

Project: Sampling Methodologies

Purpose of the project is to compare different sampling methodologies for estimating the posterior $p(\theta|y_1, \dots, y_n)$ of a bayesian inference problem.

Data (y_1, \dots, y_n) are gene expression measurements for two genes on $n = 24$ samples where $y_i = (y_{i,1}, y_{i,2})$ represent gene expressions for sample i . Our samples are all labelled by "group", denoted (t_1, \dots, t_n) . Cell type (or mix of cell types) vary with group and we assume mean gene expression (but not variance) depends on cell type. Moreover, the expressions of different genes are independently normally distributed.

- $Y_i \sim N(\mu, \sigma^2 \mathbb{I})$ if sample i from group 1
- $Y_i \sim N(\gamma, \sigma^2 \mathbb{I})$ if sample i from group 2
- $Y_i \sim N(0.5\mu + 0.5\gamma, \sigma^2 \mathbb{I})$ if sample i from group 3
- $Y_i \sim N(\tau\mu + (1 - \tau)\gamma, \sigma^2 \mathbb{I})$ if sample i from group 4

Our model has a 6-dimensional parameter $\theta = (\sigma^2, \tau, \mu_1, \mu_2, \gamma_1, \gamma_2)$.

For all sampling methodologies, I computed 5000 samples with a burn-in of 200. The rest (step size, momentum, proposals, etc.) I discuss and treat as design choices.

1 Metropolis Hastings

To implement the Metropolis-Hastings algorithm we require the joint and transition densities to compute the hastings ratio. Below we derive the join density for our model, and treat the transition density as a design choice.

Joint density:

$$\begin{aligned}
 p(\theta|y) &\propto \prod_{i=1}^n p(y_i|\theta)p(\theta) \\
 &= \prod_{t=1}^4 \prod_{i=1}^n 1\{t_i = t\} \cdot p(y_i|\theta) \cdot p(\mu) \cdot p(\gamma) \cdot p(\tau) \cdot p(\sigma^2) \\
 &= \prod_{t_i=1} N(\mu, \sigma^2 \mathbb{I}) \cdot \prod_{t_i=2} N(\gamma, \sigma^2 \mathbb{I}) \cdot \prod_{t_i=3} N(0.5\mu + 0.5\gamma, \sigma^2 \mathbb{I}) \cdot \prod_{t_i=4} N(\tau\mu + (1 - \tau)\gamma, \sigma^2 \mathbb{I}) \cdot p(\sigma^2)
 \end{aligned}$$

Hastings Ratio: let $q(\theta_0, \theta_1)$ be our transition density and $\pi(y, \theta)$ be our joint density. Then,

$$\text{accept prob.} = \min\left(1, \frac{q(\theta_0, \theta_1)\pi(y, \theta_1)}{q(\theta_1, \theta_0)\pi(y, \theta_0)}\right)$$

```

1 def metropolis_hastings(data, n_samples, step_size, initial_position):
2     curr_theta = initial_position.copy()
3     samples = [curr_theta]
4
5     while it < n_samples:
6
7         proposed = proposal_sampler(curr_theta, step_size)
8         h_ratio = hastings_ratio(proposed, curr_theta, data)
9         accept_prob = min(1, h_ratio)
10
11         if np.random.uniform(0, 1) <= accept_prob:
12             curr_theta = proposed
13             accept_count += 1
14
15         samples.append(curr_theta)
16
17     return samples

```

The Metropolis-Hastings algorithm itself is very simple, However, there are still a number of design choices we need to make, such as (a) how to propose a new sample, (b) enforcing any constraints we have (e.g. $\tau \in [0, 1]$), and (c) choosing hyperparameters (step size, burn-in).

- (a) **Proposal selection:** If possible, we would like to pick a symmetric proposal distribution to sample from (which implies a symmetric transition kernel) since this will simplify computation and guarantee detail balance. I used a gaussian random step with mean equal to the step size and variance of 1 which worked well (achieved reasonable acceptance ratio of 0.4-0.5).

```

1 def proposal_sampler(curr_theta, step_size):
2     num_params = len(curr_theta)
3
4     while True:
5         randomness = np.random.normal(0, 1, num_params)
6         proposal = curr_theta + np.multiply(step_size, randomness)
7
8         if proposal[0] > 0 and (proposal[1] >= 0 and proposal[1] <=
9             1):
10             break
11
12     return proposal

```

Note: If this choice had not worked so well, I would have tried non-symmetric options that better mimic the expected behaviour of τ and σ^2 parameters given their constraints.

- (b) **Enforcing constraints:** We had two constraints to consider: (a) $\sigma^2 > 0$ and (b) $0 \leq \tau \leq 1$. I enforce these constraints in the proposal sampler function but simply resampling if the proposal violates either (a) or (b). Note, this would be problematic (i.e. lead to us collecting biased posterior samples) if these constraints were often binding, however, we can see in the results below (figure 1) that neither σ^2 nor τ have maximum likelihoods or significant probability density near their boundaries and so the biased-ness we introduce will be minimal.
- (c) **Hyperparameters:** There are not many hyperparameters to tune for Metropolis-Hastings, which is one of its advantages! I experimented with different step sizes (0.01, 0.05, 0.1, 0.5), and for each computed the acceptance ratio and number of effective (uncorrelated) samples for 300 sample test (after burn-in). I choose a step size of 0.05 since it maximized number of effective samples.

Step size	0.01	0.05	0.1	0.5
Acceptance ratio	0.92	0.45	0.19	0.02
Number of effective samples	4.53	16.64	9.97	6.96

I did not investigate varying initialization (used $[1., 0.5, 0., 0., 0., 0.]$) or burn-in (fixed at 200 to match what I saw in textbook examples).

Results: Using the above design choices, we produce the following samples from our posterior (figure 1). These passed basic sense checks, such as σ^2 and τ falling within their respective bounds, lower variance as we increase number of samples, and minimal density on boundary of τ as hoped.

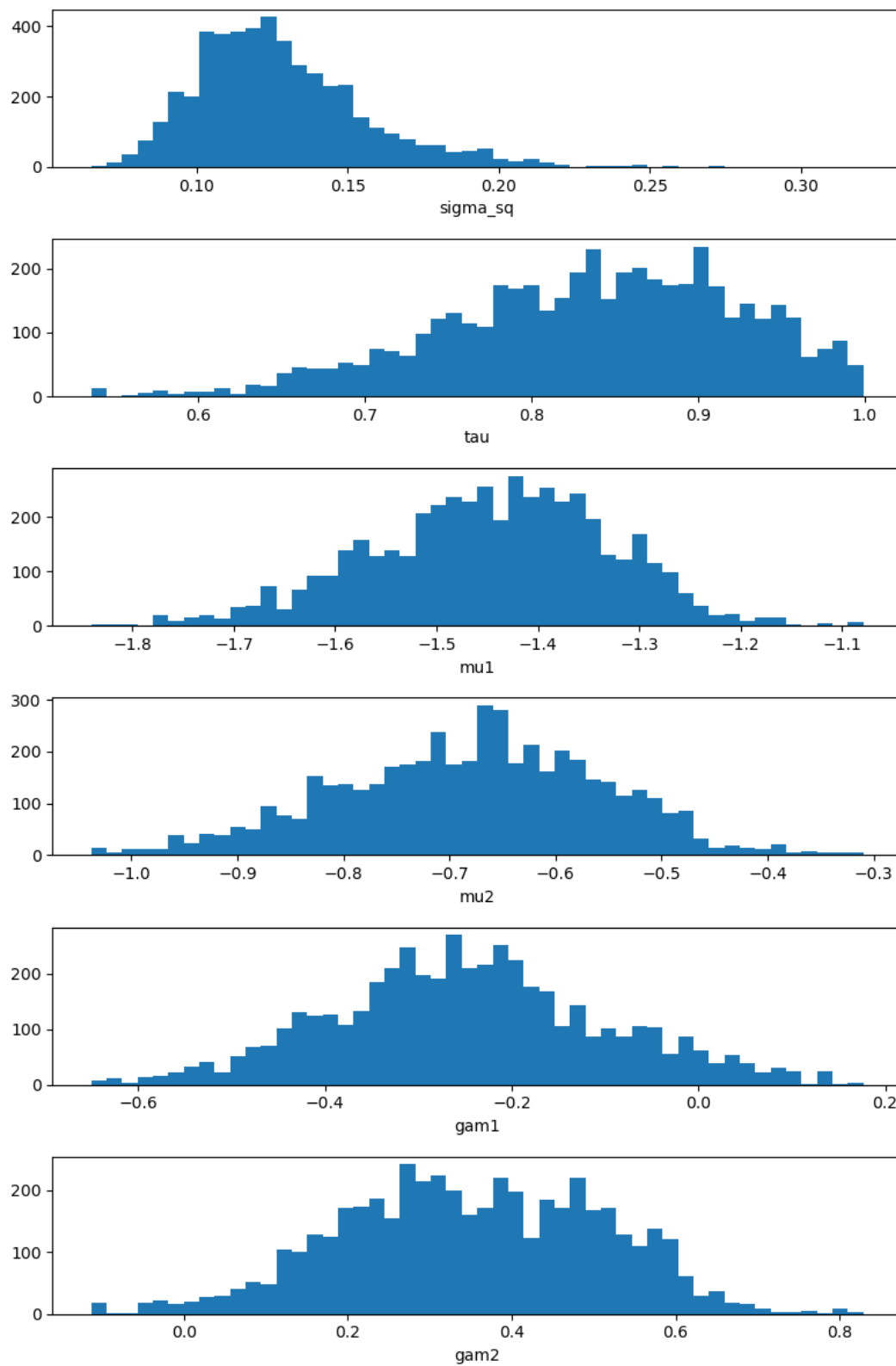


Figure 1: Histogram of Metropolis-Hastings posterior samples

The traceplots in figure 2 give an indication of how well the sampler explored the posterior density. I am comforted by the fact that there are no long periods of repeated values (getting stuck) despite an acceptance rate of only 0.45.

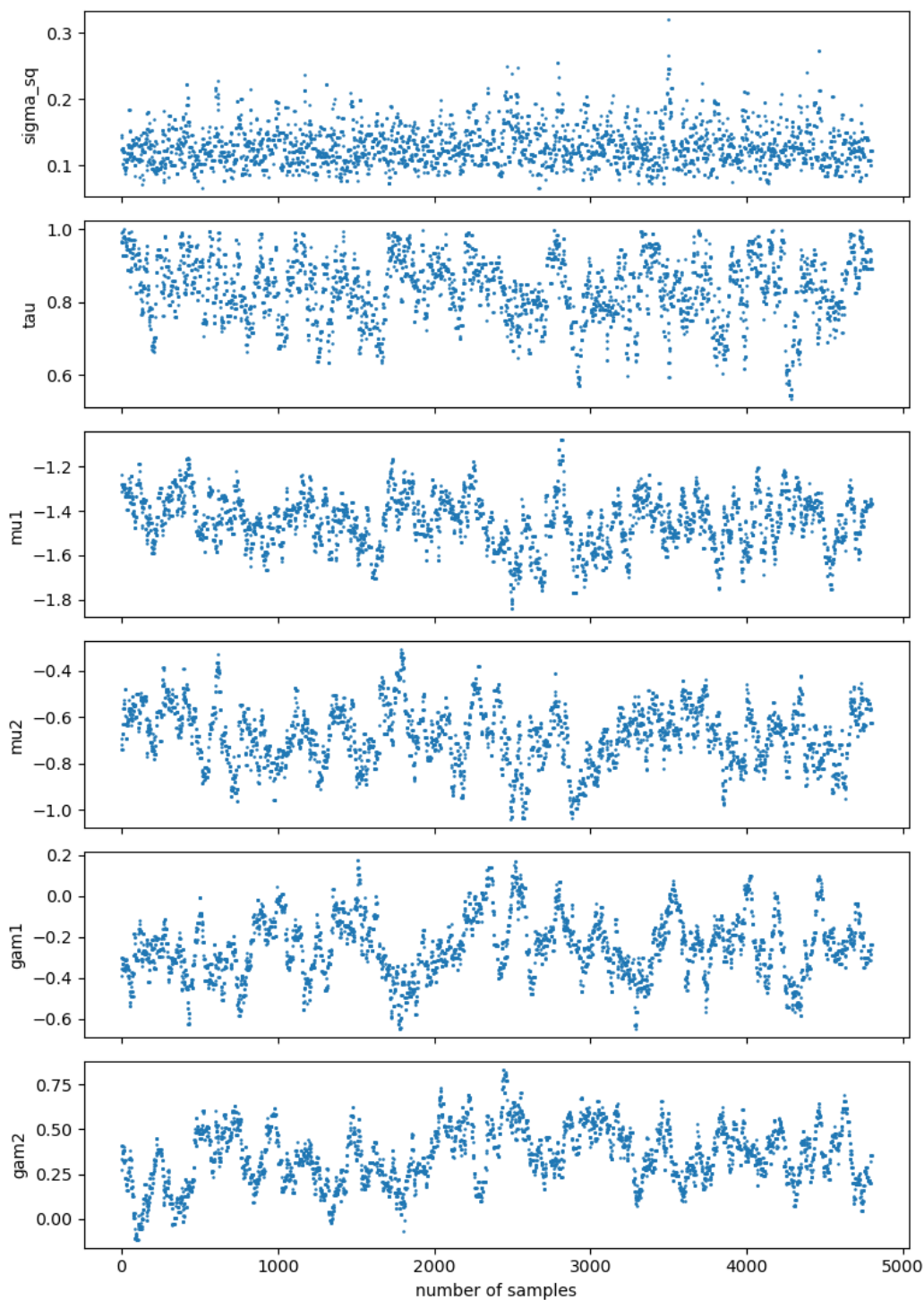


Figure 2: Traceplot for Metropolis-Hastings sampling

Final remarks. Metropolis-Hastings is simple to implement and relatively fast to run (time = 197 sec for 5000 samples), however, number of effective samples (autocorrelation) and acceptance ratio were not as good as we might expect from other techniques that take more directed paths through the posterior space (e.g. HMC).

2 Hamiltonian Monte Carlo

To implement the Hamiltonian Monte Carlo we need to compute the Hamiltonian $H(\rho, \theta)$ given independently drawn momentum ρ and our current parameter values θ .

$$\begin{aligned} H(\theta, \rho) &= -\log p(\rho, \theta) \\ &= -\log p(\rho|\theta) - \log p(\theta) \\ &= K(\rho, \theta) + V(\theta) \end{aligned} \quad \text{kinetic and potential energy}$$

We now evolve the system using the following equations from Hamiltonian mechanics. Note: $\frac{\partial V}{\partial \rho} = 0$ and if we choose our kinetic energy to be gaussian $K(\rho, \theta) = \frac{1}{2}\rho^T M^{-1}\rho + \log |M| + \text{const.}$ so we get $\frac{\partial K}{\partial \rho} = M^{-1}\rho$ and $\frac{\partial K}{\partial \theta} = 0$.

$$\begin{aligned} \frac{d\theta}{dt} &= +\frac{\partial H}{\partial \rho} = +\frac{\partial K}{\partial \rho} + \frac{\partial V}{\partial \rho} = M^{-1}\rho \\ \frac{d\rho}{dt} &= -\frac{\partial H}{\partial \theta} = -\frac{\partial K}{\partial \theta} - \frac{\partial V}{\partial \theta} = -\frac{\partial V}{\partial \theta} \end{aligned}$$

Therefore, to implement the above system, we need only to calculate the gradient of our potential energy (negative log likelihood) with respect to our parameters θ .

Negative log likelihood: let $V(\theta) = -l(\theta) = -\log p(\theta|y)$,

$$\begin{aligned} V(\theta) &= -\log \prod_{i=1}^n p(y_i|\theta)p(\theta) \\ &= -\sum_{i=1}^n \log p(y_i|\theta) - \log p(\theta) \quad \text{let } y'_i = \text{centered data} \\ &= -\sum_{i=1}^n \log \left[(2\pi)^{-k/2} \cdot |\sigma^2 \mathbb{I}|^{-1/2} \cdot \exp\left(-\frac{1}{2}y_i'^T (\sigma^2 \mathbb{I})^{-1} y'_i\right) \right] - \log \frac{1}{\sigma^2} \\ &= \frac{nk}{2} \log 2\pi + (n+1) \log \sigma^2 + \frac{1}{2\sigma^2} \sum_{i=1}^n y_i'^T \mathbb{I}^{-1} y'_i \end{aligned}$$

Gradient of $V(\theta)$ wrt θ :

$$\frac{\partial V(\theta)}{\partial \sigma^2} = \frac{n+1}{\sigma^2} - \frac{1}{2(\sigma^2)^2} \sum_{i=1}^n \|y'_i\|_2^2$$

$$\frac{\partial V(\theta)}{\partial \tau} = \frac{1}{\sigma^2} \cdot (\gamma - \mu)^T \sum_{t_i=4} y'_i$$

$$\frac{\partial V(\theta)}{\partial \mu} = -\frac{1}{\sigma^2} \cdot \left[\sum_{t_i=1} y'_i + 0.5 \sum_{t_i=3} y'_i + \tau \sum_{t_i=4} y'_i \right]$$

$$\frac{\partial V(\theta)}{\partial \gamma} = -\frac{1}{\sigma^2} \cdot \left[\sum_{t_i=2} y'_i + 0.5 \sum_{t_i=3} y'_i + (1 - \tau) \sum_{t_i=4} y'_i \right]$$

Our implementation of these hamiltonian equations employs a leapfrog algorithm to perform numerical integration. This is a second-order method as opposed to euler which is first-order. This design choice helps with stability.

```

1  def leapfrog(q, p, data, M_mat, path_len, step_size):
2      q, p = np.copy(q), np.copy(p)  # curr_theta = q
3
4      p -= step_size * dVdq(data, q) / 2
5      for _ in range(int(path_len / step_size)):
6          q, p = q_update(q, p, M_mat, step_size)
7          p -= step_size * dVdq(data, q)
8
9      q, p = q_update(q, p, M_mat, step_size)
10     p -= step_size * dVdq(data, q) / 2
11
12     # momentum flip at end
13     return q, -p
14
15 def hamiltonian_monte_carlo(data, n_samples, initial_position, m, step_size, path_1
16     samples = [initial_position]
17     size = (n_samples,) + initial_position.shape[:1]
18     M_mat = np.eye(len(initial_position)) * m
19     momentum = st.norm(0, m)
20
21     for p0 in momentum.rvs(size=size):
22         # integrate over our path to get new position and momentum
23         q_new, p_new = leapfrog(
24             samples[-1],
25             p0,
26             data,
27             M_mat=M_mat,
28             path_len=path_len,
29             step_size=step_size,
30         )
31
32         # check metropolis acceptance criterion
33         curr = joint_posterior_density(data, samples[-1]) * np.exp(-(0.5/m)*np.linalg.nor
34         prop = joint_posterior_density(data, q_new) * np.exp(-(0.5/m)*np.linalg.nor
35         alpha = min(1, prop/curr)
36
37         if np.random.uniform(0, 1) < alpha:
38             samples.append(q_new)
39         else:

```

```

40         samples.append(np.copy(samples[-1]))
41
42     return np.array(samples)

```

The Hamiltonian Monte Carlo algorithm has a number of design choices, including (a) whether to use an acceptance criterion, (b) enforcing any constraints we have (e.g. $\tau \in [0, 1]$), and (c) choosing hyperparameters (step size, momentum).

- (a) **Acceptance criterion:** My first implementation did not include an acceptance step which was faster to evaluate but did not produce sensible, unbiased posterior samples. Adding the metropolis acceptance criterion at the end of each iteration helped to correct for errors introduced via numerical integration.
- (b) **Enforcing constraints:** We had two constraints to consider: (a) $\sigma^2 > 0$ and (b) $0 \leq \tau \leq 1$. I enforce these constraints in the $q(\theta)$ update function by creating a "hard wall" or barrier, where we assume both p (momentum) and q (parameter θ) are reversed (flip sign) by same magnitude that they surpassed the constraint.

```

1  def q_update(q, p, M_mat, step_size):
2      """Helper function to update theta within bounds"""
3      q_prop = q + step_size * np.linalg.inv(M_mat) @ p
4
5      # check bounds
6      if q_prop[0] < 0:
7          p[0] = -p[0]
8          q_prop[0] = -q_prop[0]
9
10     if q_prop[1] < 0 or q_prop[1] > 1:
11         p[1] = -p[1]
12         q_prop[1] = -q_prop[1]
13
14     return q_prop, p

```

- (c) **Hyperparameters:** I experimented with different step sizes (0.005, 0.01, 0.05) and momentum variance values (1, 5, 10). For each combination I computed the acceptance ratio and number of effective (uncorrelated) samples for 300 sample test (after burn-in of 200). I choose a (step size, momentum) pair of (0.005, 10) since it maximized number of effective samples, excluding experiments with low acceptance (e.g. (0.05, 1)).

Step size	Momentum	Accept ratio	Eff. samples
0.005	1	0.98	73.8
0.005	5	0.99	139.4
0.005	10	0.99	11.5
0.01	1	0.97	66.3
0.01	5	0.98	99.8
0.01	10	0.97	55.91
0.05	1	0.004	300
0.05	15	0.64	112.7
0.05	10	0.91	74.8

I did not investigate varying initialization (used $[1., 0.5, 0., 0., 0., 0.]$), burn-in (fixed at 200 to match what I saw in textbook examples) or path length (used 1 as set number of leapfrog steps equal to path length / step size).

Results: Using the above design choices, we produce the following samples from our posterior (figure 3).

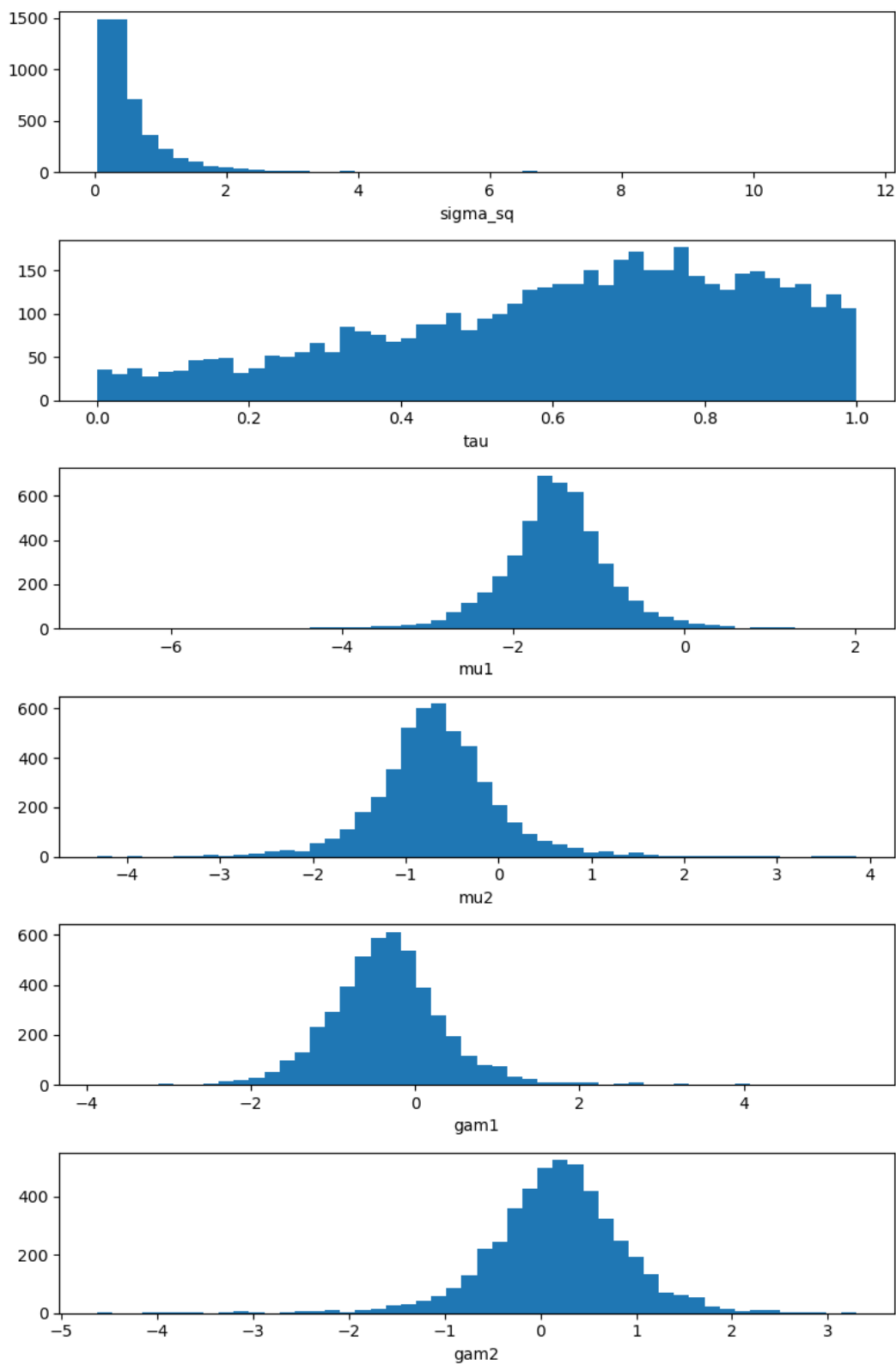


Figure 3: Histogram of Hamiltonian Monte Carlo posterior samples

The traceplots in figure 4 give an indication of how well the sampler explored the posterior density. I am comforted by the fact that there are no long periods of repeated values (getting stuck) despite us not implementing no-turn logic.

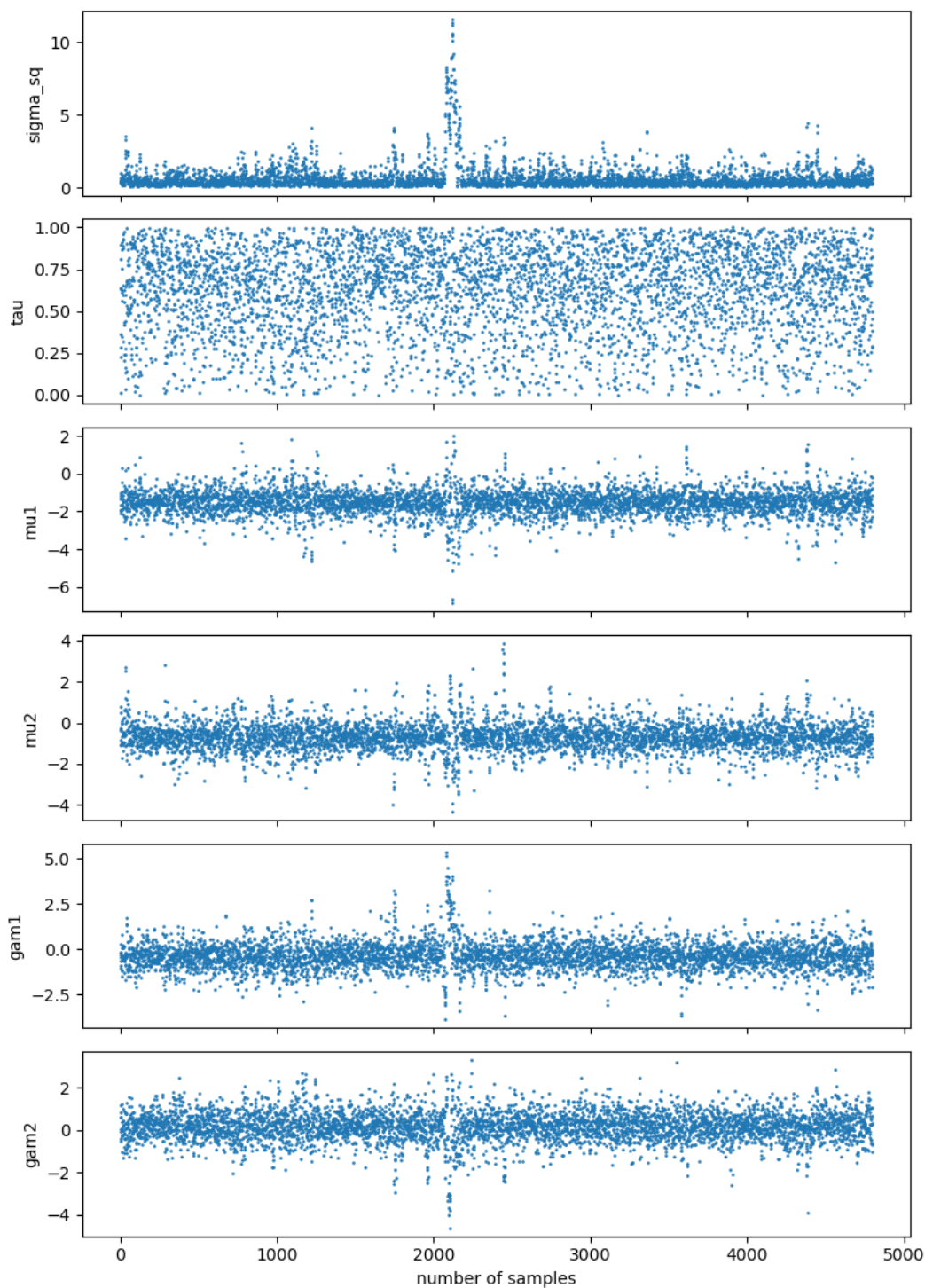


Figure 4: Traceplot for Hamiltonian Monte Carlo sampling

Final remarks. HMC was much slower to run than Metropolis- Hastings due to the gradient evaluation at each iteration (4,205 sec for 5000 samples), however, our acceptance ratio was much higher (approx. 0.95 vs 0.45). Moreover, our samples were far less likely to be autocorrelated (approx. 46 vs 5 effective samples per 100 iterations). This is because we are taking directed rather than random steps through the posterior.

3 Gibbs Sampling

To implement the Gibbs Sampling we need to derive the conditional distributions for each parameter from which to sample.

Conditional distributions Idea: start with joint posterior density, then remove constants (e.g. terms with only fixed parameters) and rearrange to derive density conditional distribution we can sample from. To simplify notation, let $\theta[-x]$ represent all parameters of θ excluding parameter x and let y'_i represent centered data (e.g. $y'_1 = y_1 - \mu$).

Derive conditional distribution for σ^2 .

$$\begin{aligned}
 p(\sigma^2|y, \theta[-\sigma^2]) &\propto \prod_{t_i=1} N(\mu, \sigma^2 \mathbb{I}) \cdot \prod_{t_i=2} N(\gamma, \sigma^2 \mathbb{I}) \cdot \prod_{t_i=3} N(0.5\mu + 0.5\gamma, \sigma^2 \mathbb{I}) \cdot \prod_{t_i=4} N(\tau\mu + (1-\tau)\gamma, \sigma^2 \mathbb{I}) \cdot p(\sigma^2) \\
 &\propto |\sigma^2 \mathbb{I}_2|^{-n/2} \cdot \frac{1}{\sigma^2} \cdot \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n y_i^T \mathbb{I}^{-1} y_i\right) \\
 &\propto \left(\frac{1}{\sigma^2}\right)^{n+1} \cdot \exp\left(-\frac{1}{\sigma^2} \cdot \frac{1}{2} \sum_{i=1}^n \|y'_i\|_2^2\right) \\
 &= x^{\alpha+1} \cdot \exp(-x\beta) \\
 \therefore \sigma^2|y, \theta[-\sigma^2] &\sim \text{InvGamma}\left(n, \frac{1}{2} \sum_{i=1}^n \|y'_i\|_2^2\right)
 \end{aligned}$$

Derive conditional distribution for τ .

$$\begin{aligned}
 p(\tau|y, \theta[-\tau]) &\propto \exp\left(-\frac{1}{2\sigma^2} \sum_{t_i=4} (y_i - (\tau\mu + (1-\tau)\gamma))^T \mathbb{I}^{-1} (y_i - (\tau\mu + (1-\tau)\gamma))\right) \\
 &\propto \exp\left(-\frac{1}{2} \cdot \frac{\|\gamma - \mu\|_2^2}{\sigma^2} \sum_{t_i=4} (\tau \vec{i} - \alpha_i)^T \mathbb{I}^{-1} (\tau \vec{i} - \alpha_i)\right) \quad \text{let } \vec{i} = (1, 1) \\
 &\propto \exp\left(-\frac{1}{2} \cdot \frac{\|\gamma - \mu\|_2^2}{\sigma^2} \sum_{t_i=4} \left(\|\tau \vec{i}\|_2^2 - 2\tau \vec{i}^T \alpha_i + \|\alpha_i\|_2^2\right)\right) \quad \|\alpha_i\|_2^2 \text{ constant} \\
 &\propto \exp\left(-\frac{1}{2} \cdot \frac{\|\gamma - \mu\|_2^2}{\sigma^2} \left(n_4 \tau^2 - 2\tau \vec{i}^T \sum_{t_i=4} \alpha_i\right)\right)
 \end{aligned}$$

$$\propto \exp \left(-\frac{1}{2} \cdot \frac{n_4 \|\gamma - \mu\|_2^2}{\sigma^2} \left(\tau - \frac{\sum_{t_i=4} \alpha_i}{n_4} \right)^2 \right) \quad \text{complete the square}$$

$$\therefore \tau|y, \theta[-\tau] \sim \text{TruncNormal} \left(\frac{\sum_{t_i=4} \alpha_i}{n_4}, \frac{\sigma^2}{n_4 \|\gamma - \mu\|_2^2}, 0, 1 \right) \quad \text{where } \alpha_i = y_i^T \mu - \gamma^T \gamma - y_i^T \gamma - \mu^T \gamma$$

Derive conditional distribution for μ .

$$\begin{aligned} p(\mu|y, \theta[-\mu]) &\propto \exp \left(-\frac{1}{2\sigma^2} \sum_{t_i \in \{1,3,4\}} (y_i - \bar{y}_i)^T \mathbb{I}^{-1} (y_i - \bar{y}_i) \right) && \bar{y}_i = \text{group mean} \\ &\propto \exp \left(-\frac{1}{2} \cdot \frac{1}{\sigma^2} \sum_{t_i \in \{1,3,4\}} (\mu - \bar{\mu}_i^{t_i})^T \mathbb{I}^{-1} (\mu - \bar{\mu}_i^{t_i}) \right) && \text{rearrange for } \mu \\ &\propto \exp \left(-\frac{1}{2} \cdot \frac{1}{\sigma^2} \sum_{t_i \in \{1,3,4\}} (\|\mu\|_2^2 - 2\mu^T \bar{\mu}_i^{t_i} + \|\bar{\mu}_i^{t_i}\|_2^2) \right) && \|\bar{\mu}_i^{t_i}\|_2^2 \text{ constant} \\ &\propto \exp \left(-\frac{1}{2} \cdot \frac{1}{\sigma^2} \left((n_1 + 0.5^2 n_3 + \tau^2 n_4) \|\mu\|_2^2 - 2\mu^T \sum_{t_i \in \{1,3,4\}} \bar{\mu}_i^{t_i} \right) \right) && \text{take } \|\mu\|_2^2 \text{ outside sum} \\ &\propto \exp \left(-\frac{1}{2} \cdot \frac{n_1 + 0.5^2 n_3 + \tau^2 n_4}{\sigma^2} \right. && \text{complete the square} \\ &\quad \left. \left(\mu - \frac{\sum_{t_i \in \{1,3,4\}} \bar{\mu}_i^{t_i}}{n_1 + 0.5^2 n_3 + \tau^2 n_4} \right)^T \mathbb{I}^{-1} \left(\mu - \frac{\sum_{t_i \in \{1,3,4\}} \bar{\mu}_i^{t_i}}{n_1 + 0.5^2 n_3 + \tau^2 n_4} \right) \right) \\ &\therefore \mu|y, \theta[-\mu] \sim \text{Normal} \left(\frac{\sum_{t_i \in \{1,3,4\}} \bar{\mu}_i^{t_i}}{n_1 + 0.5^2 n_3 + \tau^2 n_4}, \frac{\sigma^2}{n_1 + 0.5^2 n_3 + \tau^2 n_4} \right) \\ &\quad \text{where } \bar{\mu}_i^{t=1} = y_i; \quad \bar{\mu}_i^{t=3} = (y_i - 0.5\gamma)/0.5; \quad \bar{\mu}_i^{t=4} = (y_i - (1 - \tau)\gamma)/\tau \end{aligned}$$

Derive conditional distribution for γ .

$$\begin{aligned} p(\gamma|y, \theta[-\gamma]) &\propto \exp \left(-\frac{1}{2\sigma^2} \sum_{t_i \in \{2,3,4\}} (y_i - \bar{y}_i)^T \mathbb{I}^{-1} (y_i - \bar{y}_i) \right) \\ &\propto \exp \left(-\frac{1}{2} \cdot \frac{1}{\sigma^2} \sum_{t_i \in \{2,3,4\}} (\gamma - \bar{\gamma}_i^{t_i})^T \mathbb{I}^{-1} (\gamma - \bar{\gamma}_i^{t_i}) \right) \\ &\propto \exp \left(-\frac{1}{2} \cdot \frac{1}{\sigma^2} \sum_{t_i \in \{2,3,4\}} (\|\gamma\|_2^2 - 2\gamma^T \bar{\gamma}_i^{t_i} + \|\bar{\gamma}_i^{t_i}\|_2^2) \right) \\ &\propto \exp \left(-\frac{1}{2} \cdot \frac{1}{\sigma^2} \left((n_2 + 0.5^2 n_3 + (1 - \tau)^2 n_4) \|\gamma\|_2^2 - 2\gamma^T \sum_{t_i \in \{2,3,4\}} \bar{\gamma}_i^{t_i} \right) \right) \end{aligned}$$

$$\propto \exp\left(-\frac{1}{2} \cdot \frac{n_2 + 0.5^2 n_3 + (1 - \tau)^2 n_4}{\sigma^2}\right) \left(\gamma - \frac{\sum_{t_i \in \{2,3,4\}} \bar{\gamma}_i^{t_i}}{n_2 + 0.5^2 n_3 + (1 - \tau)^2 n_4}\right)^T \mathbb{I}^{-1} \left(\gamma - \frac{\sum_{t_i \in \{2,3,4\}} \bar{\gamma}_i^{t_i}}{n_2 + 0.5^2 n_3 + (1 - \tau)^2 n_4}\right)$$

$$\therefore \gamma|y, \theta[-\gamma] \sim \text{Normal}\left(\frac{\sum_{t_i \in \{2,3,4\}} \bar{\gamma}_i^{t_i}}{n_2 + 0.5^2 n_3 + (1 - \tau)^2 n_4}, \frac{\sigma^2}{n_2 + 0.5^2 n_3 + (1 - \tau)^2 n_4}\right)$$

where $\bar{\gamma}_i^{t=2} = y_i$; $\bar{\gamma}_i^{t=3} = (y_i - 0.5\mu)/0.5$; $\bar{\gamma}_i^{t=4} = (y_i - \tau\mu)/(1 - \tau)$

Having derived our conditional distributions, the gibbs implementation itself is very straight-forward. We iterate through and update one or multiple parameters at a time (see below).

```

1  def gibbs_sampling(data, n_samples, initial_position):
2      samples = [initial_position]
3
4      it = 0
5      while it < n_samples:
6          it += 1
7          curr_theta = samples[-1].copy()
8          idx = (it-1) % 4  # systematic
9
10         if idx == 0:
11             sigma_sq_proposal = sample_ssq_conditional_posterior(data, curr_theta)
12             curr_theta[0] = sigma_sq_proposal
13
14         elif idx == 1:
15             tau_proposal = sample_tau_conditional_posterior(data, curr_theta)
16             curr_theta[1] = tau_proposal
17
18         elif idx == 2:
19             mu_proposal = sample_mu_conditional_posterior(data, curr_theta)
20             curr_theta[2:4] = mu_proposal
21
22         elif idx == 3:
23             gam_proposal = sample_gam_conditional_posterior(data, curr_theta)
24             curr_theta[4:6] = gam_proposal
25
26         else:
27             print("Error: trying to update out-of-bounds parameter!")
28             samples.append(curr_theta)
29
30     return np.array(samples)

```

The Gibbs Sampling algorithm has a number of design choices, including (a) systematic vs random scan, and (b) block vs individual parameter updates. Note: there is no hyperparameter tuning for step size here because we take a completely new sample (from an adaptive proposal distribution) at each step.

(a) **Systematic vs random scan:** While random scan ensures detail balance of our

markov chain, I preferred to use a systematic scan since it was more efficient, especially over smaller sampling experiments (guarantees an equal number of updates for each).

- (b) **Block updates for mu and gamma:** Since μ_1, μ_2 and γ_1, γ_2 would always come from the same distribution I found it more efficient to update these together, drawing from a 2-dim multivariate normal rather than separately. This does mean that our proposals

Results: Using the above design choices, we produce the following samples from our posterior (figure 5).

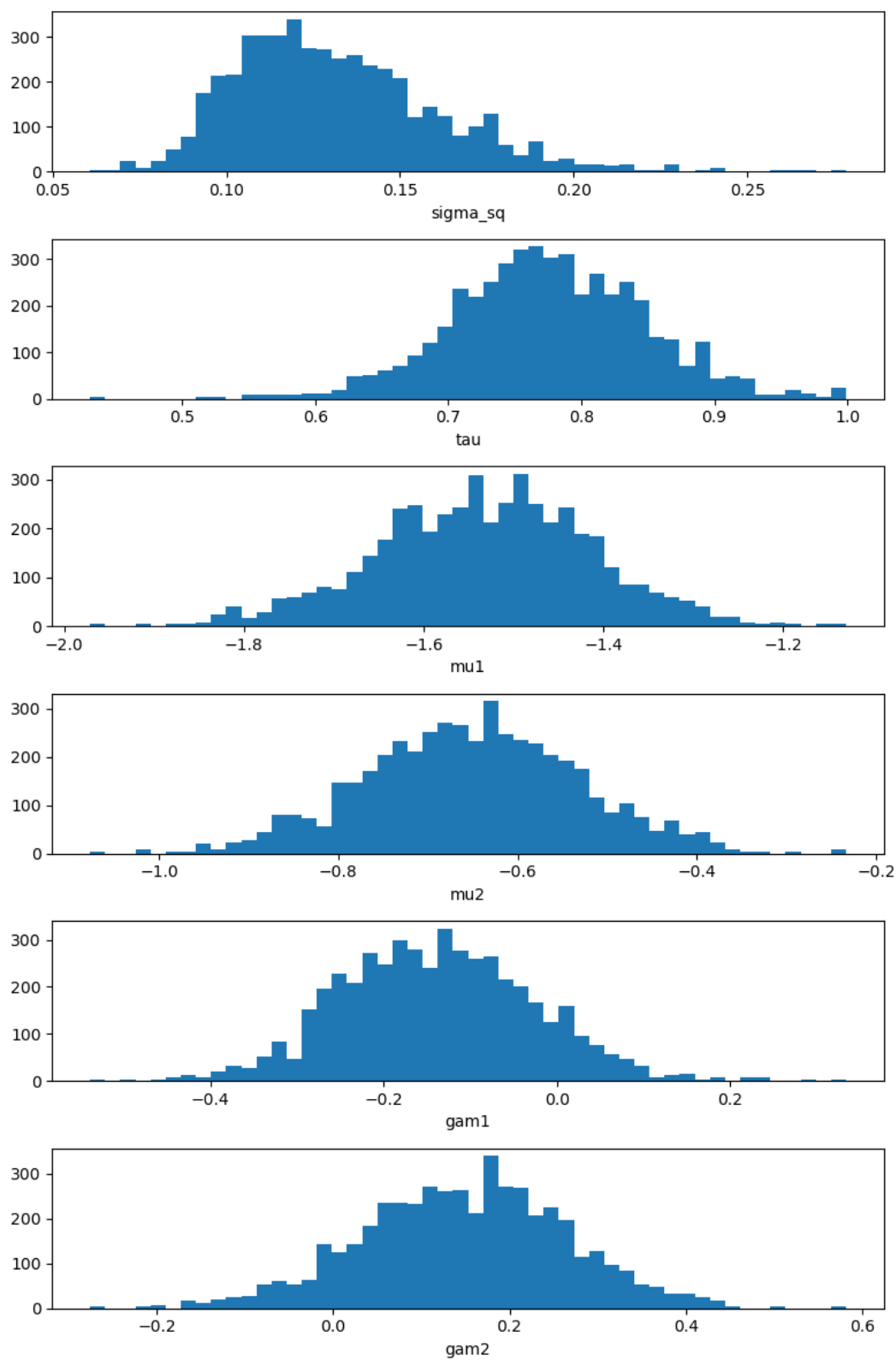


Figure 5: Histogram of Hamiltonian Monte Carlo posterior samples

The traceplots in figure 6 give an indication of how well the sampler explored the posterior density. I am comforted by the fact that there are no long periods of repeated values (getting stuck) despite us not implementing no-turn logic.

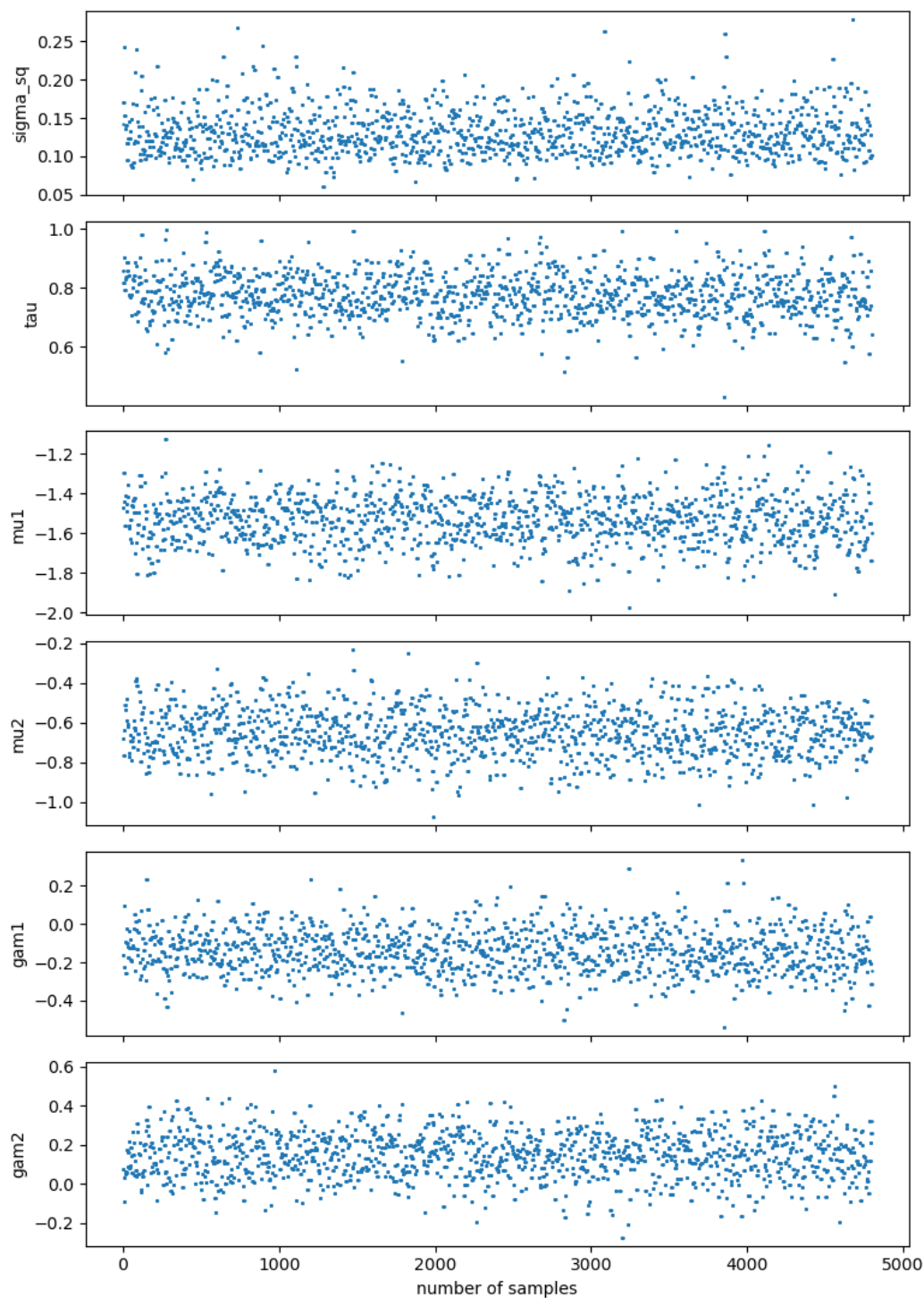


Figure 6: Traceplot for Hamiltonian Monte Carlo sampling

Final remarks. The Gibbs sampling algorithm is lightning fast compared to MH and HMC (25.0 sec!). This is because it does not execute an acceptance criterion! The main tradeoff is that our samples have significant autocorrelation (approx. 16 effective samples per 100 iterations). Note, the number of effective samples still surpasses MH but is almost 1/3 of our HMC result.

4 Importance Sampling

Importance Sampling is typically used to estimate summary statistics. For example, if $I_A(x)$ is the indicator function of x lying in some region A , and we know the target density $p(x)$, we can pick a proposal distribution Q to sample from and weight our samples in the following way.

$$E[I_A(x)] = \int I_A(x)p(x)dx = \int I_A(x)\frac{p(x)}{q(x)}q(x)dx \approx \frac{1}{n} \sum I_A(x)\frac{p(x)}{q(x)}$$

Adapting this theory to our problem, we want to derive our target density $p(\theta|y)$ (likelihood \times prior) and find a suitable proposal distribution Q that we can sample from to produce a set of samples and corresponding weights for each. Scaling each sample by its respective weight will give us posterior samples!

```

1     def multistep_importance_sampling(data, n_samples, initial_position):
2         samples, weights = [initial_position], [0]
3         for it in range(n_samples):
4
5             # sample from proposal dist q
6             theta = sample_from_proposal_dist(data)
7             samples.append(theta)
8
9             # evaluate p(theta) and q(theta) to compute weight
10            p_theta = joint_posterior_density(data, theta) # trial density
11            q_theta = compute_proposal_density(data, theta) # proposal
12            weights.append(p_theta/q_theta)
13
14     return np.array(samples), np.array(weights)

```

The importance sampling method requires us to make a number of design choices, including (a) selecting a proposal distribution, (b) whether to use a normalized scheme, and (c) choice of prior for τ .

- (a) **Proposal distribution.** Want to find a proposal distribution that is as similar as possible (but with greater variance) to distribution described by our target density. Idea: split evaluation of the posterior into two separate steps:
 - **Step 1:** Use only groups 1 and 2 to generate a closed form partial posterior (μ, γ, σ^2 only). Combine with some $p(\tau)$ to generate our proposal distribution Q

- **Step 2:** Use output from step 1 as our new prior, then update using likelihood of data from groups 3 and 4 given parameters θ to generate our target density (equivalent to joint posterior)

This two-step approach is attractive because it uses our data effectively to inform our proposal distribution. Let $\theta = (\mu, \gamma, \tau, \sigma^2)$.

$$\begin{aligned}
 p(\theta|Y_{1,2,3,4}) &\propto p(\mu, \gamma, \sigma^2|Y_{1,2}) \cdot p(\tau) \cdot L(Y_{3,4}|\theta) \\
 &\propto p(\mu, \gamma, \sigma^2|Y_{1,2}) \cdot p(\tau) \cdot \prod_{t \in 3,4} p(y_t|\theta) \\
 &\propto q(\theta) \cdot \prod_{t_i \in 3,4} p(y_i|\theta) \quad \text{choose proposal } q(\theta)
 \end{aligned}$$

Want to find closed form distribution for $p(\mu, \gamma, \sigma^2|Y_{1,2})$. First recognize we can separate σ^2 from μ and γ .

$$p(\mu, \gamma, \sigma^2|Y_{1,2}) = p(\mu, \gamma|Y_{1,2}) \cdot p(\sigma^2|\mu, \gamma, Y_{1,2})$$

Derive $p(\sigma^2|\mu, \gamma, Y_{1,2})$: σ^2 conditional on μ, γ and groups 1, 2.

$$\begin{aligned}
 p(\sigma^2|\mu, \gamma, Y_{1,2}) &\propto \frac{1}{\sigma^2} \cdot \left(\frac{1}{\sigma^2}\right)^{n_1+n_2} \exp\left(-\frac{1}{2\sigma^2}\left(\sum_{t_i=1} \|y_i - \mu\|_2^2 + \sum_{t_i=2} \|y_i - \gamma\|_2^2\right)\right) \\
 \text{let } M_{\sigma^2} &= \sum_{t_i=1} \|y_i - \mu\|_2^2 + \sum_{t_i=2} \|y_i - \gamma\|_2^2 \\
 &\propto \left(\frac{1}{\sigma^2}\right)^{n_1+n_2+1} \exp\left(-\frac{M_{\sigma^2}}{2} \cdot \frac{1}{\sigma^2}\right) \\
 &\propto \text{InvGamma}\left(n_1 + n_2, \frac{M_{\sigma^2}}{2}\right)
 \end{aligned}$$

Derive $p(\mu, \gamma|Y_{1,2})$: the marginal distribution of μ and γ .

$$\begin{aligned}
 p(\mu, \gamma|Y_{1,2}) &= \int_0^\infty p(\mu, \gamma, \sigma^2|Y_{1,2}) d\sigma^2 \\
 &\propto \int_0^\infty \left(\frac{1}{\sigma^2}\right)^{n_1+n_2+1} \exp\left(-\frac{1}{2\sigma^2}\left(\sum_{t_i=1} \|y_i - \mu\|_2^2 + \sum_{t_i=2} \|y_i - \gamma\|_2^2\right)\right) d\sigma^2 \\
 \text{recall } \frac{\Gamma(\alpha)}{\beta^\alpha} &= \int_0^\infty (\sigma^2)^{-\alpha-1} \exp\left(-\frac{\beta}{\sigma^2}\right) d\sigma^2 \\
 &\propto \Gamma(n_1 + n_2) \left(-\frac{1}{2} \sum_{t_i=1} \|y_i - \mu\|^2 + \sum_{t_i=2} \|y_i - \gamma\|^2\right)^{-(n_1+n_2)} \\
 &\propto \left(\sum_{t_i=1} \|y_i - \bar{Y}_1\|^2 + \sum_{t_i=2} \|y_i - \bar{Y}_2\|^2 + n_1 \|\bar{Y}_1 - \mu\|^2 + n_2 \|\bar{Y}_2 - \gamma\|^2\right)^{-(n_1+n_2)}
 \end{aligned}$$

$$\begin{aligned}
\text{define } M_{\mu,\gamma} &= \sum_{t_i=1} \|y_i - \bar{Y}_1\|^2 + \sum_{t_i=2} \|y_i - \bar{Y}_2\|^2 \\
&\propto (M_{\mu,\gamma} + n_1 \|\bar{Y}_1 - \mu\|^2 + n_2 \|\bar{Y}_2 - \gamma\|^2)^{-(n_1+n_2)} \\
&\propto \left(M_{\mu,\gamma} + \left[\begin{pmatrix} \mu \\ \gamma \end{pmatrix} - \begin{pmatrix} \bar{Y}_1 \\ \bar{Y}_2 \end{pmatrix} \right]^T \begin{pmatrix} n_1 & 0 & 0 & 0 \\ 0 & n_1 & 0 & 0 \\ 0 & 0 & n_2 & 0 \\ 0 & 0 & 0 & n_2 \end{pmatrix} \left[\begin{pmatrix} \mu \\ \gamma \end{pmatrix} - \begin{pmatrix} \bar{Y}_1 \\ \bar{Y}_2 \end{pmatrix} \right] \right)^{-(n_1+n_2)} \\
&\propto \left(1 + \frac{2(n_1 + n_2) - 4}{M_{\mu,\gamma}(2(n_1 + n_2) - 4)} \left[\begin{pmatrix} \mu \\ \gamma \end{pmatrix} - \begin{pmatrix} \bar{Y}_1 \\ \bar{Y}_2 \end{pmatrix} \right]^T \begin{pmatrix} n_1-1 & 0 & 0 & 0 \\ 0 & n_1^{-1} & 0 & 0 \\ 0 & 0 & n_2-1 & 0 \\ 0 & 0 & 0 & n_2-1 \end{pmatrix} \begin{pmatrix} \mu \\ \gamma \end{pmatrix} - \begin{pmatrix} \bar{Y}_1 \\ \bar{Y}_2 \end{pmatrix} \right)^{-1} \\
&\quad \left[\begin{pmatrix} \mu \\ \gamma \end{pmatrix} - \begin{pmatrix} \bar{Y}_1 \\ \bar{Y}_2 \end{pmatrix} \right] \right)^{-(n_1+n_2)} \\
&\propto \left[1 + \frac{1}{\nu} (x - \eta)^T \Sigma^{-1} (x - \eta) \right]^{-\frac{\nu+4}{2}} \quad \text{recognize t-distribution density} \\
\text{where } \nu &= 2(n_1 + n_2) + 4, \Sigma = \frac{M_{\mu,\gamma}}{2(n_1 + n_2) - 4} \begin{pmatrix} n_1-1 & 0 & 0 & 0 \\ 0 & n_1^{-1} & 0 & 0 \\ 0 & 0 & n_2-1 & 0 \\ 0 & 0 & 0 & n_2-1 \end{pmatrix}, \eta = \begin{pmatrix} \bar{Y}_1 \\ \bar{Y}_2 \end{pmatrix} \\
\therefore p(\mu, \gamma \mid Y_{1,2}) &\sim t_4 \left(\begin{pmatrix} \bar{Y}_1 \\ \bar{Y}_2 \end{pmatrix}, \frac{M_{\mu,\gamma}}{2(n_1 + n_2) - 4} \begin{pmatrix} n_1^{-1} & 0 & 0 & 0 \\ 0 & n_1^{-1} & 0 & 0 \\ 0 & 0 & n_2^{-1} & 0 \\ 0 & 0 & 0 & n_2^{-1} \end{pmatrix} \right)
\end{aligned}$$

Putting these parts together we have the following proposal distribution,

$$q(\theta) \sim t_4 \left(\begin{pmatrix} \bar{Y}_1 \\ \bar{Y}_2 \end{pmatrix}, \frac{M_{\mu,\gamma}}{2(n_1 + n_2) - 4} \begin{pmatrix} n_1^{-1} & 0 & 0 & 0 \\ 0 & n_1^{-1} & 0 & 0 \\ 0 & 0 & n_2^{-1} & 0 \\ 0 & 0 & 0 & n_2^{-1} \end{pmatrix} \right) \cdot \text{InvGamma} \left(n_1 + n_2, \frac{M_{\sigma^2}}{2} \right)$$

- (b) **Normalized importance sampling.** xx cannot solve for closed form after groups 1 and 2. Idea: let our target $p(x) = f(x)/z_p$ and $q(x) = g(x)/z_q$ where we can evaluate $f(x), g(x)$ but not $p(x), q(x)$ are z_p, z_q are constants.

If we draw x_i $i = 1, 2, \dots, n$ iid samples from Q distribution, then compute weights $u_i = f(x_i)/g(x_i)$ and apply these to our samples, we can recover the weights as if we had been able to evaluate $p(x)$ and directly compute $w_i = p(x_i)/q(x_i)$:

$$\hat{x}_i = \frac{x_i \cdot w_i}{\sum_{i=1}^n w_i} = \frac{\frac{z_p}{z_q} \cdot x_i \cdot \frac{f(x_i)}{g(x_i)}}{\sum_{i=1}^n \frac{f(x_i)}{g(x_i)}} = \frac{x_i \cdot u_i}{\sum_{i=1}^n u_i}$$

This is important for our particular problem since it is not possible to compute the closed form posterior (target density) and so instead we need to make do with some $f(x) \propto p(x)$, which we take to be the likelihood \times prior.

- (c) **Choice of tau prior.** While we were able to solve for a closed form of the posterior for groups 1 and 2, this does not give us any additional information about τ to use as a prior for Step 2. I tried both using a beta centered at zero Beta(5, 2) and a beta centered at 0.8 Beta(5, 2) where we know τ should be from our other sampling experiments.

5 Comparison of methodologies

Autocorrelation, speed to evaluate, sample efficiency, biased estimator, ...table!