

Personal notes – Bayesian machine learning

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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

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

$$\mathcal{D} = \{x_1, \dots, x_N\} \quad (2.2)$$

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

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

Likelihood

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

Prior

$$p(\theta) = \text{Beta}(\theta|a, b) \quad (2.6)$$

Posterior

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

Posterior predictive

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

Evidence

2.1.2 Derivations

2.2 Beta-binomial model

2.2.1 Summary

The model

$$N_1 \sim \text{Bin}(N, \theta) \quad (2.9)$$

$$\mathcal{D} = \{N_1, N\} \quad (2.10)$$

$$N_1 = \text{number of successes} \quad (2.11)$$

$$N = \text{total number of trials} \quad (2.12)$$

$$\tilde{\mathcal{D}} = \{\tilde{N}_1, \tilde{N}\} \quad (2.13)$$

$$\tilde{N}_1 = \text{number of successes in a new batch of data} \quad (2.14)$$

$$\tilde{N} = \text{total number of trials in a new batch of data} \quad (2.15)$$

Likelihood

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

Prior

$$p(\theta) = \text{Beta}(\theta|a, b) \quad (2.17)$$

Posterior

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

Posterior predictive

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

Evidence

2.2.2 Derivations

2.3 Dirichlet-categorical model

2.3.1 Summary

The model

$$X_i \sim \text{Cat}(\boldsymbol{\theta} = (\theta_1, \dots, \theta_K)^T), \text{ for } i \in \{1, \dots, N\} \quad (2.20)$$

$$\mathcal{D} = \{x_1, \dots, x_N\} \quad (2.21)$$

$$n_k = \sum_{i=1}^N \mathbb{I}(x_i = k) \quad (2.22)$$

Likelihood

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

Prior

$$p(\theta) = \text{Dir}(\boldsymbol{\theta}; \boldsymbol{\alpha}) \quad (2.24)$$

Posterior

$$p(\theta|\mathcal{D}) = \text{Dir}(\theta; \alpha' = \alpha + (n_1, \dots, n_K)^T) \quad (2.25)$$

Posterior predictive

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

$$= \frac{\alpha_j + n_j}{\alpha_0 + N} \quad (2.27)$$

$$\text{where } \alpha_0 = \sum_{k=1}^K \alpha_k \quad (2.28)$$

Evidence

2.3.2 Derivations

2.4 Dirichlet-multinomial model

2.4.1 Summary

The model

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

$$\mathcal{D} = \{\mathbf{n} = \text{vector of counts of successes}\} \quad (2.30)$$

$$N = \sum_{i=1}^K n_i \quad (2.31)$$

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

$$\tilde{N} = \sum_{i=1}^K \tilde{n}_i \quad (2.33)$$

Likelihood

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

Prior

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

Posterior

$$p(\theta|\mathcal{D}) = \text{Dir}(\theta; \alpha' = \alpha + (n_1, \dots, n_K)^T) \quad (2.36)$$

Posterior predictive

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

$$\text{where } \alpha_0 = \sum_{k=1}^K \alpha_k \quad (2.38)$$

Evidence

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

2.4.2 Derivations

2.5 Poisson-gamma model

2.5.1 Summary

The model

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

$$\mathcal{D} = \{x_1, \dots, x_N\} \quad (2.41)$$

Likelihood

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

Prior

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

Posterior

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

Posterior predictive

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

Evidence

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

2.5.2 Derivations

3 Sampling algorithms

3.1 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 $Z_p = \int_{\mathcal{X}} p^*(\mathbf{x}) d\mathbf{x}$). We want to achieve the following:

Problem 1 Generate samples $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(R)}\}$, $R \in \mathbb{N}$ (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 $\mathbf{x} \sim p$, $E_{\mathbf{x} \sim p} [f(\mathbf{x})]$ (we will use the shorthand notation $E[f]$ from now).

3.2 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

$$cq^*(\mathbf{x}) > p^*(\mathbf{x}) \text{ for all } \mathbf{x} \quad (3.1)$$

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 $u \sim \text{Unif}(0, cq^*(\mathbf{x}))$.
 - 3: If $u > p^*(\mathbf{x})$ it is rejected, otherwise it is accepted.
-

3.2.1 Why it works?

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

$$\mathcal{X} = \left\{ \boldsymbol{\alpha} \in \mathbb{R}^{d+1} : \alpha_{1:d} \in \mathbb{R}^d, \alpha_{d+1} \in [0, cq^*(\boldsymbol{\alpha})] \right\} \quad (3.2)$$

$$\mathcal{X}' = \left\{ \boldsymbol{\alpha} \in \mathbb{R}^{d+1} : \alpha_{1:d} \in \mathbb{R}^d, \alpha_{d+1} \in [0, p^*(\boldsymbol{\alpha})] \right\} \quad (3.3)$$

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

$$\Pr(\mathbf{x}, u) = \Pr(\mathbf{x}) \Pr(u) \quad (3.4)$$

$$= q(\mathbf{x}) \frac{1}{cq^*(\mathbf{x})} \quad (3.5)$$

$$= q(\mathbf{x}) \frac{1}{cZ_q q(\mathbf{x})} \quad (3.6)$$

$$= \frac{1}{cZ_q} \quad (3.7)$$

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

$$(\mathbf{x}, u) \sim \text{Unif}(\mathcal{X}) \quad (3.8)$$

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') :

$$(\mathbf{x}', u') = \begin{cases} (\mathbf{x}, u) & \text{if } (\mathbf{x}, u) \in \mathcal{X}' \\ \text{nothing} & \text{otherwise.} \end{cases} \quad (3.9)$$

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

$$\Pr(\mathbf{x}', u') = \begin{cases} \Pr(\mathbf{x}, u) & \text{if } (\mathbf{x}, u) \in \mathcal{X}' \\ 0 & \text{otherwise.} \end{cases} \quad (3.10)$$

which means

$$(\mathbf{x}', u') \sim \text{Unif}(\mathcal{X}') \quad (3.11)$$

Working backwards

$$\Pr(\mathbf{x}') = \frac{\Pr(\mathbf{x}', u')}{\Pr(u')} \quad (3.12)$$

$$\propto \frac{1}{1/p^*(\mathbf{x}')} \quad (3.13)$$

$$\propto p^*(\mathbf{x}') \quad (3.14)$$

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

3.3 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 $E[f]$.
-

3.3.1 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 $E[f]$, as R increases. We consider the the expectations of the numerator and denominator separately:

$$E_q[\text{numer}] = E_q \left[\sum_r w_r f(\mathbf{x}^{(r)}) \right] \quad (3.15)$$

$$= \sum_r E_q \left[w_r f(\mathbf{x}^{(r)}) \right] \quad (3.16)$$

$$= \sum_r E_q \left[\frac{p^*(\mathbf{x}^{(r)})}{q^*(\mathbf{x}^{(r)})} f(\mathbf{x}^{(r)}) \right] \quad (3.17)$$

$$= \sum_r E_q \left[\frac{Z_p p(\mathbf{x}^{(r)})}{Z_q q(\mathbf{x}^{(r)})} f(\mathbf{x}^{(r)}) \right] \quad (3.18)$$

$$= \frac{Z_p}{Z_q} \sum_r \int_{\mathbf{x}^{(r)}} p(\mathbf{x}^{(r)}) f(\mathbf{x}^{(r)}) d\mathbf{x}^{(r)} \quad (3.19)$$

$$= \frac{Z_p}{Z_q} \sum_r E_p \left[f(\mathbf{x}^{(r)}) \right] \quad (3.20)$$

$$= \frac{Z_p}{Z_q} R E_p [f(\mathbf{x})] \quad (3.21)$$

$$E_q[\text{denom}] = E_q \left[\sum_r w_r \right] \quad (3.22)$$

$$= \sum_r E_q \left[\frac{p^*(\mathbf{x}^{(r)})}{q^*(\mathbf{x}^{(r)})} \right] \quad (3.23)$$

$$= \sum_r E_q \left[\frac{Z_p p(\mathbf{x}^{(r)})}{Z_q q(\mathbf{x}^{(r)})} \right] \quad (3.24)$$

$$= \frac{Z_p}{Z_q} \sum_r \int_{\mathbf{x}^{(r)}} p(\mathbf{x}^{(r)}) d\mathbf{x}^{(r)} \quad (3.25)$$

$$= \frac{Z_p}{Z_q} R \quad (3.26)$$

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

3.3.2 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

$$\text{var}_q \left[\frac{p(\mathbf{x})}{q(\mathbf{x})} f(\mathbf{x}) \right] = \text{E}_q \left[\frac{p^2(\mathbf{x})}{q^2(\mathbf{x})} f^2(\mathbf{x}) \right] - \left(\text{E}_q \left[\frac{p(\mathbf{x})}{q(\mathbf{x})} f(\mathbf{x}) \right] \right)^2 \quad (3.27)$$

$$= \text{E}_q \left[\frac{p^2(\mathbf{x})}{q^2(\mathbf{x})} f^2(\mathbf{x}) \right] - (\text{E}_p[f(\mathbf{x})])^2 \quad (3.28)$$

The second part is independent of q so we can ignore it. By Jensen's inequality, we have $\text{E}[g(u(\mathbf{x}))] \geq g(\text{E}[u(\mathbf{x})])$ 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:

$$\text{E}_q \left[\frac{p^2(\mathbf{x})}{q^2(\mathbf{x})} f^2(\mathbf{x}) \right] \geq \left(\text{E}_q \left[\frac{p(\mathbf{x})}{q(\mathbf{x})} |f(\mathbf{x})| \right] \right)^2 = (\text{E}_p[|f(\mathbf{x})|])^2 \quad (3.29)$$

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

$$q_{\text{optimal}}(\mathbf{x}) = \frac{|f(\mathbf{x})|p(\mathbf{x})}{\int |f(\mathbf{x}')|p(\mathbf{x}') d\mathbf{x}'} \quad (3.30)$$

3.4 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

- 1: Generate samples $\{\mathbf{x}^{(r)}\}$ from q .
- 2: Calculate importance weights $\left\{w_r = \frac{p^*(\mathbf{z}^{(r)})}{q^*(\mathbf{z}^{(r)})}\right\}$.
- 3: Calculate the normalised importance weights $\left\{\hat{w}_r = \frac{w_r}{\sum_{r'} w_{r'}}\right\}$. Note that $\sum_r \hat{w}_r = 1$.
- 4: We can resample from

$$\hat{p}(d\mathbf{x}) = \sum_r \hat{w}_r \delta_{\mathbf{x}^{(r)}}(d\mathbf{x}) \quad (3.31)$$

to estimate sampling from $p(\mathbf{x})$.

3.4.1 Why it works?

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

$$N(x) = \lim_{\delta x \rightarrow 0} Rq(x)\delta x \quad (3.32)$$

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

$$\lim_{\delta x \rightarrow 0} \Pr(x \leq x^{(r)} \leq x + \delta x) = N(x) \hat{w}_r \quad (3.33)$$

$$\propto \lim_{\delta x \rightarrow 0} Rq(x) \delta x \frac{p(x)}{q(x)} \quad (3.34)$$

$$\propto \lim_{\delta x \rightarrow 0} p(x) \delta x \quad (3.35)$$

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

$$\Pr(a \leq x^{(r)} \leq b) \propto \int_a^b p(x) dx \quad (3.36)$$

$$\implies x^{(r)} \sim p \quad (3.37)$$

3.5 Particle filtering

3.5.1 Sequential importance sampling (SIS)

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

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

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

$$q(\mathbf{x}_{1:t} | \mathbf{y}_{1:t}; \boldsymbol{\theta}) = q(\mathbf{x}_t | \mathbf{x}_{1:t-1}, \mathbf{y}_{1:t}; \boldsymbol{\theta}) q(\mathbf{x}_{1:t-1} | \mathbf{y}_{1:t}; \boldsymbol{\theta}) \quad (3.38)$$

$$= q(\mathbf{x}_t | \mathbf{x}_{1:t-1}, \mathbf{y}_{1:t}; \boldsymbol{\theta}) q(\mathbf{x}_{1:t-1} | \mathbf{y}_{1:t-1}; \boldsymbol{\theta}) \quad (3.39)$$

$$= q(\mathbf{x}_t | \mathbf{x}_{t-1}, \mathbf{y}_t; \boldsymbol{\theta}) \quad (3.40)$$

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

$$p(\mathbf{x}_{1:t} | \mathbf{y}_{1:t}) = \frac{p(\mathbf{y}_{1:t} | \mathbf{x}_{1:t}) p(\mathbf{x}_{1:t})}{p(\mathbf{y}_{1:t})} \quad (3.41)$$

$$= \frac{p(\mathbf{y}_t | \mathbf{x}_{1:t}, \mathbf{y}_{1:t-1}) p(\mathbf{y}_{1:t-1} | \mathbf{x}_{1:t}) p(\mathbf{x}_{1:t})}{p(\mathbf{y}_t | \mathbf{y}_{1:t-1}) p(\mathbf{y}_{1:t-1})} \quad (3.42)$$

$$= \frac{p(\mathbf{y}_t | \mathbf{x}_{1:t}, \mathbf{y}_{1:t-1}) p(\mathbf{x}_{1:t} | \mathbf{y}_{1:t-1})}{p(\mathbf{y}_t | \mathbf{y}_{1:t-1})} \quad (3.43)$$

$$= \frac{p(\mathbf{y}_t | \mathbf{x}_{1:t}, \mathbf{y}_{1:t-1}) p(\mathbf{x}_t | \mathbf{x}_{1:t-1}, \mathbf{y}_{1:t-1}) p(\mathbf{x}_{1:t-1} | \mathbf{y}_{1:t-1})}{p(\mathbf{y}_t | \mathbf{y}_{1:t-1})} \quad (3.44)$$

$$= \frac{p(\mathbf{y}_t | \mathbf{x}_t) p(\mathbf{x}_t | \mathbf{x}_{t-1}) p(\mathbf{x}_{1:t-1} | \mathbf{y}_{1:t-1})}{p(\mathbf{y}_t | \mathbf{y}_{1:t-1})} \quad (3.45)$$

$$\propto p(\mathbf{y}_t | \mathbf{x}_t) p(\mathbf{x}_t | \mathbf{x}_{t-1}) p(\mathbf{x}_{1:t-1} | \mathbf{y}_{1:t-1}) \quad (3.46)$$

$$= g(\mathbf{y}_t | \mathbf{x}_t) f(\mathbf{x}_t | \mathbf{x}_{t-1}) p(\mathbf{x}_{1:t-1} | \mathbf{y}_{1:t-1}) \quad (3.47)$$

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

$$w_t^{(r)} \propto \frac{p(\mathbf{x}_{1:t}^{(r)} | \mathbf{y}_{1:t})}{q(\mathbf{x}_{1:t}^{(r)} | \mathbf{y}_{1:t})} \quad (3.48)$$

$$\propto \frac{p(\mathbf{y}_t | \mathbf{x}_t^{(r)}) p(\mathbf{x}_t^{(r)} | \mathbf{x}_{t-1}^{(r)}) p(\mathbf{x}_{1:t-1}^{(r)} | \mathbf{y}_{1:t-1})}{q(\mathbf{x}_t^{(r)} | \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t) q(\mathbf{x}_{1:t-1}^{(r)} | \mathbf{y}_{1:t-1})} \quad (3.49)$$

$$= w_{t-1}^{(r)} \frac{p(\mathbf{y}_t | \mathbf{x}_t^{(r)}) p(\mathbf{x}_t^{(r)} | \mathbf{x}_{t-1}^{(r)})}{q(\mathbf{x}_t^{(r)} | \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t)} \quad (3.50)$$

$$= w_{t-1}^{(r)} \frac{g(\mathbf{y}_t | \mathbf{x}_t^{(r)}) f(\mathbf{x}_t^{(r)} | \mathbf{x}_{t-1}^{(r)})}{q(\mathbf{x}_t^{(r)} | \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t)} \quad (3.51)$$

For $t = 1$

$$w_1^{(r)} \propto \frac{p(\mathbf{x}_1^{(r)} | \mathbf{y}_1)}{q(\mathbf{x}_1^{(r)} | \mathbf{y}_1)} \quad (3.52)$$

$$\propto \frac{p(\mathbf{x}_1^{(r)}, \mathbf{y}_1)}{q(\mathbf{x}_1^{(r)} | \mathbf{y}_1)} \quad (3.53)$$

$$\propto \frac{p(\mathbf{y}_1 | \mathbf{x}_1^{(r)}) p(\mathbf{x}_1^{(r)})}{q(\mathbf{x}_1^{(r)} | \mathbf{y}_1)} \quad (3.54)$$

$$= \frac{g(\mathbf{y}_1 | \mathbf{x}_1^{(r)}) \mu(\mathbf{x}_1^{(r)})}{q(\mathbf{x}_1^{(r)} | \mathbf{y}_1)} \quad (3.55)$$

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.

The reason why it works is the same as in the case of Sampling importance resampling described in section 3.4.

Algorithm 4 Sequential importance sampling

1: Sample from proposal ▷ Initialisation

$$\mathbf{x}_1^{(r)} \sim q\left(\cdot \mid \mathbf{y}_1^{(r)}, \boldsymbol{\theta}\right), r = 1, \dots, R \quad (3.56)$$

2: Compute weights

$$w_1^{(r)} \propto \frac{g\left(\mathbf{y}_1 \mid \mathbf{x}_1^{(r)}\right) \mu\left(\mathbf{x}_1^{(r)}\right)}{q\left(\mathbf{x}_1^{(r)} \mid \mathbf{y}_1\right)}, r = 1, \dots, R \quad (3.57)$$

3: Normalise weights

$$\hat{w}_1^{(r)} = \frac{w_1^{(r)}}{\sum_{r'} w_1^{(r')}}, r = 1, \dots, R \quad (3.58)$$

4: We can resample from

$$\hat{p}(\mathrm{d}\mathbf{x}_1 \mid \mathbf{y}_1, \boldsymbol{\theta}) = \sum_r \hat{w}_1^{(r)} \delta_{\mathbf{x}_1^{(r)}}(\mathrm{d}\mathbf{x}_1) \quad (3.59)$$

to estimate

$$p(\mathbf{x}_1 \mid \mathbf{y}_1, \boldsymbol{\theta}) \quad (3.60)$$

5: **for** $t = 2, \dots, T$ **do** ▷ Main loop

6: Compute weights

$$w_t^{(r)} \propto w_{t-1}^{(r)} \frac{p\left(\mathbf{y}_t \mid \mathbf{x}_t^{(r)}, \boldsymbol{\theta}\right) p\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}, \boldsymbol{\theta}\right)}{q\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t, \boldsymbol{\theta}\right)}, r = 1, \dots, R \quad (3.61)$$

7: Normalise weights

$$\hat{w}_t^{(r)} = \frac{w_t^{(r)}}{\sum_{r'} w_t^{(r')}}, r = 1, \dots, R \quad (3.62)$$

8: We can resample from

$$\hat{p}(\mathrm{d}\mathbf{x}_{1:t} \mid \mathbf{y}_{1:t}, \boldsymbol{\theta}) = \sum_r \hat{w}_t^{(r)} \delta_{\mathbf{x}_{1:t}^{(r)}}(\mathrm{d}\mathbf{x}_{1:t}) \quad (3.63)$$

to estimate

$$p(\mathbf{x}_{1:t} \mid \mathbf{y}_{1:t}, \boldsymbol{\theta}) \quad (3.64)$$

3.5.2 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:

$$S_{\text{eff}} \triangleq \frac{S}{1 + \text{var} \left[w_t^{(r)*} \right]} \quad (3.65)$$

$$\hat{S}_{\text{eff}} \approx \frac{1}{\sum_r \left(w_t^{(r)} \right)^2} \quad (3.66)$$

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.

3.5.3 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

1: Sample from proposal

▷ Initialisation

$$\mathbf{x}_1^{(r)} \sim q\left(\cdot \mid \mathbf{y}_1^{(r)}, \boldsymbol{\theta}\right), r = 1, \dots, R \quad (3.67)$$

2: Compute weights

$$w_1^{(r)} \propto \frac{p\left(\mathbf{x}_1^{(r)} \mid \mathbf{y}_1, \boldsymbol{\theta}\right)}{q\left(\mathbf{x}_1^{(r)} \mid \mathbf{y}_1, \boldsymbol{\theta}\right)}, r = 1, \dots, R \quad (3.68)$$

3: Normalise weights

$$\hat{w}_1^{(r)} = \frac{w_1^{(r)}}{\sum_{r'} w_1^{(r')}}, r = 1, \dots, R \quad (3.69)$$

4: We can resample from

$$\hat{p}(\mathrm{d}\mathbf{x}_1 \mid \mathbf{y}_1, \boldsymbol{\theta}) = \sum_r \hat{w}_1^{(r)} \delta_{\mathbf{x}_1^{(r)}}(\mathrm{d}\mathbf{x}_1) \quad (3.70)$$

to estimate

$$p(\mathbf{x}_1 \mid \mathbf{y}_1, \boldsymbol{\theta}) \quad (3.71)$$

5: **for** $t = 2, \dots, T$ **do**

▷ Main loop

6: Sample parents' indices of t^{th} generation

$$A_{t-1}^{(r)} \sim \text{Cat}(\hat{w}_{t-1}), r = 1, \dots, R \quad (3.72)$$

7: Sample t^{th} generation using corresponding parents

$$\mathbf{x}_t^{(r)} \sim q\left(\cdot \mid \mathbf{x}_{t-1}^{A_{t-1}^{(r)}}, \mathbf{y}_t, \boldsymbol{\theta}\right), r = 1, \dots, R \quad (3.73)$$

8: Compute weights

$$w_t^{(r)} \propto w_{t-1}^{(r)} \frac{p\left(\mathbf{y}_t \mid \mathbf{x}_t^{(r)}, \boldsymbol{\theta}\right) p\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{A_{t-1}^{(r)}}, \boldsymbol{\theta}\right)}{q\left(\mathbf{x}_t^{(r)} \mid \mathbf{x}_{t-1}^{A_{t-1}^{(r)}}, \mathbf{y}_t, \boldsymbol{\theta}\right)}, r = 1, \dots, R \quad (3.74)$$

9: Normalise weights

$$\hat{w}_t^{(r)} = \frac{w_t^{(r)}}{\sum_{r'} w_t^{(r')}}, r = 1, \dots, R \quad (3.75)$$

10: We can resample from

$$\hat{p}(\mathrm{d}\mathbf{x}_{1:t} \mid \mathbf{y}_{1:t}, \boldsymbol{\theta}) = \sum_r \hat{w}_t^{(r)} \delta_{\mathbf{x}_{1:t}^{(r)}}(\mathrm{d}\mathbf{x}_{1:t}) \quad (3.76)$$

to estimate

$$p(\mathbf{x}_{1:t} \mid \mathbf{y}_{1:t}, \boldsymbol{\theta}) \quad (3.77)$$

3.5.4 Particle filter animation

3.5.5 The proposal distribution

It is common to use the following proposal distribution

$$q(\mathbf{x}_{1:t}^{(r)} | \mathbf{y}_{1:t}) = q(\mathbf{x}_t^{(r)} | \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t) \quad (3.78)$$

$$= p(\mathbf{x}_t^{(r)} | \mathbf{x}_{t-1}^{(r)}) \quad (3.79)$$

$$= f(\mathbf{x}_t^{(r)} | \mathbf{x}_{t-1}^{(r)}) \quad (3.80)$$

Hence the weight equation in (3.51) becomes

$$w_t^{(r)} \propto w_{t-1}^{(r)} \frac{g(\mathbf{y}_t | \mathbf{x}_t^{(r)}) f(\mathbf{x}_t^{(r)} | \mathbf{x}_{t-1}^{(r)})}{q(\mathbf{x}_t^{(r)} | \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t)} \quad (3.81)$$

$$= w_{t-1}^{(r)} g(\mathbf{y}_t | \mathbf{x}_t^{(r)}) \quad (3.82)$$

This approach can be inefficient because the likelihood, $p(\mathbf{y}_t | \mathbf{x}_t^{(r)})$, can be very small at many places meaning many of the particles will be very small.

The optimal proposal distribution has the form

$$q(\mathbf{x}_{1:t}^{(r)} | \mathbf{y}_{1:t}) = q(\mathbf{x}_t^{(r)} | \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t) \quad (3.83)$$

$$= p(\mathbf{x}_t^{(r)} | \mathbf{x}_{t-1}^{(r)}, \mathbf{y}_t) \quad (3.84)$$

$$= \frac{p(\mathbf{y}_t | \mathbf{x}_t, \mathbf{x}_{t-1}^{(r)}) p(\mathbf{x}_t, \mathbf{x}_{t-1}^{(r)})}{p(\mathbf{x}_{t-1}^{(r)} | \mathbf{y}_t)} \quad (3.85)$$

$$= \frac{p(\mathbf{y}_t | \mathbf{x}_t) p(\mathbf{x}_t | \mathbf{x}_{t-1}^{(r)})}{p(\mathbf{y}_t | \mathbf{x}_{t-1}^{(r)})} \quad (3.86)$$

$$= \frac{g(\mathbf{y}_t | \mathbf{x}_t) f(\mathbf{x}_t | \mathbf{x}_{t-1}^{(r)})}{p(\mathbf{y}_t | \mathbf{x}_{t-1}^{(r)})} \quad (3.87)$$

The weight equation in (3.51) becomes

$$w_t^{(r)} \propto w_{t-1}^{(r)} p(\mathbf{y}_t | \mathbf{x}_{t-1}^{(r)}) \quad (3.88)$$

$$= w_{t-1}^{(r)} \int p(\mathbf{y}_t, \mathbf{x}'_t | \mathbf{x}_{t-1}^{(r)}) d\mathbf{x}' \quad (3.89)$$

$$= w_{t-1}^{(r)} \int p(\mathbf{y}_t | \mathbf{x}'_t, \mathbf{x}_{t-1}^{(r)}) p(\mathbf{x}'_t | \mathbf{x}_{t-1}^{(r)}) d\mathbf{x}' \quad (3.90)$$

$$= w_{t-1}^{(r)} \int p(\mathbf{y}_t | \mathbf{x}'_t) p(\mathbf{x}'_t | \mathbf{x}_{t-1}^{(r)}) d\mathbf{x}' \quad (3.91)$$

$$= w_{t-1}^{(r)} \int g(\mathbf{y}_t | \mathbf{x}'_t) f(\mathbf{x}'_t | \mathbf{x}_{t-1}^{(r)}) d\mathbf{x}'_t \quad (3.92)$$

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.

3.6 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 :

$$p_t(x_t) = p_{t-1}(x_{t-1})M_t(x_{t-1}, x_t) \quad (3.93)$$

Also assume that

$$\tilde{p}_t(x_{0:t}) = p_t(x_t) \sum_{k=1}^t L_k(x_k, x_{k-1}) \quad (3.94)$$

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

- 1: Initialisation, $t = 0$:
 - 2: **for** $r = 1, \dots, R$ **do** ▷ Sample.
 - 3: Sample $\tilde{x}_0^{(r)} \sim q_0(\cdot)$.
 - 4: **for** $r = 1, \dots, R$ **do**
 - 5: Calculate normalised weights $\hat{w}_0^{(r)} \propto \frac{p_0(\tilde{x}_0^{(r)})}{q_0(\tilde{x}_0^{(r)})}$, such that $\sum_r \hat{w}_0^{(r)} = 1$.
 - 6: Resample from the pmf $\sum_r \hat{w}_0^{(r)} \delta_{\tilde{x}_0^{(r)}}(\cdot)$ to get R samples $\{x_0^{(r)}\}$. ▷ Resample.
 - 7:
 - 8: Iterate, $t = 1, \dots, T$:
 - 9: **for** $t = 1, \dots, T$ **do**
 - 10: **for** $r = 1, \dots, R$ **do** ▷ Sample.
 - 11: Set $\tilde{x}_{0:t-1}^{(r)} = x_{0:t-1}^{(r)}$.
 - 12: Sample $\tilde{x}_t^{(r)} \sim M_t(\tilde{x}_{0:t-1}^{(r)}, \cdot)$.
 - 13: **for** $r = 1, \dots, R$ **do**
 - 14: Calculate normalised weights $\hat{w}_t^{(r)} \propto \frac{p_t(x_t) L_t(x_t, x_{t-1})}{p_{t-1}(x_{t-1}) M_t(x_{t-1}, x_t)}$.
 - 15: Resample from the pmf $\sum_r \hat{w}_t^{(r)} \delta_{\tilde{x}_t^{(r)}}(\cdot)$ to get R samples $\{x_t^{(r)}\}$. Reset the weights to $1/R$. ▷ Resample.
-

3.7 Markov chain Monte Carlo methods

3.7.1 Definitions

Definition 3.7.1. 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 $\mathcal{T}(\mathbf{x} \rightarrow \mathbf{x}')$ of going from \mathbf{x} to \mathbf{x}' , i.e. $\mathcal{T}(\mathbf{x} \rightarrow \mathbf{x}') = \Pr(\mathbf{x}' \mid \mathbf{x})$. 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 3.7.1 (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

$$\frac{1}{T} \sum_{t=1}^T f(\mathbf{X}_t) \xrightarrow[n \rightarrow \infty]{a.s.} \mathbb{E}[f(\mathbf{X})] \quad \text{where } \mathbf{X} \sim \pi \quad (3.95)$$

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

If further, it is aperiodic, then

$$\Pr(\mathbf{X}_T = \mathbf{x} \mid \mathbf{X}_0 = \mathbf{x}_0) \xrightarrow[n \rightarrow \infty]{} \pi(\mathbf{x}) \quad \forall \mathbf{x}, \mathbf{x}_0 \in \mathcal{X}. \quad (3.96)$$

A MC following these conditions is ergodic

Definition 3.7.2. A MC (\mathbf{X}_t) is time-homogeneous if $\Pr(\mathbf{X}_{t+1} = b \mid \mathbf{X}_t = a) = \mathcal{T}(a \rightarrow b) \forall t \in \{1, \dots, T-1\} \forall a, b \in \mathcal{X}$ for some kernel function \mathcal{T} .

Definition 3.7.3. A pmf π on \mathcal{X} is a stationary (invariant) distribution (w.r.t. \mathcal{T}) if

$$\pi(\mathbf{X} = \mathbf{x}') = \sum_{\mathbf{x} \in \mathcal{X}} \pi(\mathbf{X} = \mathbf{x}) \mathcal{T}(\mathbf{x} \rightarrow \mathbf{x}') \quad \forall \mathbf{x}' \quad (3.97)$$

Definition 3.7.4. 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 3.7.5. An irreducible MC (\mathbf{X}_t) is aperiodic if $\forall a \in \mathcal{X}$,

$$\gcd\{t : \Pr(\mathbf{X}_t = a \mid \mathbf{X}_0 = a) > 0\} = 1. \quad (3.98)$$

Definition 3.7.6. 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 3.7.2. 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 3.7.7. A finite state MC described by \mathcal{T} is reversible if there exists a unique distribution π such that, for all $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$

$$\pi(\mathbf{x})\mathcal{T}(\mathbf{x} \rightarrow \mathbf{x}') = \pi(\mathbf{x}')\mathcal{T}(\mathbf{x}' \rightarrow \mathbf{x}). \quad (3.99)$$

This equation is called the detailed balance (DB).

Proposition 3.7.1. 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 (3.99), we want to prove the stationarity equation (3.97) to ensure π is a stationary distribution of \mathcal{T} . We have

$$\sum_{\mathbf{x} \in \mathcal{X}} \pi(\mathbf{x})\mathcal{T}(\mathbf{x} \rightarrow \mathbf{x}') = \sum_{\mathbf{x} \in \mathcal{X}} \pi(\mathbf{x}')\mathcal{T}(\mathbf{x}' \rightarrow \mathbf{x}) \quad (3.100)$$

$$= \sum_{\mathbf{x} \in \mathcal{X}} \pi(\mathbf{x}') \Pr(\mathbf{x} \mid \mathbf{x}') \quad (3.101)$$

$$= \pi(\mathbf{x}') \sum_{\mathbf{x} \in \mathcal{X}} \Pr(\mathbf{x} \mid \mathbf{x}') \quad (3.102)$$

$$= \pi(\mathbf{x}') \quad (3.103)$$

which proves the equation (3.97). π is the unique stationary distribution of \mathcal{T} because of Theorem 3.7.2. \square

Proposition 3.7.2. Let $\mathcal{T}_1, \dots, \mathcal{T}_K$ be a set of kernels each of which satisfies detailed balance w.r.t. π . Let p_1, \dots, p_K be any distribution over $\{1, \dots, K\}$. 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

$$\mathcal{T}(\mathbf{x} \rightarrow \mathbf{x}') = \Pr(\mathbf{x}' \mid \mathbf{x}) \quad (3.104)$$

$$= \sum_k \Pr(\mathbf{x}', k \mid \mathbf{x}) \quad (3.105)$$

$$= \sum_k \Pr(\mathbf{x}' \mid k, \mathbf{x}) \Pr(k \mid \mathbf{x}) \quad (3.106)$$

$$= \sum_k \mathcal{T}_k(\mathbf{x} \rightarrow \mathbf{x}') p_k \quad (3.107)$$

Using this, we can prove the detailed balance as follows

$$\pi(\mathbf{x})\mathcal{T}(\mathbf{x} \rightarrow \mathbf{x}') = \pi(\mathbf{x}) \sum_k \mathcal{T}_k(\mathbf{x} \rightarrow \mathbf{x}') p_k \quad (3.108)$$

$$= \sum_k \pi(\mathbf{x}) \mathcal{T}_k(\mathbf{x} \rightarrow \mathbf{x}') p_k \quad (3.109)$$

$$= \sum_k \pi(\mathbf{x}') \mathcal{T}_k(\mathbf{x}' \rightarrow \mathbf{x}) p_k \quad (3.110)$$

$$= \pi(\mathbf{x}') \sum_k \mathcal{T}_k(\mathbf{x}' \rightarrow \mathbf{x}) p_k \quad (3.111)$$

$$= \pi(\mathbf{x}') \mathcal{T}(\mathbf{x}' \rightarrow \mathbf{x}) \quad (3.112)$$

□

Proposition 3.7.3. *Let $\mathcal{T}_1, \dots, \mathcal{T}_K$ 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

$$\mathcal{T}(\mathbf{x} \rightarrow \mathbf{x}') = \Pr(\mathbf{x}' | \mathbf{x}) \quad (3.113)$$

$$= \sum_{\mathbf{x}_{1:K-1}} \Pr(\mathbf{x}', \mathbf{x}_{K-1}, \dots, \mathbf{x}_1 | \mathbf{x}) \quad (3.114)$$

$$= \sum_{\mathbf{x}_{1:K-1}} \Pr(\mathbf{x}_K, \dots, \mathbf{x}_1 | \mathbf{x}_0) \quad (3.115)$$

$$= \sum_{\mathbf{x}_{1:K-1}} \Pr(\mathbf{x}_1 | \mathbf{x}_0) \cdots \Pr(\mathbf{x}_K | \mathbf{x}_{K-1}) \quad (3.116)$$

$$= \sum_{\mathbf{x}_{1:K-1}} \mathcal{T}_1(\mathbf{x}_0 \rightarrow \mathbf{x}_1) \cdots \mathcal{T}_K(\mathbf{x}_{K-1} \rightarrow \mathbf{x}_K) \quad (3.117)$$

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

$$\sum_{\mathbf{x} \in \mathcal{X}} \pi(\mathbf{x}) \mathcal{T}(\mathbf{x} \rightarrow \mathbf{x}') = \sum_{\mathbf{x}_0} \pi(\mathbf{x}_0) \sum_{\mathbf{x}_{1:K-1}} \mathcal{T}_1(\mathbf{x}_0 \rightarrow \mathbf{x}_1) \cdots \mathcal{T}_K(\mathbf{x}_{K-1} \rightarrow \mathbf{x}_K) \quad (3.118)$$

$$= \sum_{\mathbf{x}_{0:K-1}} \pi(\mathbf{x}_0) \mathcal{T}_1(\mathbf{x}_0 \rightarrow \mathbf{x}_1) \cdots \mathcal{T}_K(\mathbf{x}_{K-1} \rightarrow \mathbf{x}_K) \quad (3.119)$$

$$= \sum_{\mathbf{x}_{0:K-1}} \mathcal{T}_1(\mathbf{x}_1 \rightarrow \mathbf{x}_0) \pi(\mathbf{x}_1) \cdots \mathcal{T}_K(\mathbf{x}_{K-1} \rightarrow \mathbf{x}_K) \quad (3.120)$$

...

$$= \sum_{\mathbf{x}_{0:K-1}} \mathcal{T}_1(\mathbf{x}_1 \rightarrow \mathbf{x}_0) \cdots \mathcal{T}_K(\mathbf{x}_K \rightarrow \mathbf{x}_{K-1}) \pi(\mathbf{x}_K) \quad (3.121)$$

$$= \pi(\mathbf{x}_K) \sum_{\mathbf{x}_{0:K-1}} \mathcal{T}_K(\mathbf{x}_K \rightarrow \mathbf{x}_{K-1}) \cdots \mathcal{T}_1(\mathbf{x}_1 \rightarrow \mathbf{x}_0) \quad (3.122)$$

$$= \pi(\mathbf{x}_K) \sum_{\mathbf{x}_{0:K-1}} \Pr(\mathbf{x}_{0:K-1} | \mathbf{x}_K) \quad (3.123)$$

$$= \pi(\mathbf{x}_K). \quad (3.124)$$

□

3.7.2 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 $q(\cdot | \mathbf{x}) \equiv q(\mathbf{x} \rightarrow \cdot)$. 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 $q^*(\mathbf{x} \rightarrow \mathbf{x}') = Z_q q(\mathbf{x} \rightarrow \mathbf{x}')$ 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 $\mathbf{x}^{(t)} \sim q(\mathbf{x}^{(t-1)} \rightarrow \cdot)$.
- 5: Accept $\mathbf{x}^{(t)}$ with the acceptance probability

$$\mathcal{A}(\mathbf{x}^{(t-1)} \rightarrow \mathbf{x}^{(t)}) = \min \left(1, \frac{\pi^*(\mathbf{x}^{(t)}) q^*(\mathbf{x}^{(t)} \rightarrow \mathbf{x}^{(t-1)})}{\pi^*(\mathbf{x}^{(t-1)}) q^*(\mathbf{x}^{(t-1)} \rightarrow \mathbf{x}^{(t)})} \right) \quad (3.125)$$

- 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

$$\mathcal{T}(\mathbf{x} \rightarrow \mathbf{x}') = \begin{cases} q(\mathbf{x} \rightarrow \mathbf{x}') \mathcal{A}(\mathbf{x} \rightarrow \mathbf{x}') & \text{if } \mathbf{x} \neq \mathbf{x}' \\ q(\mathbf{x} \rightarrow \mathbf{x}) + \sum_{\mathbf{x}', \mathbf{x}' \neq \mathbf{x}} q(\mathbf{x} \rightarrow \mathbf{x}') (1 - \mathcal{A}(\mathbf{x} \rightarrow \mathbf{x}')) & \text{if } \mathbf{x} = \mathbf{x}' \end{cases} \quad (3.126)$$

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

$$\pi(\mathbf{x}) \mathcal{T}(\mathbf{x} \rightarrow \mathbf{x}') = \pi(\mathbf{x}) q(\mathbf{x} \rightarrow \mathbf{x}') \min \left(1, \frac{\pi(\mathbf{x}') q(\mathbf{x}' \rightarrow \mathbf{x})}{\pi(\mathbf{x}) q(\mathbf{x} \rightarrow \mathbf{x}')} \right) \quad (3.127)$$

$$= \min (\pi(\mathbf{x}) q(\mathbf{x} \rightarrow \mathbf{x}'), \pi(\mathbf{x}') q(\mathbf{x}' \rightarrow \mathbf{x})) \quad (3.128)$$

$$= \pi(\mathbf{x}') q(\mathbf{x}' \rightarrow \mathbf{x}) \min \left(1, \frac{\pi(\mathbf{x}) q(\mathbf{x} \rightarrow \mathbf{x}')}{\pi(\mathbf{x}') q(\mathbf{x}' \rightarrow \mathbf{x})} \right) \quad (3.129)$$

$$= \pi(\mathbf{x}') \mathcal{T}(\mathbf{x}' \rightarrow \mathbf{x}) \quad (3.130)$$

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

3.7.3 Gibbs sampling

Assume we want to sample from $p(\mathbf{x}) = p(x_1, \dots, x_D)$. 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 omitted. 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** $t = 1, \dots, T$ **do**
 - 3: Sample $x_1^{(t)} \sim p(\cdot \mid x_2^{(t-1)}, x_3^{(t-1)}, \dots, x_D^{(t-1)})$
 - 4: Sample $x_2^{(t)} \sim p(\cdot \mid x_1^{(t)}, x_3^{(t-1)}, \dots, x_D^{(t-1)})$
 - 5: \vdots
 - 6: Sample $x_D^{(t)} \sim p(\cdot \mid x_1^{(t)}, x_2^{(t)}, \dots, x_{D-1}^{(t)})$
-

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 :

$$p(\mathbf{x})\mathcal{T}_i(\mathbf{x} \rightarrow \mathbf{x}') = p(\mathbf{x})p(\mathbf{x}_{-i}, x'_i \mid \mathbf{x}) \quad (3.131)$$

$$= p(\mathbf{x}_{-i}, x'_i, \mathbf{x}) \quad (3.132)$$

$$= p(\mathbf{x}, x'_i, \mathbf{x}_{-i}) \quad (3.133)$$

$$= p(\mathbf{x}')p(\mathbf{x} \mid x'_i, \mathbf{x}_{-i}) \quad (3.134)$$

$$= p(\mathbf{x}')\mathcal{T}_i(\mathbf{x}' \rightarrow \mathbf{x}) \quad (3.135)$$

This is the premise of Proposition 3.7.3, 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 $q_i(\mathbf{x} \rightarrow \mathbf{x}')$ 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.

$$\mathcal{A}(\mathbf{x} \rightarrow \mathbf{x}') = \min \left(1, \frac{p(\mathbf{x}')p(\mathbf{x} \mid \mathbf{x}')}{p(\mathbf{x})p(\mathbf{x}' \mid \mathbf{x})} \right) \quad (3.136)$$

$$= \min \left(1, \frac{p(\mathbf{x}', \mathbf{x})}{p(\mathbf{x}', \mathbf{x})} \right) \quad (3.137)$$

$$= 1 \quad (3.138)$$

3.8 Particle Markov Chain Monte Carlo

Bibliography

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