2025 May 20 : CIAO Workshop UMass Lowell

Source Detection & Statistics

VINAY KASHYAP
CfA / CXC-Calibration

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Basics of high-energy Astrostatistics

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Outline

- Why bother?
- What to bother about
  - errors, uncertainties, and appropriateness
  - detection, fitting :: deciding, estimating
- Where CIAO/Sherpa is doing the bothering for you

In the space of one hundred and seventy-six years the Lower Mississippi has shortened itself two hundred and forty-two miles. Therefore, any calm person, who is not blind or idiotic … can see that seven hundred and forty-two years from now the lower Mississippi will be only a mile and three-quarters long.

There is something fascinating about science. One gets such wholesale returns of conjecture out of such a trifling investment of fact.

–Mark Twain, Life on the Mississippi

Lessons from Sam Clemens

- Generalization is the foundational cornerstone of science, especially of astronomy, and it is trivially easy to shoot yourself in the foot
- It is easy to run into situations where fluctuations can ruin an observation, or you push your model of the Universe too far into realms where it is not applicable
- We must pay attention to errors and uncertainties in the data, on the quality of the models we build to explain them, and how we make decisions and draw inferences

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- Interpretation of observations needs a model
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- Astrostatistics is a system to
    - quantify uncertainty
    - extend inference to complex systems
    - make decisions

Error bars

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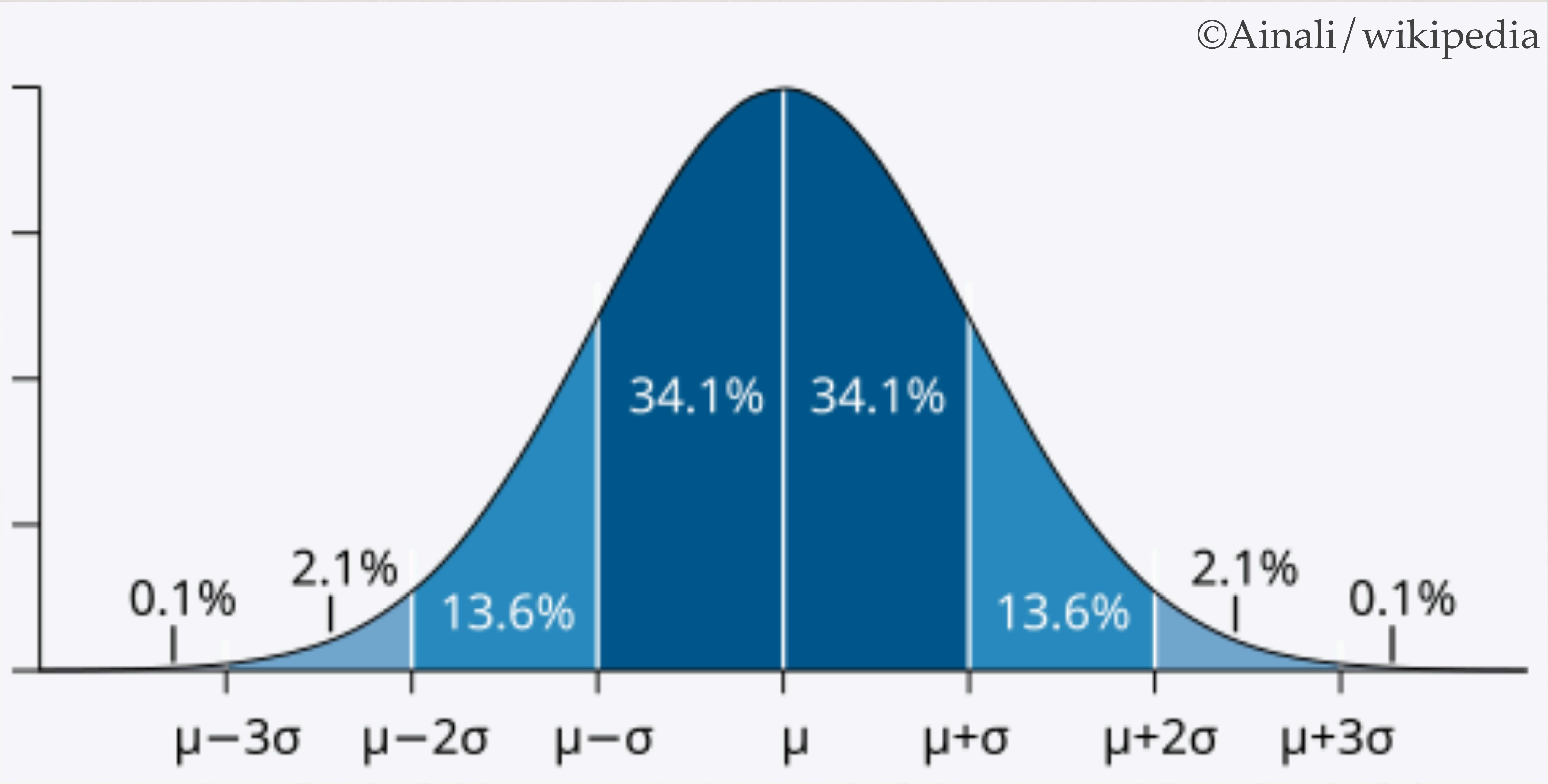
- Invented by Gauss while figuring out where Ceres would reappear after coming around the Sun:
  - Measurement uncertainties follow a "normal" distribution, with deviations being symmetrical, large discrepancies being less frequent, and the average represents the likely value



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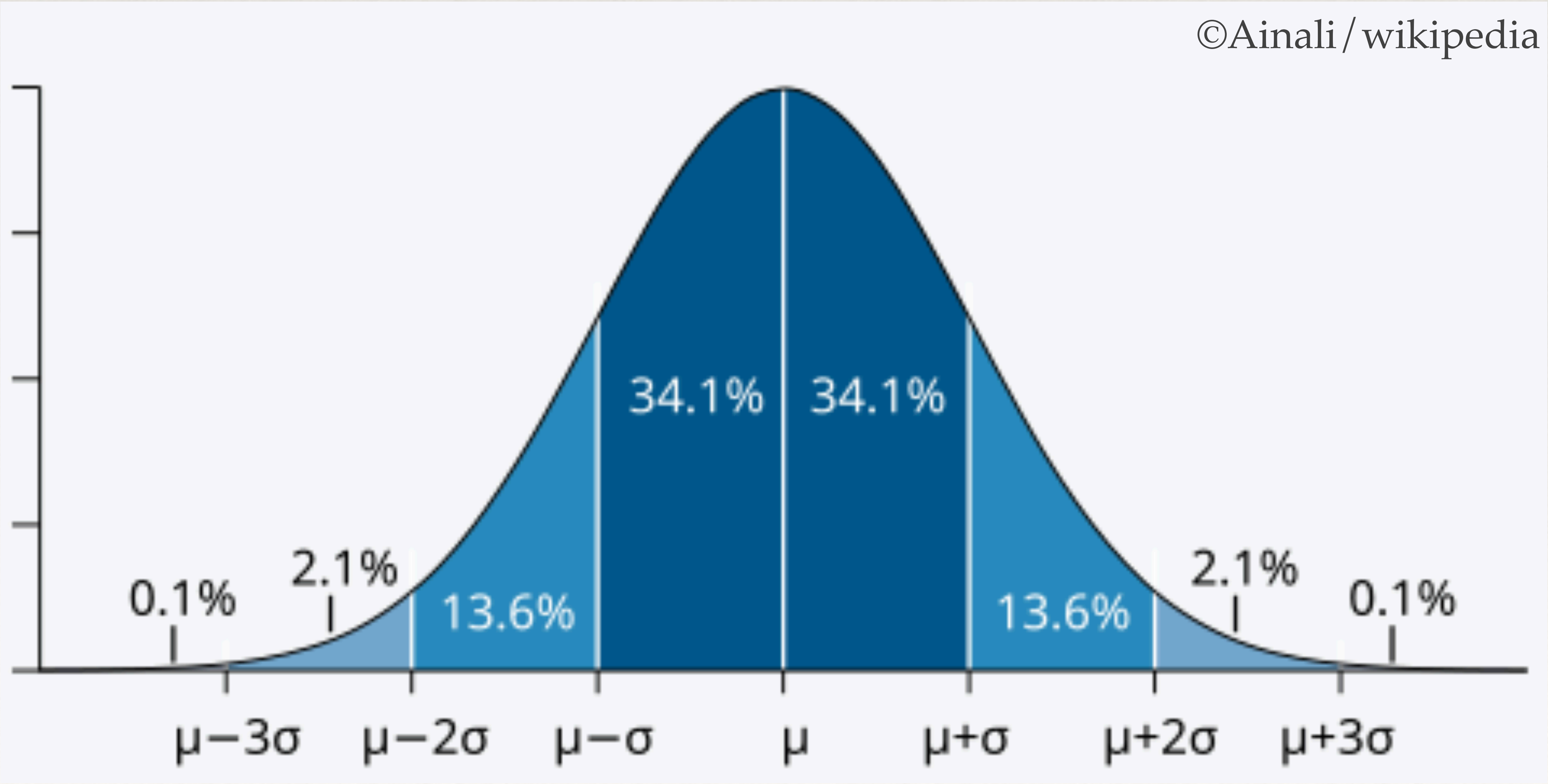

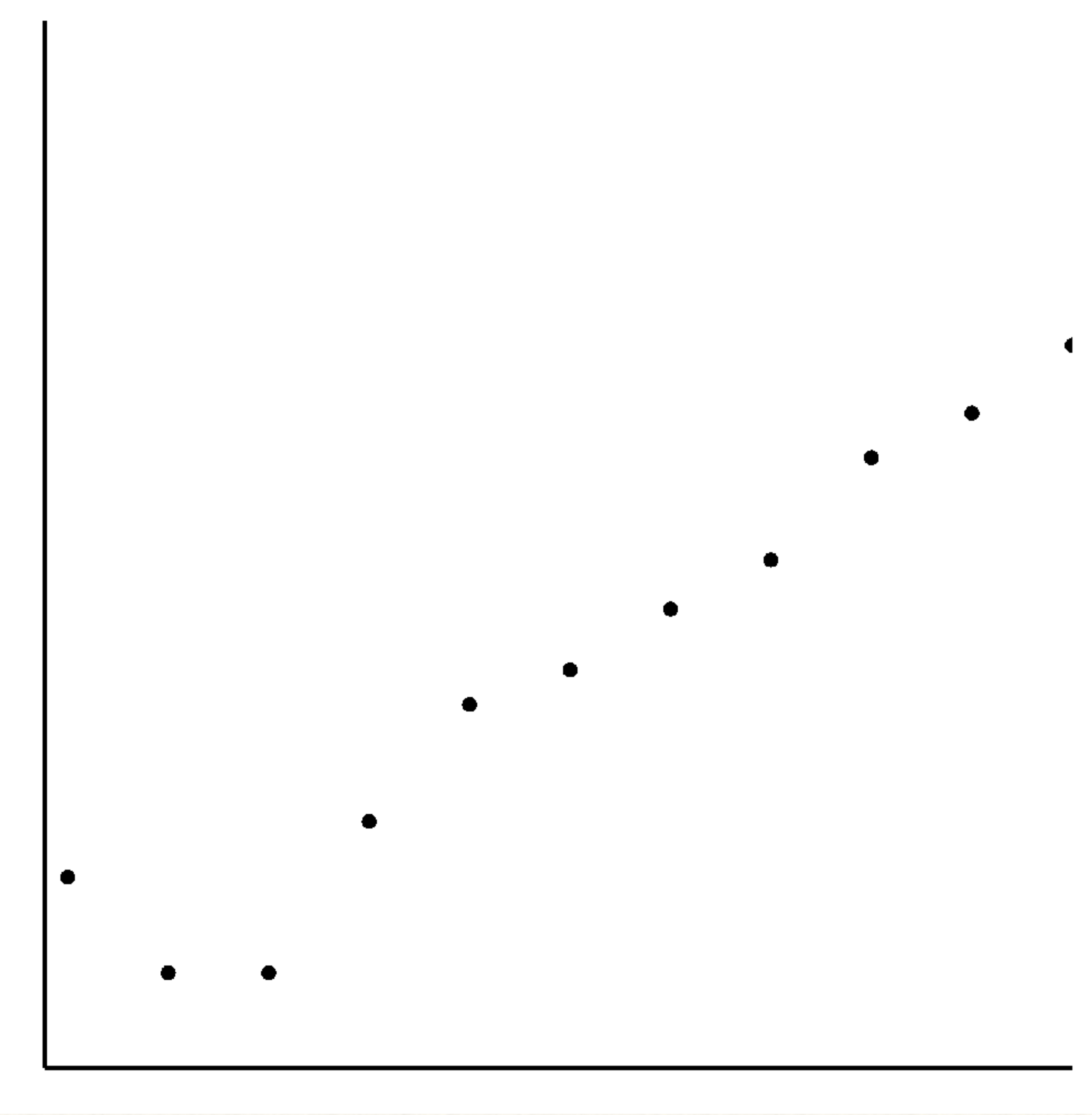

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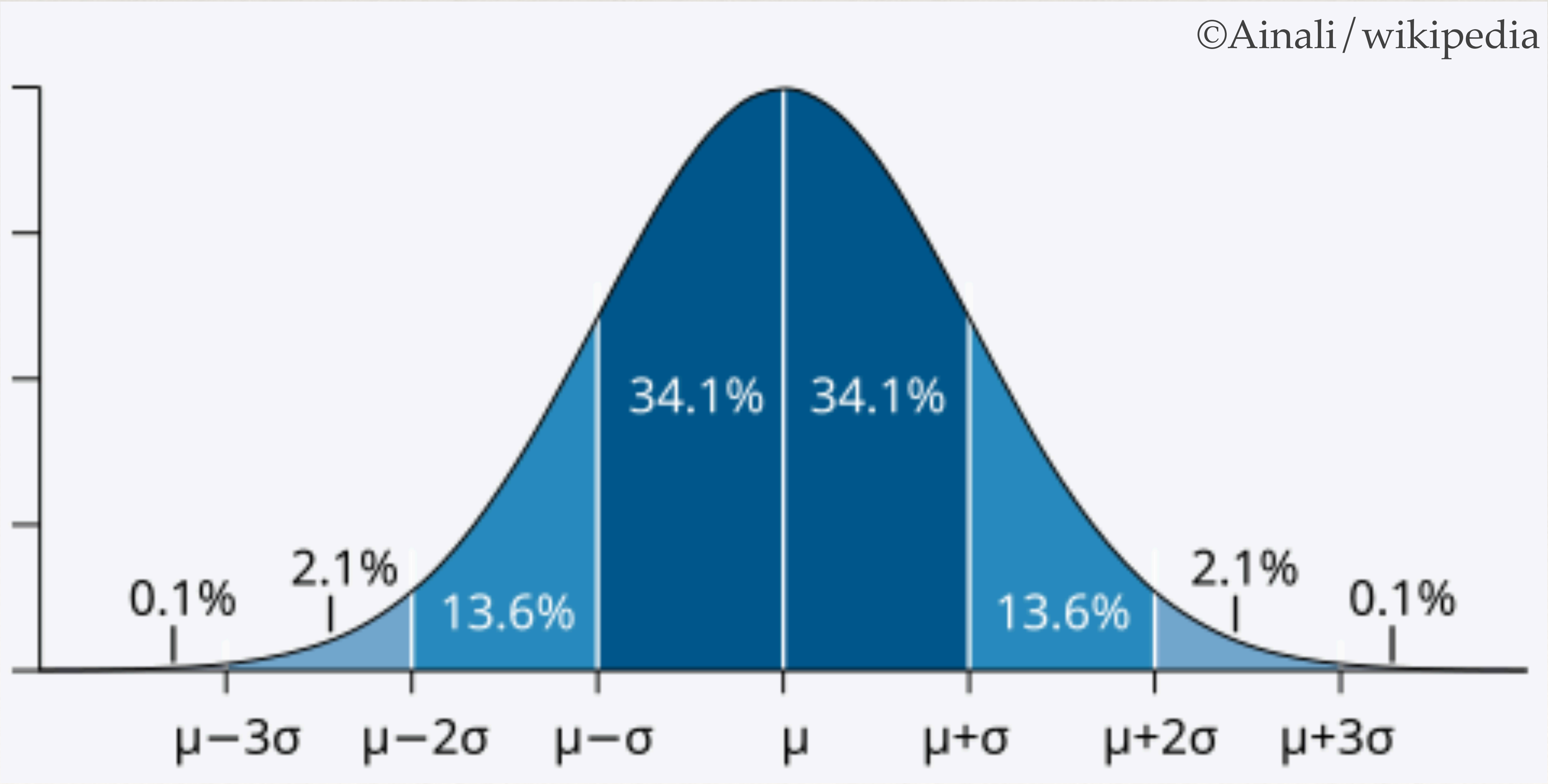

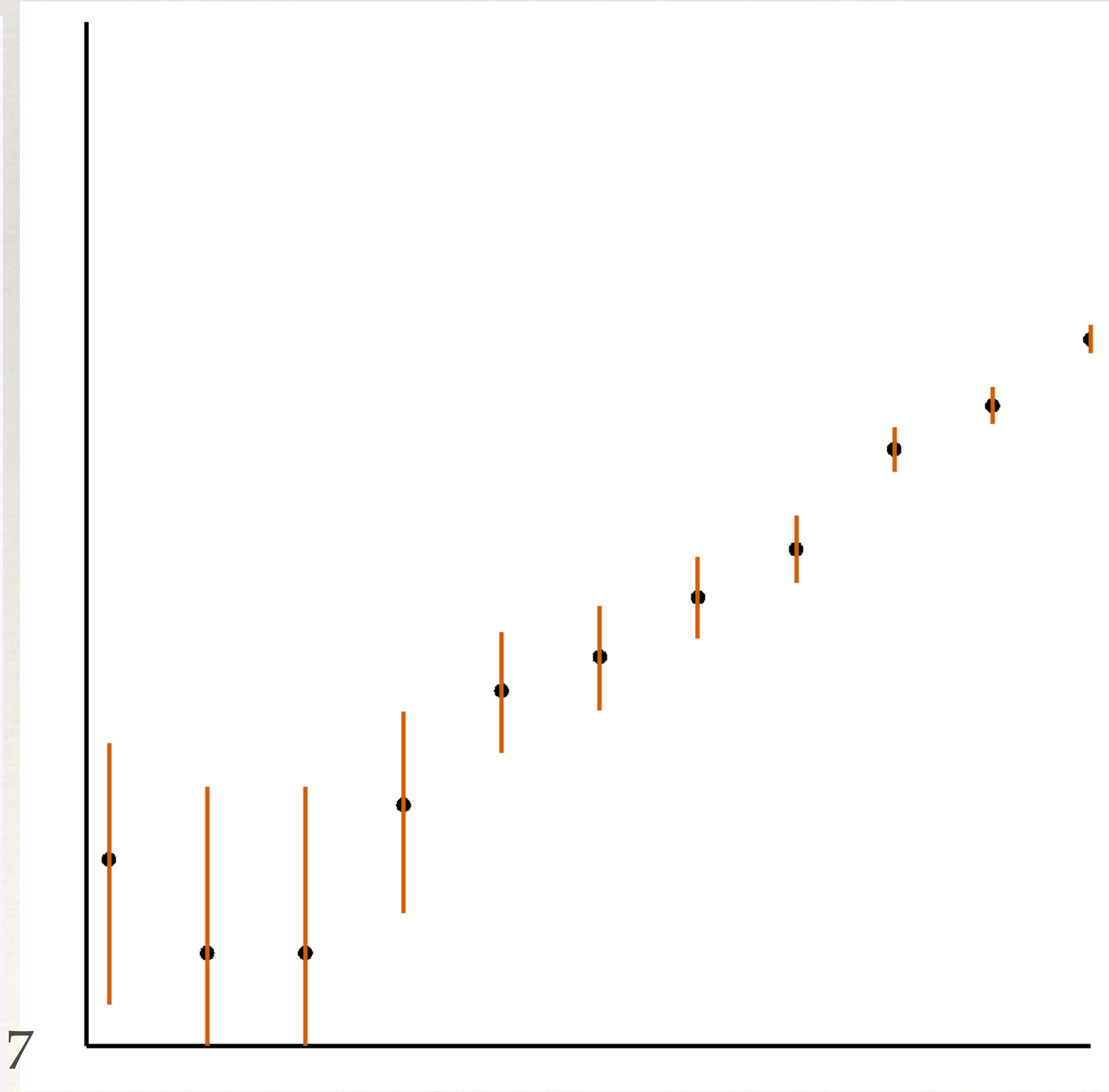

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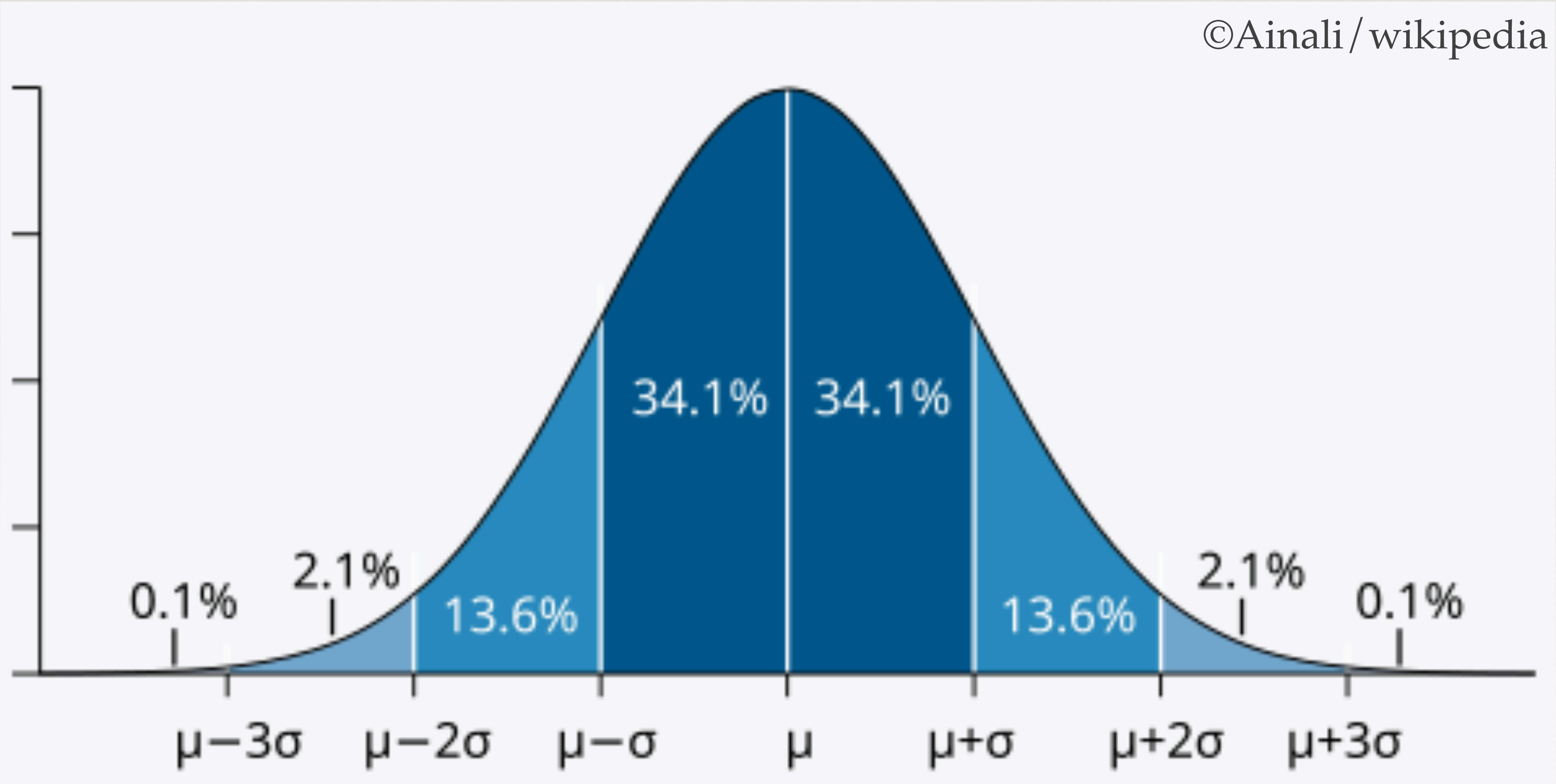
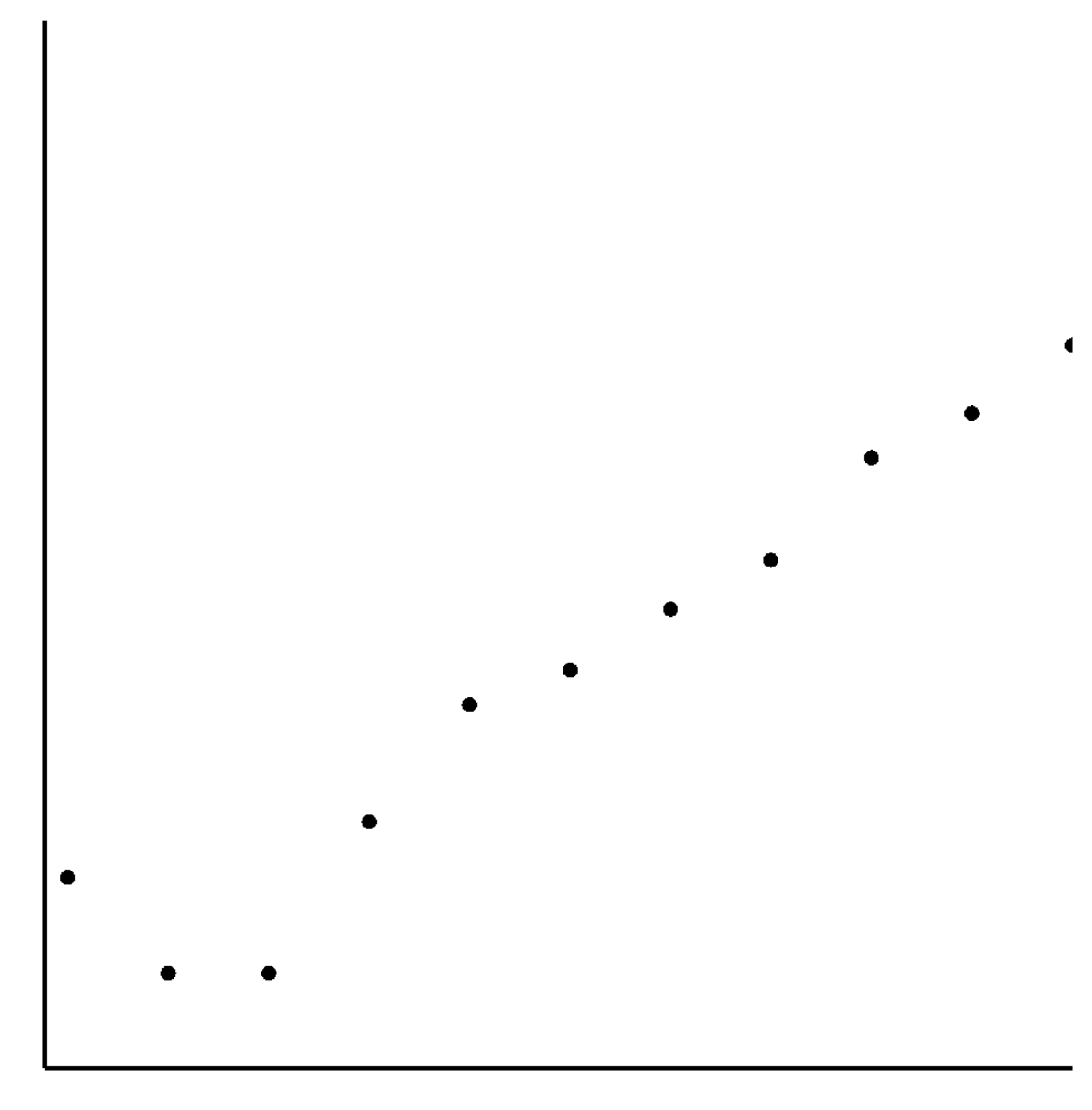
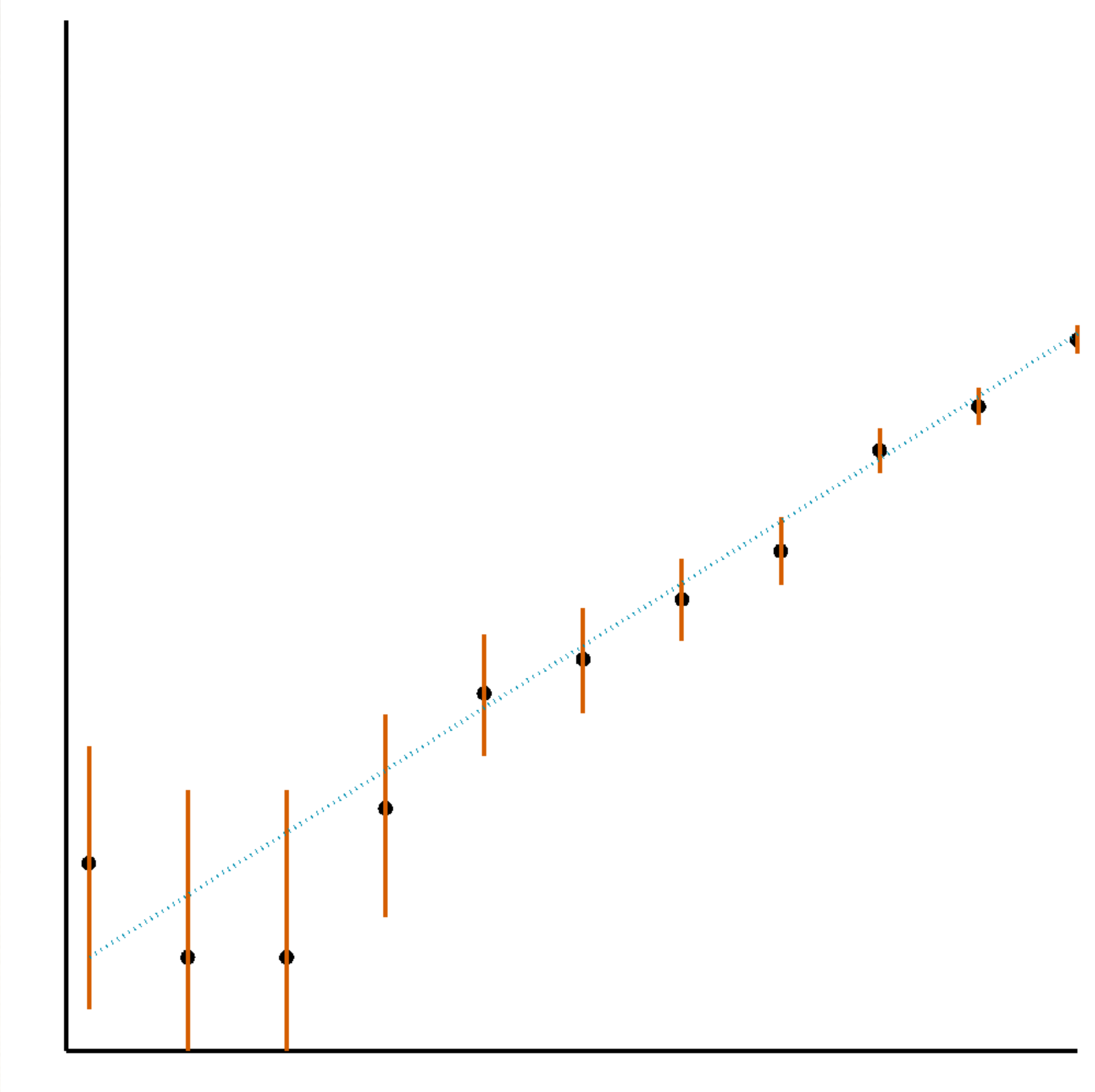
  - Lets you fit a simplified model curve to the data by minimizing the squared deviations of residuals







Error propagation : Gaussian

- How to propagate uncertainty from one stage to another — if $g = f(x)$, and σ_x is known, what is σ_g =?= $f(\sigma_x)$
- Simple case: if everything is distributed as a Gaussian, and has well-defined means and standard deviations, then at "best fit" values a_i, $g = g(a_i)$

$$\sigma_g^2 = \sum_i \frac{1}{N} \sum_k (g_k(a_i + \delta a_i) - g_k(a_i))^2$$ for all data points k=1..N and independent variables i

and expand as Taylor series and sum over k to get to the 2nd order

$$\sigma_g^2 = \sum_i \sum_j \frac{\partial g}{\partial a_i} \frac{\partial g}{\partial a_j} \sigma_{a_i a_j}$$ where i, j are variables

or ignoring correlations amongst the $\{a_i\}$, $\sigma_{a_i a_j} = \sigma_{a_i}^2 \delta_{ij}$

$$\sigma_g^2 \approx \sum_i \left(\frac{\partial g}{\partial a_i} \right)^2 \sigma_{a_i}^2$$

Error propagation : Examples

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$$g = C \cdot a \;\rightarrow \sigma_g = C \cdot \sigma_a$$

uncertainties scale (counts → count rate)

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$$g = a + b \rightarrow \sigma_g^2 = \sigma_a^2 + \sigma_b^2$$

errors square-add

Uncertainty intervals

- Equal tail
- Highest density (also the shortest interval)
- "1σ" ⇒ 68% ≡ 16th–84th percentile
- 5th–95th ≡ 90% ≡ 1.6σ
- 2.5th–97.5th ≡ 95% ≡ 2σ
- "3σ" ⇒ p=0.003

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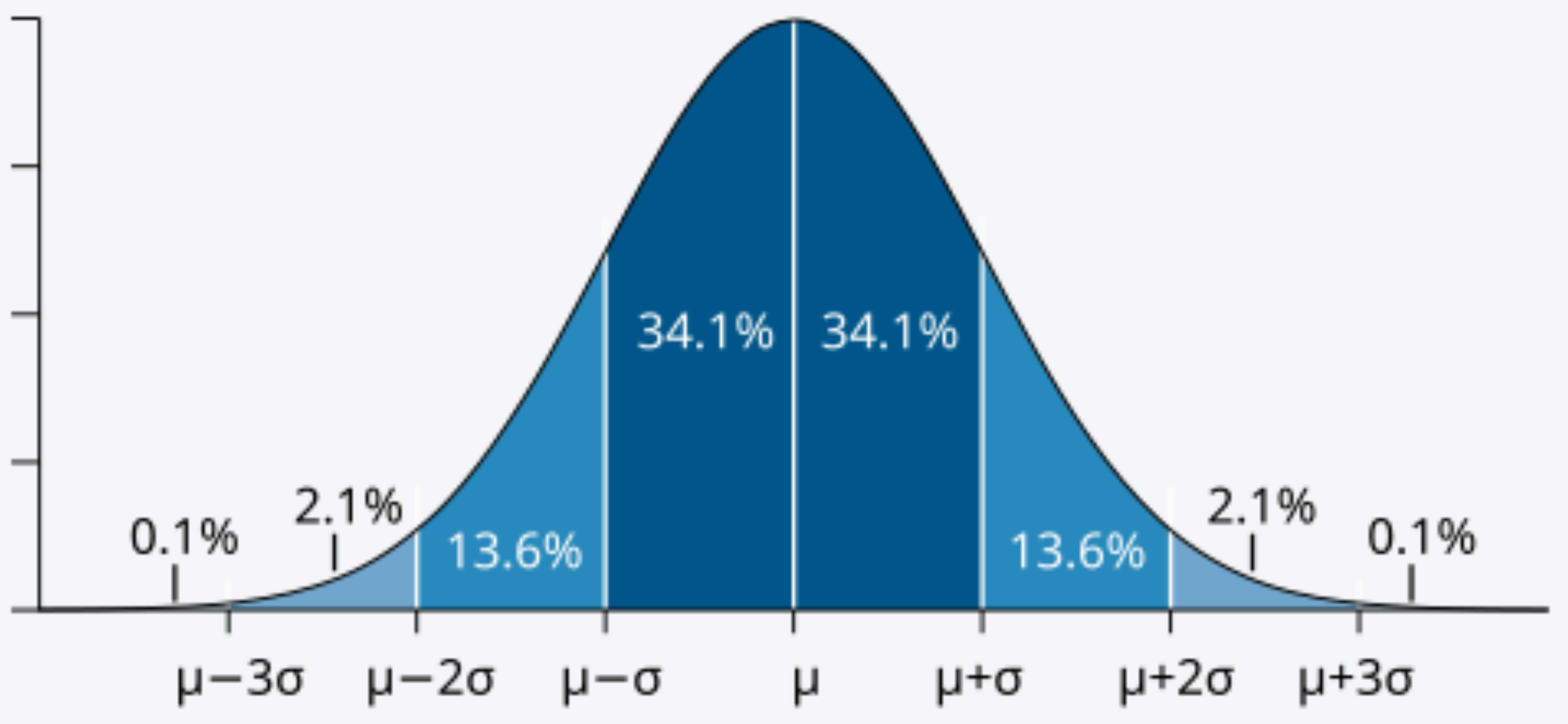

Distributions

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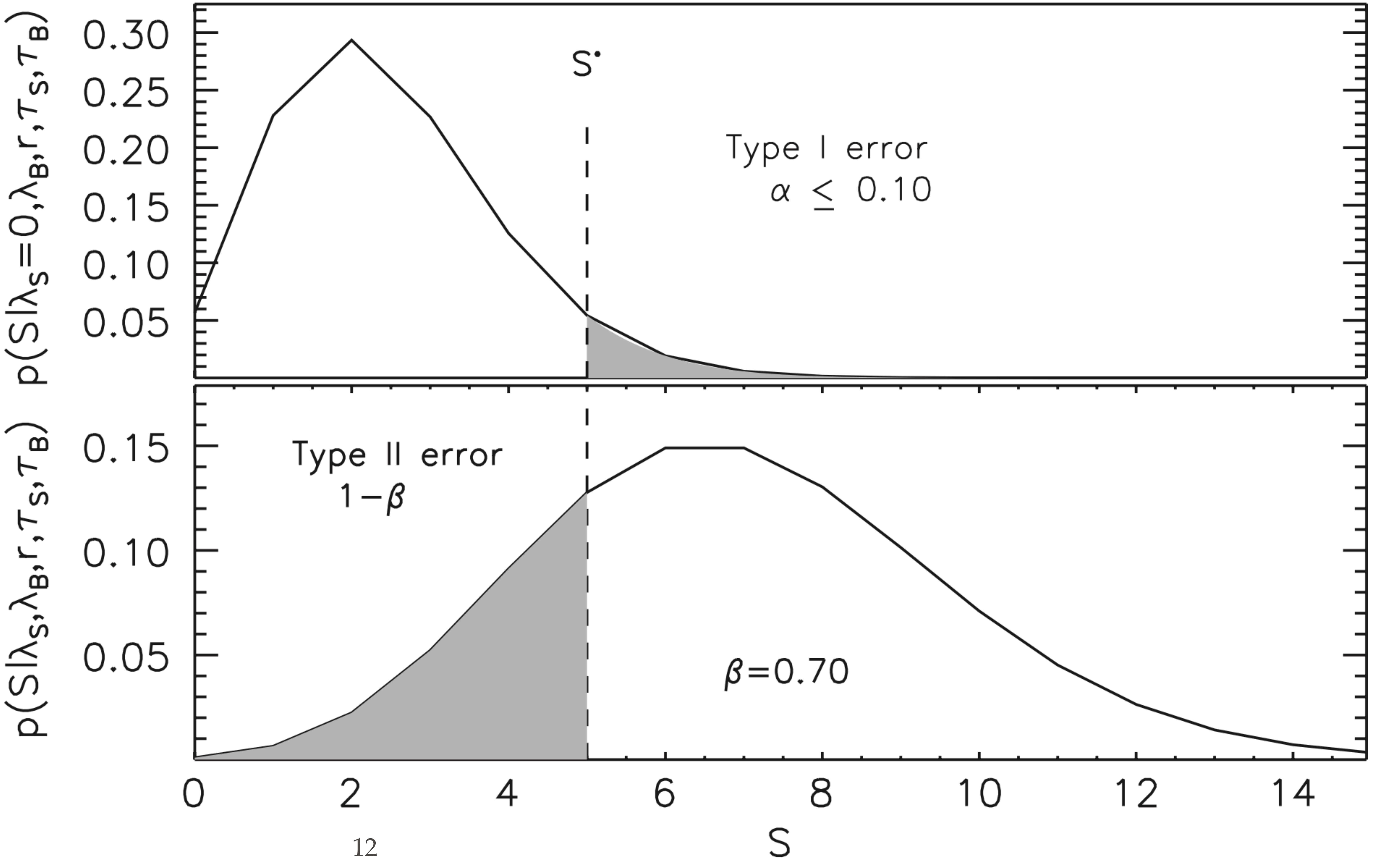
Delta: $\delta(x - x_0) = 0$ for $x \neq x_0$, and $\int dx\ \delta(x - x_0) = 1$

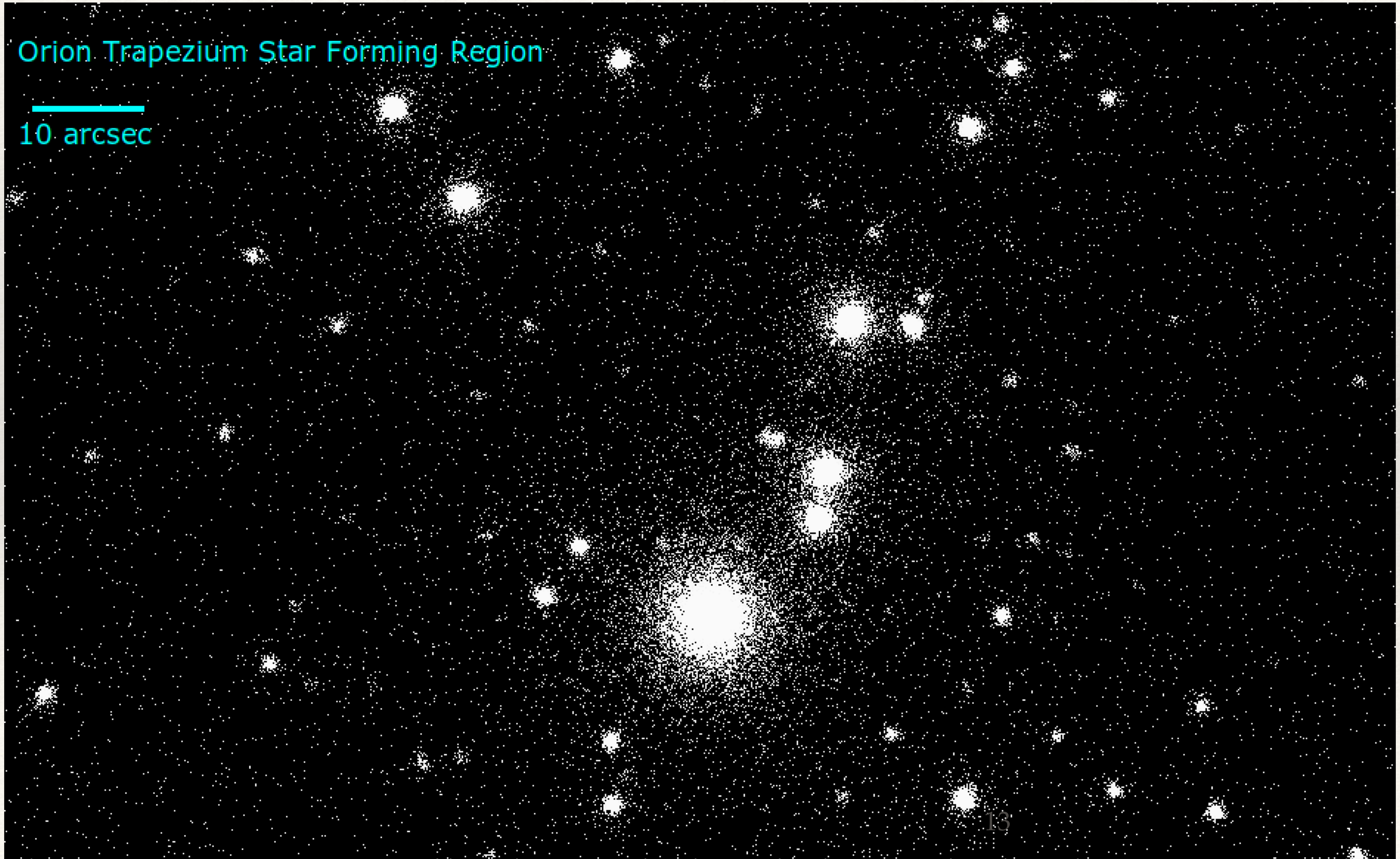
p-values, false +ves, and false –ves

- *p*-value: the tail integral of a distribution
- False +ve ≡ Type I error: the *p*-value at which a threshold is set for a *null* distribution
- False –ve ≡ Type II error: the fraction of the *alternate* distribution that falls below the threshold



Detection and Estimation

An observation that falls in the tail of the null distribution where the p-value is small enough that the risk of false +ve is deemed acceptable



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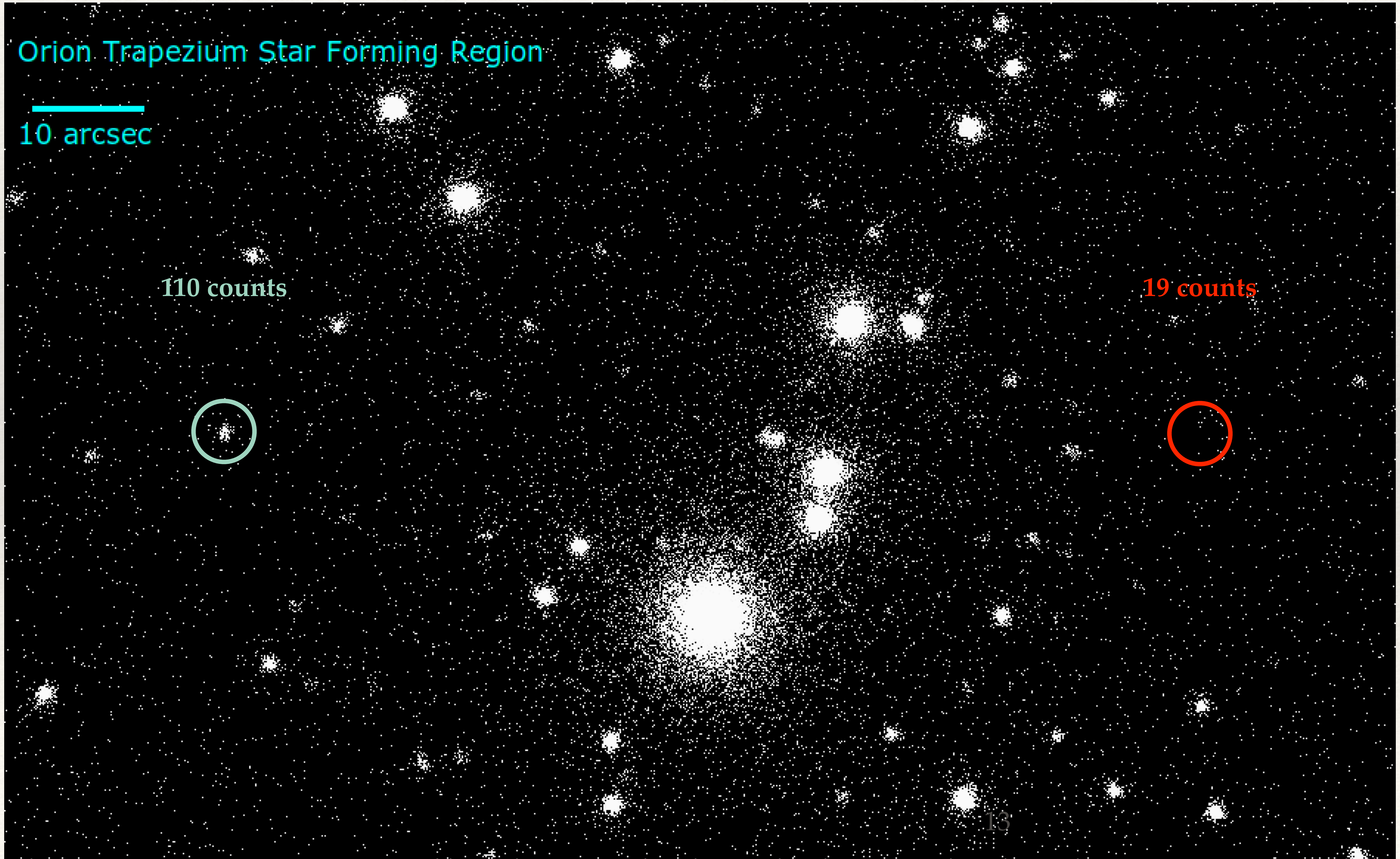

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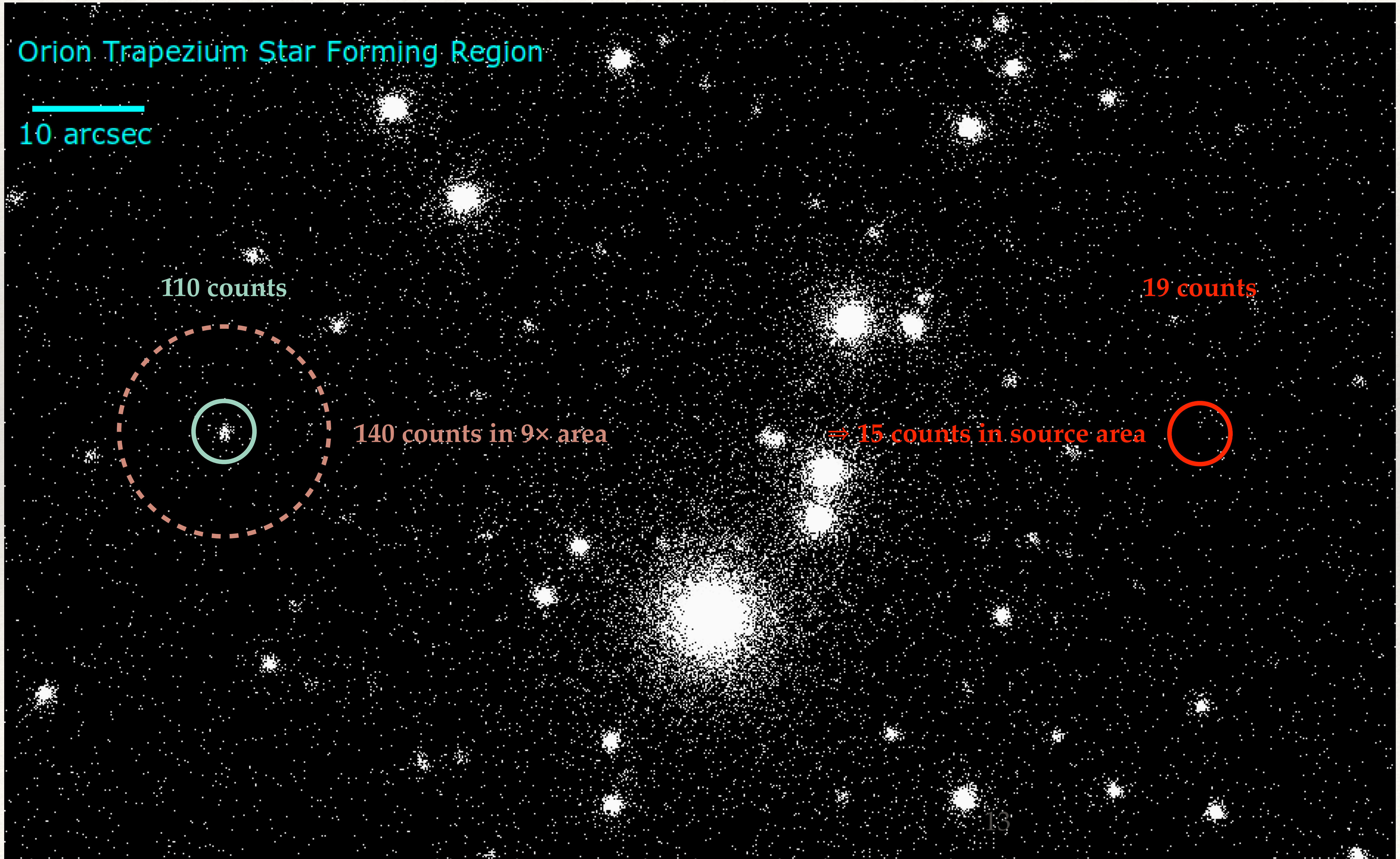

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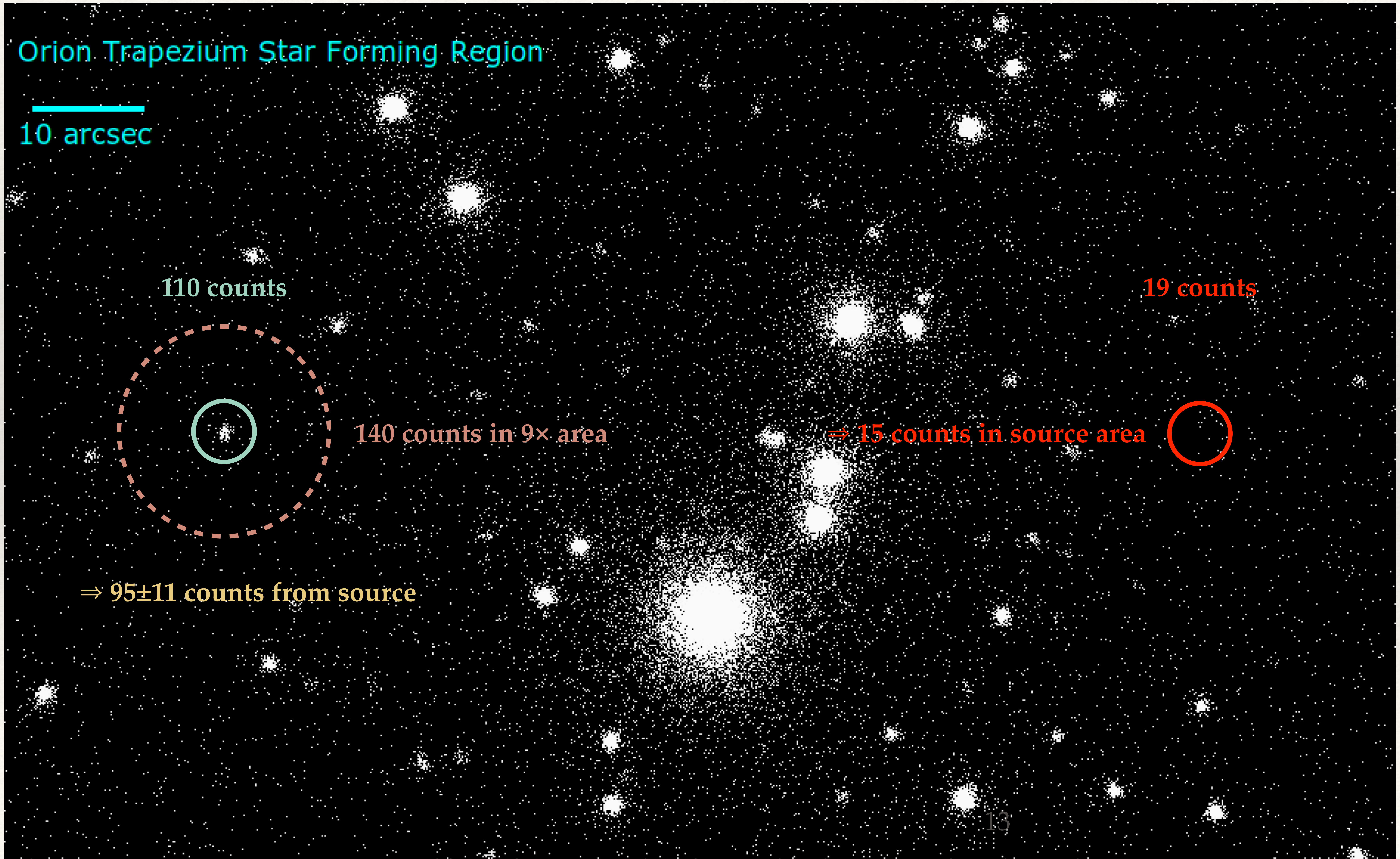

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Net = $N_S - N_B / \mathbb{B}$

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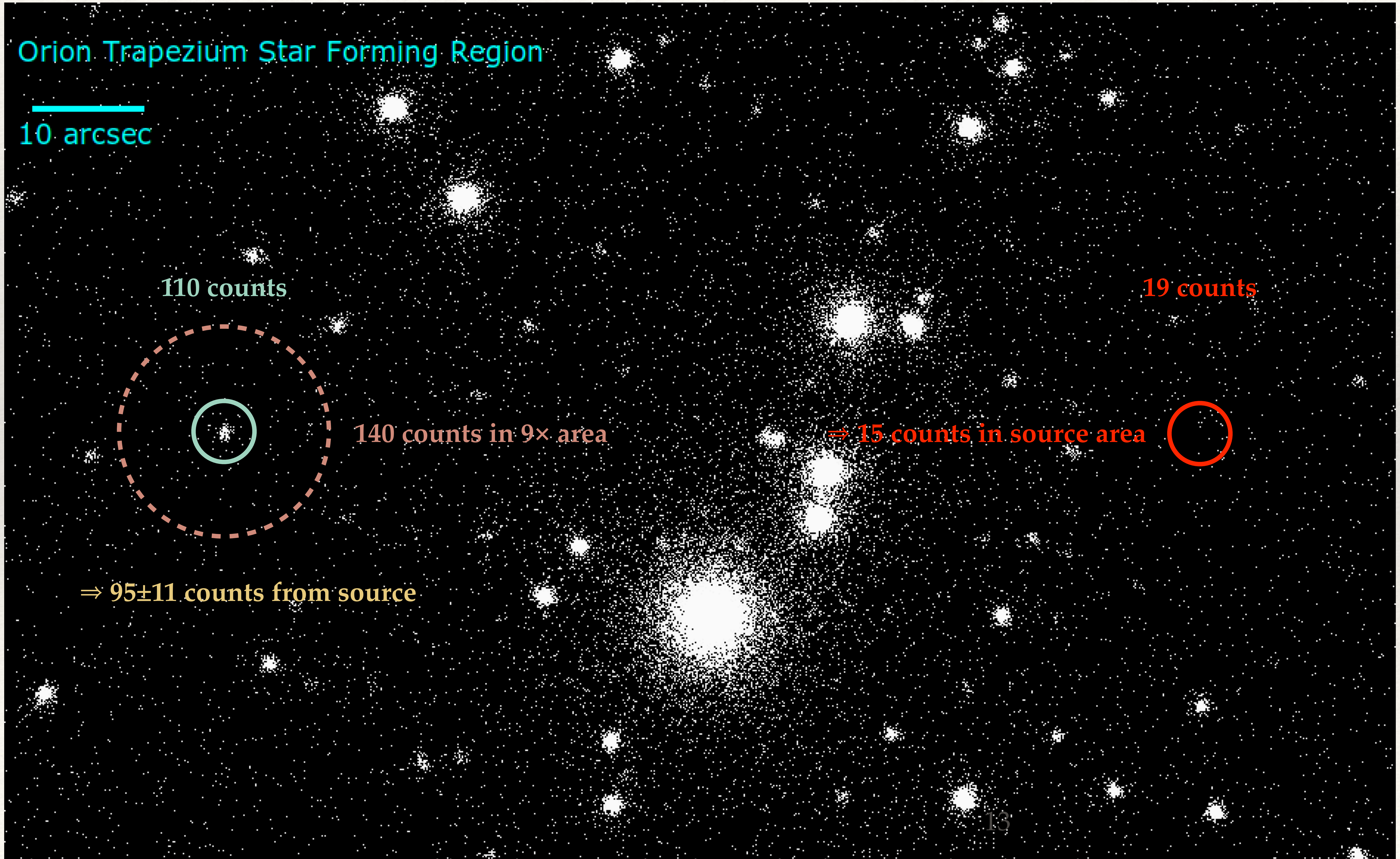

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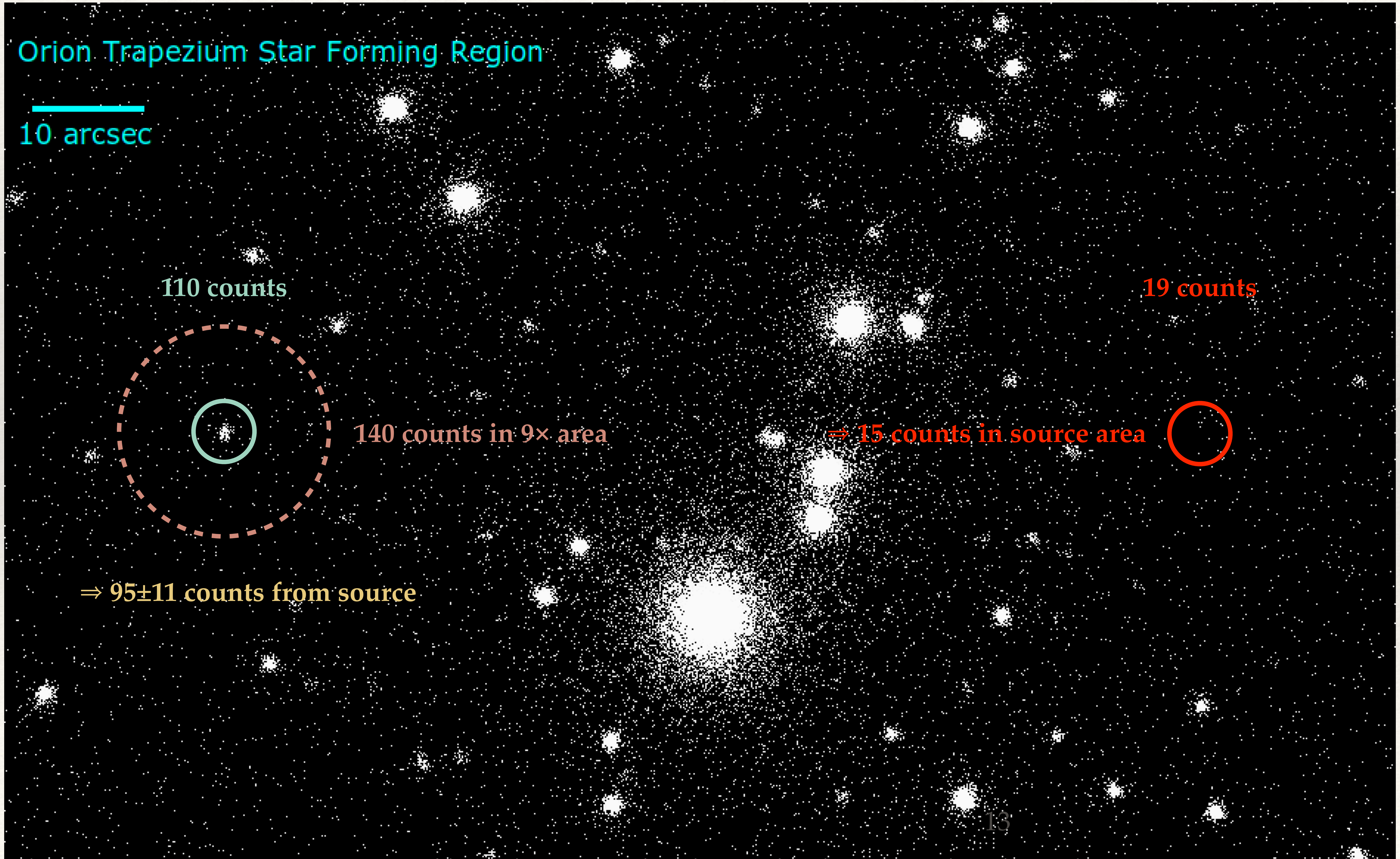

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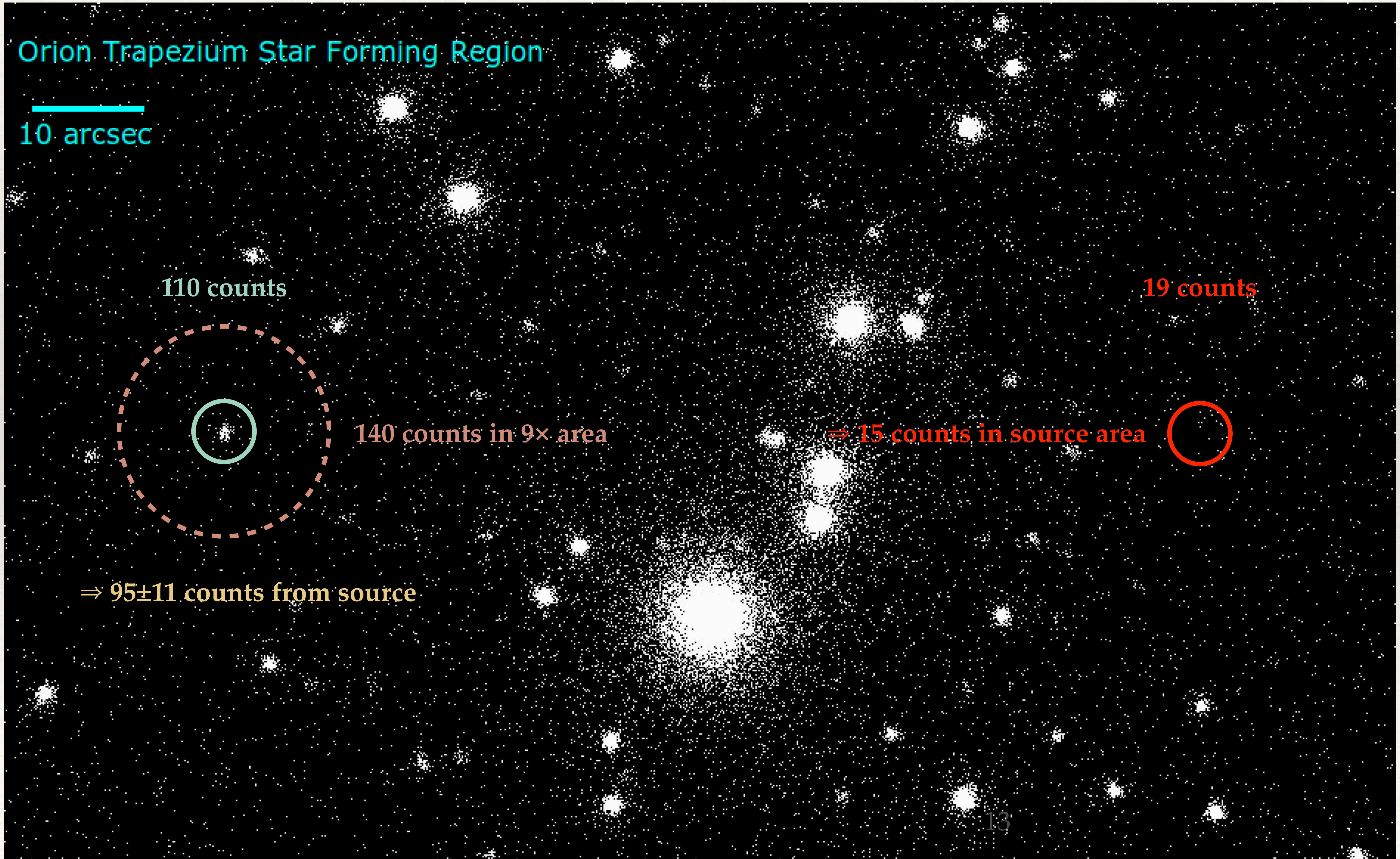

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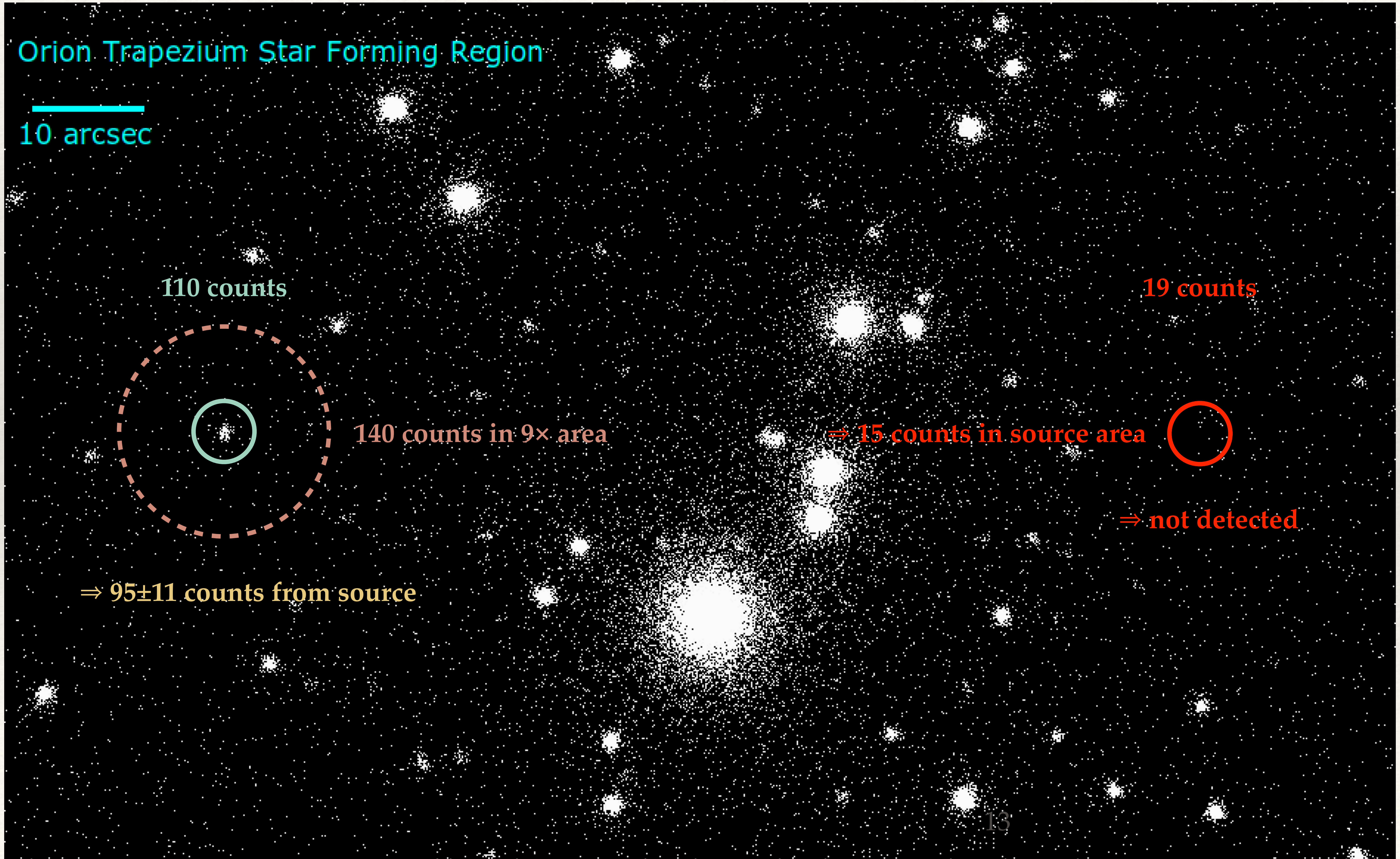

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$\gg$ typical threshold p

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b̅a̅r̅ and ĥât̂ to indicate sample averages and best-fit values

Γρεεκ letters for model quantities, Roman for data quantities

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- **Covariance errors** aka curvature errors aka inverse of the Hessian

  For Gaussian, $\frac{\partial^2 \ln L_{\text{Gauss}}}{\partial x^2} \propto \frac{1}{\sigma^2}$

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- **$\Delta\chi^2$**

  Difference from best-fit χ^2 value is itself a χ^2 distribution with dof=1, so look for percentiles of that distribution:

  $\Delta\chi^2$=+1 ≡ 68% (1σ)

  $\Delta\chi^2$=+2.71 ≡ 90% (1.6σ)

  + more robust than curvature

  – gets complicated if parameters are correlated

  – higher computational cost

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- When the observed $\chi^2 \sim \text{dof} \pm \sqrt{2 \cdot \text{dof}}$, the model is doing a good job of matching the data. The farther it is from this range, the less likely it is that the model is a good description of the data
  - But always use your judgement, because this is a *probabilistic* rule!
  - Watch out for how σ^2 is defined (model variance is better)

Fitting: `cstat`

- Recall Poisson log Likelihood: $\ln L_{\text{Pois}} = -\ln\Gamma(k+1) + k\ln\lambda - \lambda$
- χ^2 is $-2\ln L_{\text{Gauss}}$, `cstat` is $-2\ln\dfrac{L_{\text{Pois}}}{L_{\text{Saturated Pois}}}$

  $$\texttt{cstat} = 2\sum_i M_i - D_i + D_i \cdot (\ln D_i - \ln M_i)$$

  where D_i are observed counts, and M_i are model predicted counts in bin i and Saturated Poisson means λ is set to k, or a model where M_i is set to D_i. `cstat` can also be derived as an approximate form of the L_{Pois}, using Stirling's approximation for $\Gamma(\cdot)$
- Watch out: `cstat` is only asymptotically χ^2, not quite the Poisson likelihood, 0s are thrown away, background must be explicitly modeled
- unbiased for low counts compared to χ^2, asymptotically χ^2, rudimentary goodness-of-fit exists (Kaastra 2017, A&A 605, A51)

[AnetaS] https://cxc.cfa.harvard.edu/ciao/workshop/oct20_egypt_virt/cstat_vs_chisq_SimsNotebook.ipynb

[AnetaS] https://cxc.cfa.harvard.edu/ciao/workshop/oct20_egypt_virt/data_for_cstat_vs_chisq_SimsNotebook.tar.gz

Handbook of X-ray Astronomy (Arnaud, Smith, Siemiginowska): https://doi.org/10.1017/CBO9781139034234.008

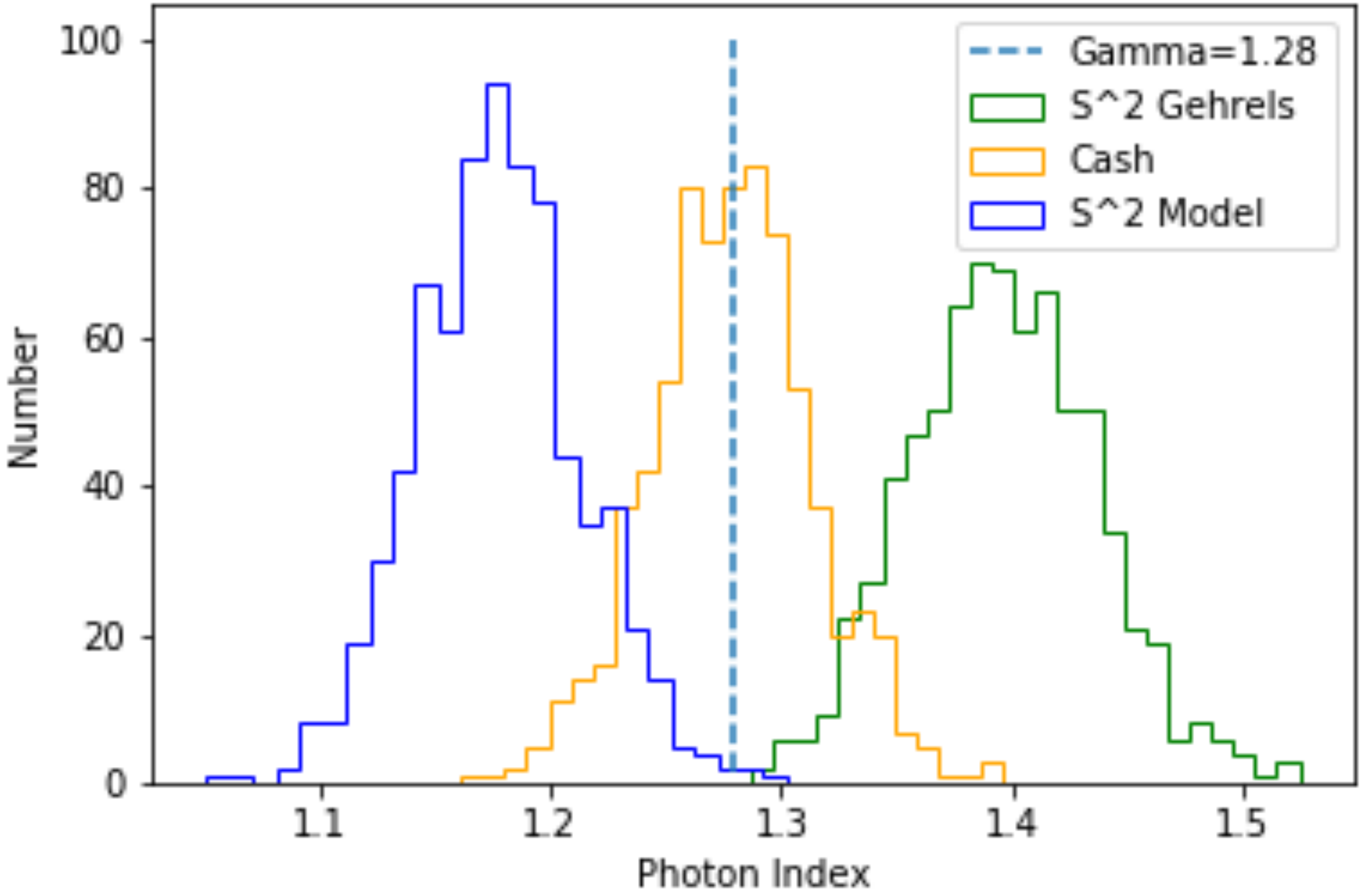

Fig. 7.3 Distributions of a photon index parameter γ obtained by fitting simulated X-ray spectra with 60 00 counts and using the three different statistics: S^2_{Pearson}, S^2 and C (i.e. the Poisson likelihood) statistics. The true value of the simulated photon index is marked with a dashed line and it was set at $\gamma = 1.28$

Statistical Tools in CIAO/Sherpa

- **fit**: non-linear minimization fitting
- **conf/covar**: uncertainty intervals and error bars
- **resample_data**: to get bootstrap distribution of model parameter draws when *data errors are asymmetric*
- **bootstrap/sample_flux/sample_photon_flux/sample_energy_flux**: with replacement/parametric bootstrap to get Monte Carlo distribution accounting for parameter uncertainties
- **get_draws**: Markov Chain Monte Carlo (MCMC) engine pyBLoCXS (Bayesian Low-Counts X-ray Spectral analysis; van Dyk et al. 2001, ApJ 548, 224)
- **calc_mlr, calc_ftest**: model comparison via Likelihood Ratio Test (LRT)/F-test
- **plot_pvalue, plot_pvalue_results**: to do posterior predictive p-value checks (Protassov et al. 2002, ApJ 571, 545)
- **glvary**: light curve modeling (Gregory & Loredo 1992, ApJ 398, 146)
- **celldetect/wavdetect/vtpdetect/mkvtpbkg**: source detection in images
- **aprates**: Bayesian aperture photometry also used in **srcflux** (Primini & Kashyap 2014, ApJ 796, 24)
- the python interpreter in Sherpa gives access to python libraries, and can be used to call upon packages and libraries in R, which are written by statisticians for statisticians

Statistics is a tool; it can be misused

- "All models are wrong, but some are useful." — George Box, c.1987
- Tak, H., et al., 2024, ApJS 275, 30 https://doi.org/10.3847/1538-4365/ad8440 — be aware of
  - where the data are coming from, what sort of filtering they have been subjected to
  - conditions under which a particular theorem is proven to be valid and make sure they apply under the scenario you are considering
  - assumptions made about the nature and range of model parameters and model complexity, and always do sanity checks and sensitivity analyses
  - limitations of hypothesis tests, and always consider the power of the tests and false detection rates

Some useful reading material

- Larry Bretthorst (1988), Bayesian Fourier analysis, https://bayes.wustl.edu/glb/book.pdf
- Tom Loredo (1990), monograph on neutrinos from 87A, http://hosting.astro.cornell.edu/staff/loredo/bayes/L90-LaplaceToSN1987A-scan.pdf
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- Buchner & Boorman (2023), Statistical aspects of X-ray spectroscopy, https://arxiv.org/abs/2309.05705
- Tak et al. (2024), Six Maxims of Statistical Acumen for Astronomical Data Analysis, ApJS 275, 30 https://doi.org/10.3847/1538-4365/ad8440