Statistical Inference

Lecture 09b

ANU - RSFAS

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Beyond Point Estimation - Interval Estimation

- Never be satisfied with a point estimate! We want to know something about the uncertainty!
- This leads to interval estimation.
- Construction methods for interval estimates:
 - parametric "exact" intervals
 - parametric asymptotic intervals
 - Bayesian intervals
 - non-parametric intervals
- Some general approaches (mostly for the frequentist parametric case(s)):
 - Inverting a test statistic
 - Pivotal Quantities
 - Pivoting the CDF

Definition: An interval estimate of a real-valued parameter θ is any pair of functions L(x) and U(x), of a sample that satisfy

$$L(\mathbf{x}) \leq U(\mathbf{x}) \quad \forall \ \mathbf{x} \in \mathcal{X}.$$

- If X = x is observed, the inference $L(x) \le \theta \le U(x)$ is made.
- The random interval [L(X), U(X)] is called an interval estimator.
- We can have one-sided estimates:

$$(-\infty, U(\mathbf{x})] \Rightarrow \theta \leq U(\mathbf{x})$$
$$[L(\mathbf{x}), \infty) \Rightarrow \theta \geq L(\mathbf{x})$$

 There is a strong relationship between hypothesis testing and interval estimation. In general, every confidence set corresponds to a test and vice versa.

Eg. $X_1, \ldots, X_n \stackrel{\text{iid}}{\sim} \text{normal}(\mu, \sigma^2)$, where σ^2 is known. Consider testing:

$$H_0: \mu = \mu_0 \quad \textit{vs} \quad \mu \neq \mu_0$$

$$R = \left\{ \left| \frac{\bar{X} - \mu_0}{\sigma / \sqrt{n}} \right| \ge z_{\alpha/2} \right\}$$

• Now we know that under H_0 $P(R) = \alpha$. So the probability that H_0 is accepted is $1 - \alpha$:

$$P\left(-z_{\alpha/2} \le \frac{\bar{X} - \mu_0}{\sigma/\sqrt{n}} \le z_{\alpha/2}\right) = 1 - \alpha$$

• Now fix α and determine the acceptance region. This is an interval estimator.

$$\begin{split} P\left(-z_{\alpha/2} \leq \frac{\bar{X} - \mu}{\sigma/\sqrt{n}} \leq z_{\alpha/2}\right) &= 1 - \alpha \\ P\left(-z_{\alpha/2} \left(\sigma/\sqrt{n}\right) \leq \bar{X} - \mu \leq z_{\alpha/2} \left(\sigma/\sqrt{n}\right)\right) &= 1 - \alpha \\ P\left(-\bar{X} - z_{\alpha/2} \left(\sigma/\sqrt{n}\right) \leq -\mu \leq -\bar{X} + z_{\alpha/2} \left(\sigma/\sqrt{n}\right)\right) &= 1 - \alpha \\ P\left(\bar{X} + z_{\alpha/2} \left(\sigma/\sqrt{n}\right) \geq \mu \geq \bar{X} - z_{\alpha/2} \left(\sigma/\sqrt{n}\right)\right) &= 1 - \alpha \\ P\left(\bar{X} - z_{\alpha/2} \left(\sigma/\sqrt{n}\right) \leq \mu \leq \bar{X} + z_{\alpha/2} \left(\sigma/\sqrt{n}\right)\right) &= 1 - \alpha \end{split}$$

• A $100(1-\alpha)\%$ confidence estimator for μ is:

$$[\bar{X}-z_{\alpha/2}\;(\sigma/\sqrt{n}),\;\bar{X}+z_{\alpha/2}\;(\sigma/\sqrt{n})]$$

ullet Remember, $oldsymbol{X}$ is random not $\mu!!$

Theorem: For each $\theta_0 \in \Theta$, let $A(\theta_0)$ be the acceptance region of a level α test of $H_0: \theta = \theta_0$.

• For each $x \in X$, define a set C(x) in the parameter space by

$$C(\mathbf{x}) = \{\theta_0 : \mathbf{x} \in A(\theta_0)\}\$$

The random set C(X) is a $1 - \alpha$ confidence set.

• Conversely, let $C(\mathbf{X})$ be a $1-\alpha$ confidence set for any $\theta \in \Theta_0$,

$$A(\theta_0) = \{ \boldsymbol{x} : \theta_0 \in C(\boldsymbol{x}) \}$$

Then $A(\theta_0)$ be the acceptance region of a level α test of $H_0: \theta = \theta_0$

$$A(\theta_0) \iff C(\mathbf{x})$$

Eg. $X_1, \ldots, X_n \stackrel{\text{iid}}{\sim} \text{normal}(\mu, \sigma^2)$, where σ^2 is unknown. Consider testing:

$$H_0: \mu = \mu_0 \quad vs \quad \mu \leq \mu_0$$

Based on a Likelihood Ratio Test we can find a rejection region of:

$$R = \left\{ \frac{\bar{X} - \mu_0}{s / \sqrt{n}} \le -t_{n-1,\alpha} \right\}$$

• This leads to an acceptance region of:

$$A(\mu_0) = \left\{ \mathbf{x} : \frac{\bar{X} - \mu_0}{s / \sqrt{n}} \ge -t_{n-1,\alpha} \right\}$$
$$= \left\{ \bar{\mathbf{x}} \ge \mu_0 - t_{n-1,\alpha} \left(s / \sqrt{n} \right) \right\}$$

ullet This leads to a (1-lpha) upper bound confidence set for μ :

$$C(\mathbf{x}) = \{ \mu_0 : \bar{\mathbf{x}} + t_{n-1,\alpha} \ (s/\sqrt{n}) \ge \mu_0 \}$$

= $(-\infty, \bar{\mathbf{x}} + t_{n-1,\alpha} \ (s/\sqrt{n})]$

Example: Suppose that 2.6, 1.2 and 4.9 are a random sample from a normal distribution whose mean is zero and whose variance σ^2 is unknown. Derive and compute a central 99% confidence interval for σ^2 .

• Approach 1:

$$\left(\frac{X_i - \mu}{\sigma}\right)^2 = \left(\frac{X_i}{\sigma}\right)^2 \sim Z^2 = \chi_1^2$$

$$\sum_{i=1}^{3} \left(\frac{X_i}{\sigma} \right)^2 = \frac{1}{\sigma^2} \sum_{i=1}^{3} X_i^2 \sim \chi_3^2$$

• Let $Y = \sum_{i=1}^{3} X_i^2$.

$$P\left(\chi_{1-\alpha/2,3}^{2} \le \frac{Y}{\sigma^{2}} \le \chi_{\alpha/2,3}^{2}\right) = 1 - \alpha$$

$$P\left(\frac{1}{\chi_{1-\alpha/2,3}^{2}} \ge \frac{\sigma^{2}}{Y} \ge \frac{1}{\chi_{\alpha/2,3}^{2}}\right) = 1 - \alpha$$

$$P\left(\frac{Y}{\chi_{\alpha/2,3}^{2}} \le \sigma^{2} \le \frac{Y}{\chi_{1-\alpha/2,3}^{2}}\right) = 1 - \alpha$$

$$\begin{bmatrix} \frac{Y}{\chi_{\alpha/2,3}^2} & , & \frac{Y}{\chi_{1-\alpha/2,3}^2} \\ \frac{32.21}{12.8381} & , & \frac{32.21}{0.0717212} \end{bmatrix}$$

$$\begin{bmatrix} 2.51 & , & 449 \end{bmatrix}$$

 Note: R does probability to the left for quantiles while C&B does probability to the right.

```
qchisq(0.01/2, 3)
```

[1] 0.07172177

qchisq(1-0.01/2, 3)

[1] 12.83816

Approach 2:

$$\frac{(n-1)S^2}{\sigma^2} \sim \chi_{n-1}^2$$

$$P\left(\chi_{1-\alpha/2,2}^{2} \le \frac{(n-1)S^{2}}{\sigma^{2}} \le \chi_{\alpha/2,2}^{2}\right) = 1 - \alpha$$

$$P\left(\frac{(n-1)S^{2}}{\chi_{\alpha/2,2}^{2}} \le \sigma^{2} \le \frac{(n-1)S^{2}}{\chi_{1-\alpha/2,2}^{2}}\right) = 1 - \alpha$$

Approach 3:

$$\begin{split} \left(\frac{\bar{X} - \mu}{\sigma/\sqrt{n}}\right)^2 &= \left(\frac{\bar{X}}{\sigma/\sqrt{n}}\right)^2 = \frac{n\bar{X}^2}{\sigma^2} \sim Z^2 = \chi_1^2 \\ P\left(\chi_{1-\alpha/2,1}^2 \leq \frac{n\bar{X}^2}{\sigma^2} \leq \chi_{\alpha/2,1}^2\right) &= 1 - \alpha \\ P\left(\frac{n\bar{X}^2}{\chi_{\alpha/2,1}^2} \leq \sigma^2 \leq \frac{n\bar{X}^2}{\chi_{1-\alpha/2,1}^2}\right) &= 1 - \alpha \\ \left[\frac{n\bar{X}^2}{\chi_{\alpha/2,1}^2} \ , \ \frac{n\bar{X}^2}{\chi_{1-\alpha/2,1}^2}\right] \\ \left[\frac{(3)2.9^2}{7.87944} \ , \ \frac{(3)2.9^2}{0.0000393}\right] \\ [3.202 \ , \ 642468.3] \end{split}$$

 All three approaches, and everything we have considered thus far have a nice property. The distribution of the statistic does not contain parameters!

Definition: A random variable $Q(X, \theta)$ is a pivotal quantity (or a pivot) if the distribution of $Q(X, \theta)$ is independent of all parameters.

• If $\mathbf{X} \sim f(\mathbf{x}|\theta)$ then $Q(\mathbf{X},\theta)$ has the same distribution for all values of θ .

$$\hat{\theta} \stackrel{\cdot}{\sim} \text{normal}(\theta, I(\theta)^{-1})$$

$$\frac{\hat{\theta} - \theta}{1/\sqrt{I(\theta)}} \stackrel{\cdot}{\sim} \operatorname{normal}(0, 1)$$

• We have a pivotal quantity. Based on the same approach as before we can construct an asymptotic $100(1-\alpha)\%$ confidence interval as:

$$\left[\hat{\theta} - z_{\alpha/2} \frac{1}{\sqrt{I(\hat{\theta})}} , \ \hat{\theta} + z_{\alpha/2} \frac{1}{\sqrt{I(\hat{\theta})}}\right]$$

• If we are interested in a function of θ , say $\tau(\theta)$, then we have:

ullet We can construct an asymptotic 100(1-lpha)% confidence interval as:

$$\left[\tau(\hat{\theta}) - z_{\alpha/2} \frac{\tau'(\hat{\theta})}{\sqrt{I(\hat{\theta})}} , \ \tau(\hat{\theta}) + z_{\alpha/2} \frac{\tau'(\hat{\theta})}{\sqrt{I(\hat{\theta})}}\right]$$

Example: Let $X_1, \ldots, X_n \stackrel{\text{iid}}{\sim} \operatorname{exponential}(\theta)$:

$$f(x|\theta) = \theta \exp(-\theta x)$$

• Provide an equal tailed 95% CI for $\tau(\theta) = \theta^{-1}$.

$$\ell = nlog(\theta) - \theta \sum x_{i}$$

$$\ell' = \frac{n}{\theta} - \sum x_{i}$$

$$\Rightarrow \frac{n}{\theta} - \sum x_{i} = 0$$

$$\hat{\theta} = \frac{1}{\bar{x}} \Rightarrow \widehat{\left(\frac{1}{\theta}\right)} = \frac{1}{\hat{\theta}} = \bar{x}$$

$$\ell'' = -\frac{n}{\theta^2}$$
Fisher Information: $I(\theta) = -E\left[-\frac{n}{\theta^2}\right] = \frac{n}{\theta^2}$

$$CRLB(\theta^{-1}) = \frac{\left[\frac{d}{d\theta}\frac{1}{\theta}\right]^2}{\frac{n}{\theta^2}} = \frac{\left[-\frac{1}{\theta^2}\right]^2}{\frac{n}{\theta^2}} = \frac{1}{n\theta^2}$$

$$CRLB(\hat{\theta}^{-1}) = \frac{1}{n\hat{\theta}^2} = \frac{\bar{x}^2}{n}$$

• We end with the following interval for $\frac{1}{\theta}$:

$$\left[\bar{x}-z_{\alpha/2}\frac{\bar{x}}{\sqrt{n}}\;,\;\bar{x}+z_{\alpha/2}\frac{\bar{x}}{\sqrt{n}}\right]$$

• Note: $\tau(\hat{\theta}) = \bar{X}$, so why not use the following interval?

$$\left[\bar{x}-z_{\alpha/2}\frac{s}{\sqrt{n}}\;,\;\bar{x}+z_{\alpha/2}\frac{s}{\sqrt{n}}\right]$$

- If the data truly are exponentially distributed, then the previous interval will be more accurate.
- Of course, the this interval will be valid even in the case that the data are not truly exponentially distributed.

- Now suppose we are interested in a CI for θ :
- We constructed an interval $\tau=\frac{1}{\theta}$, so why not just take the the inverse? We can.

$$[u^{-1}, I^{-1}]$$

• So we have for θ :

$$\left[\left\{\bar{x}+z_{\alpha/2}\frac{\bar{x}}{\sqrt{n}}\right\}^{-1},\left\{\bar{x}-z_{\alpha/2}\frac{\bar{x}}{\sqrt{n}}\right\}^{-1}\right]$$

ullet OK, but let's go back to the drawing-board and find the CI for heta from first principles:

$$\left[\bar{x}^{-1} - z_{\alpha/2} \frac{1}{\sqrt{n}\bar{X}} , \bar{x}^{-1} + z_{\alpha/2} \frac{1}{\sqrt{n}\bar{x}}\right]$$

 We see that the two approaches are not the same. This is because interval construction, as we have done it, is not functionally equivalent!!

- Can we come up with an approach which does possess the equivariance property?
 - Yes, as long as the functional transformation in question is invertible.
 - Let's consider an asymptotic likelihood-based confidence interval procedure which is parameterization equivariant.
 - Specifically, this means that if we find a confidence region, C, for θ based on this new procedure and transform all of its values [which we sometimes denote as $\tau(C) = \{\tau(\theta) : \theta \in C\}$] then we will arrive at the same confidence region as if we had applied our new procedure to the parameter τ directly.

• Let's consider the following based on the maximum likelihood ratio test, where $X_1, \ldots, X_n \stackrel{\text{iid}}{\sim} \text{exponential}(\theta)$; $f(x|\theta) = \theta \exp(-\theta x)$:

$$-2\log\left(\frac{\textit{L}(\theta|\textbf{\textit{x}})}{\textit{L}(\hat{\theta}|\textbf{\textit{x}})}\right) \stackrel{.}{\sim} \chi_1^2$$

$$-2[\ell(\theta|\mathbf{x}) - \ell(\hat{\theta}|\mathbf{x})] = 2[\ell(\hat{\theta}|\mathbf{x}) - \ell(\theta|\mathbf{x})]$$

$$= 2[nlog(\hat{\theta}) - \hat{\theta} \sum x_i - nlog(\theta) + \theta \sum x_i]$$

$$= 2[nlog(\frac{1}{\bar{x}}) - \frac{1}{\bar{x}} \sum x_i - nlog(\theta) + \theta \sum x_i]$$

$$= -2n \log(\bar{x}) - 2n\frac{\bar{x}}{\bar{x}} - 2nlog(\theta) + 2\theta n\bar{x}$$

$$= -2n \log(\bar{x}\theta) + 2n(\theta\bar{x} - 1)$$

• We reject if:

$$-2n \log(\bar{x}\theta) + 2n(\theta\bar{x} - 1) > \chi^2_{\alpha,1}$$

• We accept if:

$$-2n \log(\bar{x}\theta) + 2n(\theta\bar{x} - 1) \le \chi_{\alpha,1}^2$$

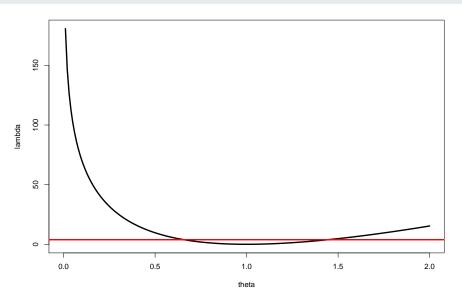
So our confidence set is:

$$C = \left\{ \theta \in \Theta : -2[\ell(\theta) - \ell(\hat{\theta})] \le \chi_{\alpha,1}^2 \right\}$$
$$= \left\{ -2n \log(\bar{x}\theta) + 2n(\theta\bar{x} - 1) \le \chi_{\alpha,1}^2 \right\}$$

- We can't solve this analytically, but let's graph it:
- Suppose $\bar{X} = 1$, n = 25, and $\alpha = 0.05$:

```
x.bar <- 1
n <- 25

theta <- seq(0,2, by =0.01)
lambda <- -2*n*log(x.bar*theta) + 2*n*(theta*x.bar - 1)
plot(theta, lambda, lwd=3, type="l")
abline(h=qchisq(1-0.05, 1), lwd=3, col="red")</pre>
```



```
min( theta[lambda <= qchisq(1-0.05, 1)])
## [1] 0.66

max( theta[lambda <= qchisq(1-0.05, 1)])</pre>
```

• So a 95% confidence interval for θ is:

[1] 1.44

 $[0.66 \ , \ 1.44]$

- Now suppose we want the interval for $au = \frac{1}{\theta}$.
- Let's reparametrize the log likelihood:

$$\ell(\tau) = \ell(\theta = \tau^{-1}) = n\log(\tau^{-1}) - \tau^{-1} \sum x_i$$
$$= -n\log(\tau) - n\frac{\bar{x}}{\tau}$$

$$\begin{array}{lcl} -2[\ell(\tau) - \ell(\hat{\tau})] & = & 2[\ell(\hat{\tau}) - \ell(\tau)] \\ & = & 2[-n\log(\hat{\tau}) - n\frac{\bar{x}}{\hat{\tau}} + n\log(\tau) + n\frac{\bar{x}}{\tau}] \\ & = & 2[-n\log(\bar{x}) - n\frac{\bar{x}}{\bar{x}} + n\log(\tau) + n\frac{\bar{x}}{\tau}] \\ & = & -2n\log(\bar{x}\tau^{-1}) + 2n(\tau^{-1}\bar{x} - 1) \end{array}$$

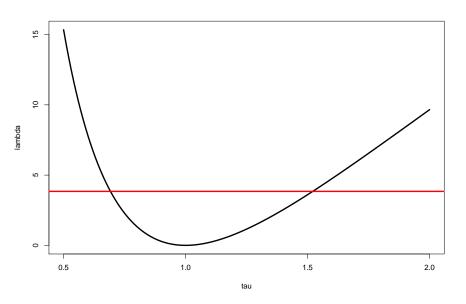
- ullet All that was done through all the math was to replace heta with $au^{-1}!$
- So our interval is:

$$[1/1.44 , 1/0.66] = [0.69 , 1.51]$$

- Let's see it in the plot
- Again, suppose $\bar{X} = 1$, n = 25, and $\alpha = 0.05$:

```
x.bar <- 1
n <- 25

tau <- seq(0.5, 2, by =0.01)
lambda <- -2*n*log(x.bar*(1/tau)) + 2*n*((1/tau)*x.bar - 1)
plot(tau, lambda, lwd=3, type="l")
abline(h=qchisq(1-0.05, 1), lwd=3, col="red")</pre>
```



```
min( tau[lambda <= qchisq(1-0.05, 1)])
## [1] 0.7

max( tau[lambda <= qchisq(1-0.05, 1)])</pre>
```

[1] 1.52

Maximimum LRT Interval Estimation

Did we have to use the asymptotic result of the LRT for our interval.
 No, but it is more straightforward.

Interval Estimation - CDF Method

- Pivoting the CDF
 - A pivot Q leads to a confidence set:

$$C(\mathbf{x}) = \{\theta_0 : a \leq Q(\mathbf{x}; \theta_0) \leq b\}$$

- If for every x the pivot is a monotone function of θ then the confidence set C(x) is guaranteed to be an interval.
- Most pivots we have considered have this property.

Interval Estimation - CDF Method

Theorem:

- Let T be a statistic with a continuous cdf $F_T(t|\theta)$ [Note: We can also work with discrete distributions see C&B].
- Let $\alpha_1 + \alpha_2 = \alpha$ with $0 < \alpha < 1$.
- Suppose that for each $t \in \mathcal{T}$, the functions $\theta_L(t)$ and $\theta_U(t)$ can be defined as:
- **1.** If $F_T(t|\theta)$ is a decreasing function of θ for each t, define $\theta_L(t)$ and $\theta_U(t)$ by:

$$F_T(t|\theta_U(t)) = \alpha_1$$
 $F_T(t|\theta_L(t)) = 1 - \alpha_2$

2. If $F_T(t|\theta)$ is an increasing function of θ for each t, define $\theta_L(t)$ and $\theta_U(t)$ by:

$$F_T(t|\theta_L(t)) = \alpha_1$$
 $F_T(t|\theta_U(t)) = 1 - \alpha_2$

Then the interval $[\theta_L(t), \theta_U(t)]$ is a $1 - \alpha$ confidence interval for θ .

• We can prove that $F_T(t|\theta)$ is monotone in θ . See C&B.

Example: Consider $X_1, \ldots, X_n \stackrel{\text{iid}}{\sim} Unif(0, \theta)$.

• So we have the following CDF for X:

$$F_X(x|\theta) = \frac{x}{\theta} \mathbb{I}_{(0 \le x \le \theta)}$$

• We know the MLE for θ is $T = max(X_1, ..., X_n)$

$$F_{T}(t|\theta) = Pr(T \le t) = Pr\{max(X_{1}, \dots, X_{n}) \le t\}$$

$$= Pr\{X_{1} \le t, \dots, X_{n} \le t\}$$

$$= Pr\{X_{1} \le t\} \times \dots \times Pr\{X_{n} \le t\}$$

$$= \{F_{X}(t|\theta)\}^{n}$$

$$= \frac{t^{n}}{\theta^{n}} \mathbb{I}_{(0 \le t \le \theta)}$$

• Note: $F_T(t|\theta)$ is a deceasing function for θ . Let $\alpha_1 = \alpha_2 = \alpha/2$. We have:

$$F_{T}(t|\theta_{U}(t)) = \alpha/2$$

$$\left(\frac{t}{\theta_{U}}\right)^{n} = \alpha/2$$

$$\theta_{U} = t(\alpha/2)^{-(1/n)}$$

$$F_{T}(t|\theta_{L}(t)) = 1 - \alpha/2$$

$$\left(\frac{t}{\theta_{L}}\right)^{n} = 1 - \alpha/2$$

$$\theta_{L} = t(1 - \alpha/2)^{-(1/n)}$$

[1] 9.873539 12.605028

```
##
set.seed(1001)
n < -15
X \leftarrow runif(n, 0, 10)
t < - max(X)
alpha <- 0.05
##
theta.u \leftarrow t*(alpha/2)^(-(1/n))
theta.l \leftarrow t*(1-alpha/2)^{-(-(1/n))}
c(theta.1, theta.u)
```

39 / 80

- Interpretation: Over repeated sampling, we expect 95% of the intervals we create to contain the true value θ .
- Let's check: We set $\alpha = 0.05$, so 95% of the intervals should contain θ .

```
set.seed(1001)
S <- 10000
coverage <- rep(0, S)
theta.true <- 10
##
n <- 15
alpha <- 0.05
##
for(s in 1:S){
##
X <- runif(n, 0, theta.true)
t <- max(X)
theta.u <- t*(alpha/2)^(-(1/n))
theta.1 <- t*(1-alpha/2)^(-(1/n))
if(theta.l < theta.true && theta.u > theta.true){coverage[s] <- 1}
}
mean(coverage)
```

[1] 0.9517

• Suppose we have data X_1, \ldots, X_n from density $f_X(x|\theta)$ along with a prior distribution $\pi(\theta)$. As we saw we use Bayes' rule to update our 'beliefs' about θ once we observe the data:

$$\pi(\theta|\mathbf{x}) = \frac{L(\theta|\mathbf{x})\pi(\theta)}{\int_{\theta\in\Theta} L(\theta|\mathbf{x})\pi(\theta)d\theta}$$
$$= \frac{L(\theta|\mathbf{x})\pi(\theta)}{m(\mathbf{x})}$$

So we have the whole distribution for

$$\pi(\theta|\mathbf{x})$$

• This is different than the frequentist approach where find an estimator for θ , say $\hat{\theta}$ and then try to determine the distribution of $\hat{\theta}$.

• To obtain an interval we simply consider:

$$P\pi(\theta|x)(C) = \int_C \pi(\theta|x)d\theta = 1 - \alpha$$

- ullet Be careful. We are using lpha quite generically. Recall that lpha does have a formal definition: The probability of a Type-I error. This is based on repeated sampling. For the Bayesian case we only think about one data set an infinite number of possible data sets.
- There are quite a lot of choices for *C*. We will consider the 3 most common.

• Equal tailed:

$$\int_{-\infty}^{\theta_L} \pi(\theta|\mathbf{x}) d\theta = \alpha/2, \quad \int_{\theta_U}^{\infty} \pi(\theta|\mathbf{x}) d\theta = \alpha/2$$

• Smallest length: We can choose C to minimize $\theta_U - \theta_L$.

• Highest posterior density region (HPD): We define C to be that set with posterior probability $1-\alpha$ which satisfies the criterion:

$$\theta_1 \in C$$
 and $\pi(\theta_2|\mathbf{x}) > \pi(\theta_1|\mathbf{x}) \Rightarrow \theta_2 \in C$

 ${\it C}$ contains the values of θ which have the highest posterior density values, so that we can determine HPD regions as the set:

$$C = \{\theta \in \Theta : \pi(\theta|\mathbf{x}) > c_{\alpha}\}\$$

 If the posterior is unimodal then this will be the smallest length interval!

Example: $X_1, \ldots, X_n \stackrel{\text{iid}}{\sim} \text{exponential}(1/\theta) \text{ and } \pi(\theta) = \theta \exp(-\theta).$

$$\pi(\theta|\mathbf{x}) \propto \left\{ \prod_{i=1}^{n} \theta \exp(-x_{i}\theta) \right\} \theta \exp(-\theta)$$

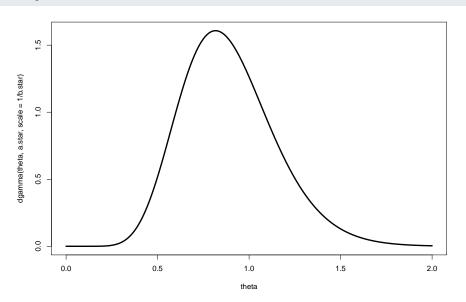
$$= \theta^{n} \exp(-\sum x_{i}\theta) \theta \exp(-\theta)$$

$$= \theta^{n+1} \exp(-\theta(n\bar{x}+1))$$

$$= \theta^{n+2-1} \exp(-\theta(n\bar{x}+1))$$

$$[\theta|\mathbf{x}] \sim gamma\left(n+2, \frac{1}{n\bar{\mathbf{x}}+1}\right)$$

• Let's plot the density for n = 10 and $\bar{x} = 1.247$.



• An equal-tailed 95% interval is given by $[\theta_I, \theta_u]$:

$$\int_0^{\theta_I} \pi(\theta | \mathbf{x}) = 0.025$$

$$F_{[\theta | \mathbf{x}]}(\theta_I) = 0.025$$

$$\int_{0}^{\theta_{u}} \pi(\theta | \mathbf{x}) = 1 - 0.025 = 0.975$$

$$F_{[\theta | \mathbf{x}]}(\theta_{u}) = 0.975$$

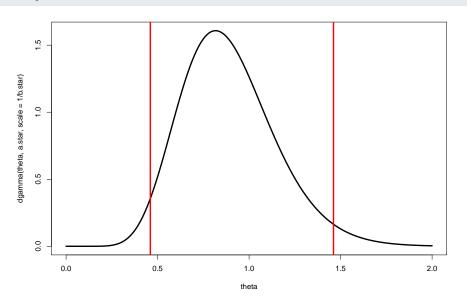
```
theta.L <- qgamma(0.025, a.star, scale=1/b.star)
theta.U <- qgamma(0.975, a.star, scale=1/b.star)

c(theta.L, theta.U)

## [1] 0.4603248 1.4611758
```

plot(theta, dgamma(theta, a.star, scale=1/b.star), type="1", 1

abline(v=c(theta.L, theta.U), lwd=3, col="red")



- If we only have tables in front of us, we can relate the gamma distribution to a χ^2 distribution as was discussed in tutorial the other week.
- If $[\theta|\mathbf{x}] \sim \operatorname{gamma}(\mathbf{a}^*, \mathbf{b}^*)$ then

$$\left[\frac{2\theta}{b^*}\middle|\mathbf{x}\right] \sim \operatorname{gamma}(a^*,2)$$
 $\sim \chi^2_{p=2a^*}$

• Using probabilities to the left. $p = 2a^* = 2n + 4$.

$$\begin{split} \left[\chi^2_{0.025,\rho} \leq & \frac{2\theta}{b^*} \middle| \mathbf{x} & \leq \chi^2_{0.975,\rho} \right] \\ \left[\chi^2_{0.025,\rho} \leq & 2\theta (n\bar{x}+1) \middle| \mathbf{x} & \leq \chi^2_{0.975,\rho} \right] \\ \left[\frac{\chi^2_{0.025,\rho}}{2(n\bar{x}+1)} \leq & \theta \middle| \mathbf{x} & \leq \frac{\chi^2_{0.975,\rho}}{2(n\bar{x}+1)} \right] \end{split}$$

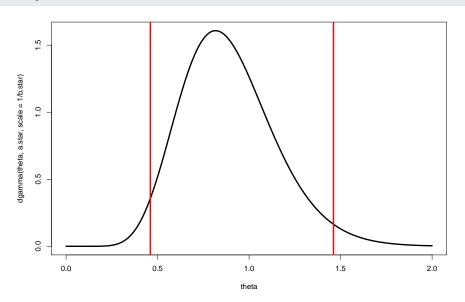
```
p <- 2*n + 4
theta.L <- qchisq(0.025, p)/(2*(n*x.bar+1))
theta.U <- qchisq(0.975, p)/(2*(n*x.bar+1))
c(theta.L, theta.U)</pre>
```

[1] 0.4603248 1.4611758

- Is the interval [0.4603, 1.4612] a HPD (highest posterior density) interval (the posterior is unimodal)?
- Recall:

$$\theta_1 \in C$$
 and $\pi(\theta_2|\mathbf{x}) > \pi(\theta_1|\mathbf{x}) \Rightarrow \theta_2 \in C$

• Let's see the density with the equal-tailed interval again.



ullet Note that the density seems to be higher for heta= 0.40 than heta= 1.4612:

```
dgamma(0.4, a.star, scale=1/b.star)
```

```
## [1] 0.1713707
```

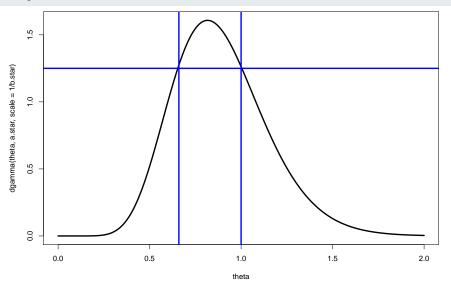
```
dgamma(1.4612, a.star, scale=1/b.star)
```

```
## [1] 0.1641042
```

• So the equal-tailed interval is not a HPD interval!

 To get the HPD interval we take horizontal slices across the density till we get the appropriate probability.

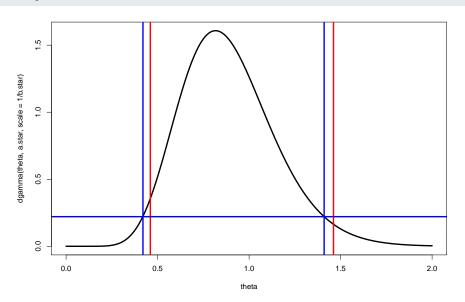
```
plot(theta, dgamma(theta, a.star, scale=1/b.star), type="l", lwd=3)
abline(h=1.25, lwd=3, col="blue")
##
theta \leftarrow seq(0, 2, by=0.01)
dens <- dgamma(theta, a.star, scale=1/b.star)
##
hpd.cut <- 1.25
theta.L <- min(theta[dens>=hpd.cut])
theta.U <- max(theta[dens>=hpd.cut])
abline(v=c(theta.L, theta.U), lwd=3, col="blue")
## interval probability
pgamma(theta.U, a.star, scale=1/b.star) -
  pgamma(theta.L, a.star, scale=1/b.star)
```



[1] 0.5062717

```
hpd.cut \leftarrow sort(seq(0.1, 1.25, by=0.0001), decreasing =TRUE)
c < -1
cred.int < -0.5063
while(cred.int<0.95){
theta.L <- min(theta[dens>=hpd.cut[c]])
theta.U <- max(theta[dens>=hpd.cut[c]])
## interval probability
cred.int <- pgamma(theta.U, a.star, scale=1/b.star) -</pre>
  pgamma(theta.L, a.star, scale=1/b.star)
c < - c + 1
HPD <- c(theta.L,theta.U)</pre>
HPD
```

[1] 0.42 1.41



- Let's check the length of each interval:
 - equal-tailed: 1.46 0.460 = 1.00
 - HPD: 1.41 0.42 = 0.99
- HPD is the shorter interval, but not by much.

- The bootstrap was used asses the bias and variability of an estimator, $\hat{\theta}$.
- The estimated standard deviation of any estimator $\hat{\theta}$ was derived by constructing some large number, B, of re-samples (with replacement) from the observed values of the sample, X_1, \ldots, X_n .
- The estimator was then applied to each of the B re-samples to construct:

$$\hat{\theta}_b^*$$
, $b = 1, \dots B$

• The estimated standard deviation was:

$$\hat{\sigma}_B(\hat{ heta}) = \sqrt{rac{1}{B-1}(\hat{ heta}_b^* - ar{ ilde{ heta}}^*)^2}$$

 We saw MLEs are asymptotically normal, and in fact many estimators are, we could just use that idea:

$$\left[\hat{\theta}-z_{\alpha/2}\hat{\sigma}_B(\hat{\theta})\right], \quad \hat{\theta}+z_{\alpha/2}\hat{\sigma}_B(\hat{\theta})$$

- For means, we relied on the Central Limit Theorem to construct intervals when we didn't know the underlying probability distribution.
- Roughly, the bootstrap interval is a natural extension to the Central Limit Theorem for estimators which are not in the form of an average.
- For small samples we still might be in trouble so why not use a Student's t-distribution quantiles instead of the standard normal quantiles?

$$t_{n-1, \alpha/2}$$

- Recall, that $\hat{\theta}_b^*$ not only provide us with estimates of the bias and standard deviation of our estimator, $\hat{\theta}$, but also of its entire distribution.
- We can use the empirical quantiles of the "bootstrap distribution". So we have:

$$P_{\hat{F}}(\hat{\theta}^* \leq \hat{\theta}_L^*) = \alpha/2, \qquad P_{\hat{F}}(\hat{\theta}^* \leq \hat{\theta}_U^*) = 1 - \alpha/2$$

• Let's consider a general third approach. Remember what we are doing:

$$\hat{F}^* \to \hat{F} \to F$$

- Instead of bootstrapping we might instead choose to bootstrap some other quantity $Q(F,\hat{F})$ and use its simulated quantiles to construct an interval.
- The simplest example of such an approach is to consider a quantity which we believe is (approximately) pivotal; for example:

$$Q = Q(F, \hat{F}) = \frac{\theta(\hat{F}) - \theta(F)}{\hat{\sigma}(F)}$$

• The trick of course is that we equate $Q(F, \hat{F})$ with $Q(\hat{F}, \hat{F}^*)$.

$$1 - \alpha = P(q_L \le Q(F, \hat{F}) \le q_U) = P(q_L \le Q(\hat{F}, \hat{F}^*) \le q_U)$$

ullet We can see that q_I and q_U can be estimated by generating re-samples:

$$\hat{Q}_b = Q(\hat{F}, \hat{F}^*)$$
 (i.e. bootstrap samples)

1. Using B re-samples, calculate \hat{Q}_b for each re-sample and approximate q_l and q_U with (where $\alpha_1 + \alpha_2 = \alpha$) using the empirical distribution of \hat{Q} :

$$\hat{q}_I = \hat{Q}_{\alpha_1}$$
 $\hat{q}_I = \hat{Q}_{1-\alpha_2}$

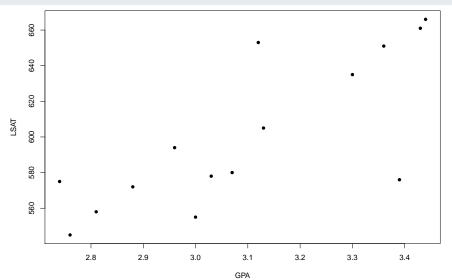
2. Construct the confidence interval using a "pivoting" argument:

$$\begin{aligned} 1 - \alpha &= P(q_L \leq Q(F, \hat{F}) \leq q_U) \\ &\approx P(\hat{q}_L \leq Q(F, \hat{F}) \leq \hat{q}_U) \\ &= P\left(\hat{q}_L \leq \frac{\theta(\hat{F}) - \theta(F)}{\hat{\sigma}(F)} \leq \hat{q}_U\right) \\ &= P\left(\theta(\hat{F}) - \hat{q}_U \hat{\sigma}(F) \leq \theta(F) \leq \theta(\hat{F}) - \hat{q}_L \hat{\sigma}(F)\right) \\ &[\theta(\hat{F}) - \hat{q}_U \hat{\sigma}(F), \theta(\hat{F}) + \hat{q}_L \hat{\sigma}(F)] \end{aligned}$$

• Let's revisit our Law School example again.

```
plot(GPA, LSAT, pch=16)

##
rho.hat <- cor(LSAT, GPA)
rho.hat</pre>
```



[1] 0.7763745

• Let's bootstrap ρ :

```
### Let's do B samples
set.seed(1001)
B <- 10000
D.B <- array(list(), B)
rho.hat.b \leftarrow rep(0, B)
for(b in 1:B){
S <- sample(1:n, n, replace = TRUE)
D.B[[b]] <- D[S,]
##
rho.hat.b[b] <- cor(D.B[[b]]$LSAT, D.B[[b]]$GPA)</pre>
```

Let's create intervals based on asymptotic normality:

$$\hat{\rho} = 0.7764$$

```
Var.B.hat <- var(rho.hat.b)
Var.B.hat

## [1] 0.01790244

## interval based on asymptotic normality
alpha <- 0.05

c(rho.hat - qnorm(1-alpha/2)*sqrt(Var.B.hat),
    rho.hat + qnorm(1-alpha/2)*sqrt(Var.B.hat))</pre>
```

[1] 0.5141313 1.0386177

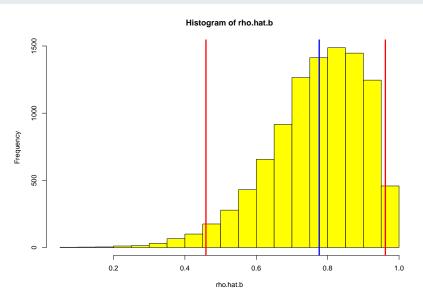
• So we have the interval:

But this extends beyond the range of ρ . Recall: $-1 \le \rho \le 1$.

• Let's just look at the density of the bootstrap values and use the bootstrap percentile method (i.e. the empirical quantiles):

```
## Now let's just examine the
## bootstrapped values and use
## the empirical values
hist(rho.hat.b, col="yellow", freq=TRUE)
alpha=0.05
qu <- quantile(rho.hat.b, c(alpha/2, 1-alpha/2))
qu
abline(v=qu, col="red", lwd=3)
abline(v=rho.hat, col="blue", lwd=3)</pre>
```

```
## 2.5% 97.5%
## 0.4589734 0.9617267
```



- We see that this interval remains within the allowable range for correlation coefficients.
- Also, that this interval is not symmetric around the point estimate $\hat{\rho}=0.7764$, which is clear from the skewness of the bootstrap histogram.

Example: In this question consider constructing a 95% interval $(\alpha_1 = \alpha_2 = \alpha/2)$ for ρ based on:

$$Q = \hat{\rho} - \rho$$

• We use the B = 10000 re-sampled values:

$$\hat{Q}_b = \hat{\rho}_b^* - \hat{\rho}$$

• Notice that the only resampled part of the equation is $\hat{\rho}_b^*$ so:

$$\hat{Q}_{\alpha/2} = \hat{\rho}_{\alpha/2}^* - \hat{\rho}, \quad \hat{Q}_{1-\alpha/2} = \hat{\rho}_{1-\alpha/2}^* - \hat{\rho}$$

• Now let's form our interval and pivot ($\alpha = 0.05$):

$$1 - \alpha = 0.95 \approx P(\hat{Q}_{\alpha/2} \le \hat{\rho} - \rho \le \hat{Q}_{1-\alpha/2})$$

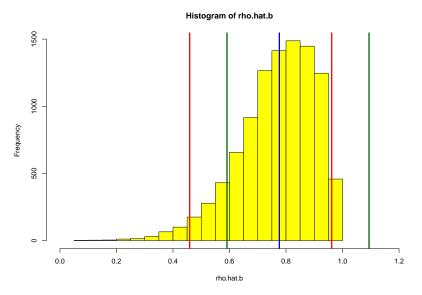
$$= P(\hat{\rho}_{\alpha/2}^* - \hat{\rho} \le \hat{\rho} - \rho \le \hat{\rho}_{1-\alpha/2}^* - \hat{\rho})$$

$$= P(\hat{\rho}_{\alpha/2}^* - 2\hat{\rho} \le -\rho \le \hat{\rho}_{1-\alpha/2}^* - 2\hat{\rho})$$

$$= P(2\hat{\rho} - \hat{\rho}_{1-\alpha/2}^* \le \rho \le 2\hat{\rho} - \hat{\rho}_{\alpha/2}^*)$$

$$\begin{split} [2\hat{\rho} - \hat{\rho}_{[1-\alpha/2]}^* \;,\; 2\hat{\rho} - \hat{\rho}_{[\alpha/2]}^*] \\ [2\times0.7764 - 0.9617 \;,\; 2\times0.7764 - 0.4590] \\ [0.5911 \;,\; 1.0938] \end{split}$$

• This interval also goes outside the range of ρ .



Properties of Intervals

- What we like:
 - Shortest intervals for a given confidence or credibility (eg. 95%).
 - Range respecting
 - Parameterization equivariance (We would like our interval construction procedures to transform appropriately if we change our focus from $x = \pi(\theta)$ to $\alpha = \alpha(\pi) = \alpha(\pi)$

$$\tau = \tau(\theta)$$
 to $\gamma = \gamma(\tau) = \gamma\{\tau(\theta)\}\$