Using Bayes Factors for Model Selection in High-Energy Astrophysics

Shandong Zhao

Department of Statistic, UCI

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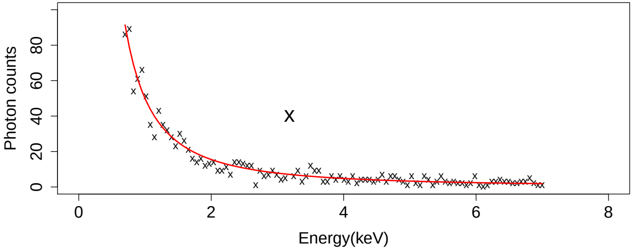
Model Comparison in Astrophysics

- Nested models (line detection in spectral analysis):



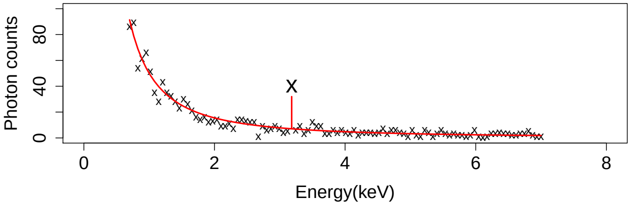
- Non-nested models:
  Powerlaw vs *Bremsstrahlung* for the red curve.
- Bottom line: need more than a confidence interval on "nesting parameter" to formally compare or select a model.

Spectral Analysis in High Energy Astrophysics

- **Goal:** Study the distribution of the energy of photons originating from a source (We use a Poisson model)
- The photon detector
  1. Counts photons into energy bins, with energy $E_1, \ldots, E_J$.
  2. May misclassify photons into wrong energy bins. (***Redistribution Matrix,* M**)
  3. Has sensitivity that varies with energy. (***effective area,*** d)
  4. Is subject to ***background contamination***, θ^B
- Mathematically: $\Xi(E_i) = \sum_{j \in \mathcal{J}} M_{ij} \Lambda(E_j) d_j + \theta_i^B$
- We ignore 2-4 in our initial simulations.

Model Selection in Spectral Analysis

- The spectral model can often be formulated as a finite mixture model. A simple form consists of a continuum and an emission line: $\Lambda(E_i) = \alpha E_i^{\beta} + \omega \mathrm{I}_{\mu == i}$



- The line detection problem:

$$\mathrm{H}_0 : \quad \Lambda(E_i) = \alpha E_i^{\beta}$$
$$\mathrm{H}_a : \quad \Lambda(E_i) = \alpha E_i^{\beta} + \omega \mathrm{I}_{\mu == i}$$

Challenges with Spectral Model Selection

- A naive method is to use the likelihood ratio test. However, the standard asymptotics of the LRT statistic do not apply.
  - μ has ***no value*** under H_0.
  - ω must be non-negative under H_a while its target tested value under H_0, ***zero***, is on the boundary of the parameter space.
- For "precise null hypotheses", *p*-values bias inference in the direction of false discovery.
  - When compared to BF or $\Pr(H_0|Y)$, *p*-values *vastly overstate the evidence* for H_1 (even using the prior most favorable to H_1)
  - Computed given data as extreme or more extreme than Y, which is *much stronger evidence* for H_1.
- Protassov et al. (ApJ, 2002) address the first set of concerns by simulating the null dist'n of the Likelihood ratio statistic and use posterior predictive *p*-values (PPP) instead.

Bayesian Model Selection

- ***Bayesian Evidence:*** The average likelihood over the prior distribution of the parameters under a specific model choice:

$$p(\boldsymbol{Y}|M) \equiv \int p(\boldsymbol{Y}|M, \boldsymbol{\theta})p(\boldsymbol{\theta}|M)d\boldsymbol{\theta}$$

  where $\boldsymbol{Y}, \theta$ and M are the observed data, parameters, and underlying models respectively.

- ***Bayes Factor (BF):*** The ratio of candidate model's Bayesian Evidence:

$$B_{01} \equiv \frac{p(\boldsymbol{Y}|M_0)}{p(\boldsymbol{Y}|M_1)}$$

Interpretation of BF

- BF and posterior probability ratio.

$$\frac{p(M_0|\boldsymbol{Y})}{p(M_1|\boldsymbol{Y})} = B_{01}\frac{p(M_0)}{p(M_1)}$$

- Interpretation against the Jeffreys' scale.

BF	Strength of evidence (toward M_0)
$1 \sim 3$	Barely worth mentioning
$3 \sim 10$	Substantial
$10 \sim 30$	Strong
$30 \sim 100$	Very strong
> 100	Decisive

Disadvantage of the Bayes Factor

- Assumes that one of the two models is true.
- Computation could be hard.
- Sensitive to prior specification.
  How does the prior dependency of BF compare to that of PPP?
- BF is ill-defined with an improper prior.
  Non-informative prior for parameters in common?

The Computation of BF

- Task is to compute $p(\boldsymbol{Y}|M) \equiv \int p(\boldsymbol{Y}|M,\boldsymbol{\theta})p(\boldsymbol{\theta}|M)d\boldsymbol{\theta}$.
    - ***Gaussian Approximation.***
      If the posterior dist'n is approximately Gaussian.
    - ***Monte Carlo Method.***
      If could get a sample from either the prior or posterior dist'n.
    - ***Nested Sampling.***
- None of the method is perfect for spectral analysis.
    - The joint posterior dist'n has many local modes.
    - Most Monte Carlo methods are inefficient.
    - Nested Sampling has bias up to 25% in simulation studies.

A New Method

- On the other hand, $B_{01} = \dfrac{p(M_0|\boldsymbol{Y})}{p(M_1|\boldsymbol{Y})} \Big/ \dfrac{p(M_0)}{p(M_1)}$
- Computing the ratio of the posterior probability is not easy.
- Challenge is to sample from $(I_{M_0}, \Theta_0, I_{M_1}, \Theta_1)$, where Θ_0 and Θ_1 might have different parameter settings and dimensions.

  Example: Θ_0 *for Powerlaw while* Θ_1 *for Bremsstrahlung.*
- It's usually straightforward, however, to sample from $p(\Theta_0|M_0, Y)$ and $p(\Theta_1|M_1, Y)$, seperately.

Jump between the Parameter Space

Assume we run $2K$ MCMC chains with half of them starting from Θ_0 and Θ_1 respectively. The parameter space for each chain is (I_M, Θ_M).

1. Run usual M-H algorithm for each chain with $q_0(\theta_0^{old}, \theta_0^{new})$ and $q_1(\theta_1^{old}, \theta_1^{new})$ being the proposal dist'n for sampling within $p(\Theta_0|M_0, Y)$ and $p(\Theta_1|M_1, Y)$, respectively.
2. For chain i, randomly pick one of the other chains, j, and propose a new draw based on its corresponding proposal dist'n. Doing so is equivalent to use the proposal dist'n of:

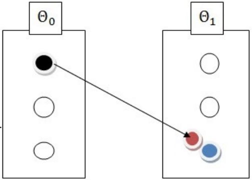
   $$\frac{1}{K-1}\sum_{j\neq i} q^j(\theta^j, \theta^{new}), \text{ where } q^j(\theta^j, \theta^{new}) = 0 \text{ if } I_M(\theta^j) \neq I_M(\theta^{new})$$

3. Combine all the chains, compute the ratio of I_{M_0}/I_{M_1} as the Monte Carlo estimate of the posterior probability ratio.

Why It Works

- The parallel MCMC algorithm was first introduced to help MCMC chain jump between modes.
- For step 2, the acceptance rate is

$$\frac{p(\theta^{new}|M(\theta^{new}),Y)}{p(\theta^{i}|M(\theta^{i}),Y)} \Big/ \frac{\sum_{j\neq i} q^j(\theta^j,\theta^{new})}{\sum_{j\neq i} q^j(\theta^j,\theta^{i})}$$



- Challenge now is to find a good local proposal dist'n.

Is Improper Prior Always Improper?

- If $\theta^\star$ only shows up in M_1, using improper prior for $\theta^\star$ is improper.

$$p(\boldsymbol{Y}|M_1) \equiv \int p(\boldsymbol{Y}|\theta^\star, \tilde{\theta}) p(\tilde{\theta}|\theta^\star) p(\theta^\star) d\tilde{\theta} d\theta^\star, \quad \Theta^1 = (\theta^\star, \tilde{\theta})$$

- What if $\theta^\star$ is one of the parameters in common?

  In the line detection problem with β, μ being fixed and assuming $p(\frac{\omega}{\alpha}) \sim U(0, \eta)$,

$$H_0 : \Lambda(E_i) = \alpha E_i^\beta \quad vs \quad H_a : \Lambda(E_i) = \alpha E_i^\beta + \omega \mathrm{I}_{\mu==i}$$

  The BFs under the prior of $p(\alpha) \sim U(0, N)$ converge as $N \to \infty$, to the BF under the prior of $p(\alpha) \propto 1$.

- What about the priors for ω and μ?

The Example

If $p(\alpha) \propto 1$,

$$BF = \eta \Big/ \int_0^{\eta} \frac{\left(1+\tilde{\omega}/E_{\mu}^{-\beta}\right)^{Y_{\mu}}}{\left(1+\tilde{\omega}/\Sigma E_i^{-\beta}\right)^{\Sigma Y_i+1}} d\tilde{\omega}$$

If $p(\alpha) \sim U(0, N)$,

$$BF_N = \eta \Big/ \int_0^{\eta} \frac{\left(1+\tilde{\omega}/E_{\mu}^{-\beta}\right)^{Y_{\mu}}}{\left(1+\tilde{\omega}/\Sigma E_i^{-\beta}\right)^{\Sigma Y_i+1}} \cdot \frac{\Pr(\tilde{z} \leq N)}{\Pr(z \leq N)} d\tilde{\omega}$$

where $z \sim Gamma(\Sigma Y_i + 1, \frac{1}{\Sigma E_i^{-\beta}})$, $\tilde{z} \sim Gamma(\Sigma Y_i + 1, \frac{1}{\Sigma E_i^{-\beta} + \tilde{\omega}})$

The Example, cont'd

Because

$$\frac{\left(1+\tilde{\omega}/E_{\mu}^{-\beta}\right)^{Y_\mu}}{\left(1+\tilde{\omega}/\Sigma E_i^{-\beta}\right)^{\Sigma Y_i+1}} \cdot \Pr(\tilde{z} \leq N) \leq \frac{\left(1+\tilde{\omega}/E_{\mu}^{-\beta}\right)^{Y_\mu}}{\left(1+\tilde{\omega}/\Sigma E_i^{-\beta}\right)^{\Sigma Y_i+1}}$$

$$\begin{aligned}
\lim_{N\to\infty} BF_N &= \lim_{N\to\infty} \int_0^{\eta} \frac{\left(1+\tilde{\omega}/E_{\mu}^{-\beta}\right)^{Y_\mu}}{\left(1+\tilde{\omega}/\Sigma E_i^{-\beta}\right)^{\Sigma Y_i+1}} \cdot \Pr(\tilde{z} \leq N) d\tilde{\omega} \Big/ \lim_{N\to\infty} \Pr(z \leq N) \\
&= \int_0^{\eta} \lim_{N\to\infty} \frac{\left(1+\tilde{\omega}/E_{\mu}^{-\beta}\right)^{Y_\mu}}{\left(1+\tilde{\omega}/\Sigma E_i^{-\beta}\right)^{\Sigma Y_i+1}} \cdot \Pr(\tilde{z} \leq N) d\tilde{\omega} \\
&= BF
\end{aligned}$$

where the second "$=$" holds by Lebegue dominated convergence theorem.

How to Assign a Proper Prior

- Compared to α and β, priors for ω and μ have much more influence on the BF. And they have to be proper.
- Different priors on ω and μ can totally change your decision based on BF. For example, with everything else held the same,
  under $p(\mu) \sim \mathrm{N}(\mu_0, \sigma_1)$, BF supports M_0
  under $p(\mu) \sim \mathrm{N}(\mu_0, \sigma_2)$, BF can't distinguish btwn the models
  under $p(\mu) \sim \mathrm{N}(\mu_0, \sigma_3)$, BF supports M_1
- Is the prior dependency always a problem?
- How does the prior influence of BF compare to that of the PPP?

Simulation Study Design

- ***Simulation Models:*** We compare a power law continuum with one delta function emission line model, with 1000 energy bins equally spaced between 0.3 to 7(keV).

$$
\begin{aligned}
\mathrm{H}_0: &\quad \Lambda(E_i) = \alpha E_i^{\beta} \\
\mathrm{H}_\mathrm{a}: &\quad \Lambda(E_i) = \alpha E_i^{\beta} + \omega \mathrm{I}_{\mu==i}
\end{aligned}
$$

  with $i = 1 \sim 1000$ and $\alpha = 50, \beta = 1.69$.

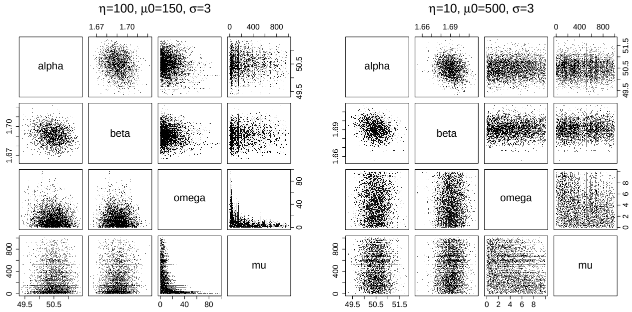
- The prior influence of α and β are negligible compared to that of ω and μ. Thus, they will be fixed in the simulation study.
- Assume:

$$\omega \sim U(0, \eta); \mu \sim \mathrm{discrete}[N(\mu_0, \sigma^2)]$$

  Using a Gamma prior for ω will have similar results.

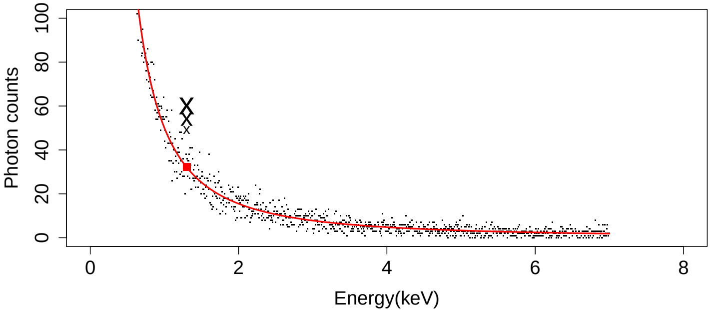
The Non-Gaussian Posterior Dist'n

- The ordinary Gibbs breaks down here because the subchain for μ does not move from its starting value, regardless of what it is. We use the **PCGS** to draw posterior samples.
- 5000 posterior draws with $\alpha = 50, \beta = 1.69, \omega = 10, \mu = 150$.



To Study The Prior Influence

- Fix α and β throughout. Calculate BF by numerical integration.
- The “true” emission line is set at bin 150, or $\mu =$ ***1.3*** keV.
- The intensity from the continuum in this bin is ***32***.
- We control the strength of data support toward $\mathrm{H_a}$ by altering the observed counts at 1.3 keV.



Prior Settings

- Recall $\omega \sim U(0, \eta)$. We control its strength by changing its upper range η.
  - η will range from 10 to 108 with a step size of 2.
- For μ, because $\mu \sim \mathrm{discrete}[N(\mu_0, \sigma^2)]$, we control both its mode μ_0 and s.d σ.
  - We use two different value for μ_0, 1.3keV and 1.97keV respectively (150 and 250 in terms of bin number).
  - For σ, it will range from 1 to 99 (bin width) with a step size of 2.

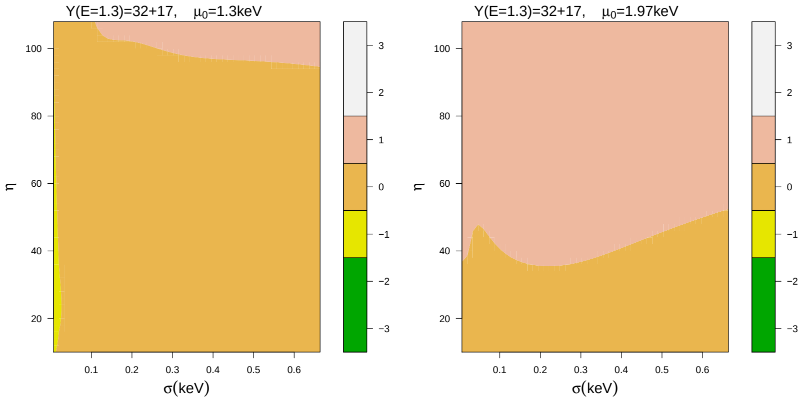
Visualize The Prior Influence

We will plot the heatmap of $\log(BF)$ against η, μ_0, and σ on the simplified Jeffrey's scale.

BF	$\log(BF)$	Evidence
> 30	> 1.5	Very strong to overwhelming for H_0
$[3, 30]$	$[0.5, 1.5]$	Substantial to strong for H_0
$[-3, 3]$	$[-0.5, 0.5]$	Not worth mentioning
$[-30, -3]$	$[-1.5, -0.5]$	Substantial to strong for H_a
< -30	< -1.5	Very strong to overwhelming for H_a

Results: A Weak Spectral Line

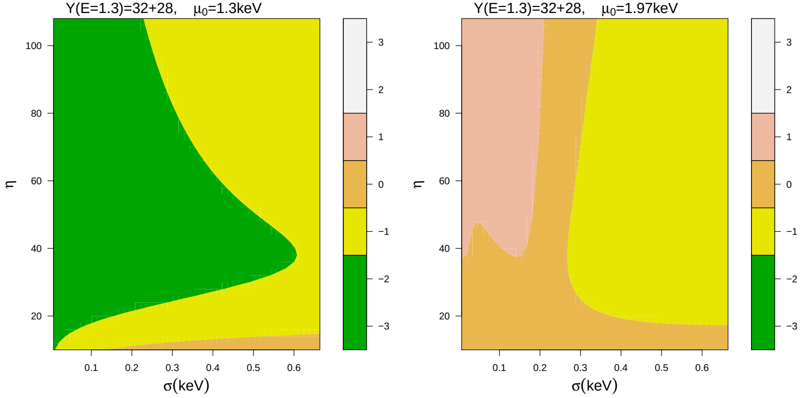
$Y(E = 1.3)$ is about 3 s.d above null model intensity.



Diffuse or misplaced priors weaken evidence

Results: A Stronger Spectral Line

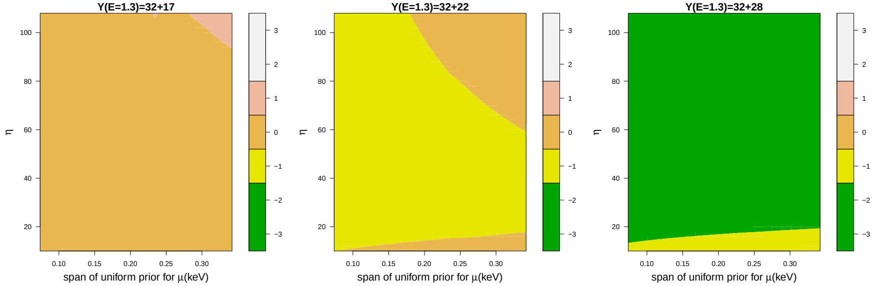
$Y(E = 1.3)$ is about 5 s.d above null model intensity.



Diffuse or misplaced priors could completely change the decision

Results: Stronger Prior

We use a stronger prior for μ: uniform prior with a span of 11 $\sim$ 51 bin width centered at the true location.

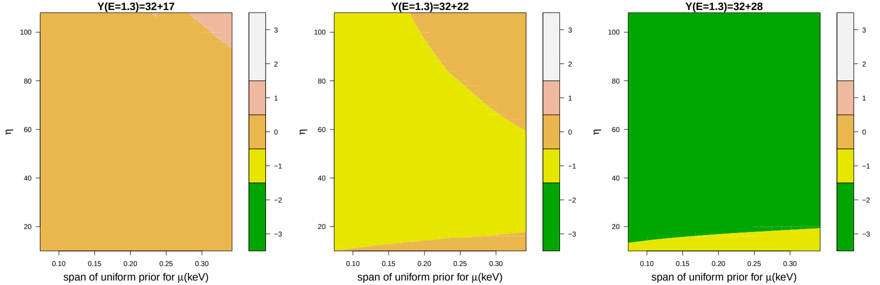


Take Home Messages

- If the data is dominantly strong, we probably don't need BF.
- The priors can reflect different scientific questions
  - $p(\mu)$: where to look for the lines
  - $p(\omega)$: how strong are the lines that we're looking for
- Even for likelihood ratio test, looking for lines
  - *at a fixed bin location,*
  - *within a restricted region,*
  - *over the whole energy range*

  will return tests with varied strength of the evidence.
- How does the prior dependency of BF compared to the PPP?

Compare BF with P-values



ppp-values (based on 1000 MC samples)

Y(E=1.3keV)	32+17	32+22	32+28
H_A: known line location	0.008	0.002	0.000
H_A: fitted line location(0.3-7.0keV)	0.539	0.184	0.006

Compare BF with P-values, cont'd

Prior on line intensity: $\omega \sim U(0, \eta)$ *and* $\mu \sim U(1.3 \pm \kappa)$.

H_A: *known* line location

- ppp-value $= 0.002$.

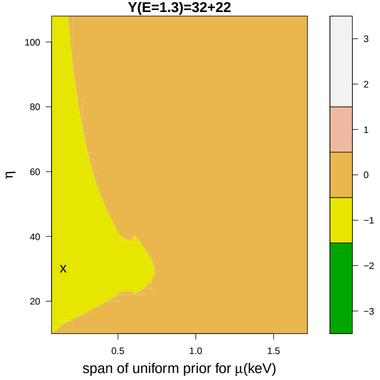
H_A: *Unknown* line location

- ppp-value $= 0.184$.

minimum Bayes Factor = 0.044 (span=0.07, $\eta = 30$)

Both ppp-value and Bayes Factor depend on where we look for line.

Can we calibrate the dependence?



Compare BF with P-values, cont'd

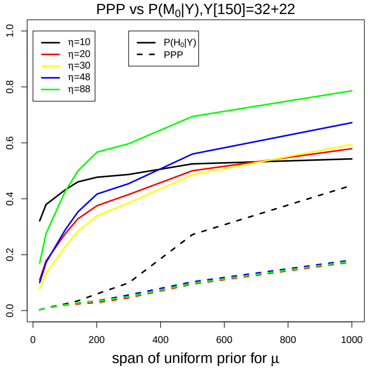
Assuming $P(M_0)/P(M_1) = 1$, we plot the PPP against $P(M_0|Y)$

Evidence decreases with more diffuse prior, for both.

BFs are more conservative.

Prior on μ

- *let's decide where to look,*
- *penalize us for looking too many place. i.e., look elsewhere effect*
- *Sensitivity of BF to prior for μ is sensible.*



A Bayesian Strategy for Line Search, Summary

Bayes Factors for Detection:

$$\text{BF} = \frac{p_0(Y)}{p_A(Y)} = \frac{\int p(Y|\theta, \omega = 0)p(\theta)d\theta}{\int p(Y|\theta, \mu, \omega)p(\theta, \mu, \omega)d\theta d\mu d\omega}$$

Setting priors

$\theta = (\alpha, \beta)$:	Non-informative / diffuse priors.
μ :	Where we want to look for the line.
ω :	How strong of a line do we want to look for?

Narrower prior ranges yield stronger results.

If strong lines are easy to see, maybe we can confine attension to weak lines.