Linear Regression and Resampling Methods for Uncertainty

Big Data y Machine Learning para Economía Aplicada

Ignacio Sarmiento-Barbieri

Universidad de los Andes

Agenda

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Predicting Well

$$y = f(X) + u \tag{1}$$

- Interest on predicting y
- Model? We treat $f()$ as a black box, and any approximation $\hat{f}()$ that yields a good prediction is good enough (*"Whatever works, works..."*).
- How do we measure "what works"?

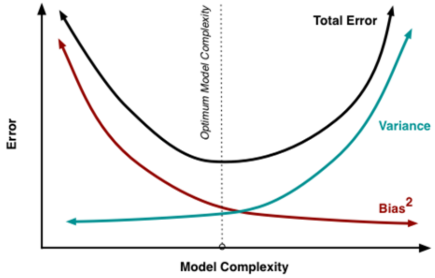
$$E(y - \hat{y})^2 = E(f(X) + u - \hat{f}(X))^2 \tag{2}$$

Predicting Well

$$E(y-\hat{y})^2 = \underbrace{[f(X)-\hat{f}(X)]^2}_{Reducible} + \underbrace{Var(u)}_{Irreducible} \tag{3}$$

$$MSE = Bias^2(\hat{f}(X)) + V(\hat{f}(X)) + \underbrace{Var(u)}_{Irreducible} \tag{4}$$

The Bias-Variance Trade-Off



Source: https://tinyurl.com/y4lvjxpc

- The best kept secret: tolerating some bias is possible to reduce $V(\hat{f}(X))$ and lower MSE

Linear Regression

$$y = f(X) + u \tag{5}$$
$$= \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + u \tag{6}$$
$$= X\beta + u \tag{7}$$

- If $f(X) = X\beta$, obtaining $f(.)$ boils down to obtaining β
- where we can obtain β minimizing RSS (SSR)

$$\hat{\beta} = (X'X)^{-1}X'y \tag{8}$$

- Involves inverting a $k \times k$ matrix $X'X$
- requires allocating $O(nk + k^2)$ if n is "big" we cannot store this in memory

Linear Regression

- Gauss-Markov Theorem
  - If it is assumed that $E(u|X) = 0$ and $E(uu'|X) = \sigma^2 I$ in the linear regression model $y = X\beta + u$, then the OLS estimator $\hat{\beta}$ is more efficient than any other linear unbiased estimator $\tilde{\beta}$, in the sense that $Var(\tilde{\beta}) - Var(\hat{\beta}$ is a positive semidefinite matrix.
- An informal way of stating this theorem is to say that $\hat{\beta}$ is the best linear unbiased estimator, or BLUE for short.
- In other words, the OLS estimator is more efficient than any other linear unbiased estimator.

Linear Regression

- Let's consider the simple case with two regressors:

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + u \tag{9}$$

- with $E(u) = 0$, $cov(x_1, u) = 0$, $cov(x_2, u) = 0$ and $E(u^2|x_1, x_2) = \sigma^2$
- OLS says we should choose the estimators $\hat{\beta}_0$,$\hat{\beta}_1$, $\hat{\beta}_2$ of β_0, β_1, β_2 such that we minimize the Sum of Square Residual (SSR) or the Residual Sum of Squares (RSS)

$$\mathcal{L} = \sum (y_i - \hat{y}_i)^2 \tag{10}$$

$$= \sum \left(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{1i} - \hat{\beta}_2 x_{2i}\right)^2 \tag{11}$$

Linear Regression

- The solution then comes from solving the FOC (and checking the SOC)

$$\frac{\partial \mathcal{L}}{\partial \hat{\beta}_0} = \sum 2\left(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{1i} - \hat{\beta}_2 x_{2i}\right)(-1) = 0 \tag{12}$$

$$\frac{\partial \mathcal{L}}{\partial \hat{\beta}_1} = \sum 2\left(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{1i} - \hat{\beta}_2 x_{2i}\right)(-x_{1i}) = 0 \tag{13}$$

$$\frac{\partial \mathcal{L}}{\partial \hat{\beta}_2} = \sum 2\left(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{1i} - \hat{\beta}_2 x_{2i}\right)(-x_{2i}) = 0 \tag{14}$$

- Solving, for example, for $\hat{\beta}_2$ we have

$$\hat{\beta}_2 = \frac{\sum(x_{1i} - \bar{x}_1)^2 \sum(x_{2i} - \bar{x}_2)y_i - \left(\sum x_{1i}x_{2i} - n\bar{x}_1\bar{x}_2\right)\sum(x_{1i} - \bar{x}_1)y_i}{\sum(x_{1i} - \bar{x}_1)^2 \sum(x_{2i} - \bar{x}_2)^2 - \left(\sum x_{1i}x_{2i} - n\bar{x}_1\bar{x}_2\right)^2} \tag{15}$$

Goodness-of-fit. In sample performance

- The mechanics of OLS lead to a very simple measure of *goodness of fit*, the R^2, or *coefficient of determination*, one of the most used and abused in the practice of econometrics and statistics.

- The starting point is the following *sum of squares decomposition*:

$$\sum \tilde{y}_i^2 = \sum \hat{\tilde{y}}_i^2 + \sum e_i^2,$$

- where $\tilde{y}_i \equiv Y_i - \bar{Y}$, $\hat{y}_i \equiv \hat{Y}_i - \bar{Y}$ and e_i are OLS residuals. The decomposition holds for any number of explanatory variables.

- where $\tilde{y}_i \equiv y_i - \bar{y}, \hat{\tilde{y}}_i \equiv \hat{\tilde{y}}_i - \bar{y}$ and e_i are OLS residuals.

- The decomposition holds for any number of explanatory variables, the derivation uses the FOC above

Goodness-of-fit. In sample performance

- To get some intuition, divide by n in both sides of the decomposition $\rightarrow$ Each term resembles sort of a variance.
- The decomposition suggests that the total variability of Y can be 'explained' by the variability in the fitted model (ESS) plus that of the error term (RSS).

$$TSS = ESS + RSS$$

- The *coefficient of determination*, or R^2 for a given regression model is defined as

$$R^2 \equiv \frac{ESS}{TSS}$$

- which we can also rewrite as

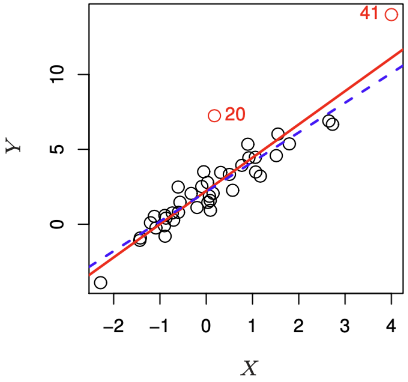
$$R^2 \equiv 1 - \frac{RSS}{TSS}$$

Goodness-of-fit. In sample performance

- R_2 is non decreasing in the number of explanatory variables

High Leverage Points

- Outliers are observations for which the response y_i is unusual given the predictor x_i.
- In contrast, observations with high leverage high have an unusual value for x_i.



High Leverage Points

- Suppose the simple model

$$y = \beta_0 + \beta_1 x + u$$

- the solution for $\hat{\beta}_1$ is

$$\hat{\beta}_1 = \frac{\sum(x_i - \bar{x})y_i}{\sum(x_i - \bar{x})^2} = \sum c_i y_i \tag{16}$$

- the solution for $\hat{\beta}_0$ is

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} = \frac{1}{n}\sum y_i - \bar{x}\sum c_i y_i \tag{17}$$

- With a bit of algebra we can write

$$\hat{y}_i = \sum \left(\frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum(x_i - \bar{x})^2} \right) y_i \tag{18}$$

$$\hat{y}_i = \sum h_i y_i \tag{19}$$

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Motivation

- The real world is messy.
- Recognizing this mess will differentiate a sophisticated and useful analysis from one that is hopelessly naive.
- This is especially true for highly complicated models, where it becomes tempting to confuse signal with noise and hence “overfit.”
- The ability to deal with this mess and noise is the most important skill you need.

Uncertainty in Linear Regression

- To get a measure of the uncertainty, precision or variability of our estimates we need a measure
- We can estimate the Variance of our estimators
- For example for

$$y_i = \beta_0 + \beta_1 x_{1i} + u \tag{20}$$

$$\hat{\beta}_1 = \frac{\sum(x_{1i} - \bar{x}_1)y_i}{\sum(x_{1i} - \bar{x}_1)^2} \tag{21}$$

$$Var(\hat{\beta}_1) = \frac{\sigma^2}{\sum(x_{1i} - \bar{x}_1)^2} = \frac{\sigma^2}{nVar(x_{1i})} \tag{22}$$

Uncertainty in Linear Regression

- Let's go back to our two variable model

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + u \tag{23}$$

- the solution for β_2 was:

$$\hat{\beta}_2 = \frac{\sum(x_{1i} - \bar{x}_1)^2 \sum(x_{2i} - \bar{x}_2)y_i - \left(\sum x_{1i}x_{2i} - n\bar{x}_1\bar{x}_2\right)\sum(x_{1i} - \bar{x}_1)y_i}{\sum(x_{1i} - \bar{x}_1)^2 \sum(x_{2i} - \bar{x}_2)^2 - \left(\sum x_{1i}x_{2i} - n\bar{x}_1\bar{x}_2\right)^2} \tag{24}$$

Uncertainty in Linear Regression

- The variance?

$$Var(\hat{\beta}_2) = \frac{\sigma^2}{nVar(x_2)(1 - R_2^2)} \tag{25}$$

- this is a special case of the very general formula

$$Var(\hat{\beta}_k) = \frac{\sigma^2}{nVar(x_k)(1 - R_k^2)} \tag{26}$$

Agenda

What are resampling methods?

- Tools that involves repeatedly drawing samples from a training set and refitting a model of interest on each sample in order to obtain more information about the fitted model
  - Parameter Assessment: estimate standard errors
  - Model Assessment: estimate test error rates
  - Model Selection: select the appropriate level of model flexibility
  - They are computationally expensive! But these days we have powerful computers

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The Bootstrap
Introduction

- Suppose we have $y_1, y_2, \ldots, y_n$ iid $Y \sim (\mu, \sigma^2)$ (both finite)
- We want to estimate

$$Var(\bar{Y}) \tag{27}$$

The Bootstrap

Introduction

- Alternative way (no formula!)
  1. From the n original data points $y_1, y_2, \ldots, y_n$ take a sample *with replacement* of size n
  2. Calculate the sample average of this *"pseudo-sample"*
  3. Repeat this B times.
  4. Compute the variance of the B means

The Bootstrap
Introduction

- The bootstrap is a widely applicable and extremely powerful statistical tool that can be used to quantify the uncertainty associated with a given estimator or statistical learning method.
- In German the expression *an den eigenen Haaren aus dem Sumpf zu ziehen* nicely captures the idea of the bootstrap – *"to pull yourself out of the swamp by your own hair."*

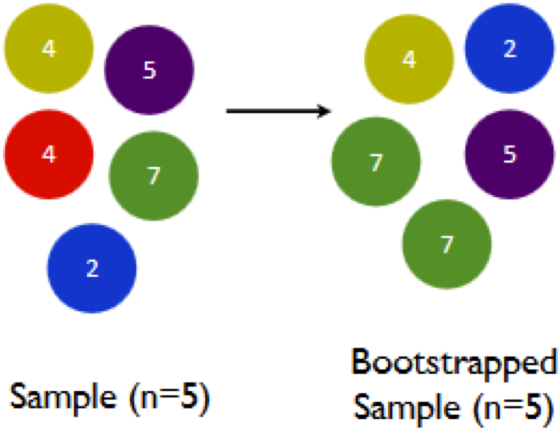
The Bootstrap
Introduction

- **Key Innovation**: The sample itself is used to assess the precision of the estimate.
- Why would this work?
- Remember that uncertainty arises from the randomness inherent to our data-generating process
- So if we can approximately simulate this randomness, then we can approximately quantify our uncertainty.

The Bootstrap
Introduction

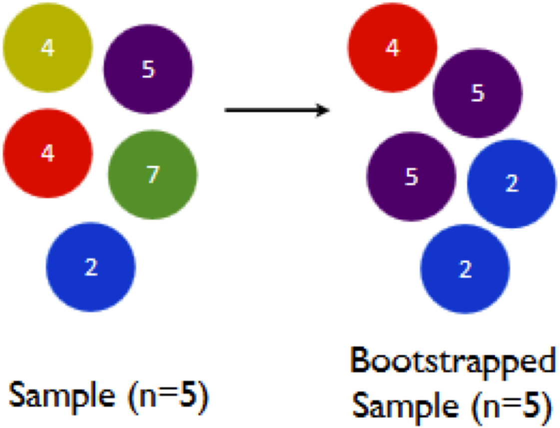
- There are two key properties of bootstrapping that make this seemingly crazy idea actually work.
  1. Each bootstrap sample must be of the same size (N) as the original sample
  2. Each bootstrap sample must be taken with replacement from the original sample

Sampling with replacement



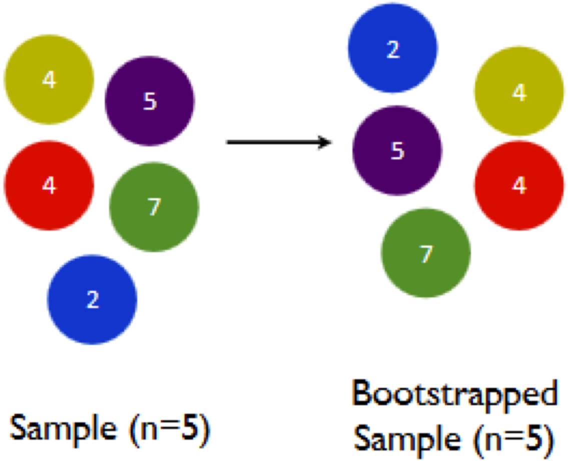
Sampling with replacement

Resampling creates synthetic variability



Sampling with replacement

Resampling creates synthetic variability

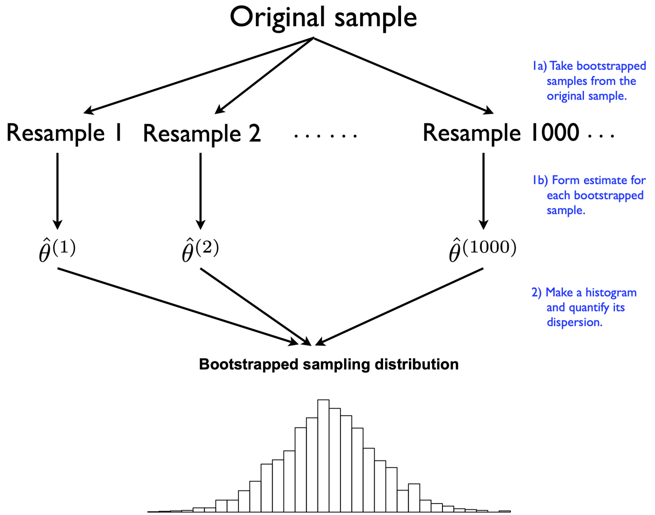


The Bootstrap

- In general terms:
  - $Y_i \; i = 1, \ldots, n$
  - θ is the magnitude of interest
- To calculate it's variance
  1. Sample of size n with replacement (*bootstrap sample*)
  2. Compute $\hat{\theta}_j \; j = 1, \ldots, B$
  3. Repeat B times
  4. Calculate

$$\hat{V}(\hat{\theta})_B = \frac{1}{B} \sum_{j=1}^{B} (\hat{\theta}_j - \bar{\hat{\theta}})^2 \tag{28}$$

The Bootstrap



Example: Elasticity of Demand for Gasoline

photo from https://www.dailydot.com/parsec/batman-1966-labels-tumblr-twitter-vine/

Review and Caveats

- The bootstrap is a widely applicable and extremely powerful statistical tool that can be used to quantify the uncertainty associated with a given estimator or statistical learning method.
- The power of the bootstrap, and resampling in general, lies in the fact that it can be easily applied to a wide range of statistical learning methods.
- In particular, it does not assume that the regression errors are iid so it can accommodate heteroscedasticity.
- Of course it does still assume that the observations are independent.
- Resampling dependent observations is an inherently more difficult task which has generated its own rather large literature.