Order statistics, quantiles & resampling

(Module 9)

Statistics (MAST20005) &
Elements of Statistics
(MAST90058)

School of Mathematics and Statistics
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Outline

Aims of this module

- Go back to **order statistics** and **sample quantiles**
- More detailed definitions
- Derive **sampling distributions** and construct **confidence intervals**
- See examples of CIs that are **not** of the form $\hat{\theta} \pm \mathrm{se}(\hat{\theta})$
- Learn some more distribution-free methods
- See how to use computation to avoid mathematical derivations

Unifying theme

- Use the data ‘directly’ rather than via assumed distributions
- Use the **sample cdf** and related summaries
  (such as order statistics)

Outline

Definition (recap)

- Sample: $X_1, \ldots, X_n$
- Arrange them in increasing order:

$$
\begin{aligned}
X_{(1)} &= \text{Smallest of the } X_i \\
X_{(2)} &= \text{2nd smallest of the } X_i \\
&\vdots \\
X_{(n)} &= \text{Largest of the } X_i
\end{aligned}
$$

- These are called the order statistics

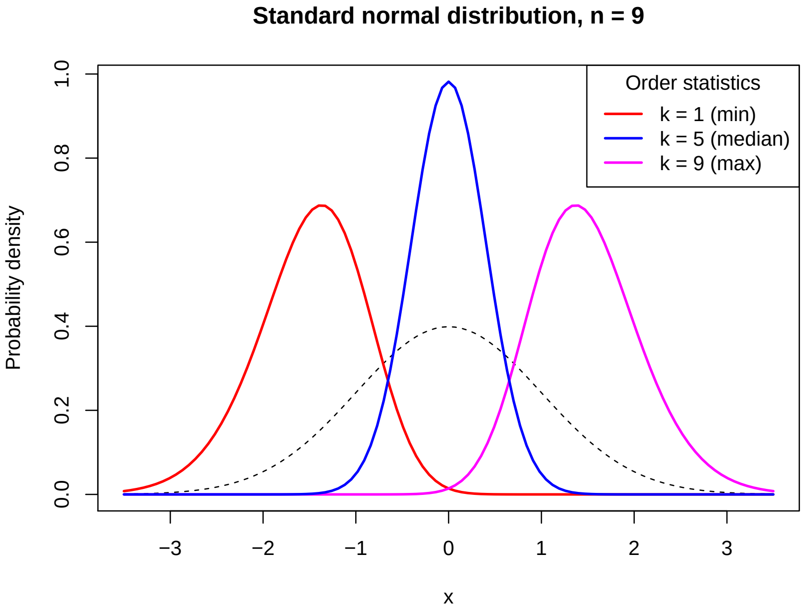
$$X_{(1)} \leqslant X_{(2)} \leqslant \cdots \leqslant X_{(n)}$$

- $X_{(k)}$ is called the kth order statistic of the sample
- $X_{(1)}$ is the minimum or sample minimum
- $X_{(n)}$ is the maximum or sample maximum

Motivating example

- Take iid samples $X \sim \mathrm{N}(0,1)$ of size $n = 9$
- What can we say about the order statistics, $X_{(k)}$?
- Simulated values:

```
      [,1]  [,2]  [,3]  [,4]  [,5]
 [1,] -0.76 -1.94 -1.32 -0.85 -1.96  <-- Minimum
 [2,] -0.32 -0.17 -0.53 -0.30 -0.98
 [3,] -0.23  0.06 -0.44  0.14 -0.83
 [4,]  0.05  0.18 -0.10  0.25 -0.63
 [5,]  0.08  0.76  0.17  0.35 -0.47  <-- Median
 [6,]  0.18  0.96  0.26  0.68  0.05
 [7,]  0.27  1.07  0.60  0.69  0.34
 [8,]  0.73  1.42  0.66  1.13  1.26
 [9,]  0.91  1.77  1.93  1.98  1.26  <-- Maximum
```


Standard normal distribution, n = 9
Order statistics
k = 1 (min)
k = 5 (median)
k = 9 (max)
Probability density
0.0
0.2
0.4
0.6
0.8
1.0
−3
−2
−1
0
1
2
3
x

Example (triangular distribution)

- Random sample: $X_1, \ldots, X_5$ with pdf $f(x) = 2x$, $0 < x < 1$
- Calculate $\Pr(X_{(4)} \leqslant 0.5)$
- Occurs if at least four of the X_i are less than 0.5,

$$\begin{aligned}\Pr(X_{(4)} \leqslant 0.5) &= \Pr(\textbf{at least 4 } X_i\text{'s less than } 0.5) \\ &= \Pr(\textbf{exactly 4 } X_i\text{'s less than } 0.5) \\ &\quad + \Pr(\textbf{exactly 5 } X_i\text{'s less than } 0.5)\end{aligned}$$

- This is a binomial with 5 trials and probability of success given by

$$\Pr(X_i \leqslant 0.5) = \int_0^{0.5} 2x\,dx = \left[x^2\right]_0^{0.5} = 0.5^2 = 0.25$$

- So we have,

$$\Pr(X_{(4)} \leqslant 0.5) = \binom{5}{4} 0.25^4\, 0.75 + 0.25^5 = 0.0156$$

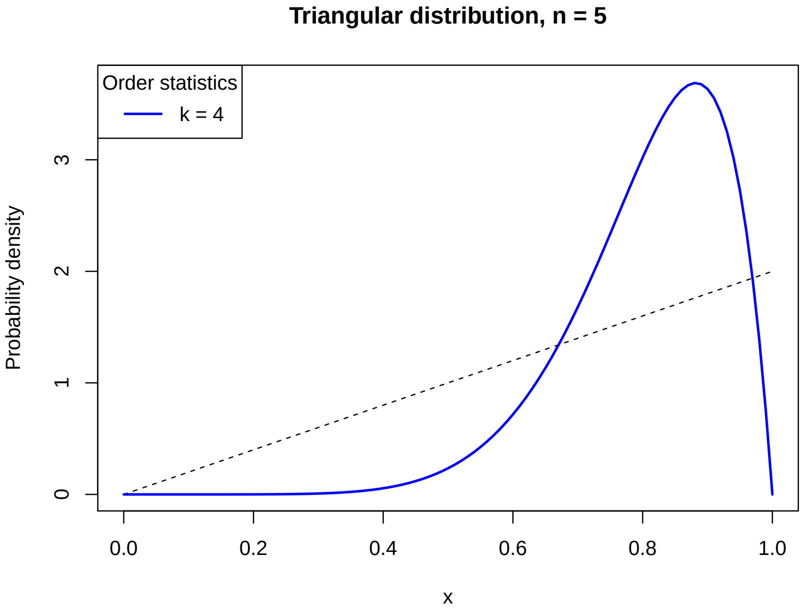
- More generally we have,

$$F(x) = \Pr(X_i \leqslant x) = \int_0^x 2t\,dt = \left[t^2\right]_0^x = x^2$$
$$G(x) = \Pr(X_{(4)} \leqslant x) = \binom{5}{4}(x^2)^4(1-x^2) + (x^2)^5$$

- Taking derivatives gives the pdf,

$$\begin{aligned} g(x) = G'(x) &= \binom{5}{4} 4(x^2)^3(1-x^2)(2x) \\ &= 4\binom{5}{4} F(x)^3\,(1-F(x))\,f(x) \end{aligned}$$

since we know that $F(x) = x^2$.



Triangular distribution, n = 5
Order statistics
k = 4
Probability density
0
1
2
3
0.0
0.2
0.4
0.6
0.8
1.0
x

Distribution of $X_{(k)}$

- Sample from a continuous distribution with cdf $F(x)$ and pdf $f(x) = F'(x)$.
- The cdf of $X_{(k)}$ is,

$$\begin{aligned} G_k(x) &= \Pr(X_{(k)} \leqslant x) \\ &= \sum_{i=k}^{n} \binom{n}{i} F(x)^i \, (1 - F(x))^{n-i} \end{aligned}$$

- Thus the pdf of $X_{(k)}$ is,

$$
\begin{aligned}
g_k(x) = G_k'(x) &= \sum_{i=k}^{n} i\binom{n}{i} F(x)^{i-1}\,(1-F(x))^{n-i}\,f(x) \\
&\quad + \sum_{i=k}^{n-1} (n-i)\binom{n}{i} F(x)^{i}\,(1-F(x))^{n-i-1}\,(-f(x)) \\
&= k\binom{n}{k} F(x)^{k-1}\,(1-F(x))^{n-k}\,f(x) \\
&\quad + \sum_{i=k+1}^{n} i\binom{n}{i} F(x)^{i-1}\,(1-F(x))^{n-i}\,f(x) \\
&\quad - \sum_{i=k}^{n-1} (n-i)\binom{n}{i} F(x)^{i}\,(1-F(x))^{n-i-1}\,f(x)
\end{aligned}
$$

- But

$$i\binom{n}{i} = \frac{n!}{(i-1)!(n-i)!} = n\binom{n-1}{i-1}$$

and similarly

$$(n-i)\binom{n}{i} = \frac{n!}{i!(n-i-1)!} = n\binom{n-1}{i}$$

which allows some cancelling of terms.

- For example, the first term of the first summation is,

$$
\begin{aligned}
(k+1)\binom{n}{k+1} F(x)^k \left(1-F(x)\right)^{n-k-1} f(x) \\
= n\binom{n-1}{k} F(x)^k \left(1-F(x)\right)^{n-k-1} f(x)
\end{aligned}
$$

- The first term of the second summation is,

$$
\begin{aligned}
(n-k)\binom{n}{k} F(x)^k \left(1-F(x)\right)^{n-k-1} f(x) \\
= n\binom{n-1}{k} F(x)^k \left(1-F(x)\right)^{n-k-1} f(x)
\end{aligned}
$$

- These cancel, and similarly the other terms do as well.

- Hence, the pdf simplifies to,

$$g_k(x) = k\binom{n}{k} F(x)^{k-1}\left(1 - F(x)\right)^{n-k} f(x)$$

- Special cases: minimum and maximum,

$$\begin{aligned} g_1(x) &= n\left(1 - F(x)\right)^{n-1} f(x) \\ g_n(x) &= n\, F(x)^{n-1} f(x) \end{aligned}$$

- Also:

$$\begin{aligned} \Pr(X_{(1)} > x) &= \left(1 - F(x)\right)^{n} \\ \Pr(X_{(n)} \leqslant x) &= F(x)^{n} \end{aligned}$$

Alternative derivation of the pdf of $X_{(k)}$

- Heuristically,

$$\Pr(X_{(k)} \approx x) = \Pr(x - \tfrac{1}{2}dy < X_{(k)} \leqslant x + \tfrac{1}{2}dy) \approx g_k(x)\, dy$$

- Need to observe X_i such that:
  - $k-1$ are in $\left(-\infty,\, x - \tfrac{1}{2}dy\right]$
  - One is in $\left(x - \tfrac{1}{2}dy,\, x + \tfrac{1}{2}dy\right]$
  - $n-k$ are in $\left(x + \tfrac{1}{2}dy,\, \infty\right)$
- Trinomial distribution (3 outcomes), event probabilities:

$$\begin{aligned}
\Pr(X_i \leqslant x - \frac{1}{2}dy) &\approx F(x) \\
\Pr(x - \frac{1}{2}dy < X_i \leqslant x + \frac{1}{2}dy) &\approx f(x)\, dy \\
\Pr(X_i > x + \frac{1}{2}dy) &\approx 1 - F(x)
\end{aligned}$$

- Putting these together,

$$g_k(x)\,dy \approx \frac{n!}{(k-1)!\,1!\,(n-k)!}F(x)^{k-1}\,(1-F(x))^{n-k}\,f(x)\,dy$$

- Dividing both sides by dy gives the pdf of $X_{(k)}$

Example (boundary estimate)

- $X_1, \ldots, X_4 \sim \text{Unif}(0, \theta)$
- Likelihood is

$$L(\theta) = \begin{cases} \left(\frac{1}{\theta}\right)^4 & 0 \leqslant x_i \leqslant \theta, \quad i = 1, \ldots, 4 \\ 0 & \text{otherwise (i.e. if } \theta < x_i \text{ for some } i\text{)} \end{cases}$$

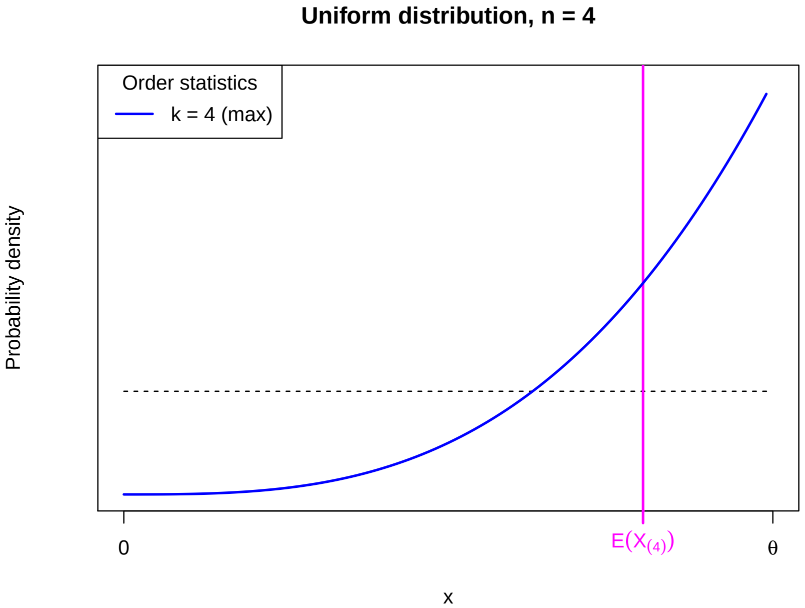
- Maximised when θ is as small as possible, so $\hat{\theta} = \max(X_i) = X_{(4)}$
- Now,

$$g_4(x) = 4\left(\frac{x}{\theta}\right)^3 \left(\frac{1}{\theta}\right) = \frac{4x^3}{\theta^4}, \quad 0 \leqslant x \leqslant \theta$$

- Then,

$$\mathbb{E}(X_{(4)}) = \int_0^\theta x \frac{4x^3}{\theta^4}\, dx = \left[\frac{4x^5}{5\theta^4}\right]_0^\theta = \frac{4}{5}\theta$$

- So the MLE $X_{(4)}$ is biased
- (But $\frac{5}{4}X_{(4)}$ is unbiased)



Uniform distribution, n = 4
Order statistics
k = 4 (max)
Probability density
0
E(X(4))
θ
x

- Deriving a one-sided CI for θ based on $X_{(4)}$:
  1. For a given $0 < c < 1$, show that,

$$1 - c^4 = \Pr(c\theta < X_{(4)} < \theta) = \Pr(X_{(4)} < \theta < X_{(4)}/c)$$

  2. Thus, a $100 \cdot (1 - c^4)$% confidence interval for θ is $\left(x_{(4)},\, x_{(4)}/c\right)$
  3. Letting $c = \sqrt[4]{0.05} = 0.47$, we have a 95% confidence interval from $x_{(4)}$ to $2.11x_{(4)}$

Outline

Population quantiles

- Informally, a **quantile** is a number that divides the range of a random variable based on the probabilities on either side.
- The p-quantile, π_p, of a continuous probability distribution with cdf F has the property:

$$p = F(\pi_p) = \Pr(X \leqslant \pi_p)$$

So, we can define it by the inverse cdf:

$$\pi_p = F^{-1}(p)$$

- More general definition (also works for discrete variables): the p-quantile is the smallest value π_p such that $p \leqslant F(\pi_p)$
- The most commonly used quantile is the median, $\pi_{0.5}$, often referred to as simply as m
- Also the first and third quartiles, $\pi_{0.25}$ and $\pi_{0.75}$

Sample quantiles

- Want a statistic which estimates π_p
- There are many ways to do this
- R implements 9 different definitions!
- See `help(quantile)`
- Previously mentioned two of these...

‘Type 6’ quantiles

- Definition:

$$\hat{\pi}_p = x_{(k)}, \quad \text{where } p = \frac{k}{n+1}$$

- Linear interpolation otherwise
- Motivated by the following relationship (see later):

$$\mathbb{E}(F(X_{(k)})) = \frac{k}{n+1}$$

- We used this previously for QQ plots

'Type 7' quantiles

- Definition:

$$\hat{\pi}_p = x_{(k)}, \quad \text{where } p = \frac{k-1}{n-1}$$

- Linear interpolation otherwise
- Motivated by the following relationship (see later):

$$\text{mode}(F(X_{(k)})) = \frac{k-1}{n-1}$$

- This is the default in R (`quantile` function)

‘Type 1’ quantiles

- Can also apply the general quantile definition to the sample cdf:

$$\hat{\pi}_p = x_{(\lceil np \rceil)}$$

- The ceiling function, $\lceil b \rceil$, is the smallest integer not less than b
- In other words,

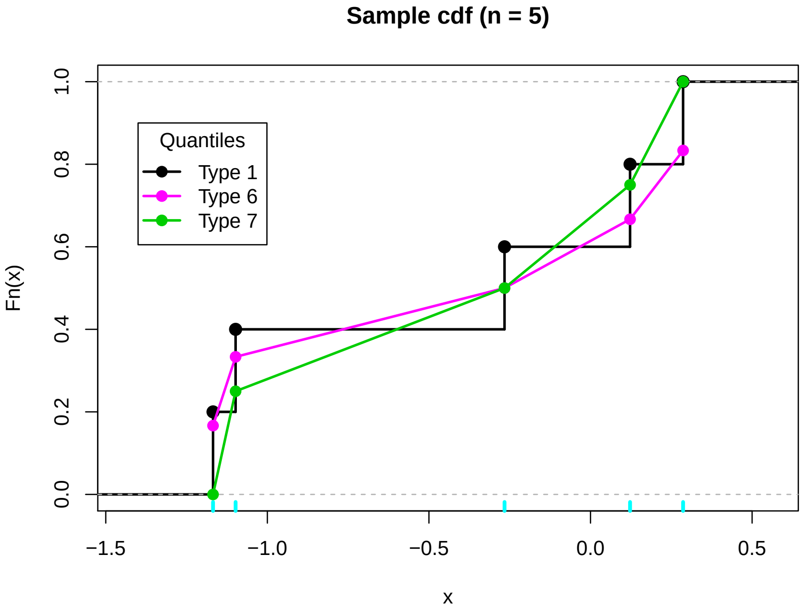
$$\hat{\pi}_p = x_{(k)}, \quad \text{if } \frac{k-1}{n} < p \leqslant \frac{k}{n}$$

- Reminder: the sample cdf is

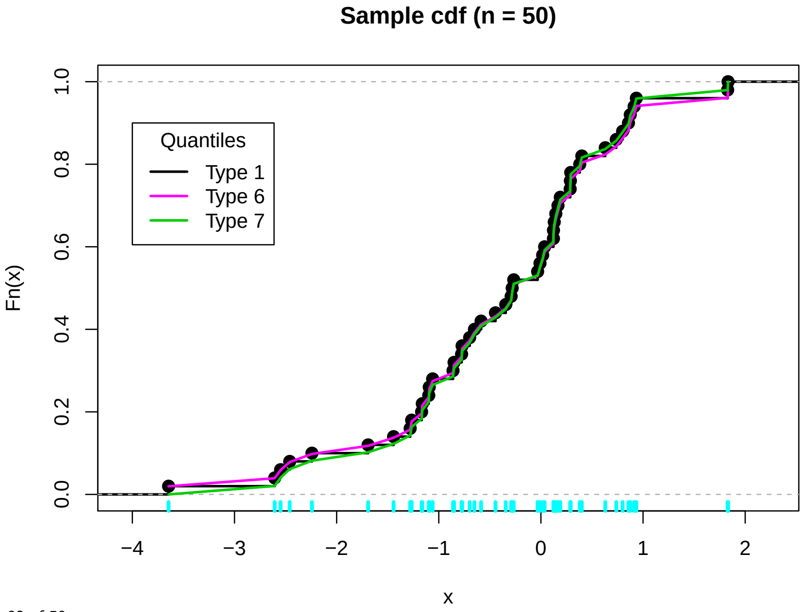
$$\hat{F}(x) = \frac{1}{n} \sum_{i=1}^{n} I(x_i \leqslant x)$$

Differences in definitions

- Different definitions imply different estimators for the cdf
- For large sample sizes, differences are negligible



Sample cdf (n = 5)
Quantiles
Type 1
Type 6
Type 7
Fn(x)
0.0
0.2
0.4
0.6
0.8
1.0
−1.5
−1.0
−0.5
0.0
0.5
x


Sample cdf (n = 50)
Quantiles
Type 1
Type 6
Type 7
Fn(x)
x
0.0
0.2
0.4
0.6
0.8
1.0
−4
−3
−2
−1
0
1
2

Distribution on the cdf scale

- Reminder: for a continuous distribution, $F(X) \sim \mathrm{Unif}(0,1)$
- Proof: for $0 \leqslant w \leqslant 1$,

$$G(w) = \Pr(F(X) \leqslant w) = \Pr(X \leqslant F^{-1}(w)) = F(F^{-1}(w)) = w$$

  so the density is

$$g(w) = G'(w) = 1, \quad 0 \leqslant w \leqslant 1$$

  so $F(X) \sim \mathrm{Unif}(0,1)$.
- Since F is non-decreasing, we have

$$F(X_{(1)}) < F(X_{(2)}) < \cdots < F(X_{(n)})$$

- So $W_i = F(X_{(i)})$ are order statistics from a $\mathrm{Unif}(0,1)$ distribution
- The cdf is $G(w) = w$, for $0 < w < 1$
- So the pdf of kth order statistic $W_k = F(X_{(k)})$ is

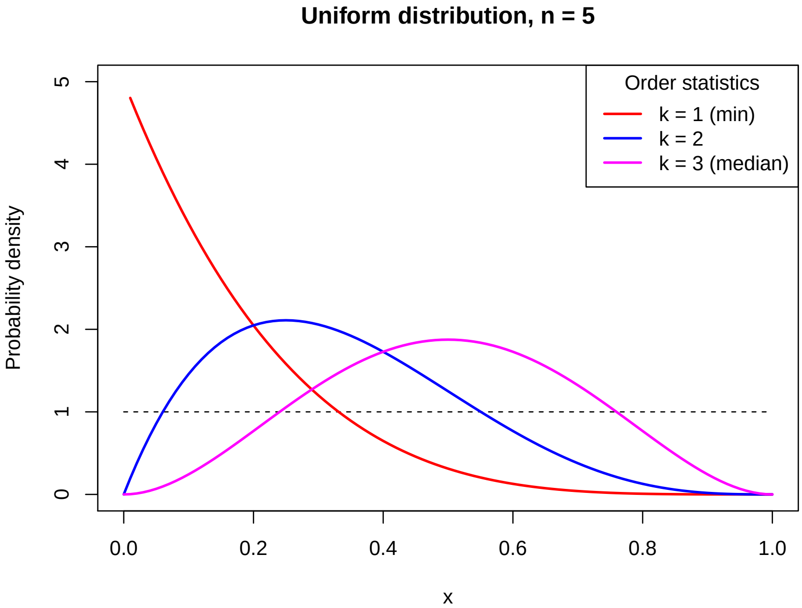
$$g_k(w) = k\binom{n}{k}w^{k-1}\,(1-w)^{n-k}$$

- This is a beta distribution,

$$F(X_k) \sim \mathrm{Beta}(k, n-k+1)$$

- We can derive that:

$$\mathbb{E}(W_k) = \frac{k}{n+1}$$
$$\text{mode}(W_k) = \frac{k-1}{n-1}$$


Uniform distribution, n = 5
Order statistics
k = 1 (min)
k = 2
k = 3 (median)
Probability density
0
1
2
3
4
5
0.0
0.2
0.4
0.6
0.8
1.0
x

Defining the estimators

- How does this relate to the definitions of the estimators?
- Consider:

$$\Pr(X \leqslant X_{(k)}) = F(X_{(k)})$$
$$\Pr(X \leqslant \pi_p) = F(\pi_p) = p$$

- Have $F(X_{(k)})$ probability to the left of $X_{(k)}$, need p probability to the left π_p
- Just need to relate them
- $F(X_{(k)})$ is the (random!) area to the left $X_{(k)}$
- We know its distribution, so can summarise it
- For example, $\mathbb{E}(F(X_{(k)})) = k/(n+1)$
- This suggests $X_{(k)}$ can be an estimator of π_p where $p = k/(n+1)$
- So, define $\hat{\pi}_p = X_{(k)}$ where $p = k/(n+1)$
- For other values of p, linearly interpolate

Sample median

- The sample median is

$$\hat{m} = \begin{cases} X_{((n+1)/2)} & \text{when } n \text{ is odd} \\ \frac{1}{2}\left(X_{(n/2)} + X_{((n/2)+1)}\right) & \text{when } n \text{ is even} \end{cases}$$

- Consistent with most definitions of the sample quantiles (not type 1!)

Asymptotic distribution

- For large sample sizes, it can be shown that

$$\hat{\pi}_p \approx \mathrm{N}\left(\pi_p,\ \frac{p(1-p)}{nf(\pi_p)^2}\right)$$

  where f is the pdf of the population distribution
- The median, $\hat{M} = \hat{\pi}_{0.5}$, is convenient special case,

$$\hat{M} \approx \mathrm{N}\left(m,\ \frac{1}{4nf(m)^2}\right)$$

Example (normal distribution)

- Random sample: $X \sim \mathrm{N}(\mu, \sigma^2)$ of size n
- Compare $\bar{X}$ and $\hat{M}$ as estimators of μ
- Already know,

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

- Now we also know,

$$\hat{M} \approx \mathrm{N}\left(m, \frac{1}{4nf(m)^2}\right)$$

- Note that $m = \mu$ and,

$$f(m) = f(\mu) = \frac{1}{\sigma\sqrt{2\pi}}$$

- This given,

$$\hat{M} \approx \mathrm{N}\left(\mu, \frac{\pi}{2}\frac{\sigma^2}{n}\right)$$

- Does the $\pi/2$ look familiar?
- . . . problem 3, week 2!
- The sample mean, $\bar{X}$, is a more efficient estimator of μ than the sample median, $\hat{M}$
- In other scenarios, it can be the other way around

Confidence intervals for quantiles

- Can we construct **distribution-free** CIs for quantiles?
- Can do so based on order statistics
- Procedure is the ‘inverse’ of the sign test

Example (CI for median)

- Take iid samples $X_1, \ldots, X_5$
- $X_{(3)}$ is an estimator of the median $m = \pi_{0.5}$
- For the median to be between $X_{(1)}$ and $X_{(5)}$ must have at least one $X_i < m$ but not five $X_i < m$
- If the distribution is continuous, $\Pr(X < m) = 0.5$
- Let W be the number of $X_i < m$, then $W \sim \mathrm{Bi}(5, 0.5)$ and

$$\begin{aligned}\Pr(X_{(1)} < m < X_{(5)}) &= \Pr(1 \leqslant W \leqslant 4) \\ &= \sum_{k=1}^{4} \binom{5}{k} \left(\frac{1}{2}\right)^k \left(\frac{1}{2}\right)^{5-k} \\ &= 1 - 0.5^5 - 0.5^5 = \frac{15}{16} \approx 0.94\end{aligned}$$

- So $(x_{(1)}, x_{(5)})$ is a 94% confidence interval for m

Confidence intervals for the median

- In general, want i and j so that, to the closest possible extent,

$$\begin{aligned}\Pr(X_{(i)} < m < X_{(j)}) &= \Pr(i \leqslant W \leqslant j-1) \\ &= \sum_{k=i}^{j-1} \binom{n}{k} \left(\frac{1}{2}\right)^k \left(\frac{1}{2}\right)^{n-k} \approx 1-\alpha\end{aligned}$$

- Need to use computed binomial probabilities (e.g. R) to determine i and j
- Or use the normal approximation to the binomial
- Note that these confidence intervals do not arise from pivots and cannot achieve 95% confidence exactly

Example (lengths of fish)

- Lengths of 9 fish (in cm), in ascending order:
  15.5, 19.0, 21.2, 21.7, 22.8, 27.6, 29.3, 30.1, 32.5
- Now,

$$\Pr(X_{(2)} < m < X_{(8)}) = \sum_{k=2}^{7} \binom{9}{k} \left(\frac{1}{2}\right)^{k} \left(\frac{1}{2}\right)^{9-k} = 0.9610$$

- In R:

```
> pbinom(7, size = 9, prob = 0.5) -
+ pbinom(1, size = 9, prob = 0.5)
[1] 0.9609375
```

- So a 96.1% confidence interval for m is (19.0, 30.1)

Confidence intervals for arbitrary quantiles

- Argument can be extended to any quantile and any order statistics,
- For example, the ith and jth,

$$
\begin{aligned}
1 - \alpha &= \Pr(X_{(i)} < \pi_p < X_{(j)}) \\
&= \Pr(i \leqslant W \leqslant j - 1) \\
&= \sum_{k=i}^{j-1} \binom{n}{k} p^k (1-p)^{n-k}
\end{aligned}
$$

Example (income distribution)

- Incomes (in \$100's) for a sample of 27 people, in ascending order:
  161, 169, 171, 174, 179, 180, 183, 184, 186,
  187, 192, 193, 196, 200, 204, 205, 213, 221,
  222, 229, 241, 243, 256, 264, 291, 317, 376
- Want to estimate the first quartile, $\pi_{0.25}$
- W is the number of the X's below $\pi_{0.25}$

- $W \sim \mathrm{Bi}(27, 0.25) \approx N(\mu = 27/4 = 6.75,\ \sigma^2 = 81/16)$
- This gives

$$\begin{aligned}
\Pr(X_{(4)} < \pi_{0.25} < X_{(10)}) \\
&= \Pr(4 \leqslant W \leqslant 9) \\
&= \Pr(3.5 < W < 9.5) \qquad \text{(continuity correction)} \\
&= \Phi\left(\frac{9.5 - 6.75}{9/4}\right) - \Phi\left(\frac{3.5 - 6.75}{9/4}\right) \\
&= 0.815
\end{aligned}$$

- So (\$17 400, \$18 700) is an 81.5% CI for the first quartile

Outline

Resampling

- What if maths is too hard?
- Try a resampling method
- Replaces mathematical derivation with brute force computation
- Used for approximating sampling distributions, standard errors, bias, etc.
- Sometimes work brilliantly, sometimes not at all

Bootstrap

- Most popular resampling method: the bootstrap
- Basic idea:
  - Use the sample cdf as an approximation to the true cdf
  - Simulate new data from the sample cdf
  - Equivalent to sampling with replacement from the actual data
- Use these bootstrap samples to infer sampling distributions of statistics of interest
- This is an advanced topic
- Only a 'taster' is presented...
- ...in the lab (week 10)