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CS 590M: Simulation Spring Semester 2020

Definition and Examples

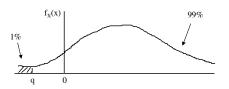
Point Estimates

Confidence Intervals

**Further Comments** 

**Checking Normality** 

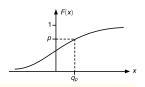
## Quantiles



#### **Example: Value-at-Risk**

- ightharpoonup X = return on investment, want to measure downside risk
- $q = \text{return s.t. } P(\text{worse return than } q) \leq 0.01$ 
  - q is called the 0.01-quantile of X
  - "Probabilistic worst case scenario"

#### Quantile Definition



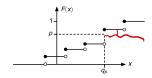
Definition of p-quantile  $q_p$ 

$$q_p = F_X^{-1}(p)$$
 (for  $0 )$ 

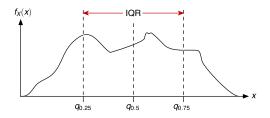
- ▶ When  $F_X$  is continuous and increasing: solve F(q) = p
- In general: Use our generalized definition of F<sup>-1</sup> (as in inversion method)

Alternative Definition of p-quantile  $q_p$ 

$$q_p = \min\{q : F_X(q) \ge p\}$$



## Example: Robust Statistics



#### Median

- ▶ Median =  $q_{0.5}$
- ▶ Alternative to means as measure of central tendency
- Robust to outliers

### Inter-quartile range (IQR)

- ► Robust measure of dispersion
- ► IQR =  $q_{0.75} q_{0.25}$



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### Point Estimate of Quantile

- ▶ Given i.i.d. observations  $X_1, \ldots, X_n \stackrel{\mathsf{D}}{\sim} F$
- ► Natural choice is *p*th sample quantile:

$$F(y) = \#\{K = x\}_n$$
  
 $F(x) = P(X = x)$ 

$$Q_n = \hat{F}_n^{-1}(p)$$

- ▶ I.e., generalized inverse of empirical cdf  $\hat{F}_n$
- Q: Can you ever use the simple (non-generalized) inverse here?
- ▶ Equivalently, sort data as  $X_{(1)} \le X_{(2)} \le \cdots \le X_{(n)}$  and set

$$Q_n = X_{(j)}, \text{ where } j = \lceil np \rceil$$

• Ex:  $q_{0.5}$  for  $\{6, 8, 4, 2\} = 4$ 

- 2,6,8
- Pc.5 4= 11
- Values), but we will stick with the above defs

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## Confidence Interval Attempt #1: Direct Use of CLT

CLT for Quantiles (Bahadur Representation)

Suppose that  $X_1, \ldots, X_n$  are i.i.d. with pdf  $f_X$ . Then for large n

$$Q_n \overset{ extsf{D}}{\sim} N\left(q_p, rac{\sigma^2}{n}
ight) \quad ext{with} \quad \sigma = rac{\sqrt{p(1-p)}}{f_X(q_p)}$$

#### Can derive via Delta Method for stochastic root-finding

- Recall: to find  $\bar{\theta}$  such that  $E[g(X,\bar{\theta})] = 0$ 
  - Point estimate  $\theta_n$  solves  $\frac{1}{n} \sum_{i=1}^n g(X_i, \theta_n) = 0$
  - ► For large n, we have  $\theta_n \approx N(\bar{\theta}, \sigma^2/n)$ , where  $\sigma^2 = \text{Var}[g(X, \bar{\theta})]/c^2$  with  $c = E[\partial g(X, \bar{\theta})/\partial \theta]$
- ▶ For quantile estimation take  $g(X, \theta) = I(X \le \theta) p$ 
  - $\bar{\theta} = q_p$  and  $\theta_n = Q_n$ , since  $E[g(X, \bar{\theta})] = P(X \leq \bar{\theta}) p = 0$
  - ►  $E[\partial g(X,\bar{\theta})/\partial \theta] = \partial E[g(X,\bar{\theta})]/\partial \theta = \partial (F_X(\bar{\theta})-p)/\partial \theta = f_X(\bar{\theta})$
  - ►  $Var[g(X, \bar{\theta})] = E[g(X, \bar{\theta})^2] = E[I^2 2pI + p^2]$ =  $E[I - 2pI + p^2] = p - 2p^2 + p^2 = p(1 - p)$

## Confidence Interval Attempt #1: Direct Use of CLT

CLT for Quantiles (Bahadur Representation)

Suppose that  $X_1, \ldots, X_n$  are i.i.d. with pdf  $f_X$ . Then for large n

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ight) \quad ext{with} \quad \sigma = rac{\sqrt{p(1-p)}}{f_X(q_p)}$$

▶ So if we can find an estimator  $s_n$  of  $\sigma$ , then  $100(1 - \delta)\%$  CI is

$$\left[Q_n-\frac{z_\delta s_n}{\sqrt{n}},Q_n+\frac{z_\delta s_n}{\sqrt{n}}\right]$$

- ▶ Problem: Estimating a pdf  $f_X$  is hard (e.g., need to choose "bandwidth" for "kernel density estimator")
- $\blacktriangleright$  So we want to avoid estimation of  $\sigma$

## Confidence Interval Attempt #2: Sectioning

- Assume that n = mk and divide  $X_1, ..., X_n$  into m sections of k observations each
- $\blacktriangleright$  m is small (around 10–20) and k is large
- Let  $Q_n(i)$  be estimator of  $q_p$  based on data in *i*th section
- ▶ Observe that  $Q_n(1), \ldots, Q_n(m)$  are i.i.d.
- ▶ By prior CLT, each  $Q_n(i)$  is approx. distributed as  $N\left(q_p, \frac{\sigma^2}{k}\right)$
- ▶ For i.i.d. normals, standard  $100(1-\delta)\%$  CI for mean is

$$\left[\bar{Q}_n - t_{m-1,\delta}\sqrt{\frac{v_n}{m}}, \bar{Q}_n + t_{m-1,\delta}\sqrt{\frac{v_n}{m}}\right]$$

- $\bar{Q}_n = (1/m) \sum_{i=1}^m Q_n(i)$
- $v_n = \frac{1}{m-1} \sum_{i=1}^m (Q_n(i) \bar{Q}_n)^2$
- $t_{m-1,\delta}$  is  $1-(\delta/2)$  quantile of Student-t distribution with m-1 degrees of freedom



# Sectioning: So What's the Problem?

Can show, as with nonlinear functions of means, that

$$E[Q_n] \approx q_p + \frac{b}{n} + \frac{c}{n^2}$$

▶ It follows that

$$E[Q_n(i)] \approx q_p + \frac{b}{k} + \frac{c}{k^2} = q_p + \frac{mb}{n} + \frac{m^2c}{n^2}$$

So

$$E[\bar{Q}_n] \approx q_p + \frac{mb}{n} + \frac{m^2c}{n^2}$$

▶ Bias of  $\bar{Q}_n$  is roughly m times larger than bias of  $Q_n$ !

## Attempt #3: Sectioning + Jackknifing

### Sectioning + Jackknifing: General Algorithm for a Statistic $\alpha$

- 1. Generate n = mk i.i.d. observations  $X_1, \ldots, X_n$
- 2. Divide observations into m sections, each of size k
- 3. Compute point estimator  $\alpha_n$  based on all observations
- 4. For i = 1, 2, ..., m:
  - 4.1 Compute estimator  $\tilde{\alpha}_n(i)$  using all observations except those in section i
  - 4.2 Form pseudovalue  $\alpha_n(i) = m\alpha_n (m-1)\tilde{\alpha}_n(i)$
- 5. Compute point estimator:  $\alpha_n^J = \frac{1}{m} \sum_{i=1}^m \alpha_n(i)$
- 6. Set  $v_n^J = \frac{1}{m-1} \sum_{i=1}^m (\alpha_n(i) \alpha_n^J)^2$
- 7. Compute 100(1  $\delta$ )% CI:  $\left[\alpha_n^J t_{m-1,\delta}\sqrt{\frac{v_n^J}{m}}, \alpha_n^J + t_{m-1,\delta}\sqrt{\frac{v_n^J}{m}}\right]$

## Application to Quantile Estimation

- $\tilde{Q}_n(i)$  = quantile estimate ignoring section i
- ▶ Clearly,  $\tilde{Q}_n(i)$  has same distribution as  $Q_{(m-1)k}$ , so

$$E[\tilde{Q}_n(i)] \approx q_p + \frac{b}{(m-1)k} + \frac{c}{(m-1)^2 k^2}$$

▶ It follows that, for pseudovalue  $\alpha_n(i)$ ,

$$E[\alpha_n(i)] = E\left[mQ_n - (m-1)\tilde{Q}_n(i)\right] \approx q_p - \frac{c}{(m-1)mk^2}$$

▶ Averaging does not affect bias, so, since n = mk,

$$E[\bar{Q}_n] = q_p + O(1/n^2)$$

General procedure is also called the "delete-k jackknife"

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#### **Further Comments**

**Checking Normality** 

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#### A confession

- ▶ There exist special-purpose methods for quantile estimation [Sections 2.6.1 and 2.6.3 in Serfling book]
- ▶ We focus on sectioning + jackknife because method is general
- Can also use bias elimination method from prior lecture

### Conditioning the data for $q_p$ when $p \approx 1$

- ▶ Fix r > 1 and get n = rmk i.i.d. observations  $X_1, ..., X_n$
- Divide data into blocks of size r
- ▶ Set  $Y_i = \text{maximum value in } j\text{th block for } 1 \leq j \leq mk$
- ▶ Run quantile estimation procedure on  $Y_1, ..., Y_{mk}$
- ► Key observation:  $F_Y(q_p) = [F_X(q_p)]^r = p^r$   $F_Y(q_p) = p(\max_i X_i \neq q_p)$ ► So p-quantile for X equals  $p^r$ -quantile for Y► Ex: if r = 50, then  $q_{0.99}$  for X equals  $q_{0.61}$  for Y• Often, reduction in sample size outside.
- Often, reduction in sample size outweighs cost of extra runs

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#### **Checking Normality**

### Checking Normality

#### Undercoverage

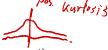
- ► E.g., when a "95% confidence interval" for the mean only brackets the mean 70% of the time
- ▶ Due to failure of CLT at finite sample sizes
- Note: If data is truly normal, then no error in CI for the mean

### Simple diagnostics



- Skewness (measures symmetry, equals 0 for normal)
  - ▶ Definition: skewness(X) =  $\frac{E[(X E(X))^3]}{(\text{var } X)^{3/2}}$
  - ► Estimator:  $\frac{n^{-1} \sum_{i=1}^{n} (X_i \bar{X}_n)^3}{\left(n^{-1} \sum_{i=1}^{n} (X_i \bar{X}_n)^2\right)^{3/2}}$





- Kurtosis (measures fatness of tails, equals 0 for normal)
  - ▶ Definition: kurtosis(X) =  $\frac{E[(X E(X))^4]}{(\text{var } X)^2} 3$
  - ► Estimator:  $\frac{n^{-1} \sum_{i=1}^{n} (X_i \bar{X}_n)^4}{\left(n^{-1} \sum_{i=1}^{n} (X_i \bar{X}_n)^2\right)^2} 3$

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## Bootstrap Confidence Intervals

### **General method works for quantiles** (no normality assumptions needed)

### Bootstrap Confidence Intervals (Pivot Method)

- 1. Run simulation *n* times to get  $\mathcal{D} = \{X_1, \dots, X_n\}$
- 2. Compute  $Q_n = \text{sample quantile based on } \mathcal{D}$
- 3. Compute bootstrap sample  $\mathcal{D}^* = \{X_1^*, \dots, X_n^*\}$
- 4. Set  $Q_n^* = \text{sample quantile based on } \mathcal{D}^*$
- 5. Set pivot  $\pi^* = Q_n^* Q_n$  ("bootstrap werld" estimate of "real world" quantity

  6. Repeat Steps 3–5 B times to create  $\pi_1^*, \ldots, \pi_B^*$   $\mathcal{A}_n \mathcal{A}_p$ )

  7. Sort pivots to obtain  $\pi_n^*, \ldots, \pi_n^*$
- 7. Sort pivots to obtain  $\pi_{(1)}^* \leq \pi_{(2)}^* \leq \cdots \leq \pi_{(B)}^*$
- 8. Set  $I = \lceil (1 \delta/2)B \rceil$  and  $u = \lceil (\delta/2)B \rceil$
- 9. Return  $100(1-\delta)\%$  CI  $[Q_n-\pi_{(I)}^*,Q_n-\pi_{(I)}^*]$