19: Sampling and the Bootstrap

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May 9, 2022

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Sampling definitions

Motivating example

N = 10,000
100,000

You want to know the true mean and variance of happiness in Bhutan.

- But you can't ask everyone.
- You poll 200 random people.
- Your data looks like this: single sample N=200

Happiness = {72, 85, 79, 91, 68, ..., 71}

- The mean of all these numbers is 83.

Is this the **true mean happiness** of Bhutanese people?

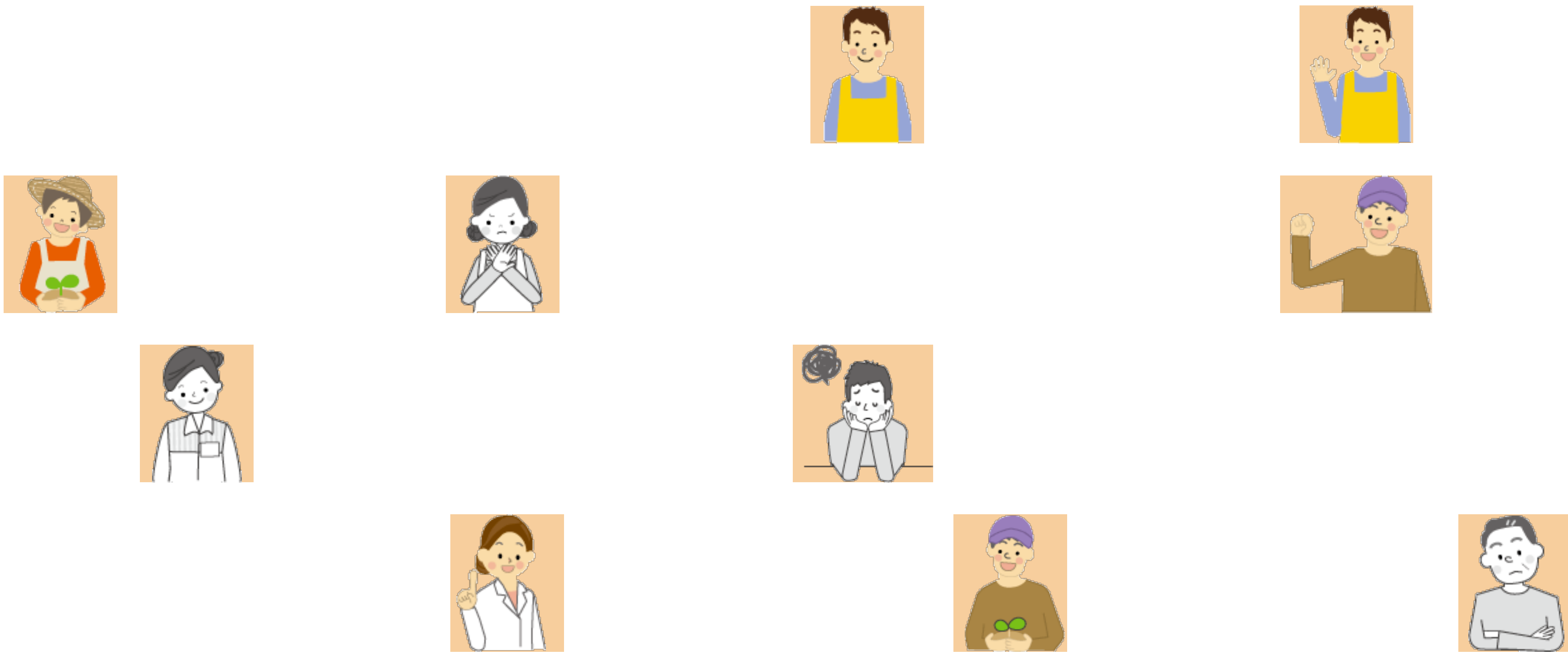
Population

This is a population.

Sample

A sample is selected from a population.

Sample



A **sample** is selected from a population.

Reasonable Questions Starting Out

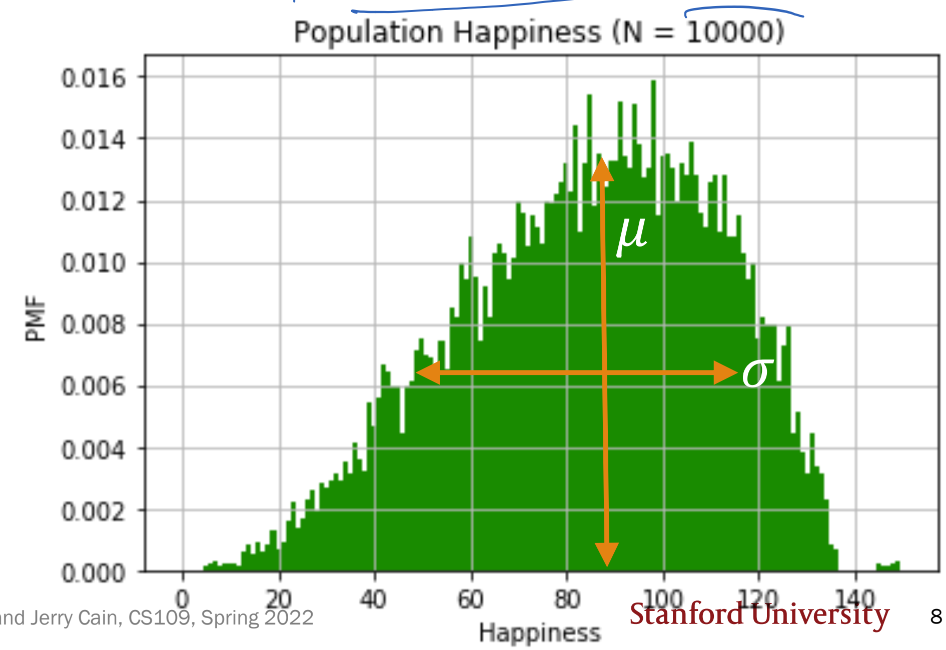
1. In situations where we can't obverse the entire population, what can we safely conclude by polling a sample drawn from that population?
2. How large does your sample need to be before your conclusions are trustworthy, and how do we express confidence with any conclusions we draw?
3. Are there alternative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

A sample, mathematically

Consider n random variables $X_1, X_2, \dots, X_n$.

The sequence $X_1, X_2, \dots, X_n$ is a **sample** from distribution F if:

- X_i are all independent and identically distributed (i.i.d.)
- X_i all have same distribution function F (the **underlying distribution**), where $E[X_i] = \mu$, $\text{Var}(X_i) = \sigma^2$



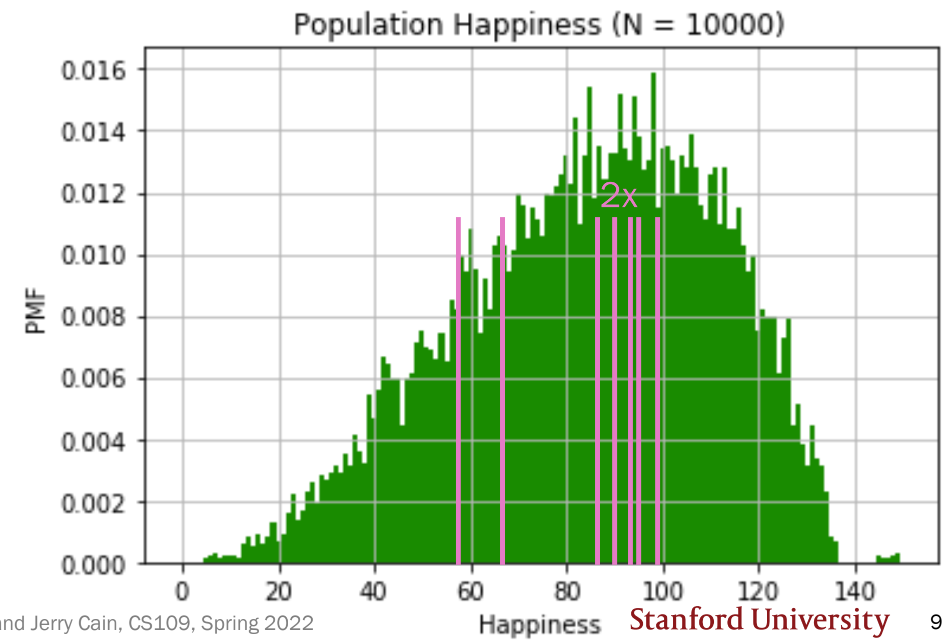
A sample, mathematically

A sample of size 8:

$(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8)$

A 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.

But we only have 200 people (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 error of these estimates?
- How do we perform something called **hypothesis testing**?

Unbiased estimators

definition

A single sample

A happy
Bhutanese person

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).

These population-level statistics are unknown:

- μ, the population mean
- σ^2, the population variance

A single sample

A happy
Bhutanese person

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 μ, the **mean happiness** of Bhutanese people?

If we only have $(X_1, X_2, \ldots, X_n)$:

The best estimate of μ is the **sample mean**:

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

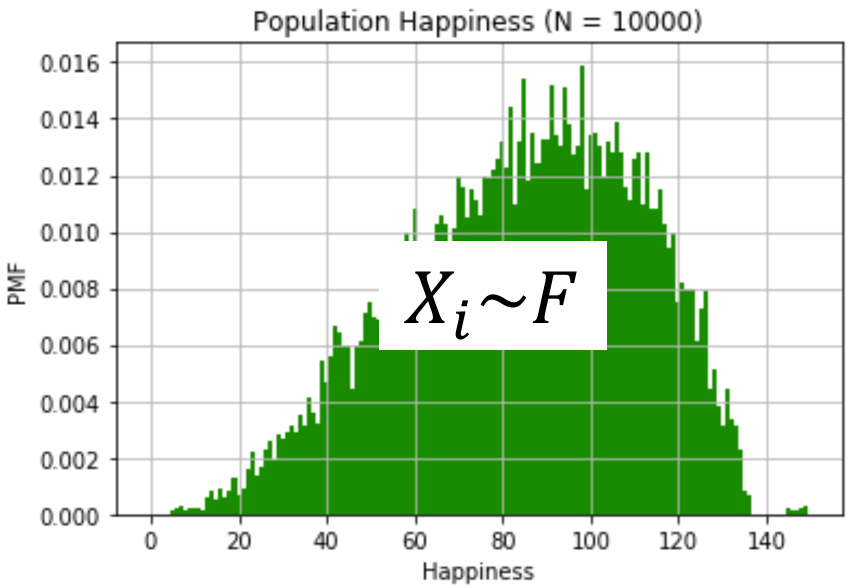
$\bar{X}$ is an <u>**unbiased estimator**</u> of the population mean μ. $\quad E[\bar{X}] = \mu$

Intuition: By the CLT, $\bar{X} \sim \mathcal{N}(\mu, \frac{\sigma^2}{n})$

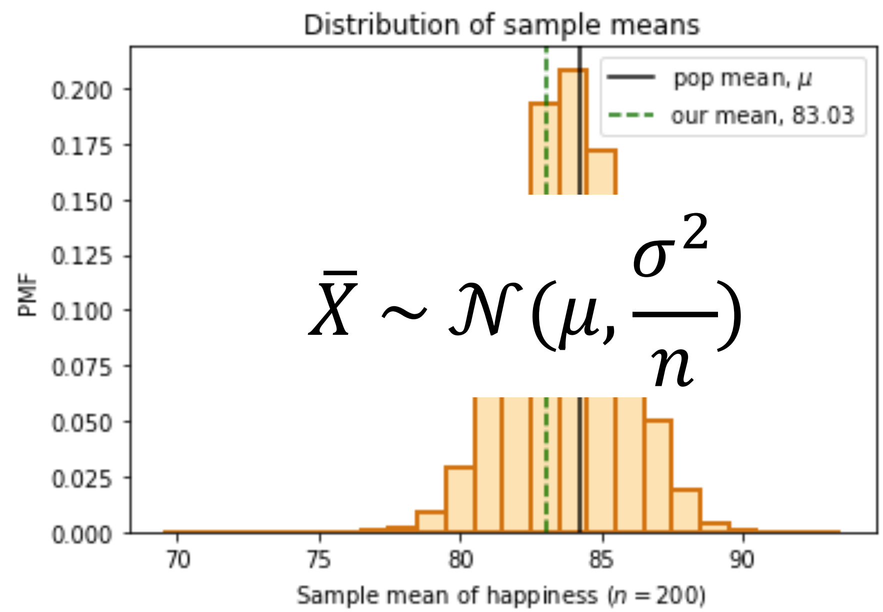
If we could take *multiple* samples of size n:

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

Sample mean



$$X_i \sim F$$



$$\bar{X} \sim \mathcal{N}\left(\mu, \frac{\sigma^2}{n}\right)$$

Even if we can't report μ, we can report our sample mean 83.03, which is an unbiased estimate of μ. $E[\bar{X}] = \mu$

Estimating the population variance

2. What is σ^2, the **variance of happiness** of Bhutanese people?

N = 700,000
10,000

If we knew the entire population $(x_1, x_2, \ldots, x_N)$:

population mean

population variance

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

perfect info access to full population

If we only have one sample: $(X_1, X_2, \ldots, X_n)$:

n = 200

sample mean

sample variance

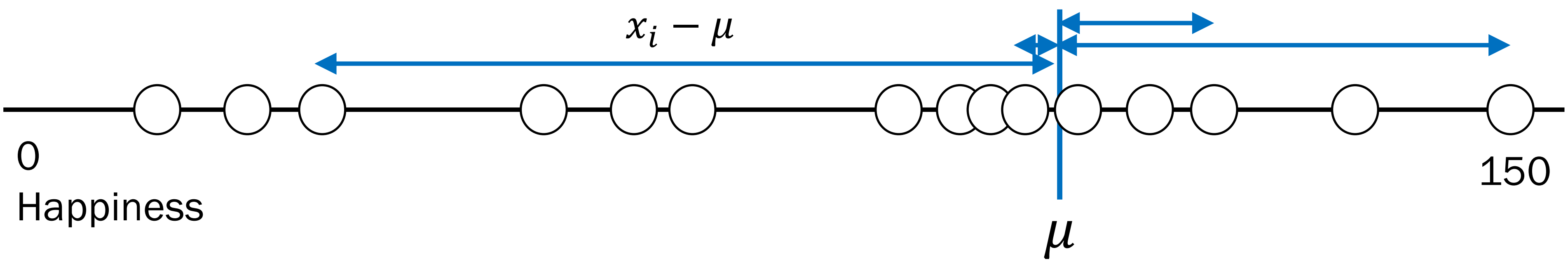
$$S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2$$

Intuition about the sample variance, S^2

Actual, σ^2

population mean

population variance $$\sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2$$

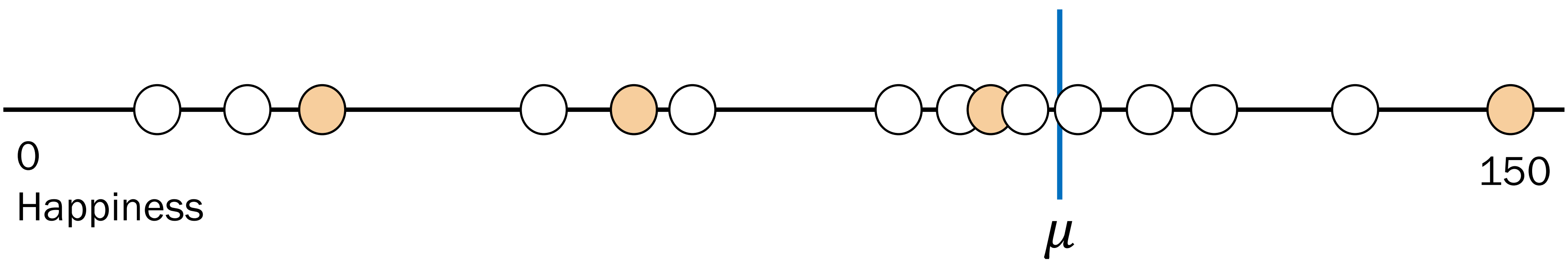


Population size, N

Calculating population statistics **exactly** requires us knowing all N datapoints.

Intuition about the sample variance, S^2

Actual, σ^2	Estimate, S^2
population mean	sample mean
population variance $\sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2$	sample variance $S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2$



Population size, N

Intuition about the sample variance, S^2

Actual, σ^2

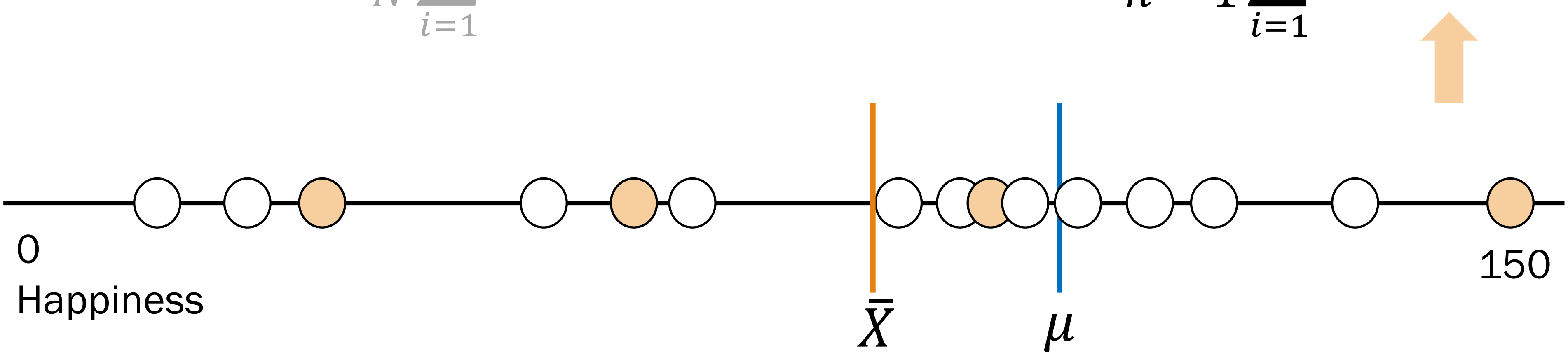
population mean

population variance $\sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2$

Estimate, S^2

sample mean

sample variance $S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2$



Population size, N

Intuition about the sample variance, S^2

Actual, σ^2

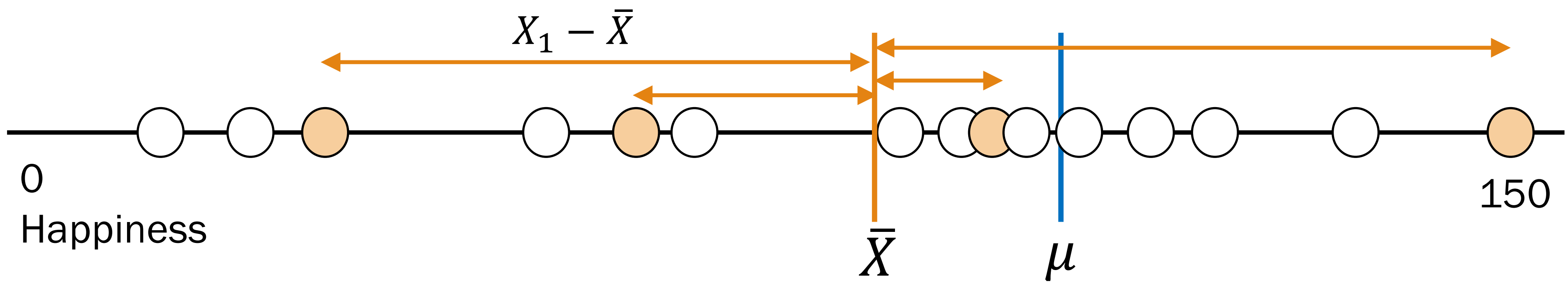
population mean

population variance $\sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2$

Estimate, S^2

sample mean

sample variance $S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2$



Population size, N

Sample variance is an estimate using an estimate, so it needs additional scaling.

Estimating the population variance

2. What is σ^2, the variance of happiness of Bhutanese people?

If we only have a sample, $(X_1, X_2, \dots, X_n)$:

The best estimate of σ^2 is the **sample variance:**

$$S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2$$

S^2 is an **unbiased estimator** of the population variance, σ^2.

$$E[S^2] = \sigma^2$$

Proof that S^2 is unbiased (just for reference)

$$E[S^2] = \sigma^2$$

$$E[S^2] = E\left[\frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2\right] \quad \Rightarrow \quad (n-1)E[S^2] = E\left[\sum_{i=1}^{n}(X_i - \bar{X})^2\right]$$

$$(n-1)E[S^2] = E\left[\sum_{i=1}^{n}\left((X_i - \mu) + (\mu - \bar{X})\right)^2\right]$$

(introduce $\mu - \mu$)

$$= E\left[\sum_{i=1}^{n}(X_i - \mu)^2 + \sum_{i=1}^{n}(\mu - \bar{X})^2 + 2\sum_{i=1}^{n}(X_i - \mu)(\mu - \bar{X})\right]$$

$$2(\mu - \bar{X})\sum_{i=1}^{n}(X_i - \mu)$$

$$2(\mu - \bar{X})\left(\sum_{i=1}^{n}X_i - n\mu\right)$$

$$2(\mu - \bar{X})n(\bar{X} - \mu)$$

$$-2n(\mu - \bar{X})^2$$

$$= E\left[\sum_{i=1}^{n}(X_i - \mu)^2 + n(\mu - \bar{X})^2 - 2n(\mu - \bar{X})^2\right]$$

$$= E\left[\sum_{i=1}^{n}(X_i - \mu)^2 - n(\mu - \bar{X})^2\right] = \sum_{i=1}^{n}E[(X_i - \mu)]^2 - nE[(\bar{X} - \mu)^2]$$

$$= n\sigma^2 - n\text{Var}(\bar{X}) = n\sigma^2 - n\frac{\sigma^2}{n} = n\sigma^2 - \sigma^2 = (n-1)\sigma^2$$

Therefore $E[S^2] = \sigma^2$

Standard error

Estimating population statistics

n=200
n=1000

A particular outcome

1. Collect a sample, $X_1, X_2, \ldots, X_n$. — $(72, 85, 79, 79, 91, 68, \ldots, 71)$, $n = 200$

random variable

2. Compute **sample mean**, $\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$. — $\bar{X} = 83$

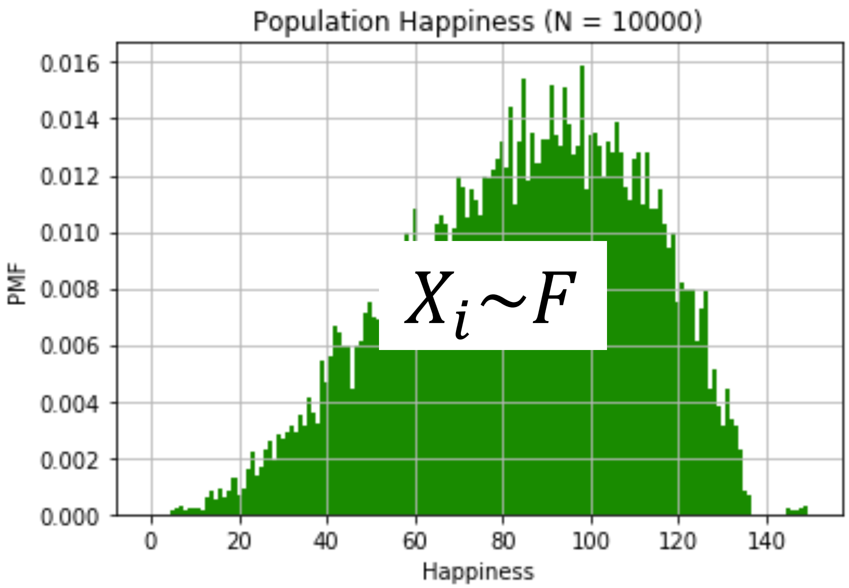
3. Compute sample deviation, $X_i - \bar{X}$. — $(-11, 2, -4, -4, 8, -15, \ldots, -12)$

random variable

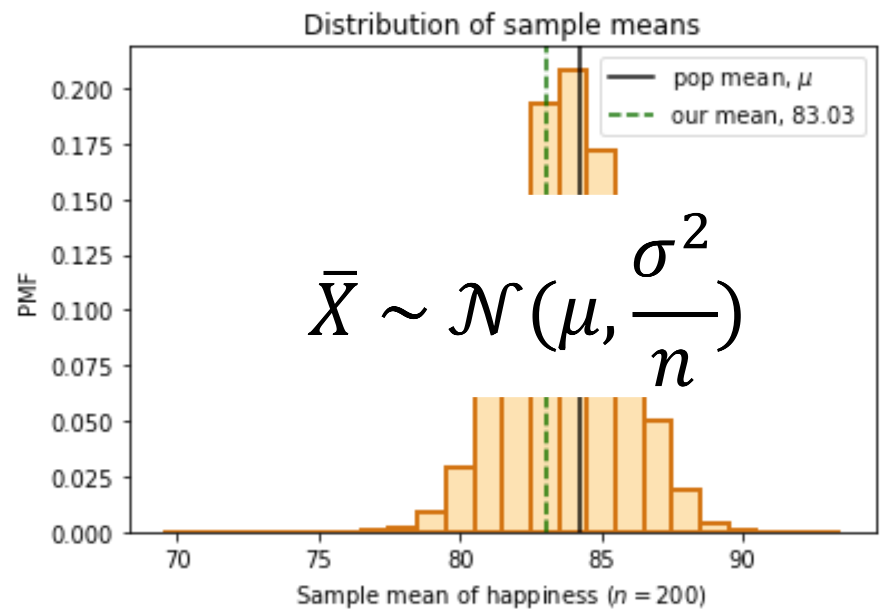
4. Compute **sample variance**, $S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2$. — $S^2 = 793$

How close are our estimates $\bar{X}$ and S^2?

Sample mean



$X_i \sim F$



$$\bar{X} \sim \mathcal{N}(\mu, \frac{\sigma^2}{n})$$

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

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

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

$$\text{Var}(\bar{X}) = \frac{\sigma^2}{n}$$

We want to estimate this

<u>def</u> The **standard error** of the mean is an estimate of the standard deviation of $\bar{X}$.

$$SE = \sqrt{\frac{S^2}{n}}$$

Intuition:

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

More info on bias of standard error: [wikipedia]

Standard error of the mean

1. Mean happiness:

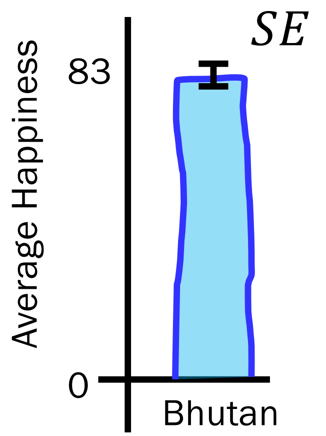
Claim: The average happiness of Bhutan is 83, with a standard error of 1.99.

this is our best estimate of μ

this is our estimate of how close we are

Closed form: $SE = \sqrt{\frac{S^2}{n}}$

error bars



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

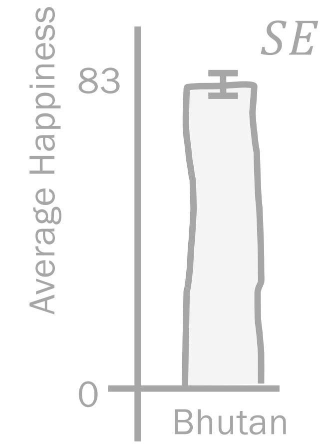
Standard error of variance?

1. Mean happiness:

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

Closed form: $SE = \sqrt{\frac{S^2}{n}}$

error bars



2. Variance of happiness:

Claim: The variance of happiness of Bhutan is 793.

this is our best estimate of σ^2

Chi-squared

Closed form: Not covered in CS109

But how close are we?

Up next: Compute Statistics with code!

Bootstrap: Sample mean

Bootstrap

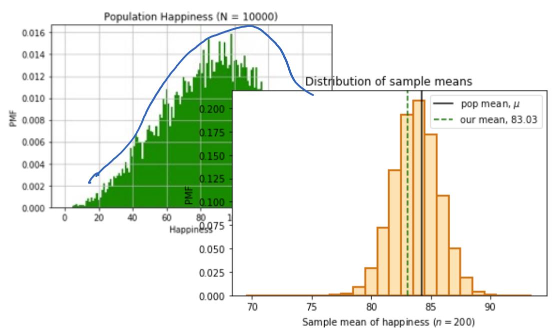
The Bootstrap:

Probability for Computer Scientists

Computing statistic of sample mean

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

Population distribution
(we don't have this)



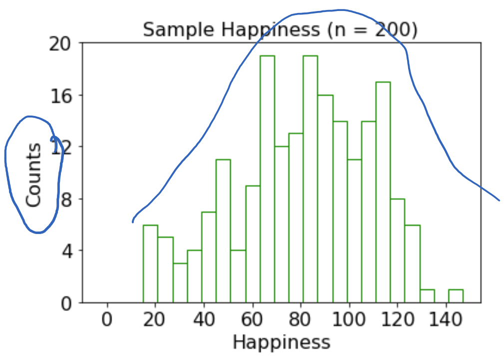
$$\frac{\sigma}{\sqrt{n}} = 1.886$$

Exact statistic
(we don't have this)

1.869

Simulated statistic
(we don't have this)

Sample distribution
(we do have this)



$$SE = \frac{S}{\sqrt{n}} = 1.992$$

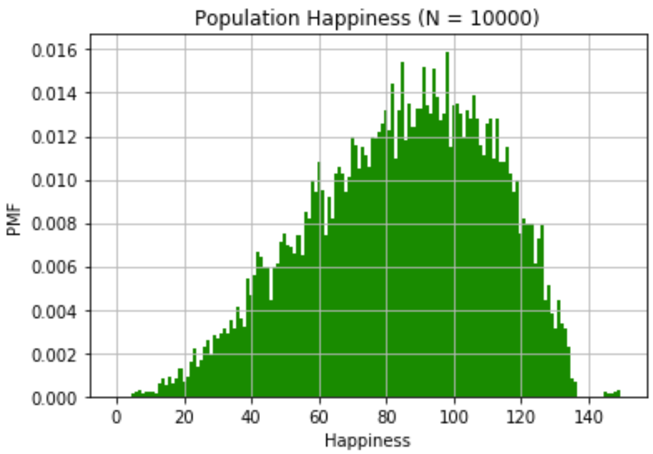
Estimated statistic, by formula, **standard error**

???

Simulated estimated statistic

Note: We don't have access to the population. But Doris is sharing the exact statistic with you.

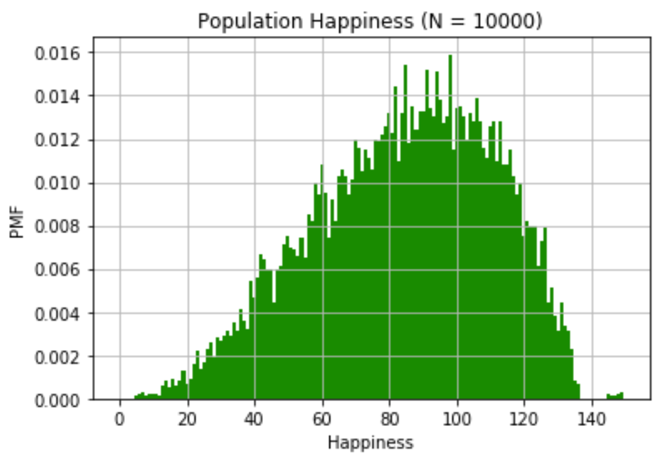
Bootstrap insight 1: Estimate the true distribution



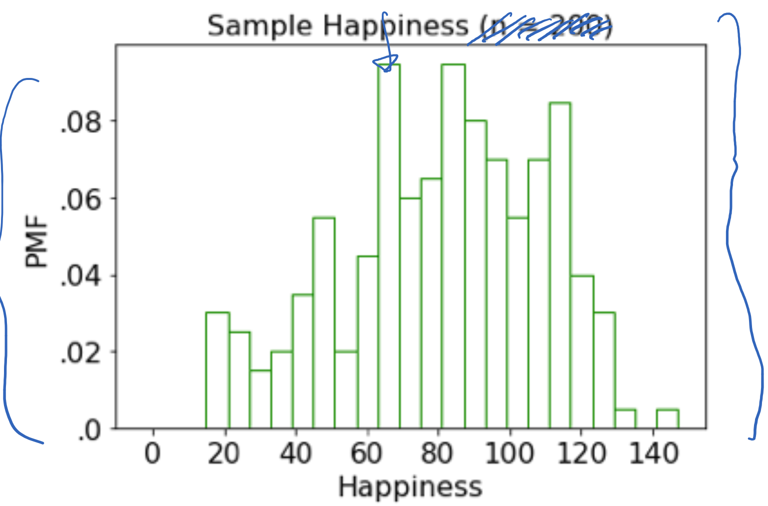
$\approx$

Bootstrap insight 1: Estimate the true distribution

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



≈



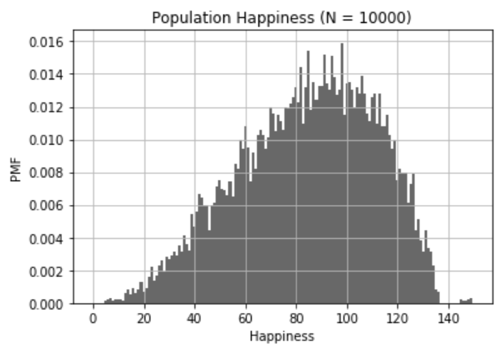
The underlying distribution → $F \approx \hat{F}$ ← the sample distribution (aka the histogram of your data)

*This is just a histogram of your data!

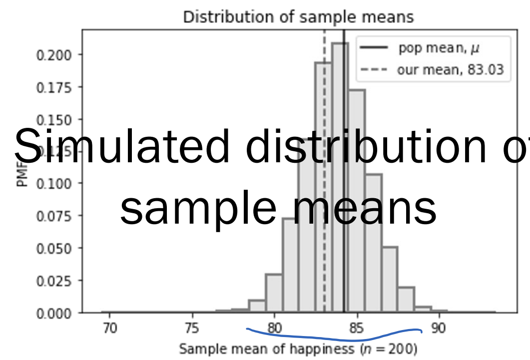
Bootstrap insight 2: Simulate a distribution

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

Population distribution
(we don't have this)



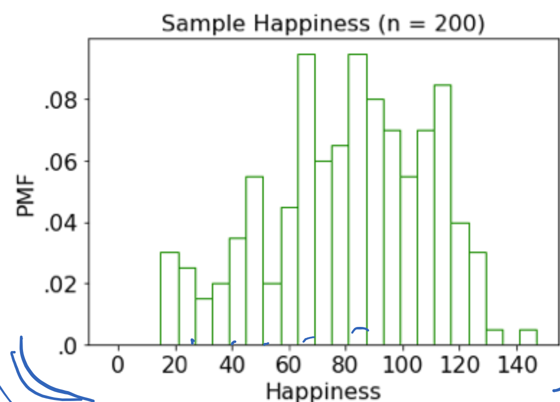
Distribution of $\bar{X}$



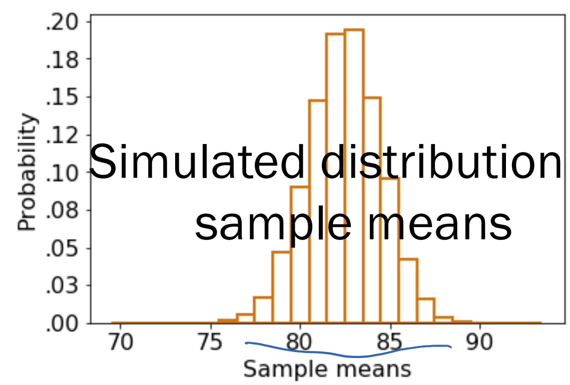
Simulated distribution of sample means

$\approx$

Sample distribution
(we do have this)



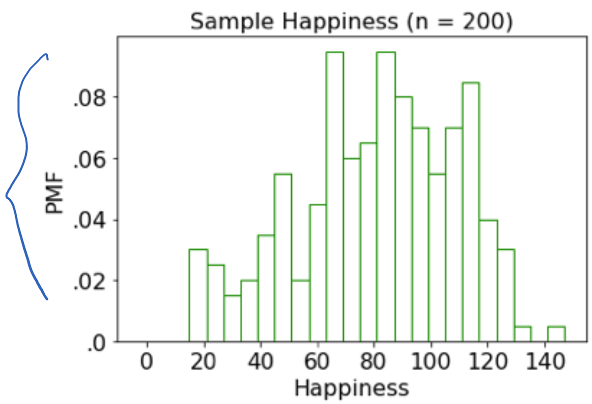
Bootstrap means



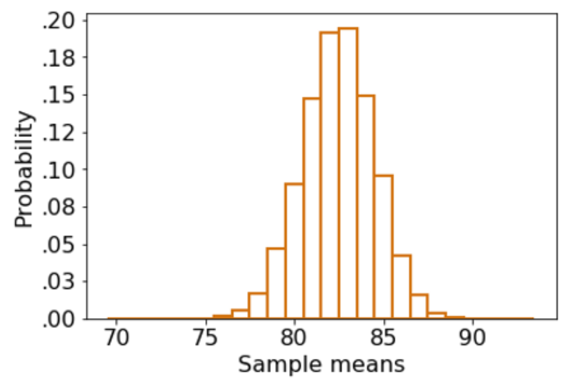
Simulated distribution of sample means

Bootstrapped sample means

```
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...

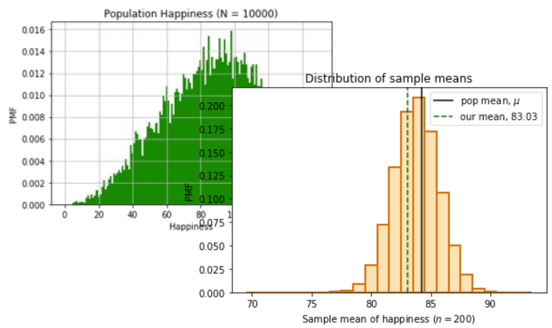
```
np.std(means)
2.003
```

...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)



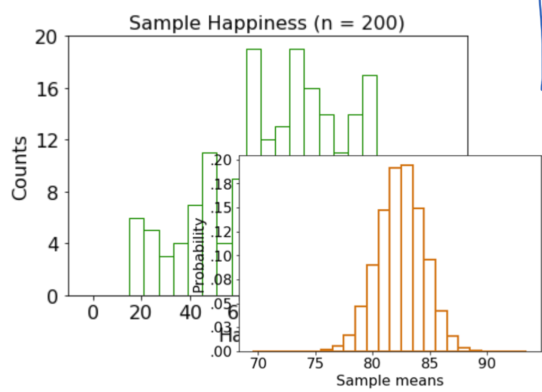
$$\frac{\sigma}{\sqrt{n}} = 1.886$$

Exact statistic
(we don't have this)

1.869

Simulated statistic
(we don't have this)

Sample distribution
(we do have this)



$$SE = \frac{S}{\sqrt{n}} = 1.992$$

Estimated statistic, by formula, **standard error**

2.003

Simulated estimated statistic, **bootstrapped standard error**

Bootstrap algorithm

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 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 either today or Wednesday!

Bootstrap algorithm

```
Bootstrap Algorithm (sample):
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
```

What is the distribution of your statistic?

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
```

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

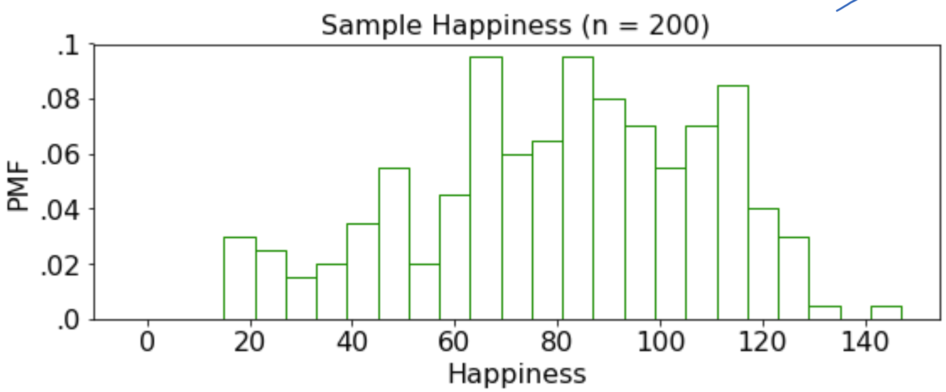
Bootstrapped sample variance

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



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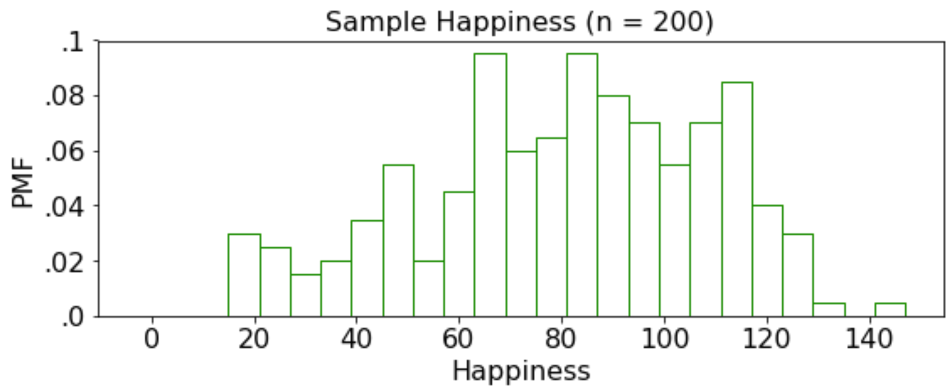
Bootstrapped variance



1. Estimate the **PMF** using the sample
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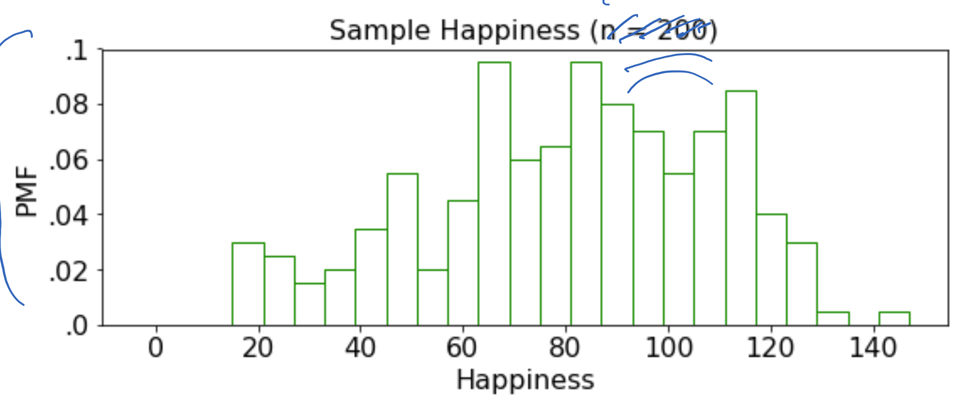
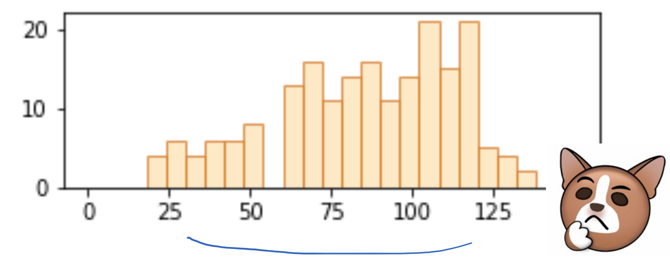
Bootstrapped variance



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



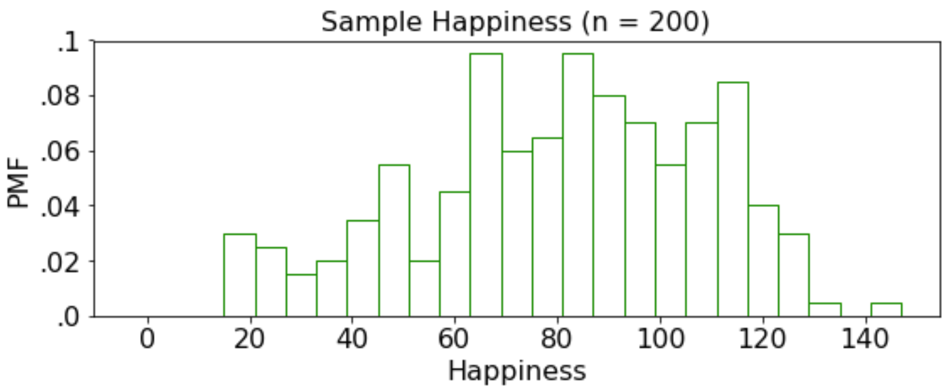
1. Estimate the **PMF** using the sample

⚠ Why are these samples **different?**

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**

This resampled sample is generated **with replacement.**

Bootstrapped variance



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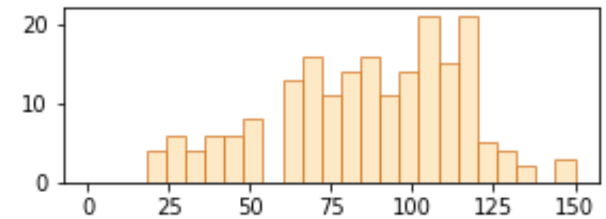
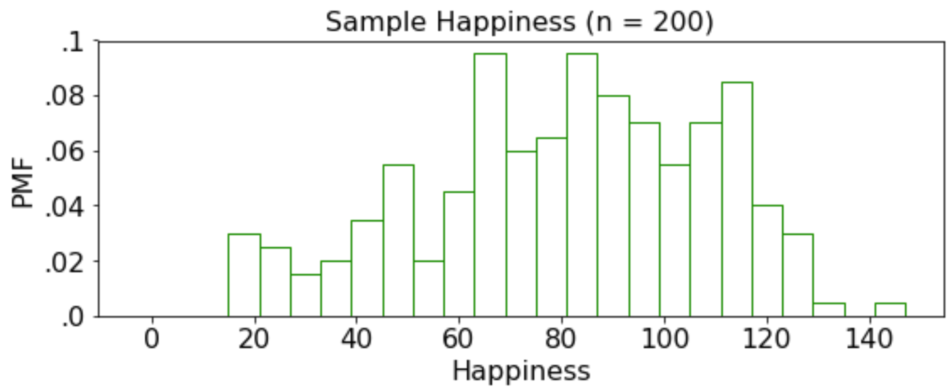


1. Estimate the **PMF** using the sample
2. Repeat **10,000** times:
   a. Resample **sample.size**() from PMF
   b. Recalculate the **sample variance** on the resample
3. You now have a **distribution of your sample variance**

```
variances = [827.4]
```

Bootstrapped variance



1. Estimate the **PMF** using the sample
2. Repeat **10,000** times:
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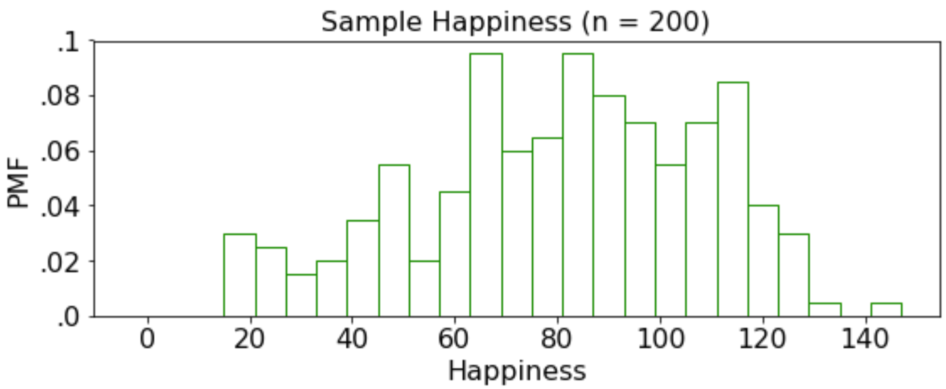
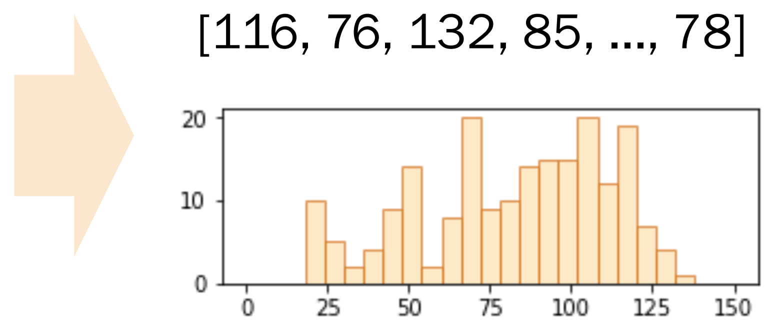
```
variances = [827.4]
```

Bootstrapped variance

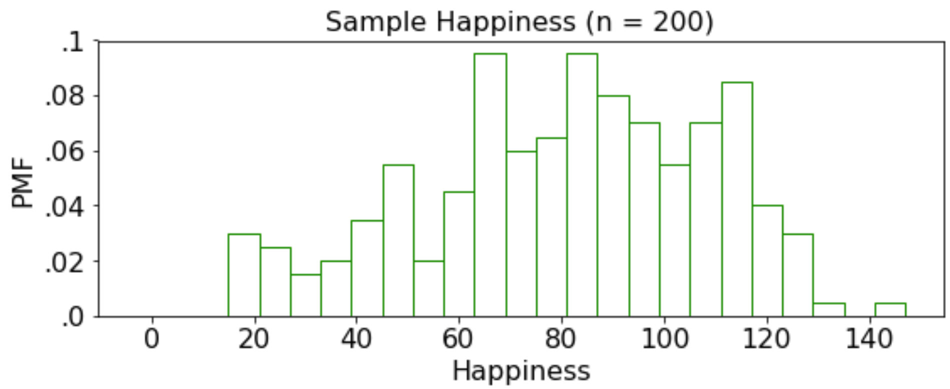




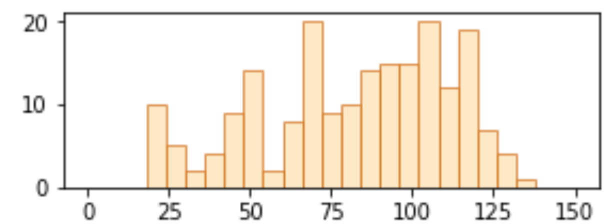
1. Estimate the **PMF** using the sample
2. Repeat **10,000** times:
   a. Resample **sample.size**() from PMF
   b. Recalculate the **sample variance** on the resample
3. You now have a **distribution of your sample variance**

```
variances = [827.4]
```

Bootstrapped variance



[116, 76, 132, 85, ..., 78]



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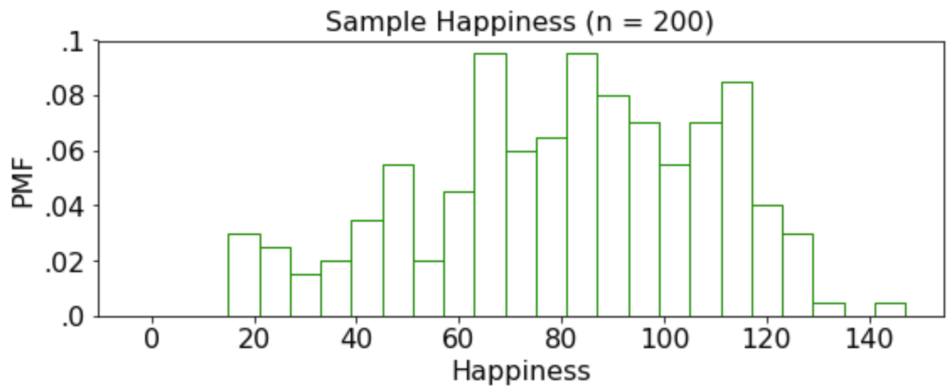
```
variances = [827.4, 846.1]
```

Bootstrapped variance



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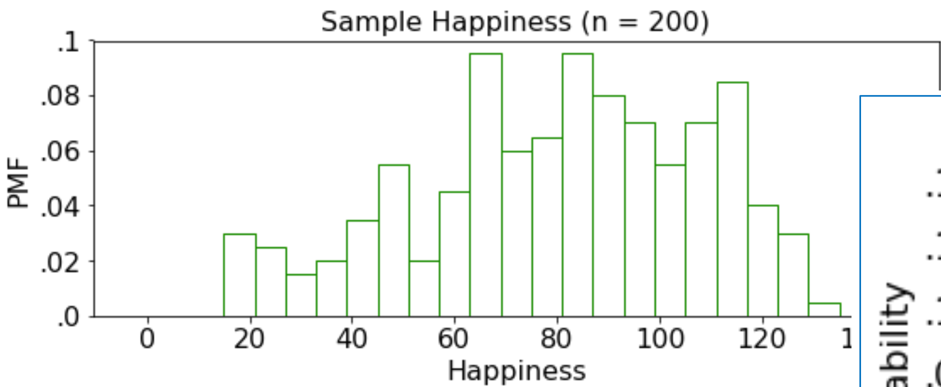
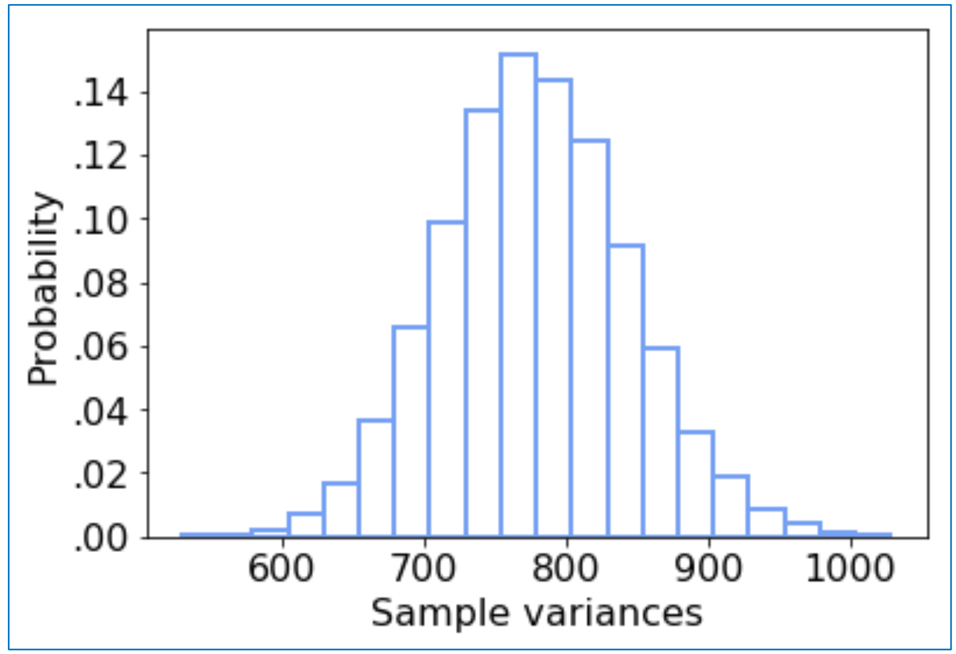
Bootstrapped variance





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

```
variances = [827.4, 846.1, 726.0, …, 860.7]
```

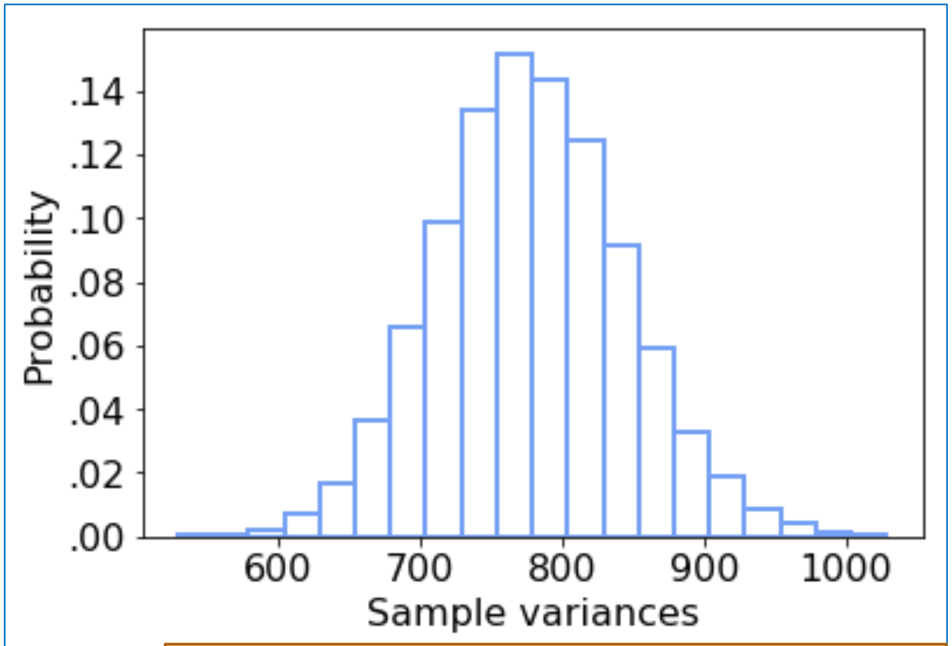
Bootstrapped variance

3. You now have a **distribution of your** **sample variance**

```
variances = [827.4,
    846.1, 726.0, …,
    860.7]
```

What is the bootstrapped standard error?

```
np.std(variances)
```



- Simulate a distribution of sample variances
- Compute standard deviation

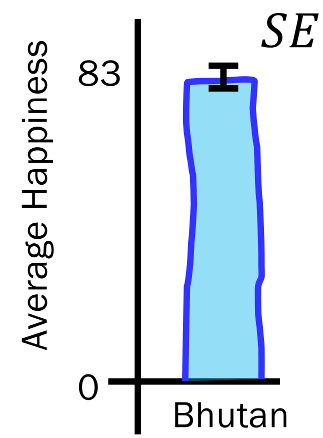
Bootstrapped standard error: 66.16

Standard error

1. Mean happiness:

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

   Closed form: $SE = \sqrt{\frac{S^2}{n}}$



2. Variance of happiness:

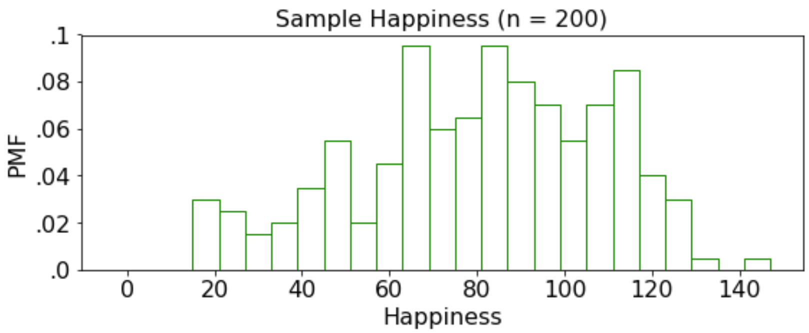
   S^2 is our best estimate of σ^2

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

   this is how close we are, calculated by bootstrapping

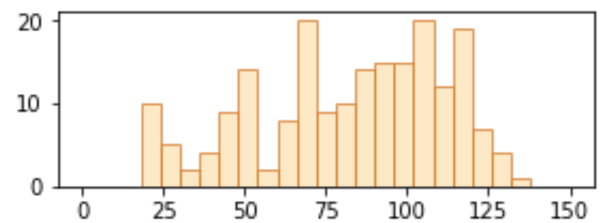
Algorithm in practice: Resampling

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**



?

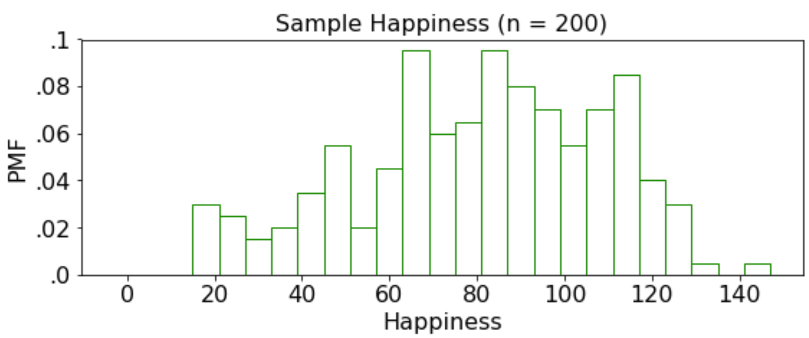
[116, 76, 132, 85, ..., 78]

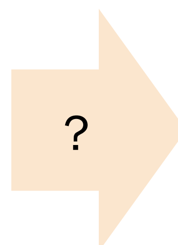


$$P(X = k) = \frac{\text{\# values in sample equal to } k}{n}$$

Algorithm in practice: Resampling

```python
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)
```





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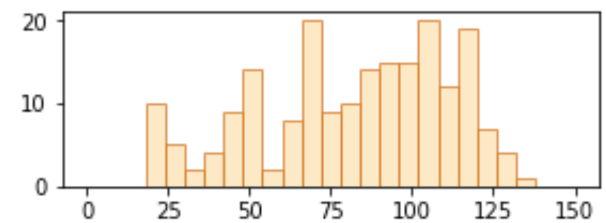


$$P(X = k) = \frac{\text{\# values in sample equal to } k}{n}$$

This resampled sample is generated **with replacement.**

To the code!

Bootstrap provides a way to calculate probabilities of statistics using code.

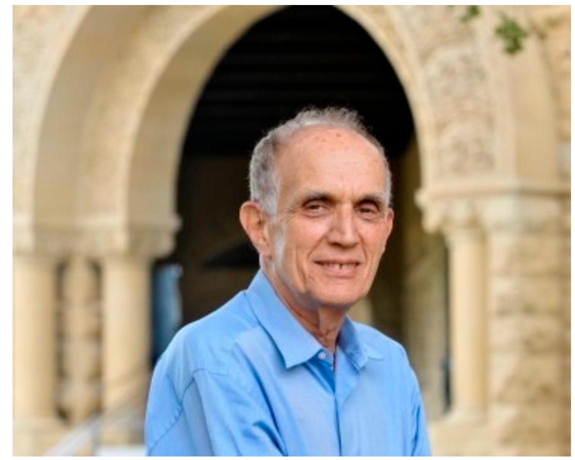
Bootstrapping works for any statistic*

*as long as your sample is i.i.d. and the underlying distribution does not have a long tail

Google colab notebook link

Bradley Efron

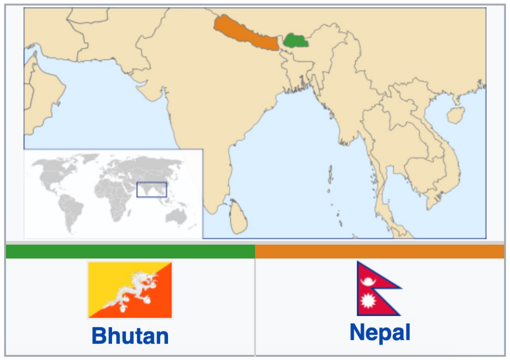
- Invented bootstrapping in 1979
- Still a professor at Stanford
- Won a National Science Medal



Efron's dice: 4 dice A, B, C, D such that

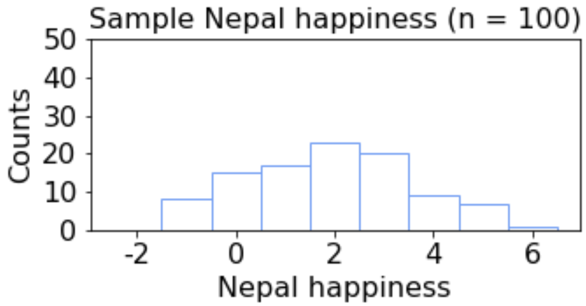
$$P(A > B) = P(B > C) = P(C > D) = P(D > A) = \frac{2}{3}$$

Bootstrap: p-value



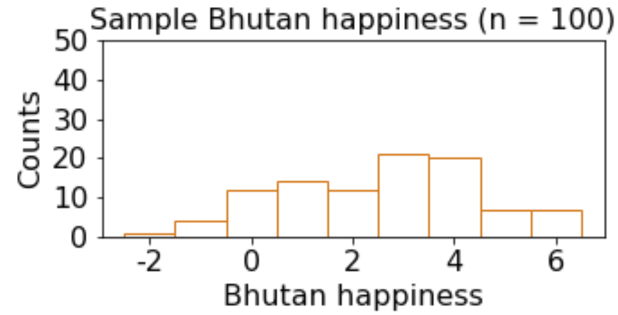
Null hypothesis test

Nepal Happiness
4.45
2.45
6.37
2.07
…
1.63



$\bar{X}_1 = 3.1$

Bhutan Happiness
0.91
0.34
1.91
1.61
…
1.08



$\bar{X}_2 = 2.4$

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

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?

Example:

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

} Null hypothesis assumes we use the same coin

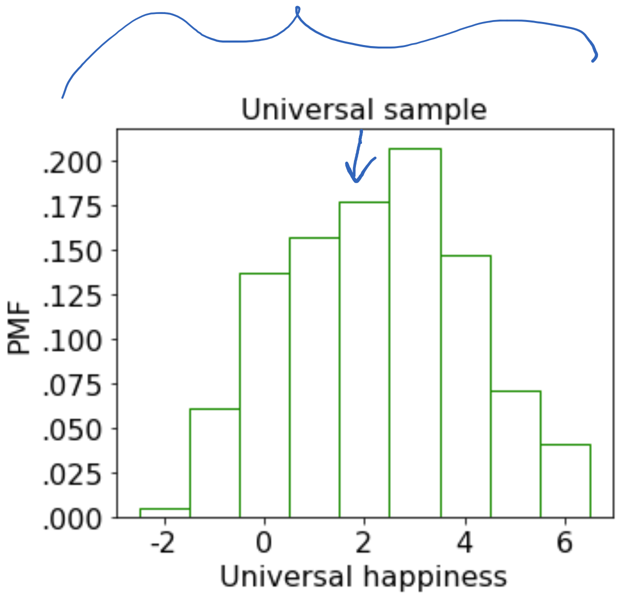
- Compute fraction of heads in both groups.
- There is a possibility we'll see the observed difference in these fractions even if we used the same coin

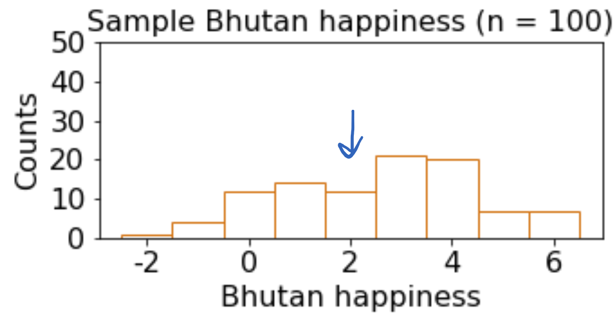
} p-value

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

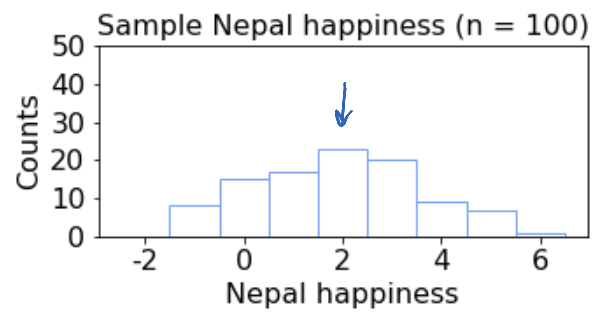
Universal sample

(this is what the null hypothesis assumes)





$\bar{X}_1 = 3.1$



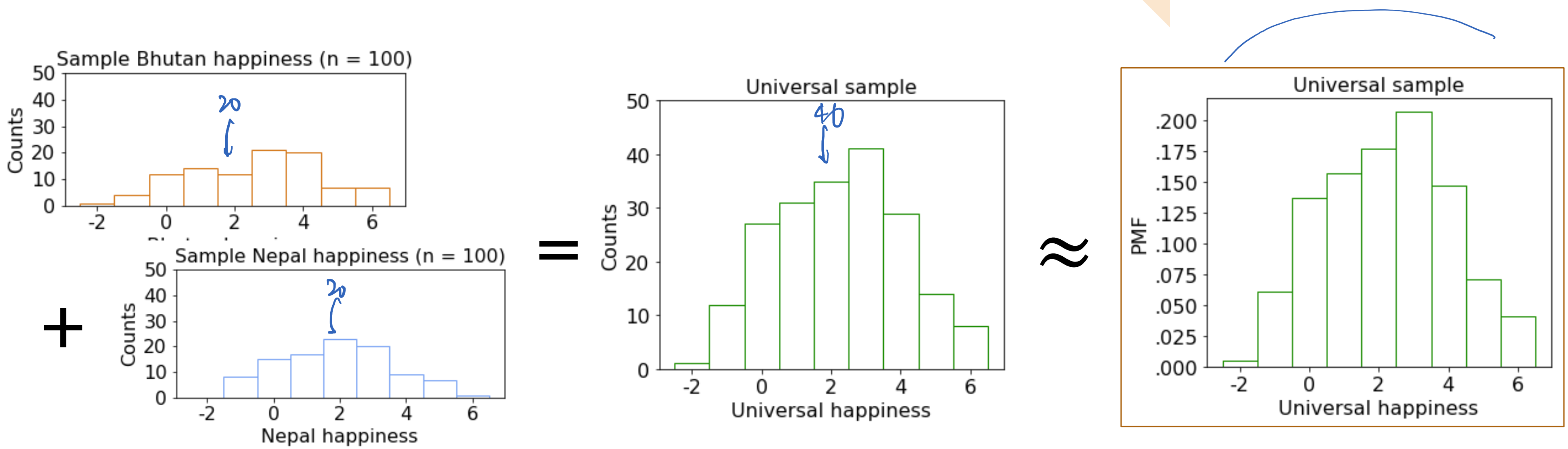
$\bar{X}_2 = 2.4$

Want p-value: probability $|\bar{X}_1 - \bar{X}_2| = |3.1 - 2.4|$ happens under null hypothesis

Bootstrap for p-values

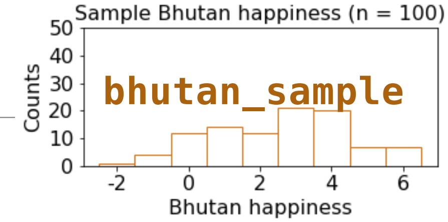
1. Create a **universal sample** using your two samples

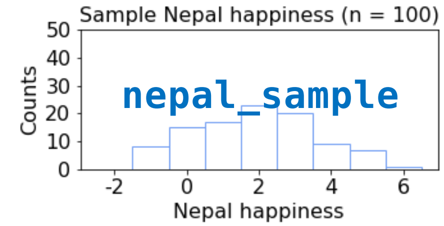
i.e., recreate the null hypothesis



Bootstrap for p-values

$|\bar{X}_1 - \bar{X}_2| \geq 0.7$





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** = $\frac{\text{\# (mean diffs >= observed diff)}}{n}$

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|   6.7

    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

1. Create a universal sample using your two samples

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def pvalue_boot(bhutan_sample, nepal_sample):
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        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):
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        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
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    uni_sample = combine bhutan_sample and nepal_sample
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    repeat 10,000 times:
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        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|

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        if diff >= observed_diff:
            count += 1

    pValue = count / 10,000
```

Bootstrap for p-values

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        if diff >= observed_diff:
            count += 1

pValue = count / 10,000
```

with replacement!

Bootstrap

Let's try it!

Google colab notebook link

Null hypothesis test

rejected by simulation

Nepal Happiness
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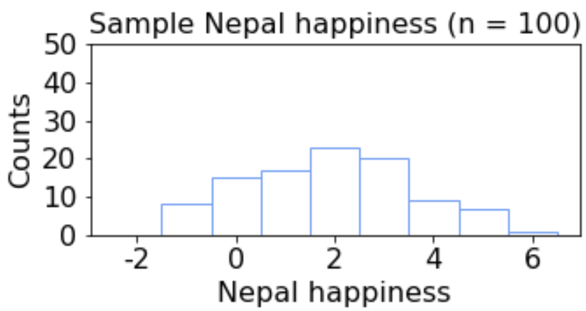
2.45
6.37
2.07
…
1.63



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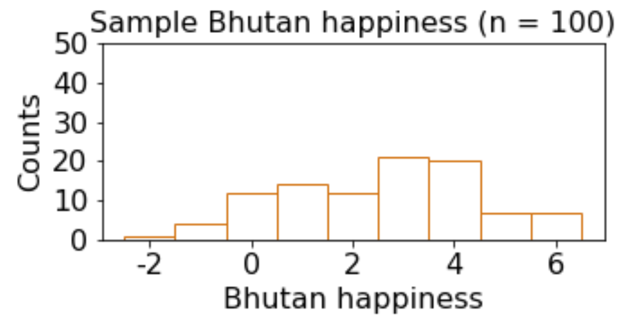

$\bar{X}_1 = 3.1$ $\bar{X}_2 = 2.4$

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

$p \approx 0.0117$