

FUNDAMENTALS OF LEARNING AND INFORMATION PROCESSING

SESSION 10: PROBABILITY THEORY (VI)

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Statistical Inference

Probability vs Statistics

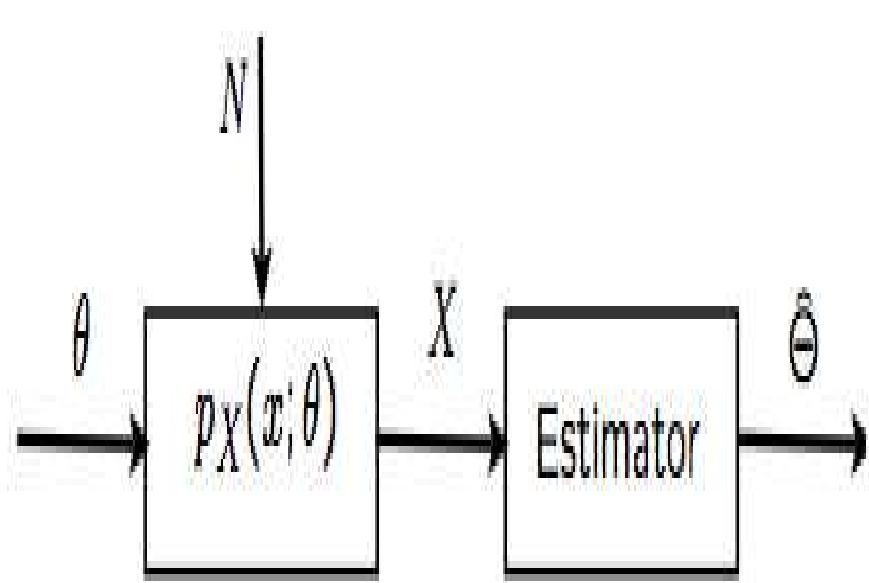
Probability

- We assume a fully specified probabilistic model that obeys the axioms.
- We then use mathematical methods to quantify the consequences of this model, or answer various questions of interest.
- Every unambiguous question has a unique correct answer, though this answer is sometimes hard to find.

Statistics

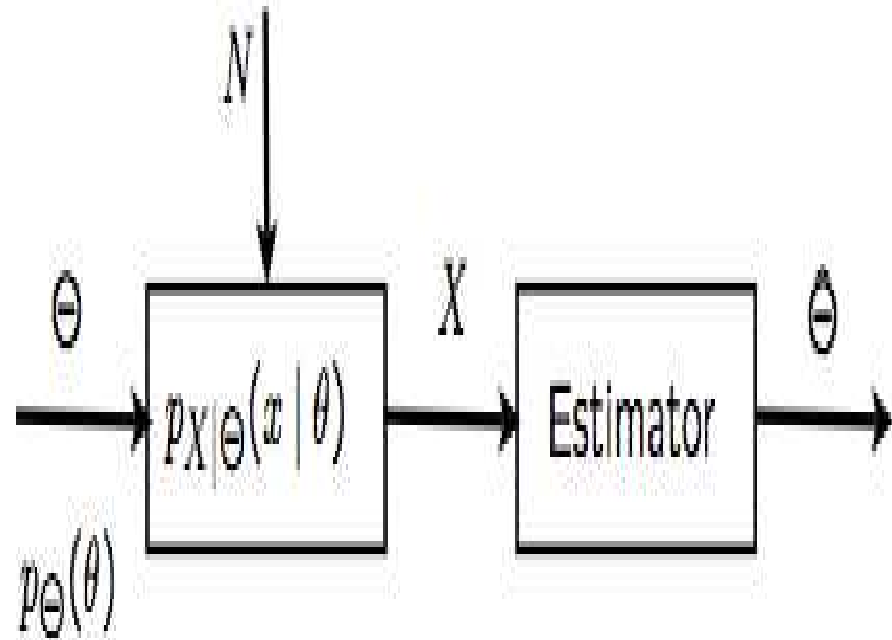
- It involves an element of art
- Several reasonable methods may exist, yielding different answers
- No principled way for selecting the ‘best’ method, unless one makes several assumptions and imposes additional constraints on the inference problem

Frequentist vs Bayesian Statistics



Frequentist Statistics

- θ is treated as deterministic quantities, that happen to be unknown
- it strives to develop an estimate of θ that as some performance guarantees.
- we are not dealing with a single probabilistic model, but rather with multiple candidate probabilistic models, one for each possible value of θ .



Bayesian Statistics

- It views the model as chosen randomly from a given model class.
- θ is treated as a random variable that characterizes the model, and by postulating a *prior* probability distribution $p_{\theta}(\theta)$.
- Use priors and Bayes rule to derive a *posterior* probability distribution $p_{\theta|X}(\theta|x)$, which captures all the information that x can provide about θ .

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Bayesian Statistics

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Bayesian Statistics

- Bayesian Statistics** treats unknown parameters as random variables with known prior distributions.
- Parameter Estimation** generates estimates that are close to the true values of the parameters in some probabilistic sense.
- Hypothesis Testing** the unknown parameter takes one of the finite number of values, corresponding to competing hypotheses; We want to choose one to achieve a small probability of error.

Bayesian Inference Methods

- MAP Rule** out of the possible parameter values/hypotheses, select one with maximum conditional or posterior probability given the data.
- Least Mean Squares (LMS)** Select an estimator/function of the data that minimizes the mean squared error between the parameter and its estimate.
- Linear Least Mean Squares (LMS)** Select an estimator/function which is a linear function of the data and minimizes the mean squared error between the parameter and its estimate.

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MAP Rule

Defn Given the value x of the observation, we select a value of θ , denoted by $\hat{\theta}$, that maximizes the posterior distribution $p_{\Theta|X}(\theta|x)$, or $f_{\Theta|X}(\theta|x)$ if Θ is continuous. This is the *Maximum a Posteriori Probability* (MAP) rule.

Priors Bayesian methods provide a way to include prior information in a systematic way: $p(\theta)$.
Non-informative Prior represent lack of information, but it has one major flaw: if it is flat in one parameterization it will not be flat in most other parameterizations.
<https://normaldeviate.wordpress.com/2012/12/08/flat-priors-in-flatland-stones-paradox/>

Single Answer If interested in a single answer, though single answers can be misleading!

MAP

$$p_{\Theta|X}(\theta^*|x) = \max_{\theta} p_{\Theta|X}(\theta|x)$$

which minimizes the probability of error, often used in hypothesis testing

Conditional Expectation

$$E[\Theta|X = y] = \int \theta f_{\Theta|X}(\theta|x) d\theta$$

Least Mean Squares (LMS) Estimation

LMS LMS estimates Θ with $\hat{\theta}$ so that the estimation error $E[(\Theta - \hat{\theta})^2]$ is least.

In the Absence of Information Estimating Θ with a constant $\hat{\theta}$, in the absence of an observation X .

- The estimation error $\hat{\theta} - \Theta$ is random, because Θ is random.
- but the *mean squared error* $E[(\Theta - \hat{\theta})^2]$ is a number that depends on $\hat{\theta}$, and can be minimized over $\hat{\theta}$.
- For any estimate $\hat{\theta}$, we have

$$E[(\Theta - \hat{\theta})^2] = var(\Theta - \hat{\theta}) + (E[\Theta - \hat{\theta}])^2 = var(\Theta) + (E[\Theta - \hat{\theta}])^2$$

- ◆ The first one from $E(Z^2) = var(Z) + (E(Z))^2$
- ◆ The second one from the $\hat{\theta}$ is a constant
- ◆ We choose $\hat{\theta}$ to minimize $(E[\Theta - \hat{\theta}])^2$, which leads to $\hat{\theta} = E[\Theta]$.

In the Observation of $X = x$ Estimating Θ with a constant $\hat{\theta}$, in the observation X .

- It is a new universe condition on $X = x$
- So the conditional expectation $E[\Theta|X = x]$ minimizes the conditional mean squared error $E[(\Theta - \hat{\theta})^2|X = x]$ over all constants $\hat{\theta}$.
- $E[\Theta|X]$ minimizes $E[(\Theta - g(X))^2]$ over all estimators $g(\cdot)$

Properties of LMS estimation Estimator: $\hat{\Theta} = E[\Theta|X]$ Estimation error: $\tilde{\Theta} = \hat{\Theta} - \Theta$

- $E(\tilde{\Theta}) = 0$, and $E(\tilde{\Theta}|X = x) = E(\hat{\Theta} - \Theta|X = x) = E(\hat{\Theta}|X) - E(\Theta|X = x) = \hat{\Theta} - \hat{\Theta} = 0$, So $\hat{\Theta}$ is unbiased.
- $E(\tilde{\Theta}h(x)|x) = h(x)E(\tilde{\Theta}|x) = 0$ From the law of iterative expectations, we have $E(\tilde{\Theta}h(x)) = 0$
- $Cov(\tilde{\Theta}h(x)) = E(\hat{\Theta}h(x)) - E(\hat{\Theta})E(h(x)) = 0$, So $Cov(\tilde{\Theta}\hat{\Theta}) = 0$.
- Since $\Theta = \hat{\Theta} - \tilde{\Theta}$, and their covariance is zero, we have $var(\Theta) = var(\hat{\Theta}) + var(\tilde{\Theta})$.

Linear Least Mean Squares Estimation

Defn

A linear estimator of a random variable Θ , based on observations X_1, \dots, X_n has the form

$$\hat{\Theta} = \alpha_1 X_1 + \dots + \alpha_n X_n + \beta$$

Given a particular choice of the scalars $\alpha_1, \dots, \alpha_n, \beta$, the corresponding mean squared error is $E[(\Theta - \alpha_1 X_1 - \dots - \alpha_n X_n - \beta)^2]$

Best linear estimator

$$\hat{\Theta}_L = E(\Theta) + \frac{Cov(X, \Theta)}{var(X)}(X - E[X])$$

- $\alpha = \frac{Cov(X, \Theta)}{var(X)} = \rho \frac{\sigma_{\Theta}}{\sigma_X}$, where $\rho = \frac{Cov(\Theta, X)}{\sigma_{\Theta} \sigma_X}$.
- With the MSE as $E[(\hat{\Theta} - \Theta)^2] = (1 - \rho^2) \sigma_{\Theta}^2$
- The formula only involves the means, variances, and the covariance of Θ and X .

Classical Statistics

Classical Statistics

Classical Statistics treats unknown parameters as constants to be determined. A separate probabilistic model is assumed for each possible value of the unknown parameter.

Parameter Estimation generates estimates that are nearly correct under any possible value of the unknown parameter.

Hypothesis Testing the unknown parameter takes finite number $m \geq 2$ of values, corresponding to competing hypotheses; We want to choose one to achieve a small probability of error under any of the possible hypotheses.

Classical Inference Methods

MLE Select the parameter that makes the observed data “most likely”, i.e., maximizes the probability of obtaining the data at hand.

Linear Regression Find the linear relation that matches best a set of data pairs, in the sense that it minimizes the sum of the squares of the discrepancies between the model and the data.

ML Estimation

Defn

Let the vector of observations $X = (X_1, \dots, X_n)$ be described by $p_X(x; \theta)$ whose form depends on an unknown parameter θ . Suppose we observe a particular value $x = (x_1, \dots, x_n)$ of X , then the *Maximum Likelihood* (ML) estimation is a value of the parameter that maximizes the *likelihood function* $p_X(x_1, \dots, x_n; \theta)$ over all θ :

$$\hat{\theta}_n = \arg \max_{\theta} p_X(x_1, \dots, x_n; \theta)$$

Example Suppose $X = (X_1, \dots, X_n)$ are i.i.d. from $\exp(\theta)$: $\theta e^{-\theta x}$

- $\max_{\theta} \prod_{i=1}^n \theta e^{-\theta x_i}$
- Take the logarithm $\max_{\theta} (n \log \theta - \theta \sum_{i=1}^n x_i)$
- $\hat{\theta}_{ML} = \frac{n}{x_1 + \dots + x_n}$

Desirable Properties Let $\hat{\theta}_n$ be an estimator of an unknown parameter θ , that is, a function of n observations X_1, \dots, X_n whose distribution depends on θ .

Estimation Error denoted by $\tilde{\theta}_n = \hat{\theta}_n - \theta$
Bias of the estimator $\hat{\theta}_n$, denoted by $b_{\theta}(\hat{\theta}) = E_{\theta}[\hat{\theta}_n] - \theta$

- **Unbiased** If $E_{\theta}[\hat{\theta}_n] = \theta$, for every possible value of θ
- **Asymptotically unbiased** if $\lim_{n \rightarrow \infty} E_{\theta}[\hat{\theta}_n] = \theta$, for every possible value of θ
- **Consistent** if the sequence $\hat{\theta}_n$ converges to the true value of θ , in probability, for every possible value of θ

MSE (Bias Variance Decomposition) $E[(\hat{\theta}_n - \theta)^2] = \text{var}(\hat{\theta}_n - \theta) + (E[\hat{\theta}_n - \theta])^2 + \sigma_{\epsilon}^2 = \text{var}(\hat{\theta}_n) + (\text{bias})^2 + \sigma_{\epsilon}^2$

Example Suppose $X = (X_1, \dots, X_n)$ are i.i.d. mean θ variance σ^2

$$X_i = \theta + W_i$$

with W_i i.i.d. mean 0, variance σ^2 .

- We have the sample mean $\hat{\theta}_n = M_n = \frac{X_1 + \dots + X_n}{n}$
 - ◆ It is unbiased $E(\tilde{\theta}) = 0$
 - ◆ From WLLN: $\hat{\theta}_n \rightarrow \theta$, so it is consistent.
 - ◆ MSE: $E[(\hat{\theta}_n - \theta)^2] = \frac{\sigma^2}{n}$

Bias-Variance Tradeoff

Defn

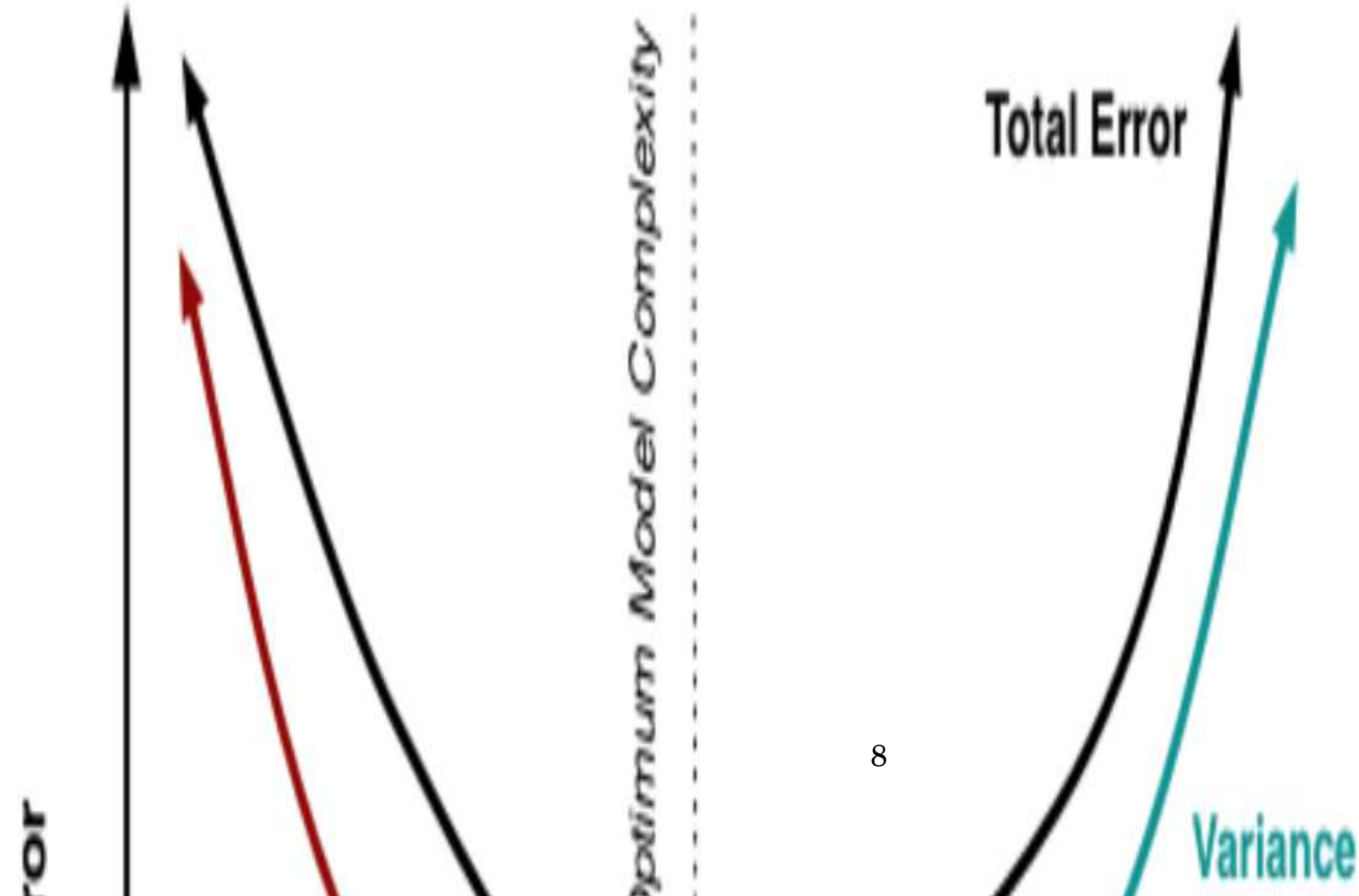
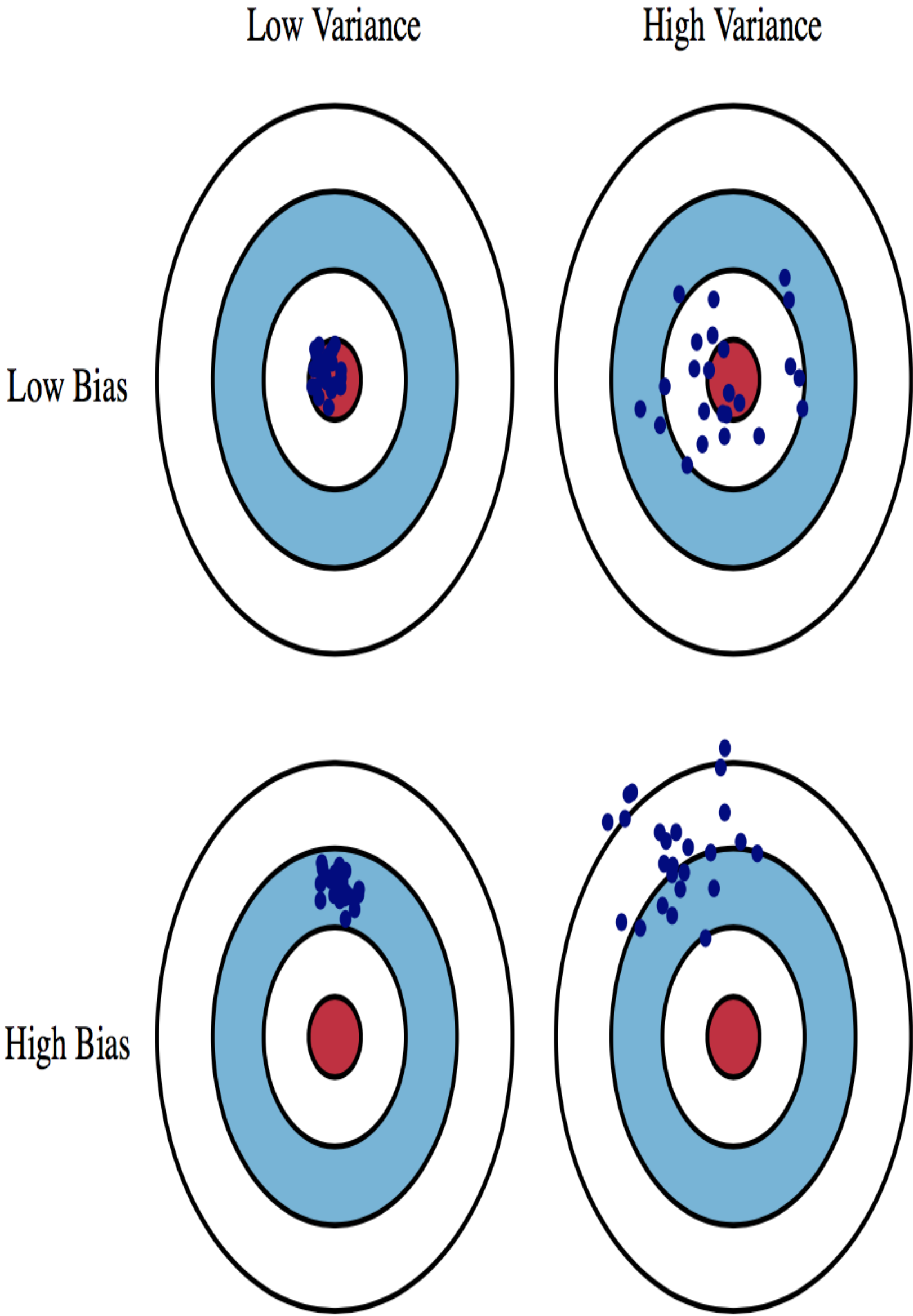
There are three kinds of errors in the estimation:
The error due to bias is taken as the difference between the expected prediction of our model and the correct value which we are trying to predict
The error due to variance is taken as the variability of a model prediction for a given data point
The irreducible error is the noise term in the true relationship that cannot fundamentally be reduced by any model

Proof.

$$\begin{aligned} E[(\hat{\theta}_n - \theta)^2] &= \text{var}(\hat{\theta}_n - \theta) + (E[\hat{\theta}_n - \theta])^2 + \sigma_{\epsilon}^2 \\ &= \text{var}(\hat{\theta}_n) + (\text{bias})^2 + \sigma_{\epsilon}^2 \\ &= \text{Variance} + \text{Bias}^2 + \text{IrreducibleError} \end{aligned}$$

□

Bias-Variance Tradeoff



Confidence Interval

Defn Let us fix a desired *confidence level*, $1 - \alpha$, where α is typically a small number. We then replace the point estimate $\hat{\theta}_n$ by a lower estimator $\hat{\theta}_n^-$ and an upper estimator $\hat{\theta}_n^+$, so that $P_\theta(\hat{\theta}_n^- \leq \theta \leq \hat{\theta}_n^+) \geq 1 - \alpha$ for every possible value of θ . Here both $\hat{\theta}_n^-$ and $\hat{\theta}_n^+$ are functions of observations, and hence random variables whose distributions depend on θ . We call $[\hat{\theta}_n^-, \hat{\theta}_n^+]$ a $1 - \alpha$ *confidence interval*.

Example Suppose $X = (X_1, \dots, X_n)$ are i.i.d., CI in estimation of the mean $\hat{\theta}_n = \frac{X_1 + \dots + X_n}{n}$

- From normal table $\Phi(1.96) = 1 - 0.05/2$
- From CLT, we have $P(\frac{|\hat{\theta}_n - \theta|}{\sigma/\sqrt{n}} \leq 1.96) \approx 0.95$
- Then we have $P(\hat{\theta}_n - \frac{1.96\sigma}{\sqrt{n}} \leq \theta \leq \hat{\theta}_n + \frac{1.96\sigma}{\sqrt{n}}) \approx 0.95$
- More generally, let z be s.t. $\Phi(z) = 1 - \alpha/2$ ^a, then $P(\hat{\theta}_n - \frac{z\sigma}{\sqrt{n}} \leq \theta \leq \hat{\theta}_n + \frac{z\sigma}{\sqrt{n}}) \approx 1 - \alpha$

Unknown σ In the case of unknown σ ,

Option 1 use the upper bound on σ , especially if X_i Bernoulli, we have $\sigma \leq 1/2$.

Option 2 use ad hoc estimate of σ , if X_i Bernoulli, we have $\sigma = \sqrt{\hat{\theta}(1 - \hat{\theta})}$

Option 3 use generic estimate of the variance.

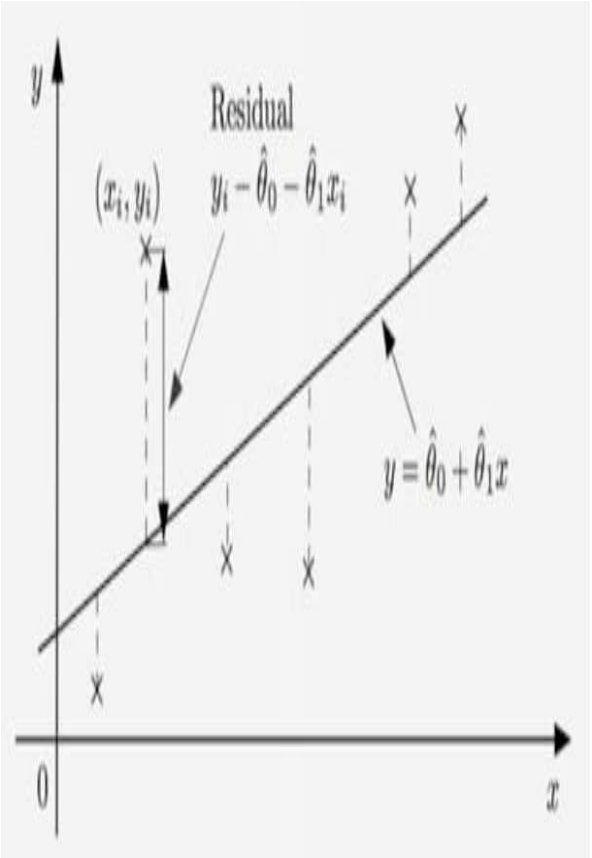
- Start from $\sigma^2 = E[(X_i - \theta)^2]$, $\hat{\sigma}_n^2 = \frac{1}{n} \sum_{i=1}^n (X_i - \theta)^2 \rightarrow \sigma^2$, but we don't know θ .
- $\hat{S}_n^2 = \frac{1}{n-1} \sum_{i=1}^n (X_i - \hat{\theta}_n)^2 \rightarrow \sigma^2$, unbiased: $E[\hat{S}_n^2] = \sigma^2$

^aWhen n is small, $\hat{\theta}_n^2$ is only an approximation to the true variance, and the random variable $T_n = \frac{\sqrt{n}(\hat{\theta}_n - \theta)}{\hat{\theta}_n}$ is not normal, but the *t-distribution with $n - 1$ degrees of freedom*. $\bar{\Phi}_{n-1}(z) = 1 - \alpha/2$, where $\bar{\Phi}_{n-1}(z)$ is the CDF of the *t-distribution* with $n - 1$ degrees of freedom. Check <http://www.sumsar.net/blog/2013/12/t-as-a-mixture-of-normals/>.

Linear Regression

Defn

We wish to model the relation between x and y , based on data set (x_i, y_i) , $i = 1, \dots, n$. Assume a linear model of the form $y \approx \theta_0 + \theta_1 x$, where θ_0 and θ_1 are unknown parameters, the objective is to solve:

$$\min_{\theta_0, \theta_1} \sum_{i=1}^n (y_i - \theta_0 - \theta_1 x_i)^2$$


One Interpretation

- $Y_i = \theta_0 + \theta_1 X_i + W_i$, with $W_i \sim N(0, \sigma^2)$
- Likelihood function is $c \cdot \exp\{-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \theta_0 - \theta_1 x_i)^2\}$.
 - Take logs, same as the linear regression objective.
 - Least squares \leftrightarrow pretend W_i is i.i.d. normal.

- Solution** $\bar{x} = \frac{x_1 + \dots + x_n}{n}$, $\bar{y} = \frac{y_1 + \dots + y_n}{n}$
- Assume W is independent of X and with zero mean
 - $E[Y] = \theta_0 + \theta_1 E[X]$ so we have $\theta_0 = E[Y] - \theta_1 E[X]$, hence, $\hat{\theta}_0 = \bar{y} - \hat{\theta}_1 \bar{x}$, though $\hat{\theta}_1$ is unknown.
 - Assume for simplicity $E[X] = E[W] = 0$, $YX = \theta_0 X + \theta_1 X^2 + XW$. Take expectation on both sides
 $Cov(X, Y) = 0 + \theta_1 Var(X) + 0$, hence, $\hat{\theta}_1 = \frac{Cov(X, Y)}{Var(X)}$.

Multiple Linear Regression $y \approx \theta_0 + \theta_1 x + \theta_2 x' + \theta_3 x''$, typically resort to linear algebra

Standard Error an estimate of σ

Explanatory Power $R^2 = \frac{Var(Y|X)}{var(Y)}$, a measure of explanatory power: when R^2 is less, it means whenever I know X , Y is well known, or X explains $1 - R^2$ percentage of Y .

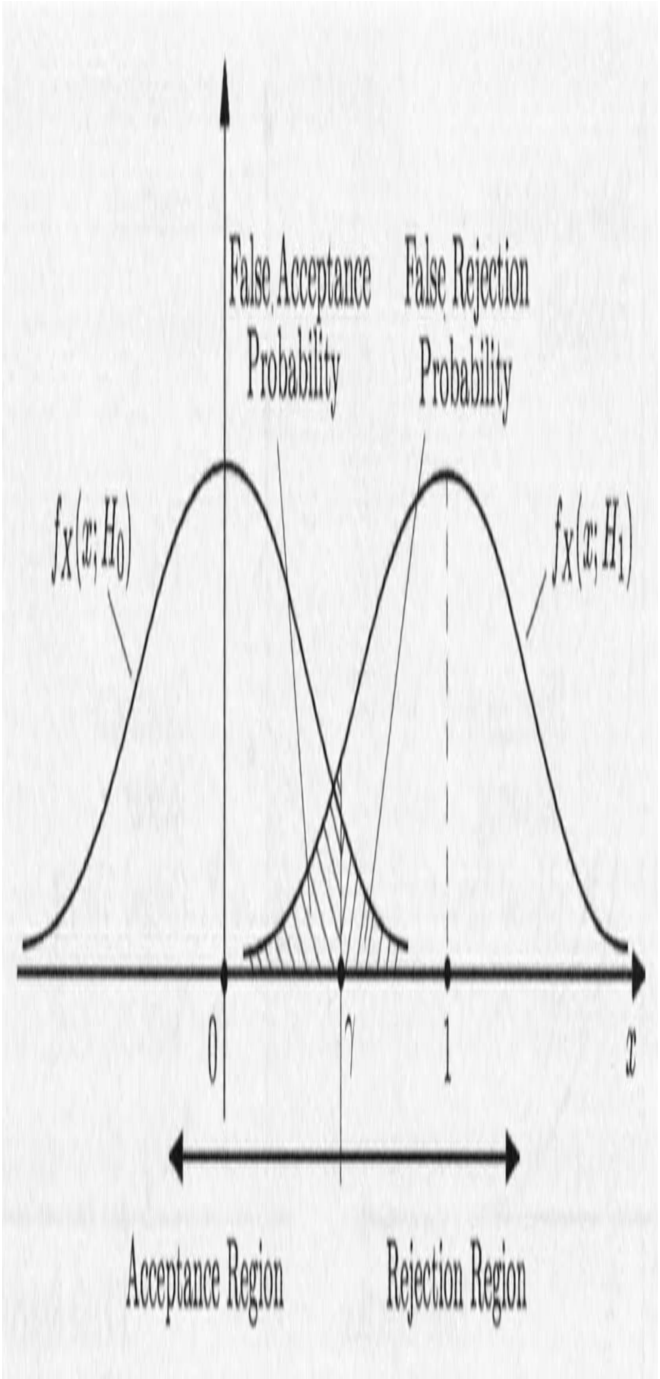
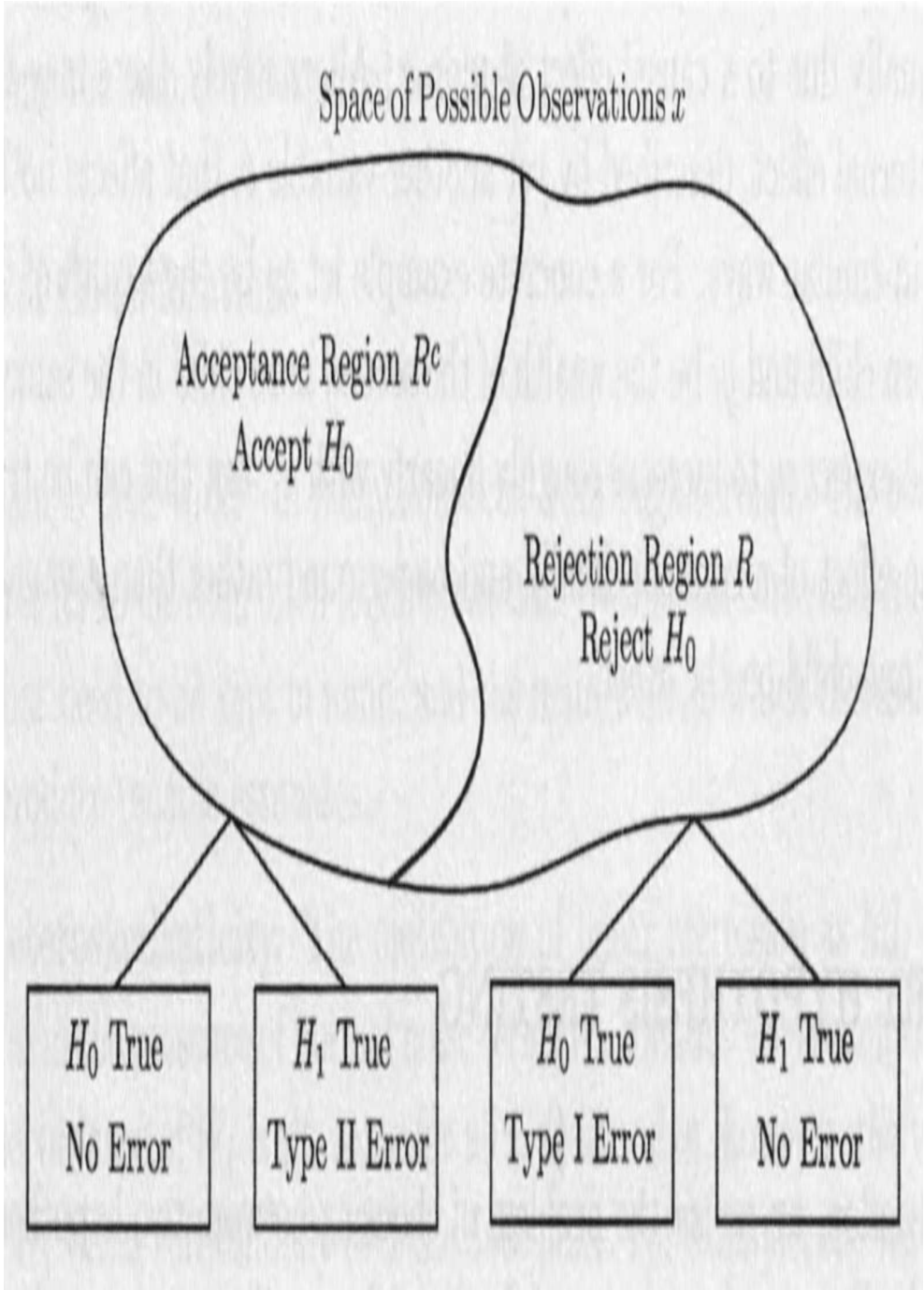
Common Pitfalls

- Heteroskedasticity** when $var(W_i)$ is strongly affected by the value of x_i .
- Multicollinearity** when two indicator variables x and x' bear a strong relation.
- Overfitting** The danger of producing a model that fits the data well, but is otherwise useless. A rule of thumb, there should be at least five or preferably ten times more data points than there are parameters to be estimated.
- Casuality** a linear relation should not be mistaken for a causal relation.

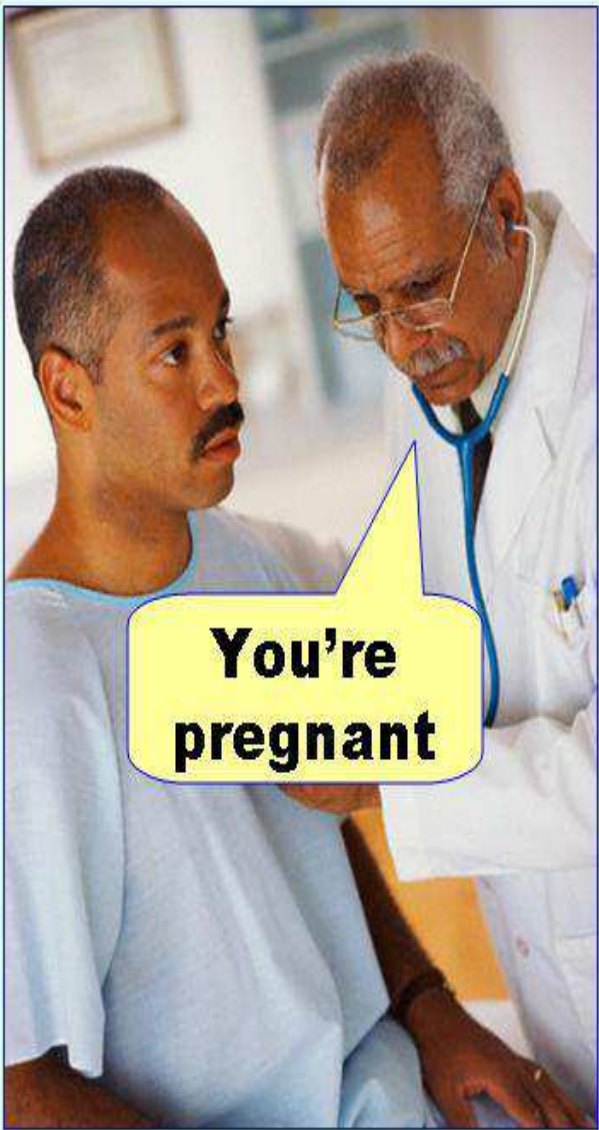
Binary Hypothesis Testing

Defn Assume no prior probability, we choose between two hypotheses H_0 and H_1 . Hypothesis H_0 is often called the *null hypothesis*, and H_1 the *alternative hypothesis*. This indicate that H_0 plays the role of a default model, to be proved or disproved on the basis of the available data.

Type I and Type II Error



Type I error
(false positive)



Type II error
(false negative)



Likelihood Ration Test (LRT)

Defn

Assume no prior probability, we choose between two hypotheses H_0 and H_1 . Define the *likelihood ratio* by

$$L(x) = \frac{p_X(x; H_1)}{p_X(x; H_0)}$$

where $p_X(x; H)$ denotes the PMF or PDF of the vector X under hypothesis H .

- Start with a target value α for the false rejection probability; typically 0.1, 0.05 or 0.01;
- Choose the *critical value* for ξ such that the false rejection probability is equal to α :

$$P(L(X) > \xi; H_0) = \alpha$$

- Once the value x of X is observed, reject H_0 if $L(X) > \xi$.

Significant Testing

Defn

When composite hypotheses involved, namely, no two well-specified alternatives, we wish to determine on the basis of observations $X = (X_1, \dots, X_n)$ whether the null hypothesis H_0 should be rejected or not.

General Steps.

- Choose a *statistic* S , namely a scalar random variable that will summarize the data to be obtained;
- Determine the *shape of the rejection region* by specifying the set of values of S for which H_0 will be rejected as a function of a yet undetermined critical value ξ
- Choose the *significance level*, namely the desired probability α of a false rejection of H_0
- Choose the *critical value* ξ so that the probability of false rejection is equal to α . At this point, the rejection region is completely determined.

Example. Got $S = 472$ heads in $n = 1000$ tosses; is this coin fair?
 H_0 : $p = \frac{1}{2}$ versus H_1 : $p \neq \frac{1}{2}$

- Choose a *statistic* S
- Determine the *rejection region*, $|S - \frac{n}{2}| > \xi$
- Choose the *significance level* $\alpha = 0.05$
- Choose the *critical value* ξ so that

$$P(\text{reject } H_0; H_0) = \alpha$$

Using the CLT, we have $\xi = 31$:

$$P(|S - 500| \leq 31; H_0) \approx 0.95$$

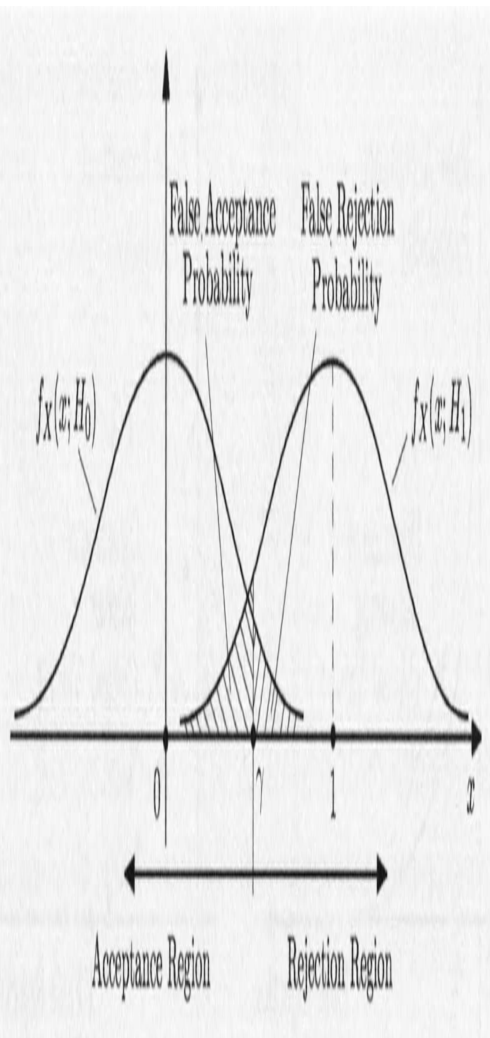
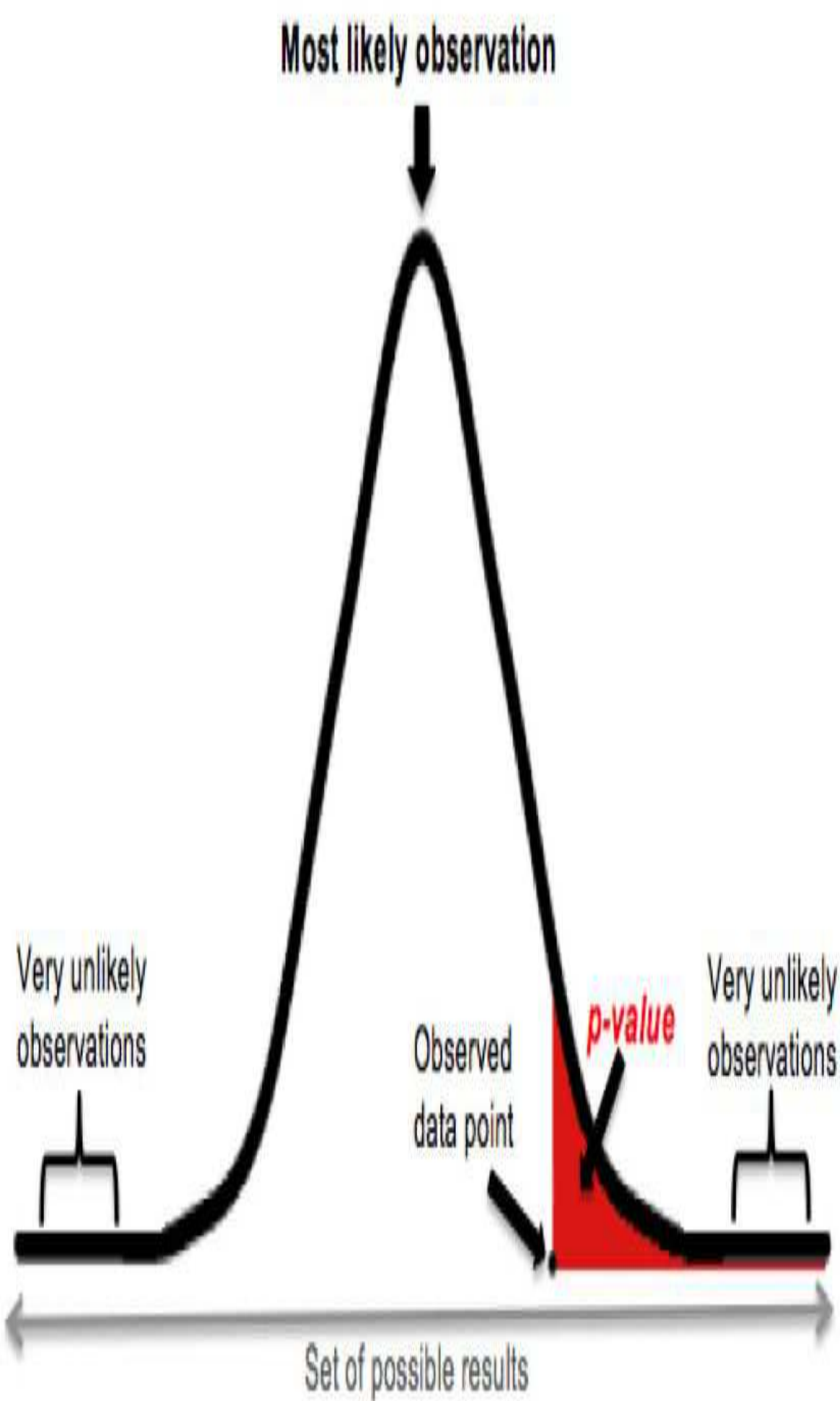
- As $|S - 500| = 28 < \xi$, so H_0 is not rejected at the 5% level.

NHST and P-Value

Defn	Warning: <i>P-values, the ‘gold standard’ of statistical validity, are not as reliable as many scientists assume.</i>
	Null Hypothesis Significance Testing (NHST) <ul style="list-style-type: none">■ State a null hypothesis: that is, there is no effect.■ Calculate the p value, which is the probability of getting results like ours - if the null hypothesis is true.■ If p is sufficiently small, reject the null hypothesis and sound the trumpets: our effect is not zero, it’s statistically significant!

Regina Nuzzo. Statistical errors. *Nature*, 506(Feburary):150–152, 2014
John P. A. Ioannidis. Why most published research findings are false. *PLoS Medicine*, 2(8):696–701, 2005
American Statistical Association. ASA statement on statistical significance and p-values. *The American Statistician*, 70(2):129–133, 2016

NHST and P-Value



A **p-value** (shaded red area) is the probability of an observed (or more extreme) result arising by chance

Defn	Consider a 2×2 table in which research findings are compared against the gold standard of true relationships.			
	Findings	True (Y)	True (No)	Total
	Find (Y)	$c(1 - \beta)R/(R + 1)$	$c\alpha/(R + 1)$	$c(R + \alpha - \beta R)/(R + 1)$
	Find (N)	$c\beta R/(R + 1)$	$c(1 - \alpha)/(R + 1)$	$c(1 - \alpha + \beta R)/(R + 1)$
	Total	$cR/(R + 1)$	$c/(R + 1)$	c

- Assume either there is only one true relationship (among many hypothesized) or the power is similar to find any of the several existing true relationships.
- Let R be the ratio of the number of “true relationships” to “no relationships” among those tested in the field. $R = \frac{P_Y}{P_N}$
- The pre-study probability of a relationship being true is $P_Y = \frac{R}{R+1}$
- The probability of a study finding a true relationship reflects the power $1 - \beta$ (one minus the Type II error rate)
- The probability of claiming a relationship when none truly exists reflects the Type I error rate, α .

When the finding shows *Yes*, how likely the truth is really *Yes*?

- The post study probability that is true is the positive predictive value (PPV), which is



$$PPV = P(Truth = Yes|Finding = Yes) = \frac{(1 - \beta)R}{(R - \beta R + \alpha)}$$

- When $(1 - \beta)R > \alpha$, we have $PPV > 50\%$, namely it is more likely true than false.
- If we take p value 0.05, namely here $\alpha = 0.05$, this means that PPV will be likely true than false when $(1 - \beta)R > 0.05$.
- If just report 0.05, it actually does not imply anything on the findings.

Questions?

Contact Information

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