Supervised Learning Methods

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Case Studies

Disease Prediction

► Al-Enhanced Blood Test for Early Parkinson's Detection

Outbreak Detection

► Machine Learning-Based COVID-19 Outbreak Detection

Personalized Medicine

► MammaPrint: 70-Gene Signature for Breast Cancer Treatment Decisions

Introduction

- Today, we'll talk about supervised learning.
- Our objective is to predict outcomes for new data based on learned patterns.
- ► The type of supervised method to use and how to evaluate how it works depends a lot on the type of outcome.
- Continuous outcomes:
 - Methods: linear regression, shrinkage linear regression methods, Support vector Regression, and Neural Networks.
 - ▶ Metrics: mean squared prediction error, median absolute deviation
- Binary outcomes:
 - Methods: logistic regression, decision trees, random forests, support vector machines.
 - Metrics: accuracy, precision, recall, F1 score, ROC curves, and AUC.

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Background: Linear Regression

- Linear Regression to model one numerical variable as a linear function of some other numeric variables.
 - the goal is to explain the variation in a variable, or to predict the value of a variable
- Two types of variables included in linear regressions
 - dependent (response, outcome) variable (Y): the variable to be predicted.
 - independent (covariates, predictors) variable (X_1, \dots, X_p) : the variables used to predict Y.
- ► The linearity is in terms of the coefficients: *Y* is a linear combination of independent variables plus some error.

$$Y = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p + \epsilon$$

Formal Definition of an SLR

- $Y = \beta_0 + \beta_1 X + \epsilon$
- \triangleright β_0, β_1 (unknown): intercept and coefficients, respectively.
- ightharpoonup ϵ : random error (commonly called the residual).
- ▶ For any given value of X, $Y \sim N(\beta_0 + \beta_1 X, \sigma^2)$
- ▶ The expected SLR line: $E[Y] = \beta_0 + \beta_1 X$
- ▶ For every one unit change in X we expect Y to change by β_1 units.
- ▶ The mean value of Y given X changes by β_1 units for every 1 unit change in X.

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Key Assumptions of Linear Regression (LINE)

- ▶ **Linearity:** Relationship between predictors and outcome is linear.
- ▶ **Independence:** Observations are independent from one another.
- ▶ **Normality:** Residuals (errors) are normally distributed.
- **Equal Variance:** Constant variance of errors across all levels of the predictors.

Violations can affect inference, prediction accuracy, or both.

Assessing Model Fit: Residual Analysis

► Residuals = observed − predicted values

$$e_i = Y_i - \hat{Y}_i$$

- Plots to examine:
 - Residuals vs. fitted: check linearity & homoscedasticity
 - Q-Q plot: check normality
 - Residuals vs. time/order: check independence
- Look for:
 - No clear pattern in plots
 - Residuals centered around 0

Line

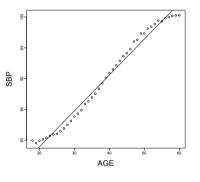
- ightharpoonup Assumption: there is a linear relationship between Y and the X's. I.e.,
 - The expected value of the residual is zero for all combinations of X's
 - $E(e_i) = 0.$
- ► How to check
 - ▶ Plot Y_i vs. X_i .
 - Plot e_i vs. \hat{Y}_i

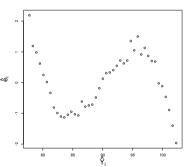
Line

Example Violation:

Corrective actions:

- Fit a different regression model.
- Add quadratic of cubic components.
- ► Transformation of *Y* and/or *X*





Normality

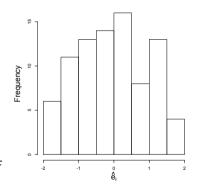
- Assumption: The residuals are normally distributed.
- ► How to check
 - Histogram of the e_i's.
 - Normal probability plot of e_i .
 - ▶ Tests of normality on e_i .
 - Outlier tests.

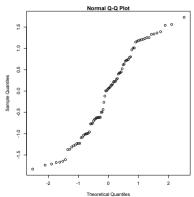
Normality

Example Violation:

Corrective actions:

- Examine outliers to determine if they are contaminated
- ► Transformation of Y and/or X



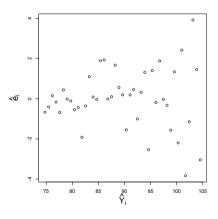


Equal Variance

- ▶ **Assumption:** the variance of the residuals is equal for all X's.
- ► How to check
 - ▶ Plot Y_i vs. X_i .
 - Plot e_i vs. \hat{Y}_i

Example Violation \Longrightarrow

- Corrective action:
 - Transformation of Y.
 - Patterned covariance model



Visual Checks for Assumptions

- ▶ **Linearity:** Scatterplots of *Y* vs. *X*, or residuals vs. fitted values
- ▶ Independence: Time series plots (look for patterns)
- ▶ Normality: Histogram or Q-Q plot of residuals
- **Equal Variance:** Residuals vs. fitted plot (look for "funnel" shape)

Residual analysis is your main tool to diagnose model issues.

The Problem of Model Selection

- ▶ In linear regression, we often have many potential predictors.
- Model selection = deciding which subset of variables to include.
- Why it matters:
 - ► Too few predictors ⇒ underfitting
 - ► Too many predictors ⇒ overfitting
- ► Goal: balance complexity and prediction accuracy

Data Example

POLAR (Predicting Outcomes of Language Rehabilitation in Aphasia) trial

- A total of 107 stroke patients with chronic aphasia (speech disorder) were randomized to one of two treatment arms.
- lacktriangle Neuroimaging data on where their stroke occurred is available on $\geq 5 imes 10^6$ voxels
- Main outcome is the Western Aphasia Battery (WAB).
- Goals of the study:
 - 1. see which treatment arm was the most effective,
 - 2. predict a person's WAB score based on their neuroimaging data,
 - 3. determine which areas of the brain with damage are related to WAB, and
 - 4. determine which areas of the brain with damage are related to treatment efficacy.

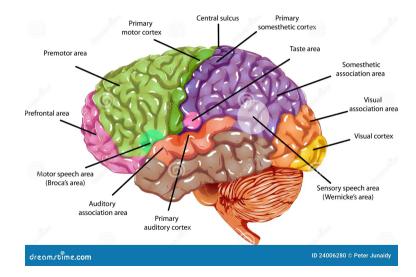
Multiple Linear Regression

- One dependent variable Y.
- p independent variables:
 - $ightharpoonup X_j = \text{proportion of voxels damaged in Region Of Interest (ROI) } j.$
- ► The model is

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p + \epsilon$$

or
$$E(Y) = X'\beta$$
.

- \triangleright β_0 : intercept;
- \triangleright $\beta_j, j = 1, \dots, p$: regression coefficients.
- $ightharpoonup E(\epsilon) = 0$ and $var(\epsilon) = \sigma^2$



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What **X** to use?

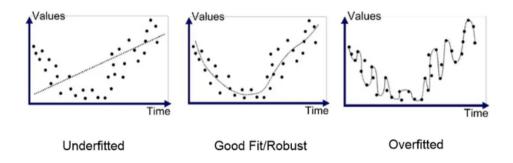
- ▶ Recall, that X_j = proportion of voxels damaged in ROI j.
- ▶ How do we define the regions? Some options:
 - 1. Harvard-Oxford Atlas, Number of ROIs (i.e., p): 48
 - 2. Automated Anatomical Labeling (AAL) Atlas, Number of ROIs: 116
 - 3. Brainnetome Atlas, Number of ROIs: 246
 - Schaefer Atlas, Number of ROIs: Varies (100, 200, 300, 400, 500, 600, 700, 800, 900, 1000)
 - 5. **Voxel level,** $p > 10^5$.

Model Selection Goals:

To make reasonable predictions or estimations, we need

- ightharpoonup accuracy ightharpoonup on average, what we estimate is equal to what we expect.
 - ▶ The predicted AQ score is equal to the average AQ score for all groups of people
- ▶ precision → small variation in prediction/estimation
 - ▶ The predicted AQ score is close to the true AQ score for all groups of people.

Underfitting vs. Overfitting



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Underfitting vs. Overfitting

- Underfitting occurs when important regressors are left out of the model. Costs:
 - deficient models (i.e., missing patterns).
 - misinterpretations of variable relationships.
- Overfitting occurs when all important regressors are in the model, but some unimportant ones are, too. Costs:
 - unneeded complexity and increased variance of the predicted values.
 - widened confidence and prediction intervals.

Common Model Selection Approaches

- ▶ Best Subset Selection: Try all combinations
- ▶ **Stepwise Selection:** Add or remove variables step-by-step
- Penalized Methods: Add penalty to control model size
 - ► LASSO (L1 penalty), Ridge (L2 penalty)

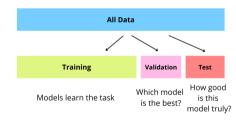
Evaluation Criteria

Evaluation Criteria

- ► Training Error: How well the model fits existing data
- ▶ **Test Error**: How well it predicts new data
- ► Cross-Validation: Estimate performance on unseen data
- Information Criteria:
 - AIC: balances fit and complexity
 - ▶ BIC: stronger penalty for complexity

Introduction to Validation

- Validation involves splitting the data into training, validation, and test sets.
- ► **Training Set:** The portion of data used to train the model.
- ➤ Validation Set: The portion of data used to tune model parameters and prevent overfitting. It's used for intermediate evaluation during model training.
- ► **Test Set:** The portion of data used to assess the final performance of the model after training and validation.



Introduction to Cross-Validation

- ▶ **Definition**: Cross-validation (CV) is a statistical method used to estimate the performance of machine learning models.
- Purpose: It helps in assessing how a model generalizes to an independent dataset.
- Why Use Cross-Validation?
 - Prevents Overfitting: Ensures model's robustness.
 - **Provides Reliable Estimates:** Offers a very good estimate of model performance.
 - ▶ **Optimizes Hyperparameters**: Helps choose parameters that can't be estimated (tuning parameters, e.g., the number of variables in a model).
 - Accuracy Measures: Any type can be used.

Evaluation Criteria

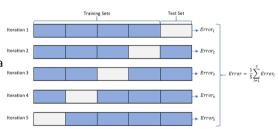
Basic Concepts

- ▶ Divide Data: Split data into training and validation (or test) sets.
- Multiple Iterations: Perform the split multiple times.
- ▶ **Aggregate Results:** Average the performance metrics.
- Types of CV:
 - K-Fold Cross-Validation
 - ► Leave-One-Out Cross-Validation (LOO)
 - Stratified K-Fold Cross-Validation
 - Time Series Split (for time-dependent data)

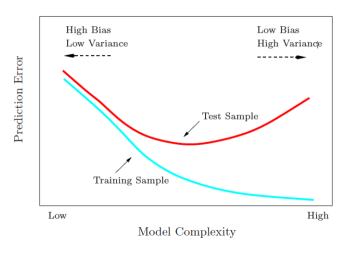
Cross-Validation Details

- Steps of K-fold cross-validation:
 - 1. Split data into K subsets (folds).
 - 2. Train/Estimate on K-1 folds and va on the remaining fold.
 - Repeat K times.
 - 4. Average the results.





Bias-Variance Tradeoff

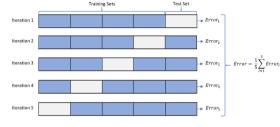


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Example: Predicting AQ with brain images (with 5-fold CV)

- 1. Put the people into 5 groups. Let $G_i = k$ if person i is in group k
- 2. Then for k = 1, 2, 3, 4, 5:
 - 2.1 Use k-1 folds to fit a linear model to every brain atlas.
 - 2.2 Using the fitted linear models, predict AQ for every person in the *k*th group, i.e., the test fold.
 - 8th group, i.e., the test fold.2.3 Get the total error for the test group for each brain atlas. For brain atlas 'a' this would be:



$$SSE_k^a = \sum_{i:G_i=k} (Y_i - \hat{Y}_i^a)^2$$

where \hat{Y}_{i}^{a} is the predicted AQ when brain atlas 'a' is used.

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Example: Predicting AQ with brain images (cont.)

3. Get the total error over all folds:

$$SSE^a = \sum_{k=1}^5 SSE_k^a$$
, $SSE^b = \sum_{k=1}^5 SSE_k^b$, $SSE^c = \sum_{k=1}^5 SSE_k^c$, etc.

4. Use the ROI that has the lowest SSE.

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CLASSIFICATION

Classification Introduction

- ▶ We'll now switch from continuous to binary (yes/no) types of outcomes.
- ► For example, the Wisconsin Breast Cancer Dataset (WBCD) was created by Dr. William H. Wolberg at the University of Wisconsin Hospitals, Madison.
- ► These data are used to predict whether a breast cancer tumor is benign or malignant based on various cell features.

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- Examples of cell features:
 - Radius (mean of distances from the center to points on the perimeter),
 - ► Texture (standard deviation of gray-scale values),
 - Perimeter, Area, etc.

Each of these features is calculated for three different metrics: mean, standard error, and the "worst" or largest value.

Classification Introduction

- Classification is the process of predicting the class label of a given input based on training data that contains input-output pairs.
- It involves building a model that learns from the training data and can predict the class of new, unseen data.
- Linear regression cannot be used for classification.
- Some Common Algorithms: logistic regression, decision trees, K-Nearest Neighbors (KNN), Naive Bayes, Neural Networks, Gradient Boosting Machines.

What is Logistic Regression?

- ightharpoonup A type of regression used when the outcome is **binary** (e.g., Yes/No, 0/1)
- ▶ Predicts the **probability** that the outcome is 1 (success)
- Output is between 0 and 1, but not linear in X
- Example: Will a patient develop a disease (Yes/No)?

The Logistic Model

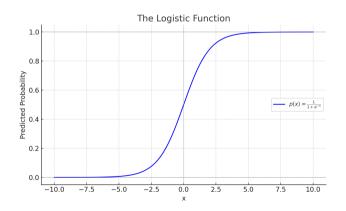
► The model uses the **logit** transformation:

$$\log\left(\frac{p}{1-p}\right) = \beta_0 + \beta_1 x_1 + \dots + \beta_k x_k$$

- ► This means:
 - ightharpoonup p = probability of success
 - ► Left-hand side = log-odds of success
- ► The inverse of this function is the **logistic curve**

The Logistic Curve

- ► S-shaped curve
- ► As predictor increases, the probability approaches 0 or 1
- ► Ensures outputs stay in the [0,1] range



Interpreting Coefficients

- lacktriangle Each eta represents the change in the **log-odds** for a 1-unit increase in the predictor
- ightharpoonup exp(eta) = odds ratio
- **Example:**
 - ▶ If $\beta_1 = 0.7$, then $\exp(0.7) \approx 2.01$
 - ightharpoonup A 1-unit increase in x_1 doubles the odds of success

When to Use Logistic Regression

- ightharpoonup Outcome is binary (0/1)
- Predictors can be continuous, binary, or categorical
- Examples in public health:
 - Predicting disease presence (yes/no)
 - Smoking status, vaccine response, hospital readmission
- Assumes independent observations and a linear relationship in the log-odds

Logistic Regression: Predicting Smoking Status from Demographic and Health Factors

Goal: Predicting Smoking Status from Demographic and Health Factors.

► Handout

Model Selection in Logistic Regression

- The same questions about model selection come up.
- For example, which of the cell features should be used for our x? Which summary measure should we use?
- ▶ AIC and BIC are two common measures of the "quality" of a model, which are general and can be used in almost any method.

└ Confounding

Introduction

- ▶ The above question on model fit are usually used for **predictive models**.
- ► However, in public health we are often more interested in determining the association between two variables.
- For example, what is the association between the use of multivitamins and mortality?

└ Confounding

Introduction

- Rarely is it reasonable to talk about the association of two variables without consideration of the impact of other variables.
- ➤ You will see a variety of labels for different etiologic and statistical phenomena that might be occurring.
- For example
 - Confounding
 - Direct Effect.
 - Indirect Effect.
 - Mediation
 - Modification/moderation
 - Interaction

Confounding

- Confounding reflects the causal association between variables in the population under study
- ► A confounder is an extraneous variable that satisfies the following criteria:
 - It is a risk factor for the study disease.
 - lt is associated with the study exposure, but is not a consequence of that exposure.
 - ▶ The association with disease must occur in the absence of exposure.
- ▶ A confounder is a risk factor for the study disease whose "control" in some appropriate way will reduce (or remove) bias in estimating the exposure—disease relationship.

└ Confounding

Confounding

- ▶ If we are interested in estimating the OR, then we could obtain a biased estimate of the OR if a confounder is not adjusted for (e.g., examining MV–MI without adjusting for age or smoking).
 - OR could be positively or negatively biased.
- How do we control/identify confounding?
 - Must have prior knowledge on potential confouders
 - ▶ Is the adjusted estimate of the OR \approx to the crude estimate of the OR?
 - ▶ People often use the 10% rule (i.e., a 10% change in the OR is a sign of confounding).

Berkley Gender Bias Case:

- ▶ Data from: "Sex Bias in Graduate Admissions: Data from Berkeley," Science 187: 398-403; 1975.
- ▶ In 1973 2,681 men and 1,835 women applied to graduate school, with 44% of men and 35% of women being admitted.
- A crude analysis finds Crude $OR = \frac{(1276/1835)}{(1486/2681)} = 1.25$ with 95% CI (1.20, 1.32).
- ▶ This difference is statistically significant (i.e., not due to chance).

Berkley Gender Bias Case:

The admission rates and RR by department

	Men		Women		
Depart.	Applicants	Admitted	Applicants	Admitted	OR _i
А	825	62%	108	82%	0.90
В	560	63%	25	68%	0.99
C	325	37%	593	34%	1.08
D	407	35%	375	34%	1.02
E	191	23%	393	26%	0.88
F	373	7%	341	6%	1.09

- ► The Summary OR is 0.97 and insignificant.
- ▶ The apparent association (OR=1.25) was due to confounding.

Mediation

- Can be thought of as a special case of a potential confounder being part of a causal pathway.
- ▶ if $E \Rightarrow M \Rightarrow D$ then we say M is a mediator.

For example:

- TAAG (Trial for Activity among Adolescent Girls)
- ▶ Interventions (*E*) effected physical activities (*D*).
- ▶ The E may have changed self-image or self-efficacy (M).
- ightharpoonup The could be a relationship between M and D.
- Important to understand why physical activity increased.

Effect modification

- ▶ When we observe that the *OR* are non-constant across strata, we say there is statistical interaction.
- Interaction (a statistical term) is related to effect modification (an epi term).
- ▶ If the effect of *E* on *D* varies with *C* we say that there *C* is an effect modifier.
 - ▶ **Effect modification:** a variable that differentially (positively and negatively) modifies the observed effect of a risk factor on disease status. Present if different groups (of *C*) have different risk estimates.
 - ► Effect modification is related to the biology of disease, not just a data observation (what makes it different from interaction).
- An obvious example of interaction is breast or prostate cancer.

Effect modification

Why study effect modification? Why do we care?

- to define high-risk subgroups for preventive actions,
- to increase precision of effect estimation by taking into account groups that may be affected differently,
- to increase the ability to compare across studies that have different proportions of effect-modifying groups, and
- to aid in developing a causal hypotheses for the disease.

Effect Modification vs Confounding

Interesting tidbit:

- ▶ If a variable C is a confounder, then the stratum specific estimates of the \widehat{OR}_i will mostly be on one side of the crude estimate of the \widehat{OR} .
- ▶ If a variable C is an effect modifier, then the crude estimate of the \widehat{OR} will be a "weighted average" of the stratum specific estimates of the \widehat{OR}_i .
- ▶ **Note:** we are comparing the crude *OR* **NOT** the adjusted estimate of the *OR*.

What to do under effect modification/confounding?

1. If a variable is a confounder, you just have to adjust for it:

$$\beta_0 + \beta_1 E + + \beta_2 C$$

2. If a variable is an effect modifier, it should go into your regression equation as an interaction term

$$\beta_0 + \beta_1 E + + \beta_2 C + \beta_3 EC$$

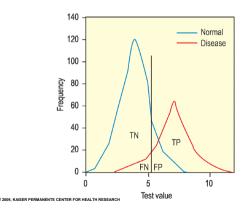
Measuring of predictive ability

- We will now take a slight detour to discuss other ways of quantifying the predictive ability of a model.
- Some of these methods will take more background than others.
- ▶ In general, they are all trying to answer the following:

Ten new subjects walk into the room (all were not in the data used to estimate $\hat{\beta}$), which model is going to give me the best estimate of the predictive probability (i.e., $\hat{\pi}_i$) for those ten subjects?

Sensitivity and specificity

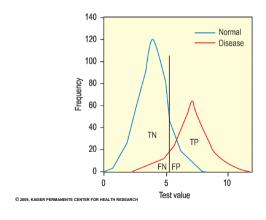
- ► Imagine a study evaluating a new test that screens people for a disease {0,1}.
- The test outcome can be positive (predicting that the person has the disease) or negative (predicting that the person does not have the disease).
- The test results for each subject may or may not match the subject's actual status.



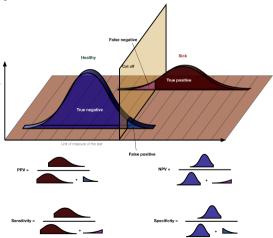
Sensitivity and specificity

In this setting, there are 4 things that could happen:

- True positive (TP): Sick people correctly diagnosed as sick
- ► False positive (FP): Healthy people incorrectly identified as sick
- ► True negative (TN): Healthy people correctly identified as healthy
- ► False negative (FN): Sick people incorrectly identified as healthy



Sensitivity, specificity, PPV, NPV

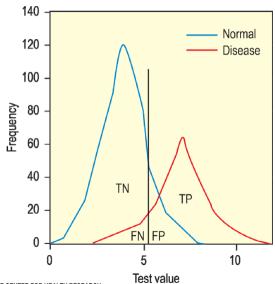


Estimating sensitivity and specificity from a logistic model

- To estimate sensitivity and specificity from a logistic model we we'll use the values of $\hat{\pi}_i$ as the results of the "test."
- Let's assume that Y=1 if the person has the disease, so that a high value of $\hat{\pi}_i$ is indicative that the person will have the disease.
- ▶ Then we can pick a value, say π_0 , such that the result of the test is

$$T_i = \begin{cases} +, & \text{if } \hat{\pi}_i > \pi_0 \\ -, & \text{if } \hat{\pi}_i \le \pi_0 \end{cases}$$

So all people with a predicted value of at least π_0 will have a test equal to "positive".



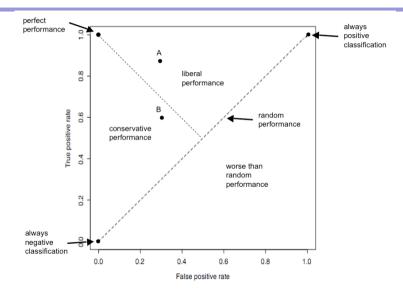
Receiver Operating Characteristic (ROC) Curves

- Receiver Operating Characteristic (ROC) Curves are a method for measuring the predictive ability of a model.
- ▶ ROC curves look at the $Sens(\pi_0)$ and $1 Spec(\pi_0)$ for all values of π_0 .
- ▶ When $\pi_0 = 0$ all tests are positive, Sens(0) = 1 and 1 Spec(1) = 1.
- ▶ When $\pi_0 = 1$ all tests are negative, Sens(1) = 0 and 1 Spec(1) = 0.

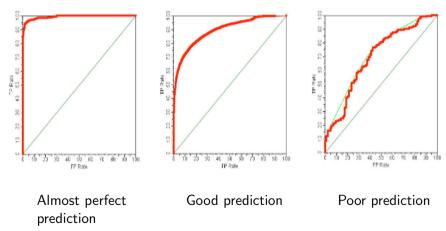
Motivation for ROC Curves

- ► For example, assume we have 100 diseased and 100 not diseased in our sample.
- Suppose that we list all 200 people from smallest to largest $\hat{\pi}_i$.
- ▶ Suppose that when I increase π_0 from 0.4 to 0.5 an additional 20 people have T^- .
- ► If the test is worthless I would expect 10 of those people to be diseased and 10 not diseased.
- ▶ In general, (If the test is worthless) as π_0 increases, 50% of the people are diseased and 50% are not diseased.

Measuring predictive ability in Classification models



ROC curve examples



Quantifying ROC curve performance

- Notice that the models that predict better have larger area under the ROC curve (AUC).
- ▶ AUC is the main way to quantify an ROC curve.
- ► The AUC is equal to the probability that the model will rank a randomly chosen diseased individual higher than a randomly chosen healthy individual.

$$\Pr(\hat{\pi}_i > \hat{\pi}_j | Y_i = 1 \text{ and } Y_j = 0)$$

AUC values

- ▶ We will interpret the AUC in terms of the discriminative ability of the model.
- ► That is, how well does the model discriminate between diseased and non-diseased individuals?

ÂÛĈ	Interpretation of discriminative ability
< 0.5	worse than expected by chance
= 0.5	no discrimination
0.7 - 0.8	acceptable discrimination
0.8 - 0.9	excellent discrimination
> 0.9	outstanding discrimination

Logistic Regression: COVID-19 Diagnosis

Goal: Distinguish COVID-19 from other respiratory illnesses

- ► Logistic regression model based on 400 patients
- ▶ 15 features, achieved 98.8% sensitivity, 97.3% specificity
- ► **Source**: PMC9277749

CART Introduction

- ▶ Suppose we have two variables X_1 and X_2 , and we are trying to classify group status.
- ▶ Tree based methods consider breaking the X_1 and X_2 space into blocks.

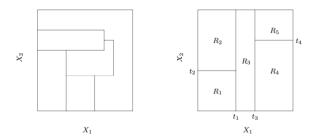


Figure: CART Example from ESL II (page 306).

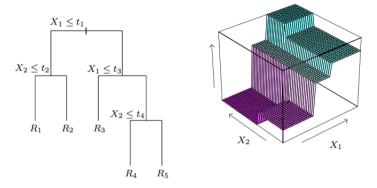


Figure: CART Example from ESL II (page 306).

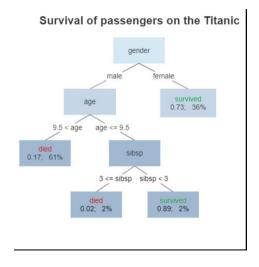
▶ The model predict population C_m for $(X_1, X_2) \in R_m$.

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Growing Trees

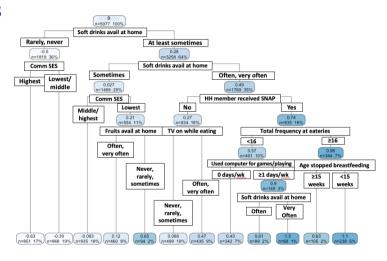
- We now turn to the question of how to grow a regression tree.
- Our data consists of p inputs and a response, for each of N observations: that is, (x_i, y_i) for i = 1, 2, ..., N, with $x_i = (x_{i1}, x_{i2}, ..., x_{ip})$.
- The algorithm decides what variable to split on and the split point.
- We split the data to maximize the differences in the outcome for the two splits.
- For example, split such that the sample means in the two groups are as different as possible.

CART: Titanic



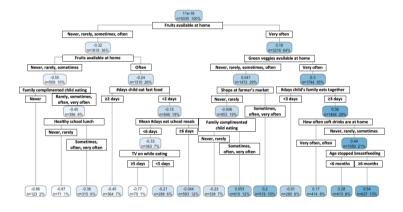
Classification and Regression Trees

CART: SSB



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CART: FVI



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CART: Predicting Influenza Risk

 $\textbf{Goal:} \ \, \mathsf{Identify} \ \, \mathsf{flu} \ \, \mathsf{patients} \ \, \mathsf{from} \ \, \mathsf{symptoms} \, + \, \mathsf{demographics}$

- ► CART used to generate fast, interpretable triage tools
- ▶ Effective alternative to lab testing in resource-limited settings
- ► **Source:** PMC5034457

CART: COVID-19 Mortality Risk

Goal: Predict severe COVID-19 outcomes in hospital patients

▶ Dataset: 5,000+ hospitalized patients

ightharpoonup CART classified mortality risk ightharpoonup clinical triage

► Source: Int J Emerg Med 2024

Summary & Discussion

- Logistic regression: good for interpretation and risk scoring
- ► CART: good for decision support and threshold-based tools
- Consider both accuracy and interpretability
- Discussion: Which would you use for your own project?