The Bootstrap¹ STA442/2101 Fall 2017

 $^{^1 \}mathrm{See}$ last slide for copyright information.





2 Bootstrap



3 Distribution-free regression example

Sampling distributions

- Let $\mathbf{x} = (X_1, \dots, X_n)$ be a random sample from some distribution F.
- $T = T(\mathbf{x})$ is a statistic (could be a vector of statistics).
- Need to know about the distribution of T.
- Sometimes it's not easy, even asymptotically.

Sampling distribution of T: The elementary version For example $T = \overline{X}$

- Sample repeatedly from this population (pretend).
- For each sample, calculate T.
- Make a relative frequency histogram of the T values you observe.
- As the number of samples becomes very large, the histogram approximates the distribution of T.

What is a bootstrap? Pull yourself up by your bootstraps



This photograph was taken by Tarquin. It is licensed under a Creative Commons Attribution - ShareAlike 3.0 Unported License. For more information, see the entry at the wikimedia site.

The (statistical) Bootstrap Bradley Efron, 1979

- Select a random sample from the population.
- If the sample size is large, the sample is similar to the population.
- Sample repeatedly from the sample. This is called *resampling*.
- Sample from the sample? Think of putting the sample data values in a jar ...
- Calculate the statistic for every bootstrap sample.
- A histogram of the resulting values approximates the shape of the sampling distribution of the statistic.

Notation

- Let $\mathbf{x} = (X_1, \dots, X_n)$ be a random sample from some distribution F.
- $T = T(\mathbf{x})$ is a statistic (could be a vector of statistics).
- Form a "bootstrap sample" \mathbf{x}^* by sampling *n* values from \mathbf{x} with replacement.
- Repeat this process B times, obtaining $\mathbf{x}_1^*, \ldots, \mathbf{x}_B^*$.
- Calculate the statistic for each bootstrap sample, obtaining T_1^*, \ldots, T_B^* .
- Relative frequencies of T_1^*, \ldots, T_B^* approximate the sampling distribution of T.

Why does it work?

$$\widehat{F}(x) = \frac{1}{n} \sum_{i=1}^{n} I\{X_i \le x\} \xrightarrow{a.s.} E(I\{X_i \le x\}) = F(x)$$

- Resampling from **x** with replacement is the same as simulating a random variable whose distribution is the empirical distribution function $\widehat{F}(x)$.
- Suppose the distribution function of T is a nice smooth function of F.
- Then as $n \to \infty$ and $B \to \infty$, bootstrap sample moments and quantiles of T_1^*, \ldots, T_B^* converge to the corresponding moments and quantiles of the distribution of T.
- If the distribution of \mathbf{x} is discrete and supported on a finite number of points, the technical issues are minor.

Quantile Bootstrap Confidence Intervals

- Suppose T_n is a consistent estimator of $g(\theta)$.
- And the distribution of T_n is approximately symmetric around $g(\theta)$.
- Then the lower $(1 \alpha)100\%$ confidence limit for $g(\theta)$ is the $\alpha/2$ sample quantile of T_1^*, \ldots, T_B^* , and the upper limit is the $1 \alpha/2$ sample quantile.
- For example, the 95% confidence interval ranges from the 2.5th to the 97.5th percentile of T_1^*, \ldots, T_B^* .

Bootstrap

Symmetry A requirement that is often ignored



The distribution of T symmetric about θ means for all d > 0, $P\{T > \theta + d\} = P\{T < \theta - d\}.$





- The distribution of T symmetric about θ means for all d > 0, $P\{T > \theta + d\} = P\{T < \theta d\}$.
- Select d so that the probability equals $\alpha/2$.

$$1 - \alpha = P\{\theta - d < T < \theta + d\}$$
$$= P\{T - d < \theta < T + d\}$$

Need to estimate d.

Estimating dThere are two natural estimates



 $1 - \alpha = P\{\theta - d < T < \theta + d\} = P\{Q_{1 - \alpha/2} < T < Q_{\alpha/2}\}$

$$\begin{split} & \widehat{\theta} - \widehat{d}_1 = \widehat{Q}_{\alpha/2} \quad \Rightarrow \quad \widehat{d}_1 = T - \widehat{Q}_{\alpha/2} \\ & \widehat{\theta} + \widehat{d}_2 = \widehat{Q}_{1-\alpha/2} \quad \Rightarrow \quad \widehat{d}_2 = \widehat{Q}_{1-\alpha/2} - T \end{split}$$

I would average them:

$$\widehat{d} = \frac{1}{2}(\widehat{d}_1 + \widehat{d}_2) = \frac{1}{2}(\widehat{Q}_{1-\alpha/2} - \widehat{Q}_{\alpha/2})$$

$$1 - \alpha = P\{T - d < \theta < T + d\}$$
Plug in an estimate of d

•
$$\hat{d}_1 = T - \hat{Q}_{\alpha/2}$$

• $\hat{d}_2 = \hat{Q}_{1-\alpha/2} - T$
• $\hat{d} = \frac{1}{2}(\hat{d}_1 + \hat{d}_2)$

Using \hat{d}_1 on the left yields

$$T - \widehat{d}_1 = T - (T - \widehat{Q}_{\alpha/2}) = \widehat{Q}_{\alpha/2}$$

Using \widehat{d}_2 on the right yields

$$T + \hat{d}_2 = T + (\hat{Q}_{1-\alpha/2} - T) = \hat{Q}_{1-\alpha/2},$$

which is the quantile confidence interval.

Maybe more reasonable: $T \pm \hat{d}$ But this is just me



where

•
$$\hat{d}_1 = T - \hat{Q}_{\alpha/2}$$

• $\hat{d}_2 = \hat{Q}_{1-\alpha/2} - T$
• $\hat{d} = \frac{1}{2}(\hat{d}_1 + \hat{d}_2)$

Justifying the Assumption of Symmetry

- Smooth functions of asymptotic normals are asymptotically normal.
- This includes functions of sample moments and MLEs.
- Delta method:

 $\sqrt{n} (T_n - \theta) \stackrel{d}{\rightarrow} T \sim N(0, \sigma^2)$ means T_n is asymptotically normal.

 $\sqrt{n} (g(T_n) - g(\theta)) \xrightarrow{d} Y \sim N(0, g'(\theta)^2 \sigma^2)$ means $g(T_n)$ is asymptotically normal too.

• Univariate and multivariate versions.

Can use asymptotic normality directly

Suppose T is asymptotically normal.

- Sample standard deviation of T_1^*, \ldots, T_B^* is a good standard error.
- Confidence interval is $T \pm 1.96 SE$.
- If T is a vector, the sample variance-covariance matrix of T_1^*, \ldots, T_B^* is useful.

Example

Let Y_1, \ldots, Y_n be a random sample from an unknown distribution with expected value μ and variance σ^2 . Give a point estimate and a 95% confidence interval for the coefficient of variation $\frac{\sigma}{\mu}$.

- Point estimate is $T = S/\overline{Y}$.
- If $\mu \neq 0$ then T is asymptotically normal and therefore symmetric.
- Resample from the data urn n times with replacement, and calculate T_1^* .
- Repeat B times, yielding T_1^*, \ldots, T_B^* .
- Percentile confidence interval for $\frac{\sigma}{\mu}$ is $(\widehat{Q}_{\alpha/2}, \widehat{Q}_{1-\alpha/2})$.
- Alternatively, since T is approximately normal, calculate $\hat{\sigma}_T = \frac{1}{B-1} \sum_{i=i}^{B} (T_i^* \overline{T}^*)^2$
- And a 95% confidence interval is $T \pm 1.96 \,\widehat{\sigma}_T$.

Example: Distribution-free regression

Independently for $i = 1, \ldots, n$, let

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i,$$

where

• X_i and ϵ_i come from unknown distributions,

•
$$E(\epsilon_i) = 0, Var(\epsilon_i) = \sigma^2,$$

- X_i and ϵ_i are independent.
- Moments of X_i will be denoted E(X), $E(X^2)$, etc.

Observable data consist of the pairs $(X_1, Y_1), \ldots, (X_n, Y_n)$.

Estimation

Estimate β_0 and β_1 as usual by

$$\widehat{\beta}_{1} = \frac{\sum_{i=1}^{n} (X_{i} - \overline{X})(Y_{i} - \overline{Y})}{\sum_{i=1}^{n} (X_{i} - \overline{X})^{2}}$$
$$= \frac{\sum_{i=1}^{n} X_{i}Y_{i} - n\overline{X}\overline{Y}}{\sum_{i=1}^{n} X_{i}^{2} - n\overline{X}^{2}} \text{ and}$$

$$\widehat{\beta}_0 = \overline{Y} - \widehat{\beta}_1 \overline{X}$$

- Consistency follows from the Law of Large Numbers and continuous mapping.
- Looks like $\widehat{\beta}_0$ and $\widehat{\beta}_1$ are asymptotically normal.
- Use this to get tests and confidence intervals.

Bootstrap approach: All by computer

- Earlier discussion implies $\hat{\beta}$ is asymptotically multivariate normal.
- Say $\widehat{\boldsymbol{\beta}} \sim N_p(\boldsymbol{\beta}, \mathbf{V}).$
- All we need is a good $\widehat{\mathbf{V}}$.
- Put data vectors $\mathbf{d}_i = (\mathbf{x}_i, Y_i)$ in a jar.
- Sample *n* vectors with replacement, yielding \mathbf{D}_1^* . Fit the regression model, obtaining $\widehat{\boldsymbol{\beta}}_1^*$.
- Repeat *B* times. This yields $\hat{\boldsymbol{\beta}}_1^* \dots \hat{\boldsymbol{\beta}}_B^*$.
- The sample covariance matrix of $\hat{\beta}_1^* \dots \hat{\beta}_B^*$ is $\hat{\mathbf{V}}$.
- Under $H_0: \mathbf{L}\boldsymbol{\beta} = \mathbf{h},$

$$(\mathbf{L}\widehat{\boldsymbol{\beta}}-\mathbf{h})^{\top}(\mathbf{L}\widehat{\mathbf{V}}^{-1}\mathbf{L}^{\top})^{-1}(\mathbf{L}\widehat{\boldsymbol{\beta}}-\mathbf{h}) \stackrel{\cdot}{\sim} \chi^2(r)$$

Remark

This is not a typical bootstrap regression.

- Usually people fit a model and then bootstrap the residuals, not the whole data vector.
- Bootstrapping the residuals applies to conditional regression (conditional on $\mathbf{X} = \mathbf{x}$).
- Our regression model is unconditional.
- The large-sample arguments are simpler in the unconditional case.

Copyright Information

This slide show was prepared by Jerry Brunner, Department of Statistics, University of Toronto. It is licensed under a Creative Commons Attribution - ShareAlike 3.0 Unported License. Use any part of it as you like and share the result freely. The LAT_EX source code is available from the course website: http://www.utstat.toronto.edu/~brunner/oldclass/appliedf17