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
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- 1.6 Categorical distribution
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2 Bayesian parameter estimation

2.1 Beta-Bernoulli model

2.1.1 Summary

The model

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

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

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

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

Posterior

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

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

$$\mathcal{D} = \{N_1, N\} \tag{2.10}$$

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

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

$$\tilde{\mathcal{D}} = \{\tilde{N}_1, \tilde{N}\} \tag{2.13}$$

$$\tilde{N}_1$$
 = 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)

Likelihood

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

Prior

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

Posterior

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

Posterior predictive

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

Evidence

2.2.2 Derivations

2.3 Dirichlet-categorical model

2.3.1 Summary

The model

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

$$\mathcal{D} = \{x_1, \dots, x_N\} \tag{2.21}$$

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

Likelihood

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

Prior

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

Posterior

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

Posterior predictive

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

$$= \frac{\alpha_j + n_j}{\alpha_0 + N}$$
(2.26)

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

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

Evidence

2.3.2 Derivations

2.4 Dirichlet-multinomial model

2.4.1 Summary

The model

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

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

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

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

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

Likelihood

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

Prior

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

Posterior

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

Posterior predictive

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

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

Evidence

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

2.4.2 Derivations

2.5 Poisson-gamma model

2.5.1 Summary

The model

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

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

Likelihood

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

Prior

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

Posterior

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

Posterior predictive

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

Evidence

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

2.5.2 Derivations

3 Sampling algorithms

3.1 Introduction

Let p be a probability distribution with pdf $p(\mathbf{x})$, 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 $Z_p = \int p^*(\mathbf{x}) d\mathbf{x}$). We want to achieve the following:

Problem 1 Generate samples $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(R)}\}$ (shorthand notation $\{\mathbf{x}^{(r)}\}$) from the probability distribution p.

Problem 2 Estimate the expectation of an arbitrary function f given that $\mathbf{x} \sim p$, $\mathrm{E}[f]$.

3.2 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

- 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].

3.2.1 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 $\mathbf{E}[f]$, as R increases. We consider the expectations of the numerator and denominator separately:

$$E_q[\text{numer}] = E_q \left[\sum_r w_r f(\mathbf{x}^{(r)}) \right]$$
(3.1)

$$= \sum_{r} E_q \left[w_r f(\mathbf{x}^{(r)}) \right]$$
 (3.2)

$$= \sum_{r} E_{q} \left[\frac{p^{*}(\mathbf{x}^{(r)})}{q^{*}(\mathbf{x}^{(r)})} f(\mathbf{x}^{(r)}) \right]$$
(3.3)

$$= \sum_{r} E_{q} \left[\frac{Z_{p} p(\mathbf{x}^{(r)})}{Z_{q} q(\mathbf{x}^{(r)})} f(\mathbf{x}^{(r)}) \right]$$
(3.4)

$$= \frac{Z_p}{Z_q} \sum_{r} \int_{\mathbf{x}^{(r)}} p(\mathbf{x}^{(r)}) f(\mathbf{x}^{(r)}) d\mathbf{x}^{(r)}$$
(3.5)

$$= \frac{Z_p}{Z_q} \sum_r \mathcal{E}_p \left[f(\mathbf{x}^{(r)}) \right]$$
 (3.6)

$$= \frac{Z_p}{Z_q} R \operatorname{E}_p \left[f(\mathbf{x}) \right] \tag{3.7}$$

$$E_q[\text{denom}] = E_q \left[\sum_r w_r \right]$$
 (3.8)

$$= \sum_{r} E_{q} \left[\frac{p^{*}(\mathbf{x}^{(r)})}{q^{*}(\mathbf{x}^{(r)})} \right]$$
(3.9)

$$= \sum_{r} E_{q} \left[\frac{Z_{p} p(\mathbf{x}^{(r)})}{Z_{q} q(\mathbf{x}^{(r)})} \right]$$
(3.10)

$$= \frac{Z_p}{Z_q} \sum_r \int_{\mathbf{x}^{(r)}} p(\mathbf{x}^{(r)}) \, d\mathbf{x}^{(r)}$$
(3.11)

$$=\frac{Z_p}{Z_q}R\tag{3.12}$$

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

3.2.2 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

$$\operatorname{var}_{q}\left[\frac{p(\mathbf{x})}{q(\mathbf{x})}f(\mathbf{x})\right] = \operatorname{E}_{q}\left[\frac{p^{2}(\mathbf{x})}{q^{2}(\mathbf{x})}f^{2}(\mathbf{x})\right] - \left(\operatorname{E}_{q}\left[\frac{p(\mathbf{x})}{q(\mathbf{x})}f(\mathbf{x})\right]\right)^{2}$$
(3.13)

$$= \operatorname{E}_{q} \left[\frac{p^{2}(\mathbf{x})}{q^{2}(\mathbf{x})} f^{2}(\mathbf{x}) \right] - \left(\operatorname{E}_{p} \left[f(\mathbf{x}) \right] \right)^{2}$$
(3.14)

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:

$$E_q\left[\frac{p^2(\mathbf{x})}{q^2(\mathbf{x})}f^2(\mathbf{x})\right] \ge \left(E_q\left[\frac{p(\mathbf{x})}{q(\mathbf{x})}|f(\mathbf{x})|\right]\right)^2 = (E_p[|f(\mathbf{x})|])^2$$
(3.15)

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

$$q_{\text{optimal}}(\mathbf{x}) = \frac{|f(\mathbf{x})|p(\mathbf{x})}{\int |f(\mathbf{x}')|p(\mathbf{x}') \, d\mathbf{x}'}$$
(3.16)

3.3 Sampling importance resampling

In Sampling importance resampling (SIR), we approximate the pdf of p as point masses and resample from them to get samples $\{\mathbf{x}^{(r)}\}$ which are approximately $\sim p$. The process is as follows:

- 1. Generate samples $\{\mathbf{z}^{(r)}\}$ 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. Resample from a probability distribution with the pmf

$$f(\mathbf{x}) = \sum_{r} \hat{w}_r \delta_{\mathbf{z}^{(r)}}(\mathbf{x}) \tag{3.17}$$

5. The resulting samples $\{\mathbf{x}^{(r)}\}$ are approximately $\sim p$.

3.3.1 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

$$N(x) = \lim_{\delta x \to 0} Rq(x)\delta x \tag{3.18}$$

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

$$\lim_{\delta x \to 0} \Pr(x \le x^{(r)} \le x + \delta x) = N(x)\hat{w}_r \tag{3.19}$$

$$\propto \lim_{\delta x \to 0} Rq(x) \delta x \frac{p(x)}{q(x)}$$
 (3.20)

$$\propto \lim_{\delta x \to 0} p(x)\delta x \tag{3.21}$$

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

$$\Pr(a \le x^{(r)} \le b) \propto \int_a^b p(x) \, \mathrm{d}x \tag{3.22}$$

$$\implies x^{(r)} \sim p \tag{3.23}$$

3.4 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

$$cq^*(\mathbf{x}) > p^*(\mathbf{x}) \text{ for all } \mathbf{x}$$
 (3.24)

The procedure that generates a sample $\mathbf{x} \sim p$ is

- 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.

3.4.1 Why it works?

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

$$\mathcal{X} = \{ \boldsymbol{\alpha} \in \mathbb{R}^{d+1} : \alpha_{1:d} \in \mathbb{R}^d, \alpha_{d+1} \in [0, cq^*(\boldsymbol{\alpha})] \}$$
(3.25)

$$\mathcal{X}' = \{ \boldsymbol{\alpha} \in \mathbb{R}^{d+1} : \alpha_{1:d} \in \mathbb{R}^d, \alpha_{d+1} \in [0, p^*(\boldsymbol{\alpha})] \}$$
(3.26)

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

$$Pr(\mathbf{x}, u) = Pr(\mathbf{x}) Pr(u)$$
(3.27)

$$= q(\mathbf{x}) \frac{1}{cq^*(\mathbf{x})} \tag{3.28}$$

$$= q(\mathbf{x}) \frac{1}{cZ_q q(\mathbf{x})} \tag{3.29}$$

$$=\frac{1}{cZ_q}\tag{3.30}$$

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

$$(\mathbf{x}, u) \sim \text{Unif}(\mathcal{X})$$
 (3.31)

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') :

$$(\mathbf{x}', u') = \begin{cases} (\mathbf{x}, u) & \text{if } (\mathbf{x}, u) \in \mathcal{X}' \\ \text{nothing} & \text{otherwise.} \end{cases}$$
(3.32)

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

$$\Pr(\mathbf{x}', u') = \begin{cases} \Pr(\mathbf{x}, u) & \text{if } (\mathbf{x}, u) \in \mathcal{X}' \\ 0 & \text{otherwise.} \end{cases}$$
 (3.33)

which means

$$(\mathbf{x}', u') \sim \text{Unif}(\mathcal{X}')$$
 (3.34)

Working backwards

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

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

$$\propto p^*(\mathbf{x}')$$
(3.35)
(3.36)

$$\propto \frac{1}{1/n^*(\mathbf{x}')} \tag{3.36}$$

$$\propto p^*(\mathbf{x}') \tag{3.37}$$

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

3.5 Particle filtering