Hidden Markov Models

Learn Bayes Methods Week
at the Karolinska Institutet

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Overview

- **First part:**

  - medical examples
  - finite mixture models
  - Markov chains
  - hidden Markov models (HMMs)
  - **simulating data in R**
  - *break*

- **Second part:**

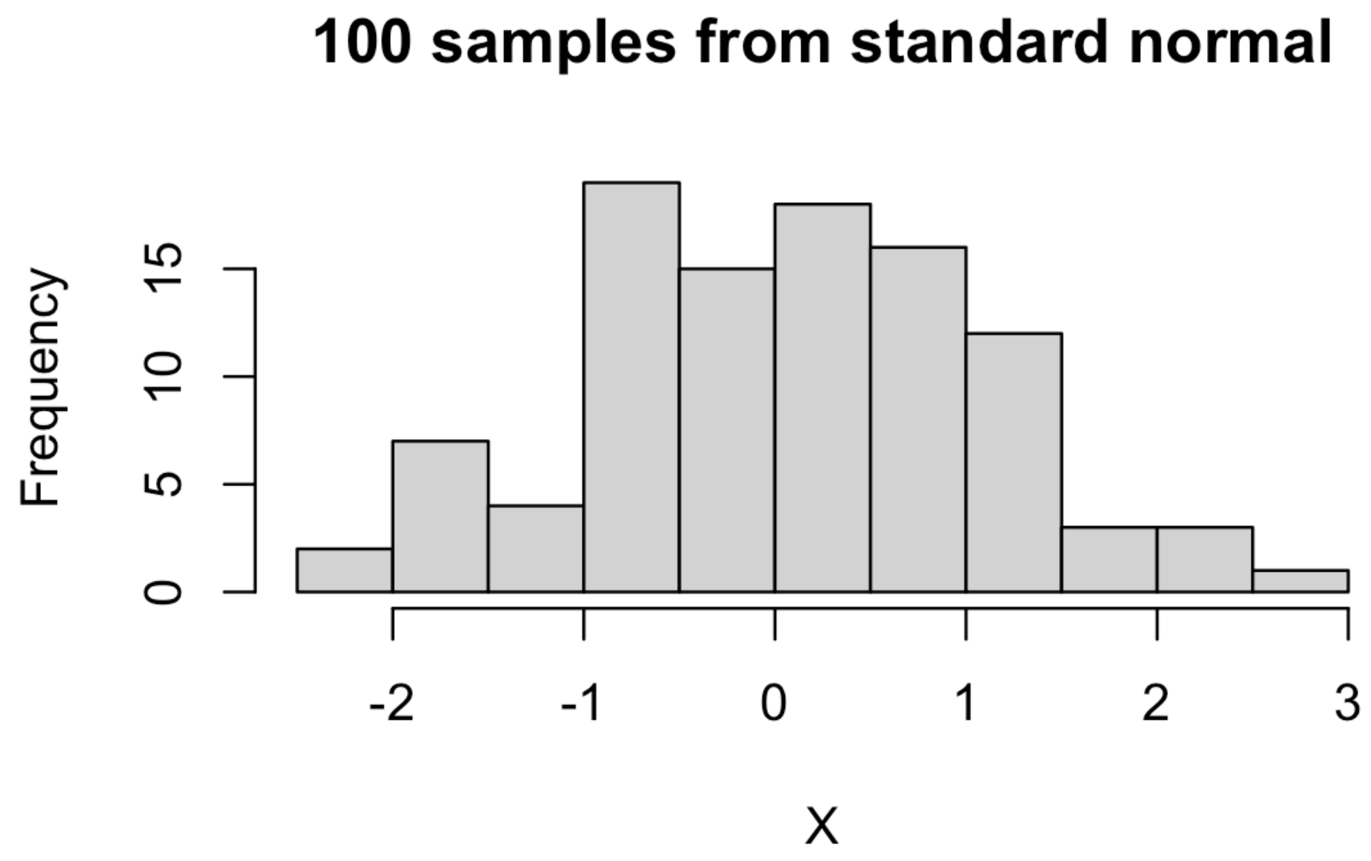
  - forward algorithm & likelihood evaluation
  - Bayesian inference
  - state decoding
  - **fitting HMMs in Stan**
  - *break*

- **Third part (discussion):**

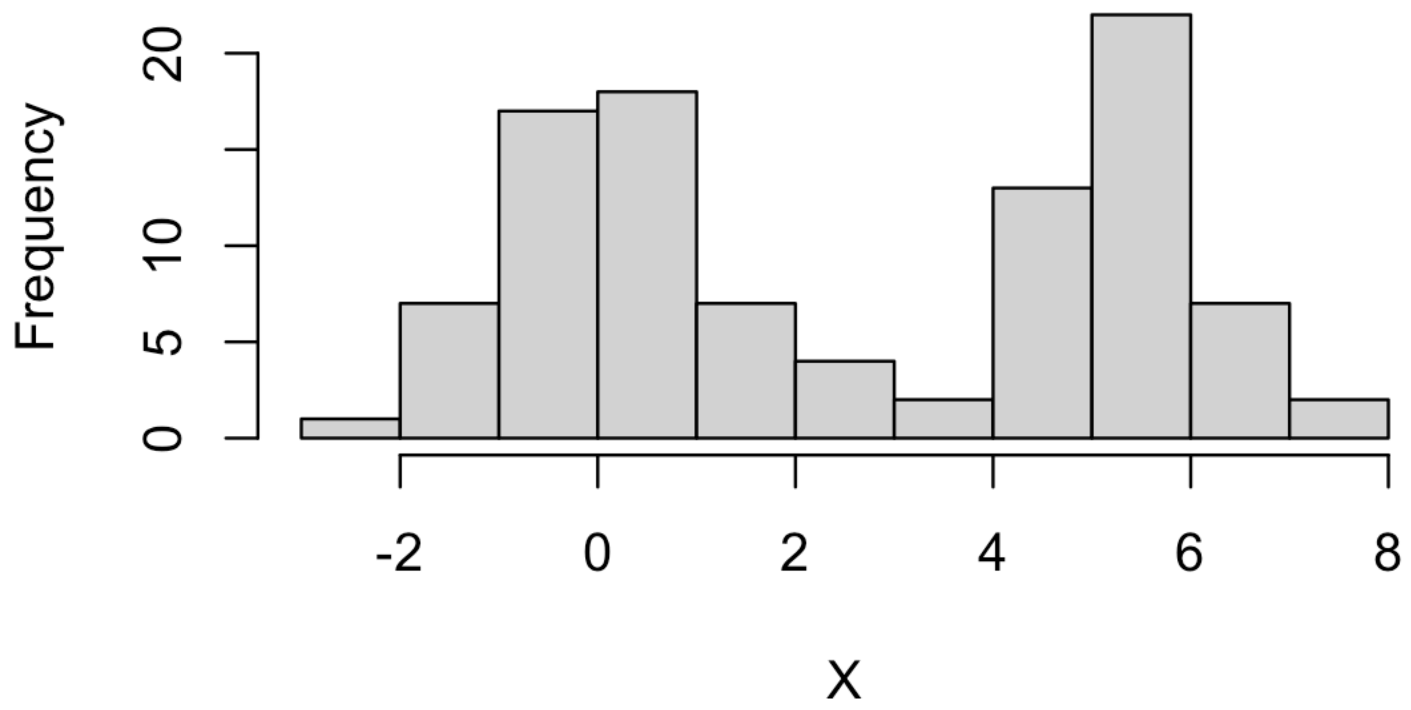
  - missing values
  - covariates
  - mixed HMMs and random effects
  - multivariate observations
  - continuous-time HMMs + other extensions

Finite Mixture Models

- Let's start with something simple, $Y \sim N(0,1)$. A histogram of a 100 samples of Y might look like:



- But what happens when our data look like:



Finite Mixture Models

- Finite mixture models (or independent mixture models) consist of a finite number of component distributions and a mechanism that ‘mixes’ them

- A finite mixture model with K components is given by:

$$f(Y) = \sum_{k=1}^{K} \pi_k f_k(Y)$$

- where $f_k(Y)$ corresponds to the k^{th} component distribution and π_k to the probability that the component is ‘active’

- $\pi_k \in (0,1)$ and $\sum_{k=1}^{K} \pi_k = 1$

- Model is fully characterized by the parameters of each of the component distributions $\left(\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_K\right)$ and $\left(\pi_1, \ldots, \pi_K\right)$

Finite Mixture Models

Likelihood evaluation + Clustering

- Given a sample of N observations, the **likelihood function** is given by:

$$\mathscr{L}(\boldsymbol{\theta}, \boldsymbol{\pi}) = \prod_{n=1}^{N} \left\{ \sum_{k=1}^{K} \pi_k f_k(y_n) \right\}$$

- **Label-switching** — a re-ordering of the labels leads to the same likelihood function/ model.

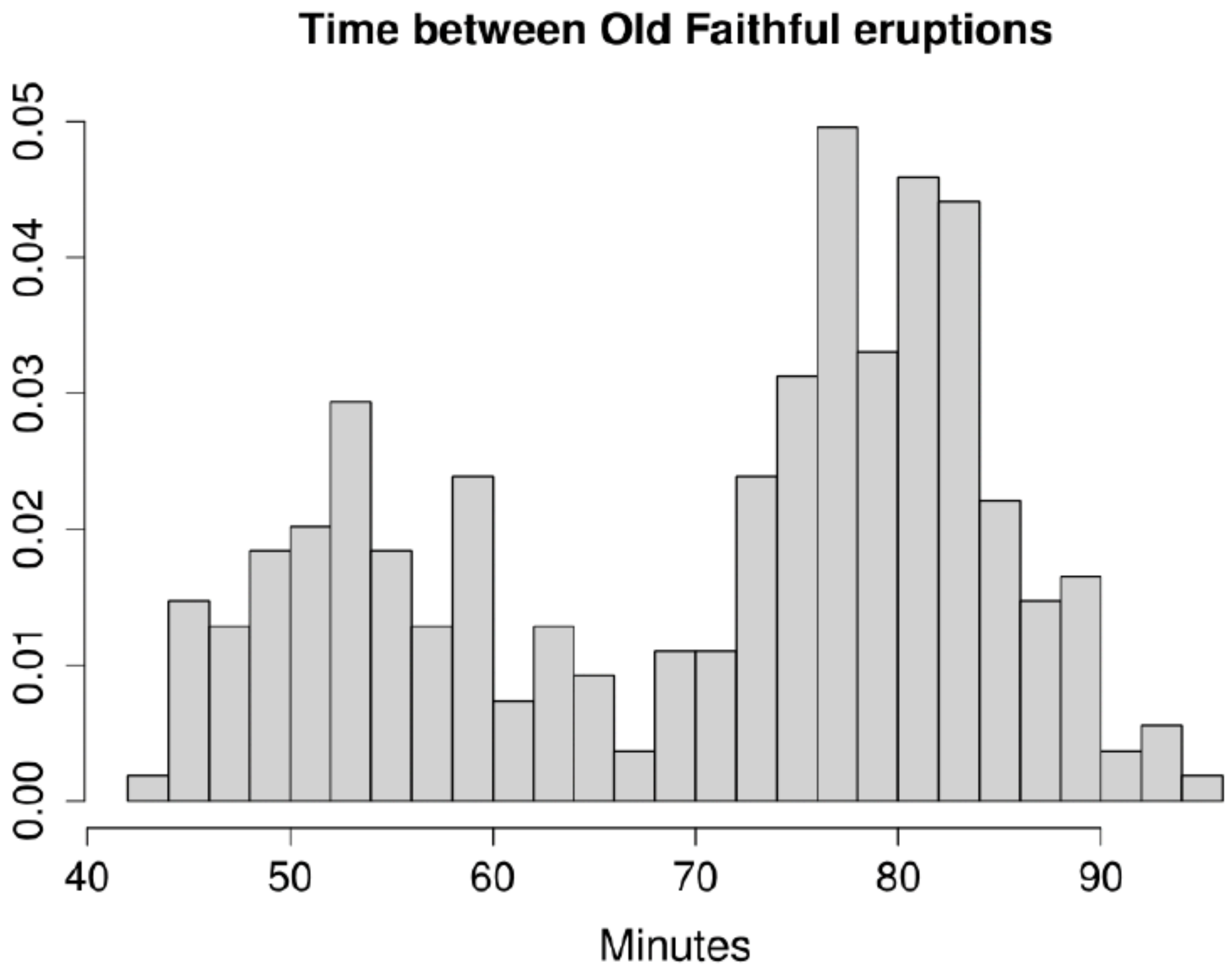
- **Clustering using Bayes' rule** — we can compute the probability that an observation was generated according to one of K possibilities by introducing random variables $\{Z_n\}_{n=1}^{N}$

$$Pr(Z_n = k \mid Y_n) = \frac{\pi_k f_k(Y_n)}{\sum_{k=1}^{K} \pi_k f_k(Y_n)}$$

Example: Time between Old Faithful eruptions

- Waiting times between eruptions for the Old Faithful geyser in Yellowstone National Park, Wyoming, USA

- The observations seem to exhibit two patterns, arising from one of two possible distributions

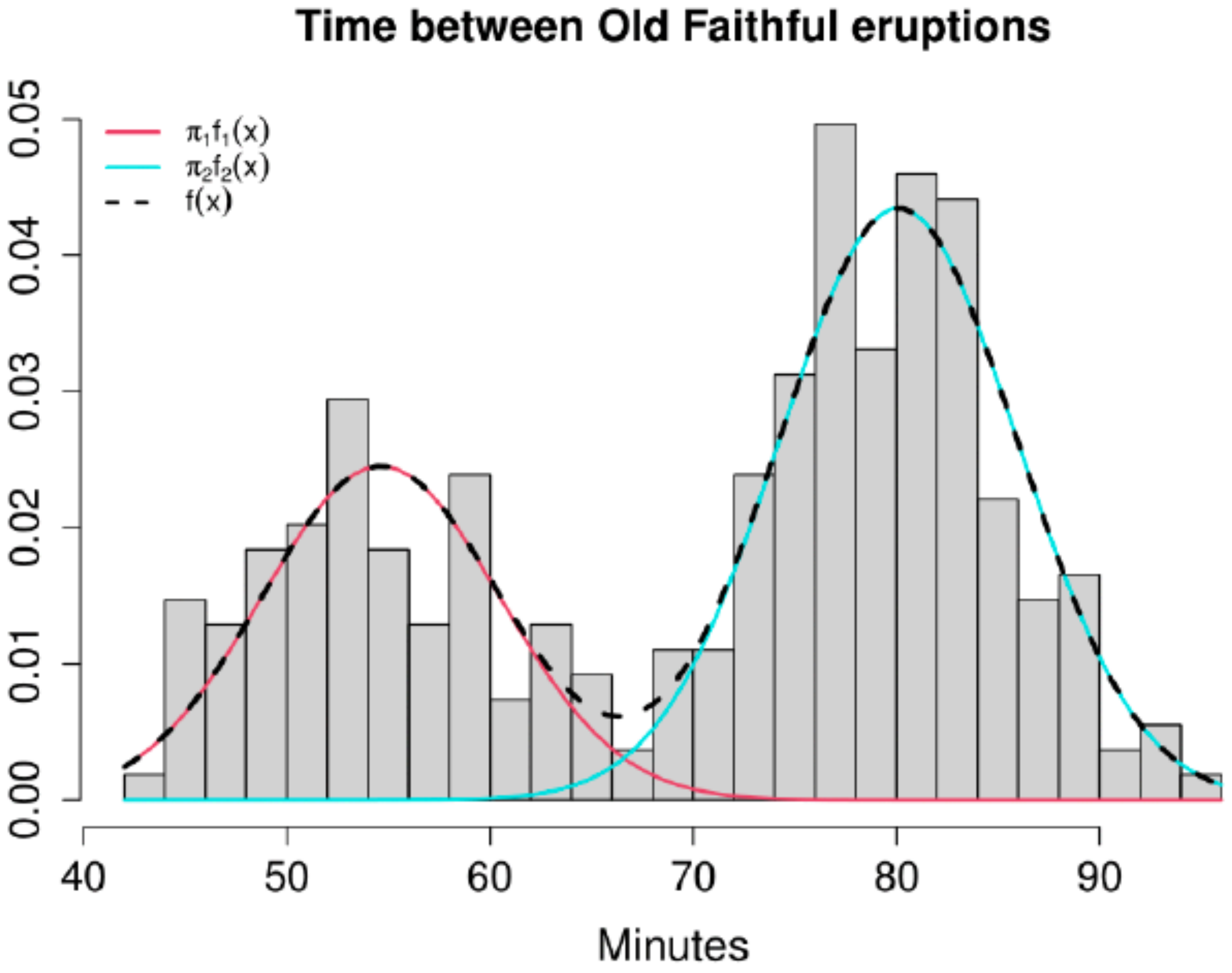


Back to Old Faithful

Point estimates

- Estimating a Gaussian mixture model for the old faithful data with 2 components:

  - $f_1(Y)$ was estimated to be $\mathcal{N}(54.6, 5.9^2)$
  - $f_2(Y)$ was estimated to be $\mathcal{N}(80.1, 5.9^2)$
  - π_1 was estimated to be 0.36
  - π_2 was estimated to be 0.64



Serial dependence

- Data collected over time or in sequence commonly show dependence between consecutive time steps
- **Dependent mixtures** better accommodate system dynamics arising from serial correlation
- In many cases it is reasonable to assume that the component distribution active at time t will more likely remain active at time $t + 1$
- **Markov chains** are a natural selection to model such dependence

Markov Chains

- A **discrete-time Markov chain** is a stochastic process $\{Z_t \in \{1,\ldots,K\}; t = 1,2,\ldots\}$ that satisfies the Markov property $Pr\left(Z_t \mid Z_t, Z_{t-1}, \ldots, Z_1\right) = Pr\left(Z_t \mid Z_{t-1}\right)$

- It is fully characterized by:

  - K, the number of components (which we'll denote as states from now on)

  - $\boldsymbol{\delta}$, the **initial state distribution**, with entries $Pr(Z_1 = k) = \delta_k$

  - the evolution of the states over time are governed by a transition probability matrix, $\boldsymbol{\Gamma}$, with entries $\gamma_{i,j}^{(t)} = Pr(Z_t = j \mid Z_{t-1} = i)$ for $i, j \in \{1,\ldots,K\}$

Markov Chains

- $\gamma_{i,j}^{(t)}$ is the probability that the chain enters state j at time $t+1$ given that it is in state i at time t

- The chain is called homogeneous when $\gamma_{i,j}^{(t)} = \gamma_{i,j}$ for all $t \in \{1,\ldots,T\}$

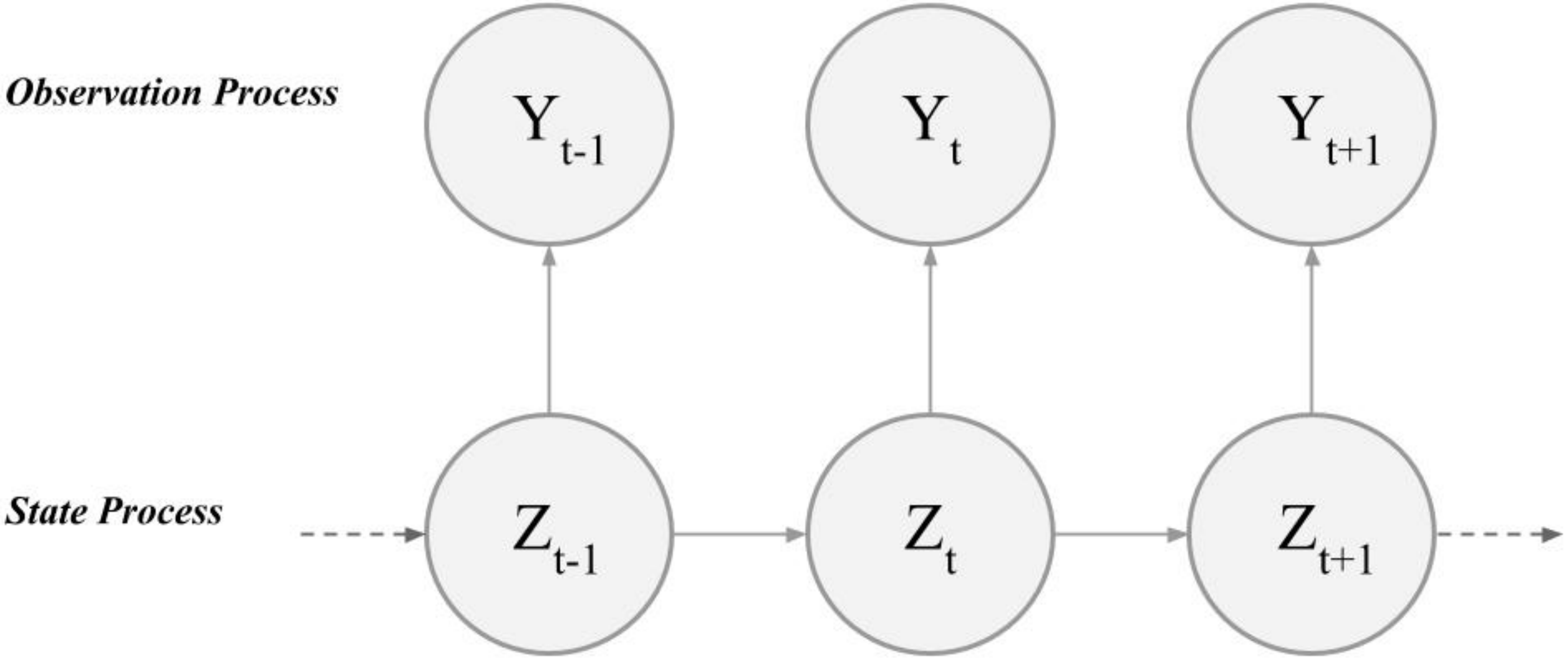
- $\mathbf{\Gamma}$ is the transition probability matrix, given by

$$\begin{pmatrix} \gamma_{1,1} & \cdots & \gamma_{1,K} \\ \vdots & \ddots & \vdots \\ \gamma_{K,1} & \cdots & \gamma_{K,K} \end{pmatrix}$$

with $\gamma_{i,j} \in [0,1]$ for all $i,j \in \{1,\ldots,K\}$ and $\sum_{j=1}^{K} \gamma_{i,j} = 1$

Hidden Markov models

Combining finite mixture models + dependence via a Markov chain



Some hidden Markov model basics

(discrete-time finite-state)

- A hidden Markov model (HMM) is a doubly stochastic process composed of an **observation process** $\{Y_t\}_{t=1}^{T}$ and a **state process** $\{Z_t\}_{t=1}^{T}$

- A basic HMM assumes **conditional independence** of the observation process given the states, $Y_k \perp Y_h | \boldsymbol{Z}$ for $k \neq h$ and $k, h \in \{1,\ldots,T\}$

Some hidden Markov model basics

(discrete-time finite-state)

- The state process is assumed to be a **first-order Markov chain** evolving in discrete-time with transition probability matrix $\mathbf{\Gamma}$, $\Gamma_{ij} = \Pr(Z_t = j \mid Z_{t-1} = i)$, and initial state distribution $\boldsymbol{\delta}$, $\delta_i = \Pr(Z_1 = i)$

- The observations are generated according to a set of **state-dependent distributions**, $f(Y_t \mid Z_t = i)$, where $i \in \{1, \ldots, N\}$ and where $N \in \mathbb{N}$ is the # of states

Simulating from a 3-State HMM

- Parameter values

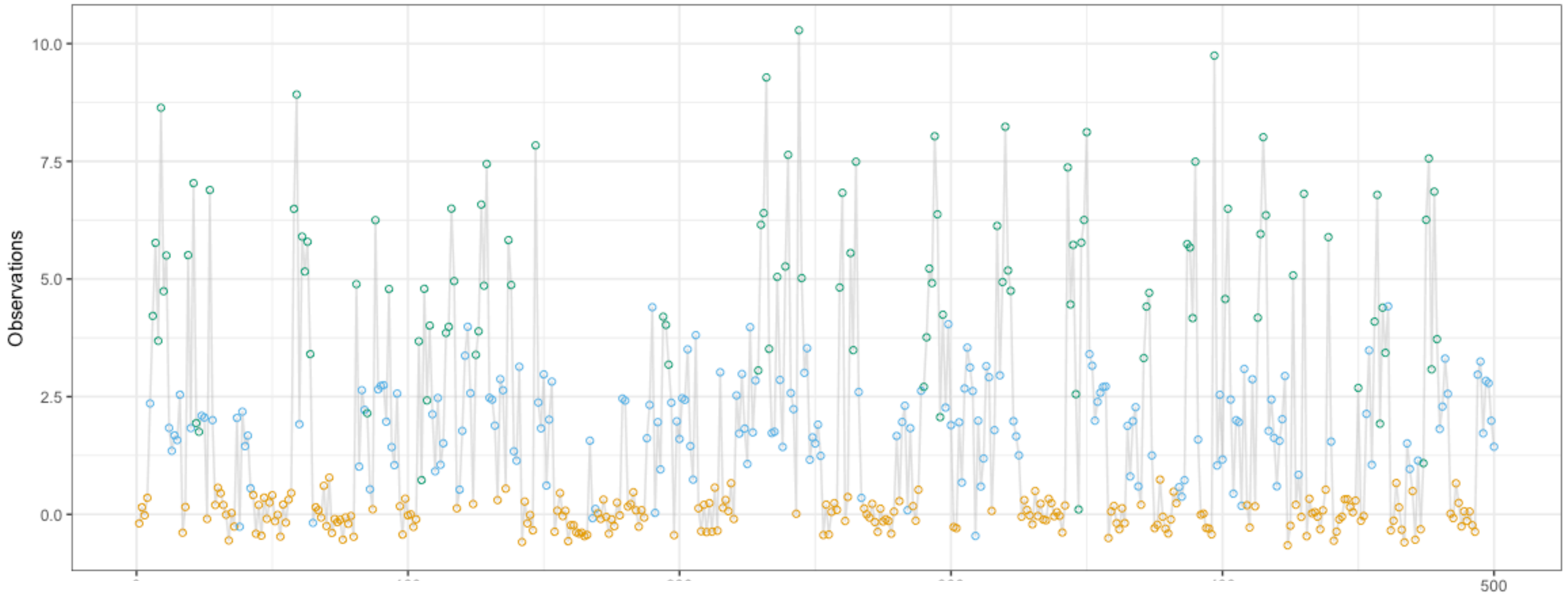
$N = 3$

$f_n(Y_t) \sim N(\mu_n, \sigma_n)$ **for** $n \in \{1,2,3\}$

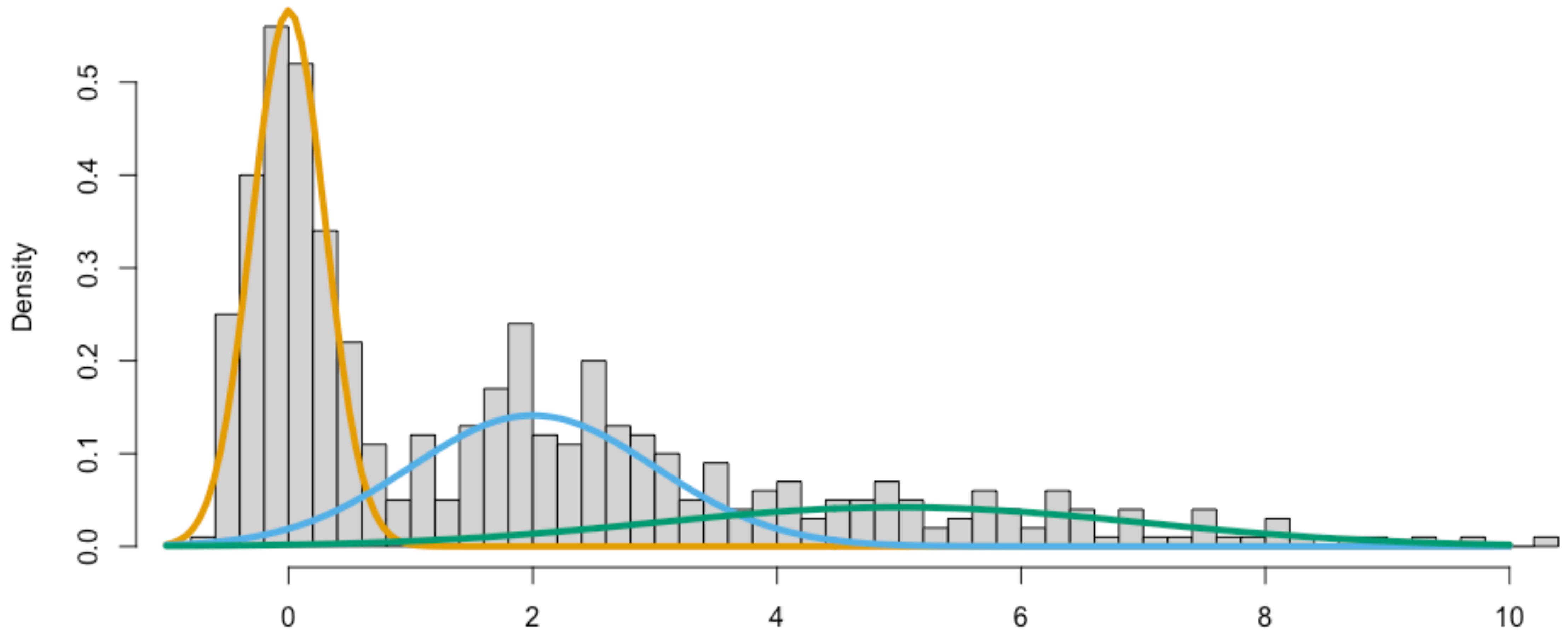
$\mu \in \{0,2,5\} \quad \sigma \in \{0.3,1,2\}$

$\boldsymbol{\delta} = [1/3, 1/3, 1/3]$

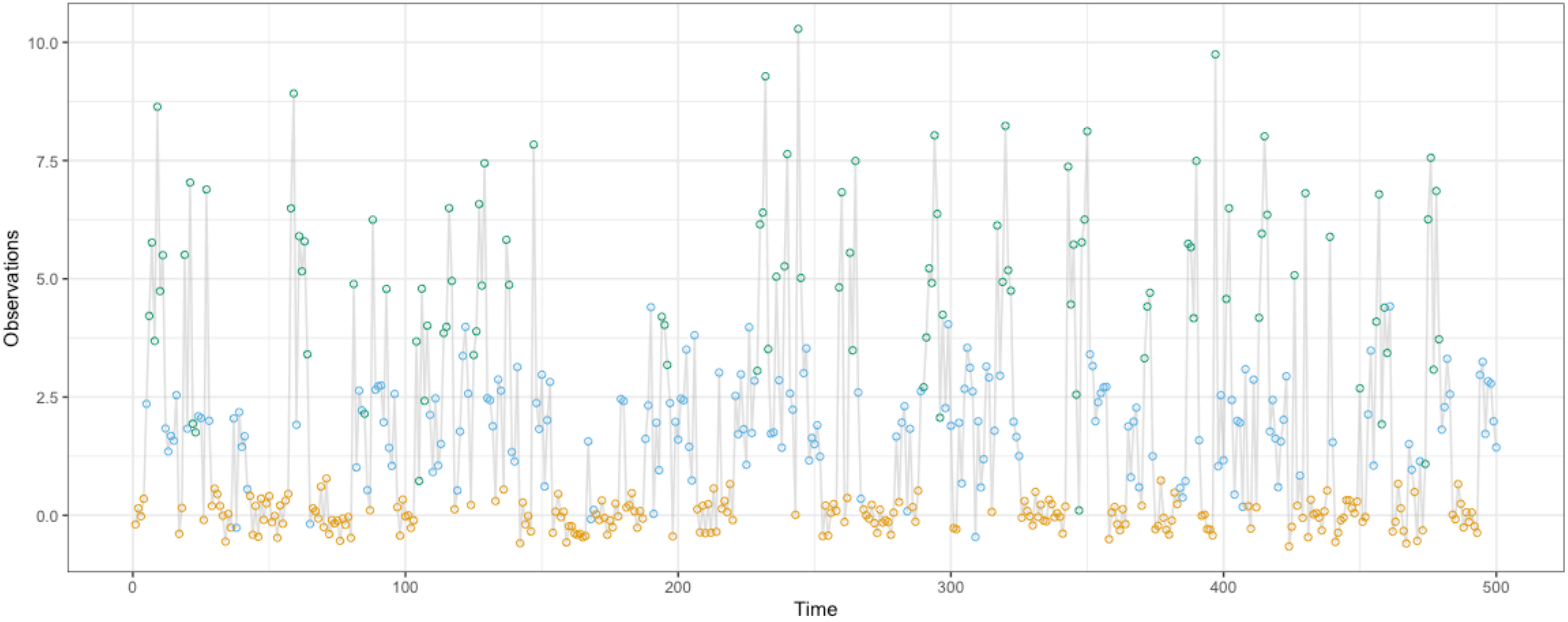
$$\boldsymbol{\Gamma} = \begin{pmatrix} 0.8 & 0.1 & 0.1 \\ 0.2 & 0.7 & 0.1 \\ 0.05 & 0.3 & 0.65 \end{pmatrix}$$



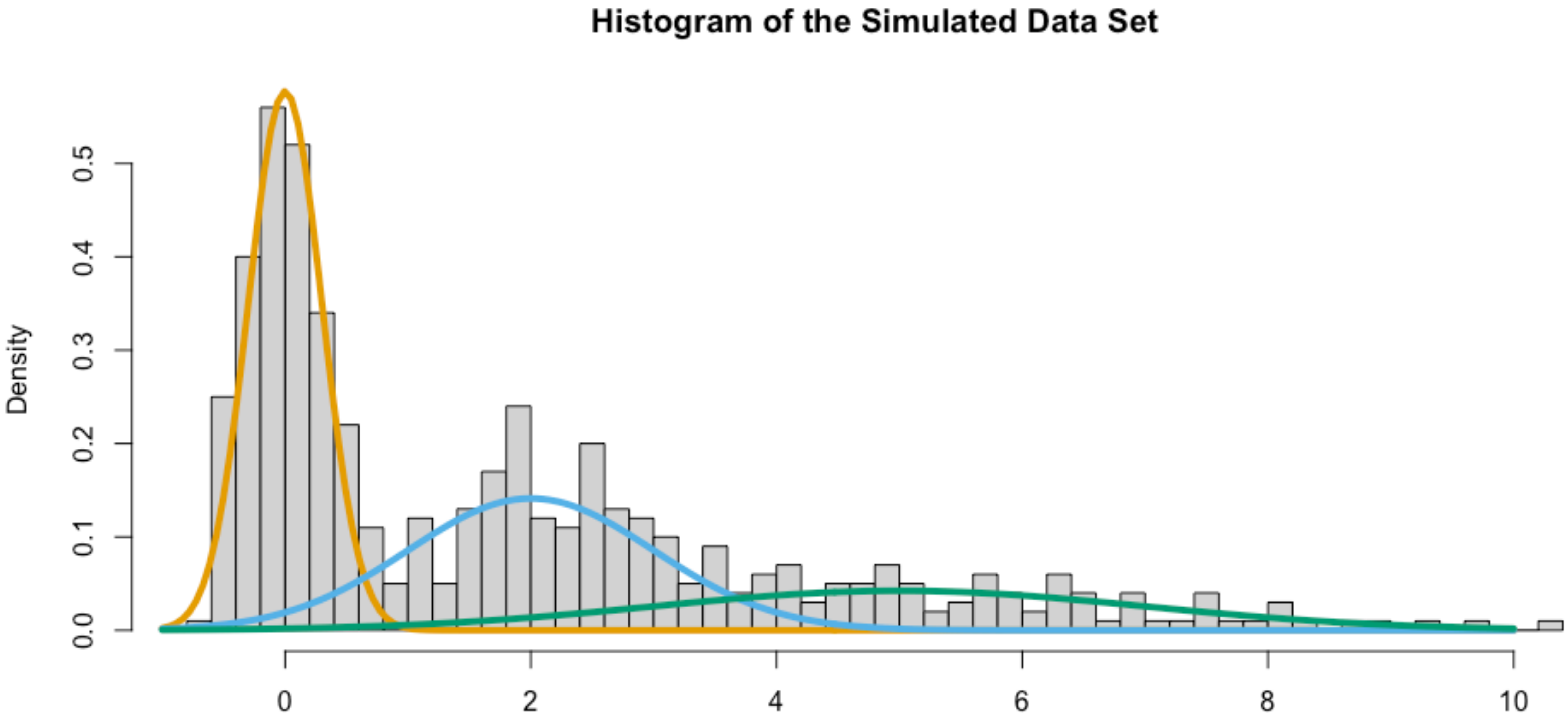
Histogram of the Simulated Data Set



Simulated data: first 500 of 2000 observations



Simulated Data: Marginal Distribution



Simulate Data from an HMM

HMM likelihoods

(Only one can be used in Stan)

- There are generally two likelihood functions used for inference in HMMs:

complete-data likelihood – $\mathscr{L}(\boldsymbol{\theta}, \boldsymbol{Z} \,|\, \boldsymbol{Y})$

likelihood – $\mathscr{L}(\boldsymbol{\theta} \,|\, \boldsymbol{Y}) = \sum_{n=1}^{N} \cdots \sum_{n=1}^{N} f(\boldsymbol{Y}, Z_1 = n, Z_2 = n, \cdots, Z_T = n \,|\, \boldsymbol{\theta})$

- The likelihood can be concisely expressed in matrix form. Let $\boldsymbol{P}(Y_t)$ = diag $\{f(Y_t \,|\, Z_t = 1), \ldots, f(Y_t \,|\, Z_t = N)\}$ and $\mathbf{1}$ be a column vector of 1's of length N, then

$$\mathscr{L}(\boldsymbol{\theta} \,|\, \boldsymbol{Y}) = \boldsymbol{\delta}^T \boldsymbol{P}(Y_1) \boldsymbol{\Gamma} \boldsymbol{P}(Y_2) \cdots \boldsymbol{\Gamma} \boldsymbol{P}(Y_T) \mathbf{1}$$

with evaluation done via the ***forward algorithm.***

Forward algorithm

- The forward algorithm is an approach to efficiently computing the likelihood of an HMM.

- We can construct 'forward variables' $\{\boldsymbol{\alpha}_t\}_{t=1}^T$ where

$$\boldsymbol{\alpha}_1 = \boldsymbol{\delta}^\top \boldsymbol{P}(Y_1) \text{ and } \boldsymbol{\alpha}_t = \boldsymbol{\alpha}_{t-1}\boldsymbol{\Gamma}\boldsymbol{P}(y_t)$$

such that $\displaystyle\sum_{k=1}^{K} \alpha_{T,k} = \mathscr{L}(\boldsymbol{\theta} \mid \boldsymbol{Y})$

- In this way, the likelihood function can be evaluated with $O(TK^2)$ operations

General HMM Application Categories

- **Unsupervised** - $\mathscr{L}(\boldsymbol{\theta} \,|\, \boldsymbol{Y})$ - no states are known/observed

→ most common in ecological applications

- **Semi-supervised** - $\mathscr{L}(\boldsymbol{\theta} \,|\, \boldsymbol{Y}, \boldsymbol{Z}_j = z_j)$ - some states are known/observed

- **Supervised** - $\mathscr{L}(\boldsymbol{\theta} \,|\, \boldsymbol{Y}, \boldsymbol{Z})$ - all states are known/observed

- In all cases, simple modifications to the likelihood function evaluation and forward algorithm can be made to adapt for different applications.

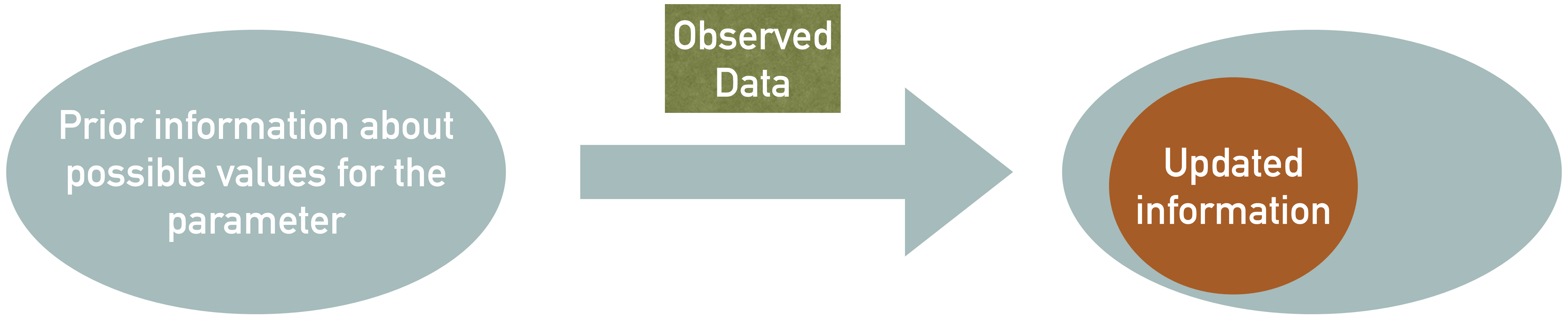
Scientific insights gained from using HMMs

- Can connect the observations to different patterns via state decoding
- We have distributions for the different patterns of interest
- Model state-switching behaviour + amount of time spent in a state before switching
- In a loose sense, we can estimate the ‘number of patterns seen’
- We can incorporate covariates to understand drivers of patterns (we’ll talk about this soon)

Bayesian inference for HMMs

- Set priors for HMMs:

  state-dependent distributions + rows of transition probability matrix



Prior information about possible values for the parameter

Observed Data

Updated information

$$\Pr(\beta) \qquad \Pr(y \mid \beta) \qquad \Pr(\beta \mid y) = \frac{\Pr(y, \beta)}{\Pr(y)}$$

Prior

Likelihood

Posterior

Calculated using ‘forward algorithm’

State Decoding

- In HMMs + extensions, assigning an observation to a state is known as state decoding

- Two common approaches:

  local state decoding — $\text{argmax}_{n \in \{1,\ldots,N\}} \Pr(Z_t = n \mid \boldsymbol{Y})$
  forward-backward algorithm

  global state decoding — $\text{argmax}_{\boldsymbol{n} \in \{1,\ldots,N\}^T} \Pr(\boldsymbol{Z} = \boldsymbol{n} \mid \boldsymbol{Y})$
  Viterbi algorithm

- Less common — taking posterior draws from the joint distribution of states via forward-filtering backward-sampling

Let’s fit an HMM to data

3-state HMM with Normal state-dependent distributions

- The choices we make when fitting an HMM in practice:

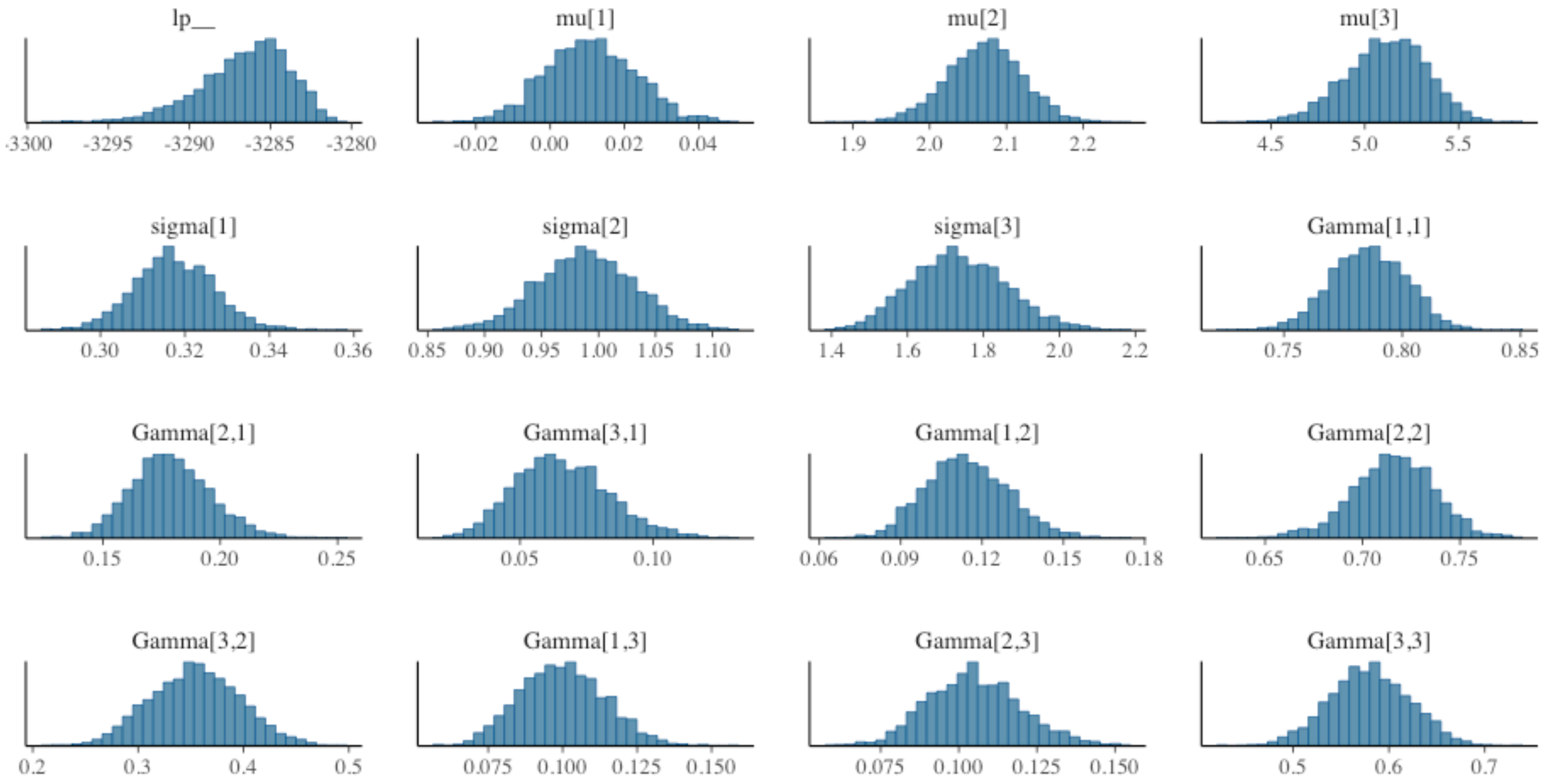
★ the number of states ⚠️

★ the forms of the state-dependent distributions⚠️

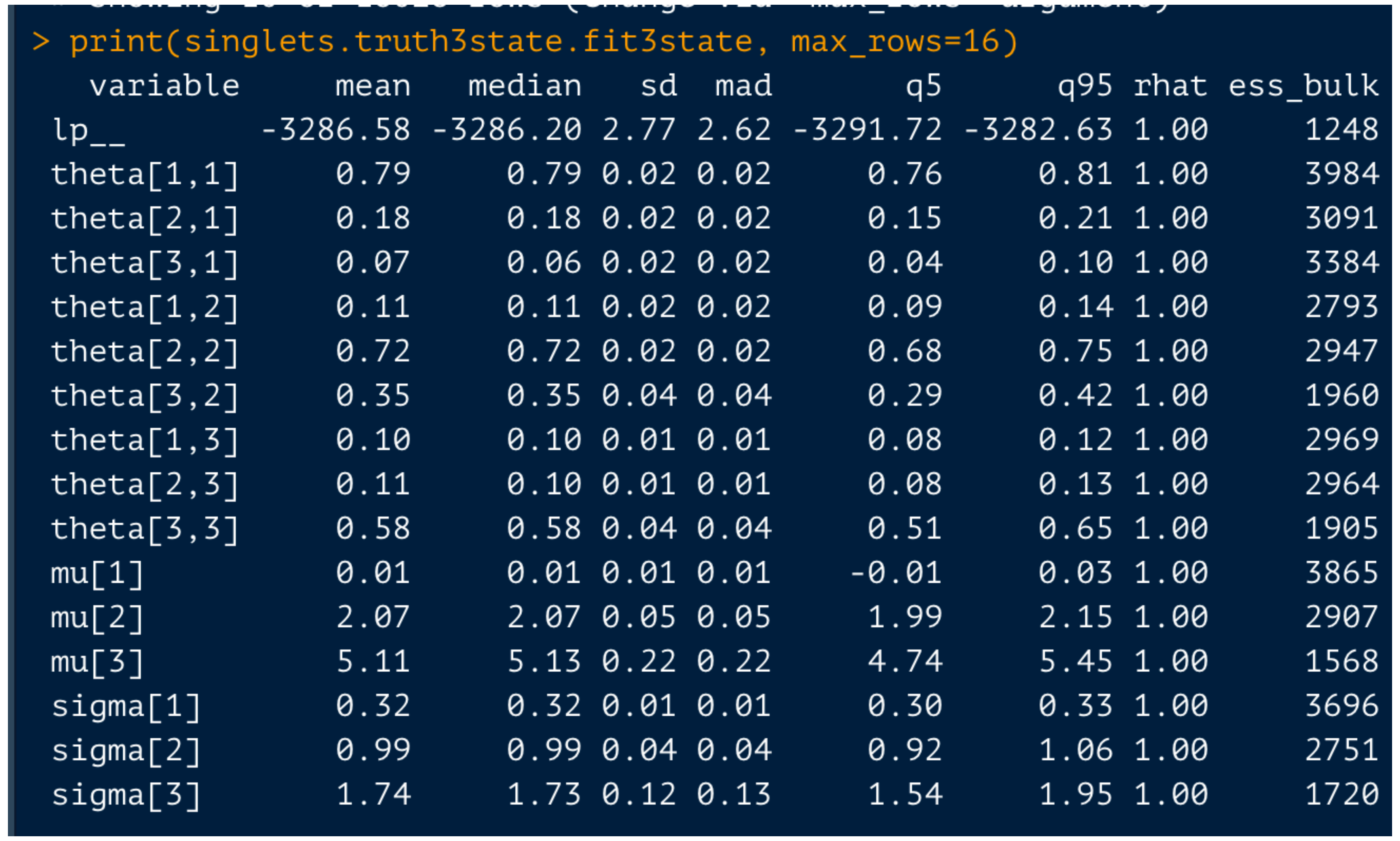
There are other assumptions but for now let’s consider that an HMM is the *true* data generating process.

When all goes well

Sampling 500 observations from true 3-state HMM



Stan output:

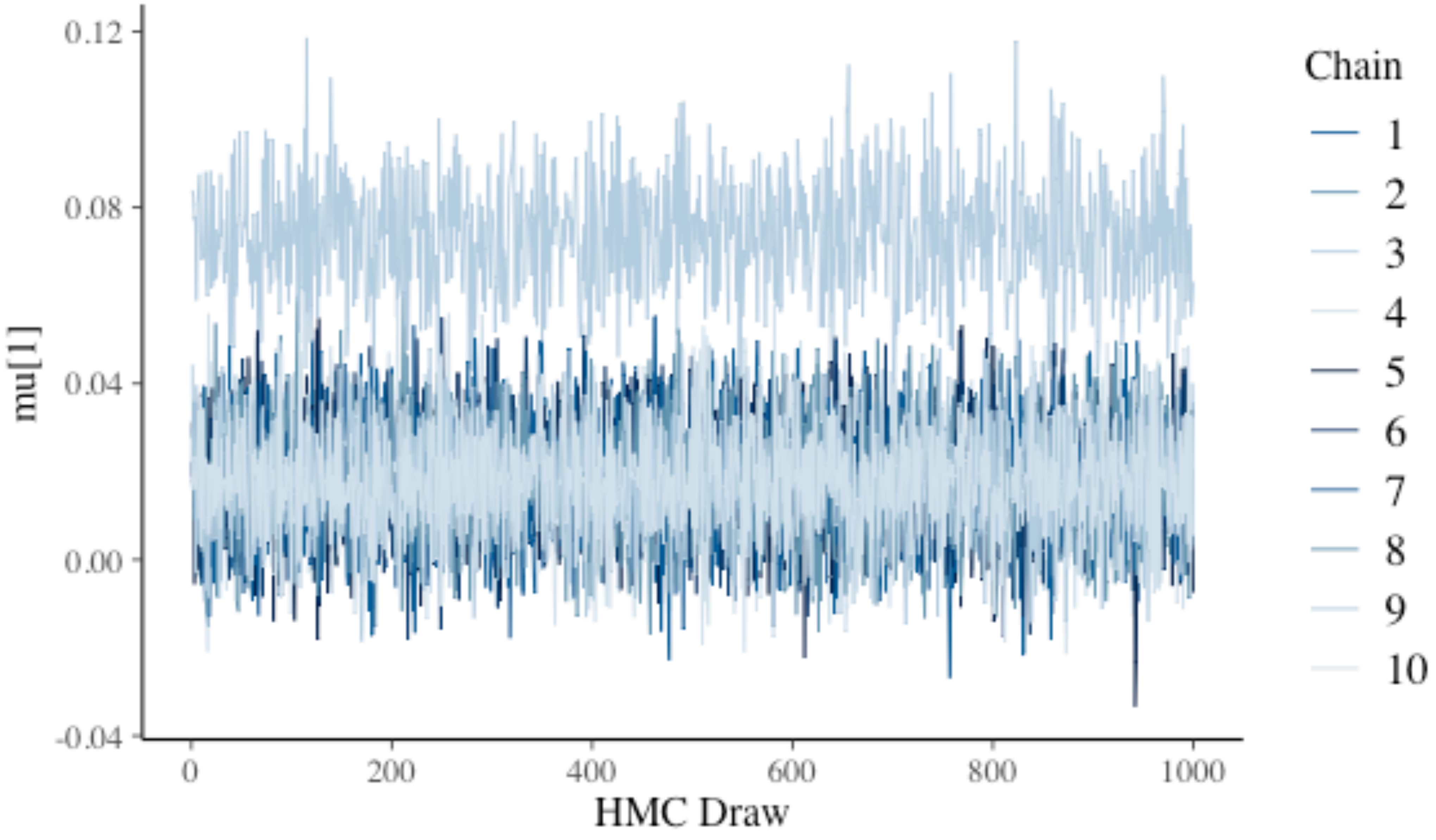


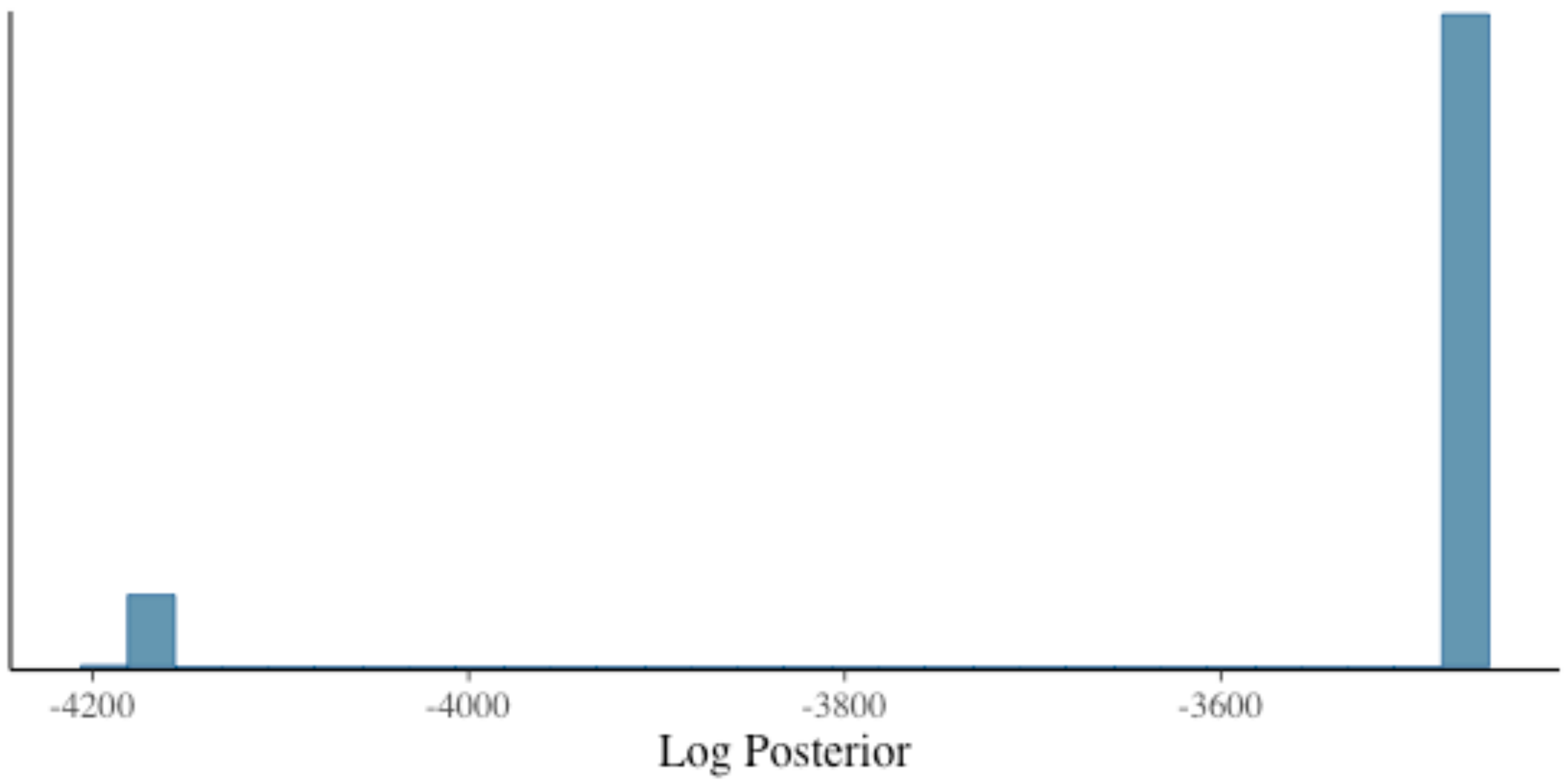
```
> print(singlets.truth3state.fit3state, max_rows=16)
   variable      mean    median   sd  mad       q5      q95 rhat ess_bulk
 lp__        -3286.58 -3286.20 2.77 2.62 -3291.72 -3282.63 1.00     1248
 theta[1,1]      0.79      0.79 0.02 0.02     0.76     0.81 1.00     3984
 theta[2,1]      0.18      0.18 0.02 0.02     0.15     0.21 1.00     3091
 theta[3,1]      0.07      0.06 0.02 0.02     0.04     0.10 1.00     3384
 theta[1,2]      0.11      0.11 0.02 0.02     0.09     0.14 1.00     2793
 theta[2,2]      0.72      0.72 0.02 0.02     0.68     0.75 1.00     2947
 theta[3,2]      0.35      0.35 0.04 0.04     0.29     0.42 1.00     1960
 theta[1,3]      0.10      0.10 0.01 0.01     0.08     0.12 1.00     2969
 theta[2,3]      0.11      0.10 0.01 0.01     0.08     0.13 1.00     2964
 theta[3,3]      0.58      0.58 0.04 0.04     0.51     0.65 1.00     1905
 mu[1]           0.01      0.01 0.01 0.01    -0.01     0.03 1.00     3865
 mu[2]           2.07      2.07 0.05 0.05     1.99     2.15 1.00     2907
 mu[3]           5.11      5.13 0.22 0.22     4.74     5.45 1.00     1568
 sigma[1]        0.32      0.32 0.01 0.01     0.30     0.33 1.00     3696
 sigma[2]        0.99      0.99 0.04 0.04     0.92     1.06 1.00     2751
 sigma[3]        1.74      1.73 0.12 0.13     1.54     1.95 1.00     1720
```

Challenges

People think I’m an expert in HMMs, I say

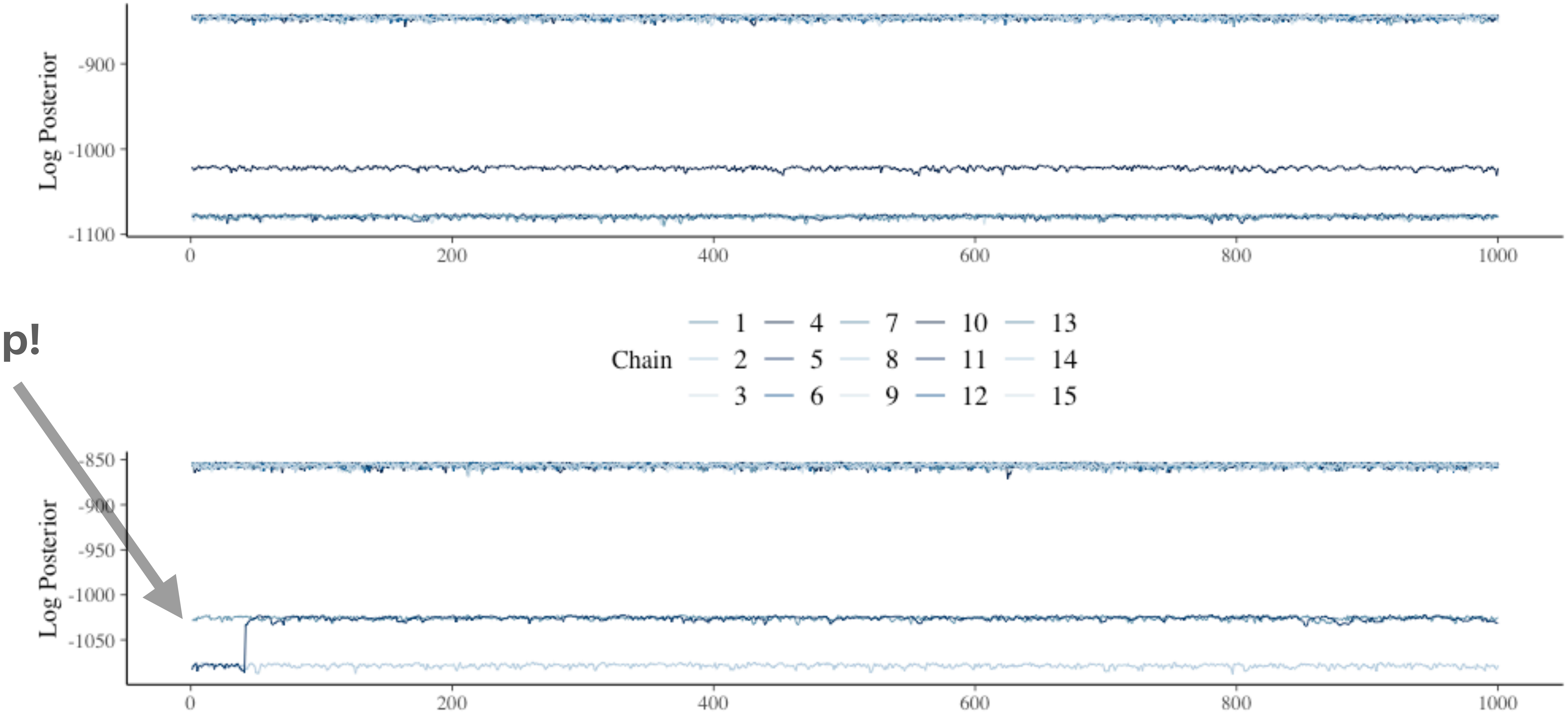
I’m an expert in failing to fit hidden Markov models





Fitting misspecified HMMs

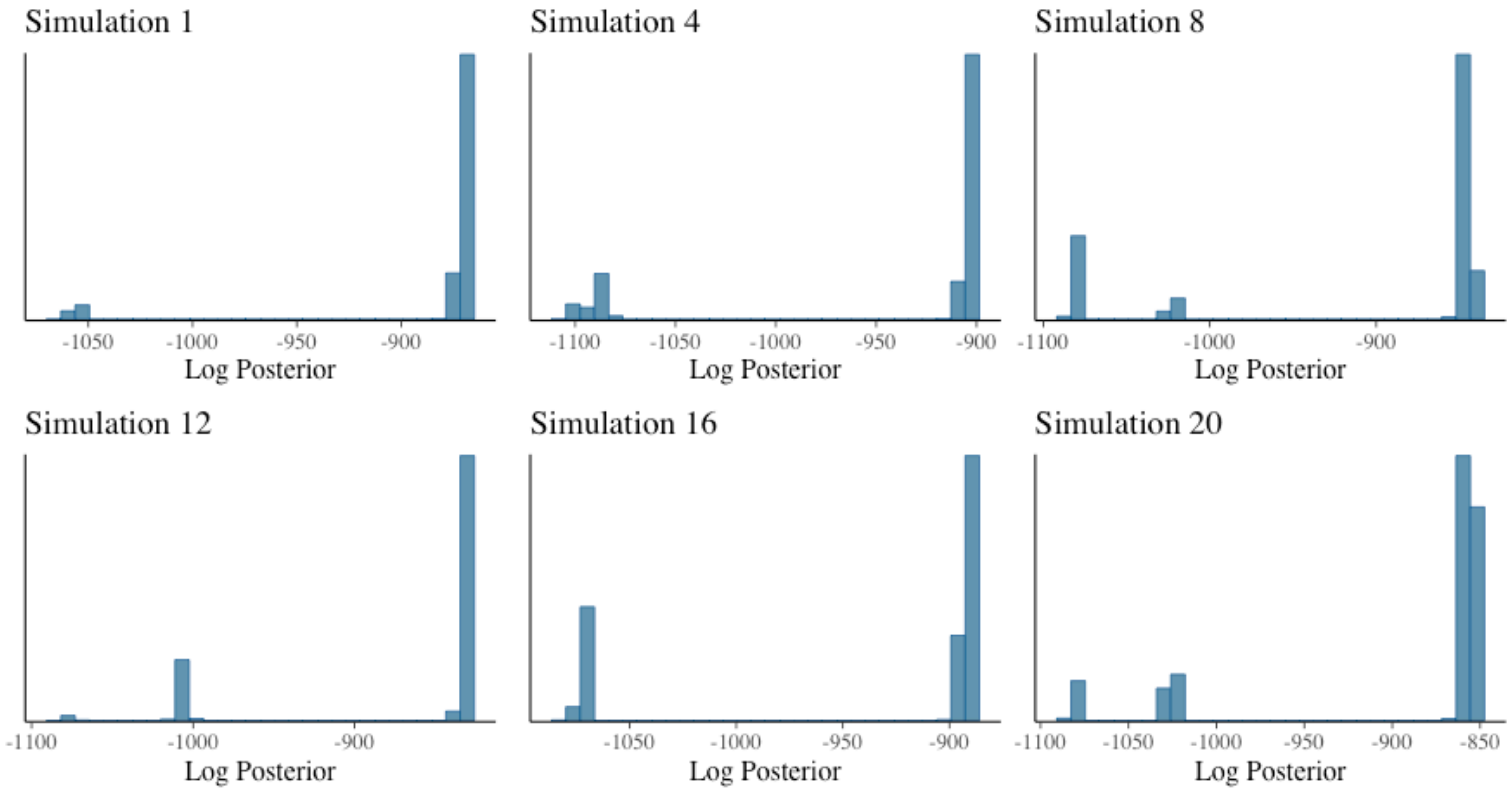
2-state HMM when truth is a 3-state HMM



Jump!

Fitting misspecified HMMs

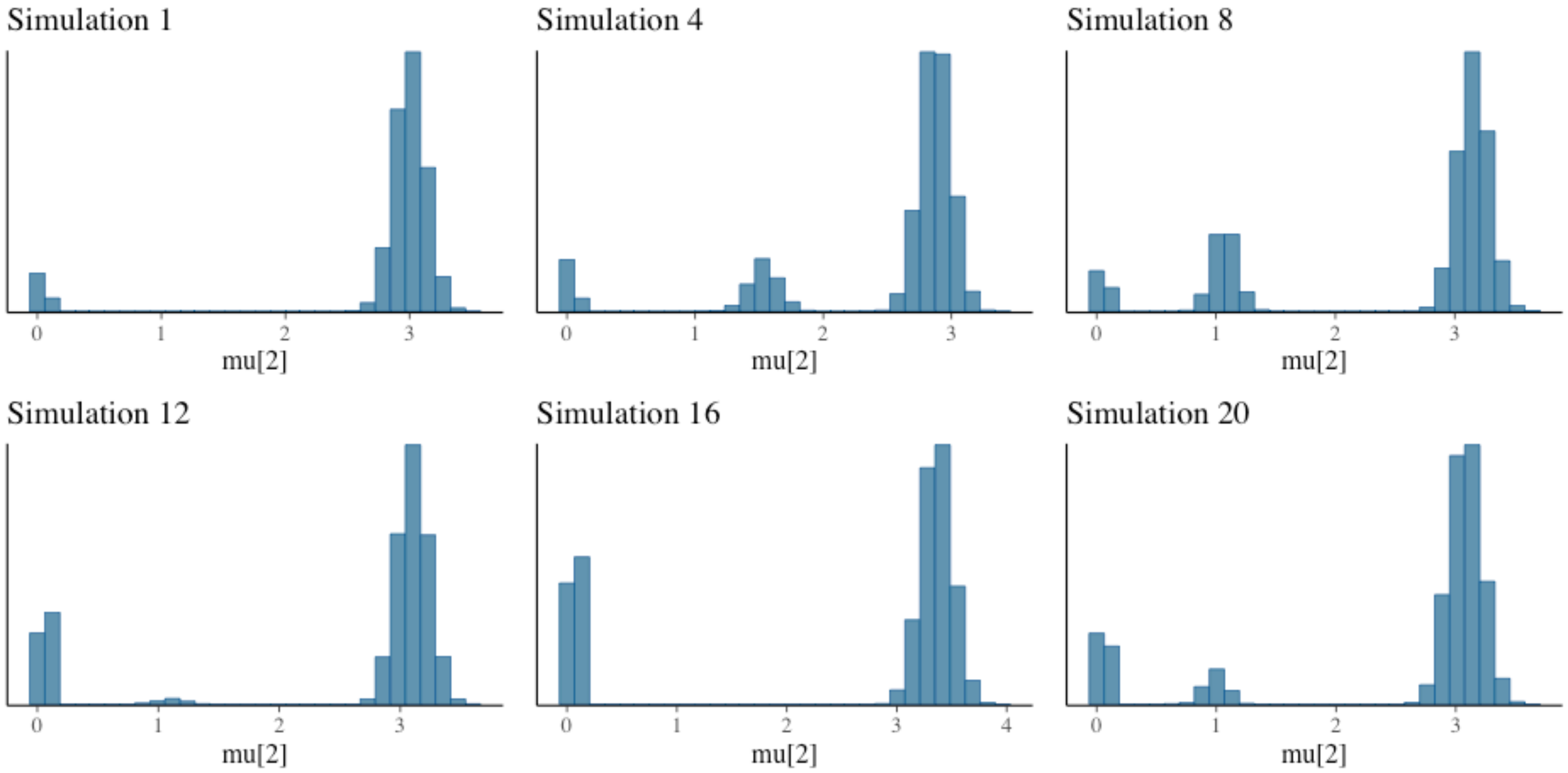
Log-posterior: $p(\boldsymbol{\theta} \mid \boldsymbol{y})$



- **Multi-modal log-posterior**
- **Each mode corresponds to different sets of parameter values that could have generated the data**
- **Not clear how much probability is associated with each mode**

Fitting misspecified HMMs

Posterior draws for μ_2 across 6 simulations:



- **These are NOT marginal distributions of μ_2**
- **These ARE values of μ_2 that are consistent with the data (and prior spec.)**

Building intuition behind misspecification

- Fitting (increasingly complex) HMM to complex data often leads to multimodal posteriors along the way

- Simulating data and fitting under misspecification helps build intuition of how to do model building when things are seemingly ‘going wrong’

- For me, I really wanted to understand — **how do different misspeficiations manifest themselves in terms of the behaviour of the likelihood/posterior distribution?** Stan is really helpful here.

Label-switching affects Bayesian inference

Fit HMMs using Bayesian inference in Stan

Extras

- Missing values

- Covariates

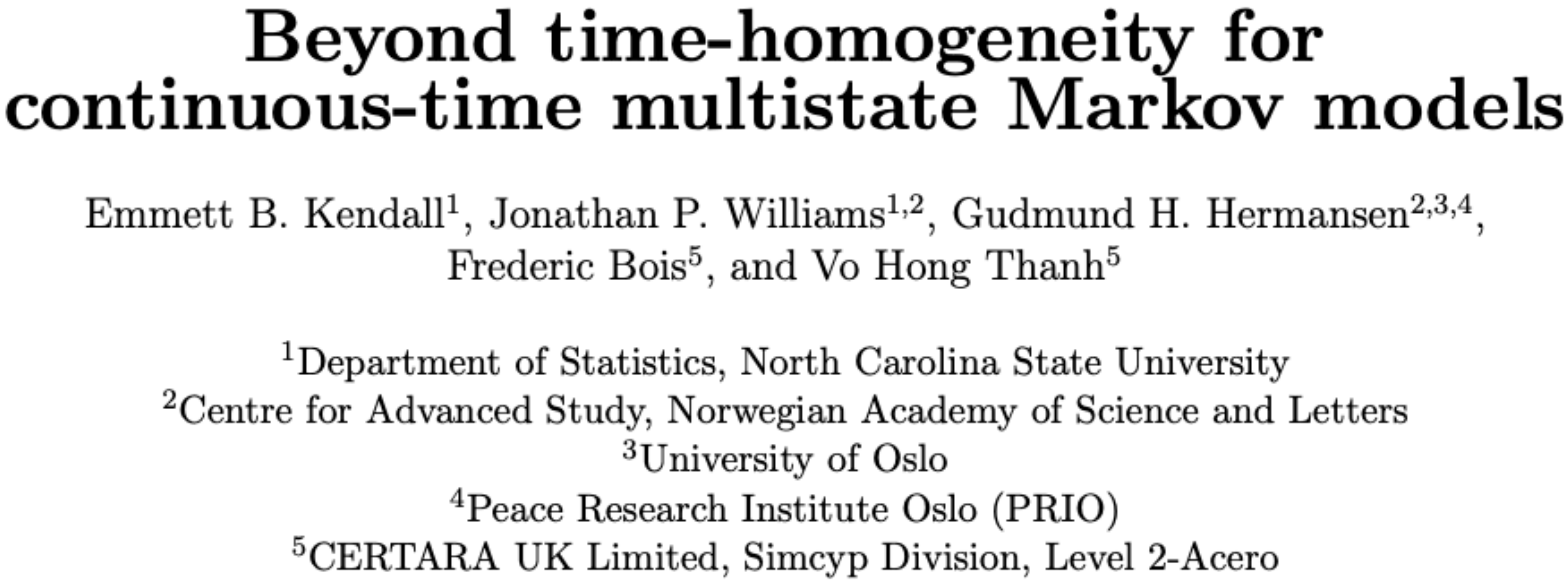
- Multivariate observations

Extras

- Mixed HMMs + random effects

- Continuous-time HMMs + more

Continuous-time HMMs



Beyond time-homogeneity for continuous-time multistate Markov models

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