Intractable Posteriors

LSST Discovery Fellowship Program Day 5

Greg Gilbert | LSST Discovery Workshop | 24 May 2025

Modeling choices

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

Statistical
Are data i.i.d.?
Is there correlated noise?
Do you account for data collection?

Model specification
Parameterization
Priors
Convergence criteria

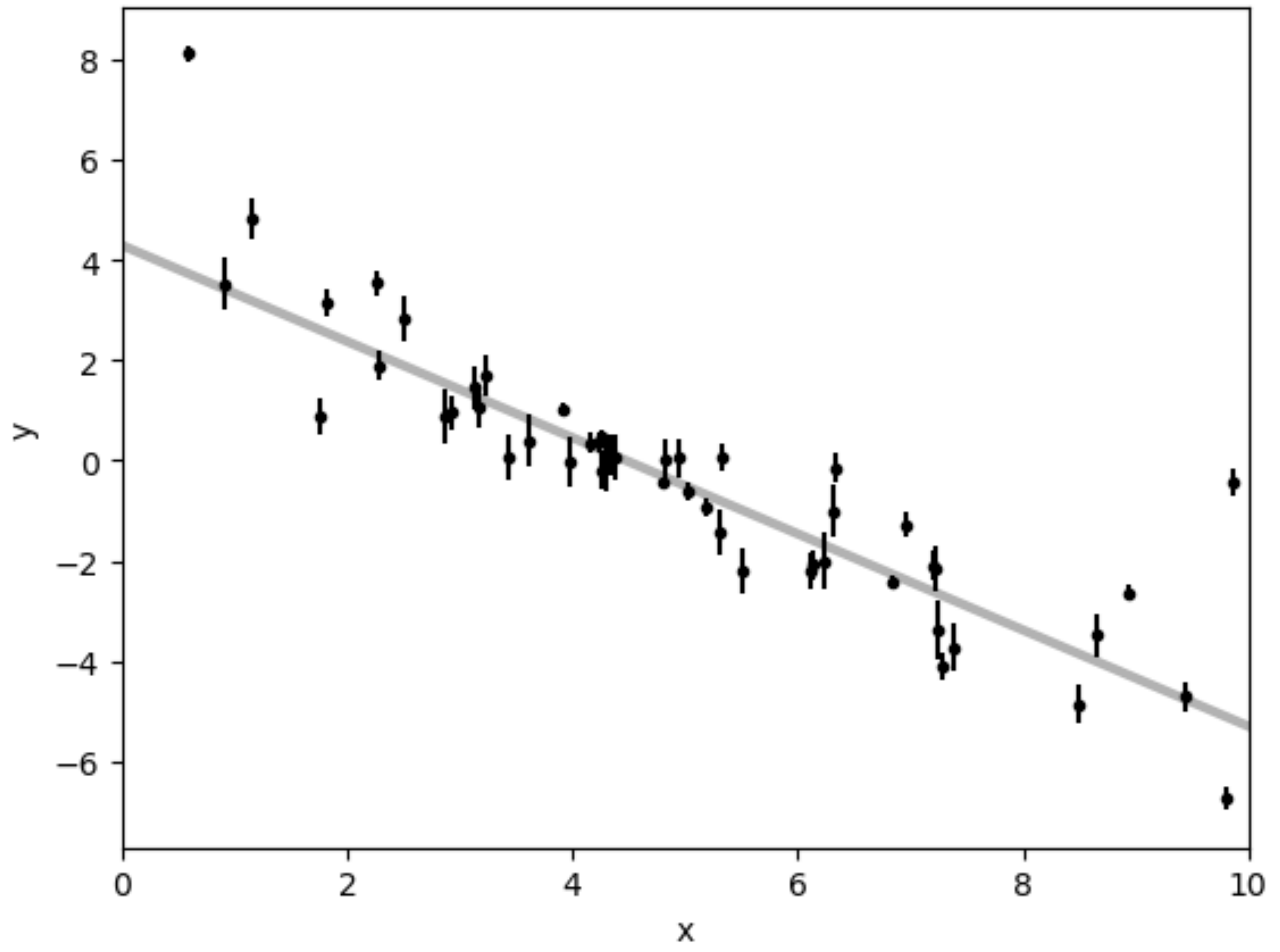
Sampler
Grid search
Maximum likelihood
Markov Chain Monte Carlo
Nested Sampling

Linear Model

Let's parameterize the obvious way

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

How can the model <u>specification</u> be improved?

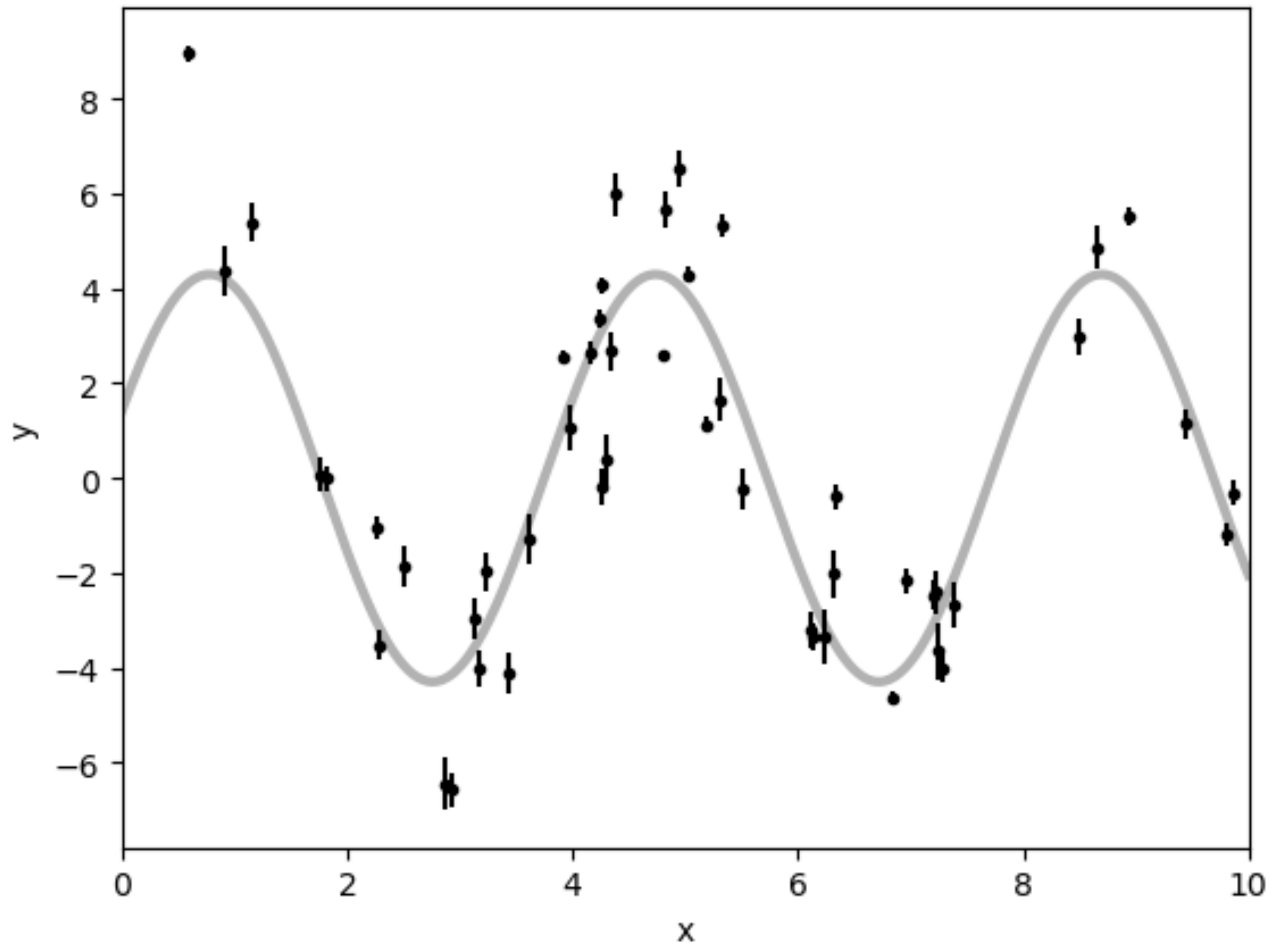


Sinusoid Model

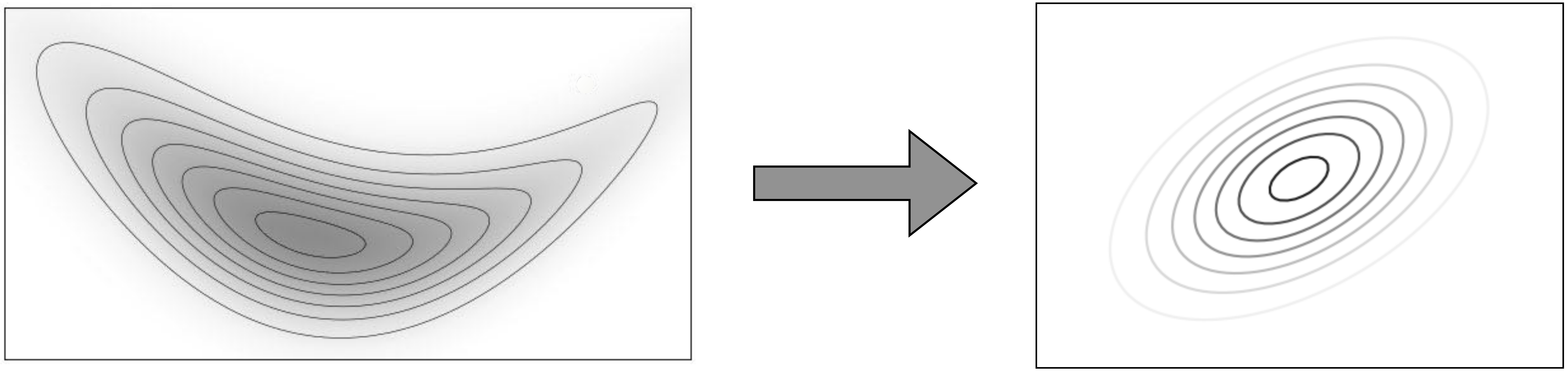
Let's parameterize the obvious way

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

How can the model <u>specification</u> be improved?



Transform to a (nearly) Orthogonal Basis

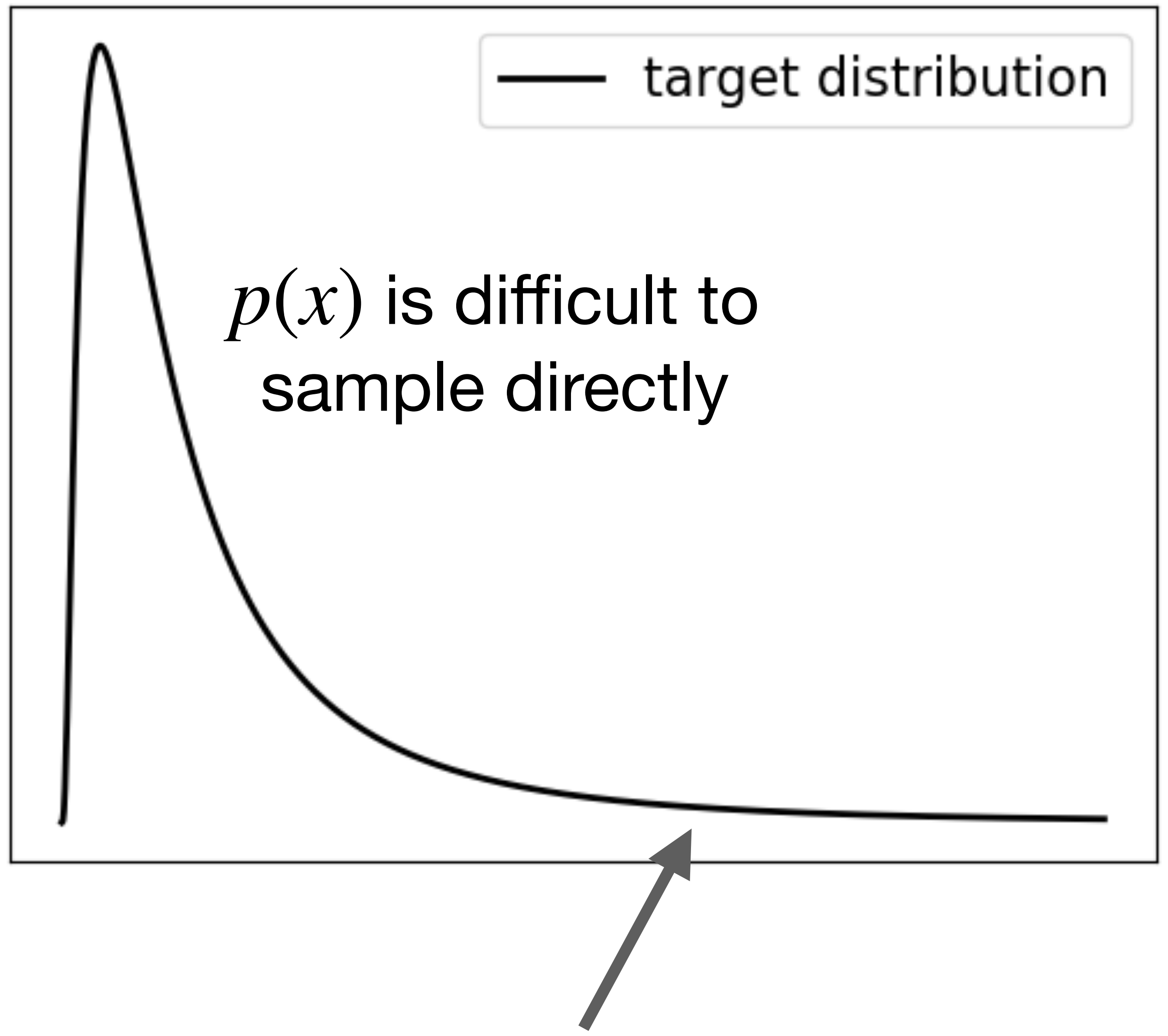


- Warps the posterior topology to be closer to Gaussian
- Reduces covariances and broadens funnels
- More efficient AND more accurate sampling results

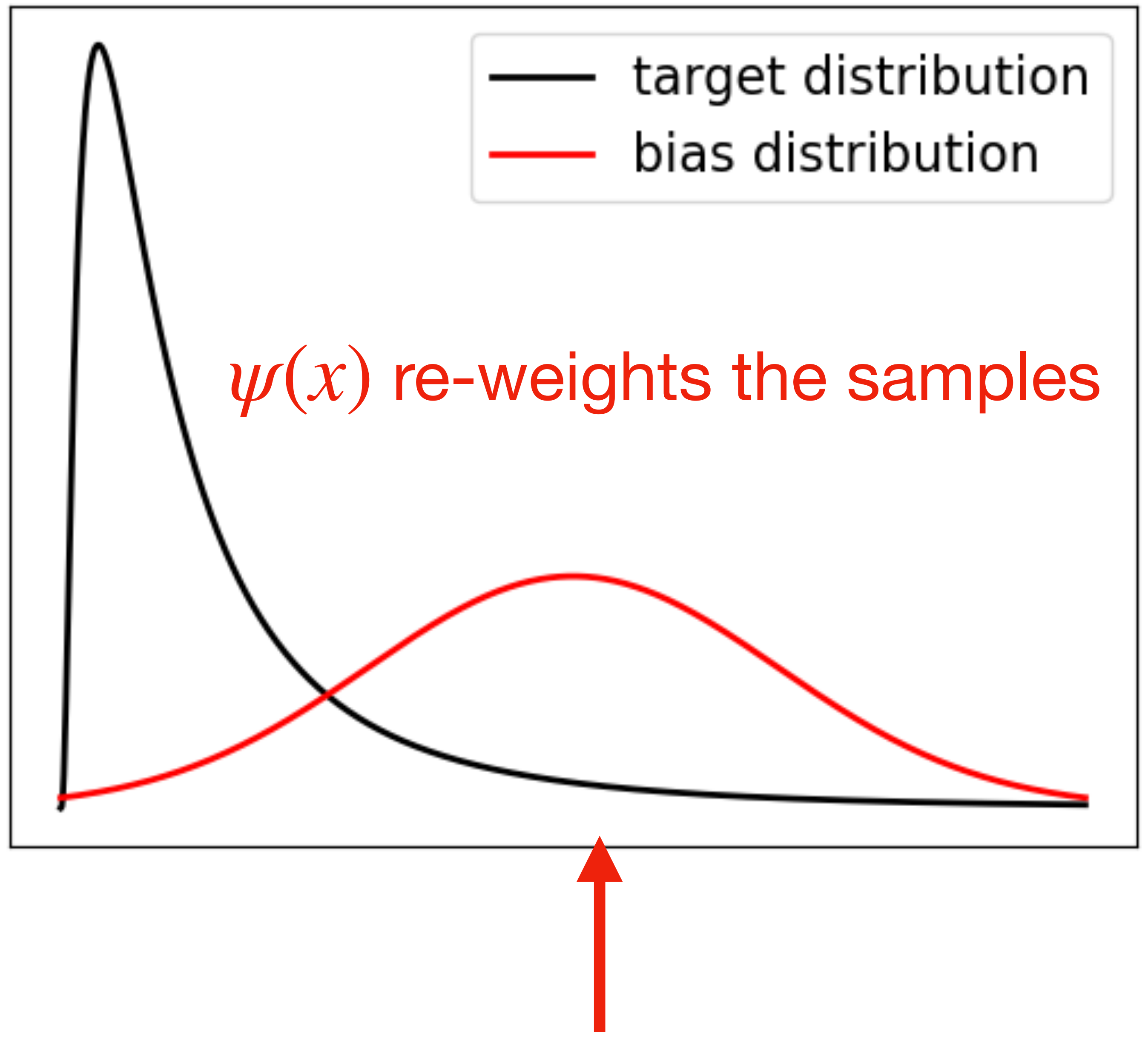
Warning: parameter transformations can introduce implicit priors

Don’t forget to incorporate the appropriate Jacobian

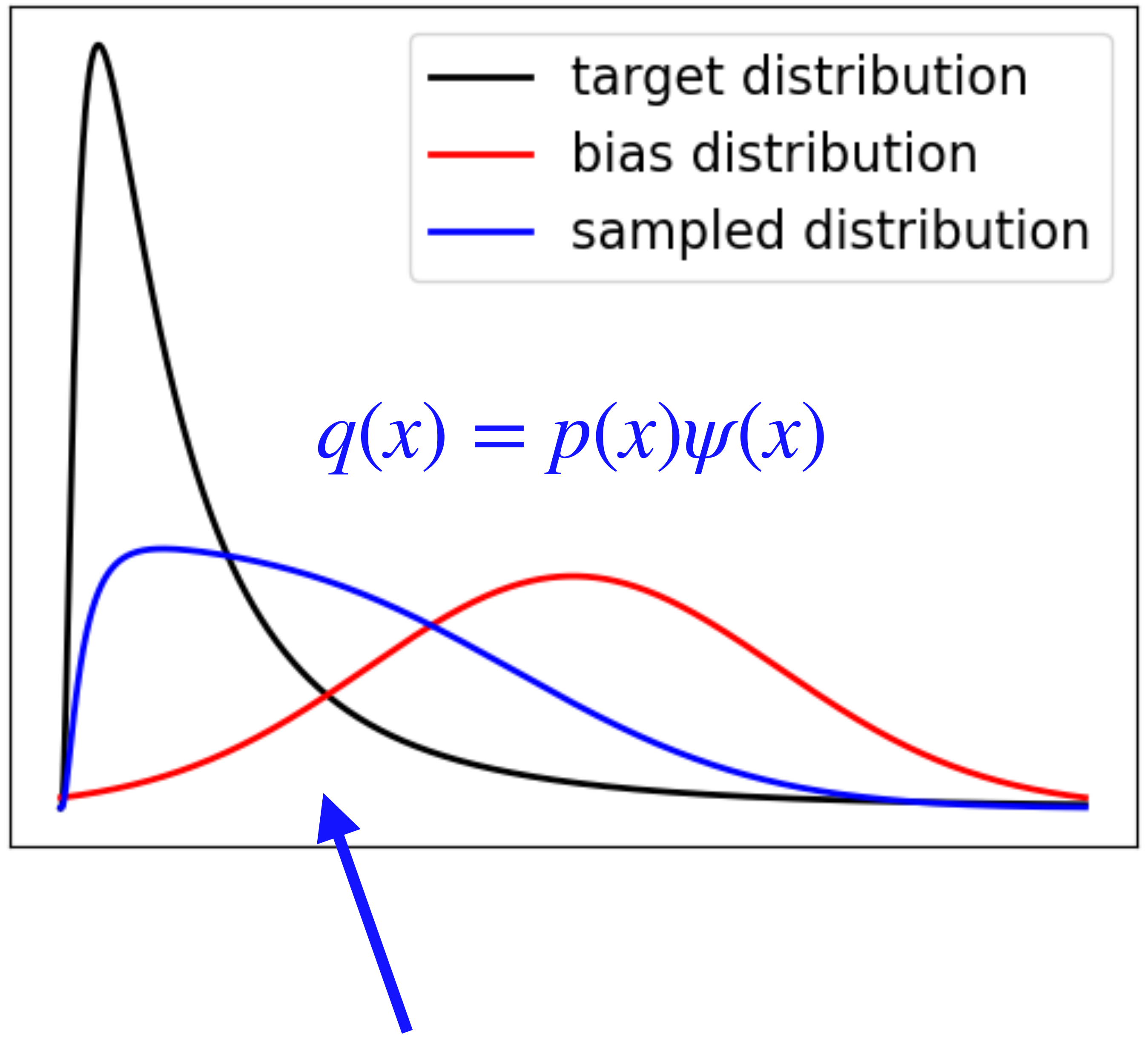
Importance Sampling



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



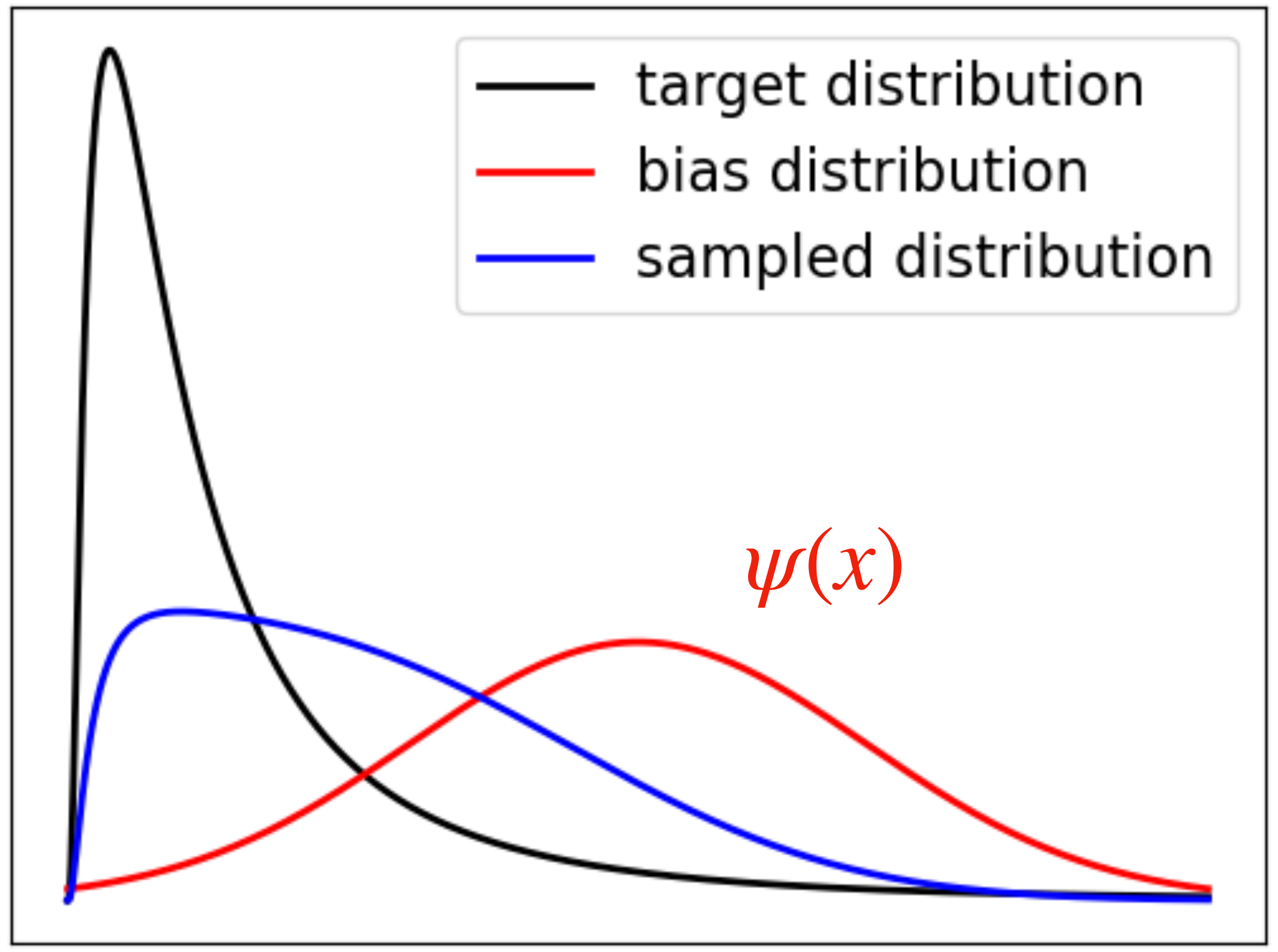
A user-specified bias function guides the sampler toward low-probability regions



The new distribution is easier to sample from

Bayesian Interpretation

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



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

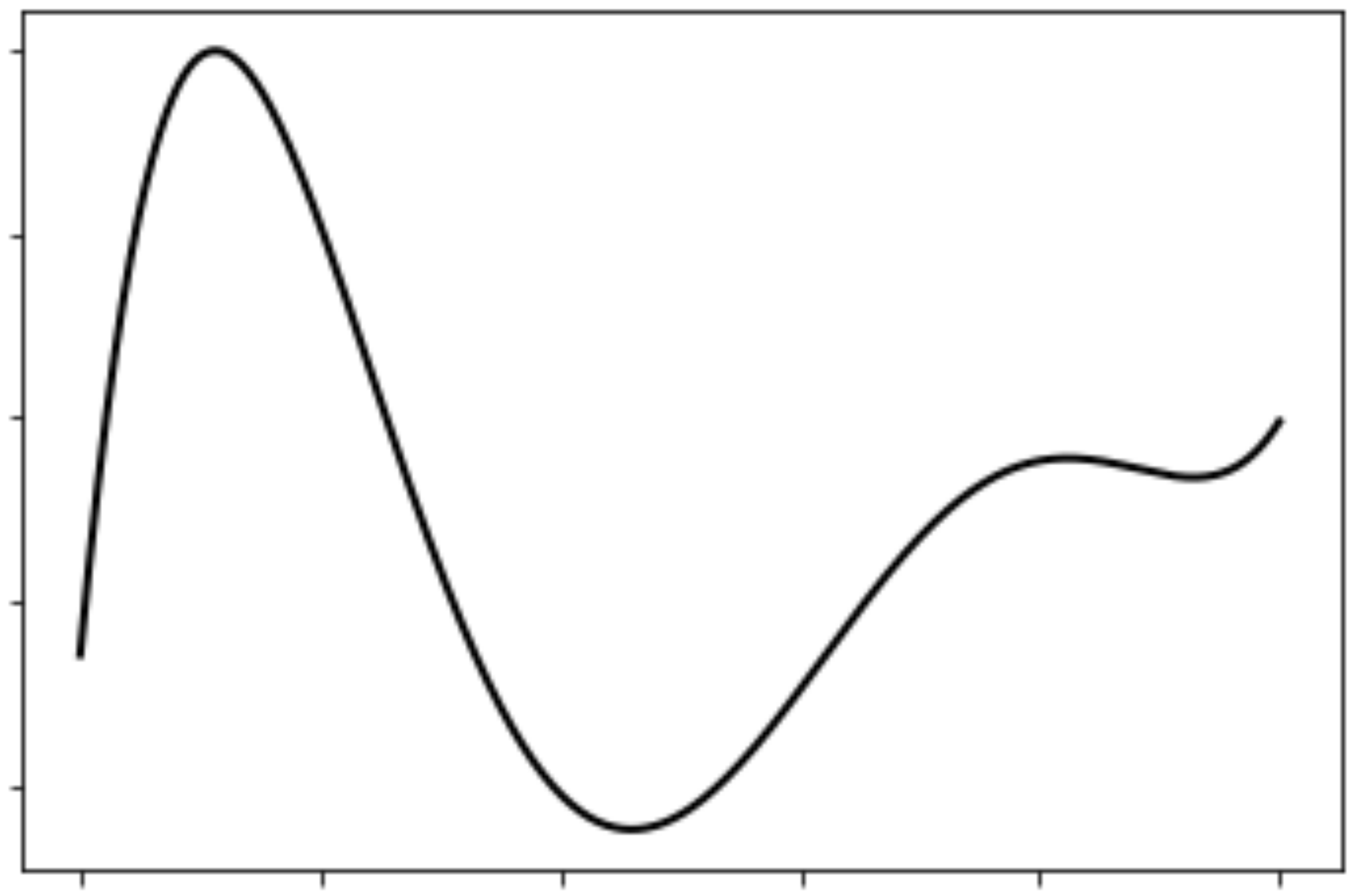
Some less spicy advice

Always state your priors

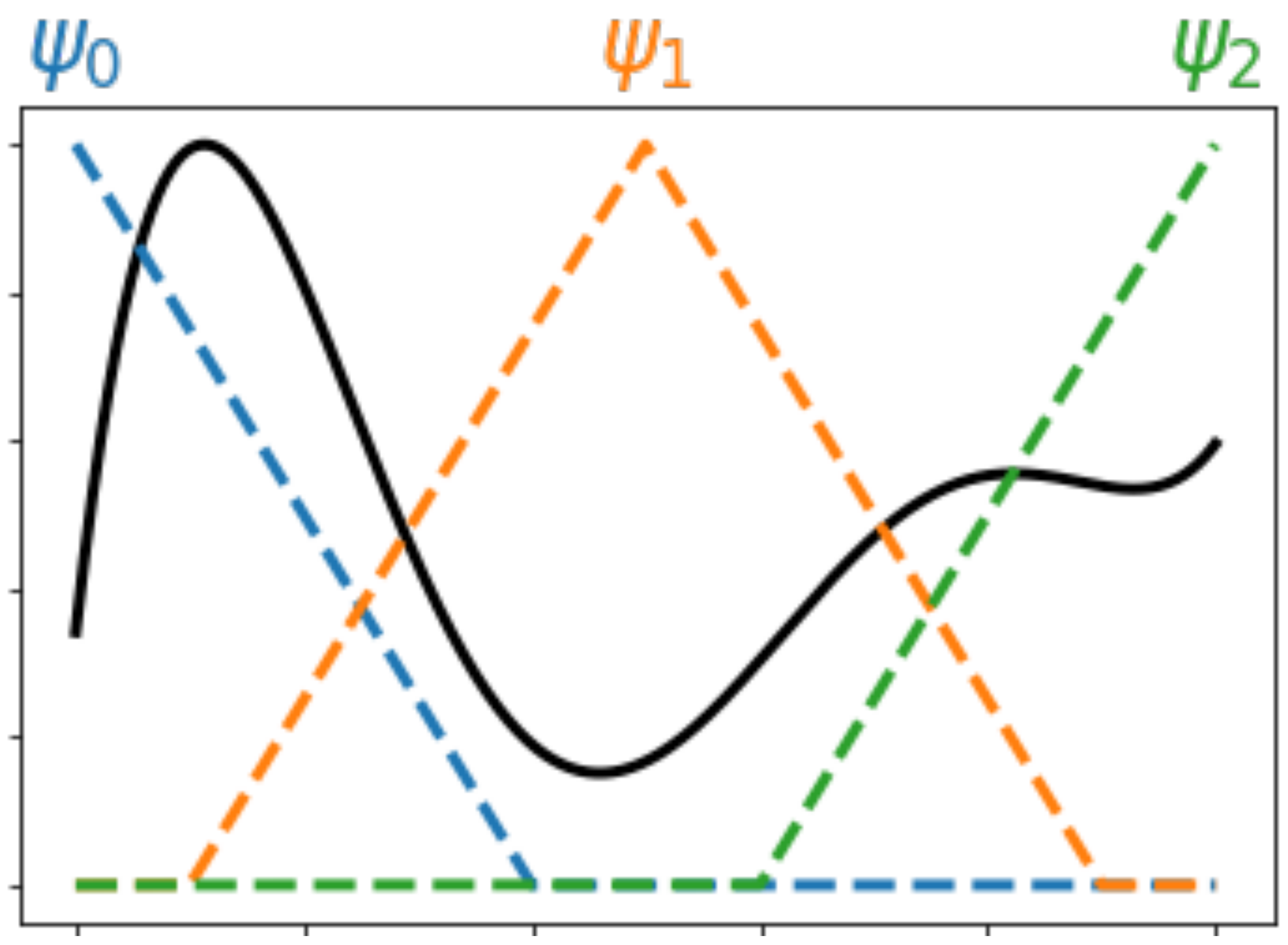
Be mindful of parameter covariances

Choose priors such that the full posterior is explored

Umbrella Sampling

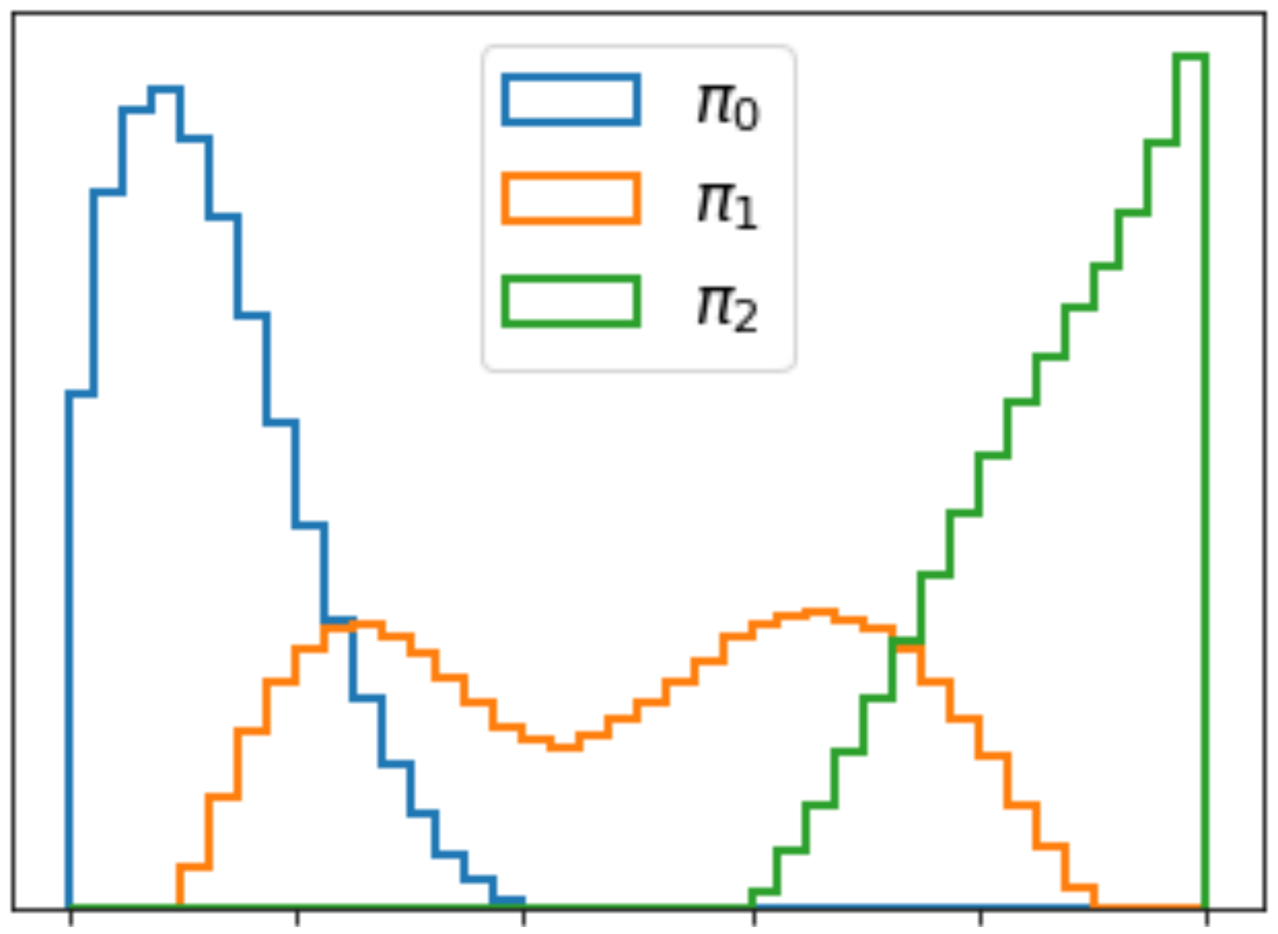


We have a complicated posterior with a narrow “bottleneck” that stymies most MCMC samplers



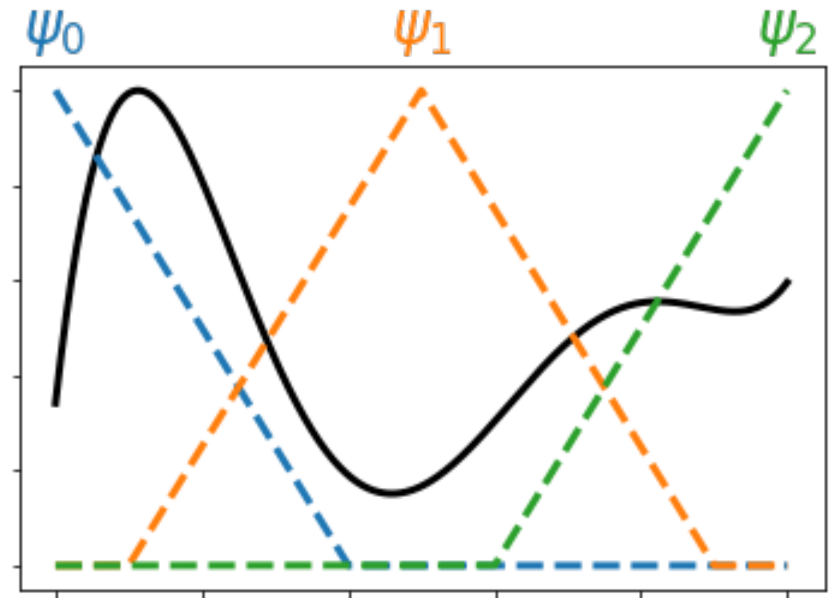
Split the posterior into three regions using bias functions

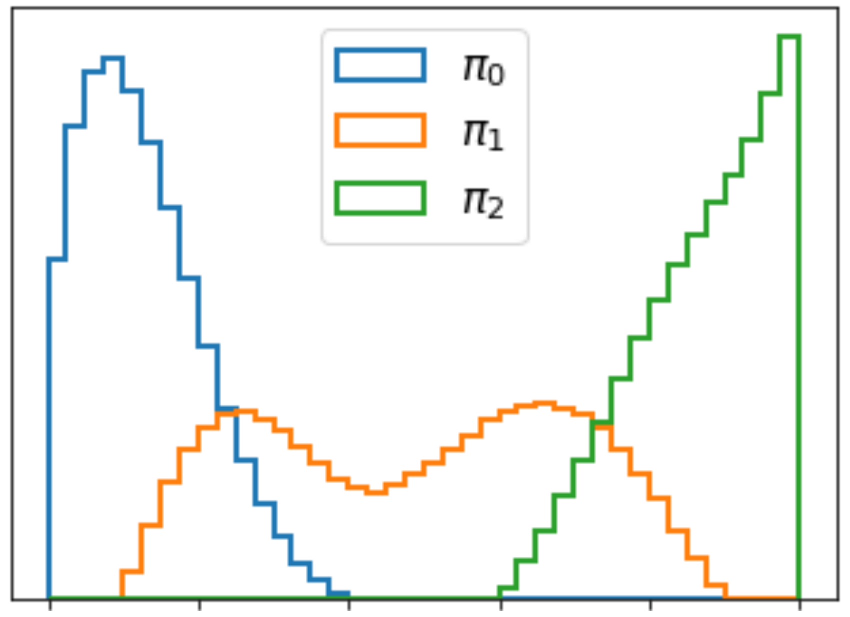
You’ll need to run the sampler three times



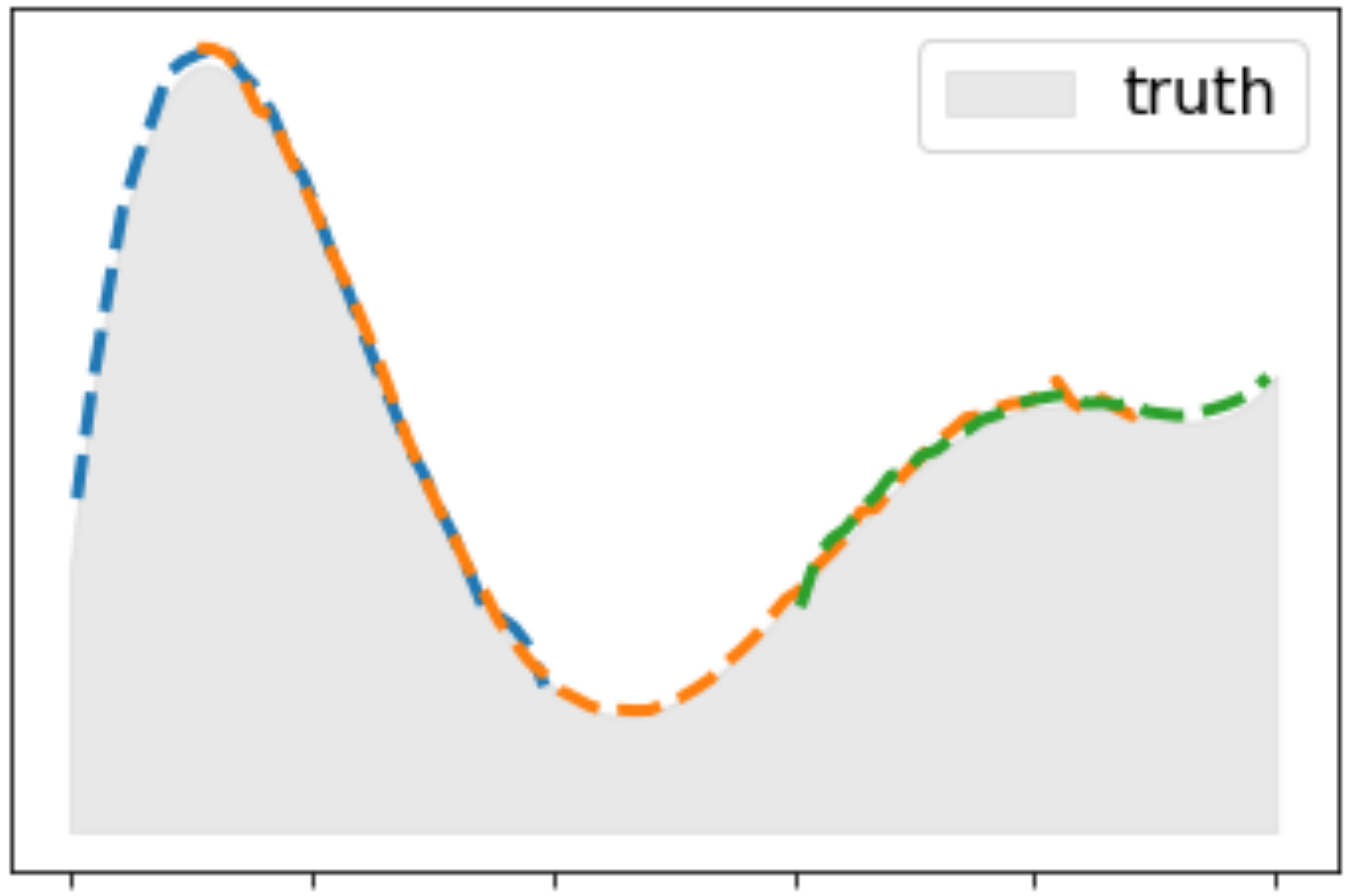
We now have three sets of (weighted) samples that need to be recombined

Umbrella Sampling





$$z_i = \int \psi_i(x)\pi(x)dx = \langle \psi_i \rangle_\pi$$

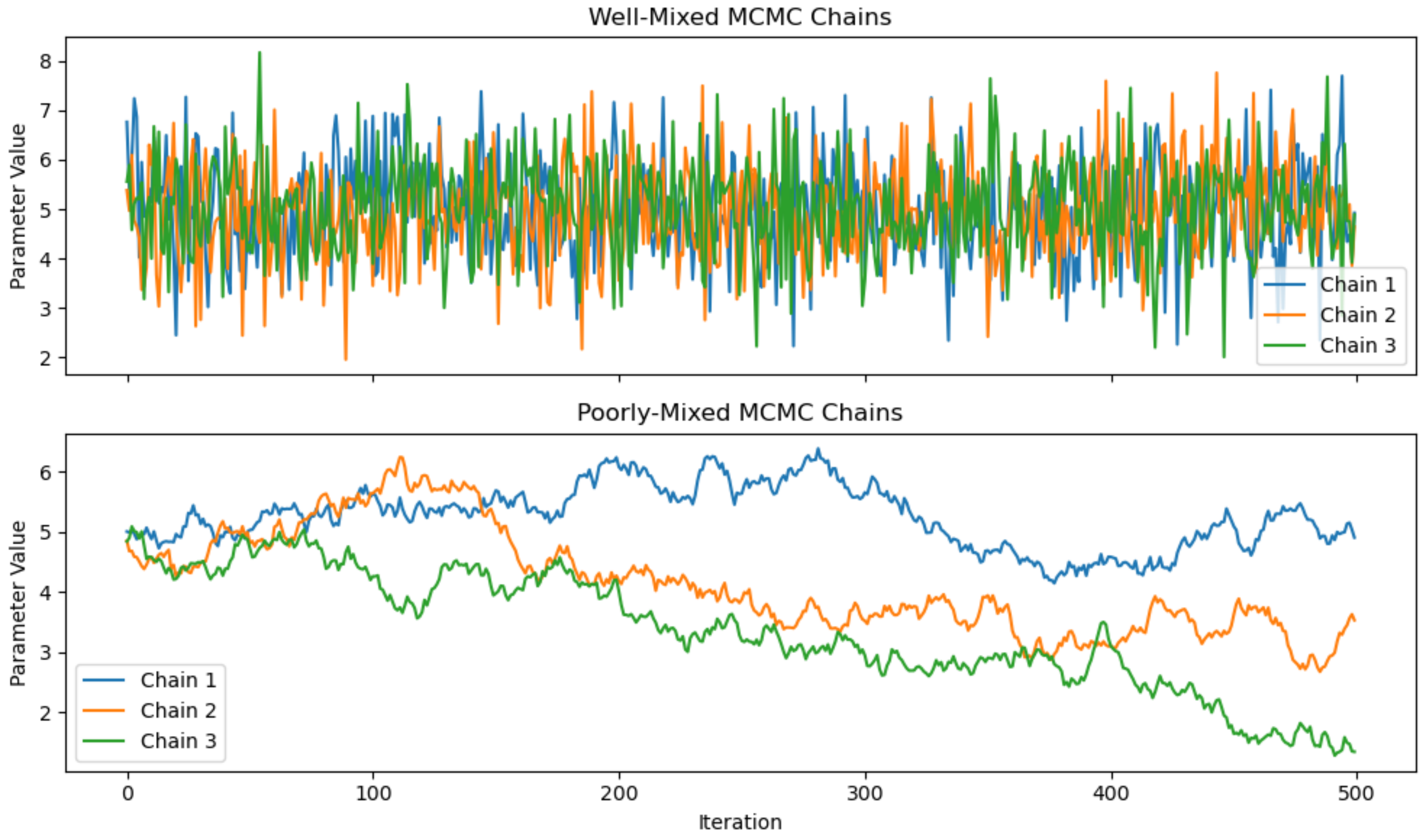


Estimating the overlap matrix *F*

$$z_i = \sum_{i=1}^{N} \left\langle \frac{\psi_i(x)}{\sum_{j=1}^{N} \psi_j(x)/z_j} \right\rangle_{\pi_i} \qquad F_{ij} = \left\langle \frac{\psi_j/z_i}{\sum_{k=1}^{N} \psi_k/z_k} \right\rangle_{\pi_i} \qquad F = \begin{bmatrix} 0.83 & 0.07 & 0 \\ 0.39 & 0.72 & 0.31 \\ 0 & 0.08 & 0.8 \end{bmatrix}$$

For a full walkthrough of the mathematics, see https://gjgilbert.github.io/tutorials/umbrella_sampling/

How do we assess convergence?



Gelman-Rubin statistic

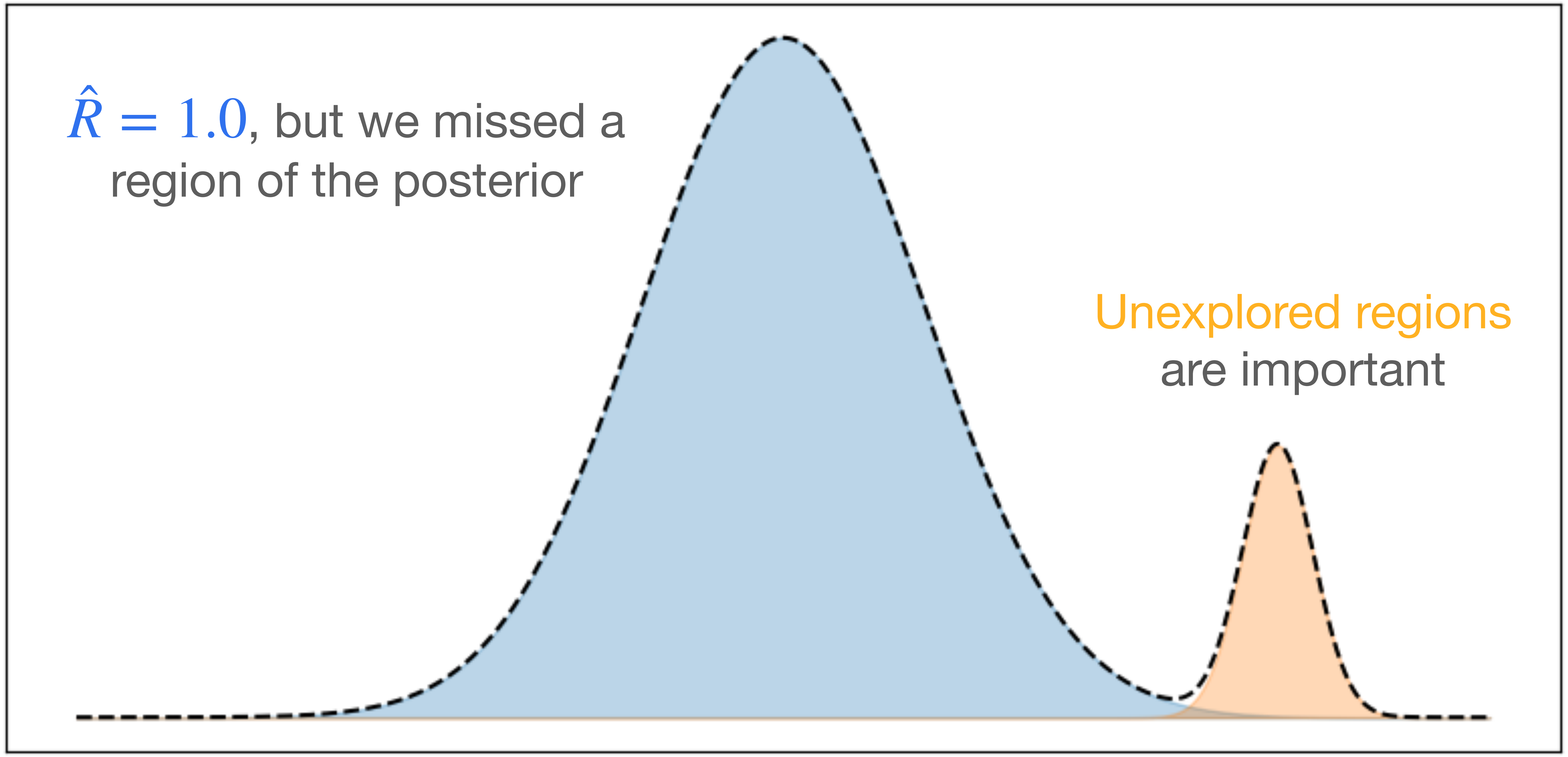
$$\hat{R} \sim \frac{W + B/L}{W}$$

Within-chain variance

Between-chain variance

Length of chain

How do we assess convergence?



How do we identify unknown unknowns?

Domain expertise

Exploratory runs

Umbrella sampling

Your sampler alone will not save you!

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