



Stan

Software Ecosystem for Modern Bayesian Inference

github.com/jgabry/lander-stan-class-2024

CNA Bayes + Stan Class
Lander Analytics
December 2024

Instructor

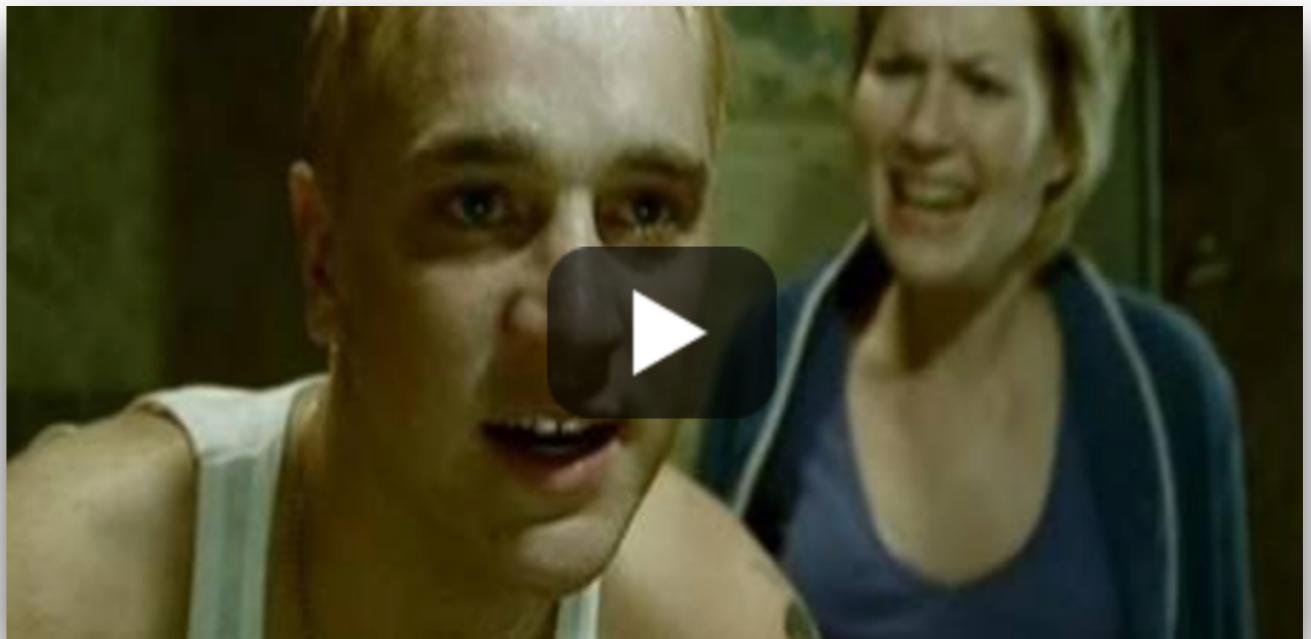
Jonah Gabry

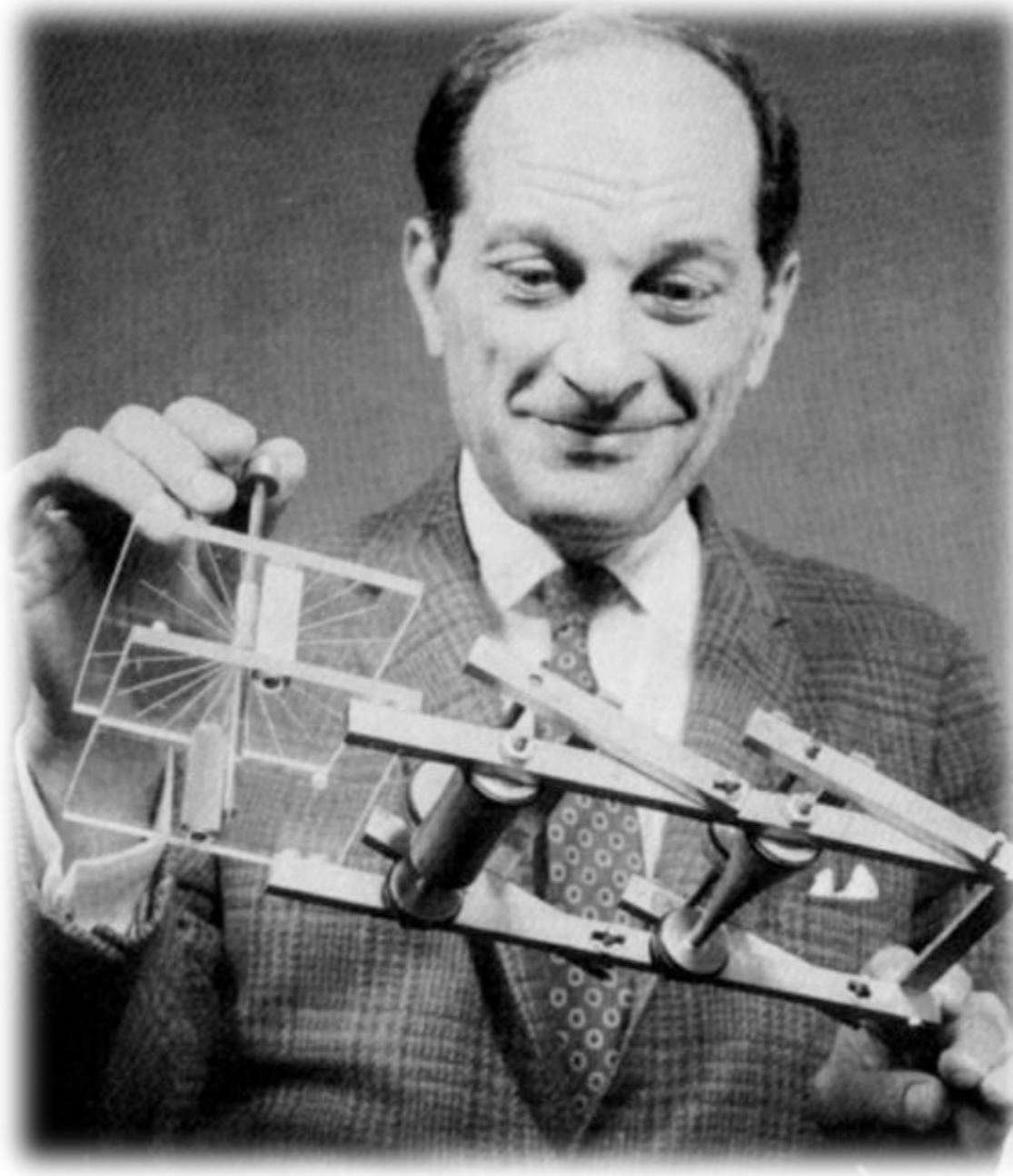
**Lander Analytics
Columbia University
Stan Development Team**

[linkedin](#)
[website](#)

Why Bayes?

Why “Stan”? suboptimal SEO





Stanislaw Ulam
(1909–1984)

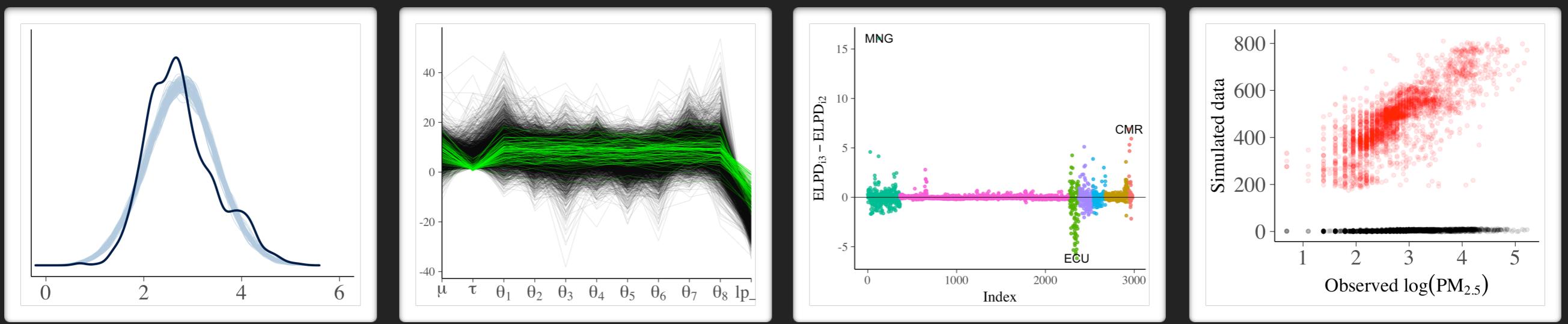
Monte Carlo
Method

H-Bomb

What is Stan?

- Open source probabilistic **programming language, inference algorithms**
- Stan **program**
 - declares data and (constrained) parameter variables
 - defines log posterior (or penalized likelihood)
- Stan **inference**
 - MCMC for full Bayes
 - VB/Pathfinder for approximate Bayes
 - Optimization for (penalized) MLE or MAP
- Stan **ecosystem**
 - language, math library (C++)
 - interfaces and tools (R, Python, Julia, and more)
 - documentation (reference manual and user guide, case studies, R package vignettes, and more)
 - online community (Stan Forums on Discourse)

Visualization in Bayesian workflow



Jonah Gabry

Columbia University
Stan Development Team

A Bayesian modeler commits to an *a priori joint distribution*

$$p(\mathbf{y}, \boldsymbol{\theta}) = p(\mathbf{y} \mid \boldsymbol{\theta})p(\boldsymbol{\theta}) = p(\boldsymbol{\theta} \mid \mathbf{y})p(\mathbf{y})$$

Likelihood x Prior

Posterior x Marginal Likelihood

The diagram illustrates the decomposition of a joint probability. On the left, the joint probability $p(\mathbf{y}, \boldsymbol{\theta})$ is shown as a product of two terms: $p(\mathbf{y} \mid \boldsymbol{\theta})$ and $p(\boldsymbol{\theta})$. This is labeled "Likelihood x Prior". Arrows point from the labels "Data (observed)" and "Parameters (unobserved)" to the terms $p(\mathbf{y} \mid \boldsymbol{\theta})$ and $p(\boldsymbol{\theta})$ respectively. On the right, the joint probability is shown as a product of two terms: $p(\boldsymbol{\theta} \mid \mathbf{y})$ and $p(\mathbf{y})$. This is labeled "Posterior x Marginal Likelihood". Arrows point from the labels "Posterior" and "Marginal Likelihood" to the terms $p(\boldsymbol{\theta} \mid \mathbf{y})$ and $p(\mathbf{y})$ respectively.

Data (observed) **Parameters (unobserved)**

Workflow

Bayesian data analysis

- Exploratory data analysis
- *Prior* predictive checking
- Model fitting and algorithm diagnostics
- *Posterior* predictive checking
- Model comparison (e.g., via cross-validation)

Gabry, J., Simpson, D., Vehtari, A., Betancourt, M., and Gelman, A. (2019).

Visualization in Bayesian workflow.

Journal of the Royal Statistical Society Series A

Journal version: rss.onlinelibrary.wiley.com/doi/full/10.1111/rssc.12378

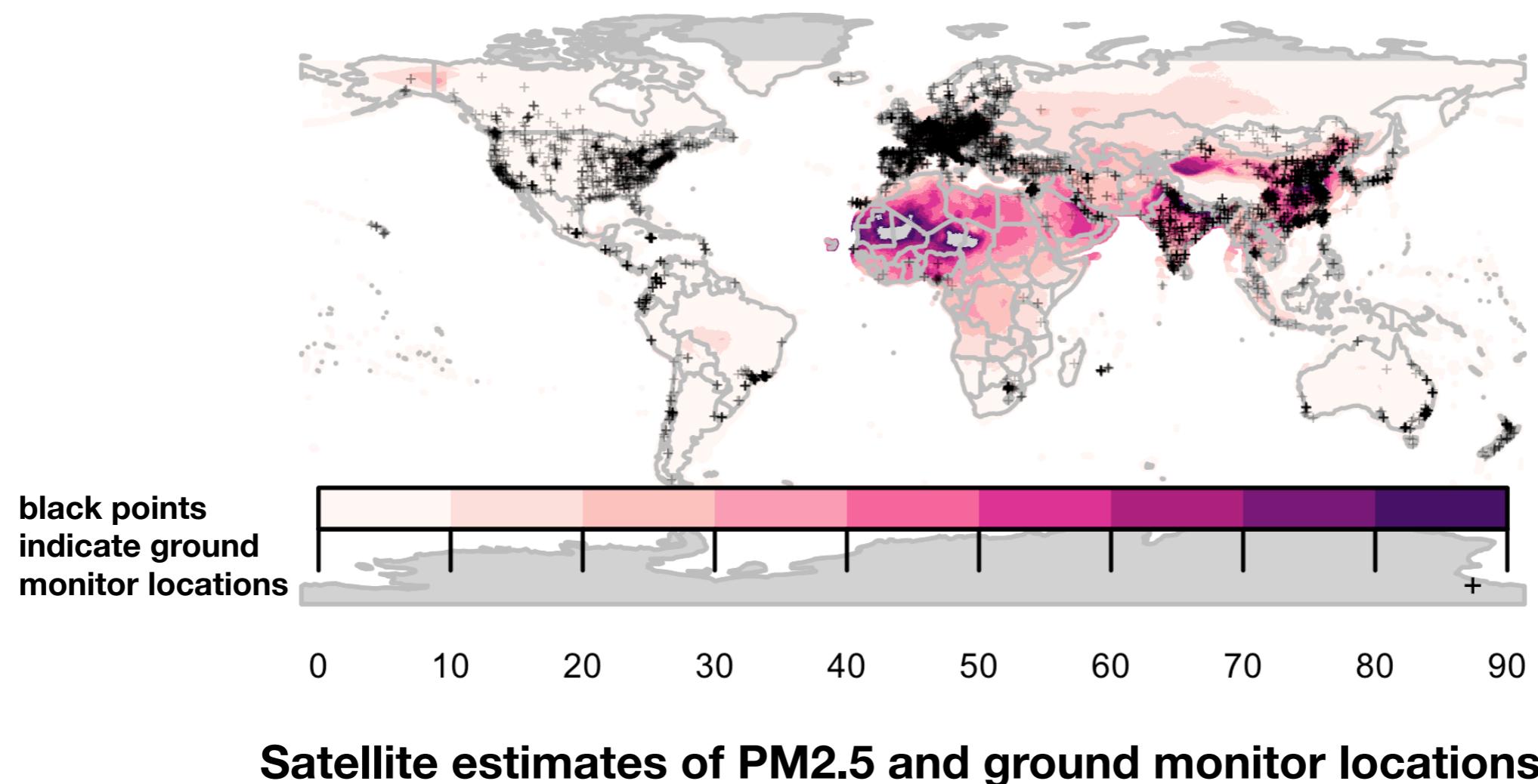
arXiv preprint: arxiv.org/abs/1709.01449

Code: github.com/jgabry/bayes-vis-paper

Example

Goal Estimate global PM2.5 concentration

Problem Most data from noisy satellite measurements (ground monitor network provides sparse, heterogeneous coverage)

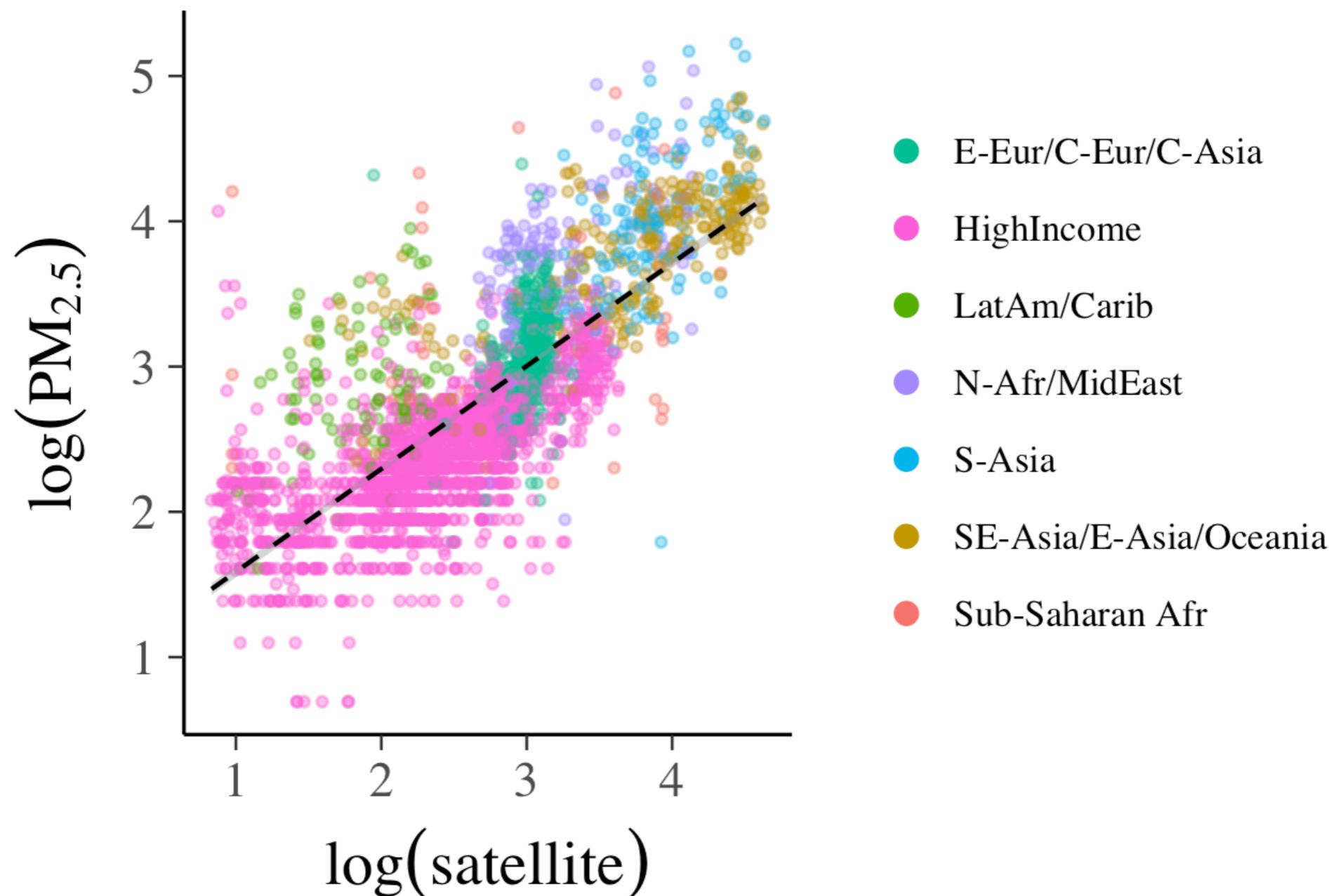


Exploratory Data Analysis

Building a network of models

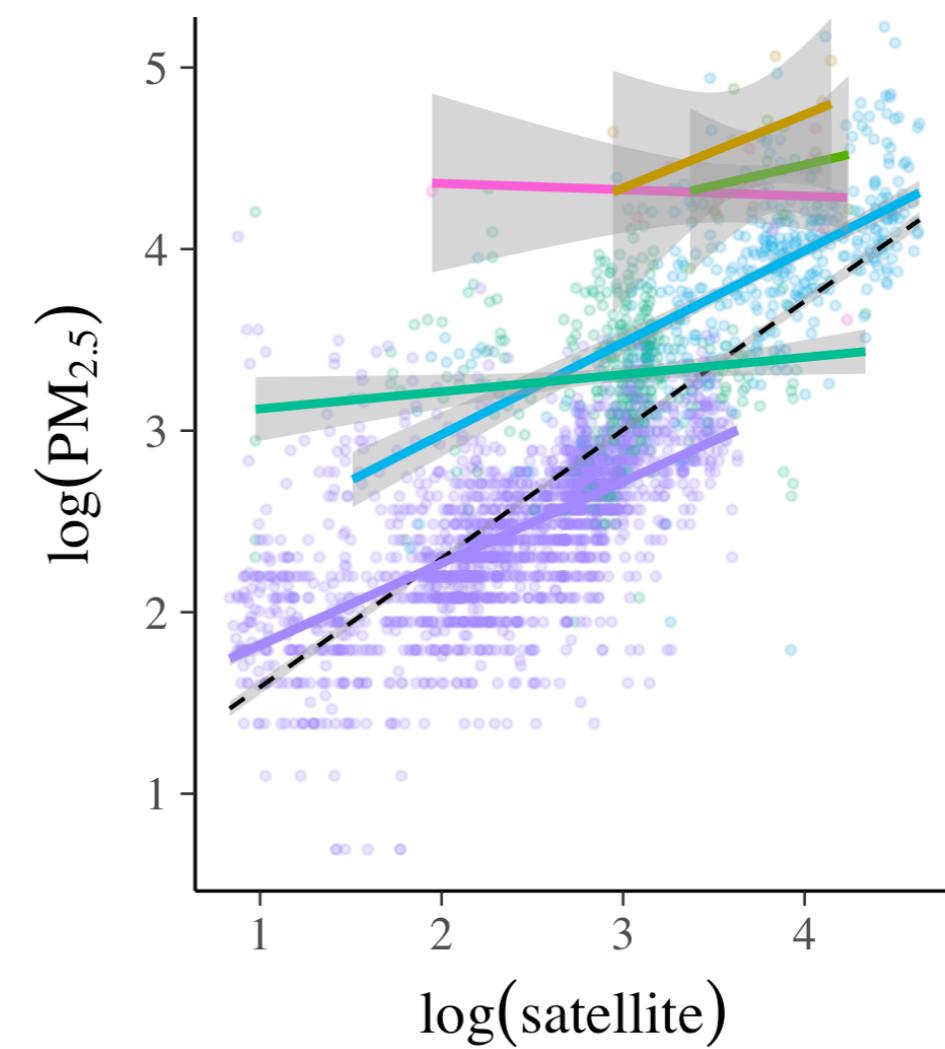
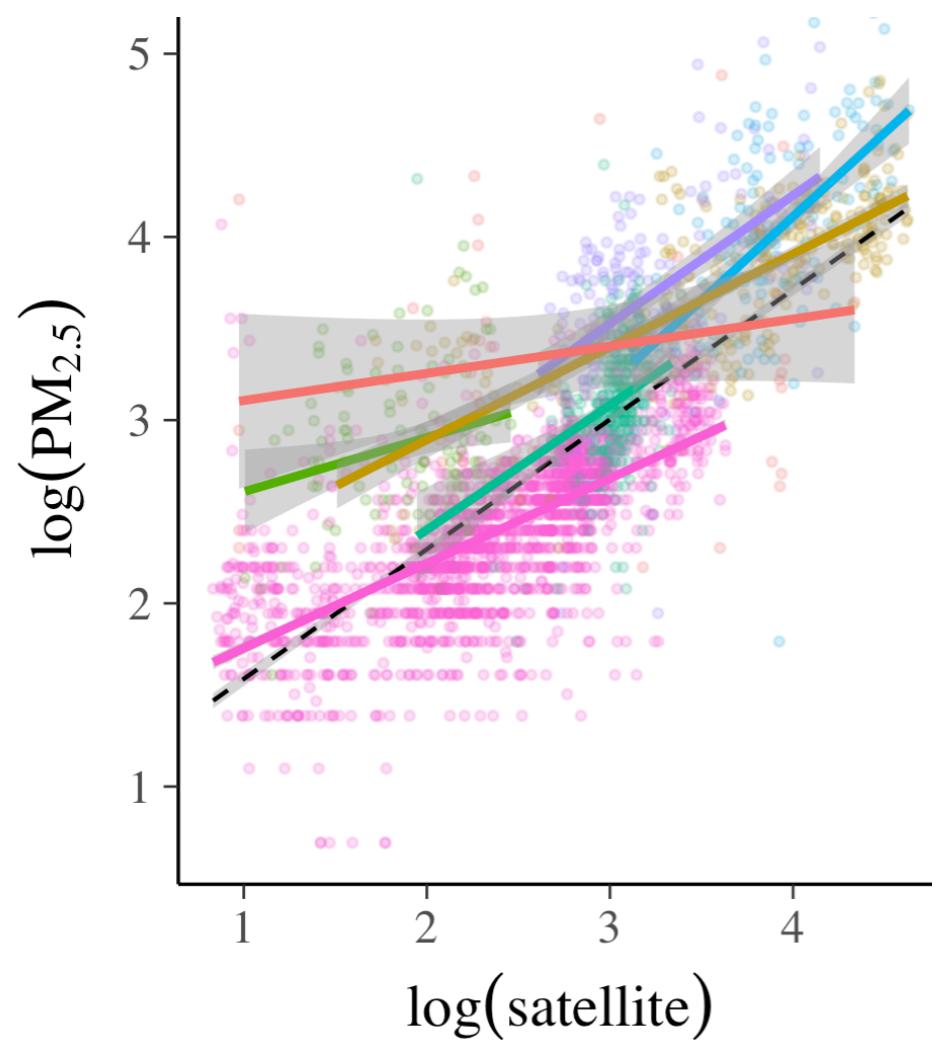
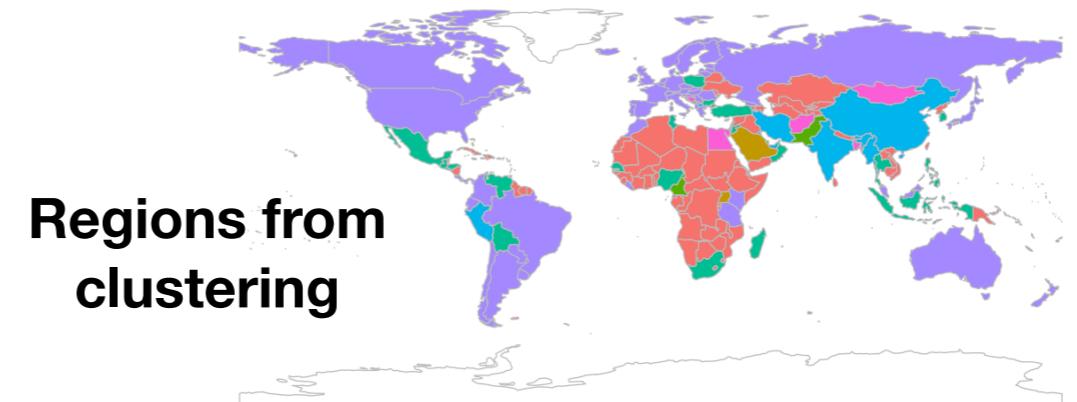
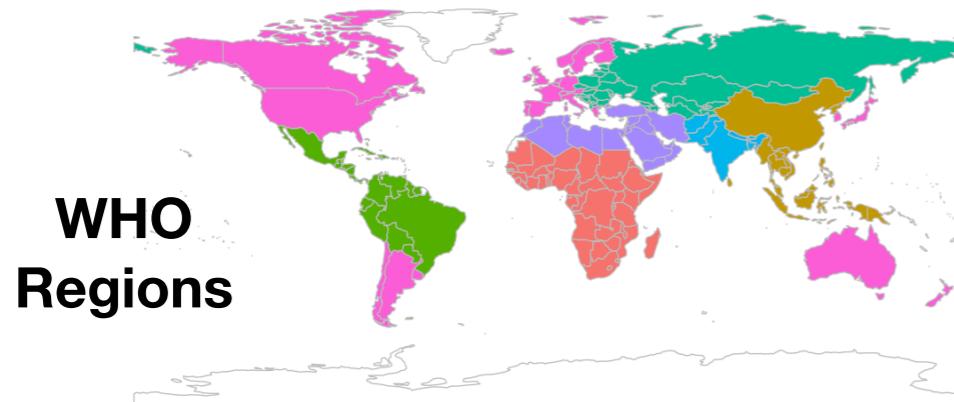
Exploratory data analysis

building a network of models



Exploratory data analysis

building a network of models



Exploratory data analysis

building a network of models

For measurements $n = 1, \dots, N$

and regions $j = 1, \dots, J$

Model 1

$$\log(\text{PM}_{2.5,nj}) \sim N(\alpha + \beta \log(\text{sat}_{nj}), \sigma)$$

Exploratory data analysis

building a network of models

For measurements $n = 1, \dots, N$

and regions $j = 1, \dots, J$

Models 2 and 3

$$\log(\text{PM}_{2.5,nj}) \sim N(\mu_{nj}, \sigma)$$

$$\mu_{nj} = \boxed{\alpha_0 + \alpha_j} + \boxed{(\beta_0 + \beta_j)} \log(\text{sat}_{nj})$$

$$\alpha_j \sim N(0, \tau_\alpha) \quad \beta_j \sim N(0, \tau_\beta)$$

Prior predictive checks

Fake data can be almost as valuable as real data

Prior predictive checking: fake data is almost as useful as real data

- Used to understand the role of the prior in the data generating process
- Even people who don't have strong feelings about a specific prior know what their observed data shouldn't look like (i.e., pollution levels aren't so thick that we can't move, so the model should reflect that)
 1. Use either observed x or generate reasonable values for x
 2. Sample from your prior (assuming a proper prior)
 3. Calculate the predicted y for that x and that particular random draw from the prior
 4. Repeat 2 & 3 many times
 5. Compute summaries / visualize

Prior predictive checking: fake data is almost as useful as real data

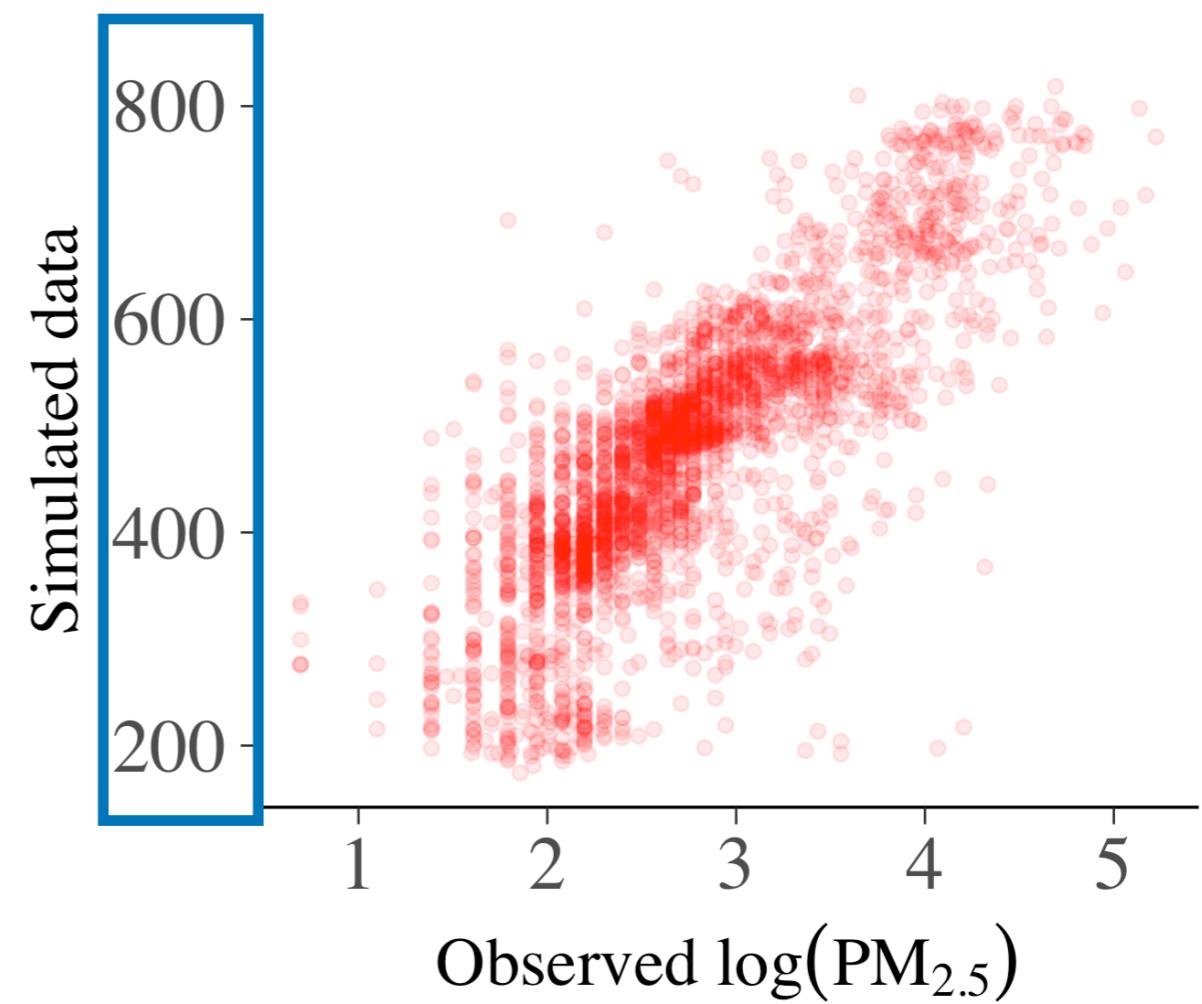
*What do vague/non-informative priors imply
about the data our model can generate?*

$$\alpha_0 \sim N(0, 100)$$

$$\beta_0 \sim N(0, 100)$$

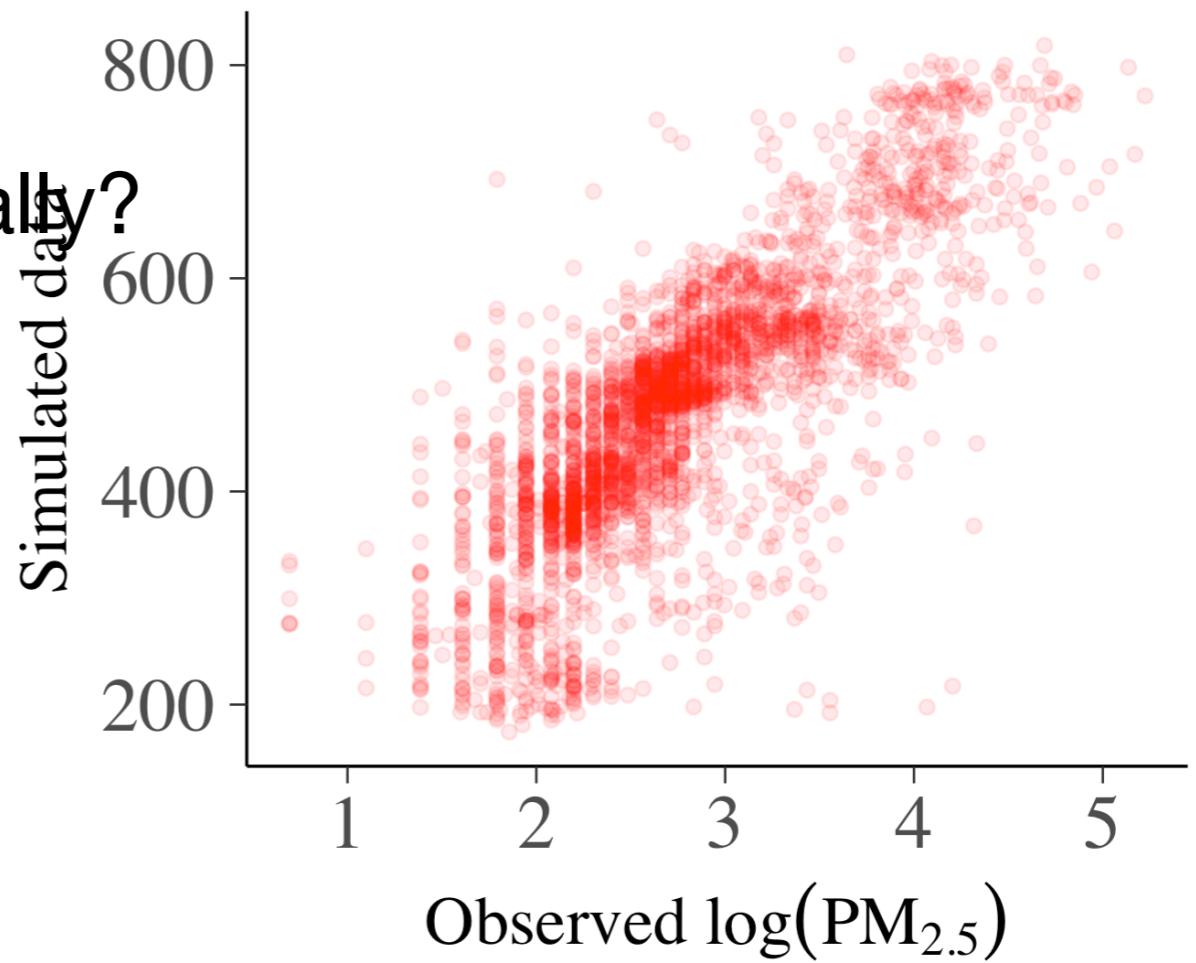
$$\tau_\alpha^2 \sim \text{InvGamma}(1, 100)$$

$$\tau_\beta^2 \sim \text{InvGamma}(1, 100)$$



Prior predictive checking: fake data is almost as useful as real data

- The prior model is **two orders of magnitude** off the real data
- Two orders of magnitude **on the log scale!**
- What does this mean practically?
- The data will have to overcome the prior...



Prior predictive checking: fake data is almost as useful as real data

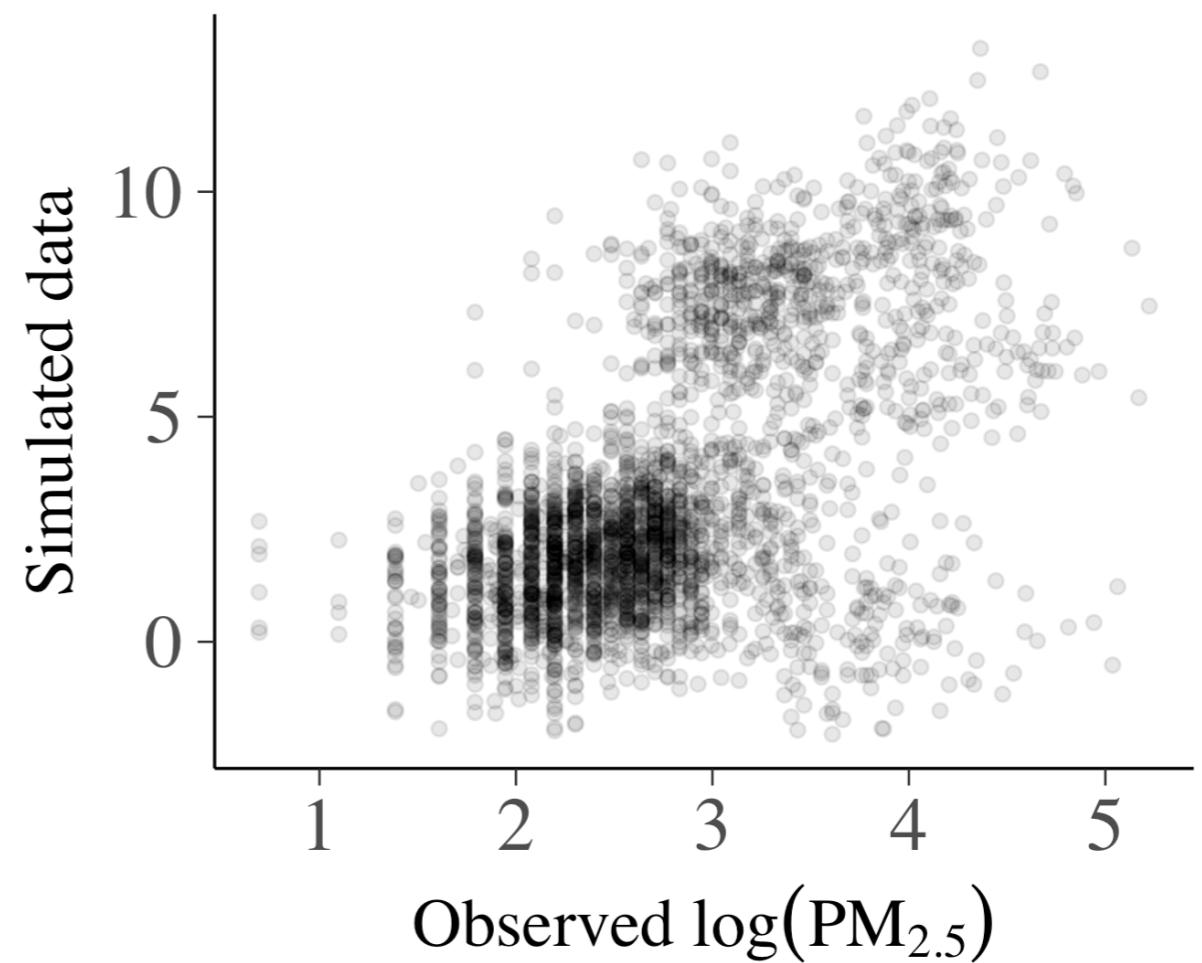
*What are better priors for the global intercept and slope
and the hierarchical scale parameters?*

$$\alpha_0 \sim N(0, 1)$$

$$\beta_0 \sim N(1, 1)$$

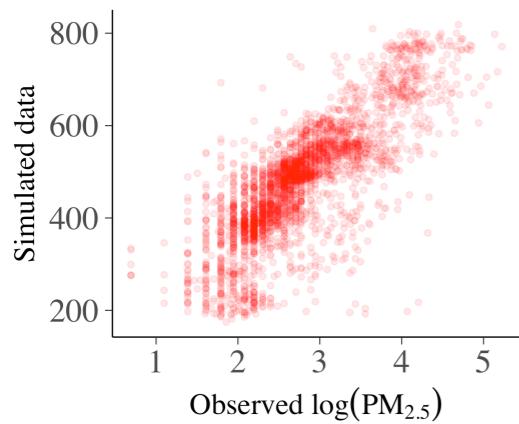
$$\tau_\alpha \sim N_+(0, 1)$$

$$\tau_\beta \sim N_+(0, 1)$$

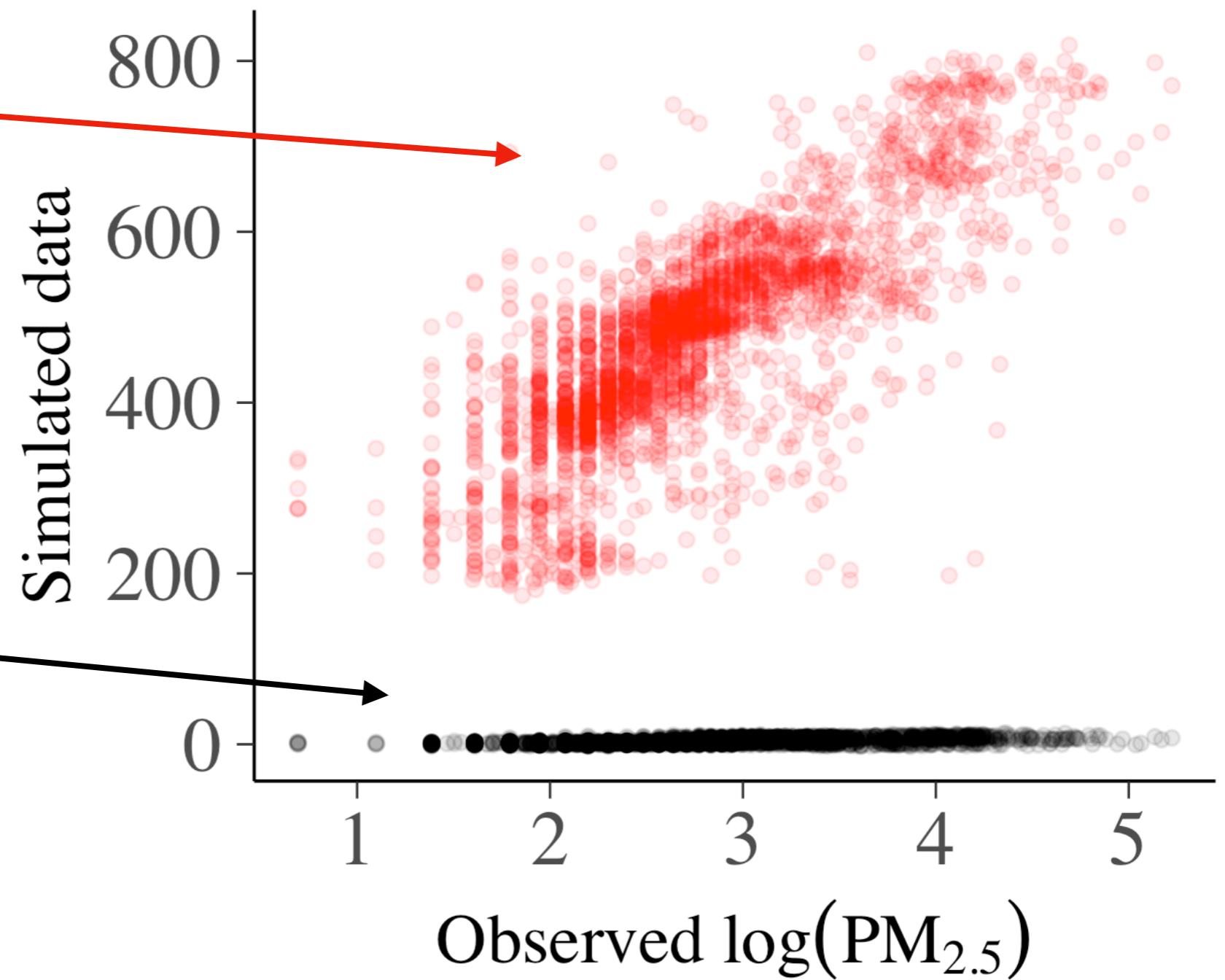
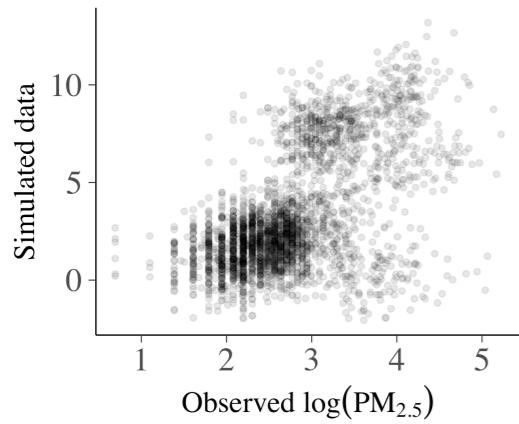


Prior predictive checking: fake data is almost as useful as real data

Non-informative



Weakly informative



What is the problem with “vague” priors?

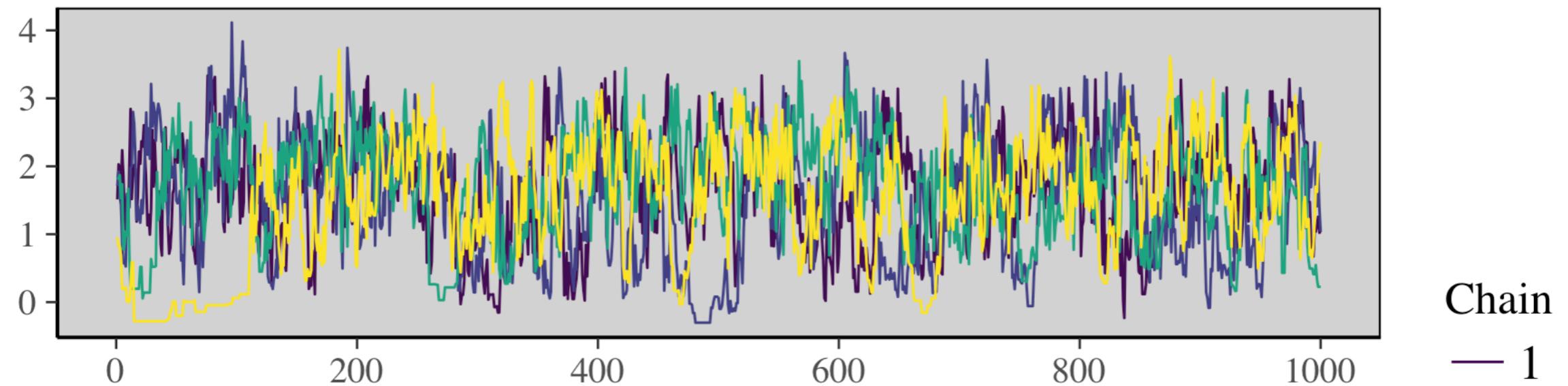
- If we use an *improper* prior, then we do not specify a joint model for our data and parameters
- More importantly, we do not specify a data generating mechanism $p(\mathbf{y})$
- By construction, these priors do not regularize inferences, which is quite often a bad idea
- Proper but diffuse is better than improper but is still often problematic

MCMC diagnostics

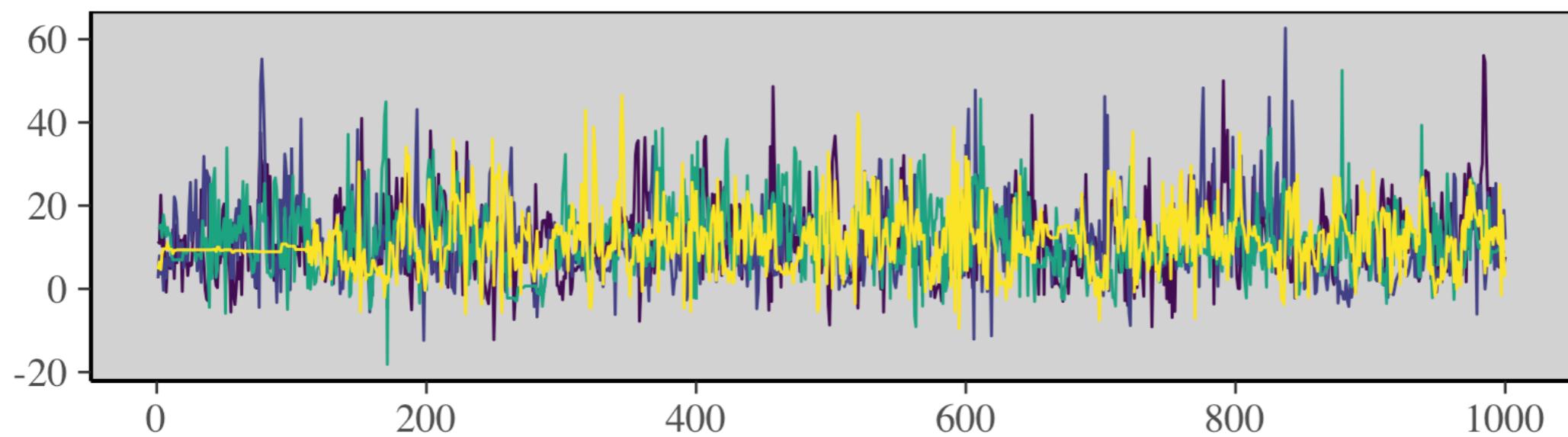
Beyond trace plots

<https://chi-feng.github.io/mcmc-demo/>

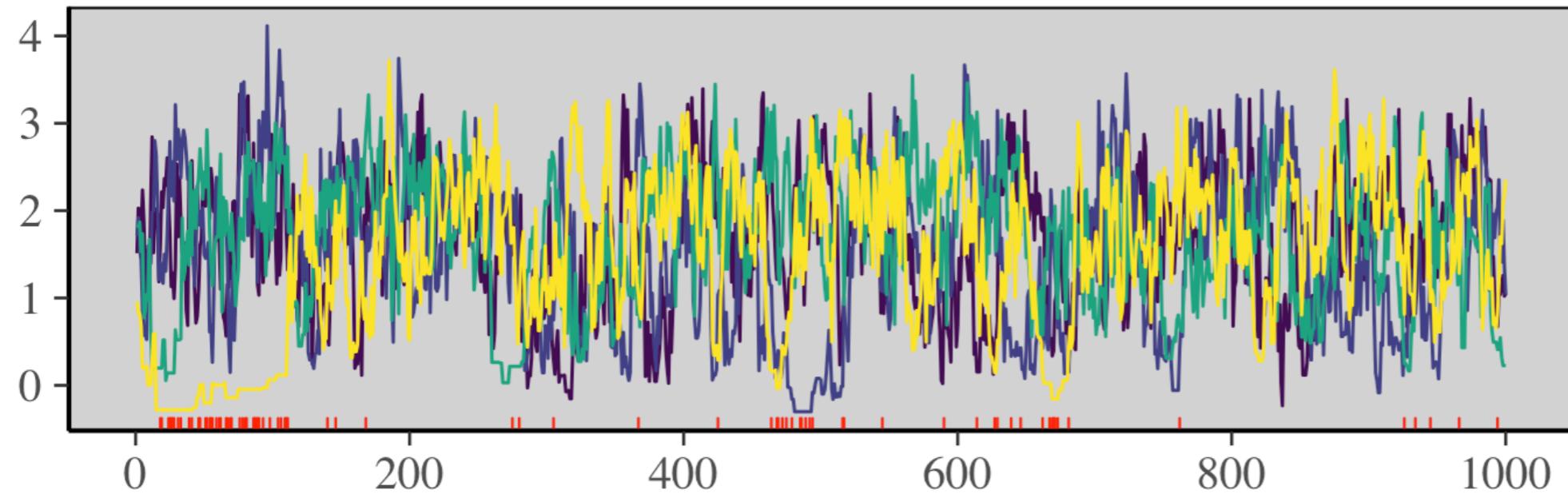
$\log(\tau)$



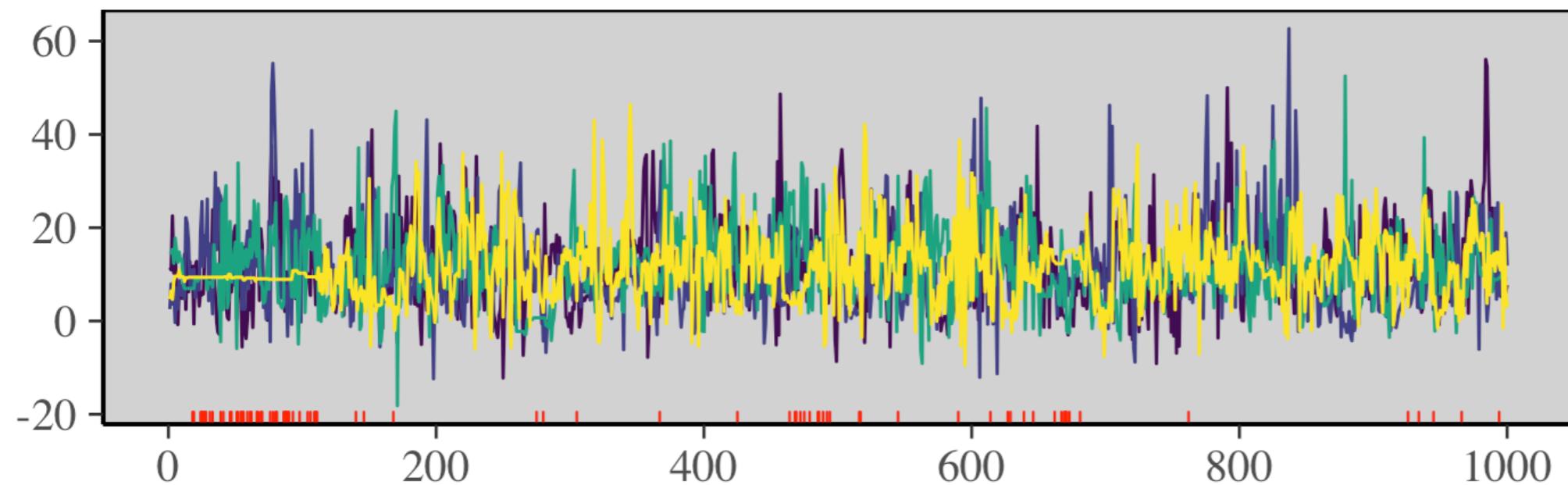
$\theta[1]$



$\log(\tau)$



$\theta[1]$



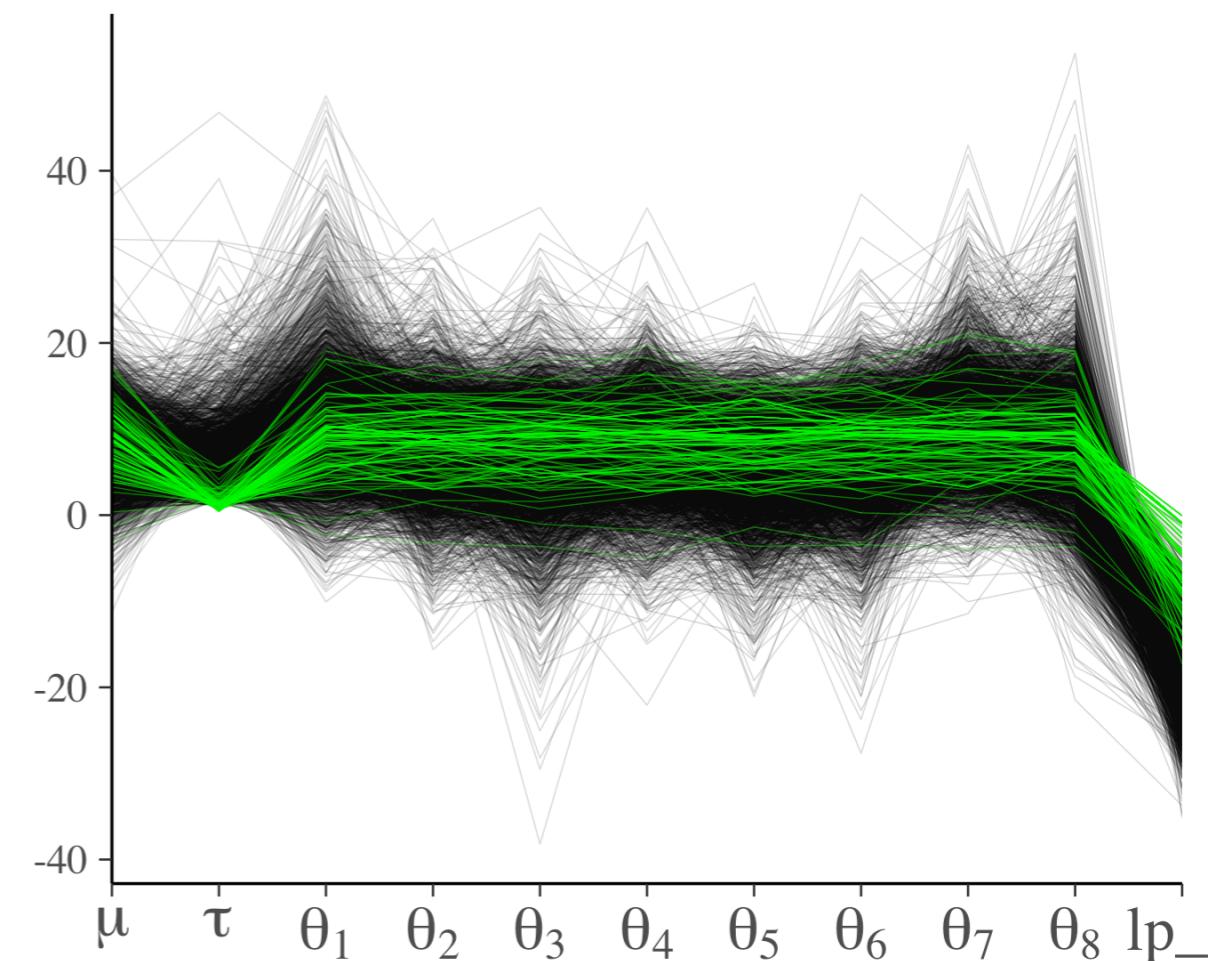
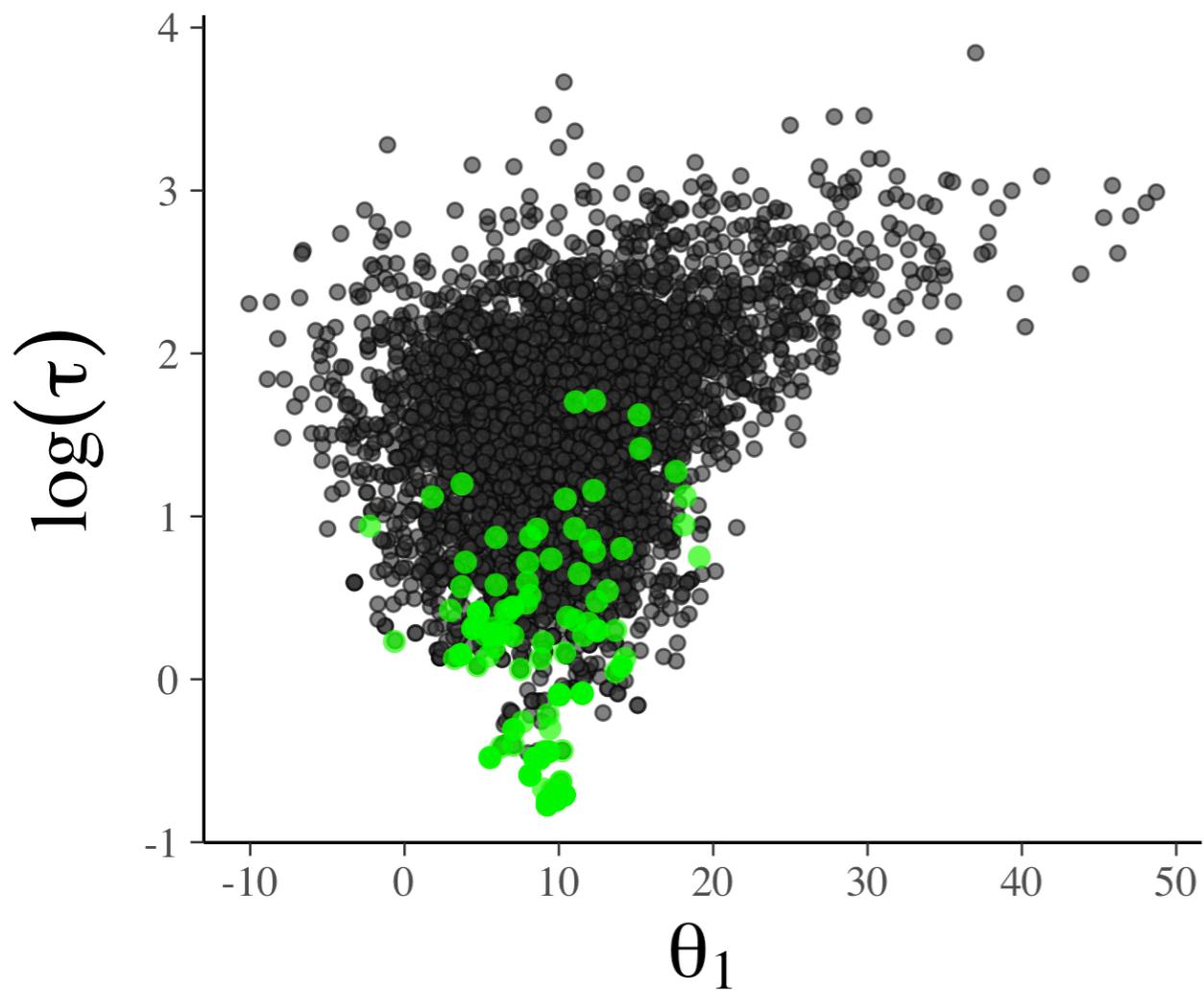
Chain

- 1
- 2
- 3
- 4

— Divergence

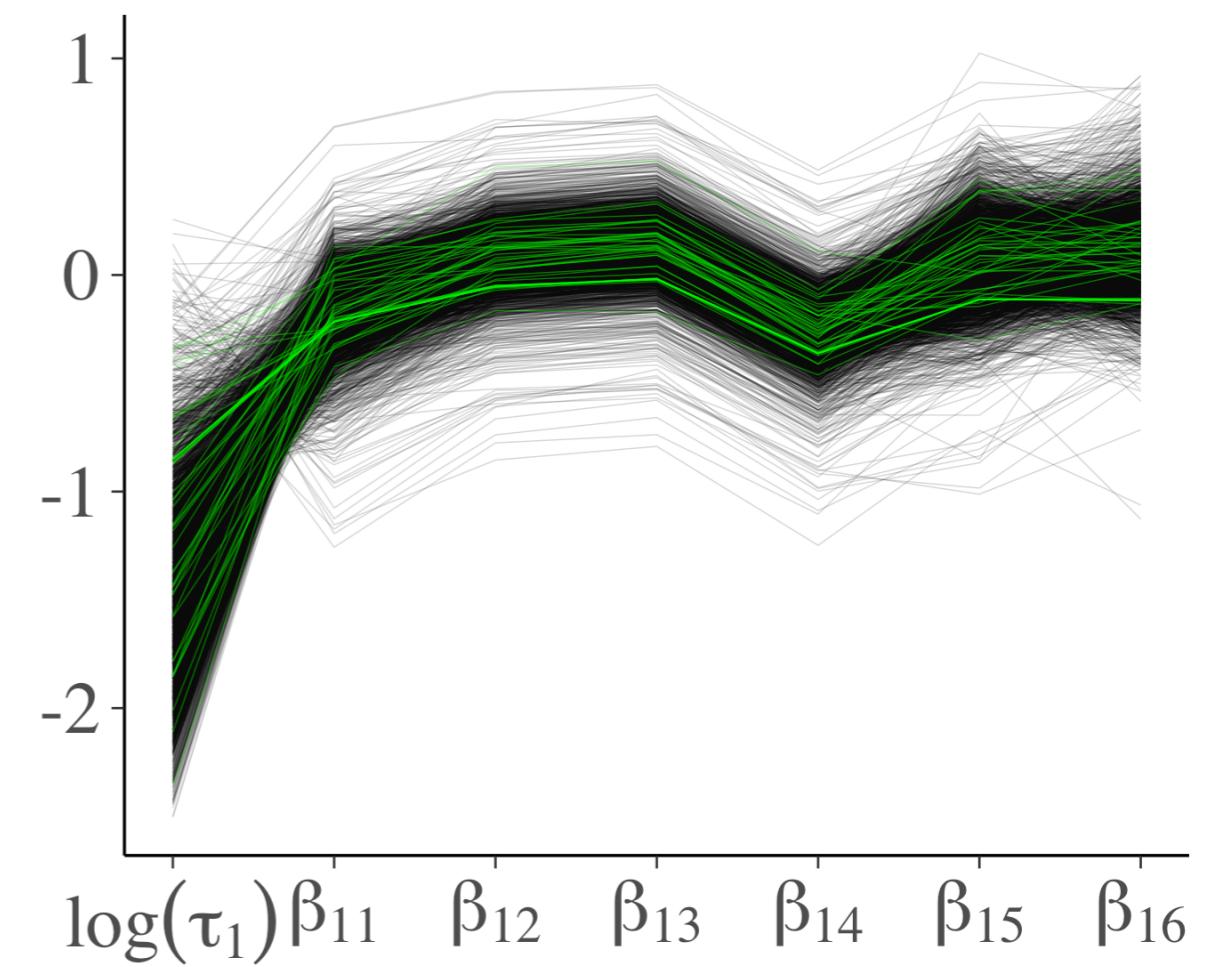
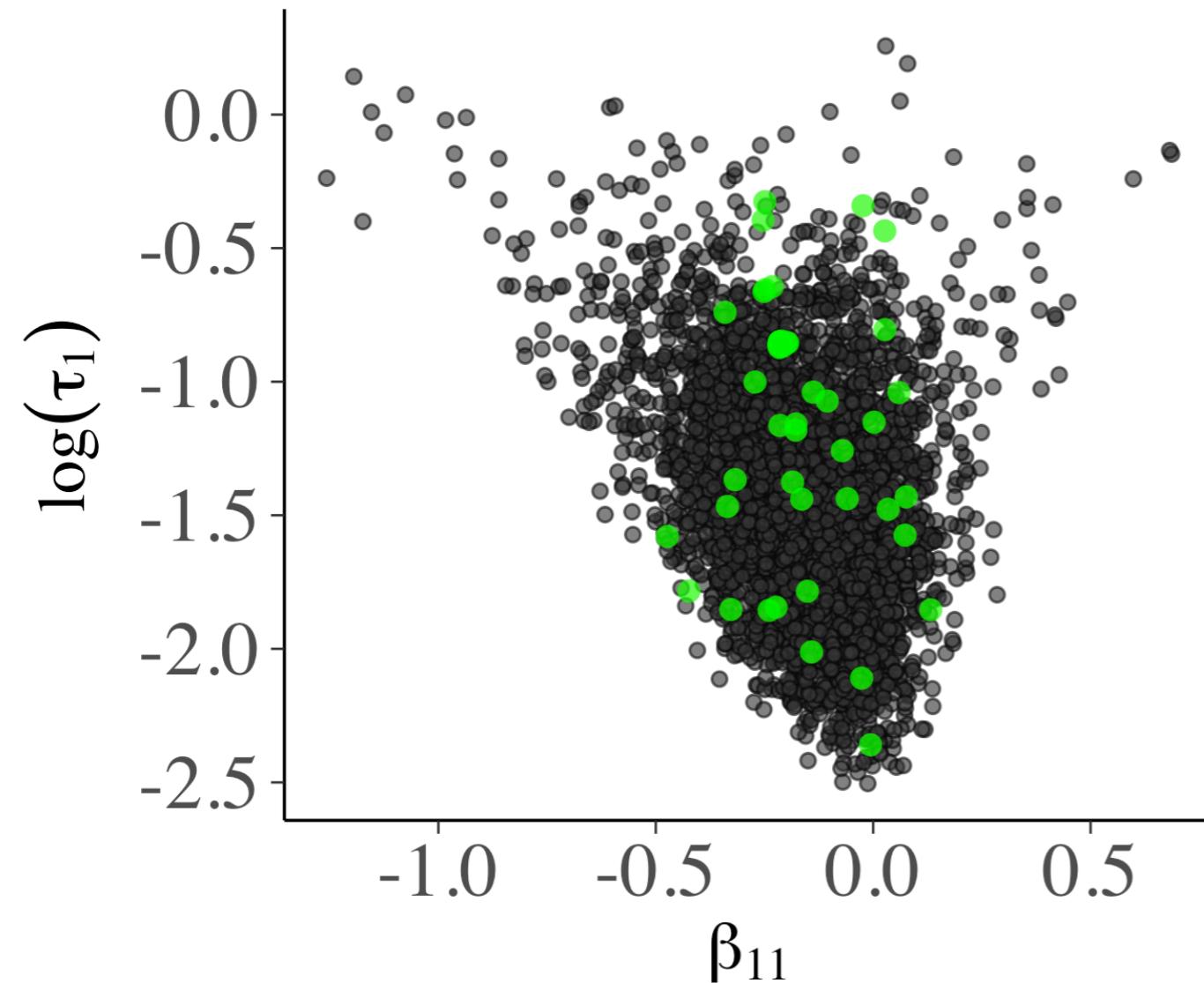
MCMC diagnostics

beyond trace plots

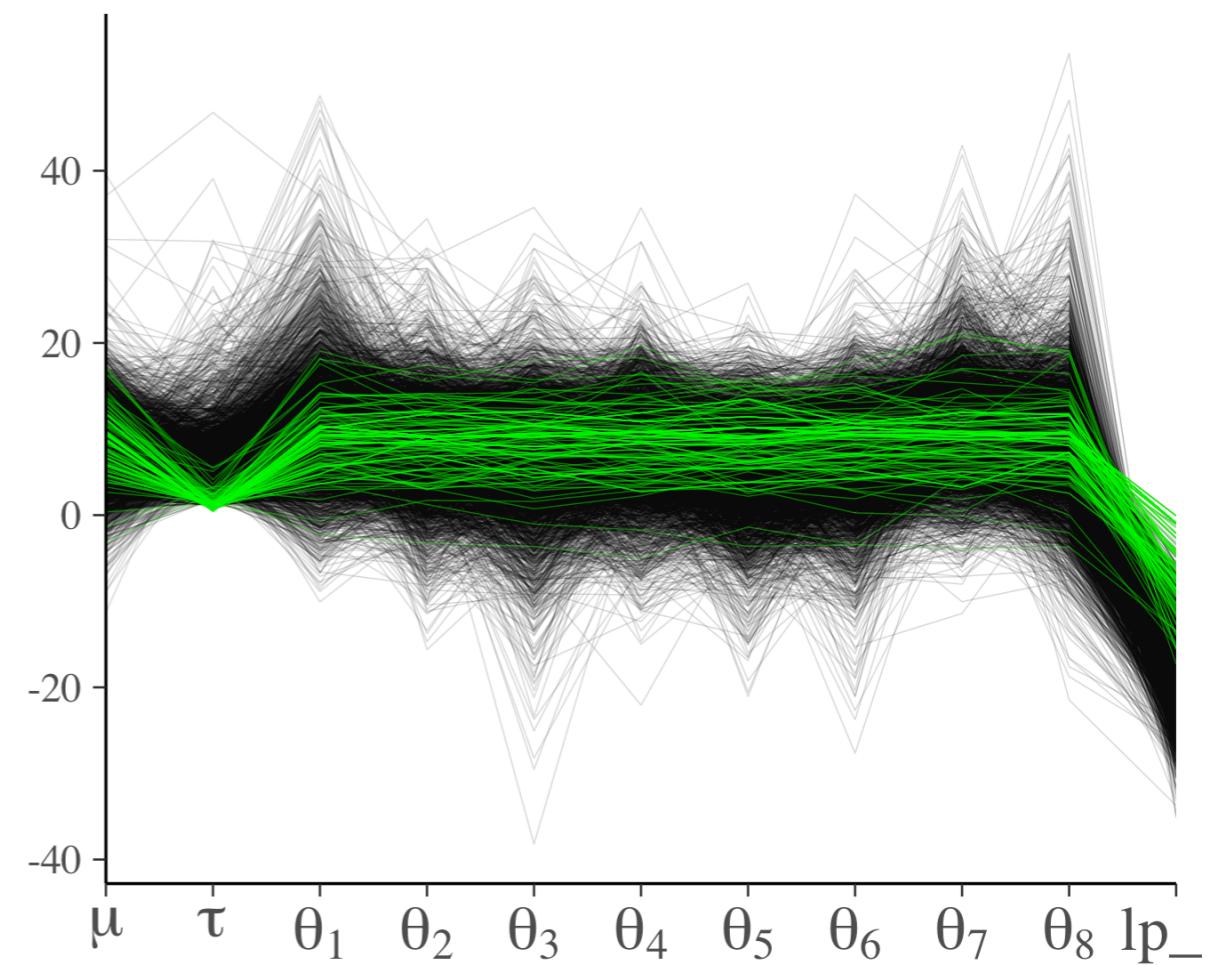
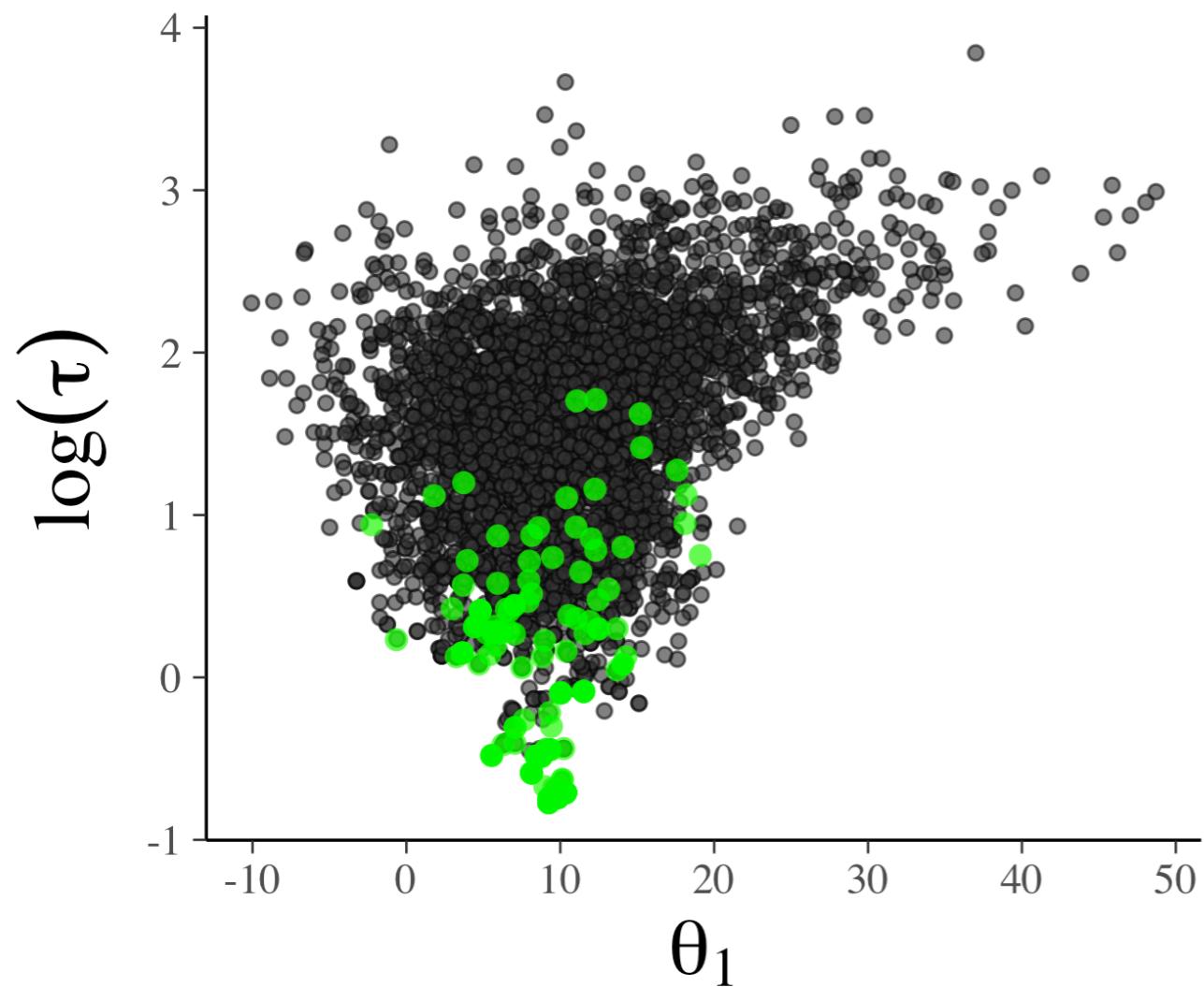


MCMC diagnostics

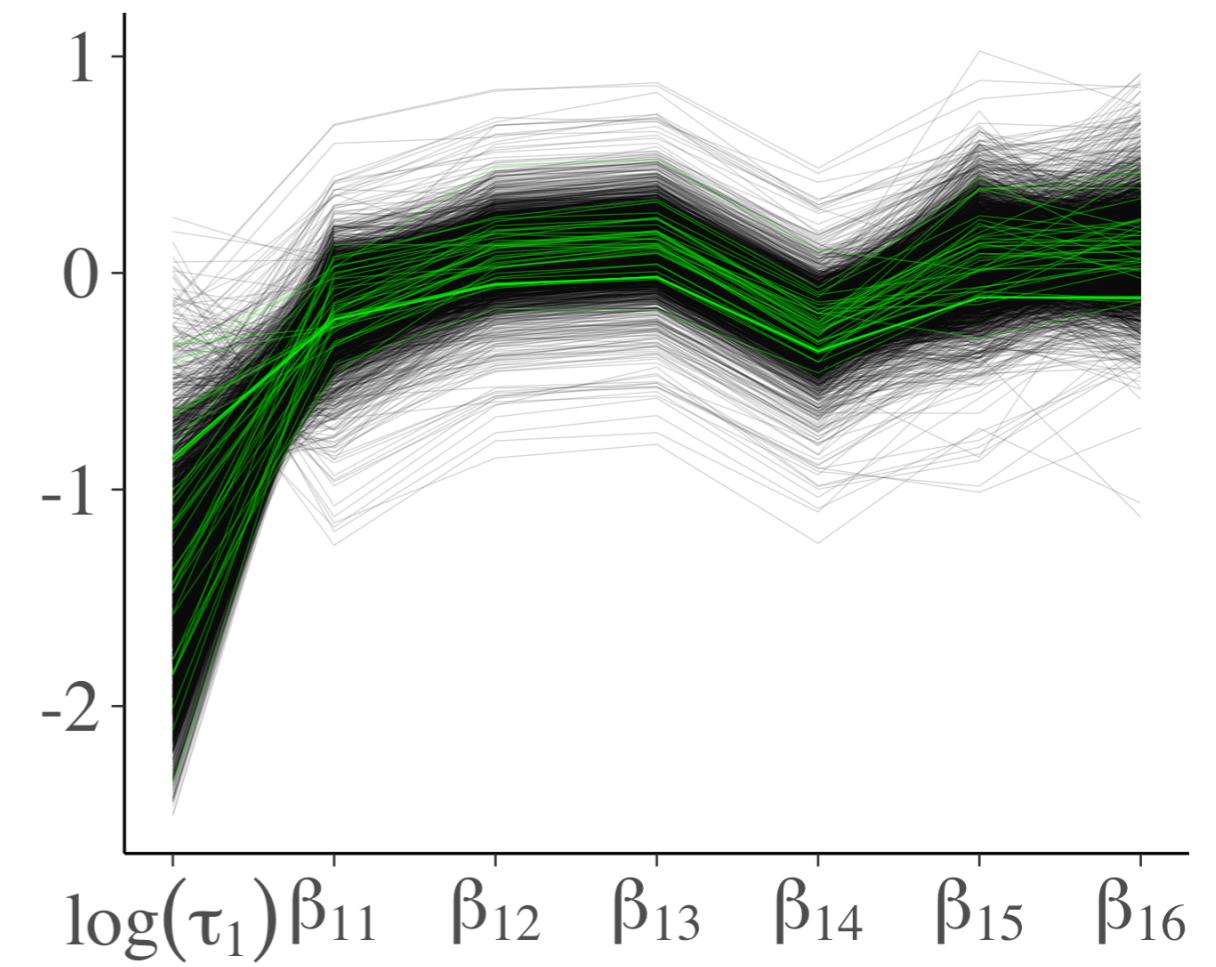
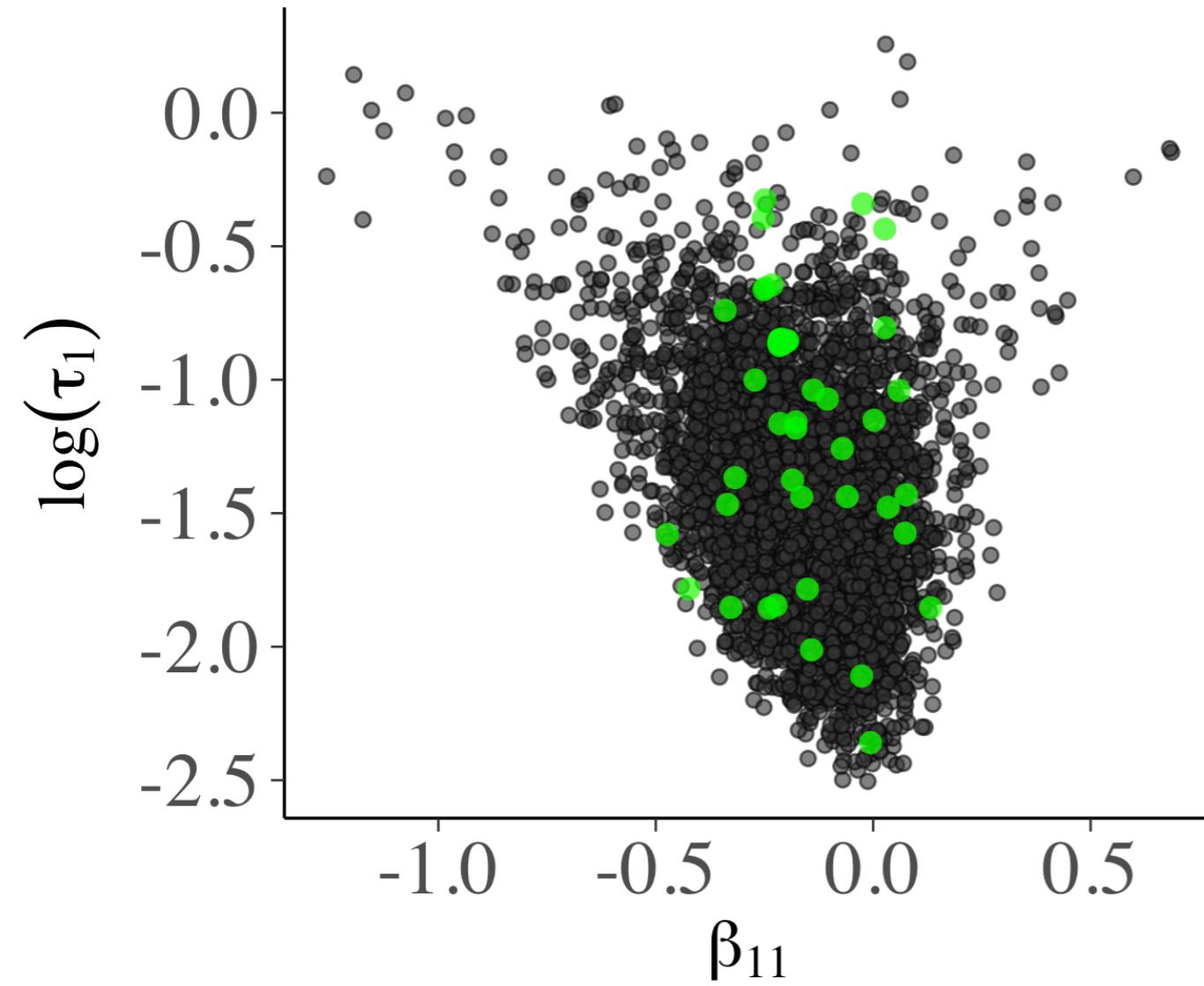
beyond trace plots



Pathological geometry



“False positives”



Posterior predictive checks

Visual model evaluation

Posterior predictive checking

visual model evaluation

- Misfitting and overfitting both manifest as tension between measurements and predictive distributions
- Graphical posterior predictive checks visually compare the observed data to the predictive distribution

Posterior predictive checking

visual model evaluation

The *posterior predictive distribution* is the average data generation process over the entire model

$$p(\tilde{y}|y) = \int p(\tilde{y}|\theta) p(\theta|y) d\theta$$

Posterior predictive checking

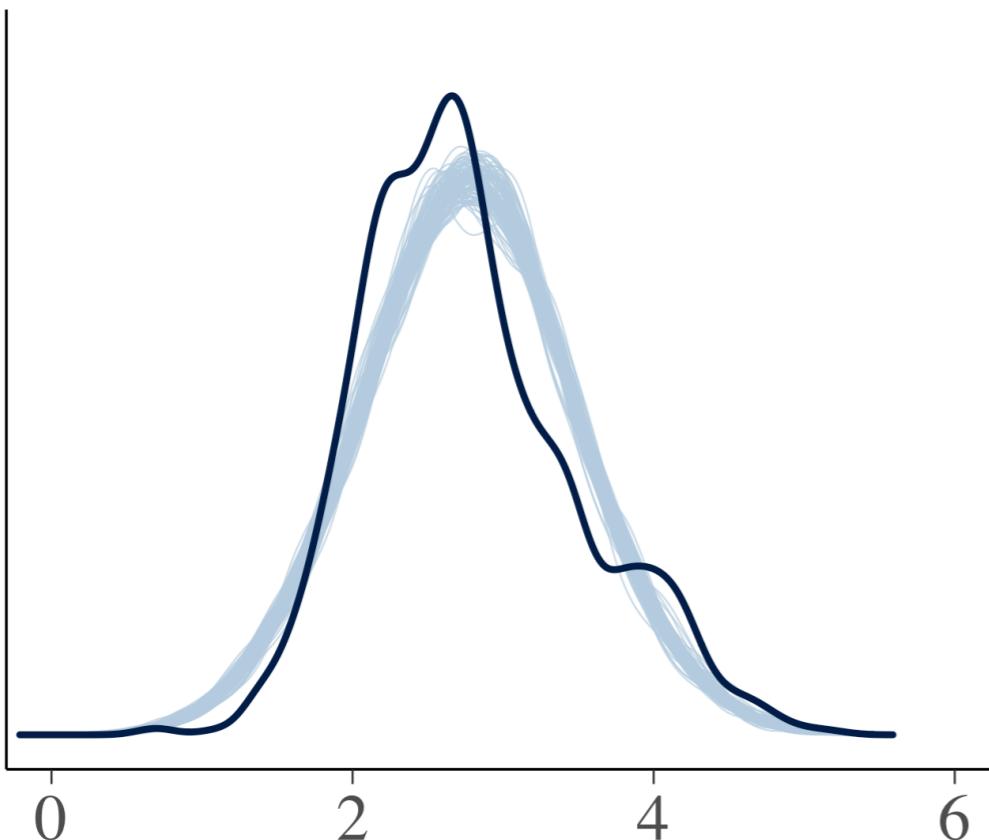
- Used to understand the fit of the model
- Procedure:
 1. Sample from your posterior
 2. Use observed x
 3. Calculate the predicted y for that x and that particular random draw from the posterior
 4. Repeat 2 & 3 many times
 5. Compute summaries / visualize

Posterior predictive checking

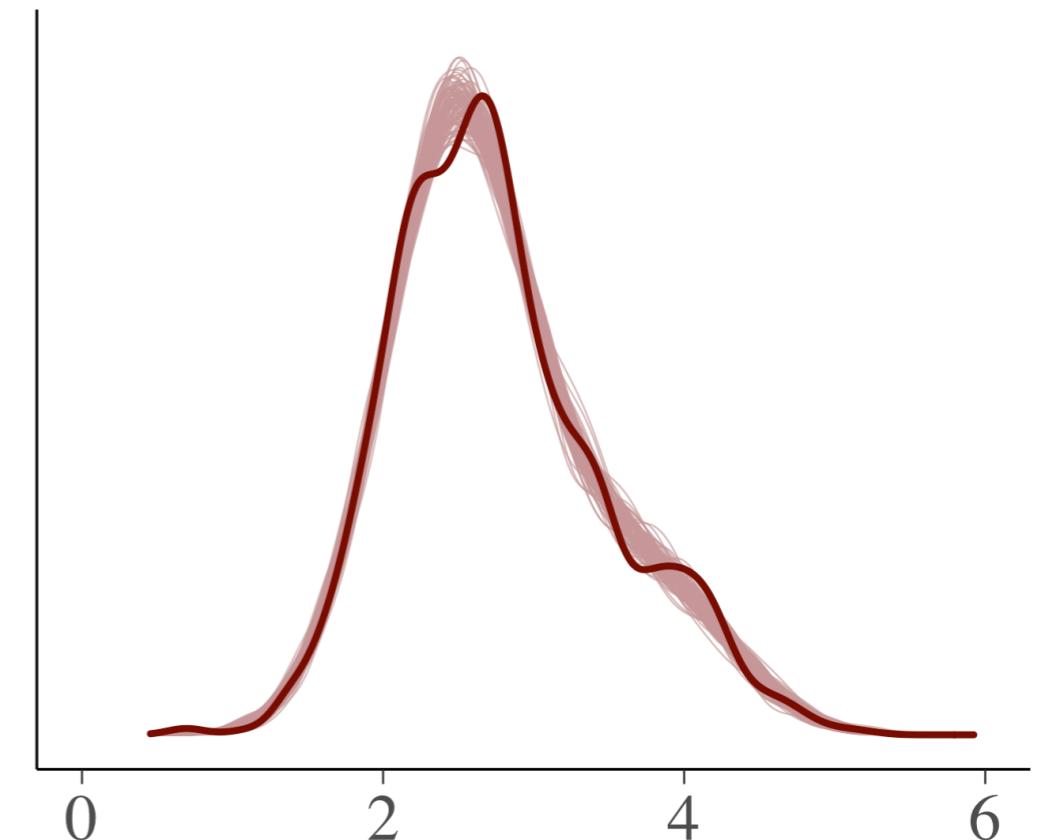
visual model evaluation

Observed data vs posterior predictive simulations

Model 1 (single level)



Model 3 (multilevel)

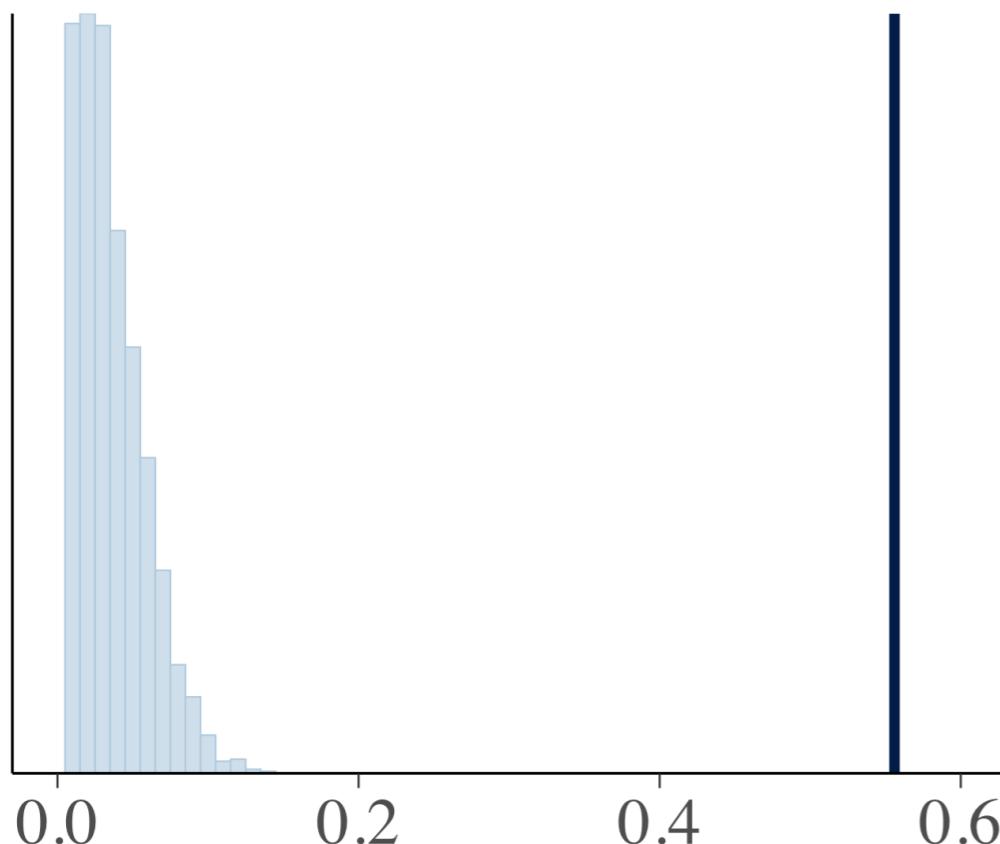


Posterior predictive checking

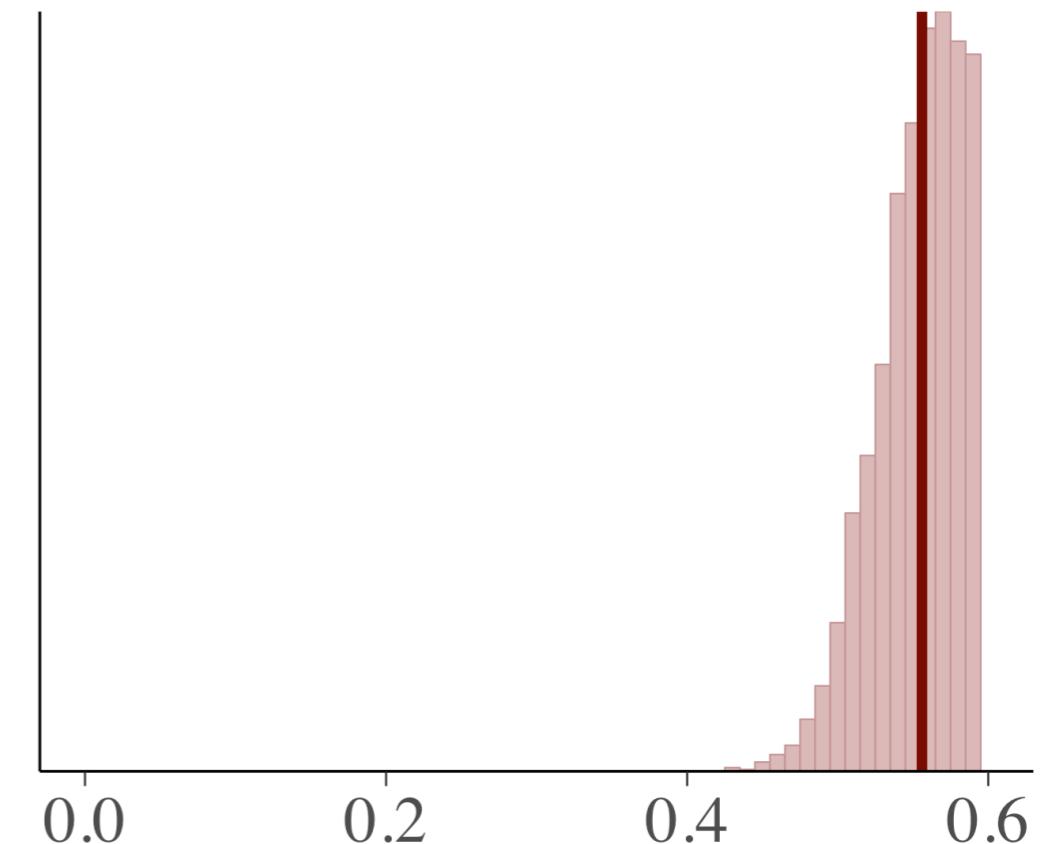
visual model evaluation

Observed statistics vs posterior predictive statistics

Model 1 (single level)

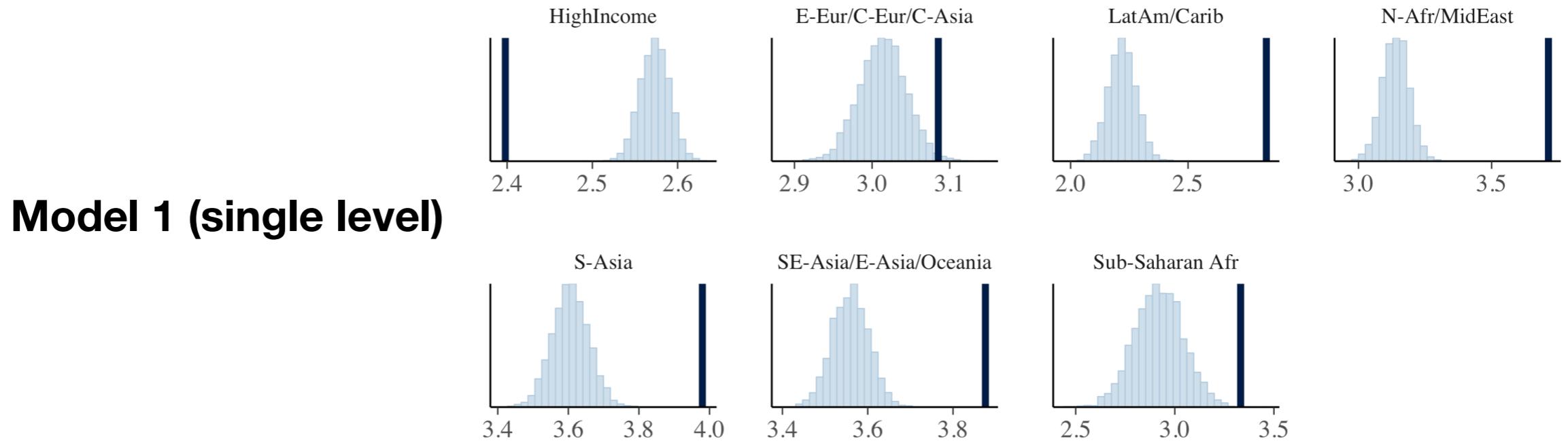


Model 3 (multilevel)

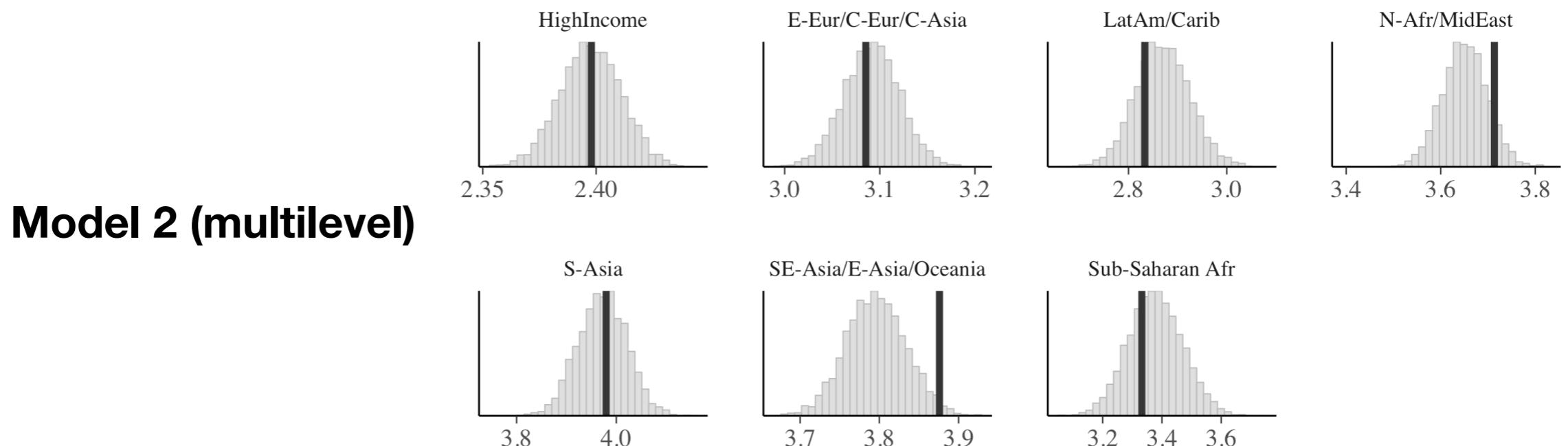


$$T(y) = \text{skew}(y)$$

Posterior predictive checking: visual model evaluation



$$T(y) = \text{med}(y|\text{region})$$



Model comparison

Pointwise predictive comparisons & LOO-CV

Model comparison

pointwise predictive comparisons & LOO-CV

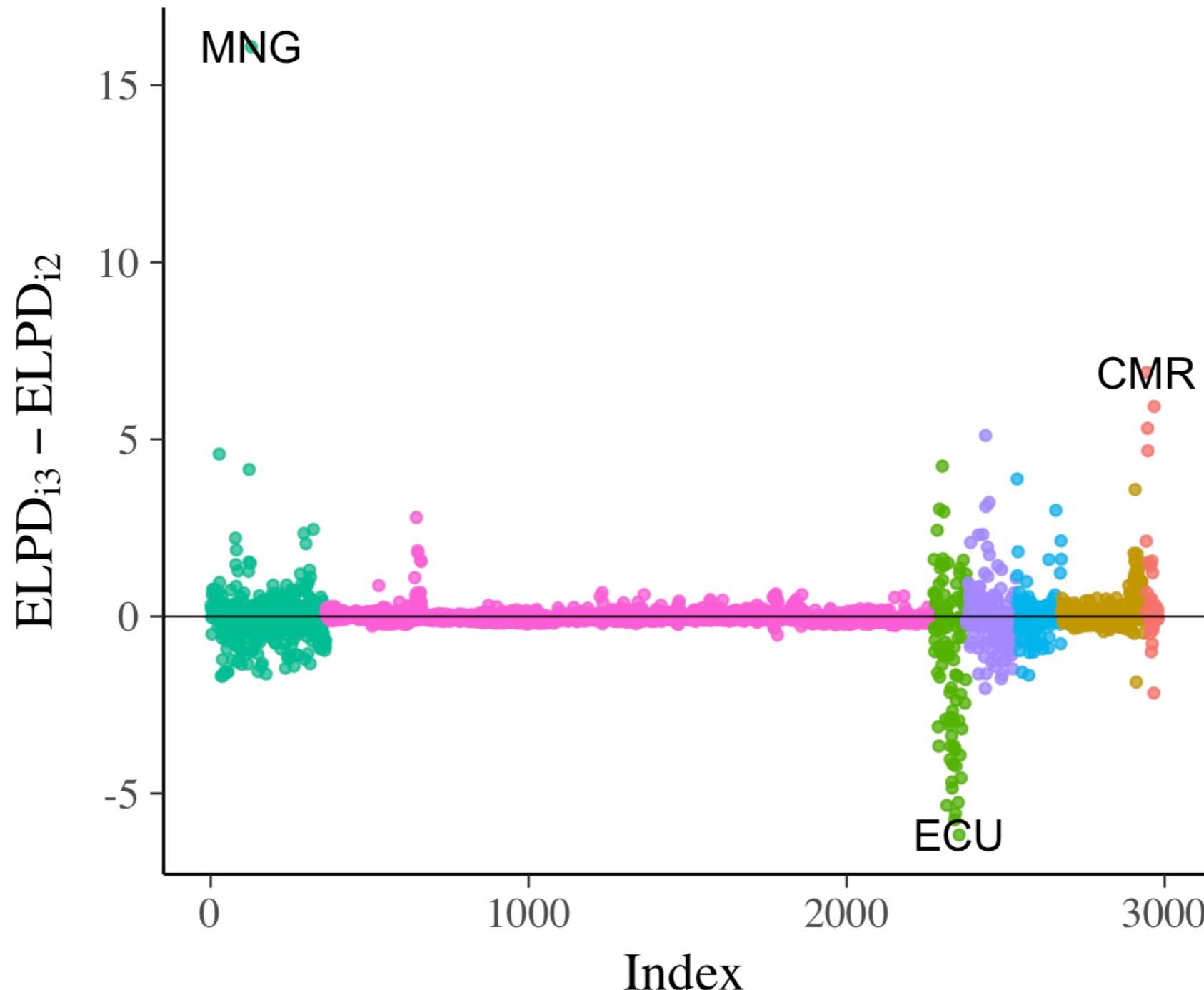
- Visual PPCs can also identify unusual/influential (outliers, high leverage) data points
- We like using cross-validated leave-one-out predictive distributions

$$p(y_i | y_{-i})$$

- Which model best predicts each of the data points that is left out?

Model comparison

pointwise predictive comparisons & LOO-CV



Model comparison

Efficient approximate LOO-CV

- How do we compute LOO-CV without fitting the model N times?
- Fit once, then use Pareto smoothed importance sampling (PSIS-LOO)
- Has finite variance property of truncated IS
- And less bias (replace largest weights with order stats of generalized Pareto)
- Assumes posterior not highly sensitive to leaving out single observations
- Asymptotically equivalent to WAIC
- Advantage: PSIS-LOO CV more robust + has diagnostics (check assumptions)

Vehtari, A., Gelman, A., and Gabry, J. (2017).

Practical Bayesian model evaluation using leave-one-out cross-validation and WAIC.

Statistics and Computing. 27(5), 1413–1432.

doi: [10.1007/s11222-016-9696-4](https://doi.org/10.1007/s11222-016-9696-4)

Diagnostics

Shape parameter of generalized Pareto distribution & influential observations

