Personal notes – Bayesian machine learning

Tuan Anh Le

September 11, 2014

Contents

1 Probability distributions

1.1 Uniform distribution

1.2 Beta distribution

1.3 Bernoulli distribution

1.4 Binomial distribution

1.5 Beta-binomial distribution

1.6 Categorical distribution

1.7 Dirichlet distribution

1.8 Multinomial distribution

1.9 Pareto distribution

2 Bayesian parameter estimation

2.1 Beta-Bernoulli model

2.1.1 Summary

The model

$$X_i \sim \mathrm{Ber}(\theta), \text{for } i \in \{1, \dots, N\} \tag{2.1}$$

$$\mathcal{D} = \{x_1, \dots, x_N\} \tag{2.2}$$

$$N_1 = \sum_{i=1}^{N} \mathbb{I}(x_i = 1) \tag{2.3}$$

$$N_0 = \sum_{i=1}^{N} \mathbb{I}(x_i = 0) \tag{2.4}$$

Likelihood

$$p(\mathcal{D}|\theta) = \theta^{N_1}(1-\theta)^{N_0} \tag{2.5}$$

Prior

$$p(\theta) = \mathrm{Beta}(\theta|a, b) \tag{2.6}$$

Posterior

$$p(\theta|\mathcal{D}) = \mathrm{Beta}(\theta|a' = N_1 + a, b' = N_0 + b) \tag{2.7}$$

Posterior predictive

$$p(\tilde{x} = 1|\mathcal{D}) = \frac{a'}{a' + b'} \tag{2.8}$$

Evidence

2.1.2 Derivations

2.2 Beta-binomial model

2.2.1 Summary

The model

$$N_1 \sim \mathrm{Bin}(N, \theta) \tag{2.9}$$

$$\begin{aligned}
\mathcal{D} &= \{N_1, N\} && (2.10)\\
N_1 &= \text{number of successes} && (2.11)\\
N &= \text{total number of trials} && (2.12)\\
\tilde{\mathcal{D}} &= \{\tilde{N}_1, \tilde{N}\} && (2.13)\\
\tilde{N}_1 &= \text{number of successes in a new batch of data} && (2.14)\\
\tilde{N} &= \text{total number of trials in a new batch of data} && (2.15)
\end{aligned}$$

Likelihood

$$p(\mathcal{D}|\theta) = \mathrm{Bin}(N_1|N, \theta) \tag{2.16}$$

Prior

$$p(\theta) = \mathrm{Beta}(\theta|a, b) \tag{2.17}$$

Posterior

$$p(\theta|\mathcal{D}) = \mathrm{Beta}(\theta|a' = N_1 + a, b' = N_0 + b) \tag{2.18}$$

Posterior predictive

$$p(\tilde{\mathcal{D}}|\mathcal{D}) = \mathrm{Bb}(\tilde{N}_1; a', b', \tilde{N}) \tag{2.19}$$

Evidence

2.2.2 Derivations

2.3 Dirichlet-categorical model

2.3.1 Summary

The model

$$\begin{aligned}
X_i &\sim \mathrm{Cat}\left(\boldsymbol{\theta} = (\theta_1, \ldots, \theta_K)^T\right), \text{for } i \in \{1, \ldots, N\} && (2.20)\\
\mathcal{D} &= \{x_1, \ldots, x_N\} && (2.21)\\
n_k &= \sum_{i=1}^{N} \mathbb{I}(x_i = k) && (2.22)
\end{aligned}$$

Likelihood

$$p(\mathcal{D}|\theta) = \prod_{k=1}^{K} \theta_k^{n_k} \tag{2.23}$$

Prior

$$p(\theta) = \mathrm{Dir}(\boldsymbol{\theta}; \boldsymbol{\alpha}) \tag{2.24}$$

Posterior

$$p(\theta|\mathcal{D}) = \text{Dir}\left(\boldsymbol{\theta}; \boldsymbol{\alpha}' = \boldsymbol{\alpha} + (n_1, \ldots, n_K)^T\right) \tag{2.25}$$

Posterior predictive

$$p(\tilde{X} = j|\mathcal{D}) = \frac{\alpha'_j}{\sum_{k=1}^{K} \alpha'_i} \tag{2.26}$$

$$= \frac{\alpha_j + n_j}{\alpha_0 + N} \tag{2.27}$$

$$\text{where } \alpha_0 = \sum_{k=1}^{K} \alpha_k \tag{2.28}$$

Evidence

2.3.2 Derivations

2.4 Dirichlet-multinomial model

2.4.1 Summary

The model

$$\mathbf{N} \sim \text{Mult}(N, \boldsymbol{\theta}) \in \mathbb{R}^K \tag{2.29}$$

$$\mathcal{D} = \{\mathbf{n} = \text{vector of counts of successes}\} \tag{2.30}$$

$$N = \sum_{i=1}^{K} n_i \tag{2.31}$$

$$\tilde{\mathcal{D}} = \{\tilde{\mathbf{n}} = \text{vector of counts of successes in a new batch of data}\} \tag{2.32}$$

$$\tilde{N} = \sum_{i=1}^{K} \tilde{n}_i \tag{2.33}$$

Likelihood

$$p(\mathcal{D}|\theta) = \text{Mult}(\mathbf{n}; N, \boldsymbol{\theta}) \tag{2.34}$$

Prior

$$p(\theta) = \text{Dir}(\boldsymbol{\theta}; \boldsymbol{\alpha}) \tag{2.35}$$

Posterior

$$p(\theta|\mathcal{D}) = \text{Dir}\left(\boldsymbol{\theta}; \boldsymbol{\alpha}' = \boldsymbol{\alpha} + (n_1, \ldots, n_K)^T\right) \tag{2.36}$$

Posterior predictive

$$p(\tilde{\mathcal{D}}|\mathcal{D}) = \frac{\Gamma(\alpha_0 + N)}{\Gamma(\alpha_0 + N + \tilde{N})} \prod_{k=1}^{K} \frac{\Gamma(\alpha_k + n_k + \tilde{n}_k)}{\Gamma(\alpha_k + n_k)} \tag{2.37}$$

$$\text{where } \alpha_0 = \sum_{k=1}^{K} \alpha_k \tag{2.38}$$

Evidence

$$p(\mathcal{D}|\boldsymbol{\alpha}) = \frac{\Gamma(\alpha_0)}{\Gamma(\alpha_0 + N)} \prod_{k=1}^{K} \frac{\Gamma(\alpha_k + n_k)}{\Gamma(\alpha_k)} \tag{2.39}$$

2.4.2 Derivations

2.5 Poisson-gamma model

2.5.1 Summary

The model

$$x \sim \text{Poi}(\lambda) \tag{2.40}$$

$$\mathcal{D} = \{x_1, \ldots, x_N\} \tag{2.41}$$

Likelihood

$$p(\mathcal{D}|\lambda) = \prod_{i=1}^{N} \frac{\lambda^{x_i}}{x_i!} \exp(-\lambda) \tag{2.42}$$

Prior

$$p(\lambda) = \text{Gamma}(\lambda; a, b) \tag{2.43}$$

Posterior

$$p(\lambda|\mathcal{D}) = \text{Gamma}\left(\lambda; a' = a + \sum_{i=1}^{N} x_i, b' = b + N\right) \tag{2.44}$$

Posterior predictive

$$p(\tilde{x}|\mathcal{D}) = \text{NB}\left(\tilde{x}|a', \frac{1}{1 + b'}\right) \tag{2.45}$$

Evidence

$$p(\mathcal{D}) = \tag{2.46}$$

2.5.2 Derivations

3 Advanced models

3.1 Gaussian mixture model

3.2 Factor analysis

3.3 Hidden Markov model

3.4 Linear regression

3.5 Logistic regression

3.6 Latent Dirichlet allocation

3.7 Linear dynamical systems

3.8 Principal components analysis

3.9 Independent components analysis

4 Sampling algorithms

4.1 Introduction

Let p be a probability distribution with a pdf $p(\mathbf{x}), \mathbf{x} \in \mathcal{X}$ (usually $\mathcal{X} = \mathbb{R}^D, D \in \mathbb{N}$), which we assume can be evaluated within a multiplicative factor (i.e. we can only evaluate $p^*(\mathbf{x}) = Z_p p(\mathbf{x})$, where $Z_p = \int_{\mathcal{X}} p^*(\mathbf{x})\,\mathrm{d}\mathbf{x}$). We want to achieve the following:

Problem 1 Generate samples $\{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(R)}\}, R \in \mathbb{N}$ (we will use the shorthand notation $\{\mathbf{x}^{(r)}\}$ from now) from the probability distribution p.

Problem 2 Estimate the expectation of an arbitrary function f given $\mathbf{x} \sim p$, $\mathrm{E}_{\mathbf{x}\sim p}[f(\mathbf{x})]$ (we will use the shorthand notation $\mathrm{E}[f]$ from now).

4.2 Rejection sampling

Assume we can sample from a proposal distribution q with a pdf $q(\mathbf{x})$, which can be evaluated within a multiplicative factor (i.e. we can only evaluate $q^*(\mathbf{x}) = Z_q q(\mathbf{x})$). Also assume we know the value of a constant c such that

$$cq^*(\mathbf{x}) > p^*(\mathbf{x}) \text{ for all } \mathbf{x} \tag{4.1}$$

The procedure that generates a sample $\mathbf{x} \sim p$ is described in Algorithm 1 below.

Algorithm 1 Rejection sampling

```
1: Generate $\mathbf{x} \sim q$.
2: Generate $u \sim \mathrm{Unif}(0, cq^*(\mathbf{x}))$.
3: If $u > p^*(\mathbf{x})$ it is rejected, otherwise it is accepted.
```

4.2.1 Why it works?

Assume $\mathbf{x} \in \mathbb{R}^D$. Define sets $\mathcal{X}$ and $\mathcal{X}'$ to be

$$\mathcal{X} = \left\{\boldsymbol{\alpha} \in \mathbb{R}^{d+1} : \alpha_{1:d} \in \mathbb{R}^d, \alpha_{d+1} \in [0, cq^*(\boldsymbol{\alpha})]\right\} \tag{4.2}$$

$$\mathcal{X}' = \left\{\boldsymbol{\alpha} \in \mathbb{R}^{d+1} : \alpha_{1:d} \in \mathbb{R}^d, \alpha_{d+1} \in [0, p^*(\boldsymbol{\alpha})]\right\} \tag{4.3}$$

Note that $\mathcal{X}' \subseteq \mathcal{X}$.

By definition, $\mathcal{X}$ is the support of $(\mathbf{x}, u)$. The probability of $(\mathbf{x}, u)$ can be expressed as

$$\Pr(\mathbf{x}, u) = \Pr(\mathbf{x}) \Pr(u) \tag{4.4}$$

$$= q(\mathbf{x}) \frac{1}{cq^*(\mathbf{x})} \tag{4.5}$$

$$= q(\mathbf{x}) \frac{1}{cZ_q q(\mathbf{x})} \tag{4.6}$$

$$= \frac{1}{cZ_q} \tag{4.7}$$

which is constant w.r.t. $(\mathbf{x}, u)$, i.e.

$$(\mathbf{x}, u) \sim \text{Unif}(\mathcal{X}) \tag{4.8}$$

Let $(\mathbf{x}', u')$ be the value of $(\mathbf{x}, u)$ that gets accepted. By definition, $\mathcal{X}'$ is the support of $(\mathbf{x}', u')$:

$$(\mathbf{x}', u') = \begin{cases} (\mathbf{x}, u) & \text{if } (\mathbf{x}, u) \in \mathcal{X}' \\ \text{nothing} & \text{otherwise.} \end{cases} \tag{4.9}$$

The probability of $(\mathbf{x}', u')$ can be expressed as

$$\Pr(\mathbf{x}', u') = \begin{cases} \Pr(\mathbf{x}, u) & \text{if } (\mathbf{x}, u) \in \mathcal{X}' \\ 0 & \text{otherwise.} \end{cases} \tag{4.10}$$

which means

$$(\mathbf{x}', u') \sim \text{Unif}(\mathcal{X}') \tag{4.11}$$

Working backwards

$$\Pr(\mathbf{x}') = \frac{\Pr(\mathbf{x}', u')}{\Pr(u')} \tag{4.12}$$

$$\propto \frac{1}{1/p^*(\mathbf{x}')} \tag{4.13}$$

$$\propto p^*(\mathbf{x}') \tag{4.14}$$

Hence the accepted $\mathbf{x}$, $\mathbf{x}'$ is $\sim p$.

4.3 Importance sampling

Assume we can sample from a proposal distribution q with a pdf $q(\mathbf{x})$, which can be evaluated within a multiplicative factor (i.e. we can only evaluate $q^*(\mathbf{x}) = Z_q q(\mathbf{x})$). To solve problem 2, we follow Algorithm 2 below.

Algorithm 2 Importance sampling

```
1: Generate samples from $q$, $\{\mathbf{x}^{(r)}\}$.
2: Calculate importance weights $w_r = \frac{p^*(\mathbf{x}^{(r)})}{q^*(\mathbf{x}^{(r)})}$.
3: $\hat{\mathbf{y}} = \frac{\sum_r w_r f(\mathbf{x}^{(r)})}{\sum_r w_r}$ is the estimator of $\mathrm{E}[f]$.
```

4.3.1 Convergence of estimator as R increases

We want to prove that if $q(\mathbf{x})$ is non-zero for all $\mathbf{x}$ where $p(\mathbf{x})$ is non-zero, the estimator $\hat{\mathbf{y}}$ converges to $\mathrm{E}[f]$, as R increases. We consider the the expectations of the numerator and denominator separately:

$$
\begin{aligned}
\mathrm{E}_q[\text{numer}] &= \mathrm{E}_q\left[\sum_r w_r f(\mathbf{x}^{(r)})\right] && (4.15)\\
&= \sum_r \mathrm{E}_q\left[w_r f(\mathbf{x}^{(r)})\right] && (4.16)\\
&= \sum_r \mathrm{E}_q\left[\frac{p^*(\mathbf{x}^{(r)})}{q^*(\mathbf{x}^{(r)})} f(\mathbf{x}^{(r)})\right] && (4.17)\\
&= \sum_r \mathrm{E}_q\left[\frac{Z_p p(\mathbf{x}^{(r)})}{Z_q q(\mathbf{x}^{(r)})} f(\mathbf{x}^{(r)})\right] && (4.18)\\
&= \frac{Z_p}{Z_q}\sum_r \int_{\mathbf{x}^{(r)}} p(\mathbf{x}^{(r)}) f(\mathbf{x}^{(r)})\,\mathrm{d}\mathbf{x}^{(r)} && (4.19)\\
&= \frac{Z_p}{Z_q}\sum_r \mathrm{E}_p\left[f(\mathbf{x}^{(r)})\right] && (4.20)\\
&= \frac{Z_p}{Z_q} R\,\mathrm{E}_p\left[f(\mathbf{x})\right] && (4.21)\\
\mathrm{E}_q[\text{denom}] &= \mathrm{E}_q\left[\sum_r w_r\right] && (4.22)\\
&= \sum_r \mathrm{E}_q\left[\frac{p^*(\mathbf{x}^{(r)})}{q^*(\mathbf{x}^{(r)})}\right] && (4.23)\\
&= \sum_r \mathrm{E}_q\left[\frac{Z_p p(\mathbf{x}^{(r)})}{Z_q q(\mathbf{x}^{(r)})}\right] && (4.24)\\
&= \frac{Z_p}{Z_q}\sum_r \int_{\mathbf{x}^{(r)}} p(\mathbf{x}^{(r)})\,\mathrm{d}\mathbf{x}^{(r)} && (4.25)\\
&= \frac{Z_p}{Z_q} R && (4.26)
\end{aligned}
$$

Hence $\hat{\mathbf{y}}$ converges to $\mathrm{E}_p[f]$ as R increases (but is not necessarily an unbiased estimator because $\mathrm{E}_q[\hat{\mathbf{y}}]$ is not necessarily $= \mathrm{E}_p[f]$).

4.3.2 Optimal proposal distribution

Assuming we can evaluate $p(\mathbf{x})$ and $q(\mathbf{x})$, we want to find a proposal distribution q to minimise the variance of the weighted samples

$$
\mathrm{var}_q\left[\frac{p(\mathbf{x})}{q(\mathbf{x})} f(\mathbf{x})\right] = \mathrm{E}_q\left[\frac{p^2(\mathbf{x})}{q^2(\mathbf{x})} f^2(\mathbf{x})\right] - \left(\mathrm{E}_q\left[\frac{p(\mathbf{x})}{q(\mathbf{x})} f(\mathbf{x})\right]\right)^2 \qquad (4.27)
$$

$$= \mathrm{E}_q\left[\frac{p^2(\mathbf{x})}{q^2(\mathbf{x})} f^2(\mathbf{x})\right] - \left(\mathrm{E}_p\left[f(\mathbf{x})\right]\right)^2 \tag{4.28}$$

The second part is independent of q so we can ignore it. By Jensen's inequality, we have $\mathrm{E}\left[g(u(\mathbf{x}))\right] \geq g\left(\mathrm{E}\left[u(\mathbf{x})\right]\right)$ for $u(\mathbf{x}) \geq 0$ where $g : x \mapsto x^2$. Setting $u(\mathbf{x}) = p(\mathbf{x})|f(\mathbf{x})|/q(\mathbf{x})$, we have the following lower bound:

$$\mathrm{E}_q\left[\frac{p^2(\mathbf{x})}{q^2(\mathbf{x})} f^2(\mathbf{x})\right] \geq \left(\mathrm{E}_q\left[\frac{p(\mathbf{x})}{q(\mathbf{x})}|f(\mathbf{x})|\right]\right)^2 = \left(\mathrm{E}_p[|f(\mathbf{x})|]\right)^2 \tag{4.29}$$

with the equality when $u(\mathbf{x}) = \text{const.} \implies q_{\text{optimal}}(\mathbf{x}) \propto |f(\mathbf{x})|p(\mathbf{x})$. Taking care of normalisation, we get

$$q_{\text{optimal}}(\mathbf{x}) = \frac{|f(\mathbf{x})|p(\mathbf{x})}{\int |f(\mathbf{x}')|p(\mathbf{x}')\,\mathrm{d}\mathbf{x}'} \tag{4.30}$$

4.4 Sampling importance resampling

In Sampling importance resampling (SIR), we approximate the pdf of p as point masses and resample from them to get samples approximately $\sim p$. The process is described in Algorithm 3 below.

Algorithm 3 Sampling importance resampling

```
Generate samples $\left\{\mathbf{x}^{(r)}\right\}$ from $q$.
Calculate importance weights $\left\{w_r = \frac{p^*(\mathbf{z}^{(r)})}{q^*(\mathbf{z}^{(r)})}\right\}$.
Calculate the normalised importance weights $\left\{\hat{w}_r = \frac{w_r}{\sum_{r'} w_{r'}}\right\}$. Note that $\sum_r \hat{w}_r = 1$.
We can resample from
    $\hat{p}(\mathrm{d}\mathbf{x}) = \sum_r \hat{w}_r \delta_{\mathbf{x}^{(r)}}(\mathrm{d}\mathbf{x})$        (4.31)
  to estimate sampling from $p(\mathbf{x})$.
```

4.4.1 Why it works?

We consider the univariate case (to do: general case) as the number of proposal samples (particles) $R \to \infty$. We can express the number of proposal samples that are in the interval $\lim_{\delta x \to 0}[x, x + \delta x]$, $N(x)$, to be

$$N(x) = \lim_{\delta x \to 0} Rq(x)\delta x \tag{4.32}$$

We can express the probability of the one final sample, $x^{(r)}$ being in the interval $\lim_{\delta x \to 0}[x, x + \delta x]$ to be

$$\lim_{\delta x \to 0} \Pr(x \leq x^{(r)} \leq x + \delta x) = N(x)\hat{w}_r \tag{4.33}$$

$$\propto \lim_{\delta x \to 0} Rq(x)\delta x \frac{p(x)}{q(x)} \tag{4.34}$$

$$\propto \lim_{\delta x \to 0} p(x)\delta x \tag{4.35}$$

Hence (to do: why exactly does that result in an integral)

$$\begin{aligned}
\Pr(a \leq x^{(r)} \leq b) &\propto \int_a^b p(x)\,\mathrm{d}x && (4.36)\\
\implies x^{(r)} &\sim p && (4.37)
\end{aligned}$$

4.5 Particle filtering

4.5.1 Sequential importance sampling (SIS)

Assume the probabilistic graphical model similar to the one in HMMs, where

- $\mathrm{x}_t, \mathrm{x}_t \subset \mathcal{X}^D$ and $\mathbf{y}_t, \mathbf{y}_t \subset \mathcal{Y}^D$ are the hidden and observed random variables at time $t, t = 1, \ldots, T$.
- The initial state is characterised by $\mathrm{x}_1 \sim \mu(\cdot \mid \boldsymbol{\theta})$ for some known parameter $\boldsymbol{\theta} \subset \Theta$.
- The transitions are characterised by $\mathrm{x}_t \mid \mathrm{x}_{t-1} \sim f(\cdot \mid \mathrm{x}_{t-1}; \boldsymbol{\theta})$.
- The emmissions are characterised by $\mathbf{y}_t \mid \mathrm{x}_t \sim g(\cdot \mid \mathrm{x}_t; \boldsymbol{\theta})$.

We want to sample from the distribution $p(\mathrm{x}_{1:t} \mid \mathbf{y}_{1:t}; \boldsymbol{\theta})$. Assume we can sample from the probability distribution with the pdf of the following form

$$\begin{aligned}
q(\mathrm{x}_{1:t} \mid \mathbf{y}_{1:t}; \boldsymbol{\theta}) &= q(\mathrm{x}_t \mid \mathrm{x}_{1:t-1}, \mathbf{y}_{1:t}; \boldsymbol{\theta}) q(\mathrm{x}_{1:t-1} \mid \mathbf{y}_{1:t}; \boldsymbol{\theta}) && (4.38)\\
&= q(\mathrm{x}_t \mid \mathrm{x}_{1:t-1}, \mathbf{y}_{1:t}; \boldsymbol{\theta}) q(\mathrm{x}_{1:t-1} \mid \mathbf{y}_{1:t-1}; \boldsymbol{\theta}) && (4.39)\\
&= q(\mathrm{x}_t \mid \mathrm{x}_{t-1}, \mathbf{y}_t; \boldsymbol{\theta}) && (4.40)
\end{aligned}$$

If we express the pdf of p for $t = 1, \ldots, T$ in the form of (for convenience, we drop the conditional dependency on $\boldsymbol{\theta}$):

$$\begin{aligned}
p(\mathrm{x}_{1:t} \mid \mathbf{y}_{1:t}) &= \frac{p(\mathbf{y}_{1:t} \mid \mathrm{x}_{1:t}) p(\mathrm{x}_{1:t})}{p(\mathbf{y}_{1:t})} && (4.41)\\
&= \frac{p(\mathbf{y}_t \mid \mathrm{x}_{1:t}, \mathbf{y}_{1:t-1}) p(\mathbf{y}_{1:t-1} \mid \mathrm{x}_{1:t}) p(\mathrm{x}_{1:t})}{p(\mathbf{y}_t \mid \mathbf{y}_{1:t-1}) p(\mathbf{y}_{1:t-1})} && (4.42)\\
&= \frac{p(\mathbf{y}_t \mid \mathrm{x}_{1:t}, \mathbf{y}_{1:t-1}) p(\mathrm{x}_{1:t} \mid \mathbf{y}_{1:t-1})}{p(\mathbf{y}_t \mid \mathbf{y}_{1:t-1})} && (4.43)\\
&= \frac{p(\mathbf{y}_t \mid \mathrm{x}_{1:t}, \mathbf{y}_{1:t-1}) p(\mathrm{x}_t \mid \mathrm{x}_{1:t-1}, \mathbf{y}_{1:t-1}) p(\mathrm{x}_{1:t-1} \mid \mathbf{y}_{1:t-1})}{p(\mathbf{y}_t \mid \mathbf{y}_{1:t-1})} && (4.44)\\
&= \frac{p(\mathbf{y}_t \mid \mathrm{x}_t) p(\mathrm{x}_t \mid \mathrm{x}_{t-1}) p(\mathrm{x}_{1:t-1} \mid \mathbf{y}_{1:t-1})}{p(\mathbf{y}_t \mid \mathbf{y}_{1:t-1})} && (4.45)\\
&\propto p(\mathbf{y}_t \mid \mathrm{x}_t) p(\mathrm{x}_t \mid \mathrm{x}_{t-1}) p(\mathrm{x}_{1:t-1} \mid \mathbf{y}_{1:t-1}) && (4.46)
\end{aligned}$$

$$= g(\mathbf{y}_t \mid \mathbf{x}_t) f(\mathbf{x}_t \mid \mathbf{x}_{t-1}) p(\mathbf{x}_{1:t-1} \mid \mathbf{y}_{1:t-1}) \tag{4.47}$$

we can write the weight of the sample $\mathbf{x}_{1:t}^{(r)}$ from the proposal q to be

$$w_t^{(r)} \propto \frac{p\left(\mathbf{x}_{1:t}^{(r)} \mid \mathbf{y}_{1:t}\right)}{q\left(\mathbf{x}_{1:t}^{(r)} \mid \mathbf{y}_{1:t}\right)} \tag{4.48}$$

$$\propto \frac{p\left(\mathbf{y}_t \mid \mathbf{x}_t^{(r)}\right) p\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}\right) p\left(\mathbf{x}_{1:t-1}^{(r)} \mid \mathbf{y}_{1:t-1}\right)}{q\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t\right) q\left(\mathbf{x}_{1:t-1}^{(r)} \mid \mathbf{y}_{1:t-1}\right)} \tag{4.49}$$

$$= w_{t-1}^{(r)} \frac{p\left(\mathbf{y}_t \mid \mathbf{x}_t^{(r)}\right) p\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}\right)}{q\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t\right)} \tag{4.50}$$

$$= w_{t-1}^{(r)} \frac{g\left(\mathbf{y}_t \mid \mathbf{x}_t^{(r)}\right) f\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}\right)}{q\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t\right)} \tag{4.51}$$

For $t = 1$

$$w_1^{(r)} \propto \frac{p\left(\mathbf{x}_1^{(r)} \mid \mathbf{y}_1\right)}{q\left(\mathbf{x}_1^{(r)} \mid \mathbf{y}_1\right)} \tag{4.52}$$

$$\propto \frac{p\left(\mathbf{x}_1^{(r)}, \mathbf{y}_1\right)}{q\left(\mathbf{x}_1^{(r)} \mid \mathbf{y}_1\right)} \tag{4.53}$$

$$\propto \frac{p\left(\mathbf{y}_1 \mid \mathbf{x}_1^{(r)}\right) p\left(\mathbf{x}_1^{(r)}\right)}{q\left(\mathbf{x}_1^{(r)} \mid \mathbf{y}_1\right)} \tag{4.54}$$

$$= \frac{g\left(\mathbf{y}_1 \mid \mathbf{x}_1^{(r)}\right) \mu\left(\mathbf{x}_1^{(r)}\right)}{q\left(\mathbf{x}_1^{(r)} \mid \mathbf{y}_1\right)} \tag{4.55}$$

Note that second line is proportional to the first line with respect to $p(\mathbf{y}_1)$ which is justifiable because the the constant of proportionality cancels out during the normalisation step. The algorithm for SIS is shown in Algorithm 4 below.

Algorithm 4 Sequential importance sampling

```
1: Sample from proposal                                        ▷ Initialisation
       $$\mathbf{x}_1^{(r)} \sim q\left(\cdot \mid \mathbf{y}_1^{(r)}, \boldsymbol{\theta}\right), r = 1, \ldots, R \tag{4.56}$$
2: Compute weights
       $$w_1^{(r)} \propto \frac{g\left(\mathbf{y}_1 \mid \mathbf{x}_1^{(r)}\right) \mu\left(\mathbf{x}_1^{(r)}\right)}{q\left(\mathbf{x}_1^{(r)} \mid \mathbf{y}_1\right)}, r = 1, \ldots, R \tag{4.57}$$
```

```
Normalise weights
    $$\hat{w}_1^{(r)} = \frac{w_1^{(r)}}{\sum_{r'} w_1^{(r')}}, r = 1, \dots, R \tag{4.58}$$
We can resample from
    $$\hat{p}(\mathrm{d}\mathbf{x}_1 \mid \mathbf{y}_1, \boldsymbol{\theta}) = \sum_r \hat{w}_1^{(r)} \delta_{\mathbf{x}_1^{(r)}}(\mathrm{d}\mathbf{x}_1) \tag{4.59}$$
to estimate
    $$p(\mathbf{x}_1 \mid \mathbf{y}_1, \boldsymbol{\theta}) \tag{4.60}$$
for $t = 2, \dots, T$ do                                              ▷ Main loop
    Compute weights
        $$w_t^{(r)} \propto w_{t-1}^{(r)} \frac{g\left(\mathbf{y}_t \mid \mathbf{x}_t^{(r)}, \boldsymbol{\theta}\right) f\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{A_{t-1}^{(r)}}, \boldsymbol{\theta}\right)}{q\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{A_{t-1}^{(r)}}, \mathbf{y}_t, \boldsymbol{\theta}\right)}, r = 1, \dots, R \tag{4.61}$$
    Normalise weights
        $$\hat{w}_t^{(r)} = \frac{w_t^{(r)}}{\sum_{r'} w_t^{(r')}}, r = 1, \dots, R \tag{4.62}$$
    We can resample from
        $$\hat{p}(\mathrm{d}\mathbf{x}_{1:t} \mid \mathbf{y}_{1:t}, \boldsymbol{\theta}) = \sum_r \hat{w}_t^{(r)} \delta_{\mathbf{x}_{1:t}^{(r)}}(\mathrm{d}\mathbf{x}_{1:t}) \tag{4.63}$$
    to estimate
        $$p(\mathbf{x}_{1:t} \mid \mathbf{y}_{1:t}, \boldsymbol{\theta}) \tag{4.64}$$
```

The reason why it works is the same as in the case of Sampling importance resampling described in section 4.4.

4.5.2 The degeneracy problem

Because the support of the pdf we are approximating ($p(\mathbf{x}_{1:t} \mid \mathbf{y}_{1:t})$) is growing, the constant number of weights we use (R) won't be sufficient after a while. This is because many weights will become very negligible, wasting our resources. An **effective sample size** is used to measure this degeneracy is defined to be and approximated by the following:

$$S_{\text{eff}} \triangleq \frac{S}{1 + \operatorname{var}\left[{w_t^{(r)}}^*\right]} \tag{4.65}$$

$$\hat{S}_{\text{eff}} \approx \frac{1}{\sum_r \left(w_t^{(r)}\right)^2} \tag{4.66}$$

where $w_t^{(r)^*} = p(\mathbf{x}_t^{(r)} \mid \mathbf{y}_{1:t}) / q(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t)$ is the “true weight” of particle r.

There are (among others) two solutions to this problem – introduce the resampling step, and using a good proposal distribution.

4.5.3 The resampling step

Whenever the effective sample size drops below some threshold, resample to get new R samples from the approximation of the pdf. This step is also called **rejuvenation**. The full algorithm for a generic particle filter is shown in Algorithm 5 below in which we resample during every tie step.

Algorithm 5 Generic particle filter

```
Sample from proposal                                              ▷ Initialisation
        $\mathbf{x}_1^{(r)} \sim q\left(\cdot \mid \mathbf{y}_1^{(r)}, \boldsymbol{\theta}\right), r = 1, \dots, R \qquad (4.67)$
Compute weights
        $w_1^{(r)} \propto \frac{p\left(\mathbf{x}_1^{(r)} \mid \mathbf{y}_1, \boldsymbol{\theta}\right)}{q\left(\mathbf{x}_1^{(r)} \mid \mathbf{y}_1, \boldsymbol{\theta}\right)}, r = 1, \dots, R \qquad (4.68)$
Normalise weights
        $\hat{w}_1^{(r)} = \frac{w_1^{(r)}}{\sum_{r'} w_1^{(r')}}, r = 1, \dots, R \qquad (4.69)$
We can resample from
        $\hat{p}(\mathrm{d}\mathbf{x}_1 \mid \mathbf{y}_1, \boldsymbol{\theta}) = \sum_r \hat{w}_1^{(r)} \delta_{\mathbf{x}_1^{(r)}}(\mathrm{d}\mathbf{x}_1) \qquad (4.70)$
    to estimate
        $p(\mathbf{x}_1 \mid \mathbf{y}_1, \boldsymbol{\theta}) \qquad (4.71)$
for $t = 2, \dots, T$ do                                           ▷ Main loop
    Sample parents' indices of $t^{\text{th}}$ generation
        $A_{t-1}^{(r)} \sim \text{Cat}\left(\hat{w}_{t-1}\right), r = 1, \dots, R \qquad (4.72)$
    Sample $t^{\text{th}}$ generation using corresponding parents
        $\mathbf{x}_t^{(r)} \sim q\left(\cdot \mid \mathbf{x}_{t-1}^{A_{t-1}^{(r)}}, \mathbf{y}_t, \boldsymbol{\theta}\right), r = 1, \dots, R \qquad (4.73)$
    Compute weights
        $w_t^{(r)} \propto w_{t-1}^{(r)} \frac{g\left(\mathbf{y}_t \mid \mathbf{x}_t^{(r)}, \boldsymbol{\theta}\right) f\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{A_{t-1}^{(r)}}, \boldsymbol{\theta}\right)}{q\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{A_{t-1}^{(r)}}, \mathbf{y}_t, \boldsymbol{\theta}\right)}, r = 1, \dots, R \qquad (4.74)$
    Normalise weights
        $\hat{w}_t^{(r)} = \frac{w_t^{(r)}}{\sum_{r'} w_t^{(r')}}, r = 1, \ldots, R \qquad (4.75)$
    We can resample from
        $\hat{p}(\mathrm{d}\mathbf{x}_{1:t} \mid \mathbf{y}_{1:t}, \boldsymbol{\theta}) = \sum_{r} \hat{w}_t^{(r)} \delta_{\mathbf{x}_{1:t}^{(r)}}(\mathrm{d}\mathbf{x}_{1:t}) \qquad (4.76)$
  to estimate
        $p(\mathbf{x}_{1:t} \mid \mathbf{y}_{1:t}, \boldsymbol{\theta}) \qquad (4.77)$
```

4.5.4 Particle filter animation

4.5.5 The proposal distribution

It is common to use the following proposal distribution

$$\begin{aligned} q\left(\mathbf{x}_{1:t}^{(r)} \mid \mathbf{y}_{1:t}\right) &= q\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t\right) && (4.78) \\ &= p\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}\right) && (4.79) \\ &= f\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}\right) && (4.80) \end{aligned}$$

Hence the weight equation in (4.51) becomes

$$\begin{aligned} w_t^{(r)} &\propto w_{t-1}^{(r)} \frac{g\left(\mathbf{y}_t \mid \mathbf{x}_t^{(r)}\right) f\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}\right)}{q\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t\right)} && (4.81) \\ &= w_{t-1}^{(r)} g\left(\mathbf{y}_t \mid \mathbf{x}_t^{(r)}\right) && (4.82) \end{aligned}$$

This approach can be **i**nefficient because the likelihood, $p\left(\mathbf{y}_t \mid \mathbf{x}_t^{(r)}\right)$, can be very small at many places meaning many of the particles will be very small.

The optimal proposal distribution has the form

$$\begin{aligned} q\left(\mathbf{x}_{1:t}^{(r)} \mid \mathbf{y}_{1:t}\right) &= q\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t\right) && (4.83) \\ &= p\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t\right) && (4.84) \\ &= \frac{p\left(\mathbf{y}_t \mid \mathbf{x}_t, \mathbf{x}_{t-1}^{(r)}\right) p\left(\mathbf{x}_t, \mathbf{x}_{t-1}^{(r)}\right)}{p\left(\mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t\right)} && (4.85) \\ &= \frac{p\left(\mathbf{y}_t \mid \mathbf{x}_t\right) p\left(\mathbf{x}_t \mid \mathbf{x}_{t-1}^{(r)}\right)}{p\left(\mathbf{y}_t \mid \mathbf{x}_{t-1}^{(r)}\right)} && (4.86) \\ &= \frac{g\left(\mathbf{y}_t \mid \mathbf{x}_t\right) f\left(\mathbf{x}_t \mid \mathbf{x}_{t-1}^{(r)}\right)}{p\left(\mathbf{y}_t \mid \mathbf{x}_{t-1}^{(r)}\right)} && (4.87) \end{aligned}$$

The weight equation in (4.51) becomes

$$\begin{aligned} w_t^{(r)} &\propto w_{t-1}^{(r)} p\left(\mathbf{y}_t \mid \mathbf{x}_{t-1}^{(r)}\right) && (4.88) \\ &= w_{t-1}^{(r)} \int p\left(\mathbf{y}_t, \mathbf{x}_t' \mid \mathbf{x}_{t-1}^{(r)}\right) \mathrm{d}\mathbf{x}' && (4.89) \\ &= w_{t-1}^{(r)} \int p\left(\mathbf{y}_t \mid \mathbf{x}_t', \mathbf{x}_{t-1}^{(r)}\right) p\left(\mathbf{x}_t' \mid \mathbf{x}_{t-1}^{(r)}\right) \mathrm{d}\mathbf{x}' && (4.90) \\ &= w_{t-1}^{(r)} \int p\left(\mathbf{y}_t \mid \mathbf{x}_t'\right) p\left(\mathbf{x}_t' \mid \mathbf{x}_{t-1}^{(r)}\right) \mathrm{d}\mathbf{x}' && (4.91) \end{aligned}$$

$$= w_{t-1}^{(r)} \int g\left(\mathbf{y}_t \mid \mathbf{x}'_t\right) f\left(\mathbf{x}'_t \mid \mathbf{x}_{t-1}^{(r)}\right) \mathrm{d}\mathbf{x}' \tag{4.92}$$

The proposal distribution is optimal because for any fixed $\mathbf{x}_{t-1}^{(r)}$, the new weight $w_t^{(r)}$ takes the same value regardless of the value drawn for $\mathbf{x}_t^{(r)}$. Hence, conditional on the old values, the variance of true weights is zero.

4.6 Sequential Monte Carlo

(to do: improve to be more rigorous)

Assume that at time t, we can extend a particle's path using a Markov kernel M_t:

$$p_t(x_t) = p_{t-1}(x_{t-1}) M_t(x_{t-1}, x_t) \tag{4.93}$$

Also assume that

$$\tilde{p}_t(x_{0:t}) = p_t(x_t) \sum_{k=1}^{t} L_k(x_k, x_{k-1}) \tag{4.94}$$

where $\{L_k\}$ is a sequence of auxiliary Markov transition kernels.

The generic algorithm for Sequential Monte Carlo (SMC) can be found in Algorithm 6.

Algorithm 6 Generic Sequential Monte Carlo

```
Initialisation, $t = 0$:
for $r = 1, \dots, R$ do                                                ▷ Sample.
    Sample $\tilde{x}_0^{(r)} \sim q_0(\cdot)$.
for $r = 1, \dots, R$ do
    Calculate normalised weights $\hat{w}_0^{(r)} \propto \frac{p_0\left(\tilde{x}_0^{(r)}\right)}{q_0\left(\tilde{x}_0^{(r)}\right)}$, such that $\sum'_r \hat{w}_0^{(r')} = 1$.
Resample from the pmf $\sum_r \hat{w}_0^{(r)} \delta_{\tilde{x}_0^{(r)}}(\cdot)$ to get $R$ samples $\left\{x_0^{(r)}\right\}$.      ▷ Resample.

Iterate, $t = 1, \dots, T$:
for $t = 1, \dots, T$ do
    for $r = 1, \dots, R$ do                                            ▷ Sample.
        Set $\tilde{x}_{0:t-1}^{(r)} = x_{0:t-1}^{(r)}$.
        Sample $\tilde{x}_t^{(r)} \sim M_t\left(\tilde{x}_{0:t-1}^{(r)}, \cdot\right)$.
    for $r = 1, \dots, R$ do
        Calculate normalised weights $\hat{w}_t^{(r)} \propto \frac{p_t(x_t) L_t(x_t, x_{t-1})}{p_{t-1}(x_{t-1}) M_t(x_{t-1}, x_t)}$.
    Resample from the pmf $\sum_r \hat{w}_t^{(r)} \delta_{\tilde{x}_t^{(r)}}(\cdot)$ to get $R$ samples $\left\{x_t^{(r)}\right\}$. Reset the
weights to $1/R$.                                                       ▷ Resample.
```

4.7 Markov chain Monte Carlo methods

4.7.1 Definitions

Definition 4.7.1. Markov chain *(MC) is defined via a state space $\mathcal{X}$ and a model that defines, for every state $\mathbf{x} \in \mathcal{X}$ a next-state distribution over $\mathcal{X}$. More precisely, the transition model $\mathcal{T}$ specifies for each pair of state $\mathbf{x}, \mathbf{x}'$ the probability $\mathcal{T}(\mathbf{x} \to \mathbf{x}')$ of going from $\mathbf{x}$ to $\mathbf{x}'$, i.e. $\mathcal{T}(\mathbf{x} \to \mathbf{x}') = \Pr(\mathbf{x}' \mid \mathbf{x})$. This transition probability applies whenever the chain is in state $\mathbf{x}$.*

If the MCMC generates a sequence of states $\mathbf{x}_0, \dots, \mathbf{x}_T$, the state at time t, $\mathbf{x}_t$ can be viewed as a random variable $\mathbf{X}_t$ for $t = 1, \dots, T$.

Theorem 4.7.1 (Ergodic Theorem for MC (simplified))**.** *If $(\mathbf{X}_0, \dots, \mathbf{X}_T)$ is an* irreducible*,* time-homogeneous *discrete space MC with* stationary distribution *π, then*

$$\frac{1}{T}\sum_{t=1}^{T} f(\mathbf{X}_t) \xrightarrow[n\to\infty]{a.s.} \mathrm{E}[f(\mathbf{X})] \qquad \textit{where } \mathbf{X} \sim \pi \tag{4.95}$$

for any bounded function $f : \mathcal{X} \mapsto \mathbb{R}$.

If further, it is aperiodic*, then*

$$\Pr(\mathbf{X}_T = \mathbf{x} \mid \mathbf{X}_0 = \mathbf{x}_0) \xrightarrow[n\to\infty]{} \pi(\mathbf{x}) \qquad \forall\, \mathbf{x}, \mathbf{x}_0 \in \mathcal{X}. \tag{4.96}$$

A MC following these conditions is ergodic

Definition 4.7.2. *A MC $(\mathbf{X}_t)$ is* time-homogeneous *if* $\Pr(\mathbf{X}_{t+1} = b \mid \mathbf{X}_t = a) = \mathcal{T}(a \to b)$ $\forall\, t \in \{1, \dots, T-1\}$ $\forall\, a, b \in \mathcal{X}$ *for some kernel function $\mathcal{T}$.*

Definition 4.7.3. *A pmf π on $\mathcal{X}$ is a* stationary (invariant) distribution *(w.r.t. $\mathcal{T}$) if*

$$\pi(\mathbf{X} = \mathbf{x}') = \sum_{\mathbf{x} \in \mathcal{X}} \pi(\mathbf{X} = \mathbf{x}) \mathcal{T}(\mathbf{x} \to \mathbf{x}') \qquad \forall\, \mathbf{x}' \tag{4.97}$$

Definition 4.7.4. *A MC $(\mathbf{X}_t)$ is* irreducible *if $\forall\, a, b \in \mathcal{X}$ $\exists\, t \geq 0$ s.t.* $\Pr(\mathbf{X}_t = b \mid \mathbf{X}_0 = a) > 0$.

Definition 4.7.5. *An* irreducible *MC $(\mathbf{X}_t)$ is* aperiodic *if $\forall\, a \in \mathcal{X}$,*

$$\gcd\{t : \Pr(\mathbf{X}_t = a \mid \mathbf{X}_0 = a) > 0\} = 1. \tag{4.98}$$

Definition 4.7.6. *A MC is* regular *if there exists some number k such that, for every $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$, the probability of getting from $\mathbf{x}$ to $\mathbf{x}'$ in exactly k steps is > 0.*

Theorem 4.7.2. *If a finite state MC described by $\mathcal{T}$ is* regular*, then it has a unique* stationary distribution*.*

A MC being *ergodic* is equivalent to it being *regular* [1, p. 510].

Definition 4.7.7. *A finite state MC described by* $\mathcal{T}$ *is* reversible *if there exists a unique distribution* π *such that, for all* $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$

$$\pi(\mathbf{x})\mathcal{T}(\mathbf{x} \to \mathbf{x}') = \pi(\mathbf{x}')\mathcal{T}(\mathbf{x}' \to \mathbf{x}). \tag{4.99}$$

This equation is called the detailed balance *(DB).*

Proposition 4.7.1. *If a finite state MC described by* $\mathcal{T}$ *is* regular *and satisfies the* detailed balance *equation relative to* π*, then* π *is the* unique stationary distribution *of* $\mathcal{T}$*.*

Proof. Assuming the DB equation (4.99), we want to prove the stationarity equation (4.97) to ensure π is a stationary distribution of $\mathcal{T}$. We have

$$\begin{aligned}\sum_{\mathbf{x}\in\mathcal{X}} \pi(\mathbf{x})\mathcal{T}(\mathbf{x} \to \mathbf{x}') &= \sum_{\mathbf{x}\in\mathcal{X}} \pi(\mathbf{x}')\mathcal{T}(\mathbf{x}' \to \mathbf{x}) &(4.100)\\ &= \sum_{\mathbf{x}\in\mathcal{X}} \pi(\mathbf{x}')\Pr(\mathbf{x} \mid \mathbf{x}') &(4.101)\\ &= \pi(\mathbf{x}')\sum_{\mathbf{x}\in\mathcal{X}} \Pr(\mathbf{x} \mid \mathbf{x}') &(4.102)\\ &= \pi(\mathbf{x}') &(4.103)\end{aligned}$$

which proves the equation (4.97). π is the unique stationary distribution of $\mathcal{T}$ because of Theorem 4.7.2. □

Proposition 4.7.2. *Let* $\mathcal{T}_1, \ldots, \mathcal{T}_K$ *be a set of kernels each of which satisfies detailed balance w.r.t.* π*. Let* $p_1, \ldots, p_K$ *be any distribution over* $\{1, \ldots, K\}$*. The mixture MC* $\mathcal{T}$*, which at each step takes a step sampled from* $\mathcal{T}_k$ *with probability* p_k *also satisfies the detailed balance equation relative to* π*.*

Proof. The aggregate kernel can be written as

$$\begin{aligned}\mathcal{T}(\mathbf{x} \to \mathbf{x}') &= \Pr(\mathbf{x}' \mid \mathbf{x}) &(4.104)\\ &= \sum_k \Pr(\mathbf{x}', k \mid \mathbf{x}) &(4.105)\\ &= \sum_k \Pr(\mathbf{x}' \mid k, \mathbf{x})\Pr(k \mid \mathbf{x}) &(4.106)\\ &= \sum_k \mathcal{T}_k(\mathbf{x} \to \mathbf{x}')p_k &(4.107)\end{aligned}$$

Using this, we can prove the detailed balance as follows

$$\begin{aligned}\pi(\mathbf{x})\mathcal{T}(\mathbf{x} \to \mathbf{x}') &= \pi(\mathbf{x})\sum_k \mathcal{T}_k(\mathbf{x} \to \mathbf{x}')p_k &(4.108)\\ &= \sum_k \pi(\mathbf{x})\mathcal{T}_k(\mathbf{x} \to \mathbf{x}')p_k &(4.109)\end{aligned}$$

$$
\begin{aligned}
&= \sum_k \pi(\mathbf{x}')\mathcal{T}_k(\mathbf{x}' \to \mathbf{x})p_k && (4.110)\\
&= \pi(\mathbf{x}') \sum_k \mathcal{T}_k(\mathbf{x}' \to \mathbf{x})p_k && (4.111)\\
&= \pi(\mathbf{x}')\mathcal{T}(\mathbf{x}' \to \mathbf{x}) && (4.112)
\end{aligned}
$$

□

Proposition 4.7.3. *Let $\mathcal{T}_1, \ldots, \mathcal{T}_K$ be a set of kernels each of which satisfies detailed balance w.r.t. π. The aggregate MC, $\mathcal{T}$, where each step consists of a sequence of K steps, with step k being sampled from $\mathcal{T}_k$ has π as its stationary distribution.*

Proof. The aggregate kernel can be written as

$$
\begin{aligned}
\mathcal{T}(\mathbf{x} \to \mathbf{x}') &= \Pr(\mathbf{x}' \mid \mathbf{x}) && (4.113)\\
&= \sum_{\mathbf{x}_{1:K-1}} \Pr(\mathbf{x}', \mathbf{x}_{K-1}, \ldots, \mathbf{x}_1 \mid \mathbf{x}) && (4.114)\\
&= \sum_{\mathbf{x}_{1:K-1}} \Pr(\mathbf{x}_K, \ldots, \mathbf{x}_1 \mid \mathbf{x}_0) && (4.115)\\
&= \sum_{\mathbf{x}_{1:K-1}} \Pr(\mathbf{x}_1 \mid \mathbf{x}_0) \cdots \Pr(\mathbf{x}_K \mid \mathbf{x}_{K-1}) && (4.116)\\
&= \sum_{\mathbf{x}_{1:K-1}} \mathcal{T}_1(\mathbf{x}_0 \to \mathbf{x}_1) \cdots \mathcal{T}_K(\mathbf{x}_{K-1} \to \mathbf{x}_K) && (4.117)
\end{aligned}
$$

where we've used the substitution $\mathbf{x} = \mathbf{x}_0$ and $\mathbf{x}' = \mathbf{x}_K$. Using this, we can prove that π is the stationary distribution as follows

$$
\begin{aligned}
\sum_{\mathbf{x} \in \mathcal{X}} \pi(\mathbf{x})\mathcal{T}(\mathbf{x} \to \mathbf{x}') &= \sum_{\mathbf{x}_0} \pi(\mathbf{x}_0) \sum_{\mathbf{x}_{1:K-1}} \mathcal{T}_1(\mathbf{x}_0 \to \mathbf{x}_1) \cdots \mathcal{T}_K(\mathbf{x}_{K-1} \to \mathbf{x}_K) && (4.118)\\
&= \sum_{\mathbf{x}_{0:K-1}} \pi(\mathbf{x}_0)\mathcal{T}_1(\mathbf{x}_0 \to \mathbf{x}_1) \cdots \mathcal{T}_K(\mathbf{x}_{K-1} \to \mathbf{x}_K) && (4.119)\\
&= \sum_{\mathbf{x}_{0:K-1}} \mathcal{T}_1(\mathbf{x}_1 \to \mathbf{x}_0)\pi(\mathbf{x}_1) \cdots \mathcal{T}_K(\mathbf{x}_{K-1} \to \mathbf{x}_K) && (4.120)\\
&\cdots\\
&= \sum_{\mathbf{x}_{0:K-1}} \mathcal{T}_1(\mathbf{x}_1 \to \mathbf{x}_0) \cdots \mathcal{T}_K(\mathbf{x}_K \to \mathbf{x}_{K-1})\pi(\mathbf{x}_K) && (4.121)\\
&= \pi(\mathbf{x}_K) \sum_{\mathbf{x}_{0:K-1}} \mathcal{T}_K(\mathbf{x}_K \to \mathbf{x}_{K-1}) \cdots \mathcal{T}_1(\mathbf{x}_1 \to \mathbf{x}_0) && (4.122)\\
&= \pi(\mathbf{x}_K) \sum_{\mathbf{x}_{0:K-1}} \Pr(\mathbf{x}_{0:K-1} \mid \mathbf{x}_K) && (4.123)\\
&= \pi(\mathbf{x}_K). && (4.124)
\end{aligned}
$$

□

4.7.2 Metropolis Hastings algorithm

The Metropolis Hastings (MH) algorithm is a recipe to create a MCMC with a particular stationary distribution. Assume we can sample from a proposal distribution $q(\cdot \mid \mathbf{x}) \equiv q(\mathbf{x} \to \cdot)$. Let $p \equiv \pi$ be the required distribution (stationary distribution for this MCMC). Assume we can only evaluate q and π up to a multiplicative factor (i.e. we can only evaluate $q^*(\mathbf{x} \to \mathbf{x}') = Z_q q(\mathbf{x} \to \mathbf{x}')$ and $\pi^*(\mathbf{x}) = Z_p \pi(\mathbf{x})$). The MH algorithm is outlined in Algorithm 7.

Algorithm 7 Metropolis Hastings algorithm

```
1: Sample $\mathbf{x}^{(0)}$ from an arbitrary probability distribution over $\mathcal{X}$.
2: for $t = 1, \dots, T$ do
3:     repeat
4:         Sample $\mathbf{x}^{(t)} \sim q(\mathbf{x}^{(t-1)} \to \cdot)$.
5:         Accept $\mathbf{x}^{(t)}$ with the acceptance probability
               $$\mathcal{A}(\mathbf{x}^{(t-1)} \to \mathbf{x}^{(t)}) = \min\left(1, \frac{\pi^*(\mathbf{x}^{(t)})q^*(\mathbf{x}^{(t)} \to \mathbf{x}^{(t-1)})}{\pi^*(\mathbf{x}^{(t-1)})q^*(\mathbf{x}^{(t-1)} \to \mathbf{x}^{(t)})}\right) \quad (4.125)$$
6:     until $\mathbf{x}^{(t)}$ is accepted.
```

Why it works?

We need to prove that π is the unique stationary distribution of this MCMC.

We can express the aggregate transition model to be

$$\mathcal{T}(\mathbf{x} \to \mathbf{x}') = \begin{cases} q(\mathbf{x} \to \mathbf{x}')\mathcal{A}(\mathbf{x} \to \mathbf{x}') & \text{if } \mathbf{x} \neq \mathbf{x}' \\ q(\mathbf{x} \to \mathbf{x}) + \sum\limits_{\mathbf{x}', \mathbf{x}' \neq \mathbf{x}} q(\mathbf{x} \to \mathbf{x}')(1 - \mathcal{A}(\mathbf{x} \to \mathbf{x}')) & \text{if } \mathbf{x} = \mathbf{x}' \end{cases} \tag{4.126}$$

To prove that π is a stationary distribution of this MCMC, we make sure the DB equation holds.

For $\mathbf{x} \neq \mathbf{x}'$, we have

$$\begin{aligned} \pi(\mathbf{x})\mathcal{T}(\mathbf{x} \to \mathbf{x}') &= \pi(\mathbf{x})q(\mathbf{x} \to \mathbf{x}') \min\left(1, \frac{\pi(\mathbf{x}')q(\mathbf{x}' \to \mathbf{x})}{\pi(\mathbf{x})q(\mathbf{x} \to \mathbf{x}')}\right) && (4.127) \\ &= \min\big(\pi(\mathbf{x})q(\mathbf{x} \to \mathbf{x}'), \pi(\mathbf{x}')q(\mathbf{x}' \to \mathbf{x})\big) && (4.128) \\ &= \pi(\mathbf{x}')q(\mathbf{x}' \to \mathbf{x}) \min\left(1, \frac{\pi(\mathbf{x})q(\mathbf{x} \to \mathbf{x}')}{\pi(\mathbf{x}')q(\mathbf{x}' \to \mathbf{x})}\right) && (4.129) \\ &= \pi(\mathbf{x}')\mathcal{T}(\mathbf{x}' \to \mathbf{x}) && (4.130) \end{aligned}$$

For $\mathbf{x} = \mathbf{x}'$, the DB equation $\pi(\mathbf{x})\mathcal{T}(\mathbf{x} \to \mathbf{x}') = \pi(\mathbf{x}')\mathcal{T}(\mathbf{x}' \to \mathbf{x})$ obviously holds.

Hence π is a stationary distribution of the MCMC described via $\mathcal{T}$. Unfortunately, regularity doesn't hold in general. We need to make sure our created MCMC is regular before we can claim that π is the unique stationary distribution of this MCMC.

4.7.3 Gibbs sampling

Assume we want to sample from $p(\mathbf{x}) = p(x_1, \ldots, x_D)$. We can only sample from the conditionals $p(x_i \mid \mathbf{x}_{-i})$ where $\mathbf{x}_{-i}$ denotes $\mathbf{x}$ with the i^{th} component ommited. The Gibbs sampling algorithm (8) is given below.

Algorithm 8 Gibbs sampling algorithm

```
1: Sample $\mathbf{x}^{(0)}$ from an arbitrary probability distribution over $\mathcal{X}$.
2: for $t = 1, \ldots, T$ do
3:     Sample $x_1^{(t)} \sim p\left(\cdot \mid x_2^{(t-1)}, x_3^{(t-1)}, \ldots, x_D^{(t-1)}\right)$
4:     Sample $x_2^{(t)} \sim p\left(\cdot \mid x_1^{(t)}, x_3^{(t-1)}, \ldots, x_D^{(t-1)}\right)$
5:     $\vdots$
6:     Sample $x_D^{(t)} \sim p\left(\cdot \mid x_1^{(t)}, x_2^{(t)}, \ldots, x_{D-1}^{(t)}\right)$
```

Why it works?

Each of the sampling steps can be viewed to be governed by a different kernel with the whole process being governed by the aggregate kernel. We prove that the single kernels follow the DB equation with respect to p:

$$\begin{aligned}
p(\mathbf{x})\mathcal{T}_i(\mathbf{x} \to \mathbf{x}') &= p(\mathbf{x})p(\mathbf{x}_{-i}, x_i' \mid \mathbf{x}) && (4.131)\\
&= p(\mathbf{x}_{-i}, x_i', \mathbf{x}) && (4.132)\\
&= p(\mathbf{x}, x_i', \mathbf{x}_{-i}) && (4.133)\\
&= p(\mathbf{x}')p(\mathbf{x} \mid x_i', \mathbf{x}_{-i}) && (4.134)\\
&= p(\mathbf{x}')\mathcal{T}_i(\mathbf{x}' \to \mathbf{x}) && (4.135)
\end{aligned}$$

This is the premise of Proposition 4.7.3, hence the aggregate kernel $\mathcal{T}$ has p as its stationary distribution.

We can also view Gibbs sampling as an instance of the MH algorithm. If the proposal of MH $q_i(\mathbf{x} \to \mathbf{x}')$ is set to be $p(\mathbf{x}' \mid \mathbf{x}) = p(x_i' \mid \mathbf{x})$ the acceptance probability is one (shown below) and so it is equivalent to one sampling step in Gibbs sampling.

$$\begin{aligned}
\mathcal{A}(\mathbf{x} \to \mathbf{x}') &= \min\left(1, \frac{p(\mathbf{x}')p(\mathbf{x} \mid \mathbf{x}')}{p(\mathbf{x})p(\mathbf{x}' \mid \mathbf{x})}\right) && (4.136)\\
&= \min\left(1, \frac{p(\mathbf{x}', \mathbf{x})}{p(\mathbf{x}', \mathbf{x})}\right) && (4.137)\\
&= 1 && (4.138)
\end{aligned}$$

4.8 Particle Markov Chain Monte Carlo

4.8.1 Particle independent Metropolis Hastings (PIMH) sampler

We want to sample from $p(\mathbf{x}_{1:T} \mid \mathbf{y}_{1:T}, \boldsymbol{\theta})$.

Algorithm 9 Particle independent Metropolis Hastings sampler

```
Run SMC targetting                                                ▷ Initial sweep $s = 0$
    $$p(\mathbf{x}_{1:T} \mid \mathbf{y}_{1:T}; \boldsymbol{\theta})$$
Sample
    $$\mathbf{x}_{1:T}(0) \sim \hat{p}(\cdot \mid \mathbf{y}_{1:T}; \boldsymbol{\theta})$$
Let
    $$\hat{p}(\mathbf{y}_{1:T} \mid \boldsymbol{\theta})$$
denote the corresponding marginal likelihood estimate.
for $s = 1, \ldots, S$ do                                         ▷ Main loop
    Run SMC targeting
        $$p(\mathbf{x}_{1:T} \mid \mathbf{y}_{1:T}; \boldsymbol{\theta})$$
    Sample
        $$\mathbf{x}^*_{1:T} \sim \hat{p}(\cdot \mid \mathbf{y}_{1:T}; \boldsymbol{\theta})$$
    Let
        $$\hat{p}(\mathbf{y}_{1:T}; \boldsymbol{\theta})^*$$
denote the coresponding marginal likelihood estimate
    Sample from Ber(·) with the success probability
        $$\min\left(1, \frac{\hat{p}(\mathbf{y}_{1:T} \mid \boldsymbol{\theta})^*}{\hat{p}(\mathbf{y}_{1:T}; \boldsymbol{\theta})(s-1)}\right)$$
    if success then
        Set
            $$\mathbf{x}_{1:T}(s) = \mathbf{x}^*_{1:T}$$
            $$\hat{p}(\mathbf{y}_{1:T} \mid \boldsymbol{\theta})(s) = \hat{p}(\mathbf{y}_{1:T} \mid \boldsymbol{\theta})^*$$
    else
        Set
            $$\mathbf{x}_{1:T}(s) = \mathbf{x}_{1:T}(s-1)$$
            $$\hat{p}(\mathbf{y}_{1:T} \mid \boldsymbol{\theta})(s) = \hat{p}(\mathbf{y}_{1:T} \mid \boldsymbol{\theta})(s-1)$$
```

4.8.2 Particle marginal Metropolis Hastings (PMMH) sampler

We want to sample from $p(\boldsymbol{\theta}, \mathbf{x}_{1:T} \mid \mathbf{y}_{1:T}) \propto p(\mathbf{x}_{1:T} \mid \mathbf{y}_{1:T;\boldsymbol{\theta}})p(\boldsymbol{\theta})$.

Algorithm 10 Particle marginal Metropolis Hastings sampler

```
Set $\boldsymbol{\theta}(0)$ arbitrarily.
```

```
Run SMC targetting                                                  ▷ Initial sweep $s = 0$
        $p(\mathbf{x}_{1:T} \mid \mathbf{y}_{1:T}; \boldsymbol{\theta}(0))$
Sample
        $\mathbf{x}_{1:T}(0) \sim \hat{p}(\cdot \mid \mathbf{y}_{1:T}; \boldsymbol{\theta}(0))$
Let
        $\hat{p}(\mathbf{y}_{1:T} \mid \boldsymbol{\theta}(0))$
denote the corresponding marginal likelihood estimate.
for $s = 1, \dots, S$ do                                            ▷ Main loop
    Sample
        $\boldsymbol{\theta}^* \sim q(\cdot \mid \boldsymbol{\theta}(s-1))$
    Run SMC targeting
        $p(\mathbf{x}_{1:T} \mid \mathbf{y}_{1:T}; \boldsymbol{\theta}^*)$
    Sample
        $\mathbf{x}^*_{1:T} \sim \hat{p}(\cdot \mid \mathbf{y}_{1:T}; \boldsymbol{\theta}^*)$
    Let
        $\hat{p}(\mathbf{y}_{1:T}; \boldsymbol{\theta}^*)$
denote the coresponding marginal likelihood estimate
    Sample from Ber$(\cdot)$ with the success probability
        $\min\left(1, \frac{\hat{p}(\mathbf{y}_{1:T} \mid \boldsymbol{\theta}^*) p(\boldsymbol{\theta}^*) q(\boldsymbol{\theta}(s-1) \mid \boldsymbol{\theta}^*)}{\hat{p}(\mathbf{y}_{1:T}; \boldsymbol{\theta}(s-1)) p(\boldsymbol{\theta}(s-1)) q(\boldsymbol{\theta}^* \mid \boldsymbol{\theta}(s-1))}\right)$
    if success then
        Set
            $\boldsymbol{\theta}(s) = \boldsymbol{\theta}^*$
            $\mathbf{x}_{1:T}(s) = \mathbf{x}^*_{1:T}$
            $\hat{p}(\mathbf{y}_{1:T} \mid \boldsymbol{\theta})(s) = \hat{p}(\mathbf{y}_{1:T} \mid \boldsymbol{\theta}^*)$
    else
        Set
            $\boldsymbol{\theta}(s) = \boldsymbol{\theta}(s-1)$
            $\mathbf{x}_{1:T}(s) = \mathbf{x}_{1:T}(s-1)$
            $\hat{p}(\mathbf{y}_{1:T} \mid \boldsymbol{\theta})(s) = \hat{p}(\mathbf{y}_{1:T} \mid \boldsymbol{\theta})(s-1)$
```

4.8.3 Particle Gibbs (PG) sampler

Conditional SMC update

We want to smple from $p(\mathbf{x}_{1:T} \mid \mathbf{y}_{1:T}; \boldsymbol{\theta})$.

Algorithm 11 Conditional SMC update

```
Choose a fixed ancestral lineage $B_{1:T}$ arbitrarily.          ▷ Initialise fixed path
Let
    $\mathbf{x}_{1:T} = \left(\mathbf{x}_1^{(B_1)}, \ldots, \mathbf{x}_T^{(B_T)}\right)$
be a path associated with the ancestral lineage $B_{1:T}$.
For $r \neq B_1$, sample                                          ▷ Time $t = 1$
    $\mathbf{x}_1^{(r)} \sim q(\cdot \mid \mathbf{y}_1, \boldsymbol{\theta})$
Compute weights
    $w_1^{(r)} \propto \frac{p\left(\mathbf{x}_1^{(r)}, \mathbf{y}_1\right)}{q\left(\mathbf{x}_1^{(r)} \mid \mathbf{y}_1\right)}$
Normalise weights
    $\hat{w}_1^{(r)} = \frac{w_1^{(r)}}{\sum_{r'} w_1^{(r')}}$
We can resample from
    $\hat{p}(\mathrm{d}\mathbf{x}_1 \mid \mathbf{y}_1, \boldsymbol{\theta}) = \sum_r \hat{w}_1^{(r)} \delta_{\mathbf{x}_1^{(r)}}(\mathrm{d}\mathbf{x}_1)$
to estimate
    $p(\mathbf{x}_1 \mid \mathbf{y}_1, \boldsymbol{\theta})$
for $t = 2, \ldots, T$ do                                         ▷ Main loop
    For $r \neq B_t$, sample
        $A_{t-1}^{(r)} \sim \mathrm{Cat}\left(\hat{w}_{t-1}^{(1)}, \ldots, \hat{w}_{t-1}^{(R)}\right)$
    For $r \neq B_t$, sample
        $\mathbf{x}_t^{(r)} \sim q\left(\cdot \mid \mathbf{y}_t, \mathbf{x}_{t-1}^{(A_{t-1}^{(r)})}\right)$
    Compute weights
        $w_t^{(r)} = \frac{p\left(\mathbf{x}_{1:t}^{(r)}, \mathbf{y}_{1:t}; \boldsymbol{\theta}\right)}{p\left(\mathbf{x}_{1:t-1}^{\left(A_{t-1}^{(r)}\right)}, \mathbf{y}_{1:t-1}; \boldsymbol{\theta}\right) q\left(\mathbf{x}_n^{(r)} \mid \mathbf{y}_t, \mathbf{x}_{t-1}^{\left(A_{t-1}^{(r)}\right)}; \boldsymbol{\theta}\right)}$
    Normalise weights
        $\hat{w}_t = \frac{w_t^{(r)}}{\sum_{r'} w_t^{(r')}}$
    We can resample from
        $\hat{p}(\mathrm{d}\mathbf{x}_{1:t} \mid \mathbf{y}_{1:t}, \boldsymbol{\theta}) = \sum_r \hat{w}_t^{(r)} \delta_{\mathbf{x}_{1:t}^{(r)}}(\mathrm{d}\mathbf{x}_{1:t})$
  to estimate
        $p(\mathbf{x}_{1:t} \mid \mathbf{y}_{1:t}, \boldsymbol{\theta})$
```

Particle Gibbs sampler

We want to sample from $p(\boldsymbol{\theta}, \mathbf{x}_{1:T} \mid \mathbf{y}_{1:T})$.

Algorithm 12 Particle Gibbs sampler

```
Set $\theta(0)$, $\mathbf{x}_{1:T}(0)$, $B_{1:T}(0)$ arbitrarily.          ▷ Initialisation, $s = 0$
for Sweep $s = 1, \ldots, S$ do                                         ▷ Main loop
    Sample parameter
        $\boldsymbol{\theta}(s) \sim p\left(\cdot \mid \mathbf{y}_{1:T}, \mathbf{x}_{1:T}(s-1)\right)$
    Run conditional SMC (Algorithm 11) targetting
        $p(\mathbf{x}_{1:T} \mid \mathbf{y}_{1:T}; \boldsymbol{\theta}(s))$
  conditional on
      • $\mathbf{x}_{1:T}(s-1)$, and
      • $B_{1:T}(s-1)$.
    Sample
        $\mathbf{x}_{1:T}(s) \sim \hat{p}(\cdot \mid \mathbf{y}_{1:T}; \boldsymbol{\theta}(s))$
```

5 Nonparametric Bayesian models

5.1 Gaussian process

5.2 Dirichlet process

5.3 Chinese restaurant process

5.4 Hierarchical Dirichlet process

5.5 Hierarchical Dirichlet process

5.6 Indian buffet process

5.7 Dirichlet diffusion trees

5.8 Pitman-Yor process

Bibliography

[1] Daphne Koller and Nir Friedman. *Probabilistic Graphical Models: Principles and Techniques - Adaptive Computation and Machine Learning*. The MIT Press, 2009.