Biostatistics Preparatory Course: Methods and Computing

Lecture 6

Simulations

Methods and Computing

Harvard University

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In the group exercise 2, we were given the following model:

$$E[Y|X_1, X_2] = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2$$

where Y was birthweight, X_1 was smoking status, and X_2 was mother's weight gain.

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- Why might β_3 be of interest?
 - If you believe that the effect of mother's weight gain varies within levels of smoking status
- What are the interpretations of β_1 and β_2 ?
 - The mean change in birthweight comparing smokers to non-smokers among mother's who did not gain weight
 - The mean change in birthweight corresponding to a one unit change in mother's weight gain among non-smokers

Recap / Warm-up: Linear Regression

$$\begin{split} E[Y|X_1 &= 1, X_2] = \hat{\beta}_0 + \hat{\beta}_1 + \hat{\beta}_2 X_2 + \hat{\beta}_3 X_2 \\ E[Y|X_1 &= 0, X_2] = \hat{\beta}_0 + \hat{\beta}_2 X_2 \end{split}$$

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What is a simulation?

- Numerical technique to conduct experiments on a computer
- In statistics, we typically care about 'Monte Carlo' (MC) simulations which involve random sampling from probability distributions
- Why bother?
 - When developing a new method, it is important to establish its properties so that it can be used in practice
 - Case I: Analytical derivations of properties are not always possible
 - It is often feasible to obtain large sample approximations, but evaluation of the approximation in finite samples is necessary
 - **Case II**: If you can derive analytic results, they usually require assumptions
 - What are the properties of the method when various conditions are violated?

- An **unbiased estimator** for some parameter means that the expected value of the estimator is equal to the parameter
- A confidence interval has **nominal coverage** if it covers the true value of the parameter the correct proportion of times
- The size of a hypothesis test is equal to the probability of rejecting the null hypothesis given that the null is true
- The **power** of a hypothesis test is equal to the probability of rejecting the null hypothesis given that the null is false

MC Simulations: The usual questions

• Under what conditions is an estimator unbiased? ex. Suppose the data is generated according to

$$\mathbf{y} \sim \beta_0 + \beta_1 \mathbf{x}_1 + \beta_2 \mathbf{x}_2 + \epsilon$$

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• How does the estimator compare to other estimators? What is its sampling variability?

ex. Suppose the data is generated according to

$$\mathbf{y} \sim \alpha_0 + \alpha_1 \mathbf{x}_1 + \alpha_2 \mathbf{x}_2 + \epsilon$$

with $E(\epsilon) = 0$ and $Var(\epsilon) = \sigma^2 I$. How do the OLS estimators compare to

$$\hat{\alpha}_{1} = \frac{\sum_{i=1}^{n} (y_{i} - \bar{y})(x_{i}^{*} - \bar{x}^{*})}{\sum_{i=1}^{n} (x_{i} - \bar{x})(x_{i}^{*} - \bar{x}^{*})} \text{ and } \hat{\alpha}_{0} = \frac{\sum_{i=1}^{n} y_{i}/x_{i}}{\sum_{i=1}^{n} 1/x_{i}} - \hat{\alpha}_{1} \frac{n}{\sum_{i=1}^{n} 1/x_{i}}$$
where \bar{x}^{*} is mean of $x_{i}^{*} = 1/x_{i}$?

MC Simulations: The usual questions

- Does a confidence interval procedure attain nominal coverage? ex.
 - The sum of *n* independent Bernoulli trials with common success probability is distributed according to Bin(n, π)
 - The MLE for π is $\hat{\pi} = \frac{X}{n}$ where X is the observed number of successes
 - The Wald 95% Confidence Interval for π is given by:

$$\left(\hat{\pi} - z_{0.975}\sqrt{rac{\hat{\pi}(1-\hat{\pi})}{n}}, \hat{\pi} + z_{0.975}\sqrt{rac{\hat{\pi}(1-\hat{\pi})}{n}}
ight)$$

• The Score 95% Confidence Interval for π is given by:

$$\hat{\pi} \left(\frac{n}{n+z_{0.975}^2} \right) + \frac{1}{2} \left(\frac{z_{0.975}^2}{n+z_{0.975}^2} \right) \pm z_{0.975} \sqrt{\frac{1}{n+z_{0.975}^2} \left[\hat{\pi} (1-\hat{\pi}) \left(\frac{n}{n+z_{0.975}^2} \right) + \left(\frac{1}{2} \right) \left(\frac{1}{2} \right) \left(\frac{z_{0.975}^2}{n+z_{0.975}^2} \right) \right]}$$

How does the coverage compare for both intervals as we increase n and vary p?

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• Does a hypothesis testing procedure achieve the specified size? If so, what is the power like? How does it compare to alternative procedures?

ex. Consider the one sample t-test for

$$H_0: \mu = 0$$
 vs. $H_A: \mu \neq 0$

How does the power vary when the data is generated under some alternative hypothesis $\mu \neq \mu_0$?

How does Monte Carlo simulation help to answer these questions?

MC Simulations: Intuition

- An estimator/test statistic has a true sampling distribution under some set of conditions
- We'd like to know the true sampling distribution so we can answer the questions on the previous slide but...
 - The (finite sample) derivation is difficult

and/or

We'd like to see how well the method holds up when assumptions are violated

So, we approximate the sampling distribution of an estimator/test statistic under a particular set of conditions through simulation

How to Approximate the Sampling Distribution

- Generate *B* independent data sets according to the data generating process
- Compute the value of the estimator/test statistic T(data) for each data set $\rightarrow \{T_1, \dots, T_B\}$

If b is large enough, summary statistics using $\{T_1, \ldots, T_b\}$ should be good approximations to the true sampling properties of the estimator/test statistic under the specified conditions

ex. T_b is the value of T from the b^{th} data set, $b = 1, \ldots, B$

- The empirical mean computed with the *B* data sets is an estimate of the true mean of the sampling distribution of the estimator
- The empirical standard error computed with the *B* data sets is an estimate of the true standard deviation of the sampling distribution of the estimator

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Commonly reported quantities

Your simulation study has B replicates for some estimator T of θ .

Simulation bias

$$\operatorname{bias}(T) = \frac{1}{b} \sum_{b=1}^{B} T_{b} - \theta$$

Simulation relative bias

relative bias(
$$T$$
) = $\frac{\text{bias}(T)}{\theta}$

• Simulation standard deviation

$$\operatorname{sd}(T) = \sqrt{\frac{1}{B-1}\sum_{b=1}^{B}(T_b - \overline{T})^2}$$

Simulation mean squared error

$$MSE(T) = bias(T)^2 + sd(T)^2$$

Although omitted, you may also be interested in reporting the empirical coverage for confidence interval, power, or size.

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Tips for Running Your Own Simulation Studies

- Setting parameter values:
 - First run your code under a favorable setting (make sure it works)
 - Then choose parameter values that will challenge your method
- 2 Don't make B too large to start (\approx 500)
- Save all the estimates and not just the summary statistics
- Set the seed
- Ocument the code (i.e. comments)
- 6 Keep track of the versions of the code you use (i.e. use GitHub)
- If you use Rmarkdown, use the cache=TRUE preamble
 - Your code will only be knitted/run the first time or anytime after it updated. Saves time!

Only present what is interesting

- ex. If the bias is small, just make a comment in the text rather than making a table
- ex. If two parameter settings are similar, you don't need to include both
- In homework assignments, you will typically be told what to report
- Ø Make the results easy for the reader to understand
 - Columns meant to be compared should be side-by-side
 - Make a graph if possible

- Suppose you are interested in comparing the properties of the following 3 estimators for the mean μ for *n* iid draws $X_1, \ldots X_n$ with $X_i \sim f(x)$
 - **(1)** Sample mean, T^1
 - 2 Sample 15% trimmed mean, T^2
 - Sample median, T³

How would you expect the estimators to compare if $X_i \sim N(1, 16)$?