# Using Bayes Factors for Model Selection in High-Energy Astrophysics

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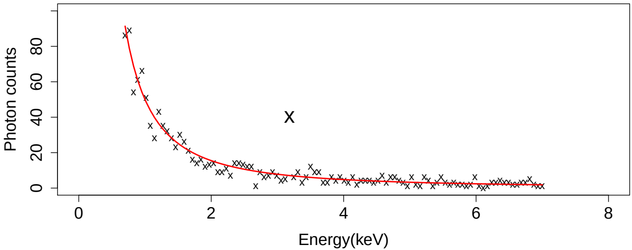
# Model Comparison in Astrophysics

- Nested models (line detection in spectral analysis):



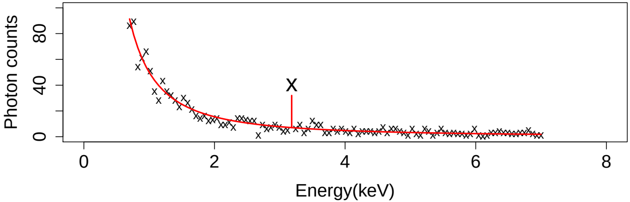

- Non-nested models:
  *Powerlaw* vs *Bremsstrahlung* for the red curve.
- Bottom line: need more than a confidence interval on “nesting parameter” to formally compare or select a model.

# 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,*** $\mathbf{M}$)
  3. Has sensitivity that varies with energy. (***effective area,*** $d$)
  4. Is subject to ***background contamination***, $\theta^B$
- 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.
  - $\mu$ has ***no value*** under $\mathrm{H}_0$.
  - $\omega$ must be non-negative under $\mathrm{H}_\mathrm{a}$ while its target tested value under $\mathrm{H}_0$, ***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 $\boldsymbol{Y}, \boldsymbol{\theta}$ 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.

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

- 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 $p(\boldsymbol{Y}|M) \equiv \int p(\boldsymbol{Y}|M,\theta)p(\theta|M)d\theta$.
  - ***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, $B_{01} = \dfrac{p(M_0|\boldsymbol{Y})}{p(M_1|\boldsymbol{Y})} \bigg/ \dfrac{p(M_0)}{p(M_1)}$
- 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 $\Theta_0$ and $\Theta_1$ might have different parameter settings and dimensions.

  **Example**: $\Theta_0$ *for Powerlaw while* $\Theta_1$ *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 $\Theta_0$ and $\Theta_1$ respectively. The parameter space for each chain is $(I_M, \Theta_M)$.

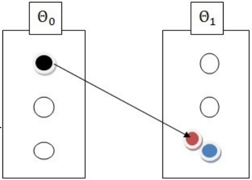
1. Run usual M-H algorithm for each chain with $q_0(\theta_0^{old}, \theta_0^{new})$ and $q_1(\theta_1^{old}, \theta_1^{new})$ being the proposal dist'n for sampling within $p(\Theta_0|M_0, Y)$ and $p(\Theta_1|M_1, Y)$, respectively.
2. For chain $i$, randomly pick one of the other chains, $j$, and propose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

   $\frac{1}{K-1}\sum_{j\neq i} q^j(\theta^j, \theta^{new})$, where $q^j(\theta^j, \theta^{new}) = 0$ 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 $\beta, \mu$ 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 $\omega$ and $\mu$?

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

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

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

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

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

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

# How to Assign a Proper Prior

- Compared to $\alpha$ and $\beta$, priors for $\omega$ and $\mu$ have much more influence on the BF. And they have to be proper.
- Different priors on $\omega$ and $\mu$ 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).

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

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

- The prior influence of $\alpha$ and $\beta$ are negligible compared to that of $\omega$ and $\mu$. Thus, they will be fixed in the simulation study.

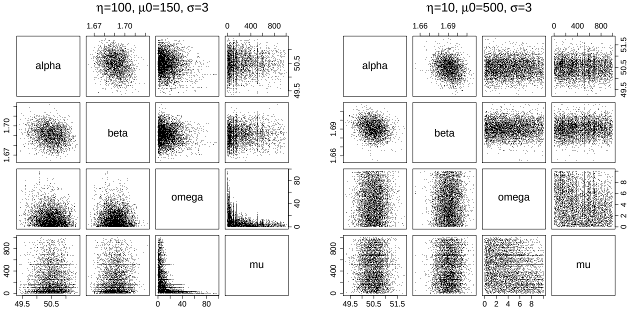
- Assume:

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

  *Using a Gamma prior for $\omega$ will have similar results.*

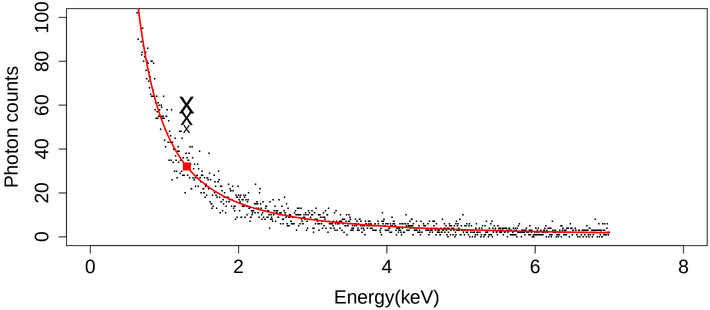
# The Non-Gaussian Posterior Dist'n

- The ordinary Gibbs breaks down here because the subchain for $\mu$ 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 $\alpha$ and $\beta$ 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 $\eta$.
  - $\eta$ will range from 10 to 108 with a step size of 2.
- For $\mu$, because $\mu \sim \mathrm{discrete}[N(\mu_0, \sigma^2)]$, we control both its mode $\mu_0$ and s.d $\sigma$.
  - We use two different value for $\mu_0$, 1.3keV and 1.97keV respectively (150 and 250 in terms of bin number).
  - For $\sigma$, it will range from 1 to 99 (bin width) with a step size of 2.

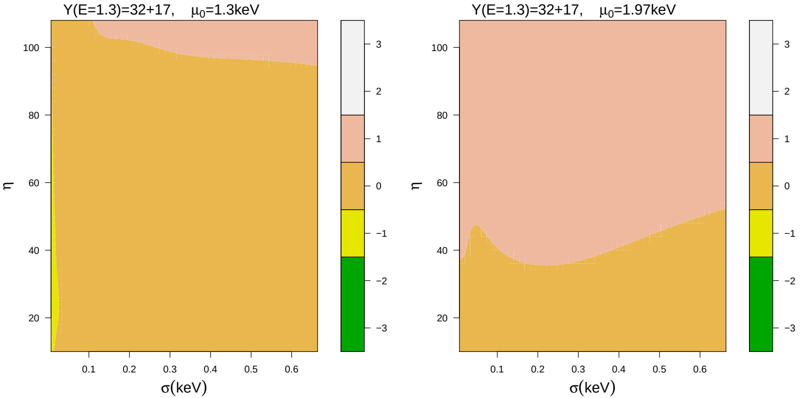
# Visualize The Prior Influence

We will plot the heatmap of $\log(BF)$ against $\eta$, $\mu_0$, and $\sigma$ 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

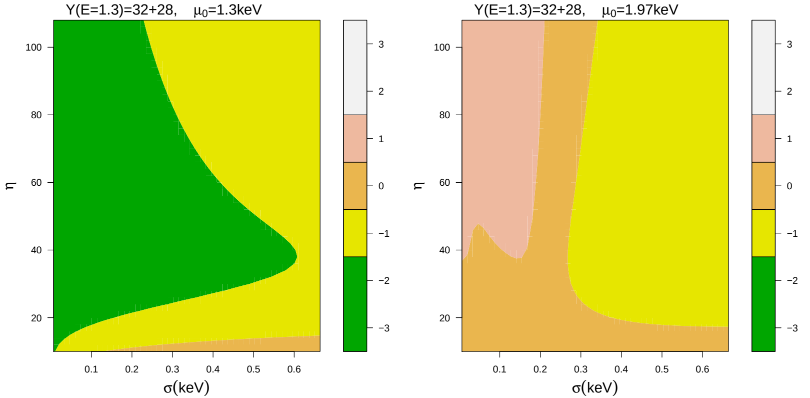
*$Y(E = 1.3)$ is about 3 s.d above null model intensity.*




*Diffuse or misplaced priors weaken evidence*

# Results: A Stronger Spectral Line

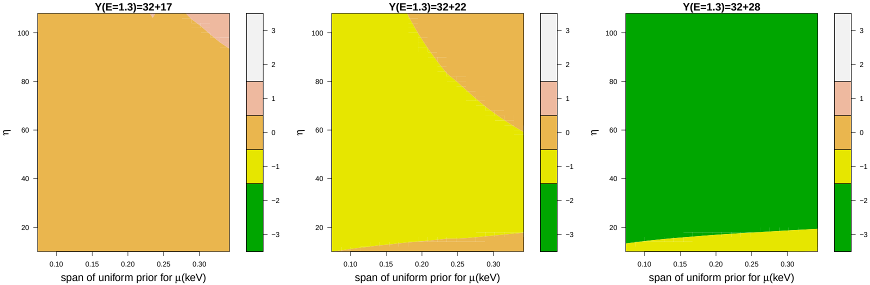
*$Y(E = 1.3)$ is about 5 s.d above null model intensity.*




*Diffuse or misplaced priors could completely change the decision*

# Results: Stronger Prior

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

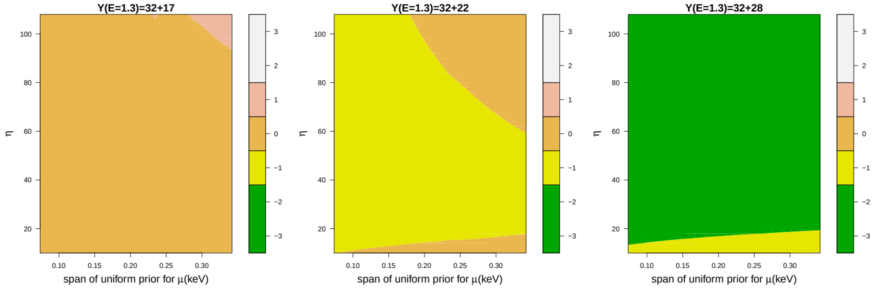


# Take Home Messages

- 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 $= 0.002$.

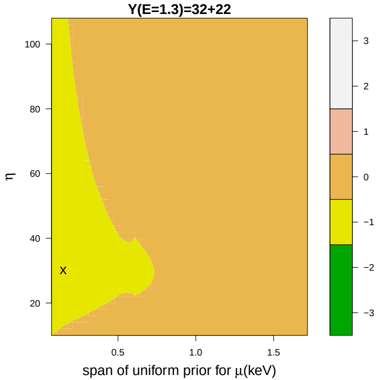
$H_A$: *Unknown* line location

- 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

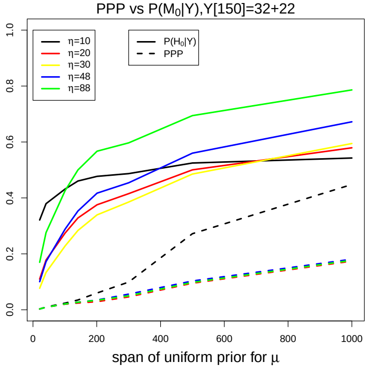
*Assuming* $P(M_0)/P(M_1) = 1$, *we plot the PPP against* $P(M_0|Y)$

***Evidence decreases with more diffuse prior, for both.***

***BFs are more conservative.***

Prior on $\mu$

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

$\mu$ : Where we want to look for the line.

$\omega$ : 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.*

# The Quasar PG 1634+706

Simulate three datasets based on the Quasar (obs47).

- source model: *xsphabs*(powlaw1d+delta1d)*
- use the ARF/RMF associated with obs47.
- $nH = 0.064, pl.ampl = 0.00043, pl.gamma = 1.99$. (sherpa fit for obs47).
- exposure$=$ 5000 (obs47 has exposure$=$ 5389.08).
- no background contamination.
- $dl.pos = 2.88$ (powlaw amplitude here$=$ 0.00005).
- $dl.ampl = 0.000005, 0.00001, 0.000025$

# Prior Setup

- When computing the BF for the real data, fix $nH, bkg.factor$ at their sherpa fitted value.
- For the simulated data, fix $nH, pl.ampl, pl.gamma$.
- For the priors,
  - $pl.ampl \sim U(0, 0.001)$
  - $pl.gamma \sim U(0, 10)$
  - $dl.pos \sim TN|_{>1}(2.88, sd)$, where $sd = n \cdot 0.025$
  - $dl.ampl \sim U(0, \eta)$, where $\eta = 0.000005 + n \cdot 0.000065/4$
  - $n = 0, 1, 2, 3, 4$

# Visualize The Prior Influence

We will plot the heatmap of $\log(BF)$ 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 $H_0$ |
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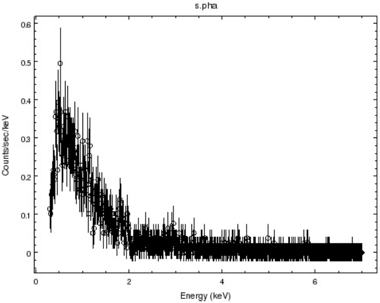
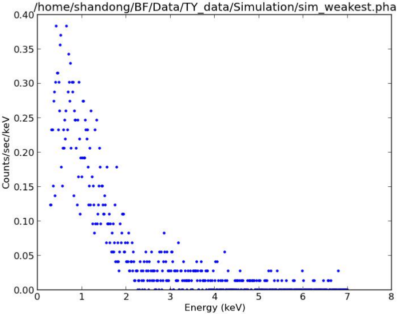
| $[-30, -3]$ | $[-1.5, -0.5]$ | Substantial to strong for $H_a$ |
| $< -30$ | $< -1.5$ | Very strong to overwhelming for $H_a$ |

# Data Visualization

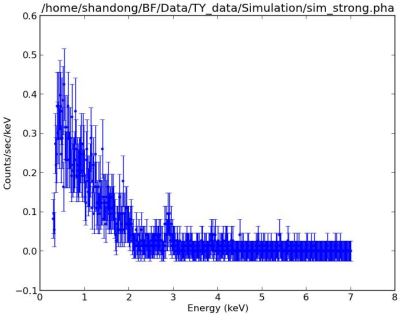
The real data and the weakest simulated case.

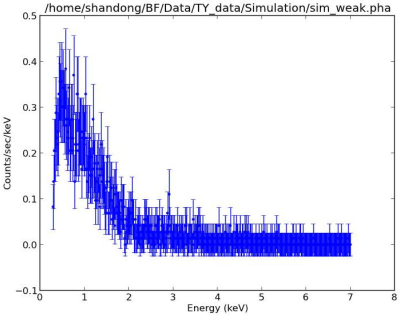


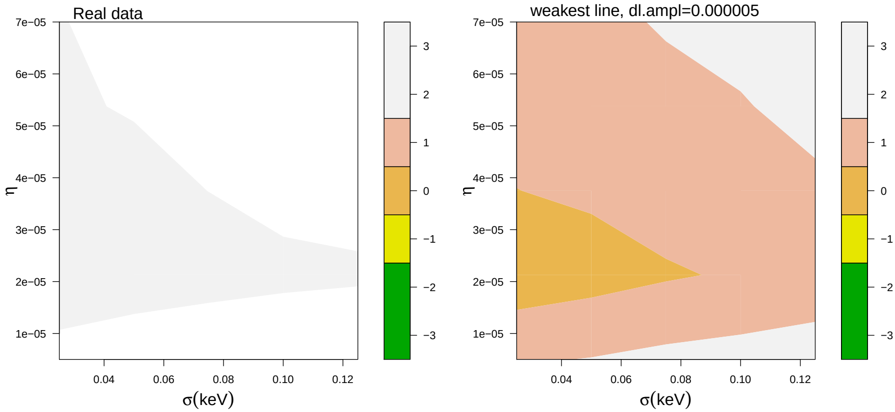
# Data Visualization, Cont'd

The strongest and modest simulated case.



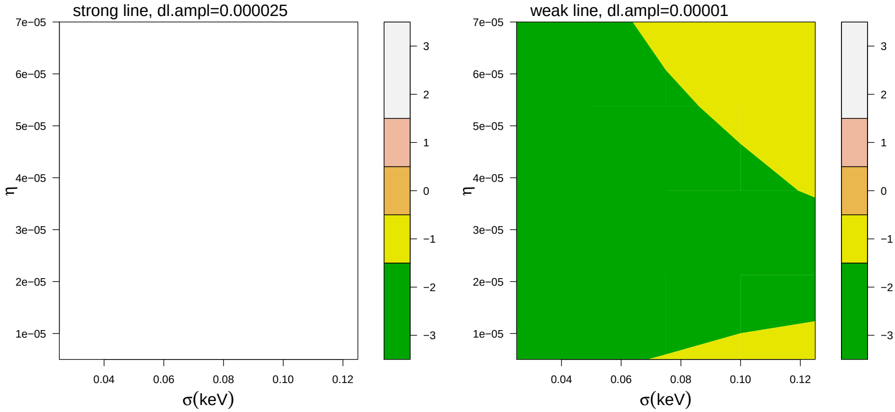



# BF and PPP



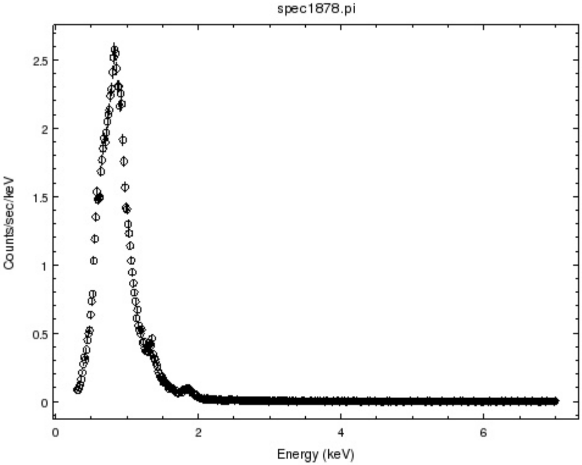

| ppp (based on 200 MC samples) | Real | Weakest |
|---|---|---|
| $H_A$: line location (1.0-7.0keV) | **0.82**/**0.09** | 0.505 |
| $H_A$: line location (2.7-3.1keV) | 0.01 | 0.065 |

# BF and PPP, Cont'd




| ppp (based on 200 MC samples) | Strong | Modest |
|---|---|---|
| $H_A$: line location (1.0-7.0keV) | 0.42 | 0.535 |
| $H_A$: line location (2.7-3.1keV) | 0.0 | 0.02 |

# Another Data: D1878




- Scientific question and prior setups for this dataset?