Sampling + Model Comparison, Part II

Universiteit van Amsterdam

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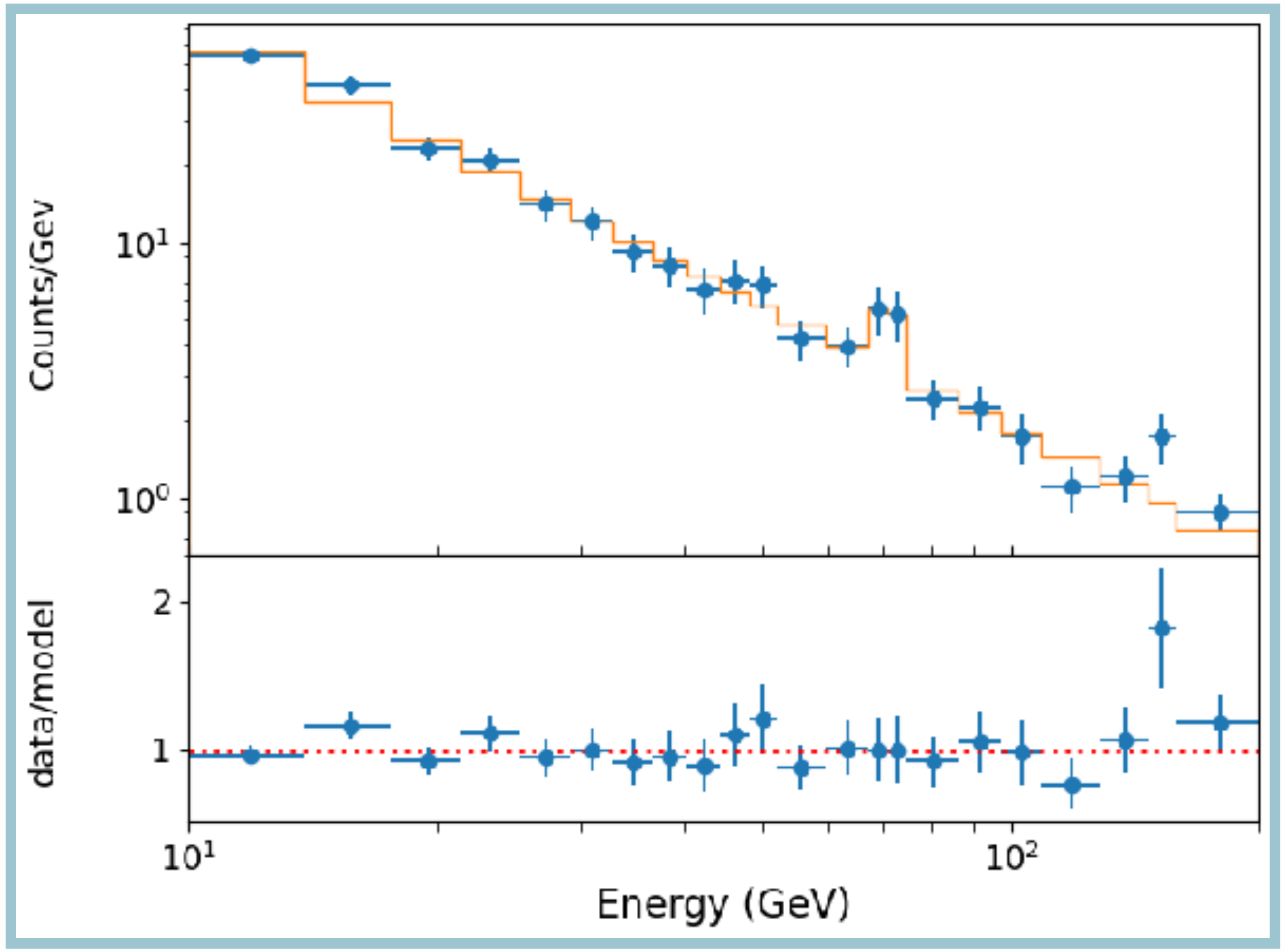
What about physics?



Data: X-ray spectrum

Model: Power law + Gaussian line

Likelihood: Poisson

Parameters: $A_{\mathrm{PL}}, \Gamma, A_{\mathrm{Line}}, E_{\mathrm{Line}}, \sigma_{\mathrm{Line}} A_{\mathrm{Line}}$

Priors: ???

What priors should we choose?

$$p(A_{\mathrm{PL}}, \Gamma, A_{\mathrm{Line}}, E_{\mathrm{Line}}, \sigma_{\mathrm{Line}} \,|\, D) = \frac{p(D \,|\, A_{\mathrm{PL}}, \Gamma, A_{\mathrm{Line}}, E_{\mathrm{Line}}, \sigma_{\mathrm{Line}}) p(A_{\mathrm{PL}}, \Gamma, A_{\mathrm{Line}}, E_{\mathrm{Line}}, \sigma_{\mathrm{Line}})}{p(D)}$$

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What assumption have we made here?

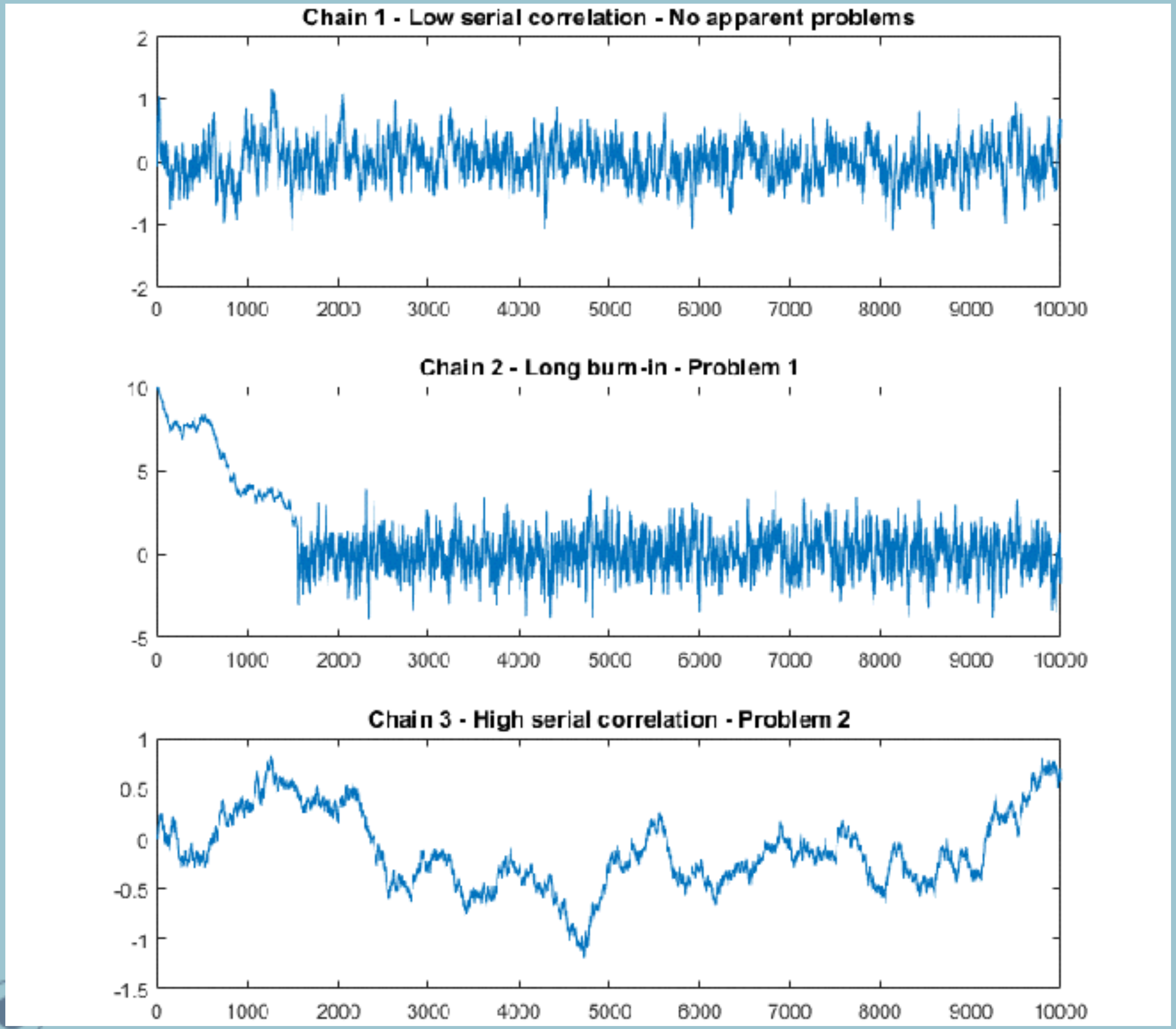
Independence of priors!

Markov Chain Monte Carlo: Assessing Convergence

Assessing Convergence:

trace plots

How do I know whether my Markov chain is sampling from the posterior?



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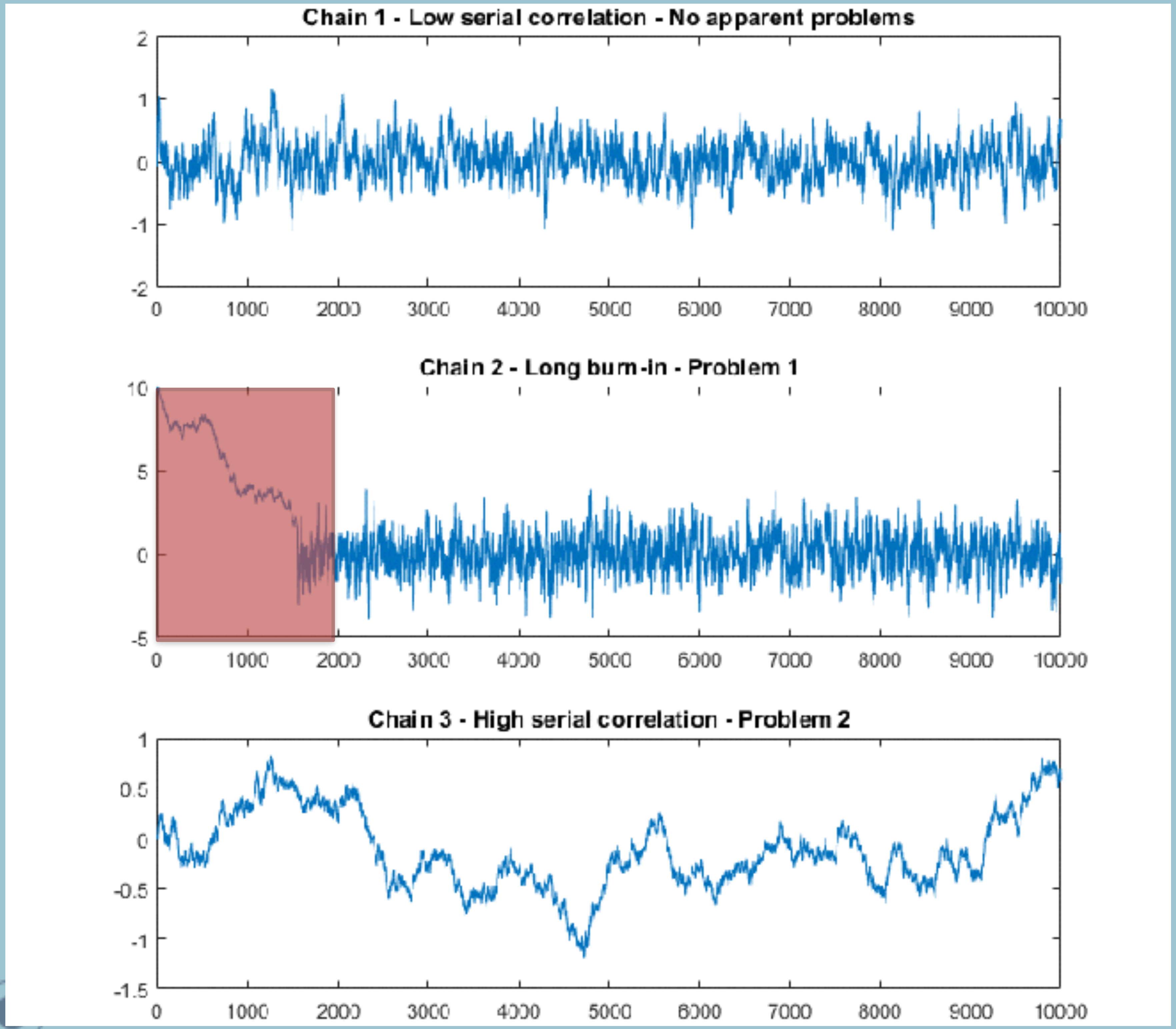

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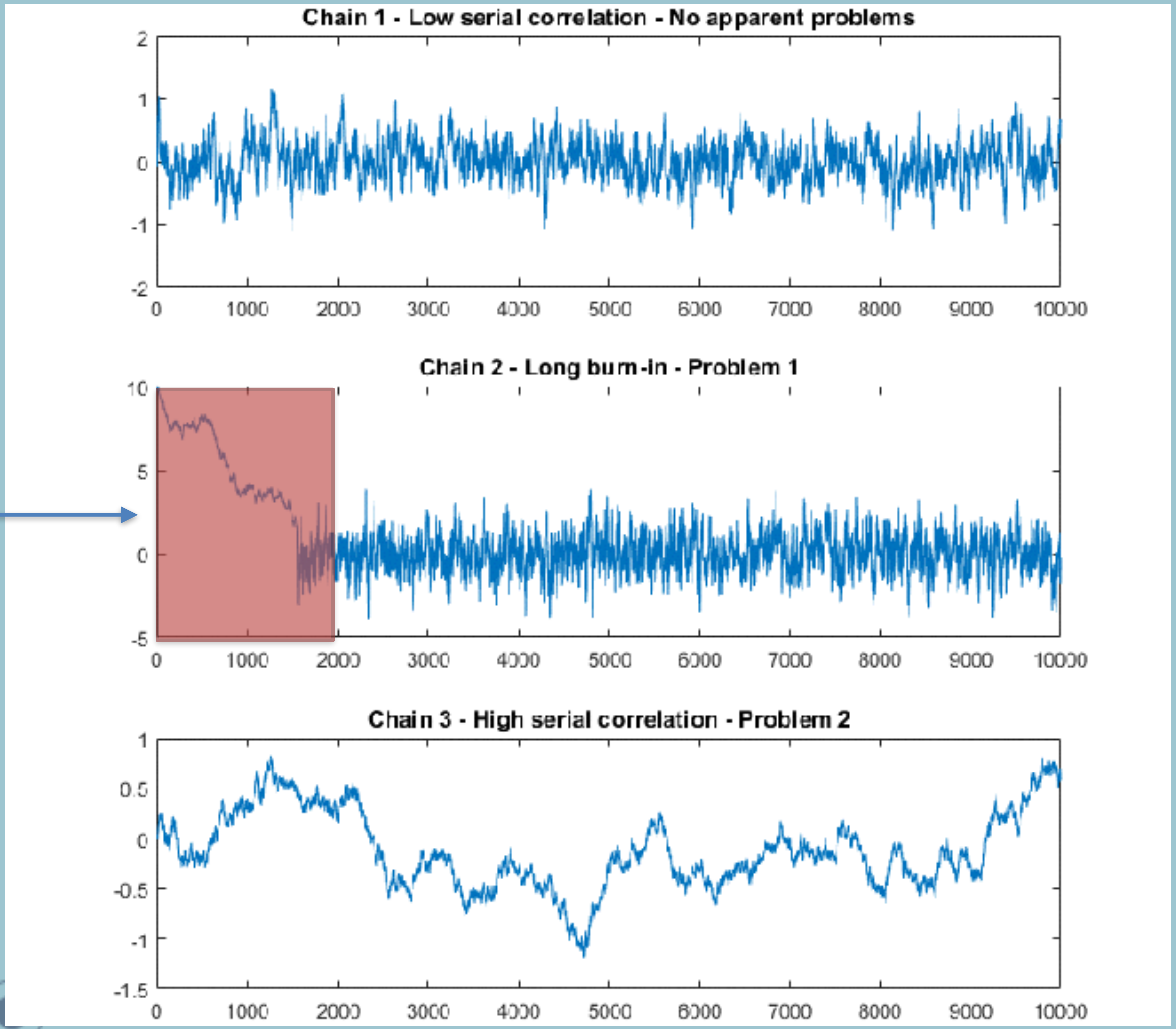

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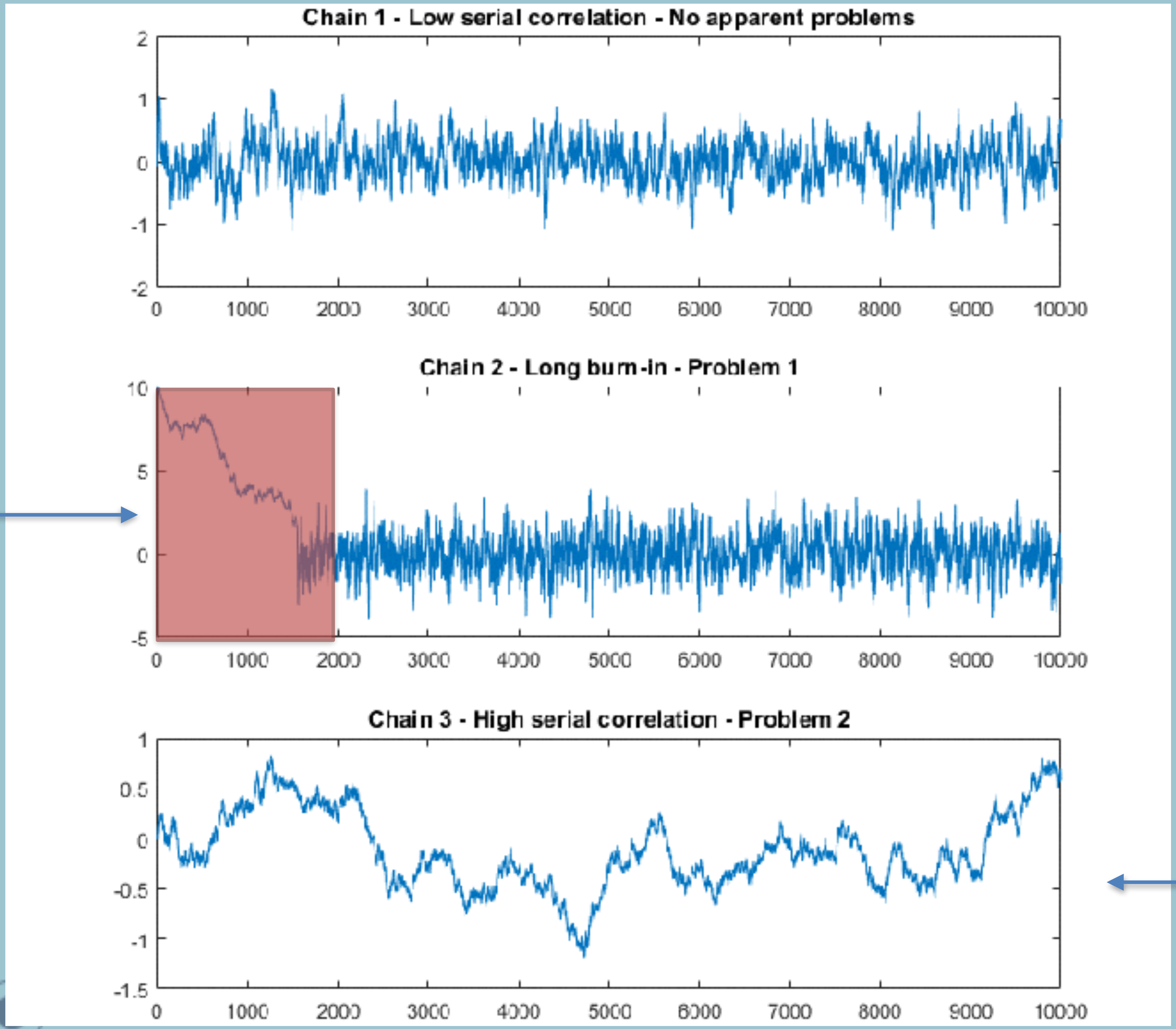

Cut out this part

Sample for much longer, change $q(\theta \mid \theta_0)$

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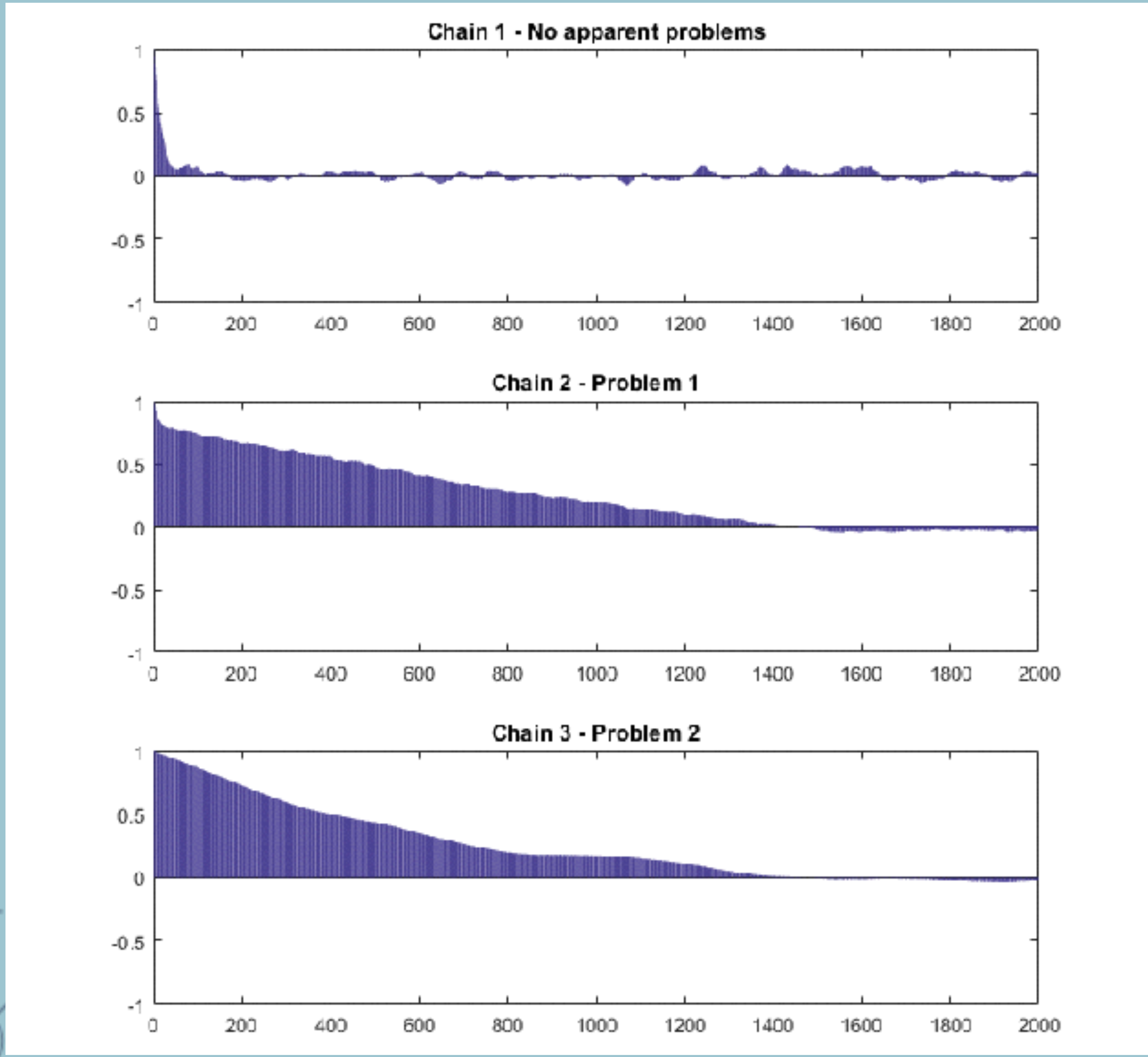
Assessing Convergence:

autocorrelation

"How long do I have to sample until I get to an independent sample?"



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Assessing Convergence:

Gelman-Rubin Statistic

Compare the variance <u>within chains</u> to the variance <u>between chains</u>

$$\bar{x}_j = \frac{1}{L}\sum_{i=1}^{L} x_i^{(j)}$$ Mean value of chain j

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$$W = \frac{1}{J}\sum_{j=1}^{J}\left(\frac{1}{L-1}\sum_{i=1}^{L}(x_i^{(j)} - \bar{x}_j)^2\right)$$ Averaged variances of the individual chains across all chains

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An estimate of the Gelman-Rubin statistic R then results as[1]

$$R = \frac{\frac{L-1}{L}W + \frac{1}{L}B}{W}.$$

When L tends to infinity and B tends to zero, R tends to 1.

Summarising Posterior Probability Distributions

You have sampled a posterior PDF, which has produced samples (vectors of parameters). What do you do now?

Summarising Posterior Probability Distributions:

Marginalised Distributions + Credible Intervals

Reminder: Marginalisation

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$$p(x) = \int_{-\infty}^{\infty} p(x, y)dy = \int_{-\infty}^{\infty} p(x \mid y)p(y)dy$$

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Reminder: Marginalisation

$$p(x) = \int_{-\infty}^{\infty} p(x, y)dy = \int_{-\infty}^{\infty} p(x \,|\, y)p(y)dy$$

$$p(\theta_1 \,|\, D) = \int_{-\infty}^{\infty} p(\theta_1, \theta_2 \,|\, D)p(\theta_1)p(\theta_2)d\theta_2$$

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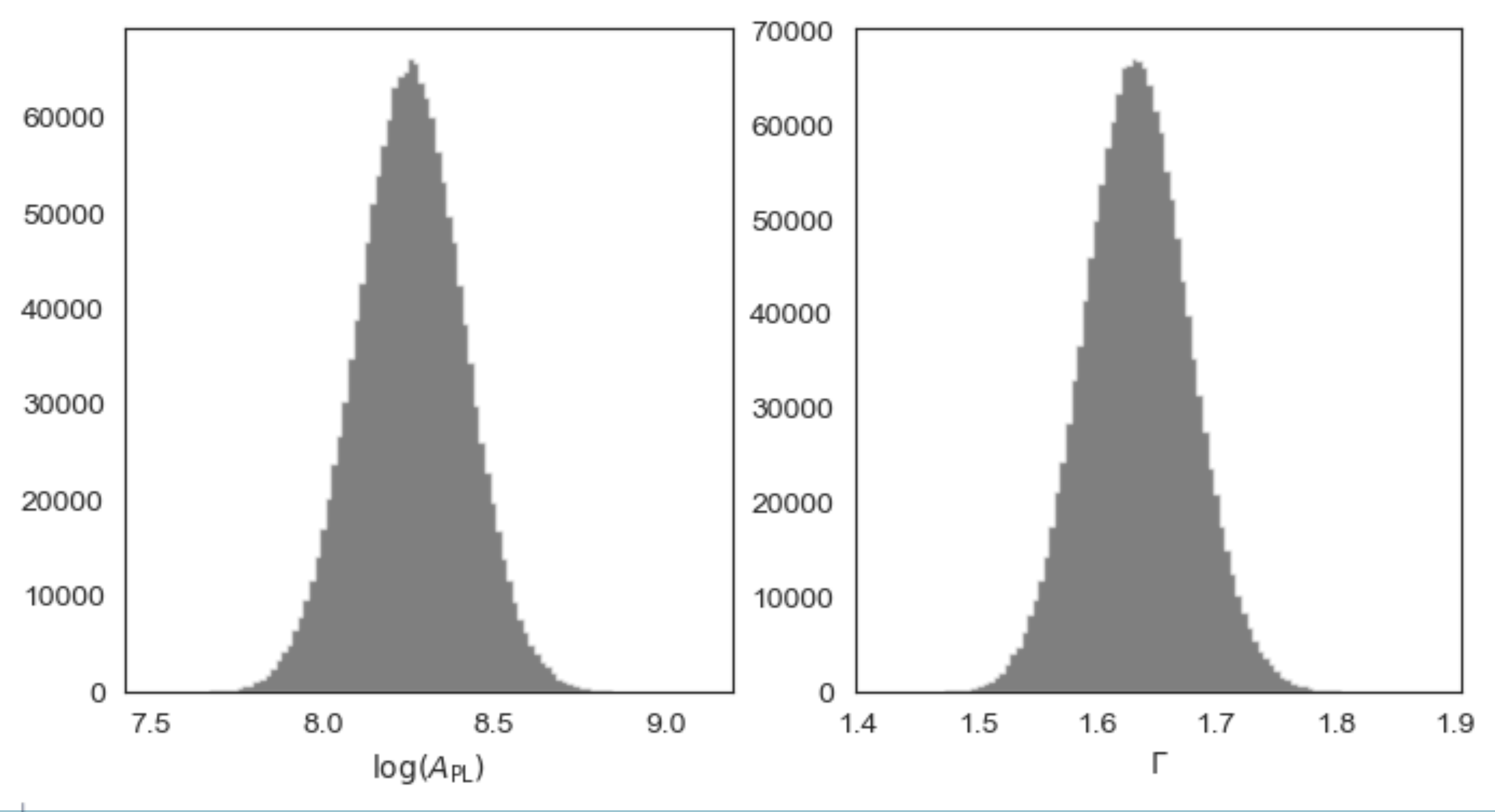

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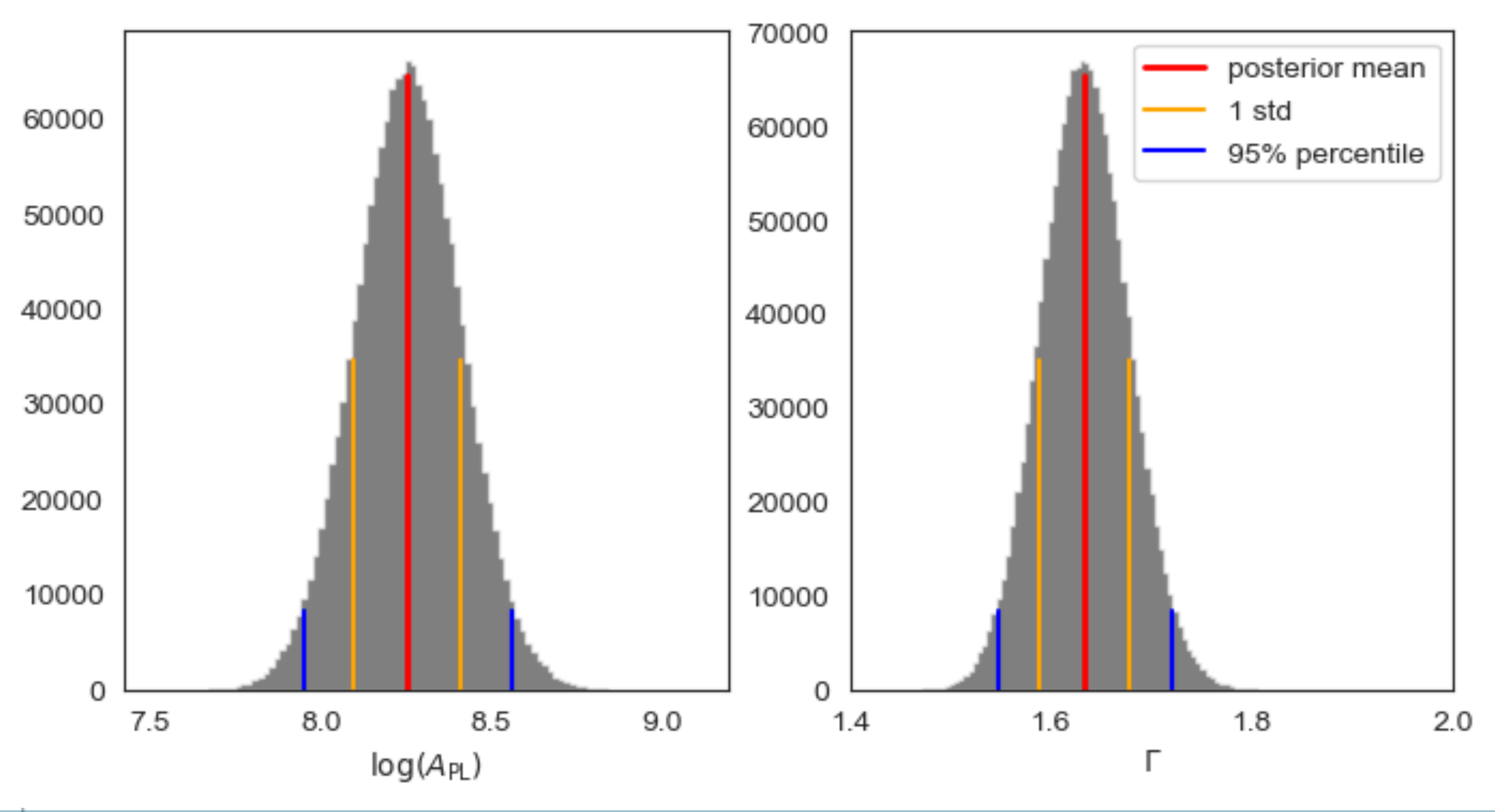

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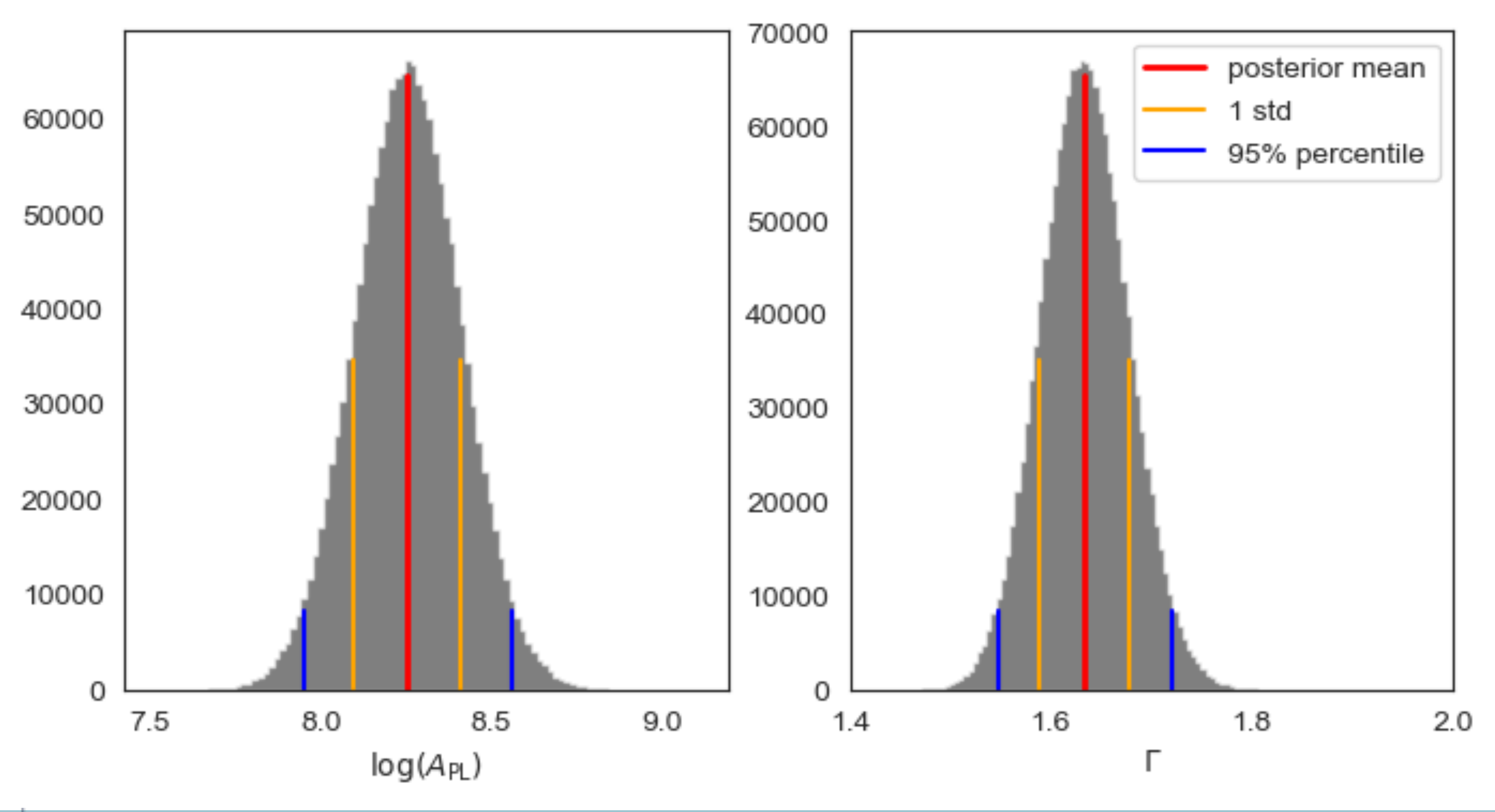
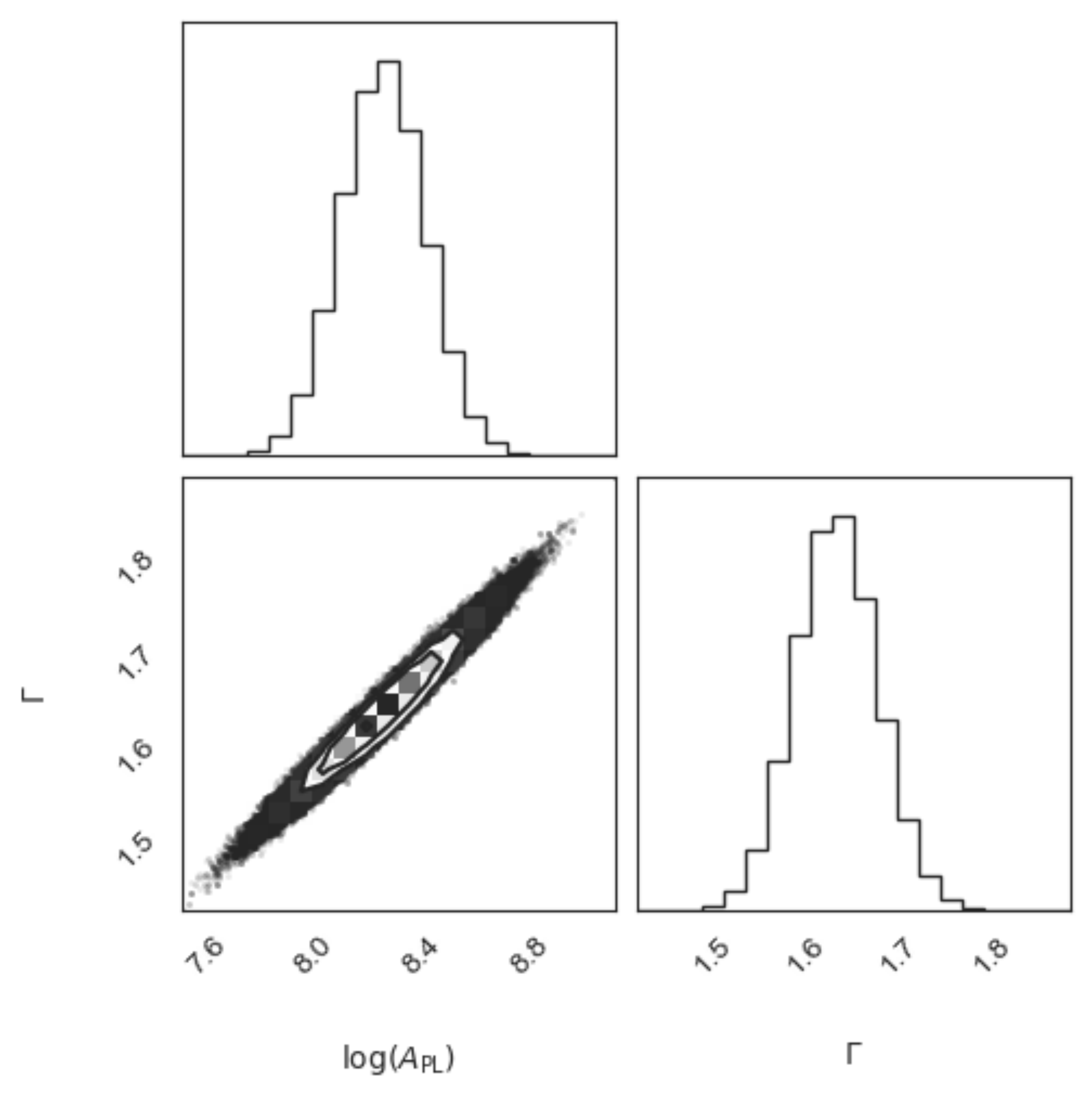


Considering just one dimension of your MCMC sample automatically marginalises over the other dimensions! Magic!

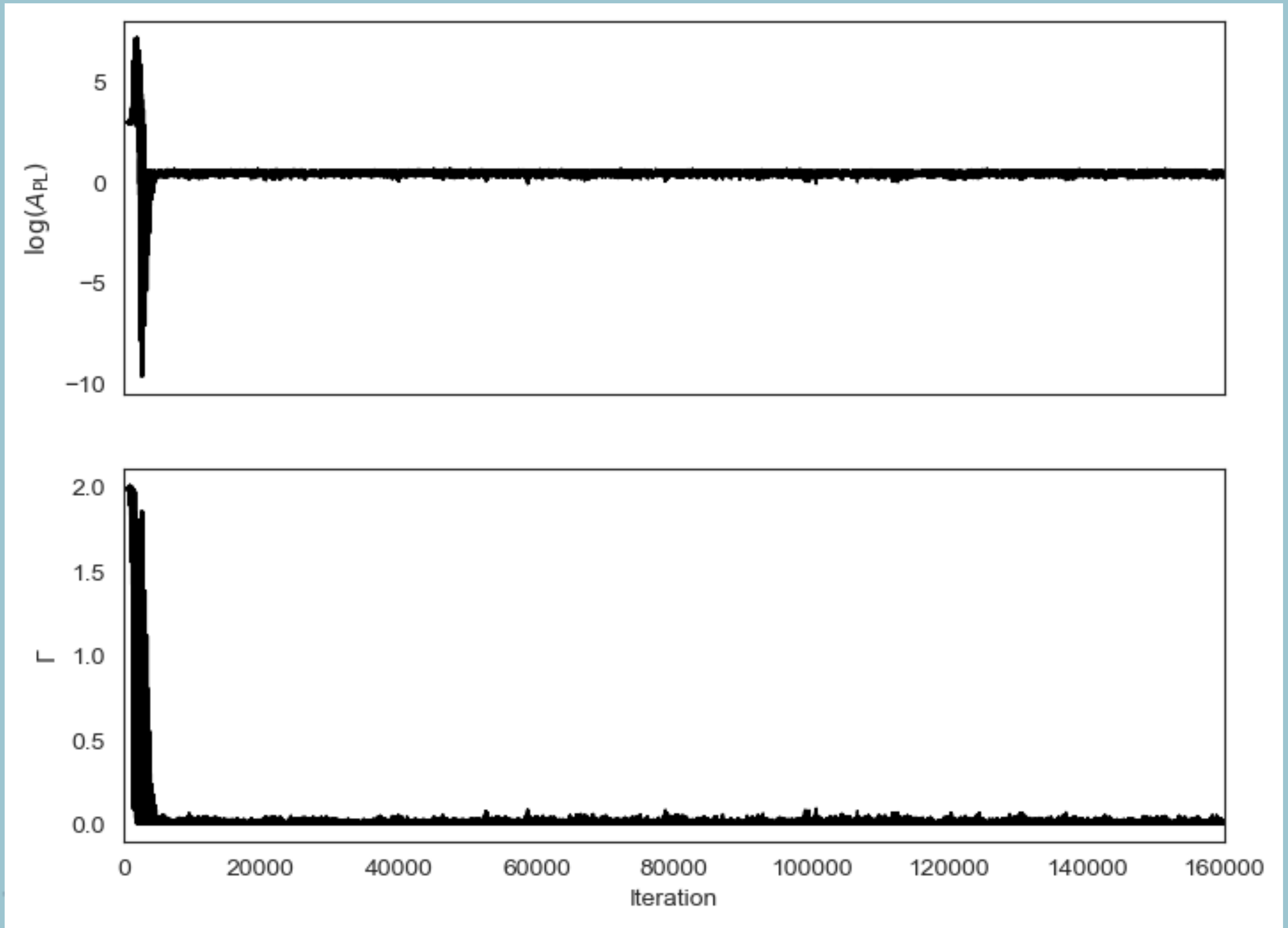
Summarising Posterior Probability Distributions:

Corner Plots or Pair Plots



How do you know if/ when things go wrong?

Earlier this week ...



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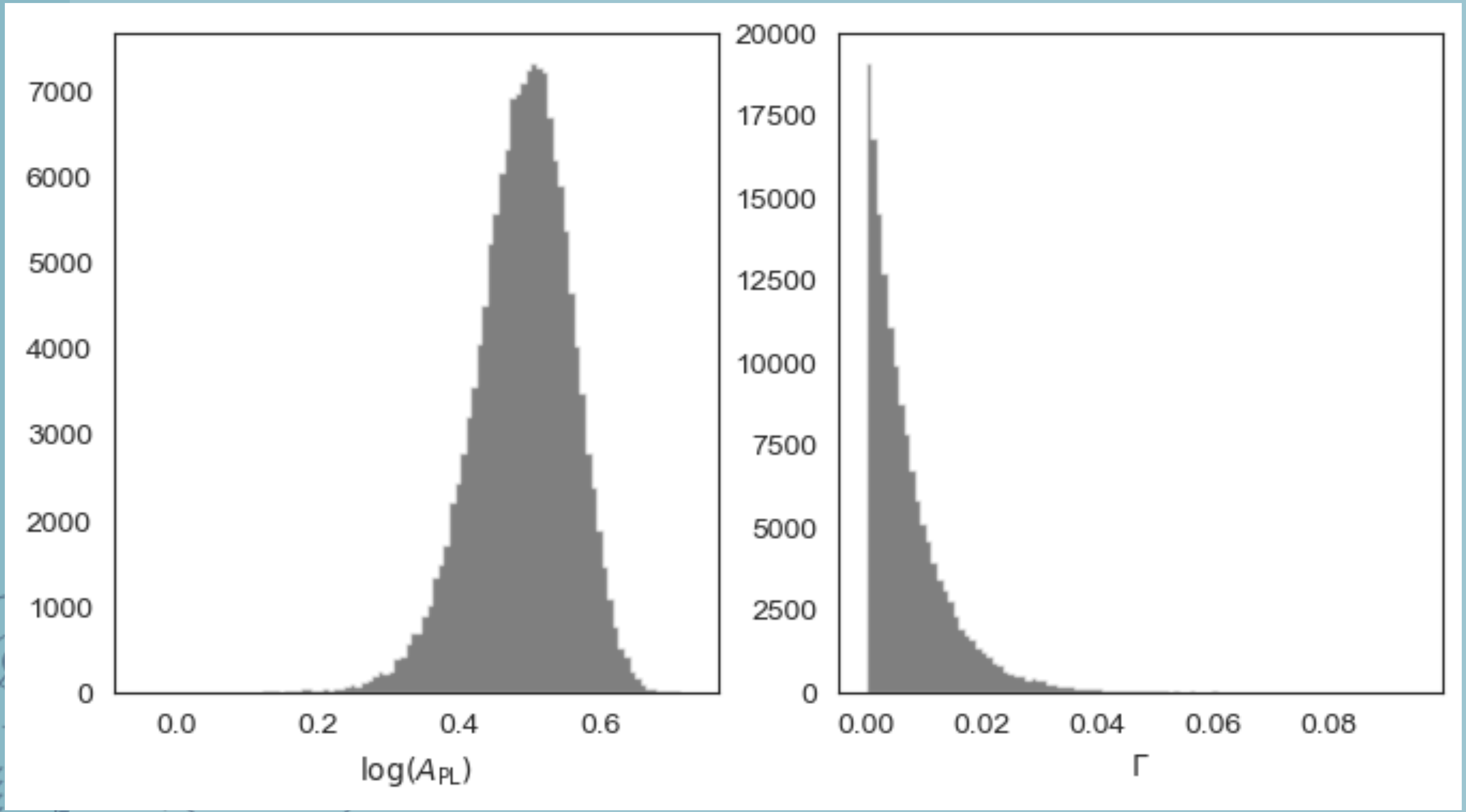

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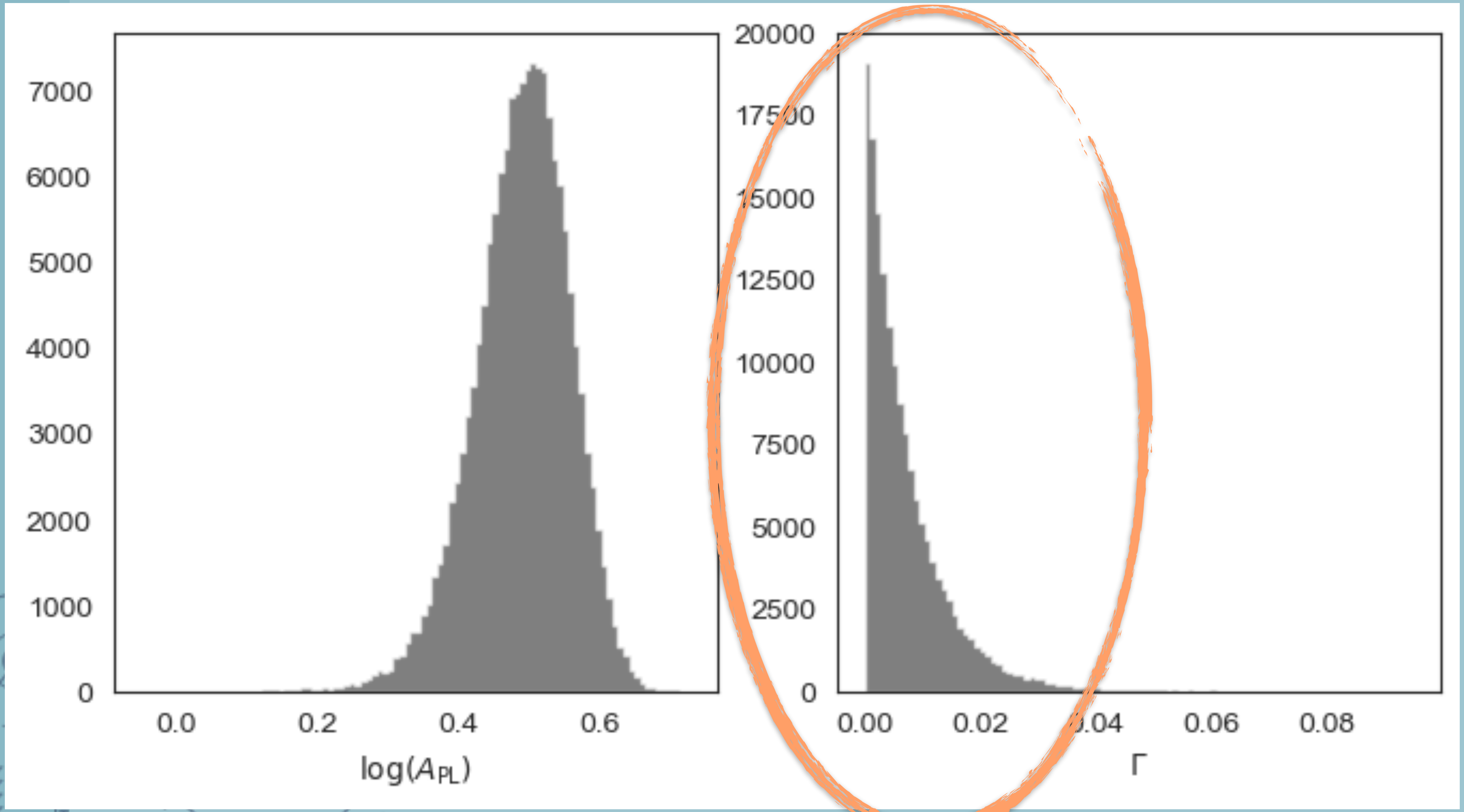
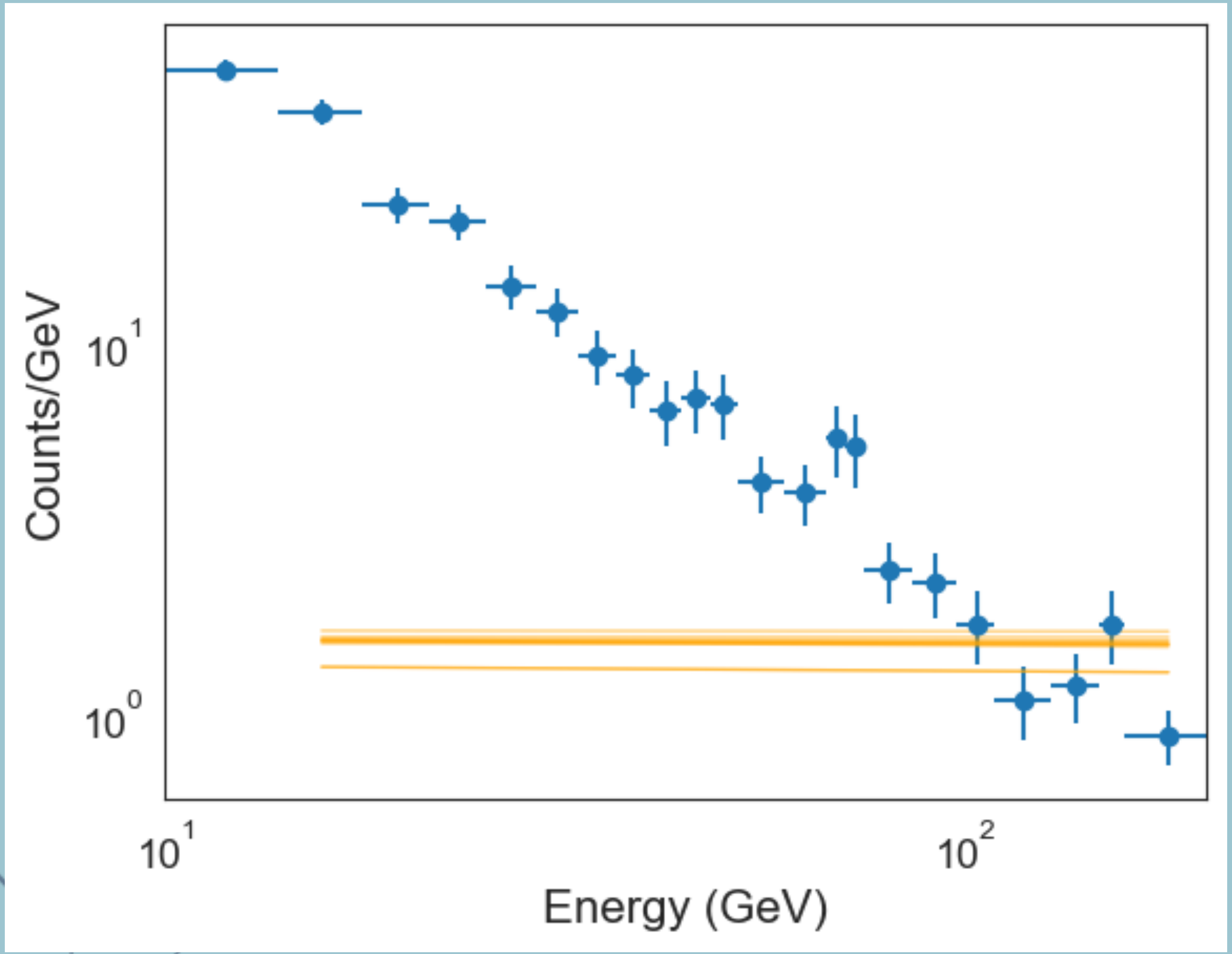


Plot posterior draws:



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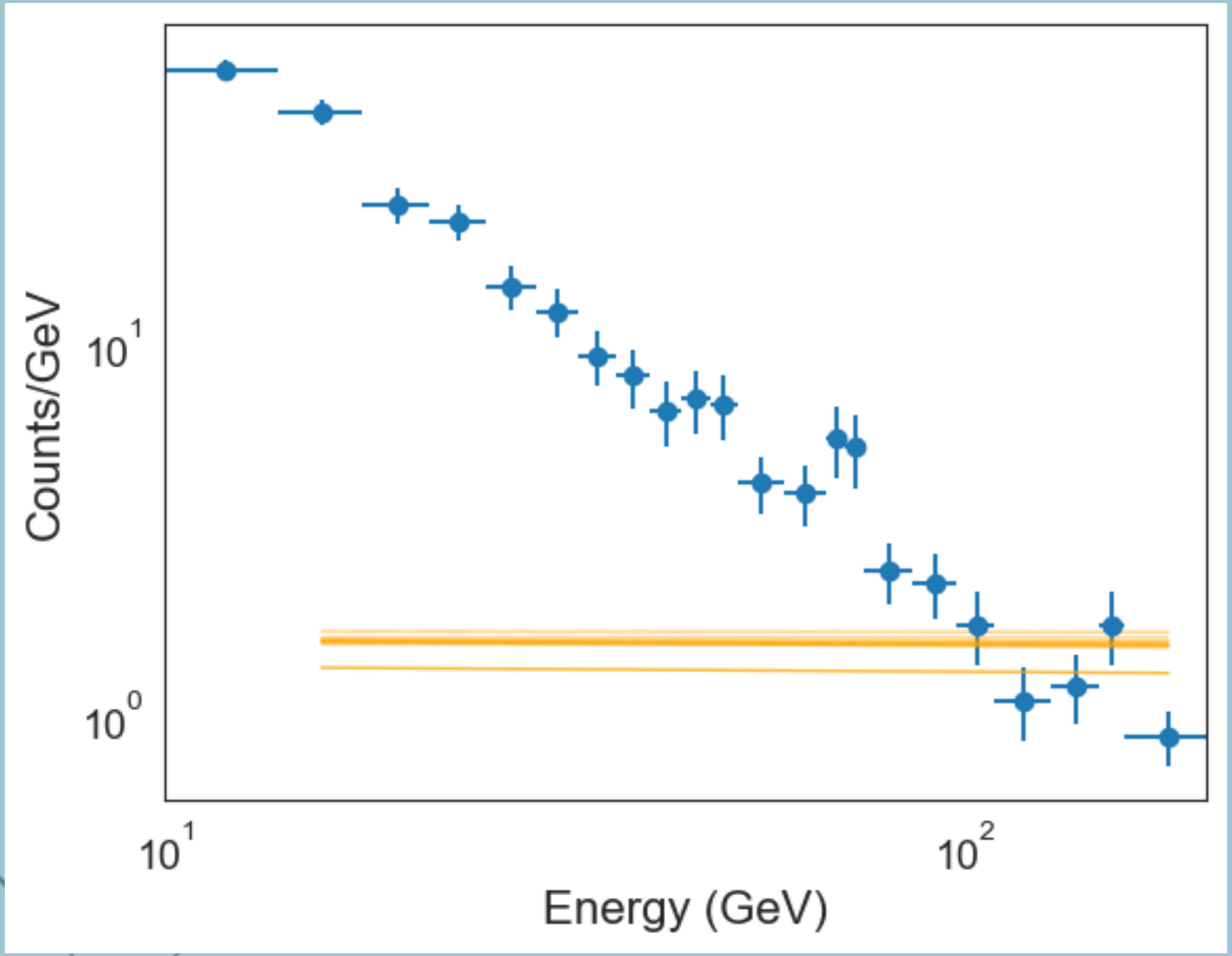
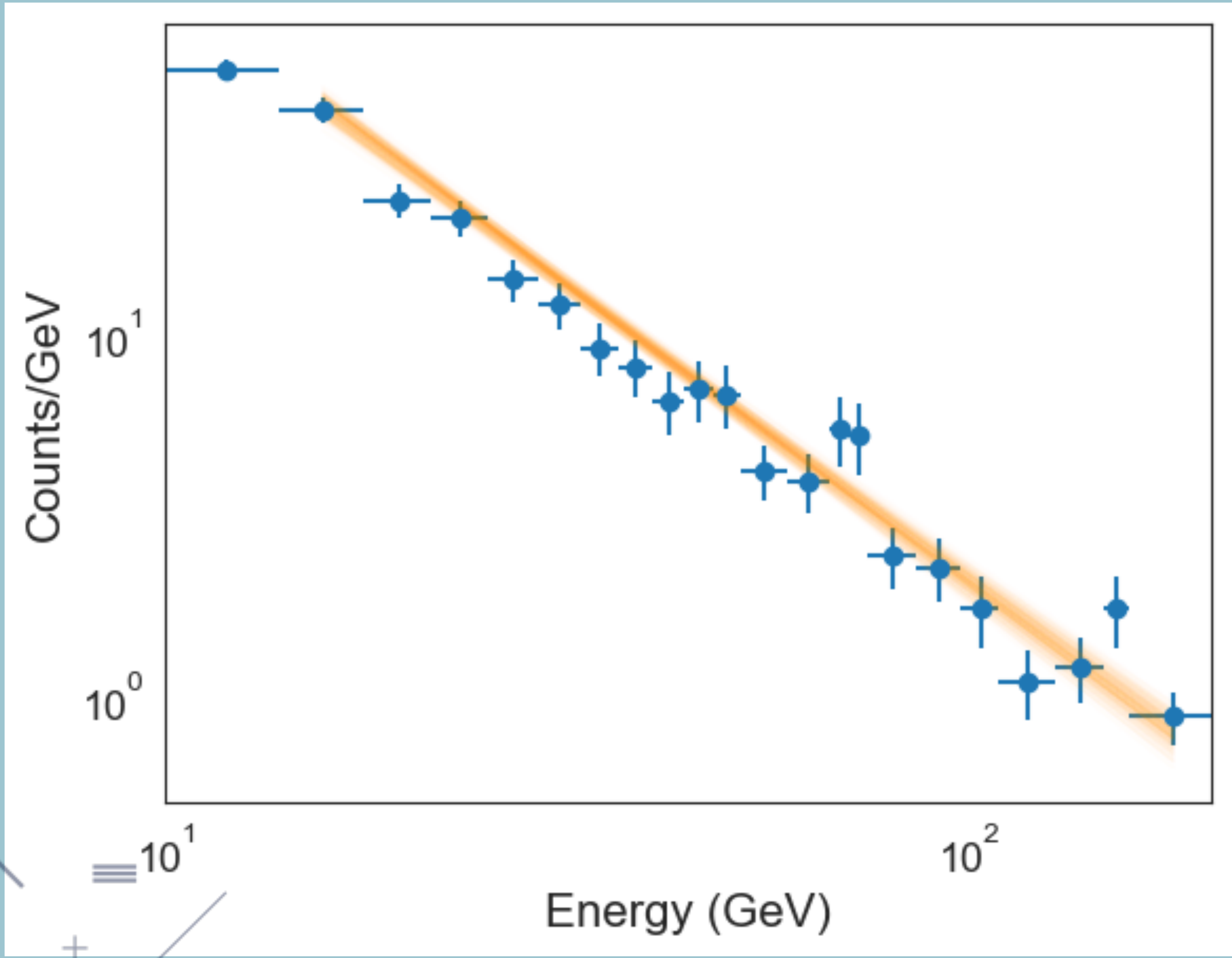


Γ was defined with the wrong sign!

Fixing Γ:



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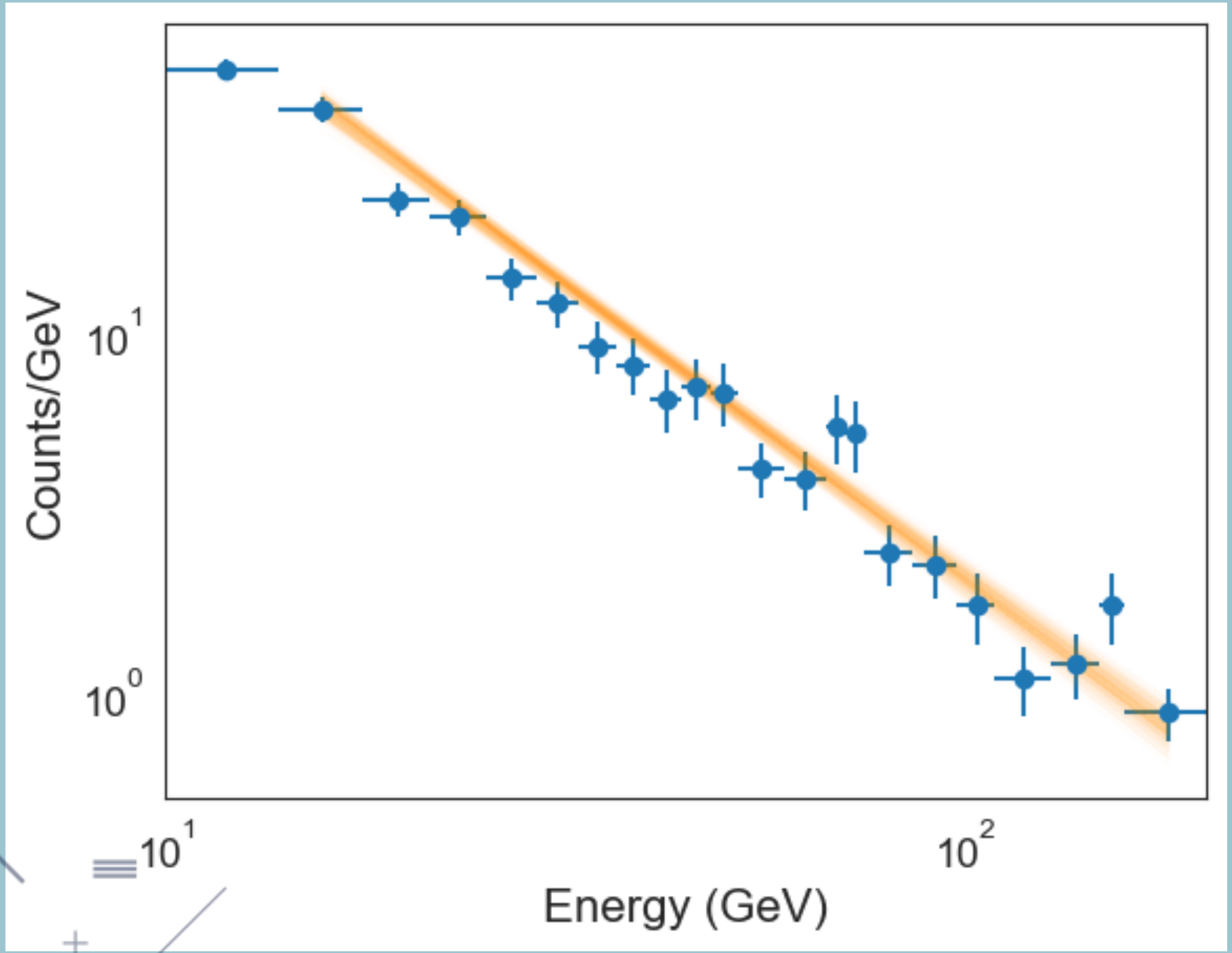

Plotting posterior draws allows you to see the range of models the posterior produces

MCMC Notes and Pitfalls

Further reading:
https://arxiv.org/pdf/1710.06068

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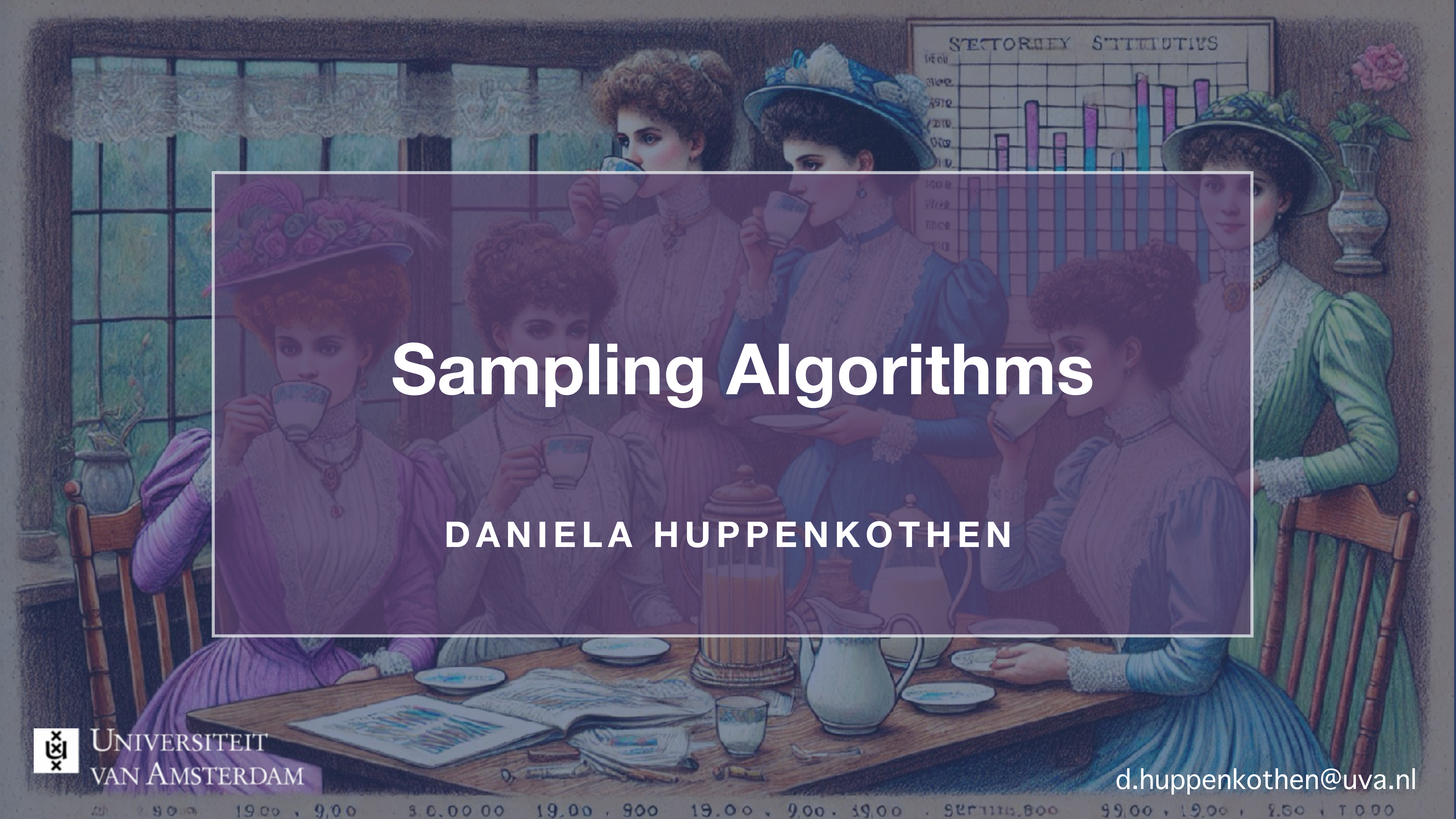
Sampling is not a one-size-fits-all solution! Different problems may do better with different sampling algorithms! And there are many (see also: Hamiltonian Monte Carlo, Importance Sampling, Slice Sampling, Gibbs Sampling, Nested Sampling, AI-supported sampling algorithms, ...)



Sampling Algorithms

DANIELA HUPPENKOTHEN

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- Can become computationally inefficient for large numbers of parameters
- Tend to get stuck in regions of parameter space for a long time, especially if high correlation in posterior and many dimensions

Slice Sampling

Further reading:

- https://www.cs.toronto.edu/pub/radford/slice-aos.pdf
- arXiv:1001.0175

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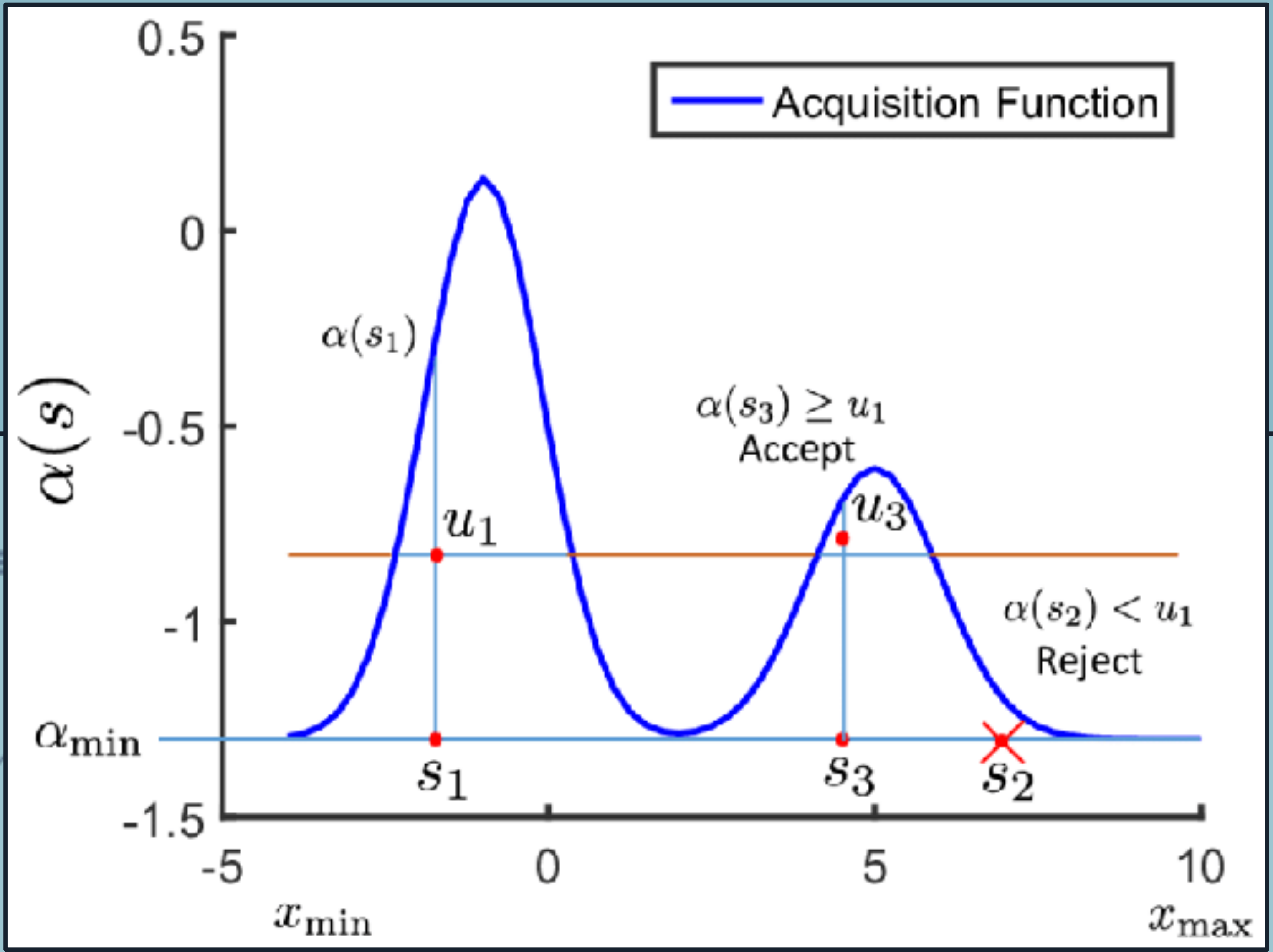

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- In 1D: easier to implement than Metropolis Hastings

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4. From all the line segments, draw a value of x uniformly.
5. Repeat from step 2 until you have as many draws as you want.

- In 1D: easier to implement than Metropolis Hastings
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Slice Sampling

Further reading:

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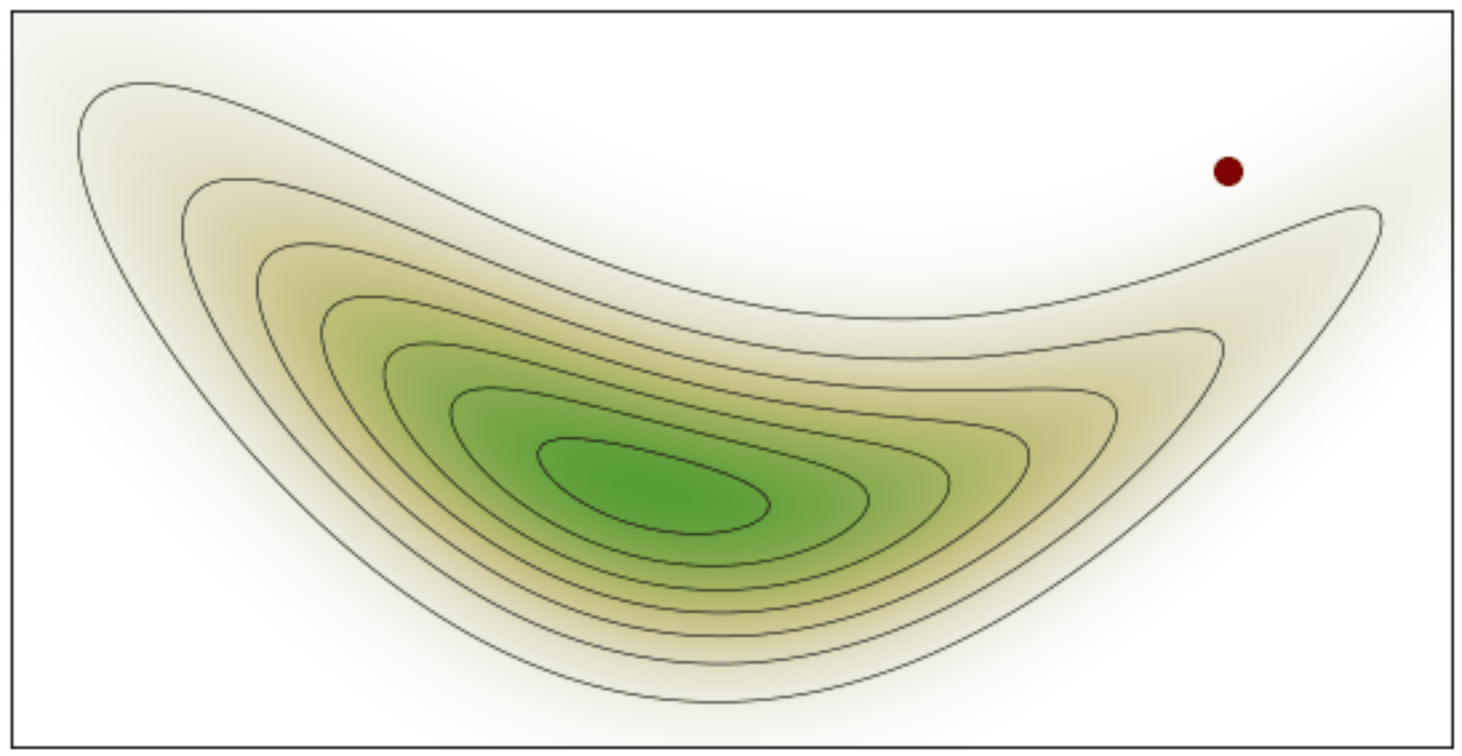
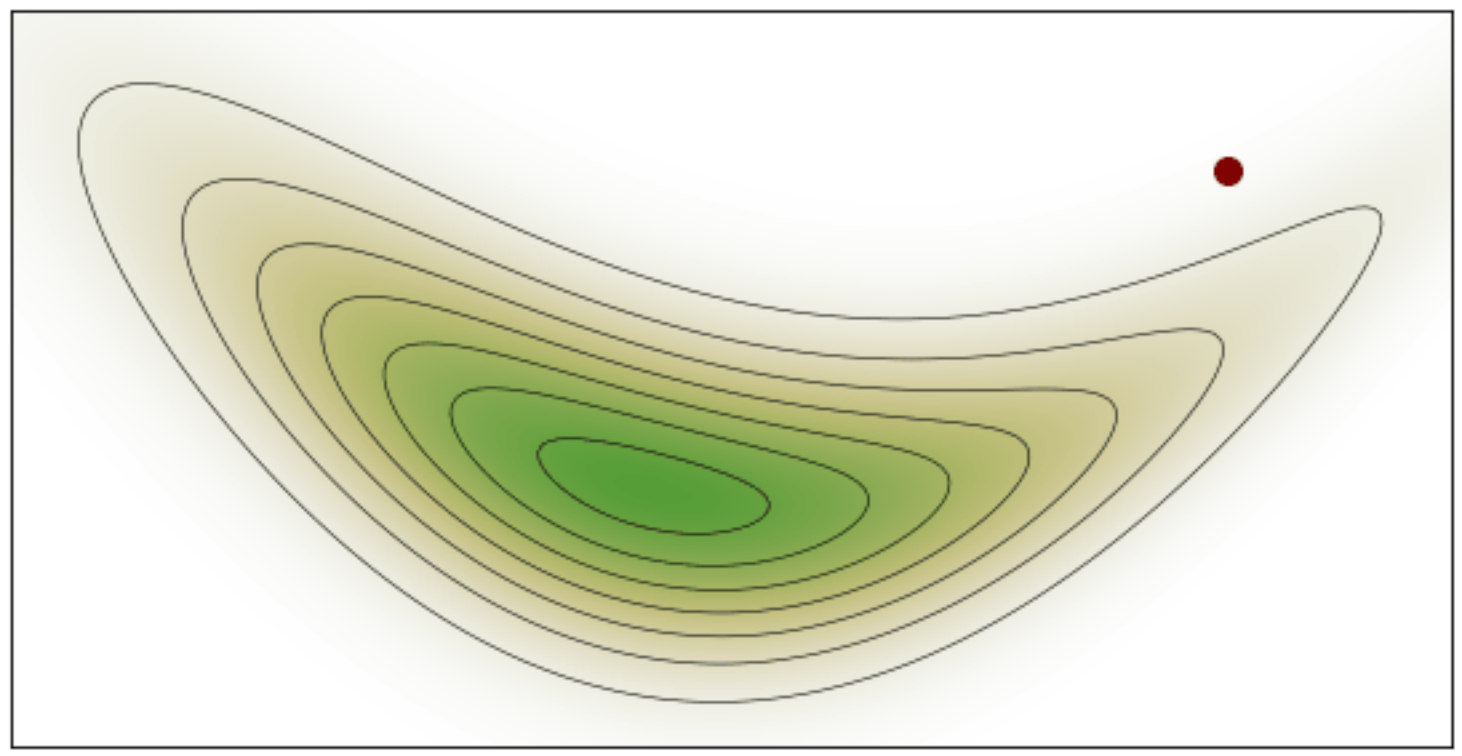
- Slice-sampling auto-adjusts the step size
- Often slower than Metropolis Hastings.
- Finding the roots of the intersection between horizontal line and distribution is pretty tricky.

Hamiltonian Monte Carlo



Hamiltonian Monte Carlo

Use Hamiltonian dynamics to propose a move to a new point in state space



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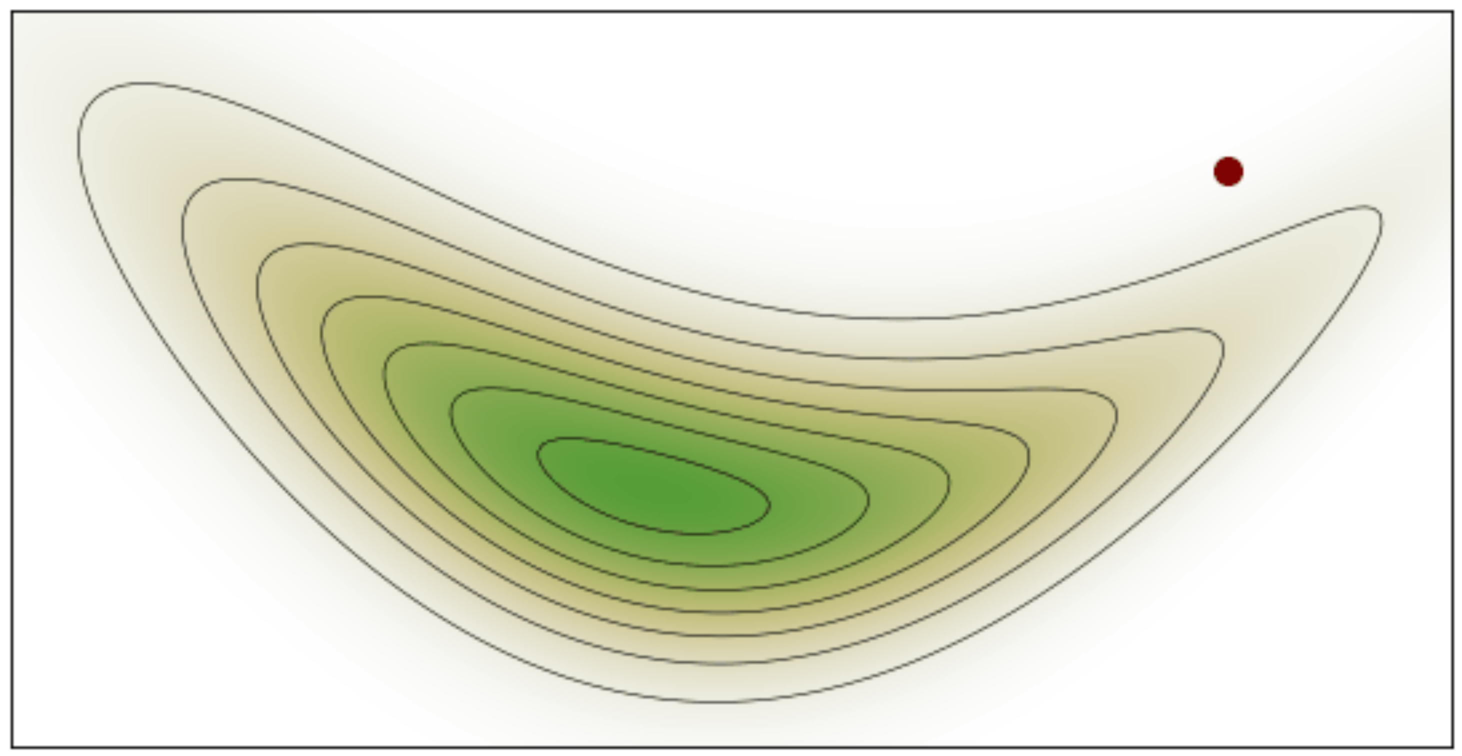
Reduces correlations between successive samples by proposing moves to distant states which maintain a high probability of acceptance



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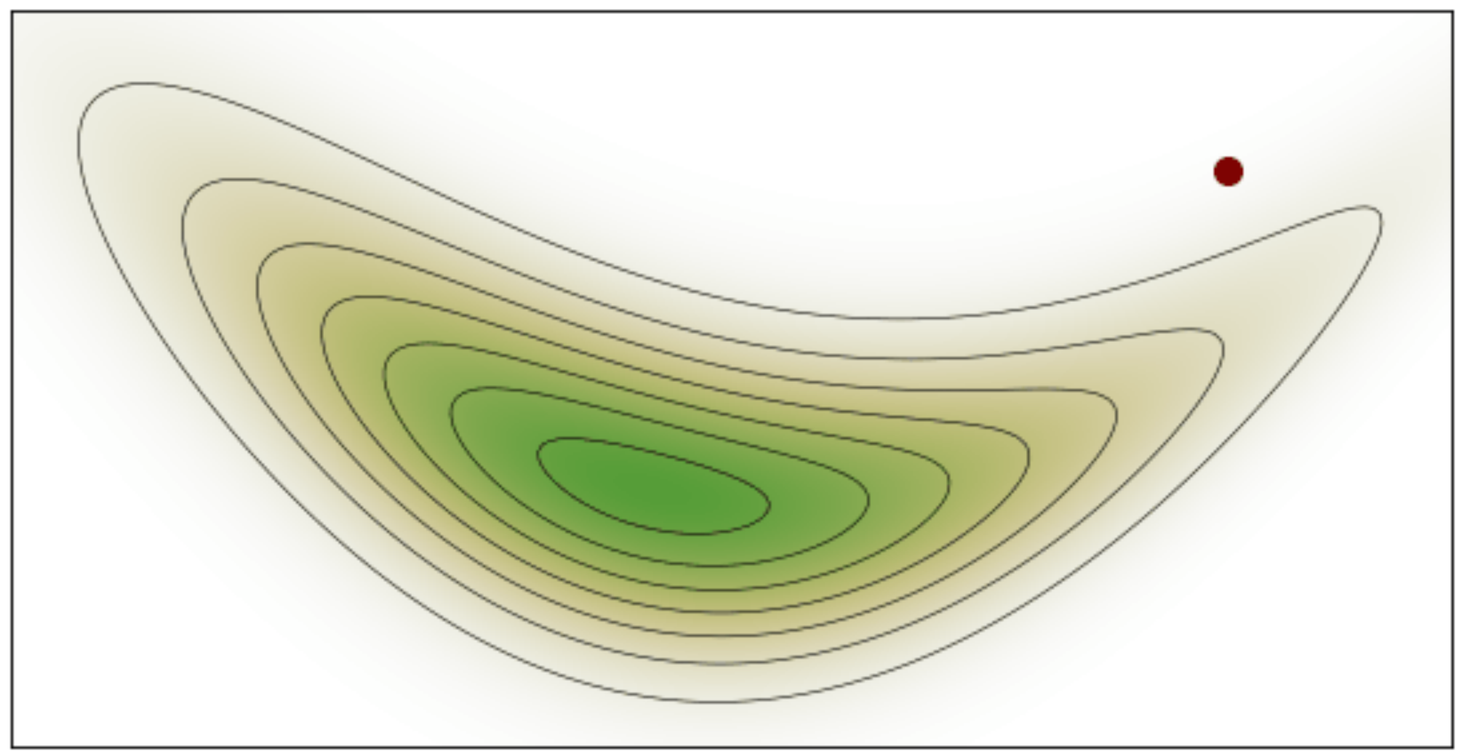

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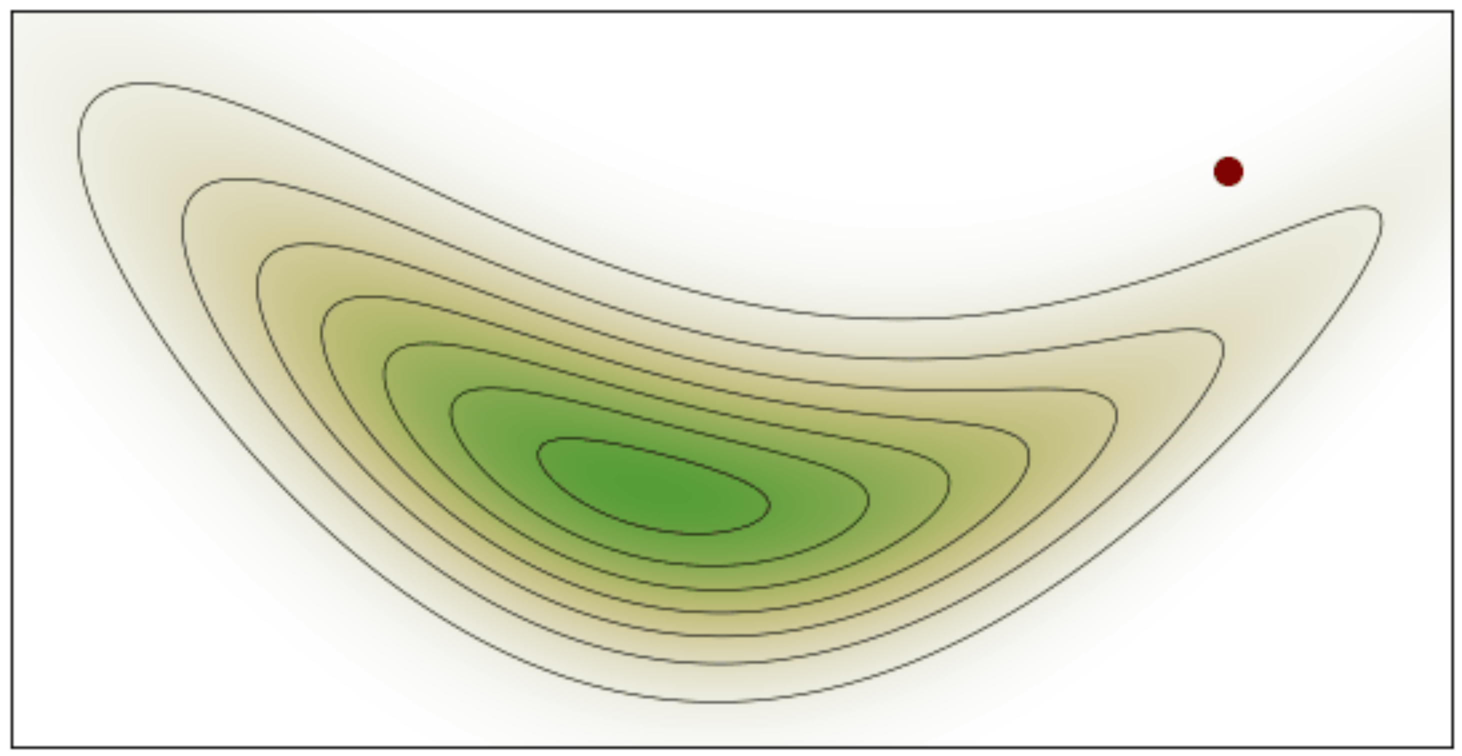

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