# Intractable Posteriors

LSST Discovery Fellowship Program Day 5

## Modeling choices

#### **Physical**

What processes do you include? What approximations do you make?

#### Model specification

Parameterization

Priors

Convergence criteria

#### **Statistical**

Are data i.i.d.?

Is there correlated noise?

Do you account for data collection?

#### Sampler

Grid search

Maximum likelihood

Markov Chain Monte Carlo

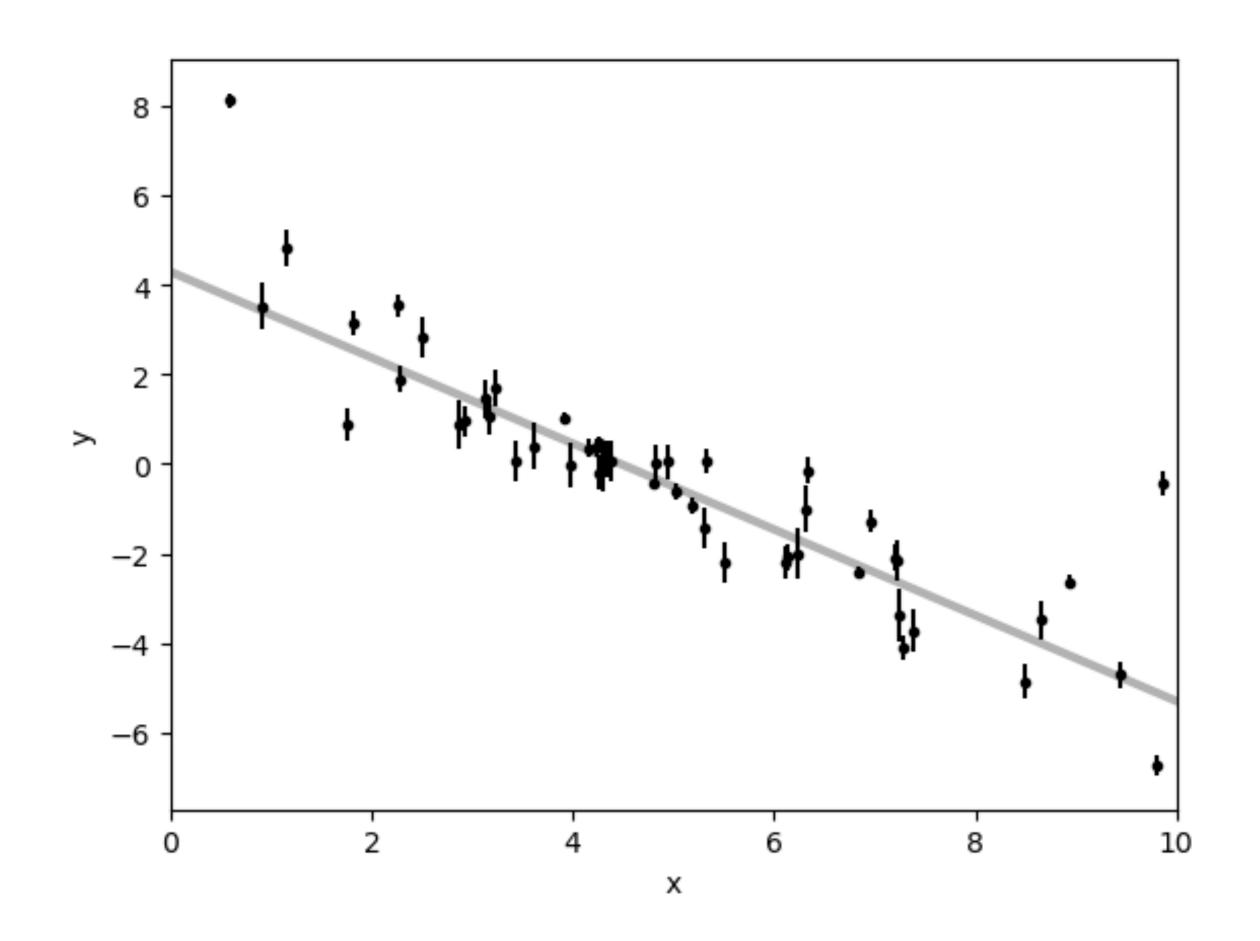
Nested Sampling

#### Linear Model

Let's parameterize the obvious way

$$y_{\text{mod}} = mx + b$$

How can the model specification be improved?

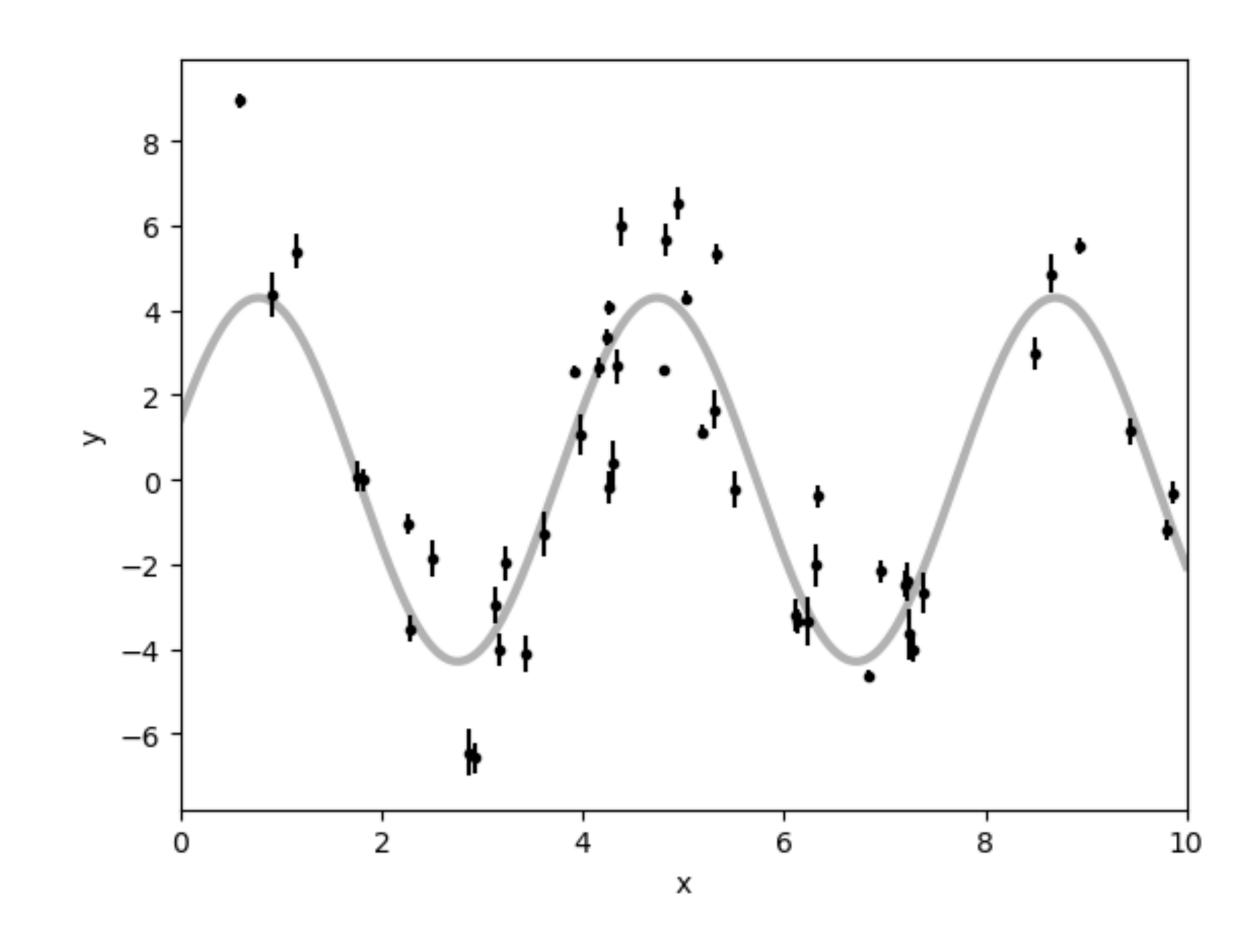


#### Sinusoid Model

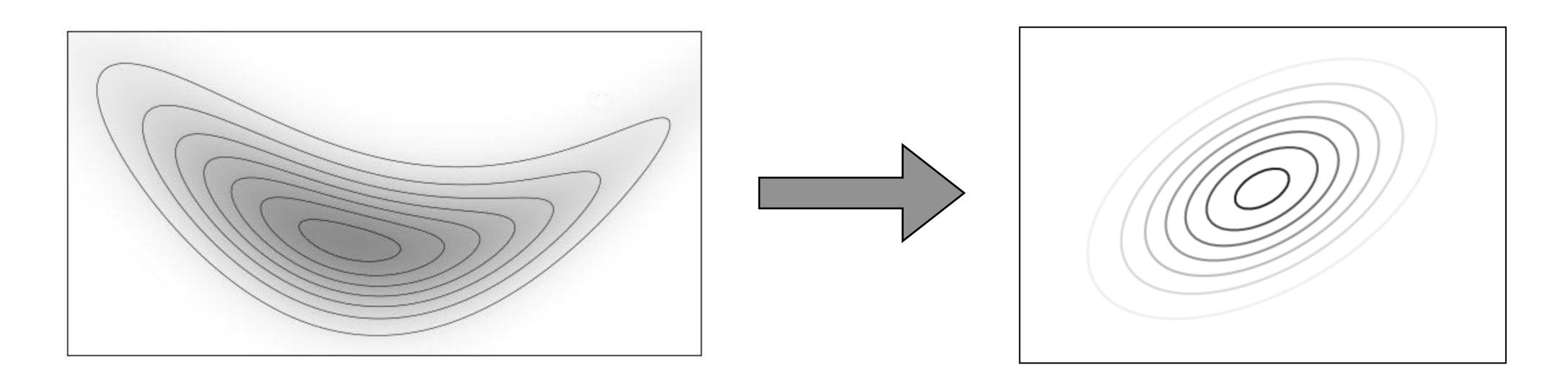
Let's parameterize the obvious way

$$y_{\text{mod}} = A \sin(\frac{2\pi t}{P} + \phi)$$

How can the model specification be improved?



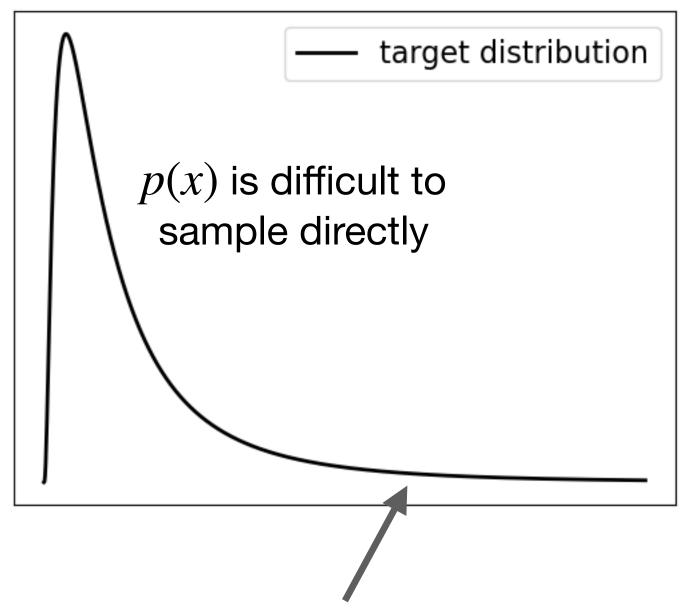
# Transform to a (nearly) Orthogonal Basis



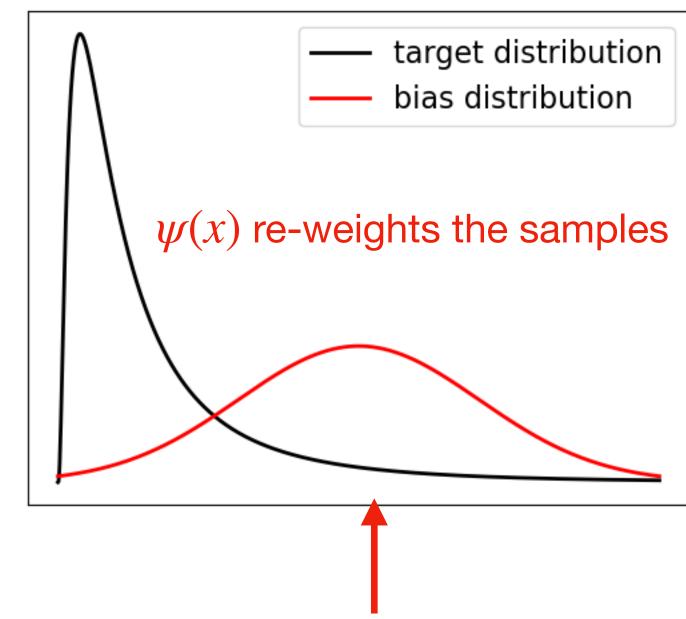
- Warps the posterior topology to be closer to Gaussian
- Reduces covariances and broadens funnels
- More efficient AND more accurate sampling results

Warning: parameter transformations can introduce implicit priors Don't forget to incorporate the appropriate Jacobian

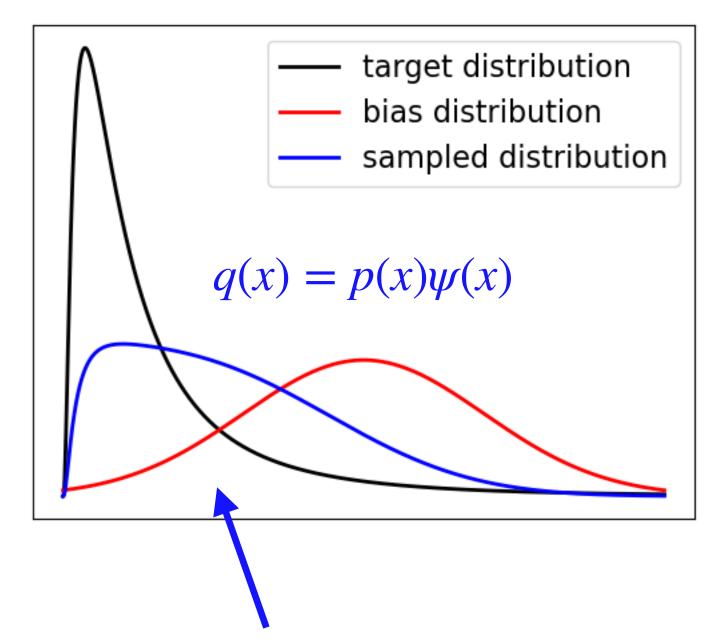
#### Importance Sampling



Samples in low-probability region strongly influence our posterior estimates of, e.g.  $\{\mu_x, \sigma_x^2\}$ 



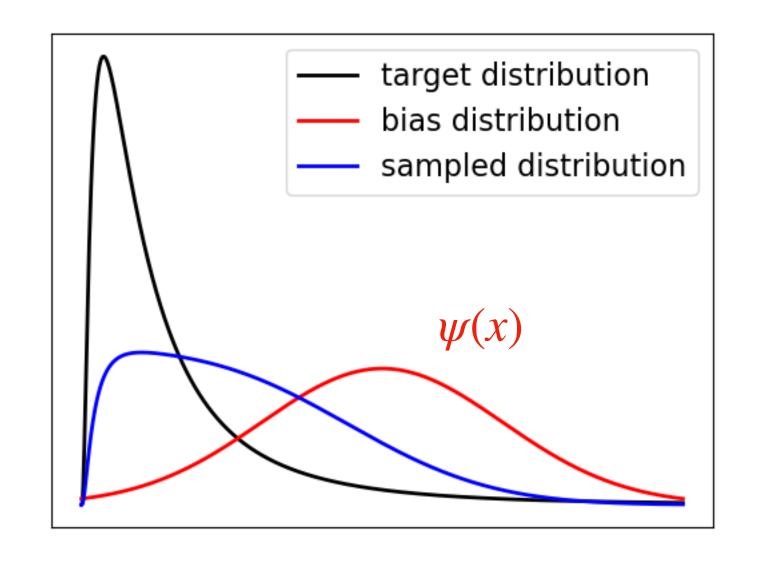
A user-specified bias function guides the sampler toward low-probability regions



The new distribution is easier to sample from

## Bayesian Interpretation

$$P(\theta \mid D) = \frac{P(D \mid \theta) P(\theta)}{P(D)}$$



In Bayesian language, imposing a bias function is equivalent to imposing a prior

Because we know the prior exactly, we can re-weight our posterior samples to remove the effect of the bias

#### Some spicy opinions on priors

There is no such thing as an "uninformative" prior

Don't get too hung up on picking a single "best" prior

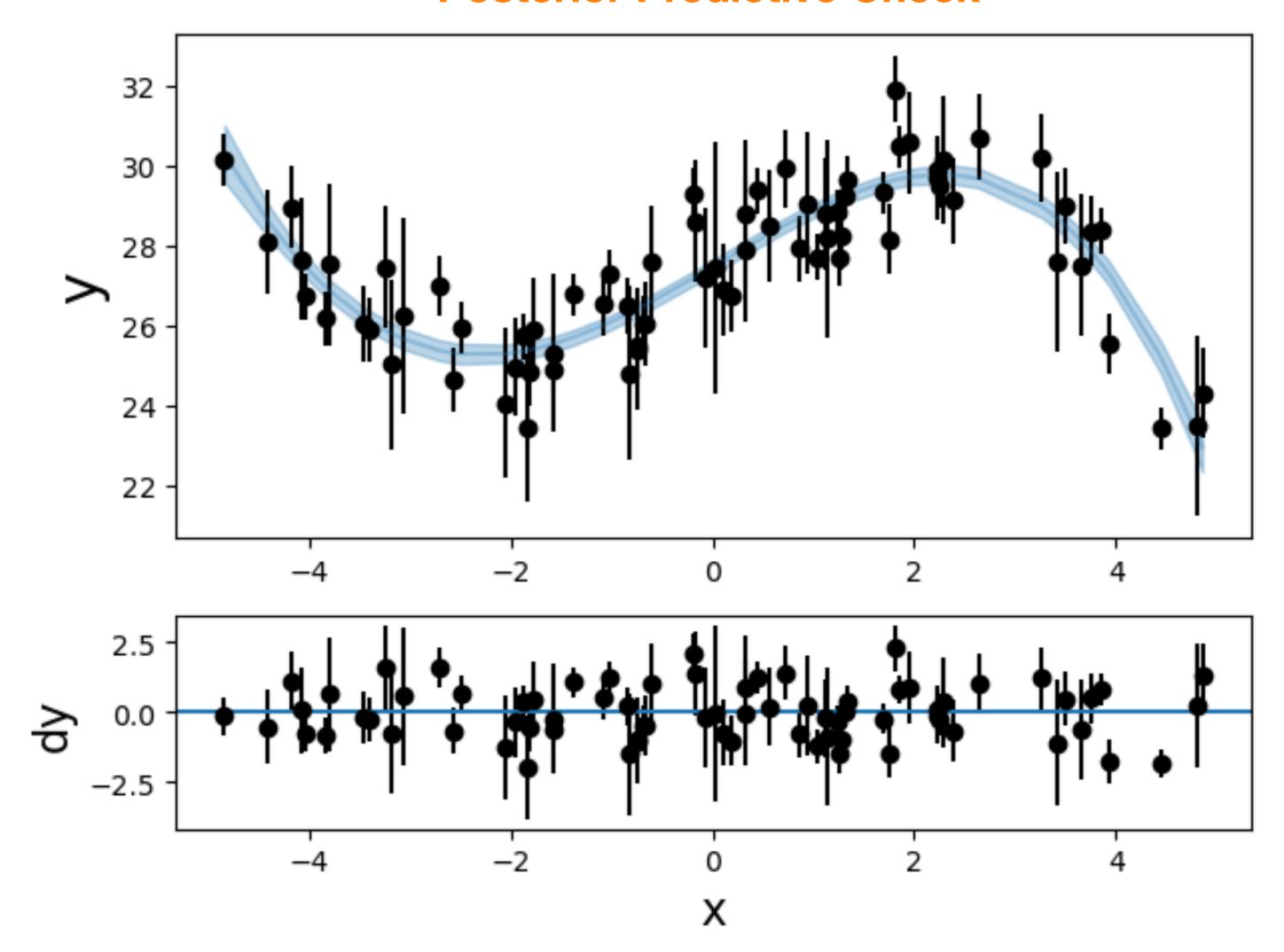
## Some less spicy advice

Always state your priors

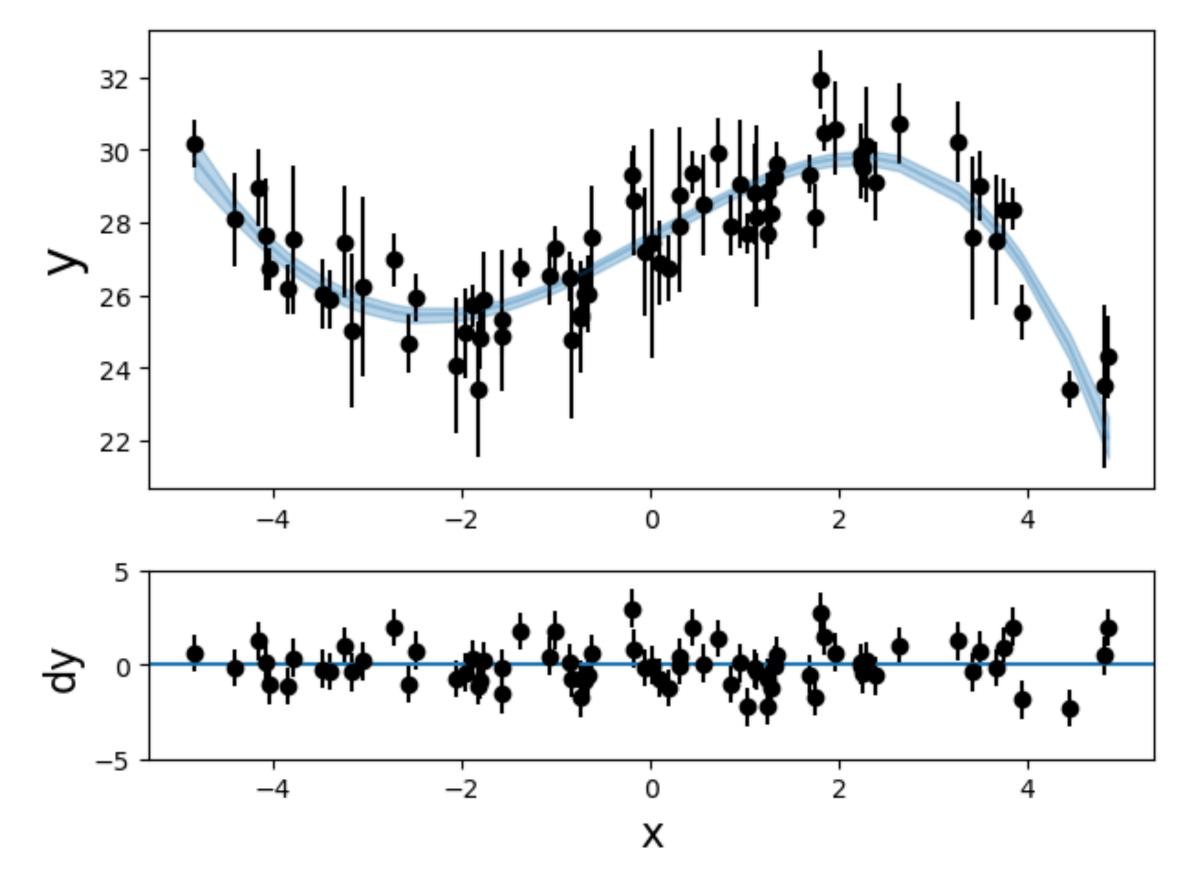
Be mindful of parameter covariances

Test to ensure the full posterior is explored

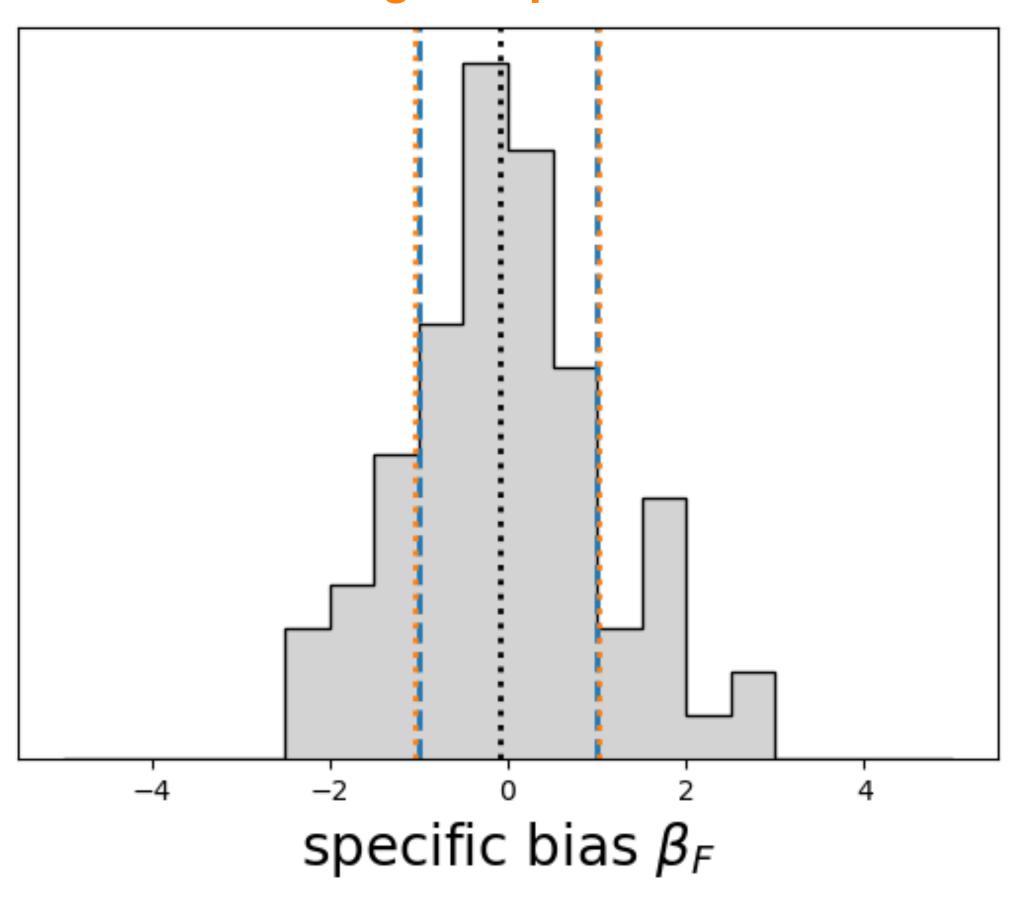
#### **Posterior Predictive Check**

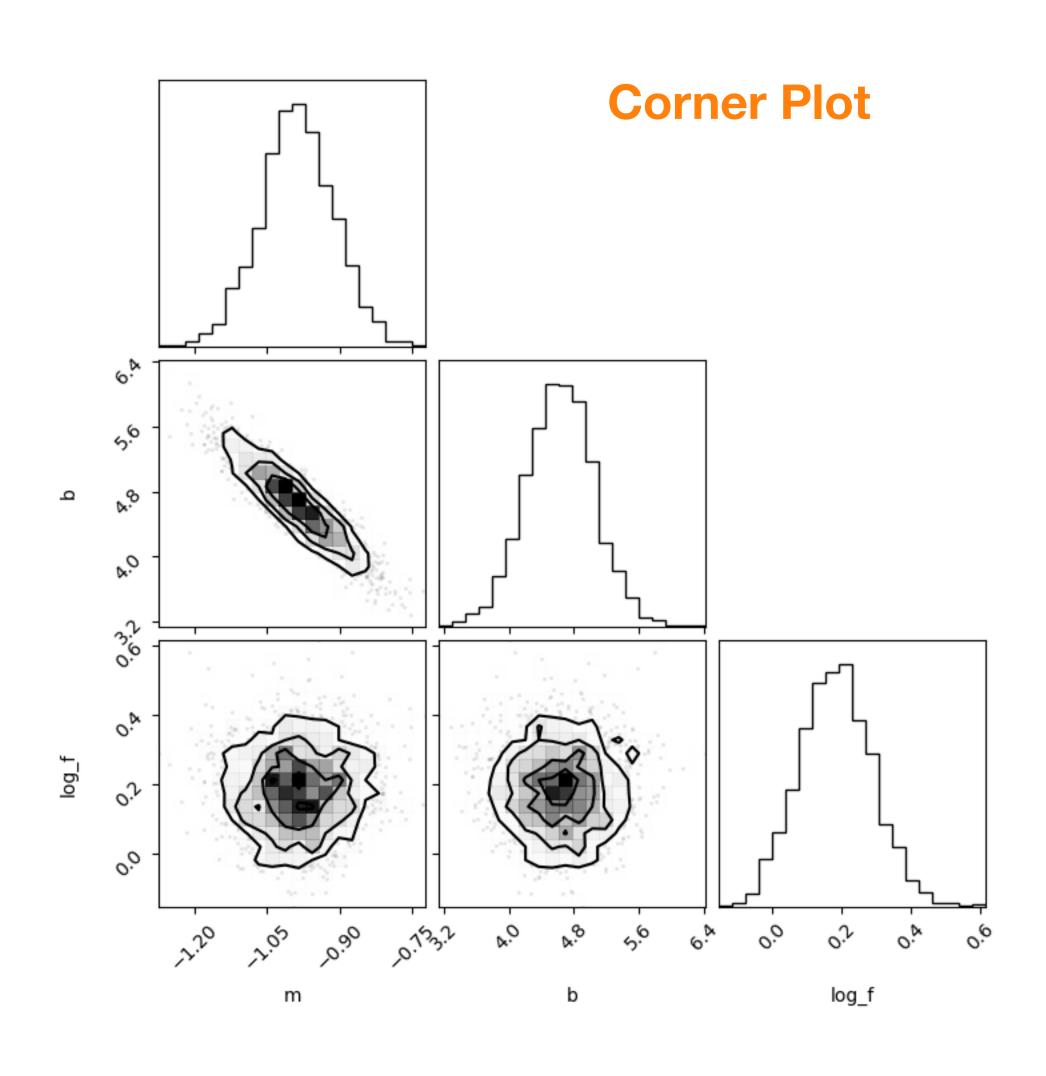






#### **Coverage & Specific Bias**





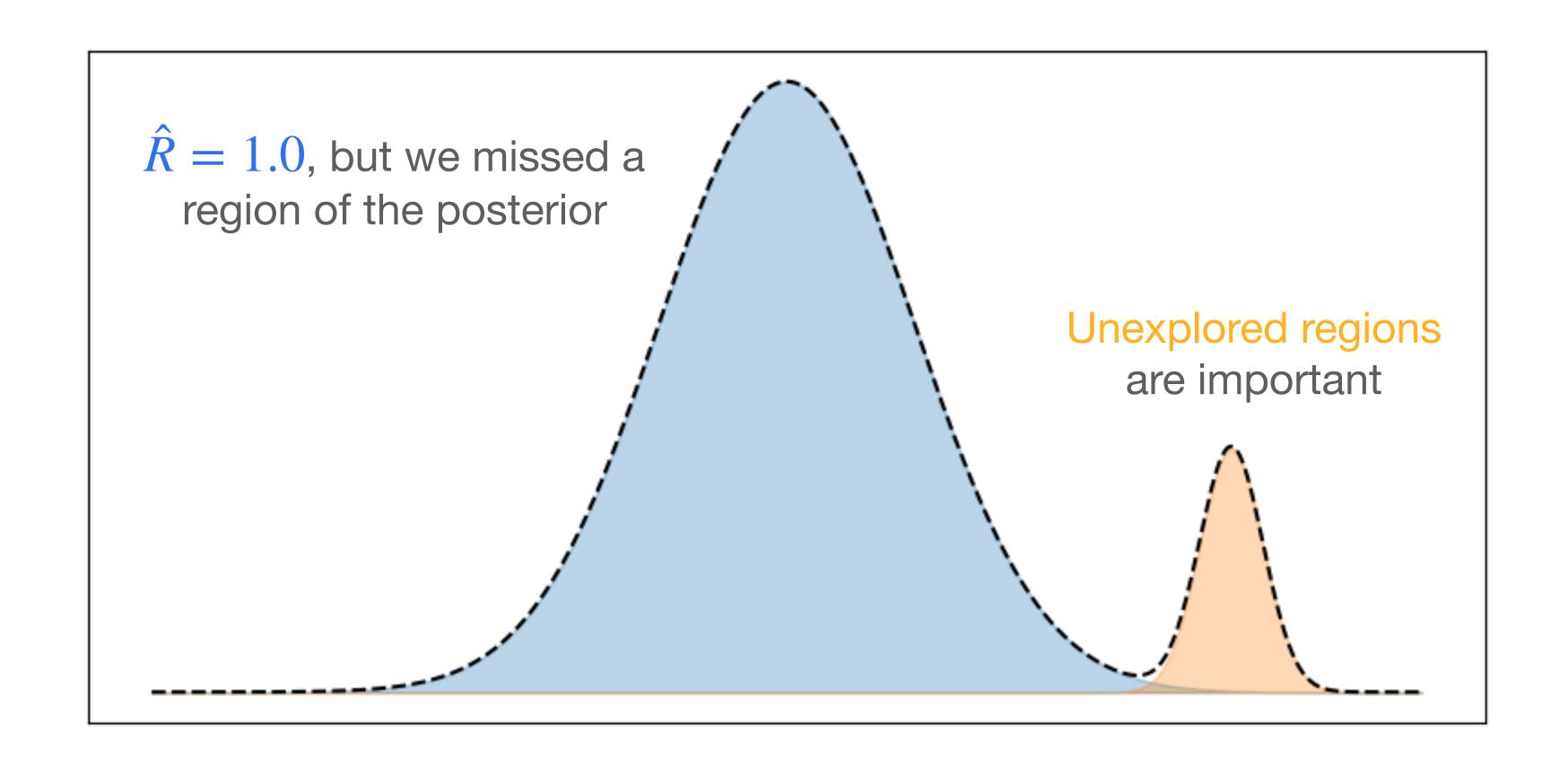


Gelman-Rubin statistic

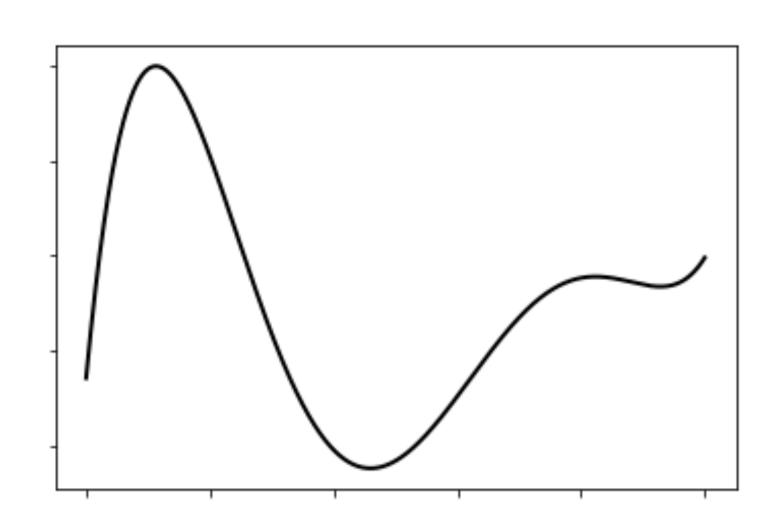
$$\hat{R} \sim \frac{W + B/L}{W}$$

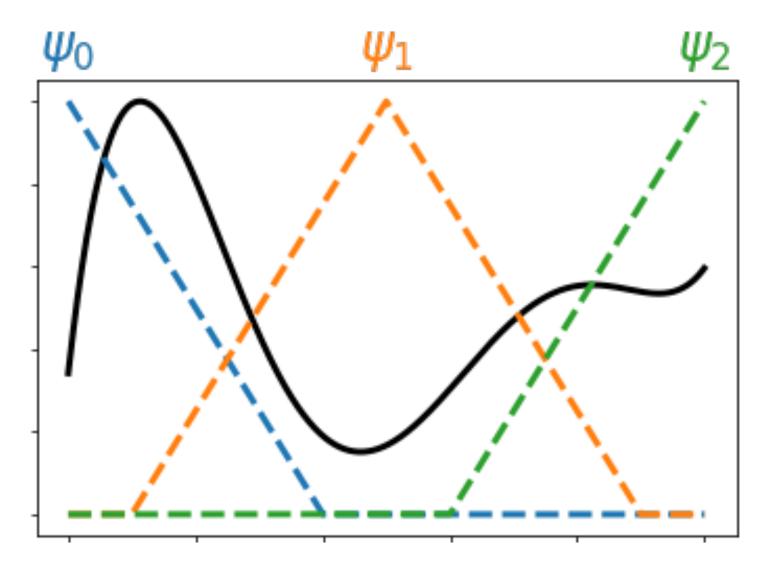
Within-chain variance
Between-chain variance
Length of chain

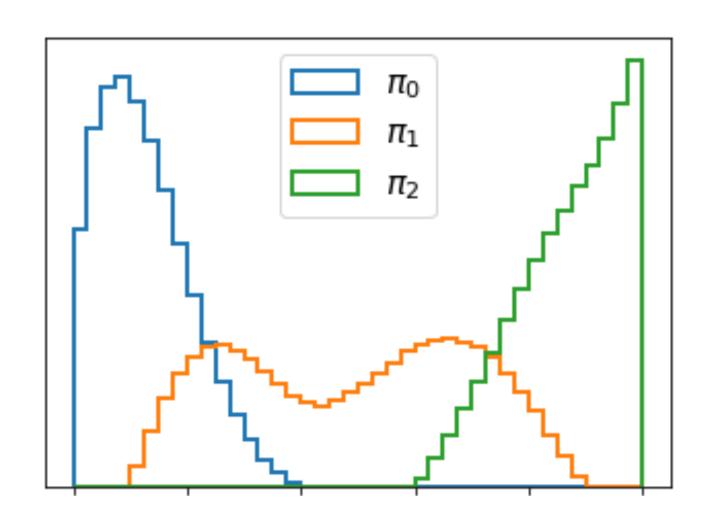
#### Convergence checks can sometimes fail!



## Umbrella Sampling







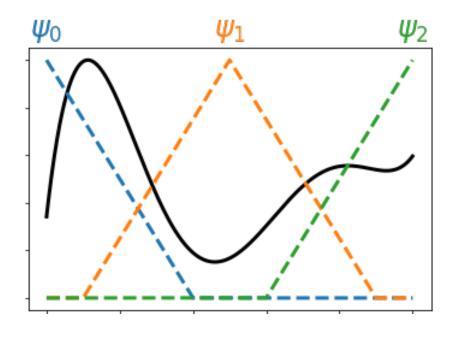
We have a complicated posterior with a narrow "bottleneck" that stymies most MCMC samplers

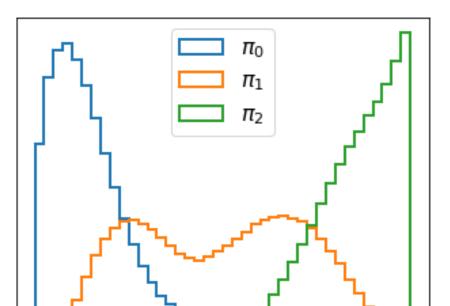
Split the posterior into three regions using bias functions

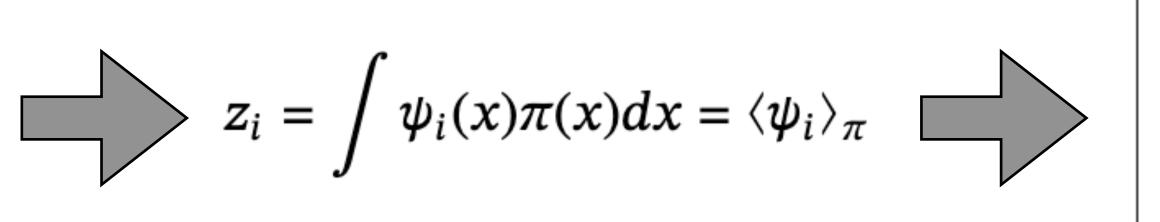
You'll need to run the sampler three times

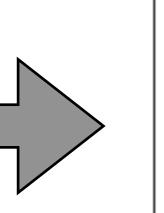
We now have three sets of (weighted) samples that need to be recombined

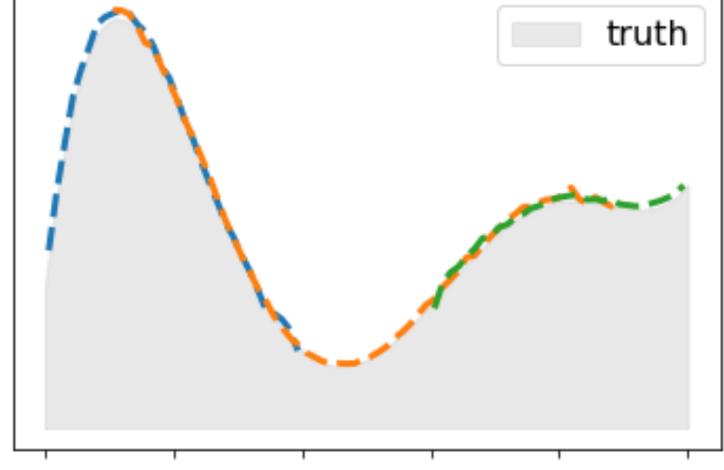
## Umbrella Sampling











#### Estimating the overlap matrix F

$$z_{i} = \sum_{i=1}^{N} \left\langle \frac{\psi_{i}(x)}{\sum_{j=1}^{N} \psi_{j}(x)/z_{j}} \right\rangle_{\pi_{i}} \qquad F_{ij} = \left\langle \frac{\psi_{j}/z_{i}}{\sum_{k=1}^{N} \psi_{k}/z_{k}} \right\rangle_{\pi_{i}} \qquad F = \begin{bmatrix} 0.83 & 0.07 & 0\\ 0.39 & 0.72 & 0.31\\ 0 & 0.08 & 0.8 \end{bmatrix}$$

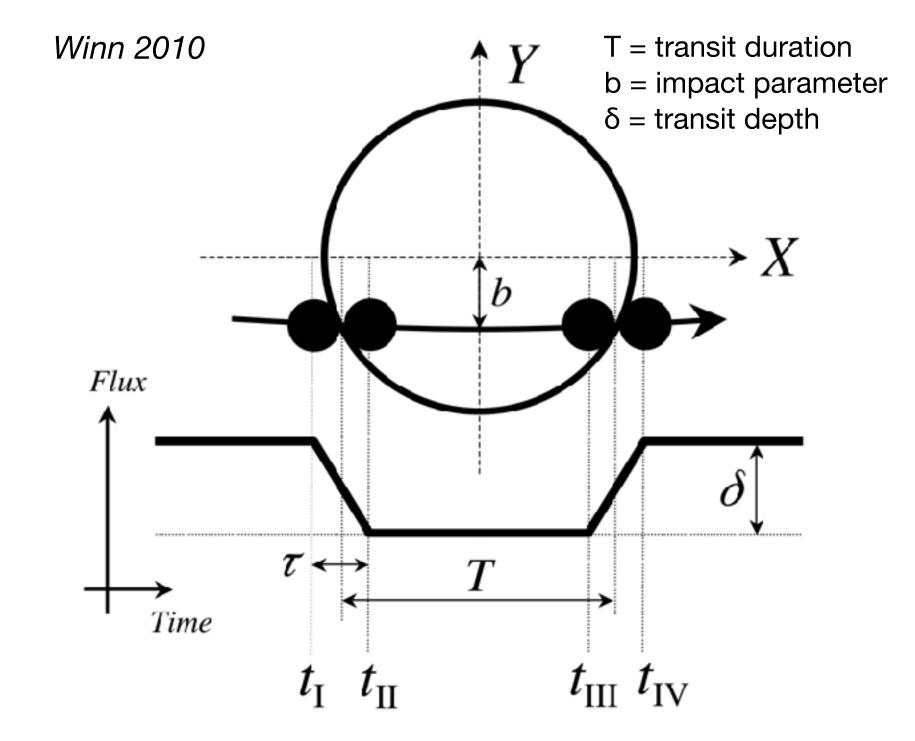
#### How do we identify unknown unknowns?

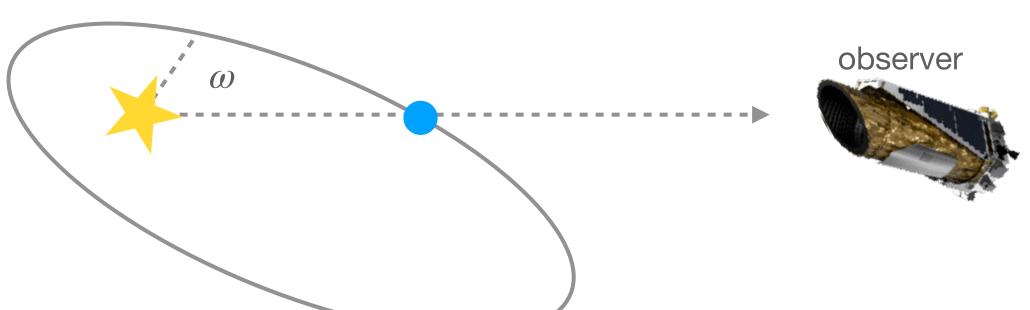
Domain expertise

Exploratory runs

Umbrella sampling

Your sampler alone will not save you!

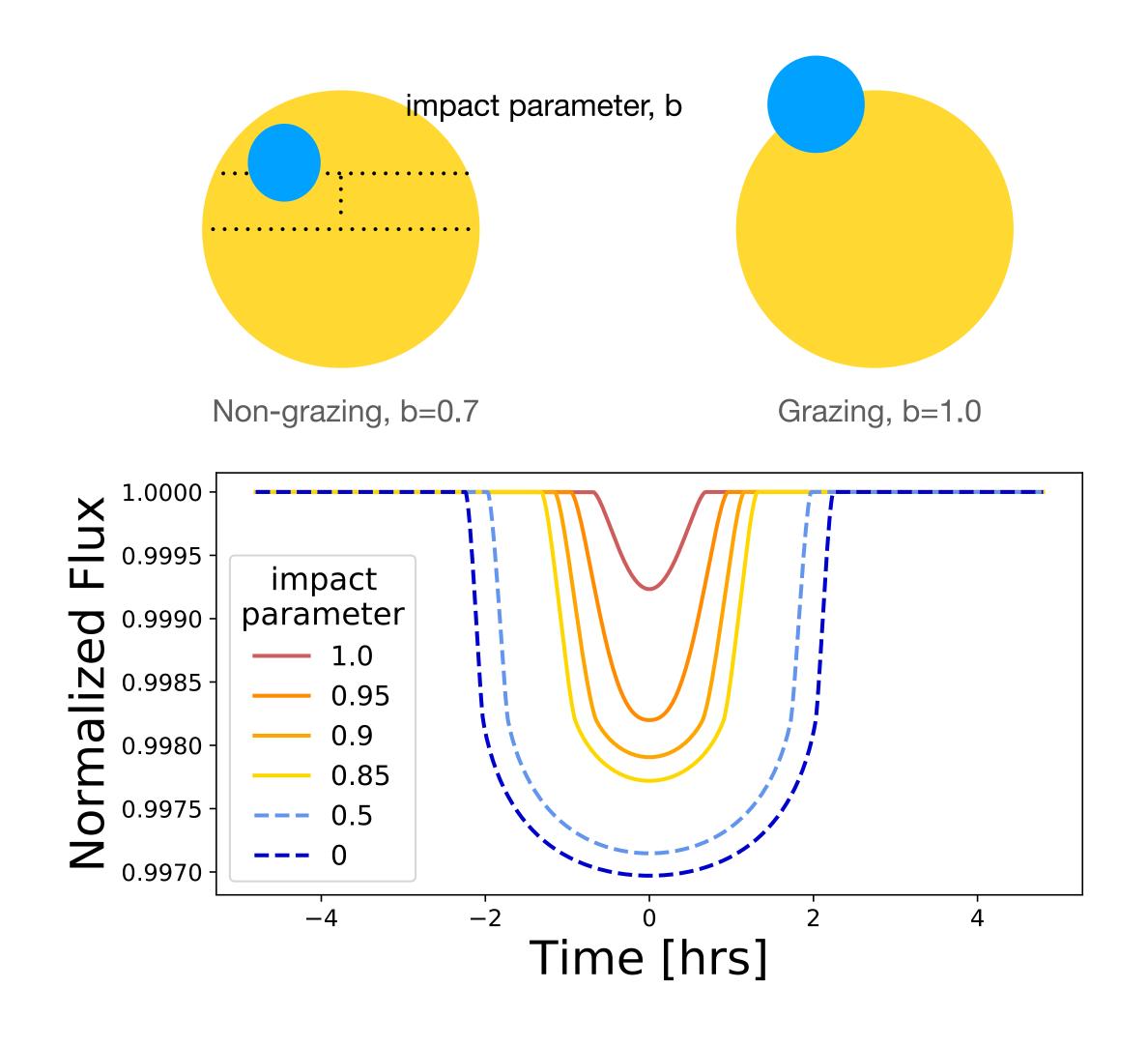


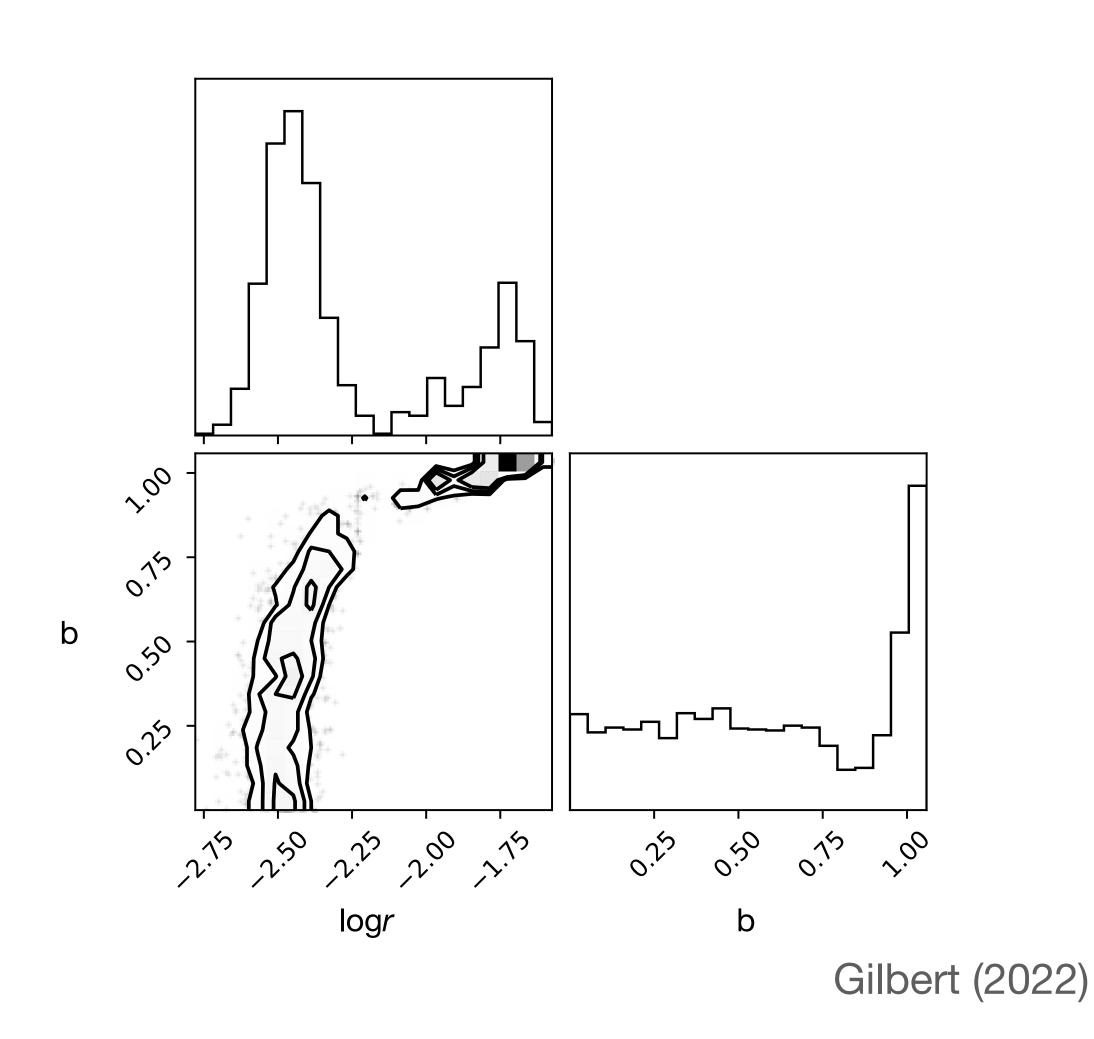


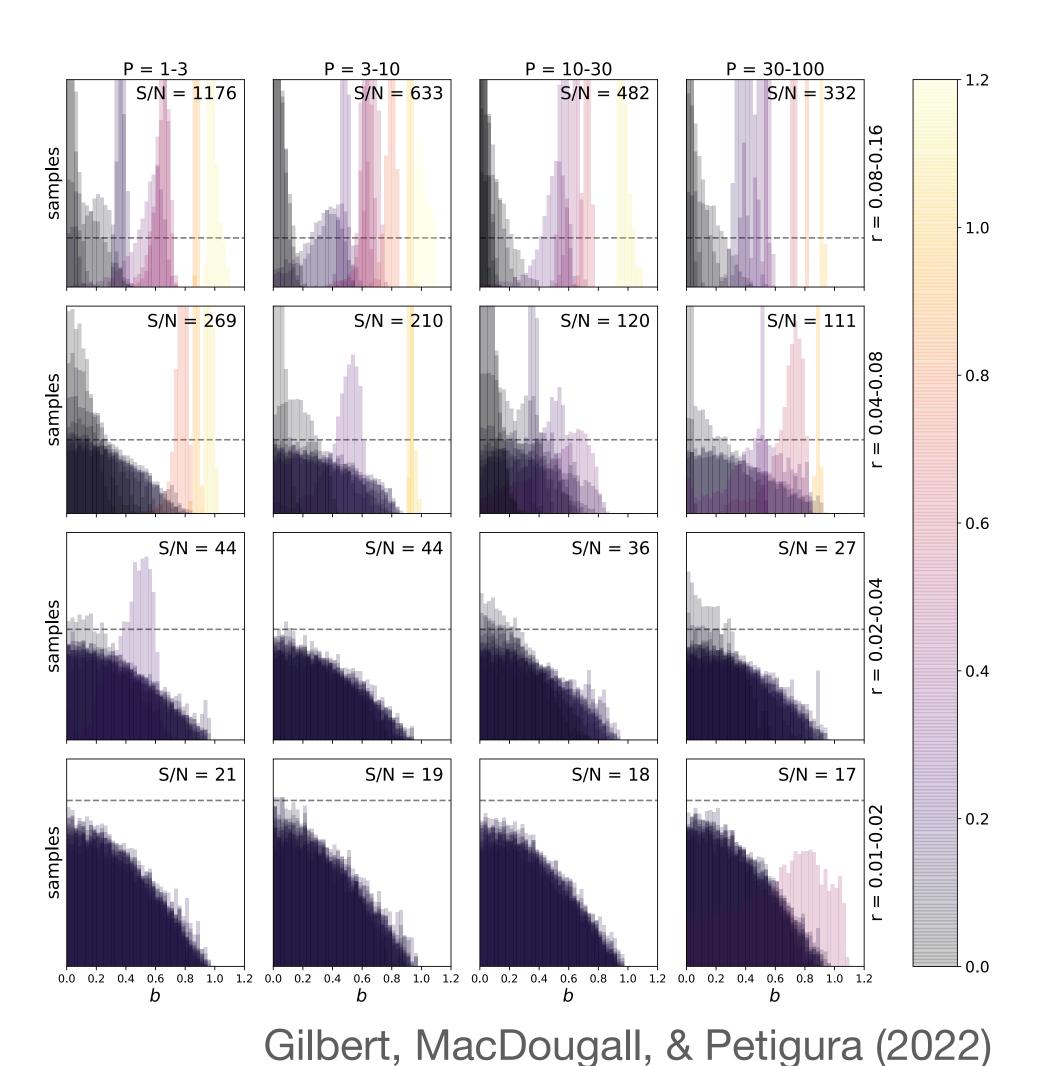
duration = 
$$\frac{\text{transit chord length}}{\text{orbital velocity}}$$

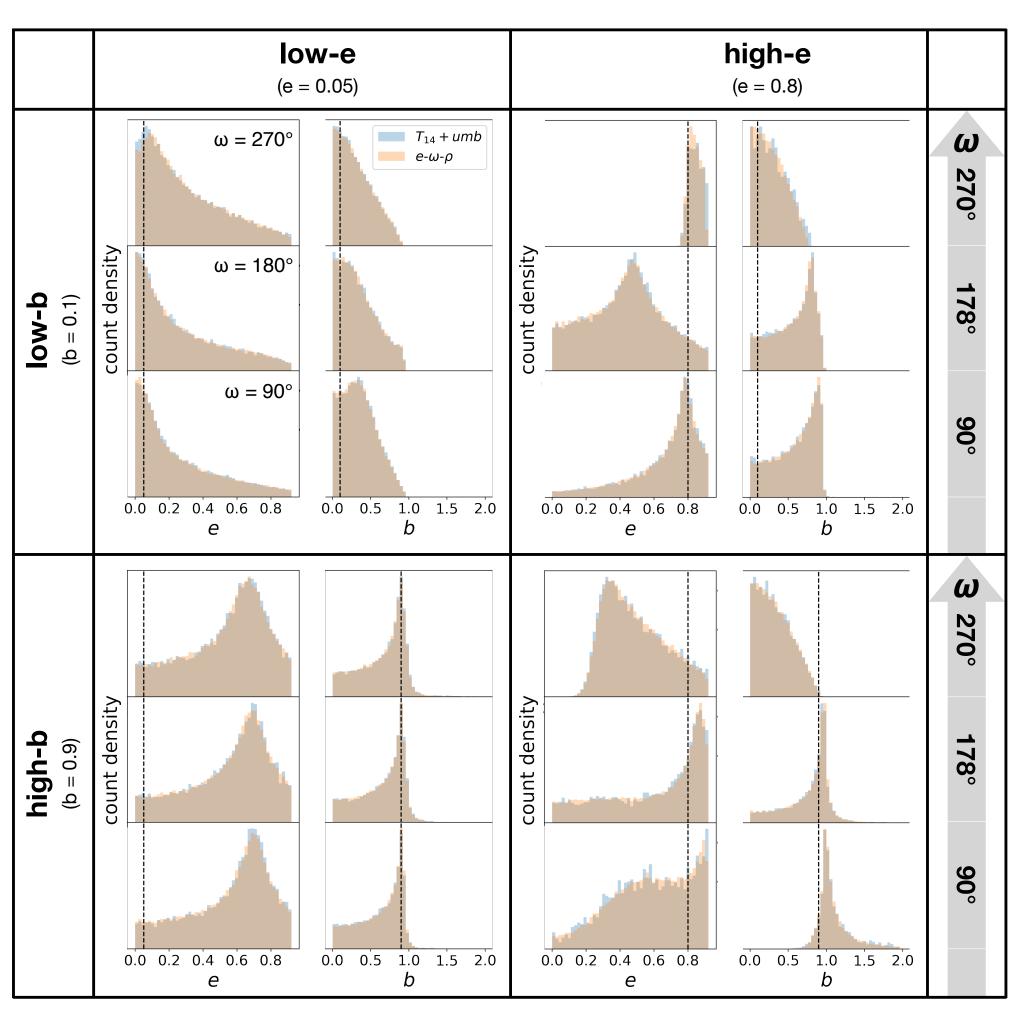
$$T_{14} \approx \frac{PR_{\star}}{\pi a} \sqrt{1 - b^2} \frac{\sqrt{1 - e^2}}{1 + e \sin \omega}$$

compare 
$$\frac{T}{T_0} \stackrel{\text{observed}}{\longleftarrow} predicted \ \text{for} \\ e=0, \ b=0$$









MacDougall, Gilbert, & Petigura (2023)

# Further reading

#### Model Parameterization

Betancourt & Girolami 2013, "Hamiltonian Monte Carlo for hierarchical models", arXiv:1312.0906

#### Importance Sampling

Bayesian Data Analysis, by A. Gelman et al. Third Edition, Boca Raton, FL: Chapman & Hall 2014

#### Umbrella Sampling

Matthews et al., 2018, "Umbrella sampling: a powerful method to sample tails of distributions", MNRAS, 480, 3

Gilbert 2022, "Accurate modeling of grazing transits using umbrella sampling", AJ, 163, 3