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# 19: Sampling and the Bootstrap <br> Jerry Cain <br> February 23, 2024 <br>  

Lecture Discussion on Ed

# Sampling definitions 

## Motivating example

 variance of happinesslin Bhutan.

- But you can't ask everyone.
- You poll 200 random people.

- Your data looks like this:

$$
\text { Happiness }=\{\underbrace{72,85,79,91, \underbrace{68, \ldots, 71}\}}
$$

- The mean of all these numbers is 83 . Is this the true mean happiness of $\wedge$ Bhutanese people?



## Population

assume for simplicity that
pepulation ic $N=100,000$


This is a population.

## Sample



A sample is selected from a population.

## Sample



A sample is selected from a population.

## Reasonable Questions Starting Out

1. In situations where we can't obverse the entire population, what can we safely infer by polling a sample drawn from that population?
2. How large does your sample need to be before your conclusions become trustworthy, and how do we express confidence in what we conclude.
3. Are there alternative ways to infer population statistics without polling entire populations?


## A sample, mathematically

Consider $n$ random variables $X_{1}, X_{2}, \ldots, X_{n}$.
The sequence $X_{1}, X_{2}, \ldots, X_{n}$ is a sample from distribution $F$ if:

- $X_{i}$ are all independent and identically distributed (iid)
- $X_{i}$ all have same distribution function $F$ (the underlying distribution), where $E\left[X_{i}\right]=\mu, \operatorname{Var}\left(X_{i}\right)=\sigma^{2}$



## A sample, mathematically

A sample of size 8:
$\left(X_{1}, X_{2}, X_{3}, X_{4}, X_{5}, X_{6}, X_{7}, X_{8}\right)$
The realization of a sample of size 8 :
( $59,87,94,99,87,78,69,91$ )


## A single sample



A happy
Bhutanese person

If we had a distribution $F$ of our entire population, we could compute exact statistics about about happiness. the distribitunform the priw slide pretends
we di kum the full ppulatem distribrtim $F$, thingh in
general we wor't hove access to it
But we only have 200 people-or rather, a sample.

Today: If we only have a single sample,

- How do we report estimated statistics?
- We're careful to call them estimated mean and estimated variance, since they're based on samples (i.e., experiments)
- How do we report estimated errors on these estimates?
- How do we perform something called hypothesis testing? Oh, and what is it?


# Unbiased estimators 

## A single sample

If we had a distribution $F$ of our entire population, we could compute exact statistics about happiness. But again, we generally do nit


A happy
Bhutanese person

But we only have 200 people (a sample).

These population-level statistics are unknown:

- $\mu$, the population mean
- $\sigma^{2}$, the population variance


## A single sample

## If we had a distribution $F$ of our entire population, we could compute exact statistics about happiness.

But we only have 200 people (a sample).

- From these 200 people, what is our best estimate of the population mean and the population variance?
- How exactly do we define best estimate?


## Estimating the population mean

1. What is our best estimate of $\mu$, the mean happiness of Bhutanese people?

If we only have $\left(X_{1}, X_{2}, \ldots, X_{n}\right)$ :

The best estimate of $\mu$ is the sample mean:

$$
\bar{X}=\frac{1}{n} \sum_{i=1}^{n} X_{i}
$$

$\bar{X}$ is an unbiased estimator of the population mean $\mu$.

$$
E[\bar{X}]=\mu
$$

Intuition: By the CLT, $\bar{X} \sim \mathcal{N}\left(\mu, \frac{\sigma^{2}}{n}\right)$
If we could take multiple samples of size $n$ :

1. For each sample, compute sample mean
2. On average, we would get the population mean

## Sample mean




Even if we can't report $\mu$, we can report our sample mean 83.03, which is an unbiased estimate of $\mu$.

## Estimating the population variance


2. What is $\sigma^{2}$, the variance of happiness of Bhutanese people?

If we knew the entire population $\left(x_{1}, x_{2}, \ldots, x_{N}\right)$ : population mean
population variance

$$
\sigma^{2}=E\left[(X-\mu)^{2}\right]=\frac{1}{N} \sum_{i=1}^{N}\left(x_{i}-\mu\right)^{2}
$$

If we only have one sample: $\left(X_{1}, X_{2}, \ldots, X_{n}\right)$ : sample mean

$$
\begin{gathered}
\text { sample } \\
\text { variance }
\end{gathered} S^{2}=\frac{1}{n-1} \sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}
$$

variance is defined in terms of anither estimate-.
the sample mean.

## Intuition about the sample variance, $S^{2}$




## Intuition about the sample variance, $S^{2}$

Actual, $\sigma^{2}$

Estimate, $S^{2}$
population mean
population
variance

$\underset{\text { variance }}{ } S^{2}=\frac{1}{n-1} \sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}$


## Intuition about the sample variance, $S^{2}$



Population size, $N$

## Intuition about the sample variance, $S^{2}$

Actual, $\sigma^{2}$
Estimate, $S^{2}$
population mean
population
variance


## Estimating the population variance


2. What is $\sigma^{2}$, the variance of happiness of Bhutanese people?

If we only have a sample, $\left(X_{1}, X_{2}, \ldots, X_{n}\right)$ :
The best estimate of $\sigma^{2}$ is the sample variance: $S^{2}=\frac{1}{n-1} \sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}$ $\frac{1}{n} \sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)$ in astimater, shats its
$S^{2}$ is an unbiased estimator of the population variance, $\sigma^{\text {biocad }, ~} E\left[S^{2}\right]=\sigma^{2}$

$$
E\left[S^{2}\right]=\sigma^{2}
$$

$$
\begin{aligned}
& E\left[S^{2}\right]=E\left[\frac{1}{n-1} \sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}\right] \Rightarrow \quad(n-1) E\left[S^{2}\right]=E\left[\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}\right] \\
& \begin{aligned}
(n-1) E\left[S^{2}\right] & =E\left[\sum_{i=1}^{n}\left(\left(X_{i}-\mu\right)+(\mu-\bar{X})\right)^{2}\right] \\
& =E\left[\sum_{i=1}^{n}\left(X_{i}-\mu\right)^{2}+\sum_{i=1}^{n}(\mu-\bar{X})^{2}+2 \sum_{i=1}^{n}\left(X_{i}-\mu\right)(\mu-\bar{X})\right]
\end{aligned} \quad \rightarrow 2(\mu-\bar{X}) \sum_{i=1}^{n}\left(X_{i}-\mu\right) \\
& \\
& =E\left[\sum_{i=1}^{n}\left(X_{i}-\mu\right)^{2}+n(\mu-\bar{X})^{2}-2 n(\mu-\bar{X})^{2}\right] \\
& =E\left[\sum_{i=1}^{n}\left(X_{i}-\mu\right)^{2}-n(\mu-\bar{X})^{2}\right]=\sum_{i=1}^{n} E\left[\left(X_{i}-\mu\right)\right]^{2}-n E\left[(\bar{X}-\mu)^{2}\right] \\
& \\
& =n \sigma_{i}^{2}-n \operatorname{Var}(\bar{X})=n \sigma^{2}-n \frac{\sigma^{2}}{n}=n \sigma^{2}-\sigma^{2}=(n-1) \sigma^{2} \quad \text { Therefore } E\left[S^{2}\right]=\sigma^{2}
\end{aligned}
$$

## Standard error

## Estimating population statistics

A particular outcome

1. Collect a sample, $X_{1}, X_{2}, \ldots, X_{n}$. (72, 85,79,79,91,68, ... 71)

$$
n=200
$$

2. Compute sample mean, $\bar{X}=\frac{1}{n} \sum_{i=1}^{n} X_{i}$.
${ }_{85-83} \quad \bar{X}=83$
3. Compute sample deviation, $X_{i}-\bar{X} . \quad(-11,2,-4,-4,8,-15, \ldots,-12)$
4. Compute sample variance, $S^{2}=\frac{1}{n-1} \sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}, \bar{x} \quad S^{2}=793$ How close are our estimates $\bar{X}$ and $S^{2}$ ?

## Sample mean



- $\operatorname{Var}(\bar{X})$ is a measure of how close $\bar{X}$ is to $\mu$.
- How do we estimate $\operatorname{Var}(\bar{X})$ ?

Distribution of sample means

if $\operatorname{Var}(\bar{X})$ is lavge, we'v rot all that onfident that $\bar{x}$ is cloce to $\mu$
conusely, if $\operatorname{Var}(\bar{x})$ is
small, then we'v mov confident it's close.

## How close is our estimate $\bar{X}$ to $\mu$ ?

$$
E[\bar{X}]=\mu
$$

$$
\begin{aligned}
& \operatorname{Var}(\bar{X})=\frac{\sigma^{2}}{n} \begin{array}{l}
\text { We want t } \\
\text { estimate }
\end{array} \\
& S D(\bar{X})=\sqrt{\operatorname{Var}(\bar{X})}=\sqrt{\frac{\partial^{2}}{n}}
\end{aligned}
$$

def The standard error of the mean is an estimate of the standard deviation of $\bar{X}$.

Intuition:

- $S^{2}$ is an unbiased estimate of $\sigma^{2}$
- $S^{2} / n$ is an unbiased estimate of $\sigma^{2} / n=\operatorname{Var}(\bar{X})$
- $\sqrt{S^{2} / n}$ can estimate $\sqrt{\operatorname{Var}(\bar{X})}$

$$
\begin{aligned}
& S E=\sqrt{\frac{S^{2}}{n}} \\
& E[S E]<S D(\bar{x}) \\
& \text { less than becaus of } \\
& \text { thebias. }
\end{aligned}
$$

More info on bias of

## Standard error of the mean

1. Mean happiness:

Claim: The average happiness of Bhutan is 83 , with a standard error of 1.99.

this is our estimate of
this is our best estimate of $\mu$
error bars


These 2 statistics give a sense of how $\bar{X}$-that is, the sample mean random variable-behaves.

## Standard error of variance?

1. Mean happiness:

Claim: The average happiness of Bhutan is 83 , with a standard error of 1.99.

$$
\begin{aligned}
& \text { Closed } \\
& \text { form: }
\end{aligned} S=\sqrt{\frac{S^{2}}{n}}
$$

2. Variance of happiness:


Claim: The variance of happiness of Bhutan is 793 .


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Up next: Compute statistics with code!

## Bootstrap: Sample mean

## Bootstrap

The Bootstrap:

## Probability for Computer Scientists

## Computing statistic of sample mean

What is the standard deviation of the sample mean $\bar{X}$ ? (sample size $n=200$ )


Note: We don't have access to the population.
But Doris is sharing the exact statistic, with cyouran Sahami, and Jery Cain, Cs109, winter 2024

## Bootstrap insight 1: Estimate the true distribution



## Bootstrap insight 1: Estimate the true distribution

You can estimate the PMF of the underlying distribution, using your sample.*



The underlying distribution

$$
F \approx \hat{F}
$$

*This is just a histogram of your datad, Chris Piech, Mehran Sahami, and Jerry Cain, CS109, Winter 2024
the sample distribution
(aka the histogram of your data) normalized tifunctum

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## Bootstrap insight 2: Simulate a distribution

Approximate the procedure of simulating a distribution of a statistic, e.g., $\bar{X}$.

Population distribution (we don't have this)


Sample distribution (we do have this)


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## Bootstrapped sample means

$$
\text { means }=[84.7, ~ 83.9, ~ 80.6, ~ 79.8, ~ 90.3, ~ . . ., ~ 85.2] ~
$$



Estimate the true PMF using our "PMF" (histogram) of our sample.

...generate a whole bunch of sample means of this estimated distribution...
np.std(means)
2.003
...and compute the standard deviation of this distribution.

## Computing statistic of sample mean

What is the standard deviation of the sample mean $\bar{X}$ ? (sample size $n=200$ )

Population distribution (we don't have this)

Sample distribution (we do have this)


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$$
\frac{\sigma}{\sqrt{n}}=1.886
$$

1.869
2.003


Exact statistic
(we don't have this)
Simulated statistic (we don't have this)

Estimated statistic, by formula, standard error

Simulated estimated statistic, bootstrapped standard error

## Bootstrap algorithm

## Bootstrap Algorithm (sample):

1. Estimate the PMF using the sample
2. Repeat $\mathbf{1 0 , 0 0 0}$ times:
a. Resample sample.size() from PMF
b. Recalculate the sample mean on the resample

3. You now have a distribution of your sample mean

What is the distribution of your sample mean?
We'll talk about this algorithm in detail with a demo!

## Bootstrap algorithm

Bootstrap Algorithm (sample):

1. Estimate the PMF using the sample
2. Repeat $\mathbf{1 0 , 0 0 0}$ times:
a. Resample sample.size() from PMF
b. Recalculate the statistic on the resample
3. You now have a distribution of your statistic

What is the distribution of your statistic?

## Bootstrapped sample variance

Bootstrap Algorithm (sample):

1. Estimate the PMF using the sample
2. Repeat $\mathbf{1 0 , 0 0 0}$ times:
a. Resample sample.size() from PMF
b. Recalculate the sample variance on the resample
3. You now have a distribution of your sample variance

What is the distribution of your sample variance?

Even if we don't have a closed form equation, we estimate statistics of sample variance with bootstrapping!

## Bootstrap: Sample variance

## Bootstrapped sample variance

Bootstrap Algorithm (sample):

1. Estimate the PMF using the sample
2. Repeat 10,000 times:
a. Resample sample.size() from PMF
b. Recalculate the sample variance on the resample
3. You now have a distribution of your sample variance

Goal What is the distribution of your sample variance?

## Bootstrapped variance



1. Estimate the PMF using the sample
2. Repeat 10,000 times:
a. Resample sample.size() from PMF
b. Recalculate the sample variance on the resample
3. You now have a distribution of your sample variance

## Bootstrapped variance



1. Estimate the PMF using the sample
2. Repeat 10,000 times:
a. Resample sample.size() from PMF
b. Recalculate the sample variance on the resample
3. You now have a distribution of your sample variance

## Bootstrapped variance



1. Estimate the PMF using the sample
2. Repeat 10,000 times:
a. Resample sample.size() from PMF
b. Recalculate the sample variance on the resample



Why are these
samples different?
3. You now have a distribution of your

This resampled sample is generated with replacement.

## Bootstrapped variance


[52, 38, 98, 107, ..., 94]

1. Estimate the PMF using the sample
2. Repeat 10,000 times:



a. Resample sample.size() from PMF
b. Recalculate the sample variance on the resample
3. You now have a distribution of your sample variance

$$
\text { variances }=\text { [827.4] }
$$

## Bootstrapped variance



1. Estimate the PMF using the sample
2. Repeat 10,000 times:
a. Resample sample.size() from PMF
b. Recalculate the sample variance on the resample 3. You now have a distribution of your sample variance
variances = [827.4]

## Bootstrapped variance




1. Estimate the PMF using the sample
2. Repeat 10,000 times:
a. Resample sample.size() from PMF
b. Recalculate the sample variance on the resample
3. You now have a distribution of your sample variance
variances = [827.4]

## Bootstrapped variance

second iteration might generale

$\begin{array}{llll}x_{1} & x_{2} & x_{3} & x_{4} \quad x_{20}\end{array}$ $[116,76,132,85, \ldots, 78]$


1. Estimate the PMF using the sample
2. Repeat $\mathbf{1 0 , 0 0 0}$ times:
a. Resample sample.size() from PMF
b. Recalculate the sample variance on the resample
3. You now have a distribution of your sample variance
variances $=$ [827.4, 846.1]

## Bootstrapped variance



1. Estimate the PMF using the sample
2. Repeat $\mathbf{1 0 , 0 0 0}$ times:
a. Resample sample.size() from PMF
b. Recalculate the sample variance on the resample
3. You now have a distribution of your sample variance
variances $=$ [827.4, 846.1]

## Bootstrapped variance



1. Estimate the PMF using the
2. Repeat 10,000 times:
a. Resample sample.size()
b. Recalculate the sample


## Bootstrapped variance

3. You now have a distribution of your sample vapiance
 860.7]

What is the bootstrapped standard error?
np.std(variances)


- Simulate a distribution of sample variances
- Compute standard deviation


## Standard error

1. Mean happiness:

Claim: The average happiness of Bhutan is 83 , with a standard error of 1.99.

$$
\begin{aligned}
& \text { Closed } \\
& \text { form: }
\end{aligned} S E=\sqrt{\frac{S^{2}}{n}}
$$

2. Variance of happiness:



Claim: The variance of happiness of Bhutan is 793, with a bootstrapped standard error of 66.16.

## Algorithm in practice: Resampling

## 1. Estimate the PMF using the sample

2. Repeat 10,000 times:
a. Resample sample.size() from PMF
b. Recalculate the statistic on the resample 3. You now have a distribution of your statistic
[116, 76, 132, 85, ..., 78]


$$
P(X=k)=\frac{\# \text { values in sample equal to } k}{n}
$$

## Algorithm in practice: Resampling

```
def resample(sample, n):
# estimate the PMF using the sample
# draw n new samples from the PMF
return np.random.choice(sample, n, replace=True)
```


$P(X=k)=\frac{\# \text { values in sample equal to } k}{n}$
$[116,76,132,85, \ldots, 78]$


This resampled sample is generated with replacement.

## To the code!

## Bootstrap provides a way to calculate probabilities of statistics using code. Bootstrapping works for any statistic*

*as long as your sample is iid and the underlying distribution does not have a long tail

Google colab notebook link

## Bradley Efron

- Invented bootstrapping in 1979
- Still a professor at Stanford
- Won a National Science Medal

Inventor of Efron's dice: 4 dice $A, B, C, D$ where:
$P(A>B)=P(B>C)=P(C>D)=P(D>A)=\frac{2}{3}$

## Bootstrap: p-value



## Null hypothesis test

Nepal
Happiness
4.45
2.45
6.37
2.07
1.63

1.08

$$
\bar{X}_{1}=3.1
$$

$$
\bar{X}_{2}=2.4
$$

Claim: The difference in mean happiness between Nepal and Bhutan is 0.7 happiness points, and this is statistically

## Null hypothesis test

def null hypothesis - Even if there is no pattern (i.e., the two samples are from identical distributions), your claim might have arisen by chance.
def $p$-value - What is the probability that the observed difference occurs under the null hypothesis? that is. is the chanc ym oberved a signiticant differene

Example:

- Flip some coin 100 times.
- Flip the same coin another 150 times.

Null hypothesis assumes we use the same coin

- Compute fraction of heads in both groups.
- There is a possibility we'll see the observed difference in these fractions even if we used the same coin


A significant p-value (<0.05) means we reject the null

## Universal sample <br> (this is what the null hypothesis assumes)



Want p-value: probability $\left|\bar{X}_{1}-\bar{X}_{2}\right|=|3.1-2.4|$ happens under null hypothesis

## Bootstrap for p-values <br> 

1. Create a universal sample using your two samples
i.e., recreate the null hypothesis


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## Bootstrap for p-values

1. Create a universal sample using your two samples
2. Repeat 10,000 times:
a. Resample both samples
b. Recalculate the mean difference between the resamples
3. p -value $=\frac{\# \text { (mean diffs }>=\text { observed diff) }}{n=1 \text { mo }}$

Probability that observed difference arose by chance

## Bootstrap for p-values

```
def pvalue_boot(bhutan_sample, nepal_sample):
    N = size of the bhutan_sample
    M = size of the nepal_sample
    observed_diff = |mean of bhutan_sample - mean of nepal_sample|
    uni_sample = combine bhutan_sample and nepal_sample
    count = 0
    repeat 10,000 times:
        bhutan_resample = draw N resamples from the uni_sample
        nepal_resample = draw M resamples from the uni_sample
        muBhutan = sample mean of the bhutan_resample
        muNepal = sample mean of the nepal_resample
        diff = |muNepal - muBhutan|
        if diff >= observed_diff:
            count += 1
```

pValue $=$ count / 10,000

## Bootstrap for p-values

def pvalue_boot(bhutan_sample, nepal_sample):

1. Create a universal sample using your two samples
```
N = size of the bhutan_sample
    M = size of the nepal_sample
    observed_diff = |mean of bhutan_sample - mean of nepal_sample|
```



```
    count = 0
    repeat 10,000 times:
        bhutan_resample = draw N resamples from the uni_sample
        nepal_resample = draw M resamples from the uni_sample
        muBhutan = sample mean of the bhutan_resample
        muNepal = sample mean of the nepal_resample
        diff = |muNepal - muBhutan|
        if diff >= observed_diff:
            count += 1
```

pValue = count / 10,000

## Bootstrap for p-values

## 2. a. Resample both samples

```
def pvalue_boot(bhutan_sample, nepal_sample):
    N = size of the bhutan_sample
    M = size of the nepal_sample
    observed_diff = |mean of bhutan_sample - mean of nepal_sample|
    uni_sample = combine bhutan_sample and nepal_sample
    count = 0
    repeat 10,000 times:
```



```
bhutan_resample = draw N resamples from the uni_sample
nepal_resample = draw M resamples from the uni_sample
muBhutan = sample mean of the bhutan_resample
muNepal = sample mean of the nepal_resample
diff = |muNepal - muBhutan|
if diff >= observed_diff:
                    count += 1
```

pValue = count / 10,000

## Bootstrap for p-values

2.b. Recalculate the mean difference b/t resamples

```
def pvalue_boot(bhutan_sample, nepal_sample):
    N = size of the bhutan_sample
    M = size of the nepal_sample
    observed_diff = |mean of bhutan_sample - mean of nepal_sample|
    uni_sample = combine bhutan_sample and nepal_sample
    count = 0
    repeat 10,000 times:
        bhutan_resample = draw N resamples from the uni_sample
        nepal_resample = draw M resamples from the uni_sample
        muBhutan = sample mean of the bhutan_resample
    muNepal = sample mean of the nepal_resample
    diff = |muNepal - muBhutan|
    if diff >= observed_diff:
    count += 1
```

pValue $=$ count / 10,000

## Bootstrap for p-values

3. $p$-value $=$ \# (mean diffs $>$ observed diff) n
```
def pvalue_boot(bhutan_sample, nepal_sample):
    N = size of the bhutan_sample
    M = size of the nepal_sample
    observed_diff = |mean of bhutan_sample - mean of nepal_sample|
    uni_sample = combine bhutan_sample and nepal_sample
    count = 0
    repeat 10,000 times:
        bhutan_resample = draw N resamples from the uni_sample
        nepal_resample = draw M resamples from the uni_sample
        muBhutan = sample mean of the bhutan_resample
        muNepal = sample mean of the nepal_resample
        diff = |muNepal - muBhutan|
        if diff >= observed_diff:
            count += 1
```

pValue $=$ count / 10,000

## Bootstrap for p-values

```
def pvalue_boot(bhutan_sample, nepal_sample):
    N = size of the bhutan_sample
    M = size of the nepal_sample
    observed_diff = |mean of bhutan_sample - mean of nepal_sample|
    uni_sample = combine bhutan_sample and nepal_sample
    count = 0
    repeat 10,000 times:
                                    with replacement!
            bhutan_resample = draw N resamples from the uni_sample
        nepal_resample = draw M resamples from the uni_sample
        muBhutan = sample mean of the bhutan_resample
        muNepal = sample mean of the nepal_resample
        diff = |muNepal - muBhutan|
        if diff >= observed_diff:
            count += 1
```

pValue $=$ count / 10,000

## Bootstrap



Let's try it!
Google colab notebook link

## Null hypothesis test

Nepal
Happiness
4.45
2.45
6.37
2.07
1.63

1.08

$$
\bar{X}_{1}=3.1
$$

$$
\bar{X}_{2}=2.4
$$

Claim: The happiness of Nepal and Bhutan have a 0.7 difference of means, and this is statistically significant ( $p<0.05$ ).

