1, Y_1), \ldots, (X_n, Y_n))$.

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- For large n, X and $X_{\hat{\imath}}$ likely to be close enough so that $\eta(X) \approx \eta(X_{\hat{\imath}})$.
- Prediction is $Y_{\hat{\imath}}$, true label is Y.
- Conditional on X and $X_{\hat{\imath}}$, what is probability that $Y_{\hat{\imath}} \neq Y$?
  - $\eta(X)(1 - \eta(X_{\hat{\imath}})) + (1 - \eta(X))\eta(X_{\hat{\imath}}) \approx 2\eta(X)(1 - \eta(X))$

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- Conclusion: expected error rate is $\mathbb{E}[\mathrm{err}(\mathrm{NN}_S)] \approx 2 \cdot \mathbb{E}[\eta(X)(1 - \eta(X))]$ for large n
  - Recall that optimal is $\mathbb{E}[\min\{\eta(X), 1 - \eta(X)\}]$.
  - So $\mathbb{E}[\mathrm{err}(\mathrm{NN}_S)]$ is at most twice optimal.
  - Never exactly optimal unless $\eta(x) \in \{0, 1\}$ for all x.

Test error rate (1)

- How to estimate error rate?
- IID model: $(X_1, Y_1), \ldots, (X_n, Y_n), (X'_1, Y'_1), \ldots, (X'_m, Y'_m), (X, Y)$ are iid
  - Training examples (that you have): $(X_1, Y_1), \ldots, (X_n, Y_n)$
  - Test examples (that you have): $(X'_1, Y'_1), \ldots, (X'_m, Y'_m)$
  - Test example (that you don't have) used to define error rate: (X, Y)
- Classifier $\hat{f}$ is based only on training examples
- Hence, **test examples are independent of** $\hat{f}$ (very important!)
- We would like to estimate $\mathrm{err}(\hat{f})$
  - Caution: since $\hat{f}$ depends on training data, it is random!
  - Convention: When we write $\mathrm{err}(\hat{f})$ where $\hat{f}$ is random, we really mean $\Pr(\hat{f}(X) \neq Y \mid \hat{f})$.
  - Therefore $\mathrm{err}(\hat{f})$ is a random variable!

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Test error rate (2)

- Conditional distribution of $S := \sum_{i=1}^{m} \mathbf{1}_{\{\hat{f}(X_i') \neq Y_i'\}}$ given training data:
  - $S \mid$ training data $\sim \mathrm{Binomial}(m, \varepsilon)$ where $\varepsilon := \mathrm{err}(\hat{f})$
  - By law of large numbers,

$$\frac{1}{m} S \to \varepsilon$$

    as $m \to \infty$
  - Therefore, test error rate

$$\frac{1}{m} \sum_{i=1}^{m} \mathbf{1}_{\{\hat{f}(X_i') \neq Y_i'\}}$$

    is close to ε when m is large
  - How accurate is the estimate? Depends on the (conditional) variance!
    - $\mathrm{var}(\frac{1}{m} S \mid \text{training data}) = \frac{\varepsilon(1-\varepsilon)}{m}$
    - Standard deviation is $\sqrt{\frac{\varepsilon(1-\varepsilon)}{m}}$

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Confusion tables

- *True positive rate* (*recall*): $\Pr(f(X) = 1 \mid Y = 1)$
- *False positive rate*: $\Pr(f(X) = 1 \mid Y = 0)$
- *Precision*: $\Pr(Y = 1 \mid f(X) = 1)$
- ...
- *Confusion table*

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	$f(x) = 0$	$f(x) = 1$
$y = 0$	# true negatives	# false positives
$y = 1$	# false negatives	# true positives

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ROC curves

- *Receiver operating characteristic (ROC) curve*
  - What points are achievable on the TPR-FPR plane?
  - Use randomization to combine classifiers

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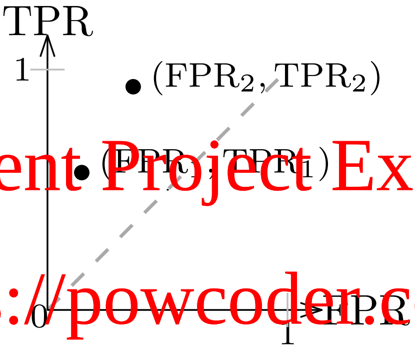

Figure 5: TPR vs FPR plot with two points

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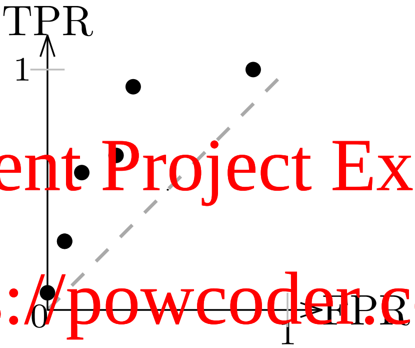

Figure 6: TPR vs FPR plot with many points

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More than two outcomes

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- What if there are $K > 2$ possible outcomes?
- Replace coin with K-sided die
- Say Y has a *categorical distribution* over $[K] := \{1, \ldots, K\}$, determined probability vector $\theta = (\theta_1, \ldots, \theta_K)$
  - $\theta_k \geq 0$ for all $k \in [K]$, and $\sum_{k=1}^{K} \theta_k = 1$
  - $\Pr(Y = k) = \theta_k$
- Optimal prediction of Y if θ is known:

$$\hat{y} := \arg\max_{k \in [K]} \theta_k$$

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Statistical model for multi-class classification

- Statistical model for labeled examples (X, Y), where Y takes values in $[K]$
  - Now, $Y \mid X = x$ has a categorical distribution with parameter vector $\eta(x) = (\eta(x)_1, \ldots, \eta(x)_K)$
  - Conditional probability function: $\eta(x)_k := \Pr(Y = k \mid X = x)$
  - Optimal classifier: $f^\star(x) = \arg\max_{k \in [K]} \eta(x)_k$
  - Optimal error rate: $\Pr(f^\star(X) \neq Y) = 1 - \mathbb{E}[\max_k \eta(X)_k]$

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Potential downsides of the IID model

- Example: Train OCR digit classifier using data from Alice's handwriting, but eventually use on digits written by Bob.
- What is a better evaluation?

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- What if we want to eventually use on digits written by both Alice and Bob?

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