Simulation and Estimation

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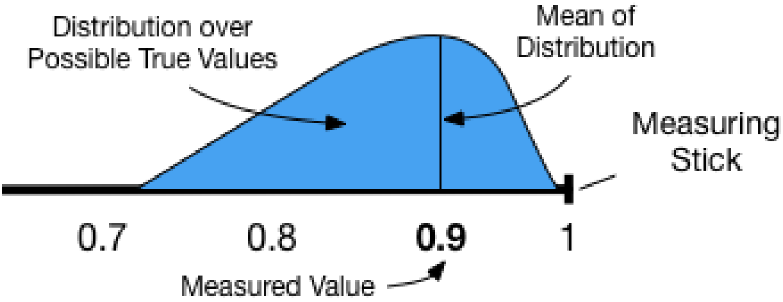
Uncertainty Propagation

All Measurements Have Error



Often assume error is symmetric and normally distributed about measured value – but it need not be.

The Problem of Uncertainty Propagation

Suppose we measured $\hat{x}$ which we assume is subject to normally distributed error such that the true value can be described by distribution $x \sim N(\hat{x}, 1)$.

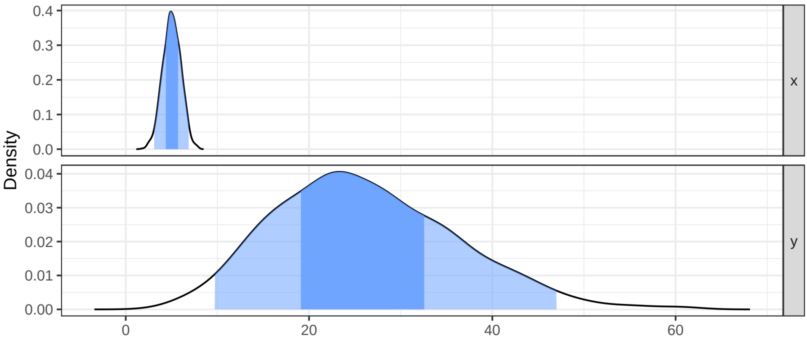
Problem Statement

Suppose we want to use x in a calculation, e.g., $y = f(x)$. How does error in x propagate into error in y?

Example

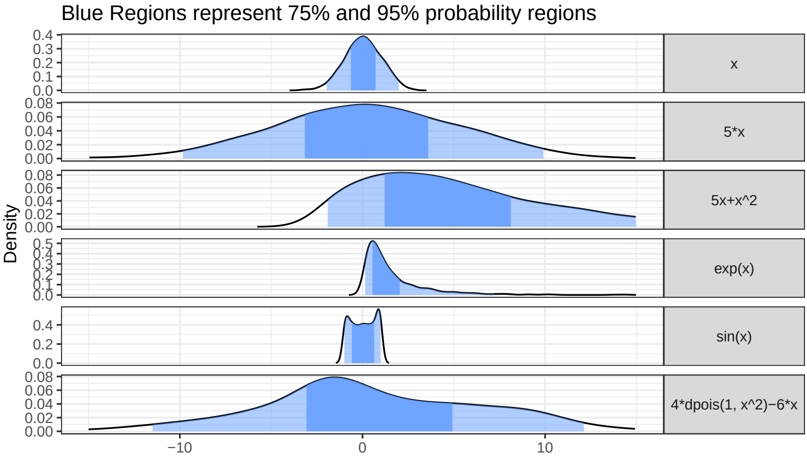
Suppose $\hat{x} = 5$ and we want to calculate $y = x^2$. What is the distribution of y?

```r
x <- rnorm(n=1000, mean=5, sd=1)
y <- x^2
```



More Examples

Suppose $x \sim N(0, 1)$ for simplicity.

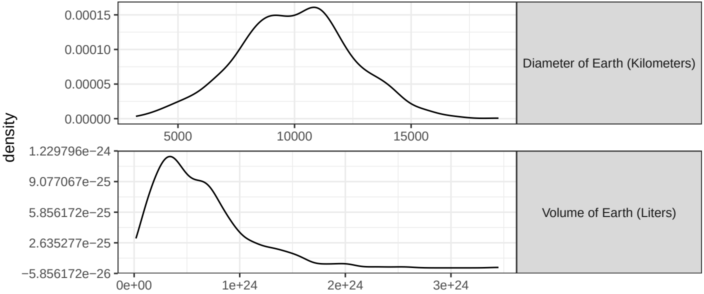


Improved Back of the Envelope Calculations

Whats the volume of the earth?

- I guessed its got a diameter of about 10,000 kilometers
- Assume my error is normally distributed, I guess a standard deviation of 2500km
  - 68% chance true value is between 7,500 and 12,500 kilometers.

```r
t <- 1000
kms <- rnorm(t, mean=10000, sd=2500)  # sample values our guessed distribution
volume.km3 <- (4/3)*pi*(kms/2)^3      # volume in cubic kilometers
liters <- volume.km3*1e12             # convert to liters
```



The true answer is 1.083e+24 (86th percentile of my guess).

Estimation and Hypothesis Testing

Estimation as Uncertainty Propagation

In (Frequentist) statistics, the sampling distribution of an estimator is a type of error propagation.

Definition (Estimator)

Any function (f) which we apply to data (x) to estimate something (μ). *An Estimator is a statistic.*

The sample mean is an estimator of the population mean:

$$\hat{\mu} = \frac{1}{N}\sum_{n=1}^{N} x_n.$$

Sampling Distribution of an Estimator

Assume that our data is *iid* from an underlying population $x_1, \ldots, x_N \sim N(\mu, \sigma^2)$.

What is the distribution of the sample mean? (Uncertainty Propagation)

This distribution is called the sampling distribution of the estimator.

From Sampling Distributions to Hypothesis Testing

Assume $x_1, \ldots, x_N \sim N(\mu, \sigma^2)$. We want to know the sampling distribution of the sample mean:

$$\hat{\mu} = \frac{1}{N} \sum_{n=1}^{N} x_n.$$

Why? (many reasons, will just pick one)

Common Statistics Logic: Use Data To Reject a (Null) Hypothesis

Suppose $H_0 : \mu = 0$, then $x_1, \ldots, x_N \sim N(0, \sigma^2)$.

Then calculate the sampling distribution of $\hat{\mu}$ and see if the value we observe is unlikely (e.g., $<$0.05% probability) under this null model. That probability value is a p-value of a hypothesis test.

But we don't know σ^2 so we can't calculate the sampling distribution of $\hat{\mu}$!

Building the t-test

Assume (under H_0, Null Hypothesis) that $x_1, \ldots, x_N \sim N(0, \sigma^2)$. We want to know the sampling distribution of the sample mean:

$$\hat{\mu} = \frac{1}{N} \sum_{n=1}^{N} x_n$$

but we can't calculate that because we don't know σ^2.

Building the t-test

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$$\hat{\mu} = \frac{1}{N} \sum_{n=1}^{N} x_n$$

but we can't calculate that because we don't know σ^2.
(Statisticians) **Let's change the statistic:**

$$t = \sqrt{N}\hat{\mu}/\hat{\sigma}$$

where $\hat{\sigma}$ is itself an unbiased estimator of the population standard deviation

$$\hat{\sigma} = \sqrt{\frac{\sum_{n=1}^{N}(x - \hat{\mu})^2}{n-1}}.$$

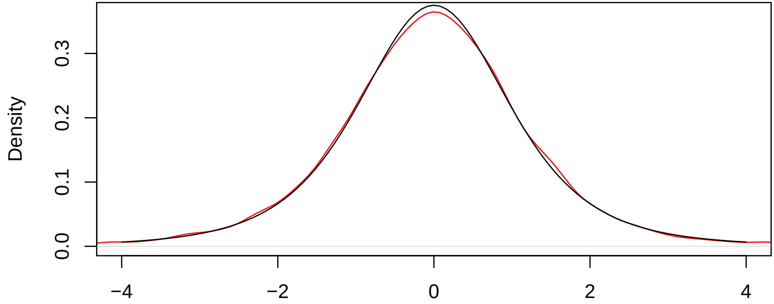
Some clever math shows that this new statistic t does not depend on any unknowns of the population (its a *pivotal quantity*):

$$t \sim t_{n-1}(\text{Student's t with } n-1 \text{ degrees of freedom}).$$

Checking Our Work 1

```
N <- 5
n.sim <- 10000
t <- rep(NA, n.sim)
for (i in 1:n.sim) {
  x <- rnorm(N, mean=0, sd=2)
  t[i] <- sqrt(N) * mean(x)/sd(x)
}
```

Plot (red) and compare to t_{N-1} density (black)



Checking Our Work 2

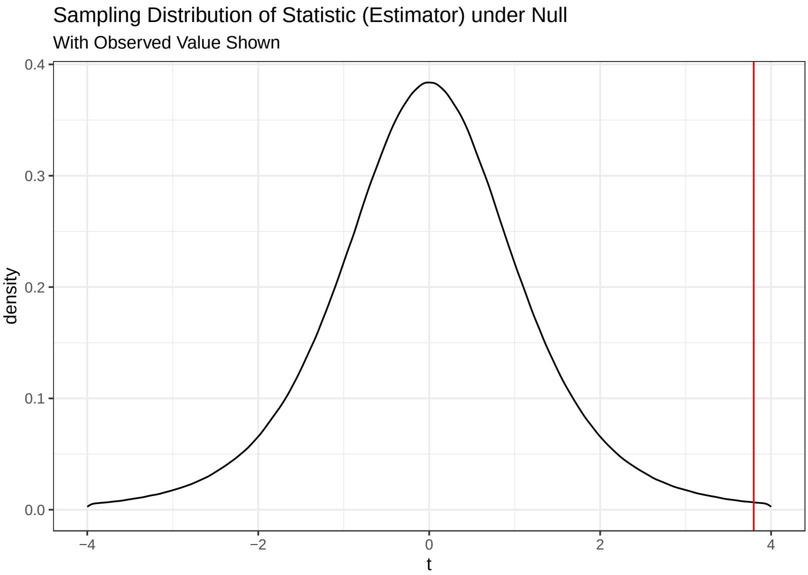
```
x <- c(3,4,3,3,1,0)

N <- length(x)
s <- sd(x) # same as sqrt(sum((x-mean(x))^2)/(N-1))
t <- sqrt(N)*mean(x)/s

## simulate sampling distribution of t (under null)
## and compare observed value
t.sim <- rt(n=10000000, df=N-1)

## calculate the number of simulations where |t|<|t.sim|
## this is the p-value
## this is the probability of the observed statistic under the null  model
sum(abs(t)<abs(t.sim))/length(t.sim)
```

```
[1] 0.0127504
```

```
## now compare to closed-form (known) solution
t.test(x)$p.value
```

```
[1] 0.0126766
```

Visualization Based on Simulation



Big Picture

(Frequentist) estimation and hypothesis testing are just clever applications of uncertainty quantification.

Differences:

- In uncertainty quantification, we typically think of randomness as arising due to measurement error.
- In estimation and hypothesis testing, we typically think of randomness as arising due to random sampling of a larger population.

Thinking of this in terms of simulation also makes it easy to do power and sample-size calculations.

Power and Sample Size Calculations

Power and Sample Size Calculation

- Up until now we have been operating under the null (sampling distribution of statistic under null).
- Now we focus on the alternative and ask one of two questions.

Power Calculations

Given my test and my belief in what the true population distribution is: for a given sample size, what is the probably that I reject the null hypothesis (the power of the test)?

Sample Size Calculations

Given my test and my belief in what the true population distribution is: what sample size do I need to achieve a desired power?

Power Calculations Made Easy (Example)

- For convenience lets use the t-test we already discussed and test the null hypothesis $H_0 : \mu = 0$.
- Suppose I believe $H_A : \mu = 5$ and $\sigma^2 = 3$.

```
n.sim <- 1000
N <- seq(3, 20)
power <- rep(NA, length(N))
for (n in 1:length(N)) {
  reject <- rep(NA, n.sim)
  for (i in 1:n.sim) {
    x <- rnorm(N[n], mean=5, sd=3)
    p.val <- t.test(x)$p.value
    reject[i] <- p.val <= 0.05
  }
  power[n] <- sum(reject)/n.sim
}
plot(N, power, type="l")
```