#### **BOQIAN MJPS\***

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Abstract.

Key words. MCMC, Markov Jump Process, Particle MCMC, Slice Sampling, infinite state

#### 1. Details of Fast Gibbs MJPs Iteration.

*Proof.* Denote the Virtual jump time as U and, true jumps as S, and true jump time as T. Denote the transition kernel of step 2 and step 3 as  $\kappa_2(S^*, T^*|S, T, W, y)$ .

$$P((S,T) \to (S^*,T^*)|W,y) = P(V^*|W,y) = P(V^*|W,y)/P(W,y)$$
 So  $P((S,T) \to (S^*,T^*)|W,y)P(S,T|W,\theta,y) = P(V^*|W,y)P(V|W,y) = P((S^*,T^*) \to (S,T)|W,y)P(S^*,T^*|W,y)$ 

So the stationary distribution of  $\kappa_2(S^*, T^*|S, T, W, y)$  is P(S, T|W, y). Then combine it with the transition kernel of step  $1\kappa_1(W^*|S,T,y)$ . So the stationary distribution of  $\kappa_2 \circ \kappa_1$  is P(S, T, W|y).

2. Details of FFBS in Gibbs Sampling on MJPs. Suppose the state space is finite and has N states, i.e.  $\mathbb{S} = \{0, 1, 2, ..., N-1\}$ . And the trajectory is  $S = [s_1, s_2, ..., s_K]$ , and  $T = [t_0, t_1, ..., t_K, t_{K+1}]$ , where  $t_0 = t_{start}$ ,  $t_{K+1} = t_{end}$ . Beside, we observe  $y = [y_1, y_2, ..., y_o]$ , at time  $\tau = [\tau_1, \tau_2, ..., \tau_o]$ . We are interested in sampling from posterior distribution  $P(s_0, S|T, y_{[0,t_{end}]})$ . The posterior distribution of  $s_0, S$  is just a markov jump process, with transition matrix  $B = \frac{A}{\Omega} + I$ . Forward Filtering:

Define 
$$\alpha_i(s) = P(S_i = s, y_{[t_0, t_i]}) = \sum_{v=0}^{N} \alpha_{i-1}(v) P(y_{[t_{i-1}, t_i]} | S_{i-1} = v) P(S_i = s | S_{i-1} = v) = \sum_{v=0}^{N} \alpha_{i-1}(v) L_{i-1}(v) P(S_i = s | S_{i-1} = v).$$
 $\alpha_0(s) = \mu(s)$ , which is the initial distribution.

$$L_i(s) = P(y_{[t_i,t_{i+1}]}|S_i = s) = \prod_{i=1}^o f(y_i|s)^{\mathbb{I}_{\{\tau_i \in [t_i,t_{i+1})\}}}, \quad i = 0,1,2,...,K \text{ where } f(.|.)$$
 is the observation probability density. Backward Sampling:

Define 
$$\beta_i(s) = P(S_i = s | S_{i+1}, y[0, t_{end})), i = 0, 1, ..., K - 1.$$

 $\beta_K(s) = P(S_K = s | y[0, t_{end})).$ 

$$\beta_K(s) \propto \alpha_K(s) \cdot L_K(s)$$
.

$$\beta_i(s) \propto \alpha_i(s) \cdot L_i(s) \cdot B_{sS_{i+1}}$$
.

Sample the new states backwardly.

3. Details of FFBS in Continuous time Gibbs Sampling on MJPs. use the same notations as the previous section.

Since in MCMC for continuous-time discrete-state systems [2012 NIPS], there is no uniformization procedure, so the posterior  $P(s_0, S|T, y_{[0,t_{end}]})$  is no longer a discretetime markov jump process.

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Denote  $\Delta t_i = ti + 1 - t_i$ .

Now, we define  $\alpha_i(s) = P(S_i = s, t_{0:i}, y_{[t_0, t_i]}) = \sum_{v=0}^{N} \alpha_{i-1}(v) P(y_{[t_{i-1}, t_i]} | S_{i-1} = v) P(\Delta t_{i-1} | S_{i-1} = v) P(S_i = s | S_{i-1} = v) = \sum_{v=0}^{N} \alpha_{i-1}(v) L_{i-1}(v) P(S_i = s | S_{i-1} = v).$ Now,  $L_i(s) = P(y_{[t_i, t_{i+1}]} | S_i = s) P(\Delta t_i | S_i = s) = \prod_{i=1}^{o} f(y_i | s)^{\mathbb{I}_{\{\tau_i \in [t_i, t_{i+1}]\}}} P(\Delta t_i | S_i = s)$ s), i = 0, 1, 2, ..., K - 1 where f(.|.) is the observation probability density.  $L_K(s) = P(y_{[t_K, t_{K+1}]} | S_i = s) e^{i B_{S_K}} \Delta t_k).$ Let  $C = I - Diag(B_0, B_1, ..., B_{N-1})^{-1} A.$ 

$$\beta_K(s) \propto \alpha_K(s) L_K(s)$$
.

$$\beta_i(s) \propto \alpha_i(s) \cdot L_i(s) \cdot C_{s,S_{i+1}}.$$

Sample the new states backwardly.

#### 4. SMC for MJPs.

Algorithm:

Basic Assumptions: We are considering the time interval [0,T], and we have N observations  $y_1, y_2, ..., y_N$ , at time  $t_1, t_2, ..., t_N$ . We assume observing time  $t_1, t_2, ..., t_N$ are known at first. The parameter  $\theta = (A, u(.), P(Y_n = .|x_n = x))$ . A is the transition matrix of the jump process.

Let's denote our proposal distribution as  $q_{\theta}(.|y_{1:N})$ .

Step 1.

At time n = 1.

Sample N particles  $X_{[0,t_1]}^k, k=1,2,...,N.$  Compute and normalize the weights.

$$w_1(X_{[0,t_1]}^k) := \frac{P_{\theta}(X_{[0,t_1]}^k, y_1)}{q_{\theta}(X_{[0,t_1]}^k|y_1)} = \frac{\mu_{\theta}(X_{[0,t_1]}^k)g_{\theta}(y_1|X_{[0,t_1]}^k)}{q_{\theta}(X_{[0,t_1]}^k|y_1)}$$

$$W_1(X_{[0,t_1]}^k) = \frac{w_1(X_{[0,t_1]}^k)}{\sum_{i=1}^N w_1(X_{[0,t_1]}^i)}$$

Step 2.

At time n = 2, 3, 4, ..., P

- (a) Sample  $A_{n-1}^k \sim Multi(.|W_{n-1}).$

(b) Sample  $X_{[t_{n-1},t_n]}^k \sim q_{\theta}^n(.|y_n,X_{[0,t_{n-1}]}^{A_{n-1}^k}).$ Then, set  $X_{[0,t_n]}^k := combine(X_{[0,t_{n-1}]}^{A_{n-1}^k},X_{[t_{n-1},t_n]}^k).$ 

(c) Calculate the weights and normalize the weights.

$$w_n(X_{[0,t_n]}^k) := \frac{P_{\theta}(X_{[0,t_n]}^k, y_{1:n})}{P_{\theta}(X_{[0,t_{n-1}]}^{A_{n-1}^k}, y_{1:n})q_{\theta}^n(X_{[t_{n-1},t_n]}^k|y_{1:n}, X_{[0,t_{n-1}]}^{A_{n-1}^k})} = \frac{f_{\theta}(X_{[t_{n-1},t_n]}^k|X_{[0,t_{n-1}]}^{A_{n-1}^k})g(y_n|X_{t_n}^k)}{q_{\theta}^n(X_{[t_{n-1},t_n]}^k|y_{1:n}, X_{[0,t_{n-1}]}^{A_{n-1}^k})}$$

$$W_n(X_{[0,t_n]}^k) = \frac{w_n(X_{[0,t_n]}^k)}{\sum_{i=1}^N w_n(X_{[0,t_n]}^i)}$$

Specify  $f_{\theta}, g_{\theta}, q_{\theta}^n$ :

1. Let  $X_{[t,t']}$  be the trajectory that is equivalent to  $S=s_0,s_1,...,s_n,\,T=t_1,t_2,...,t_n.$ 

2. 
$$f_{\theta}(X_{[t,t']}|X_{[0,t]}) = f_{\theta}(X_{[t,t']}|X_t = s_0^*) = A_{s_0^* s_1} e^{-|A_{s_0^*}|(t_1-t)} \prod_{i=2}^n (|A_{s_{i-1}}|e^{-|A_{s_{i-1}}|(t_i-t_{i-1})} A_{s_{i-1}s_i}) e^{|A_{s_n}|(t'-t_n)}.$$
  
 $3.g_{\theta}(y_n|X_{[t',t_n]}) = G(y_n|X_{t_n}).$ 

 $4.q_{\theta}^{n}$  is the important sampling proposal distribution. In our case, we just let it be the following.

$$q_{\theta}^{n}(.|y_{n},X_{[0,t_{n-1}]}) = f_{\theta}(X_{[t_{n-1},t_{n}]}|X_{t_{n-1}}).$$

$$\begin{aligned} q_{\theta}^{n}(.|y_{n},X_{[0,t_{n-1}]}) &= f_{\theta}(X_{[t_{n-1},t_{n}]}|X_{t_{n-1}}). \\ 5. \ \mu(X_{[0,t]}) &= \pi_{0}(s_{0})A_{s_{0}^{*}s_{1}}\prod_{i=2}^{n}(|A_{s_{i-1}}|e^{-|A_{s_{i-1}}|(t_{i}-t_{i-1})}A_{s_{i-1}s_{i}})e^{|A_{s_{n}}|(t-t_{n})}, \text{ with } t_{0} = 0 \end{aligned}$$

This procedure provides us at time T with an approximation of the joint posterior density  $p_{\theta}(dX_{[0,T]}|y_{1:n})$  given by

$$\hat{p_{\theta}}(dX_{[0,T]}|y_{1:n}) = \sum_{k=1}^{N} W_n^k \delta_{X^k[0:T]}(dX_{[0,T]})$$

In addition, the estimate of the marginal likelihood  $p_{\theta}(y_{1:n})$  is given by

$$\hat{p}_{\theta}(y_{1:n}) = \hat{p}_{\theta}(y_1) \prod_{i=2}^{n} \hat{p}_{\theta}(y_i|y_{i-1})$$

where

$$\hat{p}_{\theta}(y_i|y_{i-1}) = \frac{1}{N} \sum_{t=1}^{N} w_n(X_{[0,t_i]})$$

is an estimate computed at time i of

$$p_{\theta}(y_i|y_{i-1}) = \int w_n(X_{[0,t_i]}) q_{\theta}(X_{[t_{i-1},t_i]}|y_i,X_{[0,t_{i-1}]}) p_{\theta}(X_{[0,t_{i-1}]}|y_{1:i-1}) dX_{[0,t_i]}.$$

### 5. PMCMC On MJPs.

Algorithm:

Basic Assumptions: Here, we have N observations  $y_1, y_2, ..., y_N$ , at time  $t_1, t_2, ..., t_N$ . The time interval we are interested in is [0,T]. The model is Hidden Markov State

Targeting distribution:  $P(X_{[0:T]}|y_{1:N})$ .

Initialize i = 0. Run a SMC algorithm targeting  $P(X_{[0:T]}|y_{1:N})$ . Sample a trajectory  $X_{[0:T]}(0) \sim \hat{P}_{\theta}(.|y_{1:N})$ . We let  $\hat{P}_{\theta}(y_{1:N})(0)$  denote the corresponding marginal likelihood estimate.

Step2:

For iteration  $i \ge 1$ ,

- (a). Run a SMC targeting sample  $X_{[0:T]}^* \sim \hat{P}_{\theta}(.|y_{1:N})$ , and let  $\hat{P}_{\theta}(y_{1:N})^*$  denote the marginal likelihood estimate.
- (b). With probability  $1 \wedge \frac{\hat{P}_{\theta}(y_{1:N})^*}{\hat{P}_{\theta}(y_{1:N})(i-1)}$  to update  $X_{[0:T]}(i) = X_{[0:T]}^*$ ,  $\hat{P}_{\theta}(y_{1:N})(i) = X_{[0:T]}^*$  $\hat{P}_{\theta}(y_{1:N})^*$ . Otherwise,  $X_{[0:T]}(i) = X_{[0:T]}(i-1)$ ,  $\hat{P}_{\theta}(y_{1:N})(i) = \hat{P}_{\theta}(y_{1:N})(i-1)$ .

#### 6. Immigration models with capability.

Now, let's consider a immigration model as follows. We have state space 0, 1, 2, ..., N, representing the total population. The transition matrix is defined as follows.

$$A_i =: A_{i,i} = -(\alpha + i\beta), i = 0, 1, ..., N$$

$$A_{i,i+1} = \alpha, \quad i = 0, 1, ..., N-1,$$

$$A_{i,i-1} = \beta, i = 1, ..., N.$$

We already know the conditional density(given  $\alpha$ ,  $\beta$ ) of a MJP trajectory  $(s_0, S, T)$  in time interval  $[t_{start}, t_{end}]$ , with  $S = (s_1, s_2, ..., s_k)$ ,  $T = (t_1, t_2, ..., t_k)$ .

$$f(s_0, S, T | \alpha, \beta) = \prod_{i=0}^{k-1} A_{s_i, s_{i+1}} \exp(\sum_{i=0}^k A_{s_i} (t_{i+1} - t_i)),$$

where  $t_0 = t_{start}$ ,  $t_{k+1} = t_{end}$ . Let's denote some notations here.

$$U(s_0, S, T) := \sum_{i=0}^{k-1} \mathbb{I}_{\{s_{i+1} - s_i = 1\}}$$

$$D(s_0, S, T) := \sum_{i=0}^{k-1} \mathbb{I}_{\{s_{i+1} - s_i = -1\}}$$

Call them U and D for short. Let's denote the total time when the trajectory state stays at state i as  $\tau_i$ , i.e.  $\tau_i = \sum_{j=0}^k (t_{j+1} - t_j) \mathbb{I}_{\{s_j = i\}}$ , then  $\sum_{i=0}^k (t_{i+1} - t_i) s_i = \sum_{i=0}^N \tau_i i$ 

$$f(s_0, S, T | \alpha, \beta) = \exp(-\alpha (t_{end} - t_{start} - \tau_N)) \alpha^U \cdot \exp((-(\sum_{i=0}^k (t_{i+1} - t_i) s_i) \beta)) \prod_{i=1}^N i^{\sum_{j=0}^{k-1} \mathbb{I}_{s_{j+1} = i-1, s_j = i}} \beta^D$$

If we assume the prior of  $\alpha$ , and  $\beta$  are  $Gamma(\mu, \lambda)$ ,  $Gamma(\omega, \theta)$ , which are independent with each other.

$$p(\alpha) = \frac{\lambda^{\mu}}{\Gamma(\mu)} \alpha^{\mu - 1} e^{-\lambda \alpha}$$

 $p(\beta) = \frac{\theta^{\omega}}{\Gamma(\omega)} \beta^{\omega - 1} e^{-\theta \beta}$ 

. Then we can get the posterior distribution

 $f(\alpha, \beta|s_0, S, T)$ 

.

as follows.

$$f(\alpha, \beta|s_0, S, T) \propto \exp(-(\lambda + t_{end} - t_{start} - \tau_N)\alpha)\alpha^{\mu + U - 1} \cdot \exp(-(\sum_{i=0}^k (t_{i+1} - t_i)s_i + \theta)\beta)\beta^{\omega + D - 1}.$$

It means that the posterior distributions of  $\alpha$ ,  $\beta$  are still independent.

 $\alpha|s_0, S, T$  is following  $Gamma(\mu + U, \lambda + t_{end} - t_{start} - \tau_N)$ 

 $\beta|s_0, S, T$  is following  $Gamma(\omega + D, \theta + \sum_{i=0}^k (t_{i+1} - t_i)s_i)$ , which is equivalent to  $Gamma(\omega + D, \theta + \sum_{i=0}^N \tau_i i)$ 

# 7. Metropolis Hasting using FFBS within the Gibbs Sampling On MJPs(marginal mcmc version).

Assume:  $S = [S_0, S_1, ..., S_N]$ ,  $T = [T_0, T_1, ..., T_N, T_{N+1}(T_{end})]$ , and y as observations. In [JMLR-2013] FFBS frame, we have defined  $\alpha_t$  as follows.

Since after uniformization, the virtual jumps are added. Then the state process of the trajectory with virtual jumps is just a discrete time markov jump process. The key point is that we need to have  $U(virtual\ jump\ times)$  and  $T(true\ jump\ times)$ be conditioned, to get the marginal probability  $P(y_{T_0,T_{N+1}}|\theta,U,T)$  from FFBS algorithm.

$$\alpha_t^{\theta}(s) = P(S_t = s, y_{\lceil T_0, T_t \rceil}, U, T).$$

$$P(y_{[T_0,T_{N+1})}|\theta,U,T) = \sum_{s=0}^{N-1} \alpha_N^{\theta}(s) \cdot P(y_{[T_N,T_{N+1})}|S_N = s).$$

Algorithm:

Step1: Initialization, i = 0,

- (a) Set  $\theta(0)$  arbitrarily and set current trajectory [S, T](0) arbitrarily;
- (b) Uniformize [S, T](0), get a uniformized trajectory [V, W](0)
- (c) Run FFBS algorithm to get the marginal probability  $P(y_{[T_0,T_{N+1})}|\theta(0))$ .

Step2: for iteration  $i \ge 1$ ,

- (a) Propose  $\theta^* \sim q(.|\theta(i-1))$
- (b) Sample Virtual jump times  $U^* \sim P(|\theta(i-1), [S, T](i-1), y_{[T_0, T_{N+1}]})$
- (c) Sample  $W^*$   $P(.|\theta^*, U^*, T(i-1), y_{[T_0, T_{N+1})})$ , with FFBS algorithm, and recording the marginal probability  $P(y_{[T_0, T_{N+1})}|\theta^*)$ .  $[S^*, T^*]$  is the new proposed trajectory.
- (d) With probability

$$1 \wedge \frac{P(y_{[T_0,T_{N+1})}|\theta^*)p(\theta^*)}{P(y_{[T_0,T_{N+1})}|\theta(i-1))p(\theta(i-1))} \frac{q(\theta(i-1)|\theta^*)}{q(\theta^*|\theta(i-1))}$$

set  $\theta(i) = \theta^*$ ,  $[S, T](i) = [S^*, T^*]$ , and  $P(y_{[T_0, T_{N+1})} | \theta(i)) = P(y_{[T_0, T_{N+1})} | \theta^*)$ ; Otherwise, set  $\theta(i) = \theta(i-1)$ , [S, T](i) = [S, T](i-1), and  $P(y_{[T_0, T_{N+1})} | \theta(i)) = P(y_{[T_0, T_{N+1})} | \theta(i-1))$ 1)).

#### 8. Proposed Metropolis Hasting within the Gibbs Sampling On MJPs.

Denote all the parameters as  $\theta$ , observations as Y. Algorithm(iteration part):

Step1: Sample  $U^* \sim P(.|\theta, S, T, Y)$ .

Step2: Propose  $\theta^* \sim q(.|\theta)$ ., with acceptance rate  $\alpha_0$ 

$$\alpha_0 = \frac{P(\theta^*, S, U^*, T)}{P(\theta, S, U^*, T)} \frac{q(\theta|\theta^*)}{q(\theta^*|\theta)} \wedge 1$$

Step3: Sample  $W^* \sim P(.|\theta, U^*, T, Y)$ , using FFBS.

Details about acceptance rate:

We are considering a Immigration model  $(\alpha, \beta)$  with capacity N.

Assume:  $S = [s_0, s_1, ..., s_N], T = [t_0, t_1, ..., t_N, t_{N+1}(t_{end})].$ 

Also assume there are  $u_i$  virtual jumps in time interval  $[t_i, t_i + 1)$ , i = 0, 1, 2, ..., N.

$$U(s_0, S, T) := \sum_{i=0}^{k-1} \mathbb{I}_{\{s_{i+1} - s_i = 1\}}$$

$$D(s_0, S, T) := \sum_{i=0}^{k-1} \mathbb{I}_{\{s_{i+1} - s_i = -1\}}$$

Call them U and D for short. The proposal density  $q(\theta^*|\theta) = \frac{1}{\sqrt{2\pi}\sigma\alpha^*} \exp(-(\frac{\log(\alpha^*-\alpha)}{2\sigma^2})^2) \cdot \frac{1}{\sqrt{2\pi}\sigma\beta^*} \exp(-(\frac{\log(\beta^*-\beta)}{2\sigma^2})^2)$ 

$$P(\theta, S, U, T) = \pi_0(s_0) \prod_{i=1}^{N} A_{s_{i-1}, s_i} \exp((t_0 - t_{N+1})\Omega) \prod_{i=0}^{N} (\Omega + A_{s_i})^{u_i}$$

$$\frac{P(\theta^*, S, U, T)}{P(\theta, S, U, T)} = \exp((t_0 - t_{N+1})(\Omega^* - \Omega)) \cdot (\frac{\alpha^*}{\alpha})^U (\frac{\beta^*}{\beta})^D \cdot \prod_{i=0}^{N} (\frac{\Omega^* + A_{S_i}^*}{\Omega + A_{S_i}})^{u_i}$$

$$\alpha_0 = \exp((t_0 - t_{N+1})(\Omega^* - \Omega)) \cdot (\frac{\alpha^*}{\alpha})^U (\frac{\beta^*}{\beta})^D \cdot \prod_{i=0}^N (\frac{\Omega^* + A_{S_i}^*}{\Omega + A_{S_i}})^{u_i} \cdot \frac{\alpha^* \beta^*}{\alpha \beta} \wedge 1$$

# 9. Metropolis Hasting using FFBS within the Gibbs Sampling On

Assume:  $S = [S_0, S_1, ..., S_N]$ ,  $T = [T_0, T_1, ..., T_N, T_{N+1}(T_{end})]$ , and y as observations.

Proof.

In JMLR-2013 Fast MCMC Sampling for MJP and Extensions, the FFBS frame contains  $\alpha_t$  as follows.

## Algorithm 1 MH In Gibbs sampling for MJPs

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Input: observations y_{[t_0,t_{k+1})}

Initialize, i=0

(a) Set \theta(0) arbitrarily and set current trajectory [S,T](0) arbitrarily.

(b) Uniformize [S,T](0), to get virtual jumps U.

repeat

for i=1 to N do

(a) Propose \theta^* \sim q(.|\theta(i-1)).

Set \theta(i)=\theta^*, with probability \alpha=1 \wedge \frac{P(W,\theta^*|y)}{P(W,\theta(i-1)|y)} \frac{q(\theta(i-1)|\theta^*)}{q(\theta^*|\theta(i-1))};

Otherwise set \theta(i)=\theta(i-1).

(b) Use FFBS algorithm to sample states given all the jump times(both true jumps and virtual jumps). (i.e. V(i) \sim P(V|\theta(i), W(i-1), y).) Then delete all the virtual jumps to get S(i), T(i).

(c) Sample U(i) \sim P(U|\theta(i), S(i), T(i), y).

end for

until i=N
```

Since after uniformization, the virtual jumps are added. Then the state process of the trajectory with virtual jumps is just a discrete time markov jump process. The key point is that we need to have W be conditioned, to get the marginal probability  $P(y_{[T_0,T_{N+1})}|\theta,W)$  from FFBS algorithm.

$$\alpha_t^{\theta}(s) = P(S_t = s, y_{[T_0, T_t)}, U, T).$$

$$P(y_{[T_0, T_{N+1})} | \theta, W) = \sum_{s=0}^{N-1} \alpha_N^{\theta}(s) \cdot P(y_{[T_N, T_{N+1})} | S_N = s).$$

$$P(\theta, W | y) \propto P(\theta, W, y) = P(y | W, \theta) P(W | \theta) P(\theta).$$

 $P(y|W,\theta)$  is the marginal probability we get after Forward Filtering Algorithm and the  $P(W\theta)$  is the probability density for the  $poisson(\Omega)$ , because of the uniformization procedure. Let denote the kernel for (a), (b) and (c) as  $\kappa_1(\theta^*|\theta, W, T, S, y)$ ,  $\kappa_2(S^*, T^*|S, T, W, \theta^*, y)$  and  $\kappa_3(W^*|S^*, T^*, \theta^*, y)$ . For Step (a)  $\kappa_1(\theta^*|\theta, W, T, S)$ :

$$P((W,T,S,\theta) \to (W,T,S,\theta^*))P(\theta,W|y) = P(\theta^*,W|y)q(\theta|\theta^*) \land P(\theta,W|y)q(\theta^*|\theta)$$
$$= P((W,T,S,\theta^*) \to (W,T,S,\theta))P(\theta^*,W|y).$$

$$\begin{split} ((S,T,\theta,W) \to (S^*,T^*,\theta,W)|y) &= P(V^*|W,\theta,y) = P(V^*|W,\theta,y)/P(W,\theta,y) \\ P((S,T) \to (S^*,T^*)|W,\theta,y)P(S,T|W,\theta,y) &= P(V^*|W,\theta,y)P(V|W,\theta,y) \\ &= P((S^*,T^*) \to (S,T)|W,\theta,y)P(S^*,T^*|W,\theta,y) \end{split}$$

So the stationary distribution of  $\kappa_2(S^*, T^*|S, T, W, y)$  is  $P(S, T|W, \theta, y)$ . Now, let's consider  $\kappa_2 \circ \kappa_1(S^*, T^*, \theta^*|S, T, \theta, y, W)$ .

$$((S, T, \theta, W) \to (S^*, T^*, \theta^*, W)|y) = P((W, T, S, \theta) \to (W, T, S, \theta^*))P((S, T, \theta^*, W) \to (S^*, T^*, \theta^*, W)|y).$$

The stationary distribution of  $\kappa_1(S^*, T^*, U^*|S, T, U)$  is  $P(S, T, U|\theta, y)$ . And the stationary distribution of  $\kappa_2(U^*|U)$  is  $P(U|S, T, \theta, y)$ .

$$\begin{split} &P((S,T,\theta,W)\to(S^*,T^*,\theta^*,W)|y)P(S,T,\theta|W,y)\\ &=P((W,T,S,\theta)\to(W,T,S,\theta^*))\cdot P(\theta|W,y)\cdot P((S,T,\theta^*.W)\to(S^*,T^*,\theta^*,W)|y)P(S,T|\theta,W,y)\\ &=P((W,T,S,\theta^*)\to(W,T,S,\theta))\cdot P(\theta^*|W,y)\cdot P((S^*,T^*,\theta^*.W)\to(S,T,\theta^*,W)|y)P(S^*,T^*|\theta,W,y)\\ &=P((S^*,T^*,\theta^*,W)\to(S,T,\theta,W)|y)P(S,T,\theta|W,y). \end{split}$$

So the stationary distribution of  $\kappa_2 \circ \kappa_1$  is  $P(S,T,\theta|W,y)$ . Obviously,  $\kappa_3(W^*|W,S^*,T^*,\theta^*,y)$  has  $P(W|S^*,T^*,\theta^*,y)$  as stationary distribution. So  $\int \kappa_3(W^*|W,S^*,T^*,\theta^*,y)P(W,S^*,T^*,\theta^*|y)dW = P(W^*,S^*,T^*,\theta^*|y)$ . So  $\int \kappa_3 \cdot (\int \kappa_2 \circ \kappa_1 \cdot P(W,S,T,\theta|y)d\theta dS dT)dW = \int \kappa_3 P(W,S^*,T^*,\theta^*|y)dW = P(W^*,S^*,T^*,\theta^*|y)$ . So the stationary distribution of  $\kappa_3 \circ \kappa_2 \circ \kappa_1$  is  $P(W^*,S^*,T^*,\theta^*|y)$ .

#### 10. Hamiltonian MCMC On immigration model MJPs.

As we can see from last section, we can use Metropolis Hasting algorithm to sample  $\theta \sim P(\theta|W,y)$ . Hamiltonian MCMC can be applied to improve the acceptance rate. With HMC, a state proposed in this way can be distant from the current state but nevertheless have a high probability of acceptance.

Denote  $\theta = (\alpha, \beta)^{\top}$  and  $\alpha_t^{\theta}(s) = P(S_t = s, y_{[T_0, T_t)}|W)$ , and  $L_t(s) = P(y_{[T_t, T_{t+1})}|S_t = s)$  and the transition matrix of V as  $B = I + \frac{A}{\Omega}$ , with  $\Omega = \max\{\beta, \alpha\} + (d-2)\beta$ . And  $L_t(s)$  has nothing to do with  $\theta$ 

Now, consider the derivative  $\nabla_{\theta} P(y|W,\theta)$ .

We already know  $P(y_{[T_0,T_{N+1})}|W,\theta) = \sum_{s=0}^{d-1} \alpha_N^{\theta}(s) L_N(s)$ . Since

$$\alpha_t^{\theta}(s) = P(S_t = s, y_{[T_0, T_t)}|W).$$

$$= \sum_{v=0}^{d-1} \alpha_{t-1}^{\theta}(v) L_{i-1}(v) P(S_i = s|S_{i-1} = v).$$

$$= \sum_{v=0}^{d-1} \alpha_{t-1}^{\theta}(v) L_{i-1}(v) B_{vs}.$$

So we can get the following updating equations.

(10.1) 
$$\nabla_{\theta} P(y_{[T_0, T_{N+1})} | W, \theta) = \sum_{s=0}^{d-1} \nabla_{\theta} \alpha_N^{\theta}(s) L_N(s).$$

(10.2) 
$$\nabla_{\theta} \alpha_{t}^{\theta}(s) = \sum_{v=0}^{d-1} (\nabla_{\theta} \alpha_{t-1}^{\theta}(v) + \alpha_{t-1}^{\theta}(v) \nabla_{\theta} B_{vs}) L_{t-1}(v).$$

$$(10.3) \qquad \nabla_{\theta} \alpha_0^{\theta}(s) = (0,0)^{\top}.$$

(10.4)

So if we consider  $\frac{\partial}{\partial \alpha}$ ,  $\frac{\partial}{\partial \beta}$  separately, then we can get the following updating equations.

(10.5) 
$$\frac{\partial}{\partial \alpha} P(y_{[T_0, T_{N+1})} | W, \theta) = \sum_{s=0}^{d-1} \frac{\partial}{\partial \alpha} \alpha_N^{\theta}(s) L_N(s).$$

(10.6) 
$$\frac{\partial}{\partial \beta} P(y_{[T_0, T_{N+1})} | W, \theta) = \sum_{s=0}^{d-1} \frac{\partial}{\partial \beta} \alpha_N^{\theta}(s) L_N(s).$$

(10.7) 
$$\frac{\partial}{\partial \alpha} \alpha_t^{\theta}(s) = \sum_{v=0}^{d-1} \left( \frac{\partial}{\partial \alpha} \alpha_{t-1}^{\theta}(v) + \alpha_{t-1}^{\theta}(v) \frac{\partial}{\partial \alpha} B_{vs} \right) L_{t-1}(v).$$

(10.8) 
$$\frac{\partial}{\partial \beta} \alpha_t^{\theta}(s) = \sum_{v=0}^{d-1} \left( \frac{\partial}{\partial \beta} \alpha_{t-1}^{\theta}(v) + \alpha_{t-1}^{\theta}(v) \frac{\partial}{\partial \beta} B_{vs} \right) L_{t-1}(v).$$

(10.9) 
$$\frac{\partial}{\partial \beta} \alpha_0^{\theta}(s) = \frac{\partial}{\partial \alpha} \alpha_0^{\theta}(s) = 0.$$

(10.10)

Because of the special structure of the transition matrix of a immigration model, we have the following.

$$B_{sv} = \mathbb{I}_{v=s+1}B_{s,s+1} + \mathbb{I}_{v=s}B_{ss} + \mathbb{I}_{v=s-1}B_{s,s-1}$$

$$(10.11) \qquad \frac{\partial}{\partial \alpha} B_{vs} = (\mathbb{I}_{v=s+1} - \mathbb{I}_{v=s}) (\frac{1}{\Omega} - \frac{\alpha}{\Omega^2} \frac{\partial \Omega}{\partial \alpha}) + (\mathbb{I}_{v=s-1} - \mathbb{I}_{v=s}) (-\frac{\beta}{\Omega^2} \frac{\partial \Omega}{\partial \alpha} s)$$

$$(10.12) \qquad \frac{\partial}{\partial \beta} B_{vs} = (\mathbb{I}_{v=s+1} - \mathbb{I}_{v=s})(-\frac{\alpha}{\Omega^2} \frac{\partial \Omega}{\partial \beta}) + (\mathbb{I}_{v=s-1} - \mathbb{I}_{v=s})(\frac{1}{\Omega} - \frac{\beta}{\Omega^2} \frac{\partial \Omega}{\partial \beta})s$$

(10.13) 
$$\Omega = \max\{\beta, \alpha\} + (d-2)\beta$$

$$\frac{\partial \Omega}{\partial \alpha} = k \mathbb{I}_{\alpha \geqslant \beta}$$

(10.15) 
$$\frac{\partial \Omega}{\partial \beta} = k(d-2)\beta + \mathbb{I}_{\beta > \alpha}k$$

So we can get the derivative  $\nabla_{\theta} P(y_{[T_0,T_{N+1})}|W,\theta)$  from FFBS algorithm. Now briefly introduce Hamiltonian Monte Carlo. Hamilton's Equations

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}$$
$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}$$

, where H represents the total "energy", H(q,p) = U(q) + K(p), and q is the "position" and p is the momentum.

 $K(p) = p^{\top} \Sigma p$ , where  $\Sigma$  is a positive definite symmetric matrix. Usually people use  $K(p) = \sum_{i=1}^{d} \frac{p_i^2}{m_i}$ .

Leapfrog Method:

$$p_i(t + \epsilon/2) = p_i(t) - \frac{\epsilon}{2} \frac{\partial U}{q_i}(q(t))$$
$$q_i(t + \epsilon) = q_i(t) + \epsilon \frac{p_i(t + \epsilon/2)}{m_i}$$
$$p_i(t + \epsilon) = p_i(t + \epsilon/2) - \frac{\epsilon}{2} \frac{\partial U}{q_i}(q(t + \epsilon))$$

For our case,  $q = \theta = (\alpha, \beta)^{\top}$ ,  $p = (p_1, p_2)^{\top}$ .

$$\begin{split} U(\theta) &= -\log(P(\theta|W,y)) \\ K(p) &= \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} \\ H(\theta,p) &= P(\theta,p) = \frac{1}{Z} \exp(-U(\theta)) \exp(-K(p)) = \frac{1}{Z} P(\theta|W,y) e^{-\frac{p_1^2}{m_1}} e^{-\frac{p_2^2}{m_2}}. \end{split}$$

So, our

# 11. Beam Sampling for continuous time Infinite Hidden Markov Models. Model Assumptions:

We are considering a continuous time Infinite Hidden Markov Model (iHMM), with transition matrix  $A = (A_{ij})_{i,j \ge 1}$ .

$$A_i \doteq A_{ii} = -\sum_{j \neq i} A_{ij}$$
$$A_{ij} > 0 , i \neq j$$

Now, we are using the way in reference 1 to construct a MJPs with virtual jumps.

PROPOSITION 11.1. The path (W, V) returned by the thinning procedure described in algorithm 3 is equivalent to a sample (S, T) from the  $MJP(\pi_0, A)$ .

*Proof.*  $S = (s_0, s_1, ..., s_N)$ ,  $T = (t_0, t_1, ..., t_N, t_{N+1})$ . And let's call the virtual jumps as U. Denote the virtual jump times between  $(t_i, t_{i+1})$  as  $n_i$ . Then the density

## Algorithm 2 HMC In Gibbs sampling for MJPs

Input: observations  $y_{[t_0,t_{k+1})}$ 

Initialize, i = 0

- (a) Set  $\theta(0)$  arbitrarily and set current trajectory [S, T](0) arbitrarily.
- (b) Uniformize [S, T](0), to get virtual jumps U.

## repeat

for i = 1 to N do

- (a) Sample  $p_1^* \sim N(0, m_1), p_2^* \sim N(0, m_2).$
- (b) Start with the current state  $(\theta(i-1), p_1^*, p_2^*)$ , Hamilton dynamics is simulated for L steps using the leapfrog method with a stepsize  $\epsilon$  to get  $(\theta^*, p^{**})$  then propose a new state as  $(\theta^*, -p^{**})$ , where

$$H(\theta, p) = P(\theta, p) = \frac{1}{Z} \exp(-U(\theta)) \exp(-K(p)) = \frac{1}{Z} P(\theta|W, y) P(W, y) e^{-\frac{p_1^2}{m_1}} e^{-\frac{p_2^2}{m_2}}.$$

- (c) Set  $\theta(i) = \theta^*$ , with probability  $\alpha = 1 \wedge \exp(-H(\theta^*, -p^{**}) + H(\theta^*, p^*))$ ; Otherwise set  $\theta(i) = \theta(i-1)$ .
- (d) Use FFBS algorithm to sample states given all the jump times (both true jumps and virtual jumps). (i.e.  $V(i) \sim P(V|\theta(i), W, y)$ .) Then delete all the virtual jumps to get S(i), T(i).
- (e) Sample  $U(i) \sim P(U|\theta(i), S(i), T(i), y)$ .

end for

until i = N

### Algorithm 3 State-dependent thinning for MJPs

**Input:** Transition matrix  $A_{ss'}$ , and an initial distribution over states  $\pi_0$ .

Dominating Transition Rate Vector  $B_s \ge A_s$ .

**Output:** A piecewise constant trajectory  $(V, W) = ((v_i, w_i))$  on the time interval  $[t_{start}, t_{end}]$ .

Initialize,

Draw  $v_0 \sim \pi_0$  and set  $w_0 = t_{start}$ . Set i = 0.

while  $w_i < t_{end}$  do

- (a) Sample  $\tau_i \sim B_{v_i}$ .
- (b) Set  $v_{i+1} = v_i$  with probability  $1 \frac{A_{v_i}}{B_{v_i}}$  and set  $w_{i+1} = w_i + \tau_i$ .
- (c) **Else:** Set  $w_{i+1} = w_i + \tau_i$  and sample  $v_{i+1}$  with  $P(v_{i+1} = s | v_i) = A_{v_i,s}/A_{v_i}$ .
- (d) Incresement i.

end while

function of (W, V) will be as follows.

$$\begin{split} P(W,V) &= \pi_0(s_0) \prod_{i=0}^{N-1} \exp(-B_{s_i}(t_{i+1} - t_i)) B_{s_i}^{n_i} (1 - \frac{A_{s_i}}{B_{s_i}})^{n_i} B_{s_i} \frac{A_{s_i}}{B_{s_i}} \cdot \exp(-B_{s_N}(t_{N+1} - t_N)) B_{s_N}^{n_N} (1 - \frac{A_{s_N}}{B_{s_N}})^{n_N} \\ &= \pi_0(s_0) \exp(-\int_{t_0}^{t_{N+1}} B_{S_{(t)}} dt) \prod_{i=0}^{N} (B_{s_i} - A_{s_i})^{n_i} \prod_{i=0}^{N-1} A_{s_i s_{i+1}} \end{split}$$

So after integrating with respect to virtual jump times and the numbers of virtual jumps, we can get the following.

$$P(S,T) = \sum_{n_1,n_2,...,n_N \geqslant 0} \int_{t_0 \leqslant \tau_1^1 \leqslant ... \leqslant \tau_{n_1}^1 \leqslant t_1} ... \int_{t_N \leqslant \tau_1^N \leqslant ... \leqslant \tau_{n_N}^N \leqslant t_{N+1}} P(W,V) d\tau_1^1 ... d\tau_{n_1}^1 ... d\tau_1^N ... d\tau_{n_N}^N ... d\tau_{n_N}^N$$

$$= \pi_0(s_0) \exp(-\int_{t_0}^{t_{N+1}} A_{S_{(t)}} dt) \prod_{i=0}^{N-1} A_{s_i s_{i+1}}$$

So the proposition is proved.

П

The main idea of beam sampler for infinite-state continuous time Hidden Markov Model is to introduce auxiliary variables  $\mu$  such that conditioned on  $\mu$ , the number of trajectories with positive probability is finite. Then dynamic programming can be used to compute the conditional probabilities efficiently.

Assume  $W = (w_0, w_1, ..., w_{N'}, w_{N'+1}), V = (v_0, v_1, ..., v_{N'}), \mu = (\mu_1, \mu_2, ..., \mu_{N'}).$ 

$$P(\mu|W,V) = \prod_{i=1}^{N'} \frac{\mathbb{I}(0 \leqslant \mu_i \leqslant \frac{A_{v_{i-1}v_i}}{A_{v_{i-1}}})}{\frac{A_{v_{i-1}v_i}}{A_{v_{i-1}}}}$$

It indicates that conditioned on the trajectory (V, W),  $\mu_i$  is depending on A,  $v_i$ , and  $v_{i-1}$  and  $\mu_i \sim Uniform(0, \frac{A_{v_{i-1}v_i}}{A_{v_{i-1}}})$ .

Proposition 11.2. Conditioned on a trajectory (S,T) of the MJP, the virtual jump times U are distributed as a Poisson process with density  $B_{s(t)} - A_{s(t)}$ .

*Proof.*  $S = (s_0, s_1, ..., s_N)$ ,  $T = (t_0, t_1, ..., t_N, t_{N+1})$ . And let's call the virtual jumps as U. Denote the virtual jump times between  $(t_i, t_{i+1})$  as  $n_i$ . Then the density function of (W, V) will be as follows.

$$\begin{split} P(W,V) &= P(U,S,T) \\ &= \pi_0(s_0) \exp(-\int_{t_0}^{t_{N+1}} B_{S_{(t)}} dt) \prod_{i=0}^N (B_{s_i} - A_{s_i})^{n_i} \prod_{i=0}^{N-1} A_{s_i s_{i+1}} \end{split}$$

$$P(S,T,n_0,...,n_N) = \pi_0(s_0) \exp(-\int_{t_0}^{t_{N+1}} B_{S_{(t)}} dt) \prod_{i=0}^{N} \frac{((B_{s_i} - A_{s_i})(t_{i+1} - t_i))^{n_i}}{n_i!} \prod_{i=0}^{N-1} A_{s_i s_{i+1}}$$

So the conditional probability  $P(n_0, n_1, ..., n_N | S, T)$  will be as follows.

$$P(n_0, ..., n_N | S, T) = \exp(-\int_{t_0}^{t_{N+1}} (B_{S_{(t)}} - A_{S_{(t)}}) dt) \prod_{i=0}^{N} \frac{((B_{s_i} - A_{s_i})(t_{i+1} - t_i))^{n_i}}{n_i!}$$

So it indicates that conditioned on the trajectory (S,T), the virtual jump U is distributed as a non-homogeneous Poisson process with density  $B_{s(t)} - A_{s(t)}$ .  $\square$  **Sampling v**: Using the same trick used in Beam Sampling for the Infinite HMM, we can sample  $P(v_t|y,\mu,W)$ . So can we sample  $P(v_t|v_{t+1},y,W,u)$ .

First of all, consider  $P(v_i|y_{w_0,w_{i+1}}, w_{0:i}, \mu_{0:i})$ .

$$\begin{split} P(v_i, w_{0:i}, \mu_{0:i}, y_{[w_0, w_{i+1})}) &= \sum_{v_{i-1}} P(v_i, y_{[w_i, w_{i+1})}, w_i, \mu_i, v_{i-1}, w_{0:i-1}, \mu_{0:i-1}, y_{[w_0, w_i)}) \\ &= \sum_{v_{i-1}} P(v_i, y_{[w_i, w_{i+1})}, w_i, \mu_i | v_{i-1}, w_{0:i-1}, \mu_{0:i-1}, y_{[w_0, w_i)}) P(v_{i-1}, w_{0:i-1}, \mu_{0:i-1}, y_{[w_0, w_i)}) \\ &= \sum_{v_{i-1}} P(y_{[w_i, w_{i+1})} | v_i, w_i, w_{i+1}) P(\mu_i | v_i, v_{i-1}) P(v_i, w_i | v_{i-1}, w_{i-1}) P(v_{i-1}, w_{0:i-1}, \mu_{0:i-1}, y_{[w_0, w_i)}) \\ &= P(y_{[w_i, w_{i+1})} | v_i, w_i, w_{i+1}) \sum_{v_{i-1}} \frac{\mathbb{I}(0 \leqslant \mu_i \leqslant \frac{A_{v_{i-1}v_i}}{A_{v_{i-1}}})}{\frac{A_{v_{i-1}v_i}}{A_{v_{i-1}}}} \exp(-B_{v_{i-1}}(w_i - w_{i-1})) \\ &(B_{v_{i-1}} - A_{v_{i-1}})^{\mathbb{I}(v_i = v_{i-1})} A_{v_{i-1}v_i}^{\mathbb{I}(v_i v_{i-1})} P(v_{i-1}, w_{0:i-1}, \mu_{0:i-1}, y_{[w_0, w_i)}) \\ &= P(y_{[w_i, w_{i+1})} | v_i, w_i, w_{i+1}) \sum_{\Im_{i-1}} \frac{\mathbb{I}(0 \leqslant \mu_i \leqslant \frac{A_{v_{i-1}v_i}}{A_{v_{i-1}}})}{\frac{A_{v_{i-1}v_i}}{A_{v_{i-1}}}} \exp(-B_{v_{i-1}}(w_i - w_{i-1})) \\ &(B_{v_{i-1}} - A_{v_{i-1}})^{\mathbb{I}(v_i = v_{i-1})} A_{v_{i-1}v_{i-1}}^{\mathbb{I}(v_i v_{i-1})} P(v_{i-1}, w_{0:i-1}, \mu_{0:i-1}, y_{[w_0, w_i)}) \end{split}$$

Although the summation over  $v_{i-1}$  is an infinite sum, the auxiliary variable  $\mu_i$  truncates this summation to the finitely many  $v_{i-1}$ 's and  $v_i$ 's that satisfy both constrains  $\mu_i \leqslant \frac{A_{v_{i-1}v_i}}{A_{v_{i-1}}}$  and  $P(v_{i-1}|y_{[w_0,w_i)},\mu_{0:i-1}) > 0$ . This means that  $|\Im_{i-1}| < +\infty$ .

Secondly, consider  $P(v_i|v_{i+1}, y_{w_0, w_{N'+1}}, w_{0:N'+1}, \mu_{0:N'})$ .

```
\begin{split} &P(v_{i}|v_{i+1},y_{w_{0},w_{N'+1}},w_{0:N'+1},\mu_{0:N'}) \propto P(v_{i},v_{i+1},y_{w_{0},w_{N'+1}},w_{0:N'+1},\mu_{0:N'}) \\ &= P(y_{[w_{i+1},w_{N'+1})},\mu_{i+2:N},w_{i+2:N}|v_{i},v_{i+1},y_{[w_{0},w_{i+1}),w_{0:i+1},\mu_{0:i+1})})P(v_{i},v_{i+1},y_{[w_{0},w_{i+1})},w_{0:i+1},\mu_{0:i+1}) \\ &= P(y_{[w_{i+1},w_{N'+1})},\mu_{i+2:N},w_{i+2:N}|v_{i+1},w_{i+1})P(v_{i},v_{i+1},y_{[w_{0},w_{i+1})},w_{0:i+1},\mu_{0:i+1}) \\ &= Const \cdot P(v_{i},v_{i+1},y_{[w_{0},w_{i+1})},w_{0:i+1},\mu_{0:i+1}) \\ &= Const \cdot P(v_{i+1},u_{i+1},w_{i+1}|v_{i},y_{[w_{0},w_{i+1})},w_{0:i},\mu_{0:i}) \cdot P(v_{i},w_{0:i},\mu_{0:i},y_{[w_{0},w_{i+1})}) \\ &= Const \cdot P(v_{i+1},u_{i+1},w_{i+1}|v_{i},w_{0:i},\mu_{0:i}) \cdot P(v_{i},w_{0:i},\mu_{0:i},y_{[w_{0},w_{i+1})}) \end{split}
```

Finally, to sample the complete trajectory, we can sample  $P(v_{N'}|y_{w_0,w_{N'+1}},\mu_{0:N'})$  first, and then do a backward sampling using the above formula.

Theorem 11.3. Algorithm 4 has  $P(S,T,W,\mu|y)$  as a stationary distribution.

*Proof.* Firstly, prove (c) step has  $P(S, T|W, \mu, y)$  as a stationary distribution. It comes from the following detail balance condition.

$$\begin{split} P((W,S,T,\mu) \to (W,S^*,T^*,\mu))P(S,T|W,\mu,y) &= P(V^*|W,\mu,y)P(V|W,\mu,y) \\ &= P((W,S^*,T^*,\mu) \to (W,S,T,\mu))P(S^*,T^*|W,\mu,y) \end{split}$$

### Algorithm 4 Beam Sampler for continuous time Infinite Hidden Markov Models

Input: observations  $y_{[t_0,t_{k+1})}, A, B, \pi_0$ 

Initialize, i = 0

(a) Set current trajectory [S, T](0) arbitrarily.

repeat

for i = 0 to N do

- (a) Sample virtual jumps  $U(i+1) \sim Poisson\ Process(B_{s(t)} A_{s(t)})$ , given S(i), T(i).
- (b) Sample  $\mu(i+1)_j \sim Uniform(0, \frac{A_{v_{j-1}v_j}}{A_{v_{j-1}}}), j = 1, 2, ..., N'.$
- (c) Sample  $V(i+1) \sim P(V|W(i+1), \mu(i+1), y)$
- (d) Delete all the virtual jumps to get S(i+1), T(i+1)

end for

until i = N

Secondly, prove (a) and (b) step have  $P(W, \mu|S, T, y)$  as a stationary distribution.

$$\begin{split} P(W,\mu|S,T,y) &= P(U,\mu|S,T,y) = \frac{P(U,\mu,S,T,y)}{P(S,T,y)} \\ &= \frac{P(y|S,T)P(U,\mu,S,T)}{P(y|S,T)P(S,T)} = P(\mu|S,T,U)P(U|S,T) \\ &= P(\mu|V,W)P(U|S,T) \end{split}$$

We know the transition probability  $P((S, T, W, \mu) \to (S, T, W^*, \mu^*))$  is as follows.

$$P((S,T,W,\mu) \to (S,T,W^*,\mu^*)) = P(\mu^*|V^*,W^*)P(U^*|S,T)$$
  
=  $P(\mu^*|S,T,U^*)P(U^*|S,T) = P(W^*,\mu^*|S,T,y)$ 

So step(a) and (b) have  $P(W, \mu|S, T, y)$  as a stationary distribution.

Above all, this theorem is proved.

#### 12. Delayed Acceptance MH algorithm for MJPs.

*Proof.* First prove that Step (a) - (d) have  $P(\theta|W,y)P(S_a,T_a|W,\theta)$  as stationary distribution.

From step(a) to step (d), W, y, S, T stay unchanged.

Let the first stage acceptance rate

$$\begin{split} \alpha_1(. \to *) &= \alpha_1(S_a, T_a, \theta) \to (S_a^*, T_a^*, \theta^*) \\ &\doteq 1 \land \frac{P(y|S_a^*, T_a^*, \theta^*)q(\theta|\theta^*)}{P(y|S_a, T_a, \theta)q(\theta^*|\theta)}. \end{split}$$

Let the second stage acceptance rate

$$\alpha_{2}(. \to *) = \alpha_{2}(S_{a}, T_{a}, \theta) \to (S_{a}^{*}, T_{a}^{*}, \theta^{*})$$

$$\stackrel{\cdot}{=} 1 \land \frac{P(\theta^{*}|W, y)P(y|S_{a}, T_{a}, \theta)}{P(\theta|W, y)P(y|S_{a}^{*}, T_{a}^{*}, \theta^{*})}.$$

#### **Algorithm 5** Delayed Acceptance MH algorithm for MJPs

**Input:** observations  $y_{[t_0,t_{k+1})}$ 

Initialize, i = 0

- (a) Set  $\theta(0)$  arbitrarily and set current trajectory [S, T](0) arbitrarily.
- (b) Sample virtual jumps U(0) based on [S, T](0).

for i = 1 to N do

- (a) Propose  $\theta^* \sim q(\theta^*|\theta)$ .
- (b) Sample the adjoint trajectory  $S_a^*, T_a^* \sim P(S, T|W(i-1), \theta^*)$  for proposed  $\theta^*$ . Sample the adjoint trajectory  $S_a, T_a \sim P(S, T|W(i-1), \theta(i-1))$
- (c) With probability

$$1 \wedge \frac{P(y|S_a^*, T_a^*, W(i-1), \theta^*)}{P(y|S_a, T_a, W(i-1), \theta(i-1))} \frac{q(\theta(i-1)|\theta^*)}{q(\theta^*|\theta(i-1))}$$

Run the following Forward Filter algorithm. Otherwise, set  $\theta(i) = \theta(i-1)$ , then increase i and go to (e).

(d) With probability

$$1 \wedge \frac{P(\theta^*|W(i-1),y)}{P(\theta|W(i-1),y)} \frac{P(y|S_a, T_a, W(i-1), \theta(i-1))}{P(y|S_a, T_a, W(i-1), \theta^*)}$$

Set  $\theta(i) = \theta^*$ . Otherwise, set  $\theta(i) = \theta(i-1)$ .

- (e) Use FFBS algorithm to sample states given all the jump times (both true jumps and virtual jumps). (i.e.  $V(i) \sim P(V|\theta(i), W(i-1), y)$ .) Then delete all the virtual jumps to get S(i), T(i).
- (f) Sample  $U(i) \sim P(U|\theta(i), S(i), T(i), y)$ .

end for

until i = N

We know the transition probability is as follows.

$$P((S_a, T_a, \theta) \to (S_a^*, T_a^*, \theta^*)) = q(\theta^* | \theta) P(S_a^*, T_a^* | W, \theta^*) \alpha_1(. \to *) \alpha_2(. \to *).$$

First of all, we have,

$$P(y|S_a, T_a, W, \theta)q(\theta^*|\theta)\alpha_1(. \to *) = P(y|S_a, T_a, W, \theta)q(\theta^*|\theta)\alpha(. \to *) \land P(y|S_a^*, T_a^*, W, \theta^*)q(\theta|\theta^*)$$
  
=  $P(y|S_a^*, T_a^*, W, \theta^*)q(\theta|\theta^*)\alpha_1(* \to .).$ 

Secondly, we have,

$$\frac{P(\theta|W,y)P(S_a,T_a|W,\theta)P(S_a^*,T_a^*|W,\theta^*)}{P(y|S_a,T_a,W,\theta)}\alpha_2(.\to *)$$

$$= P(S_a,T_a|W,\theta)P(S_a^*,T_a^*|W,\theta^*)(\frac{P(\theta|W,y)}{P(y|S_a,T_a,W,\theta)} \wedge \frac{P(\theta^*|W,y)}{P(y|S_a^*,T_a^*,W,\theta^*)})$$

$$= \frac{P(\theta^*|W,y)P(S_a^*,T_a^*|W,\theta^*)P(S_a,T_a|W,\theta)}{P(y|S_a^*,T_a^*,W,\theta^*)}\alpha_2(*\to .).$$

#### **Algorithm 6** New MH algorithm for MJPs

```
Input: observations y_{[t_0,t_{k+1})}
Initialize, i = 0
(a) Set \theta(0) arbitrarily and set current trajectory [S, T](0) arbitrarily.
(b) Sample virtual jumps U(0) based on [S, T](0).
repeat
  for i = 1 to N do
      (a) Propose \theta^* \sim q(\theta^*|\theta).
     (b) Sample the adjoint trajectory S_a^*, T_a^* \sim P(S, T|W(i-1), \theta^*) for proposed
     \theta^*. Sample the adjoint trajectory S_a, T_a \sim P(S, T|W(i-1), \theta(i-1))
      (c) With probability
                1 \wedge \frac{P(y|S_a^*, T_a^*, W(i-1), \theta^*)}{P(y|S_a^*, T_a^*, W(i-1), \theta(i-1))} \frac{P(\theta^*)P(W(i-1)|\theta^*)}{P(\theta)P(W(i-1)|\theta(i-1))}
     Set \theta(i) = \theta^*. Otherwise, set \theta(i) = \theta(i-1).
      (d) Use FFBS algorithm to sample states given all the jump times(both true
     jumps and virtual jumps). (i.e. V(i) \sim P(V|\theta(i), W(i-1), y).) Then delete all
```

the virtual jumps to get S(i), T(i). (e) Sample  $U(i) \sim P(U|\theta(i), S(i), T(i), y)$ .

end for until i = N

So above all, we have,

$$\begin{split} &P(\theta|W,y)P(S_{a},T_{a}|\theta,W)P((S_{a},T_{a},\theta)\to(S_{a}^{*},T_{a}^{*},\theta^{*}))\\ &=P(\theta|W,y)P(S_{a},T_{a}|\theta,W)q(\theta^{*}|\theta)\alpha_{1}(.\to*)\alpha_{2}(.\to*)P(S_{a}^{*},T_{a}^{*}|W,\theta^{*})\\ &=P(y|S_{a},T_{a},W,\theta)\alpha_{1}(.\to*)q(\theta^{*}|\theta)\cdot\frac{P(\theta|W,y)P(S_{a},T_{a}|W,\theta)P(S_{a}^{*},T_{a}^{*}|W,\theta^{*})}{P(y|S_{a},T_{a},W,\theta)}\alpha_{2}(.\to*)\\ &=P(y|S_{a}^{*},T_{a}^{*},W,\theta^{*})\alpha_{1}(*\to.)q(\theta|\theta^{*})\cdot\frac{P(\theta^{*}|W,y)P(S_{a}^{*},T_{a}^{*}|W,\theta^{*})P(S_{a},T_{a}|W,\theta)}{P(y|S_{a}^{*},T_{a}^{*},W,\theta^{*})}\alpha_{2}(*\to.)\\ &=P(\theta^{*}|W,y)P(S_{a}^{*},T_{a}^{*}|\theta^{*},W)q(\theta|\theta^{*})\alpha_{1}(*\to.)\alpha_{2}(*\to.)P(S_{a},T_{a}|W,\theta)\\ &=P(\theta^{*}|W,y)P(S_{a}^{*},T_{a}^{*}|\theta^{*},W)P((S_{a}^{*},T_{a}^{*},\theta^{*})\to(S_{a},T_{a},\theta)) \end{split}$$

So Step(a) - Step(d)  $P(\theta|W,y)P(S_a,T_a|\theta)$  as stationary distribution. So if we only keep  $\theta$ , then  $\theta$ s are distributed as  $P(\theta|W,y) = \sum_{S_a,T_a} P(\theta|W,y) P(S_a,T_a,|W,\theta)$ . Then the following proof will be exactly the same as the algorithm 1 (MH In Gibbs sampling for MJPs).  $\square$ 

#### 13. New MH algorithm for MJPs.

*Proof.* First prove that Step (a) - (c) have  $P(y|W, \theta, S_a, T_a)P(S_a, T_a|W, \theta)P(W, \theta)$ as stationary distribution.

From step(a) to step (c), W, y, S, T stay unchanged.

Step (a) - (c) is exactly a pseudo marginal MH scheme.

14. Variance Analysis on MH sampler APR 21. In this section, we consider two conditional variances,  $Var(\beta|S,T)$  and  $Var(\beta|W,y)$ . If the first one is smaller, it means that the information provided from S, T is more than the information

provided from W. Then we should prefer the MH sampler instead of the Gibbs sampler. Vice versa.

Since given  $S, T, \beta$  is distributed as  $Gamma(\omega + D, \sum_{i=0}^{d-1} \tau_i i + \theta)$ , the conditional variance

$$Var(\beta|S,T) = \frac{\omega + D}{(\sum_{i=0}^{d-1} \tau_i i + \theta)^2}.$$

For immigration model, if  $\alpha < \beta$ , then the rate of W,  $\Omega = k(d-1)\beta$ .

Then  $\beta | W, \alpha < \beta \sim Gamma(\omega + |W|, k(d-1)(T_{N+1} - T_0) + \theta)$ . So the conditional variance  $Var(\beta | W, \alpha < \beta)$  will be as follows.

$$Var(\beta|W, \alpha < \beta) = \frac{\omega + |W|}{(k(d-1)(T_{N+1} - T_0) + \theta)^2}.$$

It implies that the second conditional variance is smaller, which means we should choose the Gibbs sampler instead of the MH sampler.

# 15. Generic Metropolis Hasting using FFBS within the Gibbs Sampling On MJPs MAY1.

Assume:  $S = [S_0, S_1, ..., S_N]$ ,  $T = [t_0(t_{start}), t_1, ..., t_N, t_{N+1}(t_{end})]$ , and y as observations.

We consider a specific structure of rate matrix A.  $A_{ij} = \alpha f_{ij}(\beta)$ ,  $i \neq j$ .  $A_{ii} = -\sum_{j\neq i} A_{ij}$ .  $0 \leq f_{ij} \leq 1$ . Denote  $F_i(\beta) = \sum_{j\neq i} f_{ij}(\beta)$ .

$$P(s_0, S, T | \alpha, \beta) = \pi_0(s_0) \prod_{i=1}^N A_{S_{i-1}S_i} \exp(-\int_{t_{start}}^{t_{end}} |A_{S(t)}| dt)$$
$$= \pi_0(s_0) \alpha^N \prod_{i=1}^N f_{S_{i-1}S_i} \exp(-\alpha \sum_{i=0}^N F_{S_i}(\beta)(t_{i+1} - t_i))$$

Assume the prior distributions of  $\alpha, \beta$  are  $p_1(\alpha)$  and  $p_2(\beta)$ .

Then the posterior distribution of parameters  $\alpha, \beta$  will be as follows.

$$P(\alpha, \beta | s_0, S, T) \propto \alpha^N \prod_{i=1}^N f_{S_{i-1}S_i} \exp(-\alpha \sum_{i=0}^N F_{S_i}(\beta)(t_{i+1} - t_i)) p_1(\alpha) p_2(\beta)$$

If we assume the priors of  $\alpha$ ,  $\beta$  are  $Gamma(\mu, \lambda)$ ,  $Gamma(\omega, \theta)$ , then the posterior will have a simper form as follows.

$$P(\alpha, \beta | s_0, S, T) = C\alpha^{\mu + N - 1} \exp(-\alpha(\lambda + \sum_{i=0}^{N} F_{S_i}(\beta)(t_{i+1} - t_i))) \prod_{i=1}^{N} f_{S_{i-1}S_i}\beta^{\omega - 1} \exp(-\theta\beta)$$

We notice that given  $\beta$ , S, T,  $\alpha$  is distributed as a Gamma distribution.  $\alpha|\beta, S, T, y = \alpha|\beta, S, T \sim Gamma(\mu + N, \lambda + \sum_{i=0}^{N} F_{S_i}(\beta)(t_{i+1} - t_i))$ .

## Algorithm 7 Generic Gibbs sampling for MJPs for Gamma priors

```
Input: observations y_{[t_0,t_{k+1})}
Initialize, i = 0
(a) Set \alpha(0), \beta(0) arbitrarily and set current trajectory [S, T](0) arbitrarily.
(b) Uniformize [S, T](0), to get virtual jumps U.
repeat
  for i = 1 to N do
     (a) Sample U(i) \sim P(U|\beta(i-1), \alpha(i-1), S(i-1), T(i-1), y).
     (b) Use FFBS algorithm to sample states given all the jump times (both true
     jumps and virtual jumps). (i.e. V(i) \sim P(V|\beta(i-1), \alpha(i-1), W(i), y).) Then
     delete all the virtual jumps to get S(i), T(i).
     (c) Propose \beta^* \sim q(.|\beta(i-1)).
     Set \beta(i) = \beta^*, with probability P_{acc} = 1 \wedge \frac{P(\beta^*|S(i),T(i))}{P(\beta(i-1)|S(i),T(i))} \frac{q(\beta(i-1)|\beta^*)}{q(\beta^*|\beta(i-1))}
     Otherwise set \beta(i) = \beta(i-1).
     (d) Sample \alpha(i) \sim P(.|\beta(i), S(i), T(i), y).
     It is a Gamma(\mu + N, \lambda + \sum_{i=0}^{N} F_{S_i}(\beta)(t_{i+1} - t_i)) distribution actually.
  end for
until i = N
```

```
Algorithm 8 Generic MH In Gibbs sampling for MJPs for Gamma priors
  Input: observations y_{[t_0,t_{k+1})}
   Initialize, i = 0
   (a) Set \alpha(0), \beta(0) arbitrarily and set current trajectory [S, T](0) arbitrarily.
   (b) Uniformize [S, T](0), to get virtual jumps U.
   repeat
      for i = 1 to N do
         (a) Propose \beta^* \sim q(.|\beta(i-1)).
        Set \beta(i) = \beta^*, with probability \alpha = 1 \land \frac{P(\beta^*|W(i-1),\alpha(i-1),y)}{P(\beta(i-1)|W(i-1),\alpha(i-1),y)} \frac{q(\beta(i-1)|\beta^*)}{q(\beta^*|\beta(i-1))}
         Otherwise set \beta(i) = \beta(i-1).
         The acceptance probability is as follows.
        \alpha = 1 \wedge \frac{P(y|W(i-1), \alpha(i-1), \beta^*)p_2(\beta^*)}{P(y|W(i-1), \alpha(i-1), \beta(i-1))p_2(\beta)} \frac{q(\beta(i-1)|\beta^*)}{q(\beta^*|\beta(i-1))}
         (b) Use FFBS algorithm to sample states given all the jump times(both true
        jumps and virtual jumps). (i.e. V(i) \sim P(V|\beta(i), \alpha(i-1), W(i-1), y).) Then
         delete all the virtual jumps to get S(i), T(i).
         (c) Sample U(i) \sim P(U|\beta(i), \alpha(i-1), S(i), T(i), y).
         (d) Sample \alpha(i) \sim P(.|\beta(i), S(i), T(i), y). It is a Gamma distribution actually.
      end for
   until i = N
```

But there is no conjugate distribution to sample  $\beta \sim P(\beta|s_0, S, T)$ . We will have to use Metropolis Hasting within Gibbs to sample  $\beta$ .

$$P(\beta|S,T) = C \frac{\prod_{i=1}^{N} f_{S_{i-1}S_i}(\beta)\beta^{\omega-1} \exp(-\theta\beta)}{(\lambda + \sum_{i=0}^{N} F_{S_i}(\beta)(t_{i+1} - t_i))^{\mu+N}}$$

Now, consider a MH sampler for such models.

#### Algorithm 9 Revised Generic MH In Gibbs sampling for MJPs for Gamma priors

**Input:** observations  $y_{[t_0,t_{k+1})}$ 

Initialize, i = 0

- (a) Set  $\alpha(0)$ ,  $\beta(0)$  arbitrarily and set current trajectory [S, T](0) arbitrarily.
- (b) Uniformize [S, T](0), to get virtual jumps U.

# repeat

for i = 1 to N do

- (a)
- (i) Propose  $\beta^* \sim q(.|\beta(i-1))$ .
- (ii) Set  $\Omega = max\{F_{\Omega}(\alpha(i-1), \beta(i-1)), F_{\Omega}(\alpha(i-1), \beta^*)\}.$
- (b) Sample  $U(i) \sim P_{\Omega}(U|\beta(i), \alpha(i-1), S(i), T(i), y)$ .
- (c) Set  $\beta(i) = \beta^*$ , with probability

$$\alpha = 1 \wedge \frac{P_{\Omega}(\beta^*|W(i-1), \alpha(i-1), y)}{P_{\Omega}(\beta(i-1)|W(i-1), \alpha(i-1), y)} \frac{q(\beta(i-1)|\beta^*)}{q(\beta^*|\beta(i-1))};$$

Otherwise set  $\beta(i) = \beta(i-1)$ .

The acceptance probability is as follows.

$$\alpha = 1 \wedge \frac{P_{\Omega}(y|W(i-1),\alpha(i-1),\beta^*)p_2(\beta^*)}{P_{\Omega}(y|W(i-1),\alpha(i-1),\beta(i-1))p_2(\beta)} \frac{q(\beta(i-1)|\beta^*)}{q(\beta^*|\beta(i-1))}$$

- acceptance probability is as follows:  $\alpha = 1 \wedge \frac{P_{\Omega}(y|W(i-1),\alpha(i-1),\beta^*)p_2(\beta^*)}{P_{\Omega}(y|W(i-1),\alpha(i-1),\beta(i-1))p_2(\beta)} \frac{q(\beta(i-1)|\beta^*)}{q(\beta^*|\beta(i-1))}$  (d) Use FFBS algorithm to sample states given all the jump times(both true jumps and virtual jumps). (i.e.  $V(i) \sim P(V|\beta(i), \alpha(i-1), W(i-1), y)$ .) Then delete all the virtual jumps to get S(i), T(i).
- (e) Sample  $\alpha(i) \sim P(.|\beta(i), S(i), T(i), y)$ . It is a Gamma distribution actually. end for

until i = N

- 16. Generic Metropolis Hasting using FFBS within the Gibbs Sampling On MJPs AUG 5.
  - 17. Figures and tables.
  - 18. Bibliography and BibT<sub>E</sub>X.
  - 19. Conclusion. Appendix. The use of appendices.

Appendix A. Title of appendix.

#### REFERENCES

[1] VINAYAK RAO, YEE WHYE TEH, MCMC for continuous-time discrete-state systems, NIPS, 2012.