

STA261 - Module 4

Intervals and Model Checking

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Uncertainty in Point Estimates

- In Module 2, we learned how to produce the “best” point estimates of θ possible using statistics of our data
- The “best” unbiased estimator $\hat{\theta}(\mathbf{X})$ is the one that has the lowest possible variance among all unbiased estimators of θ
- But even so, suppose we observe $\mathbf{X} = \mathbf{x}$ and calculate $\hat{\theta}(\mathbf{x})$; how do we know this is close to the true θ ?
It may not be!
- We can’t know for sure
- But we can use the data to get a range of *plausible* values of θ

Eg: still assuming STA261 heights $\sim N(\mu, 1)$. I calculate $\bar{x}_n = 5'6.5''$

Probably more plausible that $\mu \in [4'6.5'', 6'6.5'']$ than $[2', 4']$
 $= [\bar{x}_n - 1, \bar{x}_n + 1]$

Random Sets

- Suppose for now that $\Theta \subseteq \mathbb{R}$
- If $\hat{\theta}(\mathbf{X})$ is a continuous random variable, then $\mathbb{P}_\theta(\theta = \hat{\theta}(\mathbf{X})) = 0$
unless...
- But we can try to find a random set $C(\mathbf{X}) \subseteq \mathbb{R}$ based on \mathbf{X} such that
 $\mathbb{P}_\theta(\theta \in C(\mathbf{X})) = 0.95$, for example
↑ a set which is a function of the random sample \bar{X}
e.g., $[\bar{X}_{n-1}, \bar{X}_n + 1]$
- **Example 4.1:** Let $X \sim \mathcal{N}(\mu, 1)$ where $\mu \in \mathbb{R}$. Show that the region $C(X) = (X + z_{0.025}, X + z_{0.975})$ satisfies $\mathbb{P}_\mu(\mu \in C(X)) = 0.95$.

$$\begin{aligned}& \mathbb{P}_\mu(\mu \in C(X)) \\&= \mathbb{P}(X + z_{0.025} < \mu < X + z_{0.975}) \\&= \mathbb{P}(z_{0.025} < \mu - X < z_{0.975}) \\&= \mathbb{P}(z_{0.025} < Z < z_{0.975}) \quad \text{where } Z \sim N(0,1) \\&\quad (\text{check!}) \\&= \Phi(z_{0.975}) - \Phi(z_{0.025}) \\&= 0.95\end{aligned}$$

Interval Estimators and Confidence Intervals

- **Definition 4.1:** An **interval estimate** of a parameter $\theta \in \Theta \subseteq \mathbb{R}$ is any pair of statistics $L, U : \mathcal{X}^n \rightarrow \mathbb{R}$ such that $L(\mathbf{x}) \leq U(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}^n$. The random interval $(L(\mathbf{X}), U(\mathbf{X}))$ is called an **interval estimator**.
interval with random endpoints! *Note: some authors include the endpoints!*
- **Example 4.2:** $N(\mu, 1) : (X_{(1)}, X_{(n)} + 5)$ Bernoulli(p) : $(-\bar{X}_n + 4, \bar{X}_n + 5)$
- **Definition 4.2:** Suppose $\alpha \in [0, 1]$. An interval estimator $(L(\mathbf{X}), U(\mathbf{X}))$ is a **$(1 - \alpha)$ -confidence interval** for θ if $\mathbb{P}_{\theta}(L(\mathbf{X}) < \theta < U(\mathbf{X})) \geq 1 - \alpha$ for all $\theta \in \Theta$. We refer to $1 - \alpha$ as the **confidence level** of the interval.
- **Example 4.3:** $X \sim N(\mu, 1) \Rightarrow$ We showed in Example 4.1 that
$$(X + z_{0.025}, X + z_{0.975})$$
 is a 0.95 -confidence interval.

One-Sided Intervals

- **Definition 4.3:** A **lower one-sided** confidence interval is a confidence interval of the form $(L(\mathbf{X}), \infty)$. An **upper one-sided** confidence interval is a confidence interval of the form $(-\infty, U(\mathbf{X}))$.
- **Example 4.4:** Let $X_1, X_2, \dots, X_n \stackrel{iid}{\sim} \mathcal{N}(\mu, 1)$. Find a lower one-sided 0.5-confidence interval for μ .

$$0.5 = P(Z < 0) \quad \text{where } Z \sim N(0,1)$$

$$= P_{\mu}\left(\frac{\bar{X}_n - \mu}{\sqrt{1/n}} < 0\right)$$

$$= P_{\mu}(\bar{X}_n < \mu)$$

$$= P_{\mu}(\mu \in (\bar{X}_n, \infty))$$

But (\bar{X}_n, ∞) is a ~~another one!~~

So $(1-\alpha)$ -CIs are not unique.

So (\bar{X}_n, ∞) is a lower
one-sided 0.5-CI for μ

Confidence Intervals: Warmups

- The reason for the “ $\geq 1 - \alpha$ ” in the definition is that $\mathbb{P}_\theta(L(\mathbf{X}) \leq \theta \leq U(\mathbf{X}))$ may not be free of θ , depending on the choices of $L(\mathbf{X})$ and $U(\mathbf{X})$
- The lower bound means we want $1 - \alpha$ confidence even in the “worst case”; equivalently,

$$\inf_{\theta \in \Theta} \mathbb{P}_\theta(L(\mathbf{X}) \leq \theta \leq U(\mathbf{X})) \geq 1 - \alpha$$

- Example 4.5:** Let $X_1, X_2, \dots, X_n \stackrel{iid}{\sim} \text{Unif}(0, \theta)$, where $\theta > 0$. Find $a \in \mathbb{R}$ such that $(aX_{(n)}, 2aX_{(n)})$ is a 95% confidence interval for θ .

$$\begin{aligned}1 - \alpha &= \mathbb{P}_\theta(\theta \in (aX_{(n)}, 2aX_{(n)})) \\&= \mathbb{P}_\theta(aX_{(n)} < \theta < 2aX_{(n)}) \\&= \mathbb{P}\left(\frac{\theta}{2a} < X_{(n)} < \frac{\theta}{a}\right) \\&= F_{X_{(n)}}\left(\frac{\theta}{a}\right) - F_{X_{(n)}}\left(\frac{\theta}{2a}\right) \\&= \left(\frac{\theta/a}{\theta}\right)^n - \left(\frac{\theta/2a}{\theta}\right)^n = \left(\frac{1}{a}\right)^n - \left(\frac{1}{2a}\right)^n \quad \Rightarrow \text{choose } a = \left(\frac{1 - 2^{-n}}{1 - \alpha}\right)^{1/n}, \quad \alpha = 0.05\end{aligned}$$

Poll Time!

$\theta \in \mathbb{R} \Rightarrow 3 < \theta < 5$ is either T or F

$$\Rightarrow P(3 < \theta < 5) \in \{0, 1\}$$

If it's 0, then it's < 0.95

If it's 1, then it's ≥ 0.95 .

We don't know!

Some Confidence Intervals Are Better Than Others

- A confidence interval is only useful when it tells us something we didn't know before collecting the data
- Example 4.6: Suppose $X_1, X_2, \dots, X_n \stackrel{iid}{\sim} \text{Bernoulli}(\theta)$, where $\theta \in (0, 1)$. Find a 100% confidence interval for θ .

$(0, 1)$. Not helpful!

$(X_1 - 1, X_2 + 1)$ Not helpful!

$(X_1 - 200, \infty)$ Not helpful!

A 100% confidence interval doesn't tell us anything!

- A good confidence interval shouldn't be any longer than necessary
- We interpret the length of the interval as a measure of how accurately the data allow us to know the true value of θ

Bringing Back Hypothesis Tests

- In Module 3, we learned about test statistics and rejection regions for hypothesis tests
- Pick some arbitrary $\theta_0 \in \Theta$, and suppose we want a level- α test of $H_0 : \theta = \theta_0$ versus $H_A : \theta \neq \theta_0$ using a test statistic $T(\mathbf{X})$
- This means finding a rejection region R_{θ_0} such that

$$\mathbb{P}_{\theta_0}(T(\mathbf{X}) \in R_{\theta_0}) \leq \alpha$$

- This is equivalent to finding an *acceptance region* $A_{\theta_0} = R_{\theta_0}^c$ such that

$$\mathbb{P}_{\theta_0}(T(\mathbf{X}) \in A_{\theta_0}) \geq 1 - \alpha$$

Confidence Intervals Via Test Statistics

- If the statement $T(\mathbf{X}) \in A_{\theta_0}$ can be manipulated into an equivalent statement of the form $L(\mathbf{X}) < \theta_0 < U(\mathbf{X})$, then

$$\mathbb{P}_{\theta_0}(L(\mathbf{X}) < \theta_0 < U(\mathbf{X})) \geq 1 - \alpha$$

- But $\theta_0 \in \Theta$ was arbitrary!
- So if we did this right, we must have

$$\mathbb{P}_\theta(L(\mathbf{X}) \leq \theta \leq U(\mathbf{X})) \geq 1 - \alpha \quad \text{for all } \theta \in \Theta$$

- This method of finding confidence intervals is called *inverting a hypothesis test*
- You can also go the other direction: start with a $(1-\alpha)$ -CI $(L(\bar{\mathbf{x}}), U(\bar{\mathbf{x}}))$, and use it to design a level- α test (under the right conditions)

Famous Examples: Z -Intervals

- **Example 4.7:** Let $X_1, X_2, \dots, X_n \stackrel{iid}{\sim} \mathcal{N}(\mu, \sigma^2)$ where $\mu \in \mathbb{R}$ and σ^2 is known. Find a $(1 - \alpha)$ -confidence interval for μ by inverting the two-sided Z -test.
Let $\mu_0 \in \mathbb{R}$. Need a level- α test & $H_0: \mu = \mu_0$ vs $H_A: \mu \neq \mu_0$.

From Example 3.15, $R_{\mu_0} = \left\{ \bar{x}_n \in \mathcal{X}^n : \left| \frac{\bar{x}_n - \mu_0}{\sigma/\sqrt{n}} \right| > z_{1-\alpha/2} \right\}$
 $\rightarrow A_{\mu_0} = \left\{ \bar{x}_n \in \mathcal{X}^n : \left| \frac{\bar{x}_n - \mu_0}{\sigma/\sqrt{n}} \right| \leq z_{1-\alpha/2} \right\}$

Then $1 - \alpha = P_\mu(\bar{x}_n \in A_\mu)$
 $= P_\mu\left(-z_{1-\alpha/2} \leq \frac{\bar{x}_n - \mu}{\sigma/\sqrt{n}} \leq z_{1-\alpha/2}\right)$
 $= P_\mu\left(-z_{1-\alpha/2} \cdot \frac{\sigma}{\sqrt{n}} - \bar{x}_n \leq -\mu \leq z_{1-\alpha/2} \cdot \frac{\sigma}{\sqrt{n}} - \bar{x}_n\right)$
 $= P_\mu\left(\bar{x}_n - z_{1-\alpha/2} \cdot \frac{\sigma}{\sqrt{n}} \leq \mu \leq \bar{x}_n + z_{1-\alpha/2} \cdot \frac{\sigma}{\sqrt{n}}\right)$

\Rightarrow Our $(1 - \alpha)$ -CI is $\left(\bar{x}_n - z_{1-\alpha/2} \cdot \frac{\sigma}{\sqrt{n}}, \bar{x}_n + z_{1-\alpha/2} \cdot \frac{\sigma}{\sqrt{n}} \right)$

"Z-interval"

Famous Examples: One-Sided Z -Intervals

- **Example 4.8:** Let $X_1, X_2, \dots, X_n \stackrel{iid}{\sim} \mathcal{N}(\mu, \sigma^2)$ where $\mu \in \mathbb{R}$ and σ^2 is known. Find a lower one-sided $(1 - \alpha)$ -confidence interval for μ by inverting an appropriate one-sided Z -test.

Example 3.16 : $R_{p_0} = \left\{ \bar{x} \in \mathcal{X}^n : \frac{\bar{x} - p}{\sqrt{\sigma^2/n}} > z_{1-\alpha} \right\}$ gave us a size- α test
 $\Rightarrow A_{p_0} = \left\{ \bar{x} \in \mathcal{X}^n : \frac{\bar{x} - p}{\sqrt{\sigma^2/n}} \leq z_{1-\alpha} \right\}$

$$\begin{aligned}1 - \alpha &= P_p \left(\frac{\bar{X}_n - p}{\sqrt{\sigma^2/n}} \leq z_{1-\alpha} \right) \\&= P_p \left(-p \geq z_{1-\alpha} \cdot \sqrt{\frac{\sigma^2}{n}} - \bar{X}_n \right) \\&= P_p \left(p \geq \bar{X}_n - z_{1-\alpha} \cdot \sqrt{\frac{\sigma^2}{n}} \right) \\&\Rightarrow \text{choose } (\bar{X}_n - z_{1-\alpha} \cdot \sqrt{\frac{\sigma^2}{n}}, \infty)\end{aligned}$$

Famous Examples: t -Intervals

- **Example 4.9:** Let $X_1, X_2, \dots, X_n \stackrel{iid}{\sim} \mathcal{N}(\mu, \sigma^2)$ where $\mu \in \mathbb{R}$ and $\sigma^2 > 0$. Find a $(1 - \alpha)$ -confidence interval for μ by inverting the two-sided t -test.

$$\text{Example 3.17: } R_{\mu_0} = \left\{ \bar{X} \in \mathcal{X}^n : \left| \frac{\bar{X} - \mu_0}{\sqrt{s^2/n}} \right| > t_{n-1, 1-\alpha/2} \right\}$$

$$\begin{aligned} \text{So } 1 - \alpha &= P_{\mu} \left(-t_{n-1, 1-\alpha/2} \leq \frac{\bar{X}_n - \mu}{\sqrt{s^2/n}} \leq t_{n-1, 1-\alpha/2} \right) \\ &= P_{\mu} \left(\bar{X}_n - t_{n-1, 1-\alpha/2} \cdot \sqrt{s^2/n} \leq \mu \leq \bar{X}_n + t_{n-1, 1-\alpha/2} \cdot \sqrt{s^2/n} \right) \end{aligned}$$

$$\text{So choose } \left(\bar{X}_n - t_{n-1, 1-\alpha/2} \cdot \sqrt{\frac{s^2}{n}}, \bar{X}_n + t_{n-1, 1-\alpha/2} \cdot \sqrt{\frac{s^2}{n}} \right)$$

" t -Interval"

Famous Examples: One-Sided t -Intervals

- **Example 4.10:** Let $X_1, X_2, \dots, X_n \stackrel{iid}{\sim} \mathcal{N}(\mu, \sigma^2)$ where $\mu \in \mathbb{R}$ and $\sigma^2 > 0$. Find an upper one-sided $(1 - \alpha)$ -confidence interval for μ by inverting an appropriate one-sided t -test.

Consider $H_0: \mu \geq \mu_0$ vs $H_A: \mu < \mu_0$. By Example 3.18,

$B_{\mu_0} = \left\{ \bar{x} \in \mathcal{X}^n : \frac{\bar{x} - \mu_0}{\sqrt{s^2/n}} \leq t_{n-1, \alpha} \right\}$ give us a size- α test.

$$\begin{aligned}\Rightarrow 1 - \alpha &= P_{\mu} \left(\frac{\bar{x} - \mu}{\sqrt{s^2/n}} \geq t_{n-1, \alpha} \right) \\ &= P_{\mu} \left(\mu \leq \bar{x}_n - t_{n-1, \alpha} \cdot \sqrt{\frac{s^2}{n}} \right)\end{aligned}$$

So choose $(-\infty, \bar{x}_n - t_{n-1, \alpha} \cdot \sqrt{\frac{s^2}{n}})$

An LRT-Based Interval

$$F_\theta(x) = 1 - e^{-(x-\theta)}$$

- **Example 4.11:** Let X_1, X_2, \dots, X_n be a random sample from a distribution with pdf $f_\theta(x) = e^{-(x-\theta)} \cdot \mathbb{1}_{x \geq \theta}$, where $\theta \in \mathbb{R}$. Find a $(1 - \alpha)$ -confidence interval for θ by inverting an LRT.

From Example 3.21, the LRT of $H_0: \theta \leq \theta_0$ vs $H_a: \theta > \theta_0$ has rejection region

$$R_{\theta_0} = \left\{ \bar{x} \in \mathcal{X}^n : X_{(1)} \geq \theta_0 - \frac{\log(c)}{n} \text{ OR } X_{(n)} < \theta_0 \right\}.$$

$$\Rightarrow A_{\theta_0} = \left\{ \bar{x} \in \mathcal{X}^n : X_{(1)} + \frac{\log(c)}{n} < \theta_0 \text{ AND } X_{(n)} \geq \theta_0 \right\} = \left\{ \bar{x} \in \mathcal{X}^n : X_{(1)} + \frac{\log(c)}{n} < \theta_0 < X_{(n)} \right\}$$

If we can choose c to make a size- α test, then $(X_{(1)} + \frac{\log(c)}{n}, X_{(n)})$ will be a $(1-\alpha)$ -CI for θ .

How? $1 - \alpha = P_\theta \left(X_{(1)} \leq \theta - \frac{\log(c)}{n} \wedge X_{(n)} \geq \theta_0 \right)$
always true!

$$\begin{aligned} &= 1 - \left(1 - F_\theta \left(\theta - \frac{\log(c)}{n} \right) \right)^n \\ &= 1 - \left(1 - \left(1 + \exp(-[\theta - \frac{\log(c)}{n} - \theta]) \right) \right)^n \end{aligned}$$

$$= 1 - c$$

$$\Rightarrow \text{choose } c = \alpha. \text{ So } (X_{(1)} + \frac{\log(c)}{n}, X_{(n)}) \text{ is a } (1-\alpha)\text{-CI for } \theta.$$

Functions of the Data and the Parameter

- In constructing our confidence intervals, we've often encountered statements that look like

$$\mathbb{P}_\theta (a < Q(\mathbf{X}, \theta) < b) \geq 1 - \alpha,$$

where $Q : \mathcal{X}^n \times \Theta \rightarrow \mathbb{R}$ is a function of the data \mathbf{X} and the parameter θ , and a, b are constants

- We were able to choose those constants a and b because we knew exactly what the distribution of $Q(\mathbf{X}, \theta)$ was

- We could then “invert” the statement $a < Q(\mathbf{X}, \theta) < b$ to produce a confidence interval for θ

$$\text{Example 4.12: } N(\mu, \sigma^2), \sigma^2 \text{ known: } \mathbb{P}_\mu \left(-2 + z_{\alpha/2} < \frac{\bar{X}_n - \mu}{\sqrt{\sigma^2/n}} < z_{1-\alpha/2} \right) = 1 - \alpha$$

$\stackrel{= Q(\bar{X}, \mu) \sim N(0, 1) \text{ under } \mu}{\sim}$

$$\text{Example 4.13: } \text{Unif}(0, \Theta) : \mathbb{P}_\theta \left(\frac{1}{2\alpha} \leq \frac{X_{(n)}}{\theta} \leq \frac{1}{\alpha} \right) = 1 - \alpha \text{ where } \alpha \text{ chosen as before}$$

$\stackrel{= Q(\bar{X}, \theta), \text{ distribution free of } \theta}{\sim}$

Pivotal Quantities

- The key in these examples was that the *distribution* of $Q(\mathbf{X}, \theta)$ is free of θ
- **Definition 4.4:** A random variable $Q(\mathbf{X}, \theta)$ is a **pivotal quantity** (or **pivot**) for θ if its distribution is free of θ .
- So if $\mathbf{X} \sim f_{\theta_1}$ and $\mathbf{Y} \sim f_{\theta_2}$, then $Q(\mathbf{X}, \theta_1) \stackrel{d}{=} Q(\mathbf{Y}, \theta_2)$
- Every ancillary statistic is a pivotal quantity
- Example 4.14: $N(\mu, \sigma^2)$, σ^2 known: $P_y\left(-2 + \frac{\bar{X}_n - \mu}{\sqrt{\sigma^2/n}} < z_{1-\alpha}\right) = 1 - \alpha$
- Example 4.15: $\text{Exp}(\lambda)$: $Q(\bar{X}, \lambda) = \frac{\bar{X}_1}{\lambda} \sim \text{Exp}(1)$ is pivotal.

Poll Time!

Confidence Intervals from Pivotal Quantities

- **Example 4.16:** Let $X_1, X_2, \dots, X_n \stackrel{iid}{\sim} \text{Exp}(\lambda)$, $\lambda > 0$. Show that $Q(\mathbf{X}, \lambda) = 2\lambda \sum_{i=1}^n X_i$ is a pivotal quantity, and use it to find a $1 - \alpha$ confidence interval for λ .

Use mgfs! $M_{\sum X_i}(t) = \left(\frac{\lambda}{\lambda-t}\right)^n, t < \lambda$

$$\Rightarrow M_{2\lambda \sum X_i}(t) = \left(\frac{\lambda}{\lambda-2\lambda t}\right)^n = (1-2t)^{-n} \Rightarrow Q(\bar{X}, \lambda) \sim \chi^2_{(2n)} \text{ free of } \lambda!$$

So pivotal.

Set $1 - \alpha = P(a < 2\lambda \sum X_i < b)$ for some $a, b \in \mathbb{R}$

where a and b satisfy $1 - \alpha = F_{\chi^2_{(2n)}}(b) - F_{\chi^2_{(2n)}}(a)$.

Can pick, for example, $a = 0 \Rightarrow b = \chi^2_{(2n), 1-\alpha}$.

Then $1 - \alpha = P(0 < \lambda < \frac{\chi^2_{(2n), 1-\alpha}}{2 \sum X_i})$

$$\Rightarrow \text{choose } (0, \frac{\chi^2_{(2n), 1-\alpha}}{2 \sum X_i})$$

Finding Pivotal Quantities

- There's no all-purpose strategy to finding pivotal quantities, but there's a neat trick that sometimes lets us pull one out of the pdf of a statistic $T(\mathbf{X})$
- **Theorem 4.1:** Suppose that $T(\mathbf{X}) \sim f_\theta$ is univariate and continuous, such that the pdf can be expressed as

$$f_\theta(t) = g(Q(t, \theta)) \cdot \left| \frac{\partial}{\partial t} Q(t, \theta) \right|$$

for some function $g(\cdot)$ which is free of θ and some function $Q(t, \theta)$ which is continuously differentiable and one-to-one as a function of t (i.e., with θ fixed). Then $Q(T(\mathbf{X}), \theta)$ is a pivot.

Fix $\theta \in \mathbb{R}$ and let $h_\theta(q)$ be the pdf of $Q(T(\mathbf{X}), \theta)$. We'll just write $Q(T(\mathbf{x}))$. Let
Proof. $Q^{-1}(q)$ be the functional inverse of $Q(t)$. Then

$$\begin{aligned} h_\theta(q) &= f_\theta(Q^{-1}(q)) \cdot \left| \frac{\partial}{\partial q} Q^{-1}(q) \right| \\ &= f_\theta(Q^{-1}(q)) \cdot \left| \frac{\partial}{\partial t} Q(t) \Big|_{t=Q^{-1}(q)} \right|^{-1} \text{ by the inverse function theorem} \\ &= g(Q(Q^{-1}(q))) \cdot \left| \frac{\partial}{\partial t} Q(t) \Big|_{t=Q^{-1}(q)} \right| \cdot \left| \frac{\partial}{\partial t} Q(t) \Big|_{t=Q^{-1}(q)} \right|^{-1} = g(q) \text{ which is free of } \theta. \quad \square \end{aligned}$$

Finding Pivotal Quantities: Examples

- **Example 4.17:** Let $X_1, X_2, \dots, X_n \stackrel{iid}{\sim} \text{Unif}(0, \theta)$ where $\theta > 0$. Find a pivotal quantity based on $T(\mathbf{X}) = X_{(n)}$, and use it to construct a $1 - \alpha$ confidence interval for θ .

The pdf of $T(\mathbf{X}) = X_{(n)}$ is

$$\begin{aligned} & n \cdot f_\theta(t) \cdot F_\theta(t)^{n-1} \\ &= n \cdot \frac{1}{\theta} \cdot \left(\frac{t}{\theta}\right)^{n-1} \\ &= \frac{nt^{n-1}}{\theta^n} \\ &= 1 \cdot \left| \frac{\partial}{\partial t} \frac{t^n}{\theta^n} \right| \\ &\text{e.g. } Q(t, \theta) \end{aligned}$$

By Theorem 4.1,

$$Q(X_{(n)}, \theta) = \frac{X_{(n)}}{\theta^n}$$
 is a pivotal quantity.

What's its distribution? $P\left(\frac{X_{(n)}}{\theta^n} \leq x\right)$

$$\begin{aligned} &= P(X_{(n)} \leq \theta x^{\frac{1}{n}}) \\ &= F_\theta(\theta x^{\frac{1}{n}})^n \\ &= \left(\frac{\theta x^{\frac{1}{n}}}{\theta}\right)^n \\ &= x \end{aligned}$$

So $Q(X_{(n)}, \theta) \sim \text{Unif}(0, 1)$.

Choose a, b s.t. $P(a \leq \frac{X_{(n)}}{\theta^n} \leq b) = 1 - \alpha$

For example, $a = \alpha/2$, $b = 1 - \alpha/2$ works.

$$\begin{aligned} 1 - \alpha &= P\left(\frac{\alpha/2}{\theta} \leq \frac{X_{(n)}}{\theta^n} \leq \frac{1 - \alpha/2}{\theta}\right) \\ &= P\left(\frac{X_{(n)}}{1 - \alpha/2} \leq \theta^n \leq \frac{X_{(n)}}{\alpha/2}\right) \end{aligned}$$

⇒ Choose $\left(\frac{X_{(n)}}{(1 - \alpha/2)^{1/n}}, \frac{X_{(n)}}{(\alpha/2)^{1/n}}\right)$.

Finding Pivotal Quantities: Examples

- **Example 4.18:** Let $X \sim f_\theta(x) = \frac{2(\theta-x)}{\theta^2} \cdot \mathbb{1}_{0 \leq x \leq \theta}$, where $\theta > 0$. Find a pivotal quantity based on X , and use it to construct a $1 - \alpha$ confidence interval for θ .

Observe if $Q(x, \theta) = \frac{\theta-x}{\theta}$, then $f_\theta(x) = g(Q(x, \theta)) \cdot \left| \frac{\partial}{\partial x} Q(x, \theta) \right|$ where $g(x) = 2x$.

By Theorem 4.1, $Q(x, \theta) = \frac{\theta-x}{\theta}$ is a pivotal quantity, with distribution...?

$$P\left(\frac{\theta-x}{\theta} \approx x\right)$$

$$= P(X \geq (1-x)\theta)$$

$$= \int_{(1-x)\theta}^\theta \frac{2(\theta-t)}{\theta^2} dt$$

$$= x^2, \quad x \in (0, 1).$$

Plenty of choices for a, b in $1-\alpha = P(a < \frac{\theta-x}{\theta} < b) = b^2 - a^2$

If we choose $a=0$, then $b=\sqrt{1-\alpha}$. Therefore,

$$1-\alpha = P(0 < \frac{\theta-x}{\theta} < \sqrt{1-\alpha})$$

$$= P(X < \theta < \frac{x}{1-\sqrt{1-\alpha}})$$

$$\Rightarrow \text{Choose } \left(X, \frac{x}{1-\sqrt{1-\alpha}}\right).$$

$$\left. \begin{aligned} 0 &< 1 - \frac{x}{\theta} < \sqrt{1-\alpha} \\ -1 &< -\frac{x}{\theta} < \sqrt{1-\alpha} - 1 \\ -1 &> -\frac{\theta}{x} > \frac{1}{\sqrt{1-\alpha}-1} \\ -x &> -\theta > \frac{x}{\sqrt{1-\alpha}-1} \\ x &< \theta < \frac{x}{1-\sqrt{1-\alpha}} \end{aligned} \right\}$$

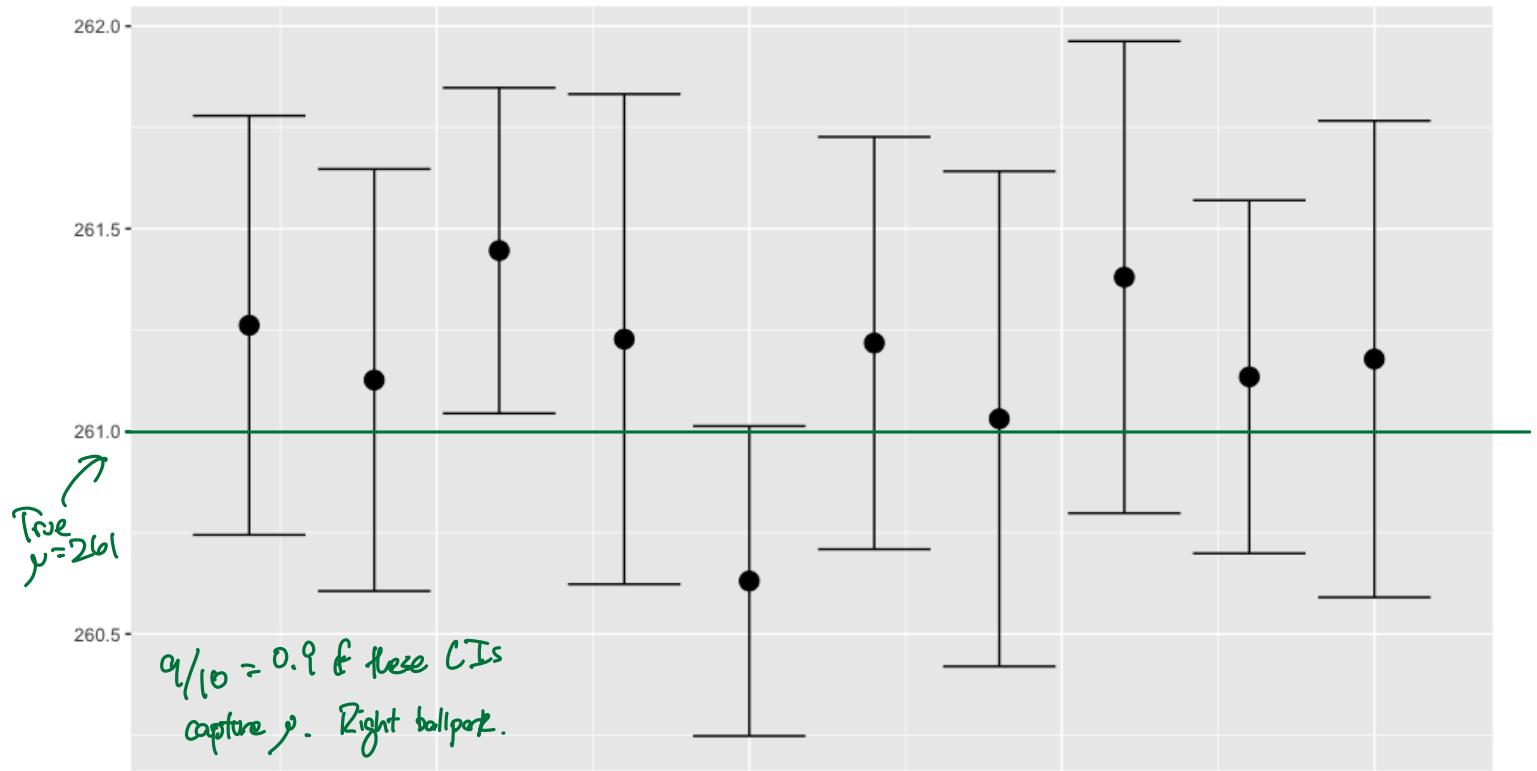
Confidence Intervals: Interpretations

- Confidence intervals are almost as widely misinterpreted as p -values
- Suppose that in a published scientific study, you see a stated 95% confidence interval such as $(0.932, 1.452)$
- How do you interpret this correctly?
- Should we be surprised if we try and reproduce the study and calculate a 95% confidence interval of $(0.824, 1.734)$?
- What about $(-0.232, 1.440)$?

Poll Time!

Confidence Intervals: Interpretations

- Here are ten observed 95% Z -intervals for μ calculated from ten random samples of size $n = 15$ from a $\mathcal{N}(\mu, 1)$ distribution:



Questioning Our Assumptions...

- All of the theory we've done up to this point has depended on the assumption of an underlying statistical model
- When we say “Suppose $X_1, X_2, \dots, X_n \stackrel{iid}{\sim} f_\theta \dots$ ”, we’re assuming the data follows one of the distributions in the parametric family $\{f_\theta : \theta \in \Theta\}$ and only the parameter θ is unknown
- If we get the statistical model wrong, then any inferences we make about θ are likely to be completely invalid
- So it’s extremely important to be able to check that statistical model assumption

Nothing Is Certain

- Of course, we can't *know* for sure that a model is correct
- Unless we generate the data, but then what's the point?
- But we can perform checks that give us confidence in our assumptions
- This is called *model checking*
- We will study two kinds of model checks: visual diagnostics and goodness-of-fit tests

Histograms: Preliminaries

- Suppose we have iid data X_1, X_2, \dots, X_n , which we hypothesize are distributed according to a cdf F_θ
- Let's group the range of the data into bins $[h_1, h_2], (h_2, h_3], \dots, (h_{m-1}, h_m]$
- By the law of large numbers,

$$\frac{1}{n} \sum_{i=1}^n \mathbb{1}_{X_i \in (h_j, h_{j+1}]} \xrightarrow{p} \mathbb{P}_\theta(X_i \in (h_j, h_{j+1}])$$

$= \mathbb{P}_\theta(h_j < X_i \leq h_{j+1})$
 $= F_\theta(h_{j+1}) - F_\theta(h_j)$

- So if n is large and we're correct about F_X , then

$$\frac{1}{n} \sum_{i=1}^n \mathbb{1}_{X_i \in (h_j, h_{j+1}]} \approx F_\theta(h_{j+1}) - F_\theta(h_j)$$

The Histogram Density Function

- If, in addition, we believe F_θ is continuous with pdf f_θ , then there exists $h^* \in (h_j, h_{j+1})$ such that

$$\frac{1}{n(h_{j+1} - h_j)} \sum_{i=1}^n \mathbb{1}_{X_i \in (h_j, h_{j+1}]} \approx \frac{F_\theta(h_{j+1}) - F_\theta(h_j)}{h_{j+1} - h_j} = f_\theta(h^*)$$

by the mean value theorem!

- **Definition 4.5:** Given data X_1, \dots, X_n and a partition $h_1 < h_2 < \dots < h_m$, the **density histogram function** is defined as

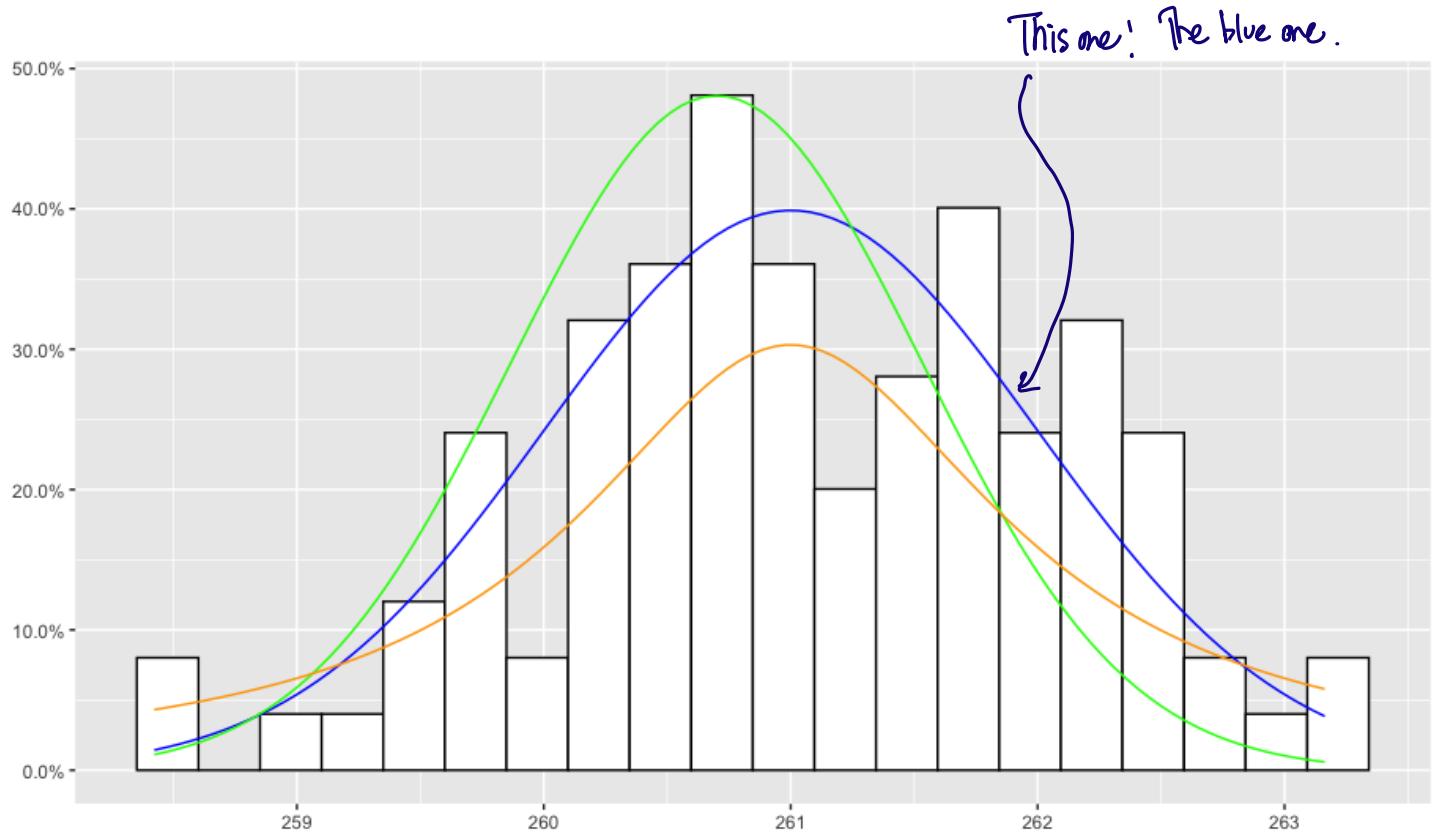
$$\hat{f}_n(t) = \begin{cases} \frac{1}{n(h_{j+1} - h_j)} \sum_{i=1}^n \mathbb{1}_{X_i \in (h_j, h_{j+1}]}, & t \in (h_j, h_{j+1}] \\ 0, & \text{otherwise} \end{cases}$$

Histograms

- If we believe that our observed data x_1, \dots, x_n are realizations of $X_1, X_2, \dots, X_n \stackrel{iid}{\sim} f_\theta$, then the observed $\hat{f}_n(t)$ should look like a “discretized” version of $f_\theta(t)$
- ...and the resemblance should improve as n gets larger and each bin size $h_{j+1} - h_j$ gets smaller
- **Definition 4.6:** A plot of a density histogram function $\hat{f}_n(t)$ with vertical lines drawn at each h_j is called a **histogram**. A histogram where each bin width $h_{j+1} - h_j = 1$ is called a **relative frequency plot**.

Histograms: An Example

- Here's a histogram ($n = 100$) overlaid with three hypothesized pdfs; which is more likely to have generated the data?



Poll Time!

Empirical CDFs

- We might prefer to deal with the cdf F_{θ} instead
- If we fix any $t \in \mathbb{R}$, then the law of large numbers says that

$$\frac{1}{n} \sum_{i=1}^n \mathbb{1}_{X_i \leq t} \xrightarrow{p} \mathbb{P}_{\theta}(X_i \leq t)$$

- So if n is large and we're correct about F_{θ} , then

$$\frac{1}{n} \sum_{i=1}^n \mathbb{1}_{X_i \leq t} \approx F_{\theta}(t)$$

- **Definition 4.7:** Given observations X_1, \dots, X_n , the **empirical distribution function (ecdf)** is defined as

$$\hat{F}_n(t) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{X_i \leq t}$$

Empirical CDFs Are Nice

- If we believe that our observed data x_1, \dots, x_n are realizations of $X_1, X_2, \dots, X_n \stackrel{iid}{\sim} F_\theta$, then $\hat{F}_n(t)$ should look like $F_\theta(t)$
- In fact, a famous result called the **Glivenko-Cantelli theorem** says that if F_X really is the true cdf, then $\hat{F}_n(t) \rightarrow F_\theta(t)$ as $n \rightarrow \infty$ in a *much* stronger sense than convergence in probability
"Uniformly almost surely" $P_\theta \left(\sup_{t \in \mathbb{R}} |\hat{F}_n(t) - F_\theta(t)| > \varepsilon \right) \rightsquigarrow 0$
- **Theorem 4.2:** For any fixed $t \in \mathbb{R}$, the ecdf $\hat{F}_n(t)$ is an unbiased estimator of $F_\theta(t)$, and it has a lower variance than $\mathbb{1}_{X_i \leq t}$.

Proof.

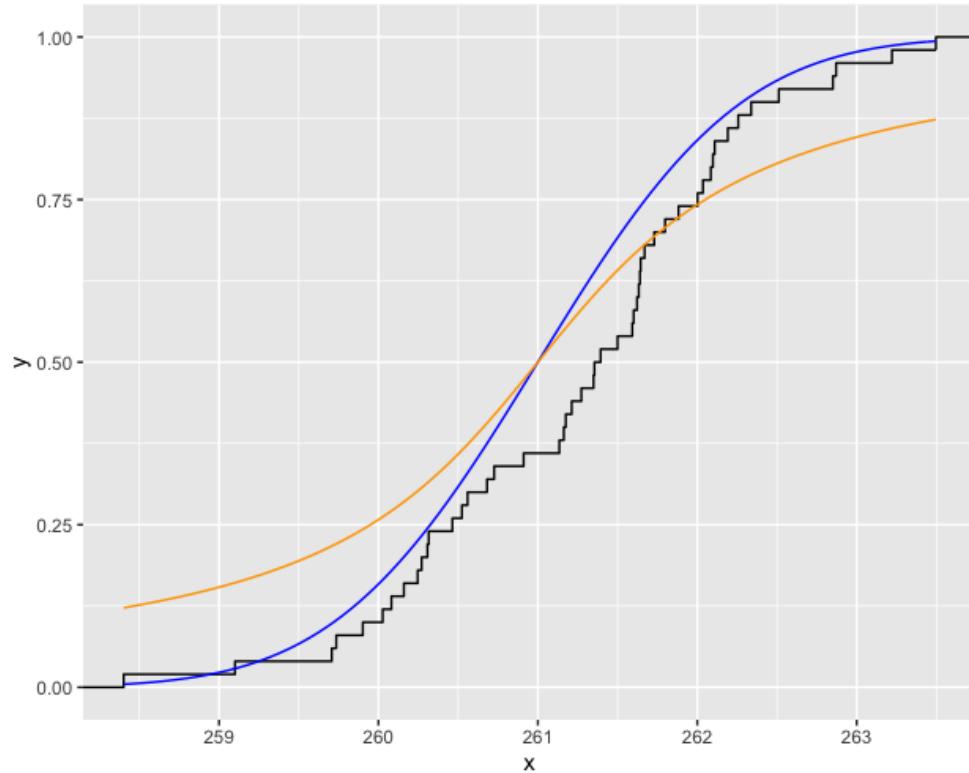
$$\begin{aligned}\mathbb{1}_{X_i \leq t} &\sim \text{Bernoulli}(P_\theta(\mathbb{1}_{X_i \leq t} = 1)) \\ &= \text{Bernoulli}(P_\theta(X_i \leq t)) \\ &= \text{Bernoulli}(F_\theta(t))\end{aligned}$$

$$\mathbb{E}_\theta[\hat{F}_n(t)] = \frac{1}{n} \sum_{i=1}^n \mathbb{E}[\mathbb{1}_{X_i \leq t}] = F_\theta(t)$$

$$\text{Var}_\theta(\hat{F}_n(t)) = \frac{1}{n} \text{Var}_\theta(\mathbb{1}_{X_i \leq t}) = \frac{1}{n} F_\theta(t) \cdot (1 - F_\theta(t)) \leq F_\theta(t) \cdot (1 - F_\theta(t)) = \text{Var}_\theta(\mathbb{1}_{X_i \leq t}). \quad \square$$

Empirical CDFs: An Example

- Here's an ecdf ($n = 50$) overlaid with two hypothesized cdfs; which is more likely to have generated the data?



Poll Time!

$X_1, \dots, X_n \stackrel{iid}{\sim} N(0, 1)$.

What's $E[\hat{F}_n(0)]$?

$$\begin{aligned} E[\hat{F}_n(0)] &= F(0) \\ &= \underline{\Phi(0)} \\ &= \frac{1}{2} \end{aligned}$$

Bringing Back Ancillarity and Sufficiency

- We know from Module 1 that if $\mathbf{X} \sim f_\theta$, the distribution of an ancillary statistic $S(\mathbf{X})$ is free of θ
- But if we've gotten the model $\{f_\theta : \theta \in \Theta\}$ wrong, $S(\mathbf{X})$ could very well depend on $\theta!$
(or some unknown parameter in the "true" model)
- So some ancillary statistics provide a model check: if our realization $S(\mathbf{x})$ is "surprising", we have evidence against the model being true
- Similarly, if $T(\mathbf{X})$ is sufficient for θ , then $\mathbf{X} | T(\mathbf{X}) = t$ shouldn't depend on θ
- This leads to the idea of **residual analysis**
- Loosely speaking, residuals are based on the information in the data that is left over after we have fit the model
(actually no formal definition of "residual"!)

Residual Plots

- **Example 4.19:** Let X_1, \dots, X_n be a random sample from a suspected $\mathcal{N}(\mu, \sigma^2)$ distribution, where $\mu \in \mathbb{R}$ and σ^2 is known. If we're correct, then $R(\mathbf{X}) = (X_1 - \bar{X}, \dots, X_n - \bar{X})$ is ancillary for μ , because

$$X_i - \bar{X} \sim \mathcal{N}\left(0, \frac{n-1}{n}\sigma^2\right), \quad i = 1, \dots, n$$

and therefore **standardized residuals**

Assignment 1 Q17

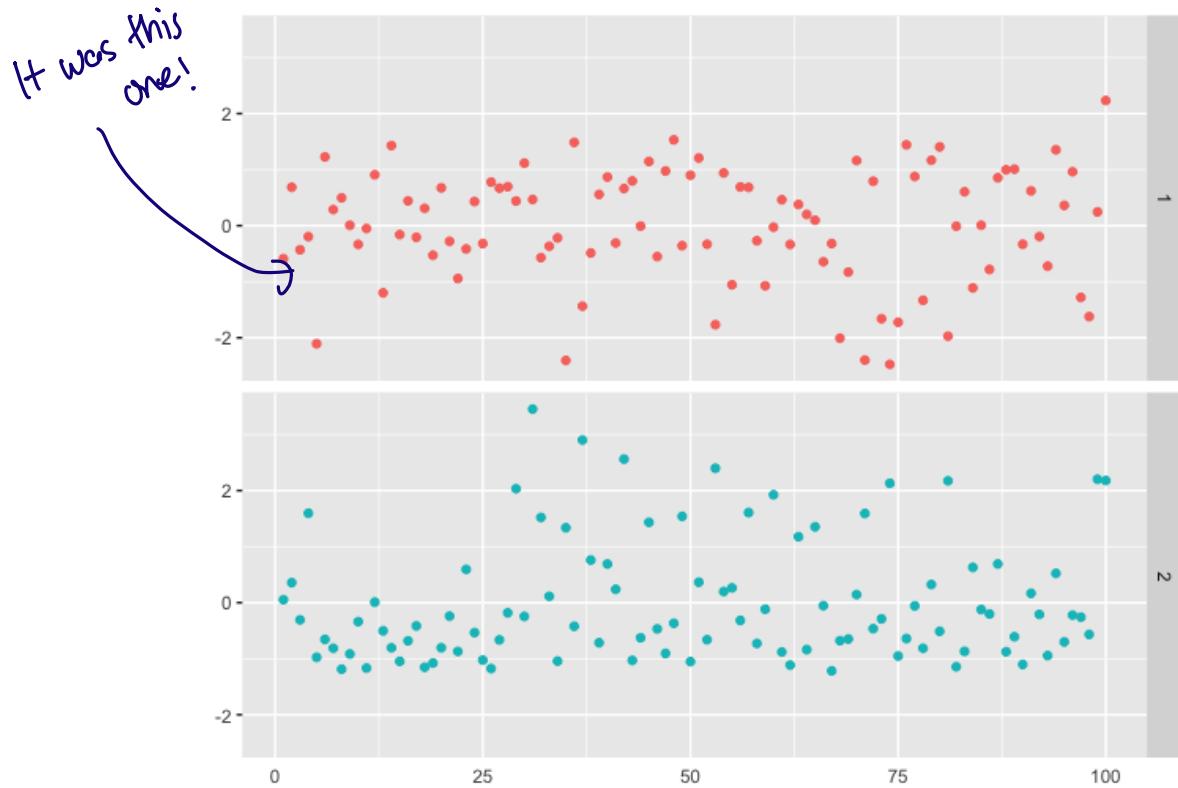
$$R_i^*(\mathbf{X}) := \frac{X_i - \bar{X}}{\sqrt{\frac{n-1}{n}\sigma^2}} \sim \mathcal{N}(0, 1).$$

So if we're right about $\mathcal{N}(\mu, \sigma^2)$, then a scatterplot of the residuals shouldn't exhibit any discernable pattern, and should mostly stay within $(-3, 3)$

If σ^2 is unknown, can swap with S^2 ,
whence $R_i^*(\bar{x}) \sim t_{n-1}$

Residual Plots

- **Example 4.20:** Here are two standardized residual plots constructed from two samples ($n = 100$) with equal variances σ^2 ; which looks more like it came from a $\mathcal{N}(\mu, \sigma^2)$ distribution?

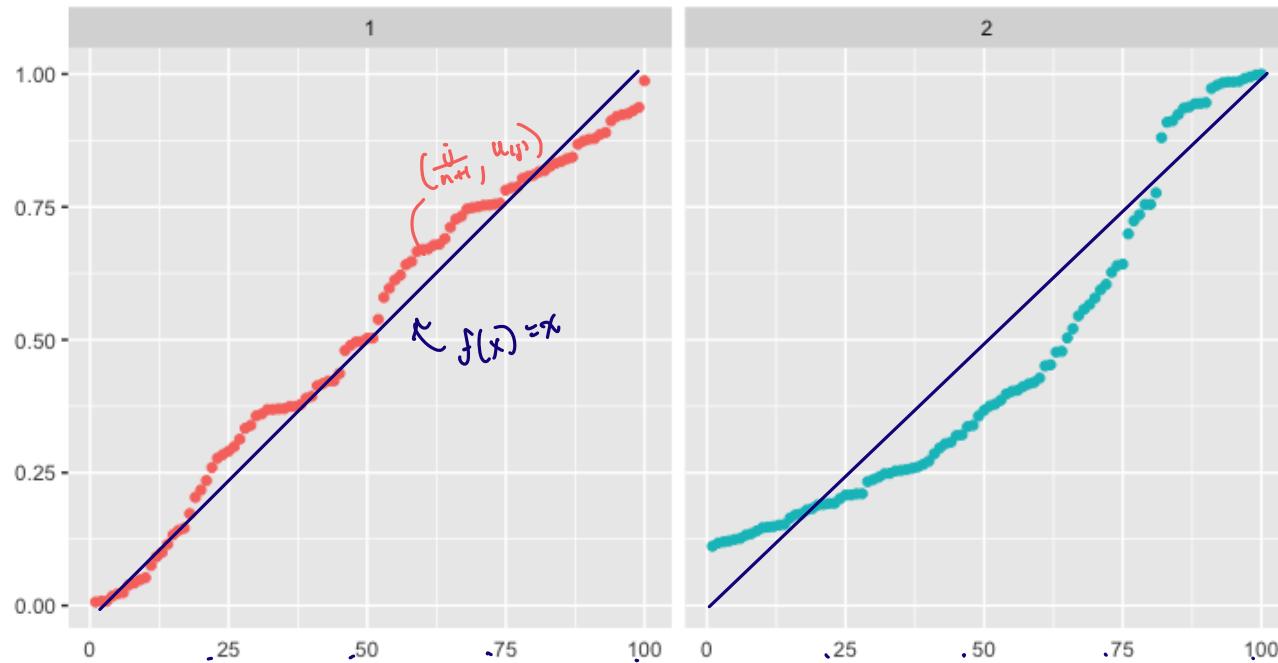


Probability Plots

- Probability plots extend this idea
- We need a fundamental result of probability theory first
- Theorem 4.3 (**Probability integral transform**): Let X be a continuous random variable with cdf $F_\theta(x)$, and let $U = F_\theta(X)$. Then $U \sim \text{Unif}(0, 1)$.
(STA257)
- The order statistics of $U_1, \dots, U_n \stackrel{iid}{\sim} \text{Unif}(0, 1)$ follow a Beta distribution: $U_{(j)} \sim \text{Beta}(j, n - j + 1)$, and so $\mathbb{E}[U_{(j)}] = \frac{j}{n+1}$ Assignment 0.
- This suggests a recipe: If we hypothesize $X_1, \dots, X_n \sim F_\theta$, then
plot $F_\theta(X_{(j)})$ versus $\frac{j}{n+1}$, $j=1, \dots, n$.
= $[F_\theta(X)]_{(j)}$ since cdfs are increasing
= $U_{(j)}$ if F_θ is correct
If it doesn't look like a straight line,
we should question F_θ .

Probability Plots

- **Example 4.21:** Here are two probability plots constructed from the standardized residuals as before, using $F_\theta(x) = \Phi(x)$. Which looks more like it came from a $\mathcal{N}(\mu, \sigma^2)$ distribution?



Q-Q Plots

- We could also go in the other direction by looking at the quantiles
- **Definition 4.8:** Let X be a random variable with cdf F_θ . The **inverse cdf** (or the **quantile function**) is defined by $F_\theta^{-1}(t) = \inf\{x : F_\theta(x) \geq t\}$.
 ↗ "generalized inverse"
- When X is continuous, the inverse cdf is simply the functional inverse of F_θ
- There are plenty of software algorithms that can estimate the quantiles from a sample x_1, \dots, x_n
- If we hypothesize $X_1, \dots, X_n \sim F_\theta$ and we can compute F_θ^{-1} , then we have another recipe for model checking:

Plot the observed quantiles versus the theoretical ones!

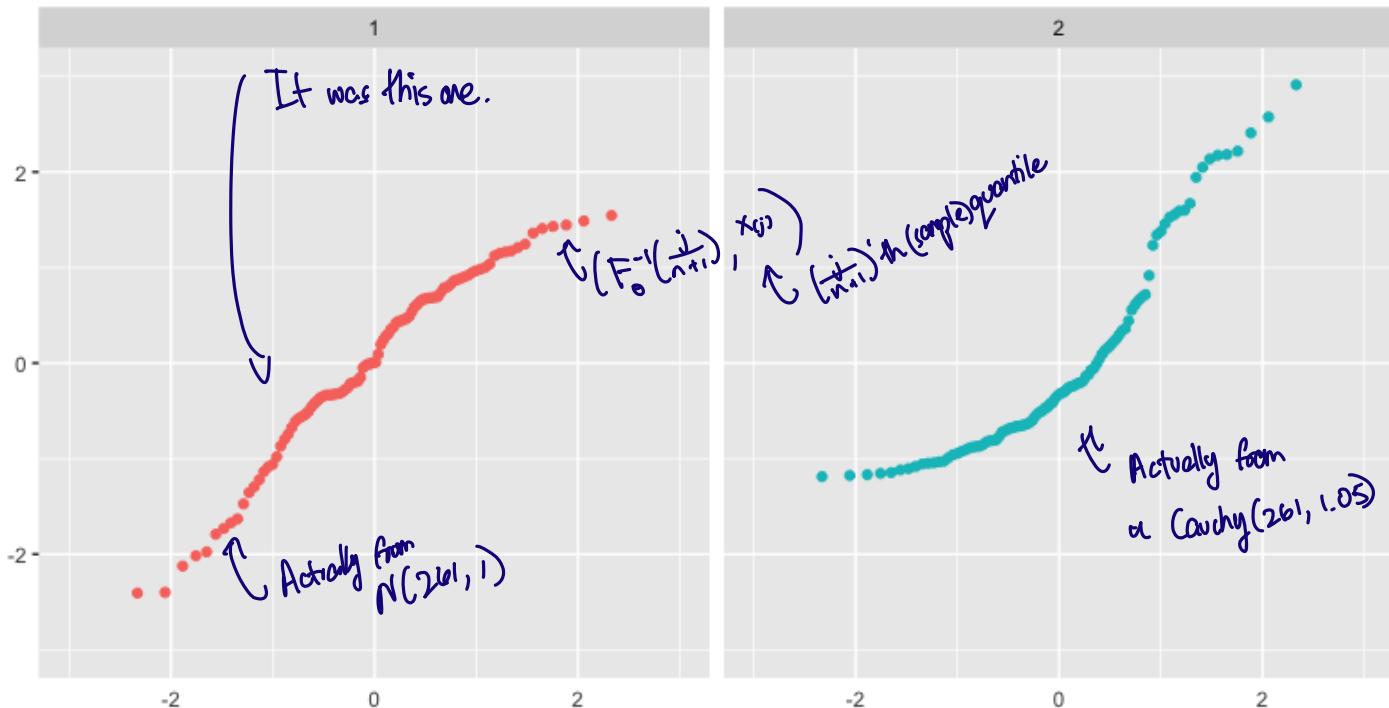
If it doesn't look like $y=x$, we should question F_θ .

Q-Q Plots

By far, the most popular use is for $F_\theta = \Phi(\cdot)$.

Want to see if the $N(0,1)$ distribution does a good job of capturing the EXTREME observations.

- Example 4.22: Here are two Q-Q plots constructed from the standardized residuals as before, using $F_\theta^{-1}(x) = \Phi^{-1}(x)$. Which looks more like it came from a $\mathcal{N}(\mu, \sigma^2)$ distribution?



Q-Q Plots

- Q-Q plots are most frequently used as a test for Normality
- But technically there's no reason why we can't use them to compare *any* two distributions, observed or hypothesized
- ...provided we can actually compute (or estimate) their quantiles, of course
- Q-Q plots are particularly useful when we want to see how the “outliers” in our data compare to the extreme values predicted by the tails of a hypothesized distribution

Goodness of Fit Tests

- Instead of using visual diagnostics, we can use hypothesis tests as model checks
- This time, the null hypothesis H_0 is that the model $\{f_\theta : \theta \in \Theta\}$ for our data is “correct”
 $H_0:$ the data is Normally distributed
 $H_0:$ the observations are independent
 $H_0:$ two distributions generating two different samples are independent
- As usual, we have a test statistic $T(\mathbf{X})$ that follows some known distribution under H_0
- An observed value $T(\mathbf{x})$ which is very unlikely under H_0 (as quantified by a p -value) provides evidence that the model is wrong
- Such hypothesis tests are called **goodness of fit tests**

Towards a Foundational Test

- Suppose we observe iid random variables W_1, W_2, \dots, W_n taking values in sample space $\mathcal{X} = \{1, 2, \dots, k\}$, which we think of as *labels* or *categories*
- We want to test whether the W_i 's are distributed according to some hypothesized probability measure \mathbb{P}_0 on \mathcal{X}
- Let $X_i = \sum_{j=1}^n \mathbb{1}_{W_j=i}$ and let $p_i = \mathbb{P}_0(\{i\})$ so that under H_0 ,

$$(X_1, X_2, \dots, X_k) \sim \text{Multinomial}(n, p_1, \dots, p_k)$$

$$X_i = \sum_{j=1}^n Y_{ij}, \quad Y_{ij} \sim \text{Bernoulli}(p_i)$$

- Now define

$$R_i = \frac{X_i - \mathbb{E}[X_i]}{\sqrt{\text{Var}(X_i)}} \stackrel{H_0}{=} \frac{X_i - np_i}{\sqrt{np_i(1-p_i)}}$$

- Since $R_i \xrightarrow{d} \mathcal{N}(0, 1)$ under H_0 , it's tempting to think $\sum_{i=1}^k R_i^2 \xrightarrow{d} \chi_{(k)}^2$, but that's not true! They're not independent!

For the multinomial,
we need $\sum_{i=1}^k X_i = n$

Pearson's Chi-Squared Test

- Instead, we have the following result
- Theorem 4.4: If $(X_1, X_2, \dots, X_k) \sim \text{Multinomial}(n, p_1, \dots, p_k)$, then

$$\sum_{i=1}^k (1 - p_i) R_i^2 = \sum_{i=1}^k \frac{(X_i - np_i)^2}{np_i} \xrightarrow{d} \chi_{(k-1)}^2.$$

Asymptotic distribution under H_0

- The statistic $\chi^2(\mathbf{X}) = \sum_{i=1}^k \frac{(X_i - np_i)^2}{np_i}$ is called a **chi-square statistic**, and it's almost always written as

$$\chi^2 = \sum_{i=1}^k \frac{(O_i - E_i)^2}{E_i}$$

O_i = "observed" i
E_i = "expected" i

- The chi-squared test is an *approximate test*, because the test statistic only has the $\chi_{(k-1)}^2$ distribution in the limit (more on this in Module 5)

A Famous Example: Fisher and Mendel's Pea Data

- Mendelian laws of inheritance establish relative frequencies of dominant and recessive phenotypes across new generations
- Gregor Mendel was known for his pioneering experiments with pea plants in the mid-1800s
- If you cross smooth, yellow male peas with wrinkled, green female peas, Mendelian inheritance predicts these relative frequencies of traits in the progeny:

	Yellow	Green
Smooth	$\frac{9}{16}$	$\frac{3}{16}$
Wrinkled	$\frac{3}{16}$	$\frac{1}{16}$

A Famous Example: Fisher and Mendel's Pea Data

- Mendel crossed 556 such pairs of peas together and recorded the following counts:

		<u>OBSERVED</u>		<u>(EXPECTED)</u>	
		Yellow	Green	Yellow	Green
		Smooth	Wrinkled	Smooth	Wrinkled
Smooth		315	108	312.75	104.25
Wrinkled		102	31	104.25	34.75

- Example 4.23: Do these results support the predicted frequencies?

$$\chi^2 = \frac{(315 - 312.75)^2}{312.75} + \frac{(108 - 104.25)^2}{104.25} + \frac{(102 - 104.25)^2}{104.25} + \frac{(31 - 34.75)^2}{34.75} \approx 0.6043$$

Our p-value is $p(\chi^2) = P(\chi_{(3)}^2 \geq 0.6043)$
 $= 1 - P(\chi_{(3)}^2 < 0.6043)$
 ≈ 0.895

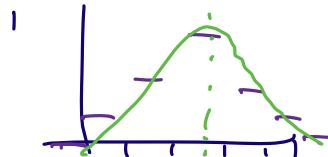
Check out the "Mendelian paradox"

So we fail to reject H_0 .

Extending the Chi-Squared Test

- What if our hypothesized distribution is not categorical, but quantitative?

- We can still use a chi-squared test – but how?



- The trick is to partition the sample space \mathcal{X} into k disjoint subsets $\mathcal{X}_1, \dots, \mathcal{X}_k$, and let $X_i = \sum_{j=1}^n \mathbb{1}_{W_j \in \mathcal{X}_i}$ and $p_i = \mathbb{P}_0(\mathcal{X}_i)$

Eg: $\mathcal{X} = \mathbb{R}$. Maybe $\mathcal{X}_1 = (-\infty, -3]$, $\mathcal{X}_2 = [-3, 3]$, $\mathcal{X}_3 = (3, 27]$, $\mathcal{X}_4 = (27, \infty)$

- The finer our partition, the better we can distinguish between distributions
- But of course, we need to increase our sample size accordingly so that each category gets sufficiently “filled” with data

Guideline: each \mathcal{X}_i should have at least 5 observations before doing this

If you have 0 observations in \mathcal{X}_i , then you can't hypothesize anything other than $p_i = 0$

A Famous Example: Testing for Uniformity

- There are many reasons why we might want to test whether some data U_1, \dots, U_n arises from a $\text{Unif}(0, 1)$ distribution
 - * Probability plot : use probability integral transform to make $U_1, \dots, U_n \stackrel{\text{iid}}{\sim} \text{Unif}(0, 1)$ under $H_0: F_\theta$. Basically quantitative version of visual probability plot check
 - * Random number generation: when simulating random data from some distribution, we need to start with $U_1, \dots, U_n \stackrel{\text{iid}}{\sim} \text{Unif}(0, 1)$ and then transform them. Can't truly generate random numbers, but we can make a sequence "look" random enough.
- We can use a chi-squared test for this by binning $[0, 1]$ into k equal-sized sub-intervals of length $1/k$, and letting $X_i = \sum_{j=1}^n \mathbb{1}_{U_j \in (\frac{i-1}{k}, \frac{i}{k}]}$ and $p_i = \frac{1}{k}$
 $= P_0(U_j \in (\frac{i-1}{k}, \frac{i}{k}]).$

A Famous Example: Testing for Uniformity

- **Example 4.24:** How can we test whether an iid sequence U_1, U_2, \dots, U_n arises from a $\text{Unif}(0, 1)$ distribution using 10 categories?

Partition $[0, 1]$ into $\left[0, \frac{1}{10}\right], \left(\frac{1}{10}, \frac{2}{10}\right], \dots, \left(\frac{9}{10}, 1\right]$

$$\text{let } X_i = \sum_{j=1}^n \mathbb{1}_{U_j \in \left[\frac{i-1}{10}, \frac{i}{10}\right]}, \quad i = 1, \dots, 10$$

OR let $V_i = \lceil 10U_i \rceil$, so V_1, \dots, V_n iid $\text{Unif}\{\{1, 2, \dots, 10\}\}$ under H_0 .

$$\text{and let } X_i = \sum_{j=1}^n \mathbb{1}_{V_j = i}$$

Then carry out a χ^2 goodness of fit test with $\chi^2 = \sum_{i=1}^{10} \frac{(X_i - \gamma_{10})^2}{\gamma_{10}} \stackrel{n}{\approx} \chi^2_{(10)}$.

Note: this is known to be a low-powered test. \therefore

There are way better randomness tests out there! The "diehard tests" are standard

Other Goodness of Fit Tests

- Pearson's chi-squared isn't the only goodness of fit test out there; there are countless others
- Many apply to one particular parametric family specifically

Eg: Normality testing: Shapiro-Wilk, Anderson-Darling, Jarque-Bera, --

- Others are completely generic and test for equality between *any* two distributions

Eg: Kolmogorov-Smirnov, Cramer-von Mises by far the most popular

- These latter tests allow us to compare an ecdf \hat{F}_n to a hypothesized cdf F_θ

Very helpful! Basically a quantitative version of the
visual ecdf-vs- F_θ check

Other Goodness of Fit Tests

- In most cases, the distribution of the test statistic under H_0 is only known in the limit as $n \rightarrow \infty$
- Even then, cutoffs often can't be calculated exactly and require simulations to approximate
- When there's more than one test out there for the same thing, it's always a good idea to read up on the benefits/drawbacks of each one before deciding which to use
- One might have a lower probability of Type I error, another might higher power for lower sample sizes, another might be more robust to outliers, and so on

Very active area & research!