

Basic Statistics and a Bit of Bootstrap

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Bias and Variance

Parameters

- Suppose we have a probability distribution P .
- Often we want to estimate some characteristic of P .
 - e.g. expected value, variance, kurtosis, median, etc...
- These things are called **parameters** of P .
- A **parameter** $\mu = \mu(P)$ is any function of the distribution P .
- Question: Is μ random?
- Answer: Nope. For example if P has density $f(x)$ on \mathbf{R} , then mean is

$$\mu = \int_{-\infty}^{\infty} xf(x) dx,$$

which is just an integral - nothing random.

- Suppose $\mathcal{D}_n = (x_1, x_2, \dots, x_n)$ is an i.i.d. sample from P .
- A **statistic** $s = s(\mathcal{D}_n)$ is any function of the data.
- A statistic $\hat{\mu} = \hat{\mu}(\mathcal{D}_n)$ is a **point estimator** of μ if $\hat{\mu} \approx \mu$.
- Question: Are statistics and/or point estimators random?
- Answer: Yes, since we're considering the data to be random.
 - The function $s(\cdot)$ isn't random, but we're plugging in random inputs.

Examples of Statistics

- Mean: $\bar{x}(\mathcal{D}_n) = \frac{1}{n} \sum_{i=1}^n x_i$.
- Median: $m(\mathcal{D}_n) = \text{median}(x_1, \dots, x_n)$
- Sample variance: $\sigma^2(\mathcal{D}_n) = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x}(\mathcal{D}_n))^2$

Fancier:

- A data histogram is a statistic.
- Empirical distribution function.
- A confidence interval.

Statistics are Random

- Statistics are random, so they have probability distributions.
- The distribution of a statistic is called a **sampling distribution**.
- We often want to know some **parameters** of the sampling distribution.
 - Most commonly the mean and the standard deviation.
- The standard deviation of the sampling distribution is called the **standard error**.
- Question: Is standard error random?
- Answer: Nope. It's a parameter of a distribution.

Bias and Variance for Real-Valued Estimators

- Let $\mu = \mu(P)$ be a real-valued parameter of distribution P .
- Let $\hat{\mu} = \hat{\mu}(\mathcal{D}_n)$ be a point estimator of μ .
- We define the **bias** of $\hat{\mu}$ to be $\text{Bias}(\hat{\mu}) = \mathbb{E}\hat{\mu} - \mu$.
- An estimator is **unbiased** if $\text{Bias}(\hat{\mu}) = \mathbb{E}\hat{\mu} - \mu = 0$.
- We define the **variance** of $\hat{\mu}$ to be $\text{Var}(\hat{\mu}) = \mathbb{E}\hat{\mu}^2 - (\mathbb{E}\hat{\mu})^2$.

Neither bias nor variance depend on a specific sample \mathcal{D}_n . We are taking expectation over \mathcal{D}_n .

- Why might we care about the bias and variance of an estimator?

Putting “Error Bars” on Estimators

- Why do we even care about estimating variance?
- May want to report a confidence interval for our point estimate, e.g.

$$\hat{\mu} \pm \sqrt{\widehat{\text{Var}}(\hat{\mu})}$$

- Where $\sqrt{\widehat{\text{Var}}(\hat{\mu})}$ is our **estimate of the standard error** of $\hat{\mu}$.

Estimating Variance of an Estimator

- To estimate $\text{Var}(\hat{\mu})$, we can use estimates of $\mathbb{E}\hat{\mu}$ and $\mathbb{E}\hat{\mu}^2$.
- Instead of a single sample \mathcal{D}_n of size n , suppose we had
 - B independent samples of size n : $\mathcal{D}_n^1, \mathcal{D}_n^2, \dots, \mathcal{D}_n^B$
- Can then estimate

$$\mathbb{E}\hat{\mu} \approx \frac{1}{B} \sum_{i=1}^B \hat{\mu}(\mathcal{D}_n^i)$$

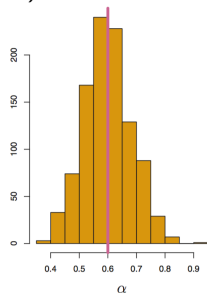
$$\mathbb{E}\hat{\mu}^2 \approx \frac{1}{B} \sum_{i=1}^B [\hat{\mu}(\mathcal{D}_n^i)]^2$$

and

$$\text{Var}(\hat{\mu}) \approx \frac{1}{B} \sum_{i=1}^B [\hat{\mu}(\mathcal{D}_n^i)]^2 - \left[\frac{1}{B} \sum_{i=1}^B \hat{\mu}(\mathcal{D}_n^i) \right]^2.$$

Histogram of Estimator

- Want to estimate $\alpha = \alpha(P) \in \mathbf{R}$ for some unknown P , and some complicated α .
- Point estimator $\hat{\alpha} = \hat{\alpha}(\mathcal{D}_{100})$ for samples of size 100.
- How to get error bars on $\hat{\alpha}$?
- Histogram of $\hat{\alpha}$ for 1000 random datasets of size 100 (estimates sampling distribution of $\hat{\alpha}$):



Pink line indicates true value of α . This is Figure 5.10 from *An Introduction to Statistical Learning, with applications in R* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

Practical Issue

- We typically get only one sample \mathcal{D}_n .
- We could divide it into B groups.
- Could use first group as point estimator $\hat{\mu} = \hat{\mu}(\mathcal{D}_{n/B}^{(1)})$,
- And use the remaining groups $\mathcal{D}_{n/B}^{(2)}, \dots, \mathcal{D}_{n/B}^{(B)}$ to get a variance estimate for $\hat{\mu}(\mathcal{D}_{n/B}^{(1)})$
- But then our point estimate only uses a fraction of the data.
- Would be much better if we used all the data: $\hat{\mu} = \hat{\mu}(\mathcal{D}_n)$.
- Can we get the best of both worlds?
 - A good point estimate AND a variance estimate?

The Bootstrap

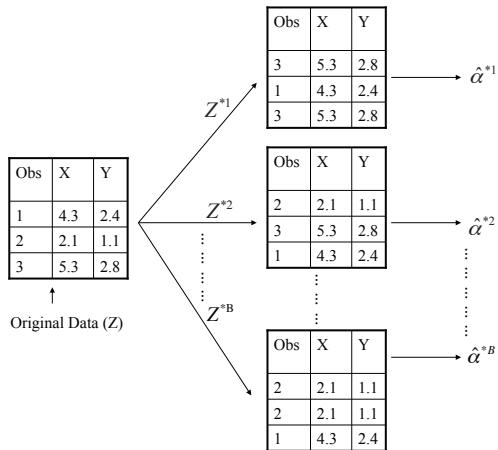
The Bootstrap Sample

- A **bootstrap sample** from $\mathcal{D}_n = (x_1, \dots, x_n)$ is a sample of size n drawn *with replacement* from \mathcal{D}_n .
- In a bootstrap sample, some elements of \mathcal{D}_n
 - will show up multiple times, and
 - some won't show up at all.
- Each x_i has a probability of $(1 - 1/n)^n$ of not being selected.
- Recall from analysis that for large n ,

$$\left(1 - \frac{1}{n}\right)^n \approx \frac{1}{e} \approx .368.$$

- So we expect $\sim 63.2\%$ of elements of \mathcal{D} will show up at least once.

The Bootstrap Sample



From *An Introduction to Statistical Learning, with applications in R* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

The Bootstrap Method

Definition

A **bootstrap method** is when you *simulate* having B independent samples from P by taking B bootstrap samples from the sample \mathcal{D}_n .

- Given original data \mathcal{D}_n , compute B bootstrap samples D_n^1, \dots, D_n^B .
- For each bootstrap sample, compute some function

$$\phi(D_n^1), \dots, \phi(D_n^B)$$

- Work with these values as though D_n^1, \dots, D_n^B were i.i.d. P .
- **Amazing fact:** Things often come out very close to what we'd get with independent samples from P .

Independent vs Bootstrap Samples

- Want to estimate $\alpha = \alpha(P)$ for some unknown P and some complicated α .
- Point estimator $\hat{\alpha} = \hat{\alpha}(\mathcal{D}_{100})$ for samples of size 100.
- Histogram of $\hat{\alpha}$ based on
 - 1000 independent samples of size 100, vs
 - 1000 bootstrap samples of size 100

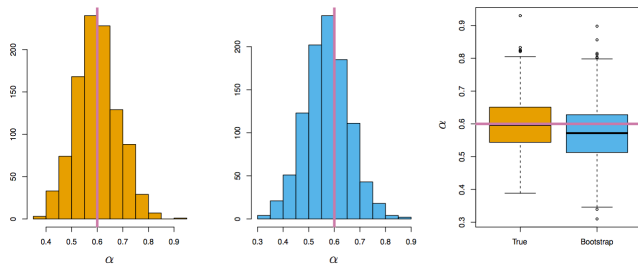


Figure 5.10 from *ISLR* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

The Bootstrap in Practice

- Suppose we have an estimator $\hat{\mu} = \hat{\mu}(\mathcal{D}_n)$.
- To get error bars, we can compute the “bootstrap variance”.
 - Draw B bootstrap samples.
 - Compute sample or empirical variance of $\hat{\mu}(\mathcal{D}_n^1), \dots, \hat{\mu}(\mathcal{D}_n^B)$..
- Could report

$$\hat{\mu}(\mathcal{D}_n) \pm \sqrt{\text{Bootstrap Variance}}$$