Goodness-of-fit in Astrophysics

Properties of C statistics

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“History” of C statistics in Astrophysics

- Cash, W., *Parameter estimation in astronomy through application of the likelihood ratio*, Astrophysical Journal, Part 1, vol. 228, Mar. 15, 1979, p. 939-947.
  - Inference: MLE & confidence intervals
  - Goodness-of-fit Test: χ^2 for difference of likelihood ratios – if there exists a hypothesized fixed subset of parameters.
- Kaastra, J. S. *On the use of C-stat in testing models for X-ray spectra*, Astronomy & Astrophysics 605 (2017): A51.
  - Goodness-of-fit Test: Approximate Gaussian
- Bonamente, Massimiliano. *Distribution of the C statistic with applications to the sample mean of Poisson data.* Journal of Applied Statistics 47.11 (2020): 2044-2065.
  - Homogeneous Poisson rates & Approximate Gaussian interval

Mathematical Notations for C-stat

Let null set be $\mathcal{S} = \{s_i(\theta), 1 \le i \le I\} \subset \mathbb{R}^I$. Under the null model, the maximum likelihood estimate for θ is

$$\hat{\theta}_I = \text{argmax}_{\theta \in \mathbb{R}^d} \left\{ L(s_1(\theta), \ldots, s_I(\theta) | N_1, \ldots, N_I) = p(N_1, \ldots, N_I | \theta) \right\}.$$

The saturated model is $N_i \overset{\text{indep.}}{\sim} \text{Poisson}(s_i)$, $1 \le i \le I$. The maximum likelihood estimate for s_i is $\hat{s}_i = N_i$. The log likelihood ratio statistics is

$$\begin{aligned} \text{LR}_I = -2 \log \Lambda_I &= -2 \log \frac{\sup_{\mathcal{S}} L(s_1, \ldots, s_I | N_1, \ldots, N_I)}{\sup_{\mathbb{R}^n} L(s_1, \ldots, s_I | N_1, \ldots, N_I)} \\ &= 2 \sum_{i=1}^{I} \left[s_i(\hat{\theta}_n) - N_i \log s_i(\hat{\theta}_I) - N_i + N_i \log N_i \right]. \end{aligned}$$

This is the `C-stat` after plugging in the MLE $\hat{\theta}_I$, i.e. $\text{LR}_I = C_I(\hat{\theta}_I)$, where the `C-stat`, denoted by $C_I(\theta)$, is defined as

$$C_I(\theta) = 2 \sum_{i=1}^{I} \left[s_i(\theta) - N_i \log s_i(\theta) - N_i + N_i \log N_i \right].$$

Likelihood Ratio Test and C-stat

The plug-in C statistic is not equal to the "true" C statistic:

Lemma (Wilk's Theorem)

For any n, $-C_n(\hat{\theta}_n) + C_n(\theta_0) = \mathrm{LR}_n^*$, where LR_n^* is given by

$$\begin{aligned} \mathrm{LR}_n^* &= -2 \log \frac{L(s_1(\theta_0), \ldots, s_n(\theta_0) | N_1, \ldots, N_n)}{L(s_1(\hat{\theta}_n), \ldots, s_n(\hat{\theta}_n) | N_1, \ldots, N_n)} \\ &= 2 \sum_{i=1}^{n} \left[N_i \log s_i(\hat{\theta}_n) - N_i \log s_i(\theta_0) + s_i(\theta_0) - s_i(\hat{\theta}_n) \right], \end{aligned}$$

which is the likelihood ratio statistics for testing the null hypothesis $H_0 : \theta = \theta_0$ versus the alternative $H_1 : \{s_i(\theta), 1 \leq i \leq n\} \in \mathcal{S}$. As $n \to \infty$, $\mathrm{LR}_n^* \xrightarrow{\mathcal{D}} \chi_d^2$.

Asymptotic Normality

Without loss of generality, we can assume that all $s_i(\boldsymbol{\theta}^\star)$ are bounded from below and n is large.

Lemma (Problem Reduction due to Infinite Divisibility)

If $\sum_{i=1}^n s_i(\boldsymbol{\theta}^\star) \to \infty$, *then there exists* $\{m_1, \ldots, m_I\}$ *such that (1)* $\sum_{i=1}^n m_i \to \infty$, *(2)* $m_i = 1$ *when* $s_i(\boldsymbol{\theta}^\star) \leq 1$, *(3)* $0.5 < s_i(\boldsymbol{\theta}^\star)/m_i < 1$ *when* $s_i(\boldsymbol{\theta}^\star) > 1$, *(4) the likelihood is equivalent to the likelihood of the following model*

$$\tilde{N}_{ij} \overset{\text{indep.}}{\sim} \text{Poisson}\left(\frac{s_i(\boldsymbol{\theta})}{m_i}\right), \quad \sum_{j=1}^{m_i} \tilde{N}_{ij} = N_i. \tag{1}$$

Under mild regularity conditions, we have

$$\frac{C_n(\hat{\boldsymbol{\theta}}) - E[C_n(\hat{\boldsymbol{\theta}})]}{\sqrt{\text{Var}(C_n(\hat{\boldsymbol{\theta}}))}} \to N(0,1), \quad \text{as} \quad n \to \infty.$$

High-Order Asymptotics

Assume s_i follows log-linear model $\boldsymbol{\eta} = \boldsymbol{X\theta}$ where $\eta_i = \log s_i$. Let $V = \text{diag}(s_i)$, $Q = (Q_{ij}) = X(X^\top VX)^{-1}X$, $\kappa_1^{(i)} = E(C_i)$, $\kappa_2^{(i)} = E(C_i - \kappa_1^{(i)})^2$, $\kappa_3^{(i)} = E(C_i - \kappa_1^{(i)})^3$, $\kappa_{11}^{(i)} = E\{(C_i - \kappa_1^{(i)})(N_i - s_i)\}$, $\kappa_{12}^{(i)} = E\{(C_i - \kappa_1^{(i)})(N_i - s_i)^2\}$, $\kappa_{21}^{(i)} = E\{(C_i - \kappa_1^{(i)})^2(N_i - s_i)\}$ and $\kappa_{03}^{(i)} = E(N_i - s_i)^3$. Then under regularity conditions,

$$E(C_{\min}|\hat{\boldsymbol{\theta}}) = \hat{\kappa}_1^{(\cdot)} - \frac{1}{2}\mathbf{1}^\top X^\top \hat{\Sigma} X(X^\top \hat{V} X)^{-1}\mathbf{1} + O(n^{-1/2}),$$

$$\text{Var}(C_{\min}|\hat{\boldsymbol{\theta}}) = \hat{\kappa}_2^{(\cdot)} - \hat{\kappa}_{11}^\top X(X^\top \hat{V} X)^{-1} X^\top \hat{\kappa}_{11} + O(n^{-1/2}),$$

where $\Sigma = \text{diag}\{\kappa_{12}^{(i)} - (\sum_j \kappa_{11}^{(j)} Q_{ji})\kappa_{03}^{(i)}\}$, $\kappa_{11} = (\kappa_{11}^{(1)}, \cdots, \kappa_{11}^{(n)})^\top$, $\kappa_1^{(\cdot)} = \sum_{i=1}^n \kappa_1^{(i)}$ and $\kappa_2^{(\cdot)} = \sum_{i=1}^n \kappa_2^{(i)}$.

Algorithms for Goodness-of-fit Assessment

Algorithm 1 Likelihood ratio with χ^2-statistics

Require: Data points: the N_i's, the number of bins n, and the number of unknown parameters to be estimated d.

1: Obtain $\hat{\boldsymbol{\theta}}$ via the following maximum likelihood estimation

$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}\in\boldsymbol{\Theta}} \log L_n(N_1, \cdots, N_n|\boldsymbol{\theta})$$

2: Calculate $s_i(\hat{\boldsymbol{\theta}}) = f_i(\hat{\boldsymbol{\theta}})$ and

$$C_{\min} = 2\sum_{i=1}^{n}[s_i(\hat{\boldsymbol{\theta}}) - N_i \log s_i(\hat{\boldsymbol{\theta}}) - N_i + N_i \log N_i]$$

3: Determine the p-value by

$$p = \max_{p}\{\chi^2_{n-d}(\frac{p}{2}) \leq C_{\min} \leq \chi^2_{n-d}(1-\frac{p}{2})\}.$$

4: **return** p

Algorithm 2 Asymptotic Normality – Bootstrap Mean/Variance

Require: Data points N_i's, the number of bins n, the number of parameters to be estimated d, and the number of bootstrap repetitions B.

1: Obtain $\hat{\boldsymbol{\theta}}$ via the maximum likelihood estimation $\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}\in\boldsymbol{\Theta}} \log L_n(N_1, \cdots, N_n|\boldsymbol{\theta})$.

2: Calculate $s_i(\hat{\boldsymbol{\theta}}) = f_i(\hat{\boldsymbol{\theta}})$ and

$$C_{\min} = 2\sum_{i=1}^{n}[s_i(\hat{\boldsymbol{\theta}}) - N_i \log s_i(\hat{\boldsymbol{\theta}}) - N_i + N_i \log N_i]$$

3: **for** $m \in \{1, 2, \cdots, B\}$ **do**

4: Generate n Poisson samples denoted by $N_i^{(m)}$, $i = 1, \cdots, n$.

5: Obtain $\hat{\boldsymbol{\theta}}^{(m)}$ via the following maximum likelihood estimation

$$\hat{\boldsymbol{\theta}}^{(m)} = \arg\min_{\boldsymbol{\theta}^{(m)}\in\boldsymbol{\Theta}} \log L_n(N_1^{(m)}, \cdots, N_n^{(m)}|\boldsymbol{\theta})$$

6: Calculate $s_i^{(m)}(\hat{\boldsymbol{\theta}}^{(m)}) = f_i(\hat{\boldsymbol{\theta}}^{(m)})$ and

$$C_{\min}^{(m)} = 2\sum_{i=1}^{n}[s_i^{(m)}(\hat{\boldsymbol{\theta}}^{(m)}) - N_i^{(m)} \log s_i^{(m)}(\hat{\boldsymbol{\theta}}^{(m)}) - N_i^{(m)} + N_i^{(m)} \log N_i^{(m)}]$$

7: **end for**

8: Determine the bootstrap mean and variance

$$\mathbb{E}_b(C_{\min}) \approx \frac{\sum_{m=1}^{B} C_{\min}^{(m)}}{B}, \mathrm{Var}_b(C_{\min}) \approx \frac{\sum_{m=1}^{B}(C_{\min}^{(m)} - \mathbb{E}_b(C_{\min}))^2}{B-1}.$$

9: Determine the p-value by

$$p = \max_{p}\left\{Z(\frac{p}{2}) \leq \frac{C_{\min} - \mathbb{E}_b(C_{\min})}{\sqrt{\mathrm{Var}_b(C_{\min})}} \leq Z(1-\frac{p}{2})\right\},$$

where Z is the cumulative distribution function of the standard normal distribution.

10: **return** p

Algorithms for Goodness-of-fit Assessment

Algorithm 3 Asymptotic Normality – High Order

Require: Data points N_i's, the number of bins n and the number of parameters to be estimated d.

1: Obtain $\hat{\boldsymbol{\theta}}$ via the following maximum likelihood estimation

$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}\in\boldsymbol{\Theta}} \log L_n(N_1, \cdots, N_n|\boldsymbol{\theta})$$

2: Calculate $s_i(\hat{\boldsymbol{\theta}}) = f_i(\hat{\boldsymbol{\theta}})$ and

$$C_{\min} = 2\sum_{i=1}^{n}[s_i(\hat{\boldsymbol{\theta}}) - N_i \log s_i(\hat{\boldsymbol{\theta}}) - N_i + N_i \log N_i]$$

3: Determine the cumulants $\hat{\kappa}_1^{(i)}$, $\hat{\kappa}_{11}^{(i)}$, $\hat{\kappa}_{12}^{(i)}$, $\hat{\kappa}_{03}^{(i)}$, $\hat{V}$, $\hat{Q}$ and $\hat{\Sigma}$ via direct summation over each Poisson data N_i.

4: Determine the theoretical asymptotic mean and variance

$$E(C_{\min}|\hat{\boldsymbol{\theta}}) = \hat{\kappa}_1^{(\cdot)} - \frac{1}{2}\mathbf{1}^\top X^\top \hat{\Sigma} X (X^\top \hat{V} X)^{-1}\mathbf{1} + O(n^{-1/2}),$$

$$\mathrm{Var}(C_{\min}|\hat{\boldsymbol{\theta}}) = \hat{\kappa}_2^{(\cdot)} - \hat{\kappa}_{11}^\top X (X^\top \hat{V} X)^{-1} X^\top \hat{\kappa}_{11} + O(n^{-1/2}).$$

5: Determine the p-value by

$$p = \max_p \left\{ Z\left(\frac{p}{2}\right) \leq \frac{C_{\min} - \mathbb{E}(C_{\min}|\hat{\boldsymbol{\theta}})}{\sqrt{\mathrm{Var}(C_{\min}|\hat{\boldsymbol{\theta}})}} \leq Z\left(1 - \frac{p}{2}\right) \right\},$$

where Z is the cumulative distribution function of the standard normal distribution.

6: **return** p

Algorithm 4 Parametric Bootstrap

Require: Data points N_i's, the number of bins n, the number of parameters to be estimated d, and the number of bootstrap repetitions B.

1: Obtain $\hat{\boldsymbol{\theta}}$ via the following maximum likelihood estimation

$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}\in\boldsymbol{\Theta}} \log L_n(N_1, \cdots, N_n|\boldsymbol{\theta})$$

2: Calculate $s_i(\hat{\boldsymbol{\theta}}) = f_i(\hat{\boldsymbol{\theta}})$ and

$$C_{\min} = 2\sum_{i=1}^{n}[s_i(\hat{\boldsymbol{\theta}}) - N_i \log s_i(\hat{\boldsymbol{\theta}}) - N_i + N_i \log N_i]$$

3: **for** $m \in \{1, 2, \cdots, B\}$ **do**

4: Generate n Poisson samples denoted by $N_i^{(m)}$, $i = 1, \cdots, n$.

5: Obtain $\hat{\boldsymbol{\theta}}^{(m)}$ via the following maximum likelihood estimation

$$\hat{\boldsymbol{\theta}}^{(m)} = \arg\min_{\boldsymbol{\theta}^{(m)}\in\boldsymbol{\Theta}} \log L_n(N_1^{(m)}, \cdots, N_n^{(m)}|\boldsymbol{\theta})$$

6: Calculate $s_i^{(m)}(\hat{\boldsymbol{\theta}}^{(m)}) = f_i(\hat{\boldsymbol{\theta}}^{(m)})$ and

$$C_{\min}^{(m)} = 2\sum_{i=1}^{n}[s_i^{(m)}(\hat{\boldsymbol{\theta}}^{(m)}) - N_i^{(m)} \log s_i^{(m)}(\hat{\boldsymbol{\theta}}^{(m)}) - N_i^{(m)} + N_i^{(m)} \log N_i^{(m)}]$$

7: **end for**

8: Rearrange $C_{\min}^{(m)}$, $m = 1, 2, \cdots, B$ such that $C_{\min}^{(1)} \leq C_{\min}^{(2)} \leq \cdots \leq C_{\min}^{(B)}$. And determine k such that $k = \min_k\{k|C_{\min}^{(k-1)} \leq C_{\min} < C_{\min}^{(k)}\}$.

9: Determine the p-value by

$$p = \frac{2}{B}\min\{k, B - k\}.$$

10: **return** p

Numerical Studies: A simple example

We consider this example: $n = 100$, $\theta_1 = 2$, $\theta_2 = 1$, and

$$s_i = \theta_1 \exp\left(\theta_2 \times i/n\right), \quad i = 1, \ldots, n.$$

Table: The p-values of five numerical studies, $\theta_1 = 2.0$.

Test	1	2	3	4	5
Bootstrap test	0.112	0.732	0.316	0.124	0.610
C_{min} test	0.109	0.730	0.302	0.113	0.649
χ^2 test	0.028**	0.184	0.063	0.025**	0.153

Numerical Studies: Systematic Comparisons

Model A: Constant Rate Poisson Model, $s_i = \mu$, $\mu = \{0.5, 2, 5, 10\}$.

Model B: Varying Rate Poisson Model

- Pareto/Powerlaw Rates: $s_i(\boldsymbol{\theta}) = \mu(1 + i \times c_0)^{-k}$, where $c_0 = \frac{1}{n}$, $\mu = \{0.5, 2, 5, 10\}$ and $k = 1$.
- Exponential Rates: $s_i(\boldsymbol{\theta}) = \mu \exp(-i\eta)$, where $\mu = 5, 10, 100$ and $\eta = n^{-1}$.

Model C: Unstructured Rate Poisson Model: $s_i \sim \Gamma(\alpha, \beta)$, where $\beta = \sqrt{\alpha}$ and $\alpha = 25, 4, 0.25$, representing large, mixed and small count settings.

Numerical Studies: Systematic Comparisons

	Alg.1			Alg.2			Alg.3			Alg.4		
Model	n=10,50,100			n=10,50,100			n=10,50,100			n=10,50,100		
A-L-B	0.07	0.06	0.03	0.05	0.05	0.05	0.05	0.05	0.03	0.05	0.04	0.04
A-M-B	0.05	0.11	0.11	0.03	0.03	0.03	0.03	0.02	0.03	0.05	0.02	0.03
A-S-B	**0**	**0**	**0**	0.04	0.03	0.02	0.06	0.03	0.10	0.02	0.02	0.02
B-P-L	0.07	0.16	0.08	0.06	0.11	0.06	0.03	0.11	0.04	0.04	0.11	0.04
B-P-M	0.01	0.16	0.19	0.04	0.08	0.09	0.03	0.07	0.07	0.04	0.09	0.09
B-P-S	0.07	0.01	0.06	**0**	**0.02**	**0.01**	0.09	0.04	0.04	0.07	0.02	0.01
B-E-L	0.08	0.08	0.09	0.05	0.05	0.07	0.05	0.05	0.07	0.05	0.06	0.06
B-E-M	0.02	0.04	0.14	0.02	0.04	0.06	0.02	0.06	0.06	0.01	0.05	0.07
B-E-S	0.13	0.06	0.11	**0.03**	**0.01**	**0.01**	0.15	0.04	0.06	0.12	0	0.01

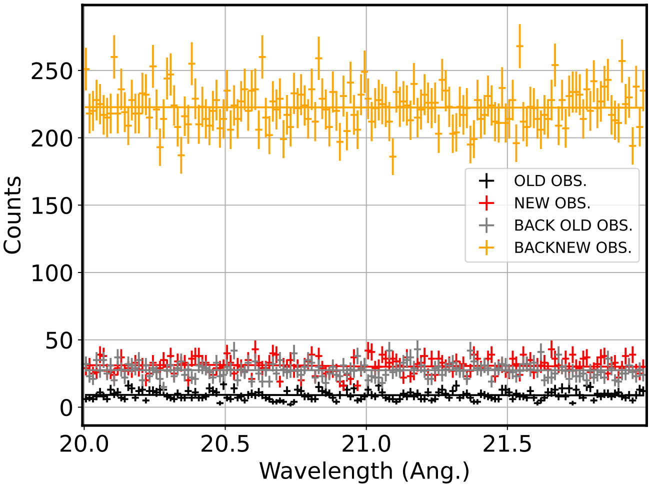
Table 1: Type I Error from 100 repeated simulation experiments with three different count settings under Models A and B: the null hypothesis is true.

Numerical Studies: Systematic Comparisons

	Alg.1			Alg.2			Alg.3			Alg.4		
Model	n=10,50,100			n=10,50,100			n=10,50,100			n=10,50,100		
C-U-L	0.90	0.43	0.21	0.92	0.41	0.22	0.92	0.42	0.21	0.93	0.47	0.25
C-U-M	0.83	0.38	0.05	0.80	0.44	0.19	0.84	0.45	0.17	0.85	0.49	0.23
C-U-S	0.79	0.38	0.19	0.61	0.16	0.01	**0.55**	**0.07**	**0**	0.70	0.18	0.02

Table 2: Type II Error from 100 repeated simulation experiments with three different count settings under Model C: the null hypothesis is not true..

Real Data Application



Real Data Application

Spectrum	$\hat{\mu}$	$C_{\min}$	Algorithm	$\mathbb{E}[C_{\min}]$	$\mathrm{Var}(C_{\min})$	p-value
Spec.I	8.962	190.72	Algo.1	158	316	0.078*
			Algo.2	162.48	338.74	0.125
			Algo.3	161.40	334.37	0.109
			Algo.4	N/A	N/A	0.128
Spec.II	30.704	167.67	Algo.1	158	316	0.568
			Algo.2	161.21	329.64	0.722
			Algo.3	158.89	321.70	0.624
			Algo.4	N/A	N/A	0.690
Spec.III	27.478	171.39	Algo.1	158	316	0.441
			Algo.2	160.81	328.85	0.560
			Algo.3	159.00	322.17	0.490
			Algo.4	N/A	N/A	0.548
Spec.IV	222.54	153.46	Algo.1	158	316	0.826
			Algo.2	159.20	324.53	0.750
			Algo.3	158.12	318.43	0.794
			Algo.4	N/A	N/A	0.760

Table 3: Performance of four test methods in each spectrum.

Thank You for Your Attention!

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