Week 03: Monte Carlo Estimation

Mark M. Fredrickson (mfredric@umich.edu)

Computational Methods in Statistics and Data Science (Stats 406)

Monte Carlo Estimation

Estimation Review

As with hypothesis testing, we want to **infer** something about a **population** based on a **sample**:

- Specific **parameters** in the distribution function.
- **Moments** of the population (mean, variance, skew, etc).
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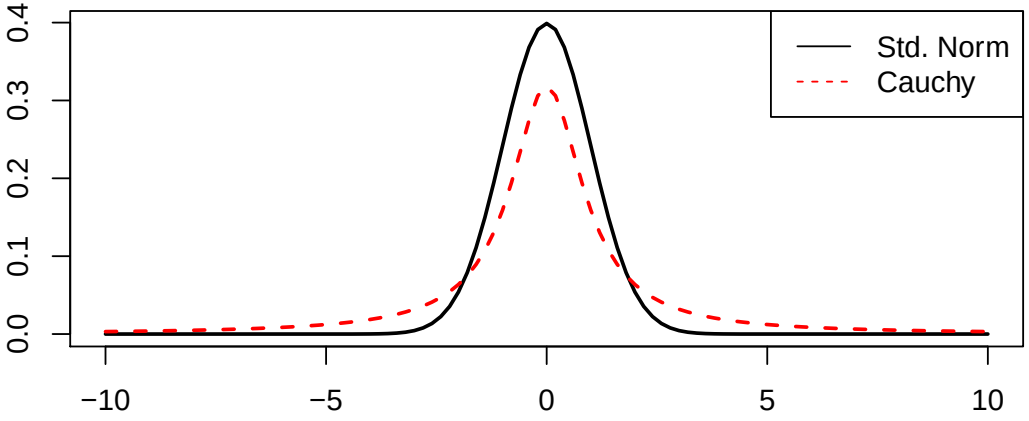
$$\hat{\theta} = \hat{\theta}(X_1, \ldots, X_n)$$

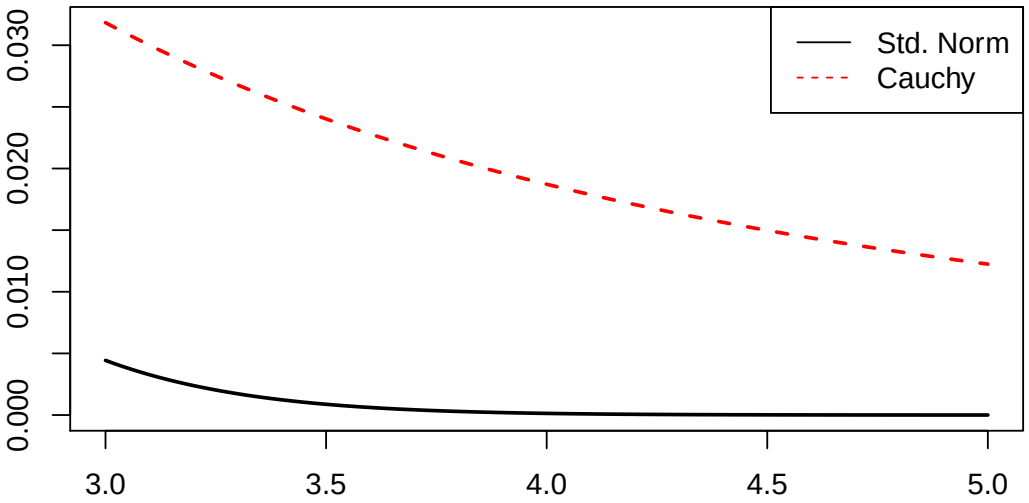
Understanding the distribution of $\hat{\theta}$ allows us to describe uncertainty and compare different estimators.

“Light” and “heavy” tails

The **Cauchy distribution** is known to have **“heavy tails”** (i.e., puts more mass away from the center).



Zooming in on the tails



Some properties of a Cauchy distribution

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Interesting fact: The Cauchy distribution does not have a mean: $E(X) = \infty$!

Suppose $X_i \overset{\text{iid}}{\sim} \text{Cauchy}(\theta)$ for $i = 1, \ldots, n$. How do we **estimate** θ?

Estimating θ

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Which of these estimators is "better?" What does it mean for an estimator to be better?

Let's investigate the **operating characteristics** of estimators: bias, variance, and mean squared error.

Sampling Distributions

Recall that our **estimators are statistics** and **have a distribution**.

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Since this distribution comes from sampling n values, we call this the **sampling distribution**. We will **estimate** the sampling distribution using **Monte Carlo techniques**.

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> median_sampling_dist <- map_dbl(samples, median)
> mean_sampling_dist <- map_dbl(samples, mean)
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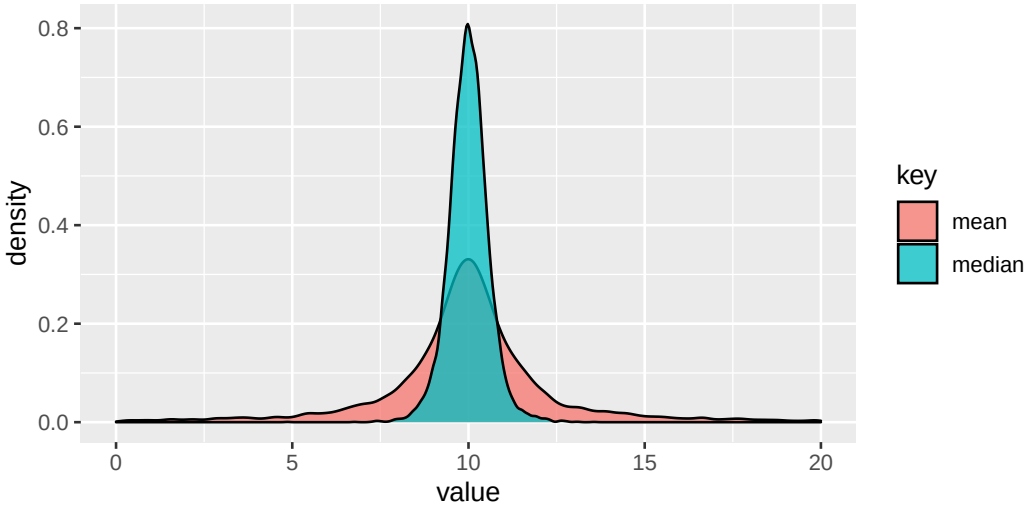

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Estimated bias of the two estimators:

```
> mean(median_sampling_dist) - true_theta
[1] 0.001323
> mean(mean_sampling_dist) - true_theta
[1] 11.77
```

More sampling distribution details

```
> summary(median_sampling_dist)

   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
   4.87    9.66   10.00   10.00   10.33   13.57

> summary(mean_sampling_dist)

   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
  -9051       9      10      22      11  119723
```

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The equivalent for estimation is the **variance of the sampling distribution**.

```
> var(median_sampling_dist)

[1] 0.3292

> var(mean_sampling_dist)

[1] 1449215
```

A better estimator

The **order statistics** of a sample are the **sorted values**:

$$X_{(1)} \leq X_{(2)} \leq \cdots \leq X_{(n)}$$

I.e., $X_{(1)}$ is the sample minimum; $X_{(n)}$ is the sample maximum.

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I.e., $X_{(1)}$ is the sample minimum; $X_{(n)}$ is the sample maximum.

Another estimator takes the average of some middle portion of the order statistics, we call this a "trimmed mean".

```
> trimmed_mean <- function(x, k) {
+   n <- length(x)
+   orderstats <- sort(x)
+   mean(orderstats[k:(n - k)])
+ }
```

How should we pick k?

```
> ks <- 1:4
> map(ks, function(k) {
+   ts <- map_dbl(samples, ~ trimmed_mean(.x,  k = k))
+   t_bias <- mean(ts) - true_theta
+   t_var  <- var(ts)
+   c(t_bias, t_var)
+ }) %>% bind_cols

# A tibble: 2 x 4
        V1     V2     V3     V4
     <dbl>  <dbl>  <dbl>  <dbl>
1    -4.22 -0.418 -0.251 -0.202
2 11534.    1.27   0.460  0.358
```

Bigger sample size n

```
> n <- 500
> k <- round(0.38 * n / 2)
> samples_500 <- data.frame(replicate(1000, rcauchy(n, true_theta)))
> median_500 <- map_dbl(samples_500, median)
> trimmed_500 <- map_dbl(samples_500, trimmed_mean, k = k)
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> median_500 <- map_dbl(samples_500, median)
> trimmed_500 <- map_dbl(samples_500, trimmed_mean, k = k)

> c(mean(median_500), var(median_500))

[1] 9.995974 0.005108

> c(mean(trimmed_500), var(trimmed_500))

[1] 9.990400 0.006029
```

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For **unbiased estimators**, then we simply prefer those with **low variance**.

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Since both were nearly unbiased, this is basically equal to variance.

Confidence Intervals for MSE

It is useful to give statements of how precise our estimates of the MSE are:

```
> t.test((median_500 - true_theta)^2)$conf.int

[1] 0.004648 0.005590
attr(,"conf.level")
[1] 0.95

> t.test((trimmed_500 - true_theta)^2)$conf.int

[1] 0.005594 0.006636
attr(,"conf.level")
[1] 0.95
```

Example: estimating upper bound of uniform distribution

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Suppose we have a sample of 20 IID draws from f. How can we **estimate** θ?

- Method of moments estimation: find θ as a function of the moments of the distribution.
- Maximum likelihood estimation: find the θ that maximizes the joint density (likelihood function).

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$$\theta = 2\mathrm{E}(X) \Rightarrow \tilde{\theta} = 2\bar{X}$$

For IID data, the likelihood in this case will be

$$L(\theta) = \prod_{i=1}^{n} I(x_i \in [0, \theta]) \frac{1}{\theta} = \frac{1}{\theta^n} \prod_{i=1}^{n} I(x_i \in [0, \theta])$$

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These two facts imply, the **MLE is the sample maximum**: $\hat{\theta} = \max_i X_i$.

Sampling distribution for $n = 20, \theta = 2$

```
> k <- 100000
> n <- 20
> theta <- 2
```

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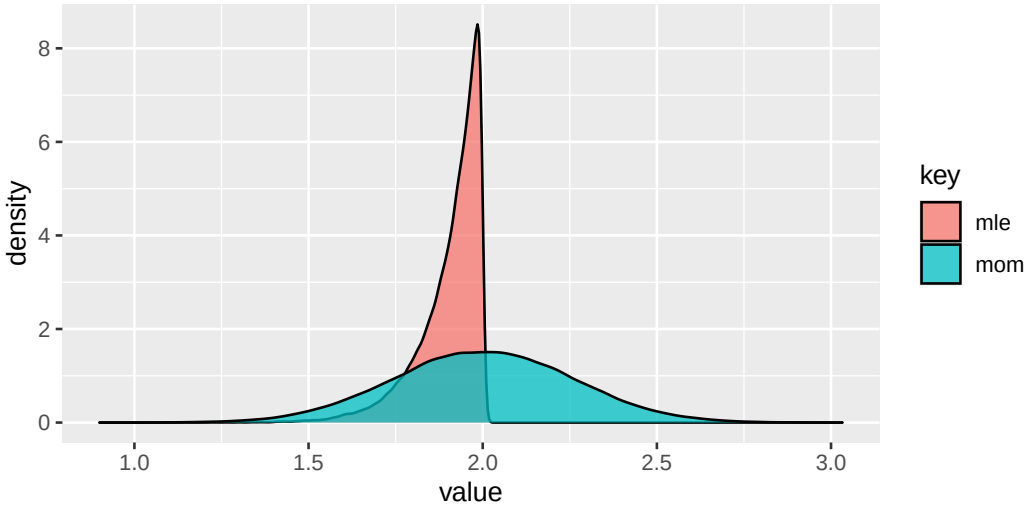
```
> k <- 100000
> n <- 20
> theta <- 2

> samples <- rerun(k, runif(n, min = 0, max = theta))
> mle_sampling_dist <- map_dbl(samples, max)
> mom_sampling_dist <- map_dbl(samples, ~ 2 * mean(.x))
```

Sampling Distributions



Operating characteristics

Bias:

```
> t.test(mle_sampling_dist - theta)$conf.int[1:2] # 1:2 silence attr
[1] -0.09571 -0.09458
> t.test(mom_sampling_dist - theta)$conf.int[1:2]
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MSE:

```
> t.test((mle_sampling_dist - theta)^2)$conf.int[1:2] # 1:2 silence attr
[1] 0.01718 0.01762
> t.test((mom_sampling_dist - theta)^2)$conf.int[1:2]
[1] 0.06617 0.06733
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- We can evaluate for **bias** and **variance** of estimators, and combine these with **mean squared error**.
- As with generating **null distributions**, we pick a distribution for the X_i, and the **estimate the distribution of** $\hat{\theta}$ (**sampling distribution**).
- Usually we wish to compare estimators or change aspects of the problem to see how the performance changes (ample size, parameter values).

Confidence Intervals

Beyond point estimates

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Point estimates are useful, but **they do not communicate uncertainty**.

When performing hypothesis tests, we started by either **accepting or rejecting the null hypothesis** and then extended this idea to computing **p-values**.

A similar concept in estimation is to construct a **confidence interval** for θ (target of inference).

Capturing Uncertainty: Confidence Intervals

A $(1-\alpha)\times 100\%$ **confidence interval** (CI) is a pair of **random variables** A and B such that

$$\Pr(A \leq \theta, B \geq \theta) > 1-\alpha \quad \text{and} \quad \Pr(A \leq B) = 1$$

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Confidence intervals are sometimes called **interval estimators** because A and B are typically functions of the data, $X_1, \ldots, X_n$:

$$A = A(X_1, \ldots, X_n) \quad B = B(X_1, \ldots, X_n)$$

Confidence interval construction

The notation $A(X_1, \ldots, X_n), B(X_1, \ldots, X_n)$ has a natural connection to **test statistics** and highlights one way of construction confidence intervals: **find the set of null hypotheses not rejected at the α-level**.

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$$B = \sup\{\theta_0 : T(X_1, \ldots, X_n) \notin \mathcal{R}(\theta_0, \alpha)\}$$

where $\mathcal{R}(\theta_0, \alpha)$ is the rejection region for T when $H_0 : \theta = \theta_0$ versus $H_1 : \theta \neq \theta_0$.

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This is called the "test inversion" method of CI construction.

Connections to hypothesis tests

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- Type I error: The **confidence coefficient/coverage** is $\Pr(\theta \in [A, B])$, which is greater than $1 - \alpha$.

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  In other words, the probability of $[A, B]$ **excluding** θ is no more than α.
- Power: No matter what θ is, we want $[A, B]$ to cover it.
  Short intervals will exclude more false null hypotheses, so we want $E(B - A)$ (**expected length**) to be small.

Connections to "estimator $\pm c$"

For $X_i \sim N(\mu, \sigma^2)$, independent with σ^2 known, let's test

$$H_0 : \mu = \mu_0 \quad \text{versus} \quad H_1 : \mu \neq \mu_0$$

at the α level using $\bar{X}$ as the statistic.

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at the α level using $\bar{X}$ as the statistic.

We accept the null if

$$-\Phi(1-\alpha/2) \leq \frac{\bar{X} - \mu_0}{\sigma/\sqrt{n}} \leq \Phi(1-\alpha/2)$$

Solving for μ_0

Solving for μ_0 gives us

$$\bar{X} - \Phi(1-\alpha/2)(\sigma/\sqrt{n}) \leq \mu_0 \leq \bar{X} + \Phi(1-\alpha/2)(\sigma/\sqrt{n})$$

or

$$\mu_0 \in \bar{X} \pm \Phi(1-\alpha/2)(\sigma/\sqrt{n})$$

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or

$$\mu_0 \in \bar{X} \pm \Phi(1-\alpha/2)(\sigma/\sqrt{n})$$

The "plus-minus" type intervals show up for **shift parameters** that change the center of the sampling distribution but not the variance or other properties.

Example: Coverage and Expected Length $X_i \sim N(\mu, \sigma^2)$

Suppose we believe we know σ^2 and

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We will use two facts (without proof):

$$\frac{\bar{X} - \mu}{\sigma/\sqrt{n}} \sim N(0, 1)$$

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This leads to two kinds of $(1-\alpha) \times 100\%$ confidence intervals:

$$\bar{X} \pm z_{\alpha/2}(\sigma/\sqrt{n}), \quad \bar{X} \pm t_{\alpha/2}(n-1)(\hat{s}/\sqrt{n})$$

Simulation to assess coverage and average width

```
> alpha <- 0.05
> k <- 10000
> n <- 20
> mu <- 2 # unknown truth
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> samples_norm <- rerun(k, rnorm(n, mean = mu, sd = sigma))
> cis_norm <- map(samples_norm,
+                 ~ mean(.x) + c(-1, 1) * qnorm(1 - alpha/2) * (sigma / sq
> cis_t <- map(samples_norm,
+              ~ mean(.x) + c(-1, 1) * qt(1 - alpha/2, df = n - 1) * (sd(.x
```

Estimating coverage

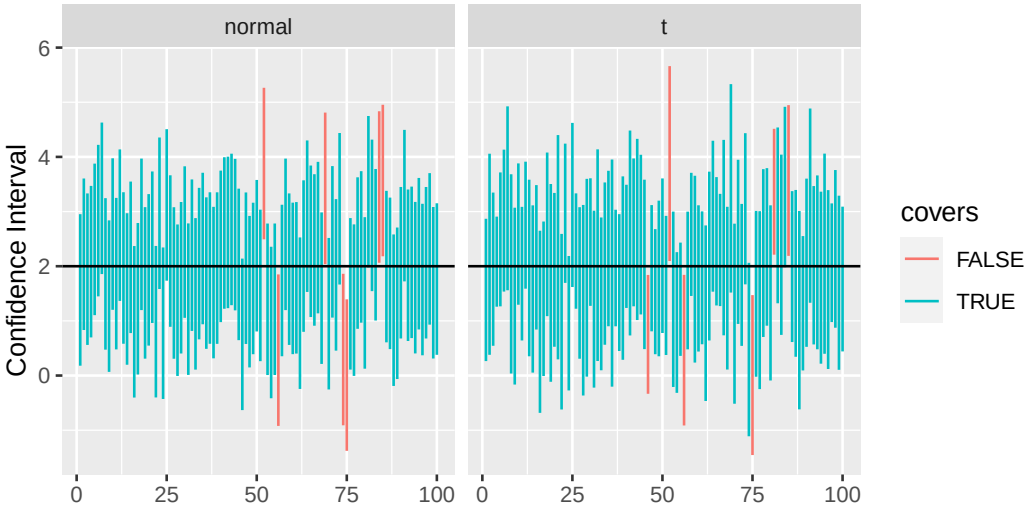
Coverage is $P(A \leq \theta \leq B)$:

```
> map_dbl(cis_norm, ~ .x[1] <= mu && mu <= .x[2]) %>% mean
[1] 0.9516
> map_dbl(cis_t, ~ .x[1] <= mu && mu <= .x[2]) %>% mean
[1] 0.9512
```

Estimating expected width

```
> map_dbl(cis_norm, ~ .x[2] - .x[1]) %>% mean
[1] 2.772
> map_dbl(cis_t, ~ .x[2] - .x[1]) %>% mean
[1] 2.918
```

Visual interpretation



Binomial proportion CI

We've already seen that if we are estimating

$$\theta = P(X \leq t)$$

using

$$\hat{\theta} = \frac{1}{n} \sum_{i=1} I(X_i \leq t)$$

the variables $Y_i = I(X_i \leq t)$ are **Bernoulli with** $P(Y_i = 1) = \theta$.

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Using the central limit theorem, if we have a large sample, then

$$\bar{Y} \approx N\left(\theta, \frac{\theta(1-\theta)}{n}\right)$$

Binomial proportion continued

Again,

$$\bar{Y} \approx N\left(\theta, \frac{\theta(1-\theta)}{n}\right)$$

so by our previous analysis the interval:

$$\bar{Y} \pm z_{\alpha/2}\sqrt{\frac{\theta(1-\theta)}{n}}$$

would be a $100 \times (1-\alpha)$ **confidence interval for** θ.

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Of course, we don't know θ, but we can stick in an **estimate**:

$$\bar{Y} \pm z_{\alpha/2}\sqrt{\frac{\bar{Y}(1-\bar{Y})}{n}}$$

This is the standard confidence interval for a proportion.

95% CI for $P(X > 1)$, $X \sim Cauchy(0)$

```
> n <- 10000
> x <- rcauchy(n)
> y <- x > 1
> ybar <- mean(y)
```

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> n <- 10000
> x <- rcauchy(n)
> y <- x > 1
> ybar <- mean(y)

> (norm_ci <- ybar + c(-1,1) * qnorm(0.975) * sqrt(ybar * (1 - ybar) / n))

[1] 0.2504 0.2676
```

Test inversion method

Let's use the duality of hypothesis tests to create another interval.

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We would accept θ_0 if either

$$a_0 < \sum_{i=1}^{n} Y_i < b_0$$

Finding a_0s and b_0s

We will search over a range of possible θ_0 values:

```
> theta_0 <- seq(0, 1, length.out = 1000)
```

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For each, compute the bounds:

```
> a0 <- qbinom(0.025, size = n, prob = theta_0)
> b0 <- qbinom(0.025, size = n, prob = theta_0,
+               lower.tail = FALSE) - 1
```

Reject or Accept θ_0

Now see for which θ_0 we would accept:

```
> w <- sum(y)
> range(theta_0[a0 < w & w < b0])
```

```
[1] 0.2513 0.2673
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Which shows that the Normal approximation is quite good a $n = 10000$:

```
[1] 0.2504 0.2676
```

Binomial proportions intervals

R provides three methods for computing binomial confidence intervals:

- `t.test`: Using a standard normal approximation
- `binom.test`: Pearson-Clapper interval (similar to exact interval earlier)
- `prop.test`: Wilson "score" interval

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Which has proper coverage? Smallest size?

MC Setup

```
> theta <- 0.25
> n <- 20
> k <- 1000
> xs <- rbinom(k, size = n, prob =  theta)
```

```
> tints <- map(xs, function(x) {
+     if (x == 0 || x == n) {
+         return(c(0, 1)) # can't estimate
+     } else {
+        return(t.test(c(rep(1, x), rep(0, n - x)))$conf.int)
+     }
+ })
```

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+     }
+ })

> bints <- map(xs, ~ binom.test(.x, n)$conf.int)
> pints <- map(xs, ~ prop.test(.x, n)$conf.int)
```

Confidence coefficient

Recall, the **confidence coefficient** is defined as

$$P(A \leq \theta, \theta \leq B)$$

```
> cover <- function(x) { x[1] <= theta && theta <= x[2] }
> (tcover <- map_dbl(tints, cover) %>% mean)

[1] 0.895

> (bcover <- map_dbl(bints, cover) %>% mean)

[1] 0.961

> (pcover <- map_dbl(pints, cover) %>% mean)

[1] 0.981
```

Expected Width

```
> (twidth <- map_dbl(tints, diff) %>% mean)
[1] 0.4053
> (bwidth <- map_dbl(bints, diff) %>% mean)
[1] 0.3944
> (pwidth <- map_dbl(pints, diff) %>% mean)
[1] 0.3893
```

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- The Pearson-Clopper method is **slightly conservative** (i.e., overcovers), which is reflected by having slightly higher average width.
- The score test inversion method has the **smallest intervals**, but also has **good coverage**.
- Important: these conclusions are for $n = 20$ and $\theta = 0.25$; other values might have other conclusions (e.g., when $\theta \approx 1$)

Confidence Intervals Summary

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- As with Type I error and power, we can **investigate the operating characteristics** of confidence intervals.
- **Confidence coefficient** (actual probability of including θ, analogous to Type I error)
- **Expected width** (ability to exclude incorrect θ, analogous to power)