



# Statistics for Astronomers: Lecture 9, 2020.10.28

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The Empirical Rule for normal distributions, the *z*-score. Student's *t*-distribution, the *t*-score. Interval estimates: the confidence interval.



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The true parameter value  $\theta$  is fixed. Repeated observations generate a distribution  $p_{\theta}(\hat{\theta})$  of point estimates  $\hat{\Theta}$  for  $\theta$ . Use this distribution to constrain the true value – interval estimate. Most common interval estimate: confidence interval (CI).



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)% CI (for  $\theta$ ) is  $[a, b]$ "  $\implies P(a \le \hat{\Theta} \le b) = \int_{a}^{b} p_{\theta}(\hat{\theta}) \ d\hat{\theta} = 1 - \alpha$   
 $\implies P(\hat{\Theta} < a) + P(\hat{\Theta} > b) = \alpha$   
(Note: definitions don't contain  $\theta$ , only its estimates)



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#### Frequentist interpretation of CI convoluted! Bayesian "credible interval" more straightforward.

"95% Cl of [-1.3, 1.3]" = fixed (unknown)  $\theta$  such that we observe  $\hat{\Theta}$  outside  $[-1.3, 1.3] \leq 5\%$  of the time.

Equivalently, if CI computed  $N \gg 1$  times using the same procedure, 95% of CIs will contain true value.

Since  $\theta$  fixed, a single CI will either trap it (probability = 1) or it won't (probability = 0).



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"A 95% CI (for  $\theta$ )" = "fraction of CIs generated in same fashion that trap true value  $\theta$  is 0.95".  $\neq$  "the probability that a single CI traps the true value is 0.95". Note: "<u>A</u> 95% CI" and not "<u>the</u> 95% CI" – for symmetric distributions, less ambiguous.



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Perform an experiment each day, trap a parameter  $\theta_j$  in a 95% CI on the  $j^{th}$  day. As long as you use the same procedure to construct the CI, it doesn't even have to be the same experiment!!. In the long run, 95% of the intervals you constructed would have trapped the true value of whatever parameter you were exploring.

BUT  $P(\text{parameter trapped in today's CI}) \in \{0, 1\}.$ 



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Example: If  $\hat{\theta}_0$  is the mean of estimates for  $\theta$ , and  $\sigma^2(\hat{\theta}_0)$  the variance around this mean,

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)% CI is such that, for some  $\ell_{\alpha/2}$ ,  $P\left(\left|\frac{\theta - \hat{\theta}_0}{\sigma(\hat{\theta}_0)}\right| \ge \ell_{\alpha/2}\right) \le \alpha$ .



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we get an approximate 100(1-lpha)% CI if we choose  $\ell_{lpha/2}=1/\sqrt{lpha}.$ 

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Example of a point estimate: MLE. Find  $\hat{\theta}_{\text{MLE}}$  such that  $\mathscr{L}(\theta)$  is maximum. If  $\mathscr{L}(\theta)$  known for all values allowed for  $\theta$ , CI computation straightforward. If not, use the CRLB to at least find lower bound on variance. Let's look at some examples for CIs using MLE.



Consider X drawn from an unknown distribution with mean  $\mu$  and variance  $\sigma^2$ . Perform a trial N times, obtain values  $\{x_i\}$   $(i = 1, \dots, N)$ .



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Uncertainty associated with each data point  $x_i$ :  $\sigma$  ("1 $\sigma$  uncertainty on a single observation"). sample mean  $\overline{x}$ , from Central Limit Theorem:  $\sigma/\sqrt{N}$  ("1 $\sigma$  uncertainty on sample mean").



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In this context, "1\sigma" is short for "one standard deviation", not to the literal value \sigma.
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In this particular example, the "1 $\sigma$  uncertainty" happens to have the value  $\sigma$  for a single observation and the value  $\sigma/\sqrt{N}$  for the sample mean.

These results are true for any distribution. If  $\sigma$  unknown, estimate from data.



Case 1:  $X \sim \mathcal{N}(\mu, \sigma^2)$ . Single observation x. MLE for  $\mu$ :

Case 2:  $X \sim \mathcal{N}(\mu, \sigma^2)$ . *N* observations  $\{x_i\}$   $(i = 1, \dots, N)$ . MLE for  $\mu$ :



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Noting  $\sum_{i=1}^{N} (x_i - \mu)^2 = \sum_{i=1}^{N} (x_i - \bar{x})^2 + \sum_{i=1}^{N} (\bar{x} - \mu)^2 = N\left(\frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})^2 + (\bar{x} - \mu)^2\right).$ 



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 $2\sigma$  CI (= 95% CI for Gaussian) centered at  $\hat{\mu}_{MLE}$  with variance  $\sigma^2(\hat{\mu}_{MLE})$ :  $\left[\hat{\mu}_{MLE} - 2\sigma(\hat{\mu}_{MLE}), \ \hat{\mu}_{MLE} + 2\sigma(\hat{\mu}_{MLE})\right]$ 



Case 1:  $X \sim \mathcal{N}(\mu, \sigma^2)$ . Single observation *x*. MLE for  $\mu$ :  $\hat{\mu}_{\text{MLE}} = x$ .

$$\mathscr{L}(\mu) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{\mu-x}{\sigma}\right)^2\right]$$

 $\Rightarrow \mathscr{L}(\mu) \propto \mathscr{N}(\hat{\mu}_{\mathrm{MLE}}, \sigma^2(\hat{\mu}_{\mathrm{MLE}})), \text{ with } \hat{\mu}_{\mathrm{MLE}} = x \text{ and } \sigma(\hat{\mu}_{\mathrm{MLE}}) = \sigma.$ 

Case 2:  $X \sim \mathcal{N}(\mu, \sigma^2)$ . N observations  $\{\overline{x_i}\}$   $(i = 1, \cdots, N)$ . MLE for  $\mu$ :  $\hat{\mu}_{\text{MLE}} = \overline{x}$ .

$$\begin{aligned} \mathscr{L}(\mu) &= \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2} \left(\frac{x_{i}-\mu}{\sigma}\right)^{2}\right] = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^{N} \exp\left[-\frac{1}{2} \sum_{i=1}^{N} \left(\frac{x_{i}-\mu}{\sigma}\right)^{2}\right]. \end{aligned}$$

$$\begin{aligned} \text{Noting } \sum_{i=1}^{N} (x_{i}-\mu)^{2} &= \sum_{i=1}^{N} (x_{i}-\overline{x})^{2} + \sum_{i=1}^{N} (\overline{x}-\mu)^{2} = N \left(\frac{1}{N} \sum_{i=1}^{N} (x_{i}-\overline{x})^{2} + (\overline{x}-\mu)^{2}\right). \end{aligned}$$

$$\begin{aligned} \mathscr{L}(\mu) \propto \exp\left[-\frac{N}{2} \left(\frac{\overline{x}-\mu}{\sigma}\right)^{2}\right] &= \exp\left[-\frac{1}{2} \left(\frac{\mu-\overline{x}}{\sigma/\sqrt{N}}\right)^{2}\right] \end{aligned}$$

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$$\begin{aligned} \Longrightarrow \mathscr{L}(\mu) \propto \mathscr{N}(\hat{\mu}_{\text{MLE}}, \sigma^{2}(\hat{\mu}_{\text{MLE}})), \text{ where } \hat{\mu}_{\text{MLE}} &= \overline{x} \text{ and } \sigma(\hat{\mu}_{\text{MLE}}) = \sigma/\sqrt{N}. \end{aligned}$$

 $2\sigma$  CI (= 95% CI for Gaussian) centered at  $\hat{\mu}_{MLE}$  with variance  $\sigma^2(\hat{\mu}_{MLE})$ :  $\left[\hat{\mu}_{MLE} - 2\sigma(\hat{\mu}_{MLE}), \ \hat{\mu}_{MLE} + 2\sigma(\hat{\mu}_{MLE})\right]$ 

$$\implies \text{Case 1: } [x - 2\sigma, x + 2\sigma]. \text{ Case 2: } \left[\overline{x} - 2\frac{\sigma}{\sqrt{N}}, \overline{x} + 2\frac{\sigma}{\sqrt{N}}\right]$$

A single measurement of the mass of a rock results in a value of 0.2 kg.

The  $1\sigma$  measurement uncertainty due to the resolution of the mass measuring device is 0.05 kg.





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Construct a 99.7% CI on the true mass of the rock.

Using the Empirical Rule, 99.7% corresponds approx. to  $3\sigma$ .

90.7% CI =  $[\widehat{\mu} - 3\sigma, \widehat{\mu} + 3\sigma] = [0.2 - 0.15, 0.2 + 0.15] = [0.05, 0.35]$  kg.

"The mass of the rock is (0.2  $\pm$  0.15) kg (3 $\sigma$ )".





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"The mass of the rock is (0.2  $\pm$  0.15) kg (3 $\sigma$ )".

Construct a 82% CI on the true mass of the rock.

$$\begin{split} &100(1-\alpha)=82 \implies \alpha=0.18.\\ &\text{scipy.stats.norm.ppf}(0.18/2)=-1.341\\ &\text{scipy.stats.norm.ppf}(1-0.18/2)=1.341 \quad \#"1.341 \text{ sigma confidence interval"}\\ &\text{Cl:} [\widehat{\mu}-1.341\sigma, \widehat{\mu}+1.341\sigma]=[0.2-0.067,0.2+0.067]\approx [0.133,0.267] \text{ kg}. \end{split}$$





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What confidence is associated with the interval [0.00545, 0.3946] kg?

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scipy.stats.norm.ppf(1-0.18/2) = 1.341 #"1.341 sigma confidence interval" Cl:  $[\hat{\mu} - 1.341\sigma, \hat{\mu} + 1.341\sigma] = [0.2 - 0.067, 0.2 + 0.067] \approx [0.133, 0.267]$  kg.

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We just said something probabilistic about a true parameter with only one data point! Assumptions: uncertainties are Gaussian, we know the standard deviation.



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### Example: CI for Gaussian uncertainties with unknown $\sigma$

Three measurements of the mass of a rock results in values of 0.2, 0.35, and 0.25 kg. As usual,  $\hat{\mu} = \overline{x}$ .

 $\sigma$  unknown, estd. from data  $\implies$  functional form of  $\mathscr{L}(\mu)$ : Student's *t*-distribution around  $\hat{\mu}$ .

m = np.array([0.2, 0.35, 0.25]); m.mean = m.mean(); m.std = m.std(ddof = 1) $\hat{\mu} = \bar{x} = 0.267 \text{ kg. } \#dof = N - 1 = 2. \ \hat{\sigma} = 0.076 \text{ kg} (Bessel-corrected).$ 





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Use methods in scipy.stats.t for the following:

Construct a 95% CI on the true mass of the rock. Find value of t (Studentised) for which  $P(|T| \le t) = 0.95$ . k95 = t.ppf((1-0.95)/2, df = 2) #number of std dev from mean 95% CI =  $[\widehat{\mu} - k95 \cdot \widehat{\sigma}, \widehat{\mu} + k95 \cdot \widehat{\sigma}]$ =  $[0.267 - 4.303 \times 0.076, 0.267 + 4.303 \times 0.076] = [0.06, 0.59]$  kg. In general, 95% CI for Student's t wider than 95% CI for Gaussian.



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What confidence is associated with the interval [-0.0484, 0.5824] kg?



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Flip a coin N = 100 times. Observe: 75 heads, 25 tails. What is P(Head)? What is the 95% CI for this estimate?



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Flip a coin N = 100 times. Observe: 75 heads, 25 tails. What is P(Head)? What is the 95% CI for this estimate?

Recall: for a Binomial distribution with N trials and k successes, if  $\theta = P(1 \text{ success})$ ,  $\mathbb{E}[k] = N\theta$ , and  $\operatorname{Var}[k] = N\theta(1 - \theta)$ .



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MLE (See <u>Lecture 6, Slide 4</u>):  $\hat{\theta}_{\rm MLE} = \frac{k}{N} = 0.75.$ 



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 $\Longrightarrow \hat{\sigma}(\hat{\theta}_{MLE}) \approx 0.043.$ 



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asymmetric function, so CI needs to be constructed with care. However, this problem satisfies conditions for a Gaussian approximation:  $\mathscr{L}(\theta) \approx \mathscr{N}\left(\hat{\theta}_{\mathrm{MLE}}, \overline{\sigma^2}(\hat{\theta}_{\mathrm{MLE}})\right) = \mathscr{N}(0.75, (0.043)^2).$ 







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A 95% CI for this problem is also a  $2\sigma$  CI:  $[0.75 - 2 \times 0.043, 0.75 + 2 \times 0.043] \approx [0.66, 0.84]$ .



Example:  $\mathscr{L}(\theta) = f \mathscr{N}(\mu_1, \sigma_1^2) + (1 - f) \mathscr{N}(\mu_2, \sigma_2^2)$  with 0 < f < 1 (mixture of Gaussians).



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Let's construct 50% CIs of each type...





A 100(1 -  $\alpha$ )% central CI is  $[\theta_-, \theta_+]$  such that  $P(\hat{\theta} \leq \theta_-) = P(\hat{\theta} \geq \theta_+) = \alpha/2$ .



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In our specific Gaussian-mixture example, the 50% central CI encloses the mean, median, and mode of the distribution.

Verify: P(left) = P(right) = 50/2 = 25%.

Central CI width for this example: 0.53 + 0.68 = 1.21.





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What happens to the central CI as its width shrinks?





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Statistics for Astronomers: Lecture 9, 2020.10.28

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Verify:  $P(\text{left}) + P(\text{right}) \approx 0.45 + (1 - 0.95) = 50\%$ . Shortest CI width for this example: 0.85 - 0.09 = 0.76.





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#### Caution!

Sharply peaked, close local maxima – shortest CI may be composed of disconnected regions.





Unlike the other two types of CI, symmetric CIs are not unique. They depend on the choice of centre.



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Verify:  $P(\text{left}) + P(\text{right}) \approx 0.45 + (1 - 0.95) = 50\%$ . Symmetric CI width for this example: 0.88 - 0.11 = 0.77.





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#### Caution!

Multimodal, (almost-)symmetric functions – MLE might pick one peak over the other!

Highly asymmetric functions: if centre of the CI is very far from median, not possible to define a symmetric CI for small  $\alpha$  (also in this example!).





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#### 95% CI: [0.043, 0.641].



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