CPSC 535 Importance Sampling Methods

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8th February 2007

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• Importance Sampling

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- Importance Sampling
- Normalized Importance Sampling.

- Importance Sampling
- Normalized Importance Sampling.
- Importance Sampling versus Rejection Sampling.

• Let $\pi(x)$ be a probability density on \mathcal{X} .

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- Monte Carlo approximation is given by

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• More precisely, we have

$$\mathbb{E}_{\left\{X^{(i)}\right\}}\left[\mathbb{E}_{\widehat{\pi}_{N}}\left(\varphi\left(X\right)\right)\right] = \mathbb{E}_{\pi}\left(\varphi\left(X\right)\right),$$
$$\mathsf{var}_{\left\{X^{(i)}\right\}}\left(\mathbb{E}_{\widehat{\pi}_{N}}\left(\varphi\left(X\right)\right)\right) = \frac{\mathsf{var}_{\pi}\left(\varphi\left(X\right)\right)}{N}.$$

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- In case where π ∝ π^{*} does not admit any standard form, we can use a proposal distribution q on X where q ∝ q^{*}.
- We need q to 'dominate' π ; i.e.

$$C = \sup_{x \in \mathcal{X}} \frac{\pi^*(x)}{q^*(x)} < +\infty.$$

Consider $C' \ge C$. Then the accept/reject procedure proceeds as follows: Accept/Reject procedure

Sample $Y \sim q$ and $U \sim \mathcal{U}(0, 1)$.

Consider $C' \geq C$. Then the accept/reject procedure proceeds as follows:

Accept/Reject procedure

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- This is a simple generic algorithm but it requires coming up with a bound *C*.
- Its performance typically degrade exponentially fast with the dimension of \mathcal{X} .
- It seems you are wasting some information by rejecting samples.
- You need to wait a random time to obtain some samples from π .
- Is it possible to "recycle" these samples?

Importance Sampling

• Consider again the target distribution π and the proposal distribution q. We only require

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where the so-called Importance Weight is given by

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It follows that

$$\mathbb{E}_{\pi}(\varphi(X)) = \int_{\mathcal{X}} \varphi(x)\pi(x)dx = \int_{\mathcal{X}} \varphi(x)\frac{\pi(x)}{q(x)}q(x)dx$$
$$= \mathbb{E}_{q}(w(X)\varphi(X))$$

• Monte Carlo approximation of q is

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• It follows that an estimate of $\mathbb{E}_{\pi}(arphi(X)) = \mathbb{E}_{q}(w(X)arphi(X))$ is

$$\mathbb{E}_{\widehat{q}_N}(w(X)\varphi(X)) = \frac{1}{N}\sum_{i=1}^N w(X^{(i)})\varphi(X^{(i)}).$$

• We have

$$\mathbb{E}_{\left\{X^{(i)}\right\}}\left[\mathbb{E}_{\widehat{q}_{N}}\left(w(X)\varphi\left(X\right)\right)\right]=\mathbb{E}_{\pi}\left(\varphi\left(X\right)\right)$$

and

$$\begin{aligned} \mathsf{var}_{\left\{X^{(i)}\right\}}\left(\mathbb{E}_{\widehat{q}_{N}}\left(\varphi\left(X\right)\right)\right) &= \frac{\mathsf{var}_{q}\left(w(X)\varphi\left(X\right)\right)}{N} \\ &= \frac{\mathbb{E}_{\pi}\left(w(X)\varphi^{2}\left(X\right)\right) - \mathbb{E}_{\pi}^{2}\left(\varphi\left(X\right)\right)}{N} \end{aligned}$$

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• We have

$$\mathbb{E}_{\left\{X^{(i)}\right\}}\left[\mathbb{E}_{\widehat{q}_{N}}\left(w(X)\varphi\left(X\right)\right)\right]=\mathbb{E}_{\pi}\left(\varphi\left(X\right)\right)$$

and

$$var_{\left\{X^{(i)}\right\}}\left(\mathbb{E}_{\widehat{q}_{N}}\left(\varphi\left(X\right)\right)\right) = \frac{var_{q}\left(w(X)\varphi\left(X\right)\right)}{N} \\ = \frac{\mathbb{E}_{\pi}\left(w(X)\varphi^{2}\left(X\right)\right) - \mathbb{E}_{\pi}^{2}\left(\varphi\left(X\right)\right)}{N}$$

• In practice, it is recommended to ensure

$$\mathbb{E}_{\pi}\left(w(X)\right) = \int \frac{\pi^{2}\left(x\right)}{q\left(x\right)} dx < \infty.$$

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• In practice, it is recommended to ensure

$$\mathbb{E}_{\pi}\left(w(X)\right) = \int \frac{\pi^{2}\left(x\right)}{q\left(x\right)} dx < \infty.$$

• Even if it is not necessary, it is actually even better to ensure that

$$\sup_{x\in\mathcal{X}}w(x)<\infty.$$



Figure: Target double exponential distributions and two IS distributions

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Figure: IS approximation obtained using a Gaussian IS distribution



Figure: IS approximation obtained using a Student-t IS distribution

• We try to compute

$$\int \sqrt{\frac{x}{1-x}} \pi(x) \, dx$$

where

$$\pi(\mathbf{x}) = \frac{\Gamma((\nu+1)/2)}{\sqrt{\nu\pi}\Gamma(\nu/2)} \left(1 + \frac{\mathbf{x}}{\nu}\right)^{-(\nu+1)/2}$$

is a t-student distribution with $\nu > 1$ (you can sample from it by composition $\mathcal{N}(0,1) / \mathcal{G}a(\nu/2,\nu/2)$) using Monte Carlo.

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• We use $q_1(x) = \pi(x)$, $q_2(x) = \frac{\Gamma(1)}{\sqrt{\nu \pi} \Gamma(1/2)} \left(1 + \frac{x}{\nu \sigma}\right)^{-1}$ (Cauchy distribution) and $q_3(x) = \mathcal{N}\left(x; 0, \frac{\nu}{\nu - 2}\right)$ (variance chosen to match the variance of $\pi(x)$)

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- It is easy to see that

$$rac{\pi\left(x
ight)}{q_{2}\left(x
ight)}<\infty$$
 and $\intrac{\pi\left(x
ight)^{2}}{q_{3}\left(x
ight)}dx=\infty,\ rac{\pi\left(x
ight)}{q_{3}\left(x
ight)}$ is unbounded



Figure: Performance for $\nu = 12$ with q_1 (solid line), q_2 (dashes) and q_3 (light dots). Final values 1.14, 1.14 and 1.16 vs true value 1.13

• We now try to compute

$$\int_{2.1}^{\infty} x^5 \pi(x) \, dx$$

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$$\int_{2.1}^{\infty} x^5 \pi\left(x\right) dx$$

 We try to use the same importance distribution but also use the fact that using a change of variables u = 1/x, we have

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$$\int_{2.1}^{\infty} x^5 \pi(x) \, dx = \int_{0}^{1/2.1} u^{-7} \pi(1/u) \, du$$
$$= \frac{1}{2.1} \int_{0}^{1/2.1} 2.1 u^{-7} \pi(1/u) \, du$$

which is the expectation of $2.1u^{-7}\pi\left(1/u\right)$ with respect to $\mathcal{U}\left[0,1/2.1\right]$.


Figure: Performance for $\nu = 12$ with q_1 (solid), q_2 (short dashes), q_3 (dots), uniform (long dashes). Final values 6.75, 6.48, 7.06 and 6.48 vs true value 6.54

Optimal Importance function

• For a given test function, one can minimize the IS variance using

$$q^{\text{opt}}(x) = \frac{|\varphi(x)| \pi(x)}{\int_{\mathcal{X}} |\varphi(x)| \pi(x) \, dx}$$

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Proof:

$$\operatorname{var}_{q}\left(w(X)\varphi\left(X\right)\right) = \int q\left(x\right)\frac{\pi^{2}\left(x\right)}{q^{2}\left(x\right)}\varphi^{2}\left(x\right)dx - \left(\int \pi\left(x\right)\varphi\left(x\right)dx\right)^{2}$$

and

$$\int q(x) \frac{\pi^2(x)}{q^2(x)} \varphi^2(x) dx \ge \left(\int q(x) \frac{\pi(x) |\varphi(x)|}{q(x)} dx \right)^2$$
$$= \left(\int \pi(x) |\varphi(x)| dx \right)^2.$$

This lower bound is attained for $q^{\text{opt}}(x)$.

Normalized Importance Sampling

• In most if not all applications we are interested in, standard IS cannot be used as the importance weights $w(x) = \pi(x) / q(x)$ cannot be evaluated in closed-form. In practice, we typically only know $\pi(x) \propto \pi^*(x)$ and $q(x) \propto q^*(x)$.

Normalized Importance Sampling

- In most if not all applications we are interested in, standard IS cannot be used as the importance weights w (x) = π (x) / q (x) cannot be evaluated in closed-form. In practice, we typically only know π (x) ∝ π* (x) and q (x) ∝ q* (x).
- Normalized IS identity is based on

$$\pi(x) = \frac{\pi^*(x)}{\int \pi^*(x) \, dx} = \frac{w^*(x) \, q^*(x)}{\int w^*(x) \, q^*(x) \, dx}$$
$$= \frac{w^*(x) \, q(x)}{\int w^*(x) \, q(x) \, dx} = \frac{w(x) \, q(x)}{\int w(x) \, q(x) \, dx}$$

where

$$w^{*}(x) = \frac{\pi^{*}(x)}{q^{*}(x)}.$$

• For any test function φ , we can also write

$$\mathbb{E}_{\pi}\left(\varphi\left(X\right)\right) = \frac{\mathbb{E}_{q}\left(w^{*}\left(X\right)\varphi\left(X\right)\right)}{\mathbb{E}_{q}\left(w^{*}\left(X\right)\right)} = \frac{\mathbb{E}_{q}\left(w\left(X\right)\varphi\left(X\right)\right)}{\mathbb{E}_{q}\left(w\left(X\right)\right)}$$

Image: A matrix

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• Given a Monte Carlo approximation of q; $\hat{q}_N(x) = \frac{1}{N} \sum_{i=1}^N \delta_{X^{(i)}}(x)$ then

$$\begin{aligned} \widehat{\pi}_{N}\left(x\right) &= \sum_{i=1}^{N} W^{(i)} \delta_{X^{(i)}}\left(x\right) \text{ where } W^{(i)} &= \frac{w^{*}\left(X^{(i)}\right)}{\sum_{j=1}^{N} w^{*}\left(X^{(j)}\right)}, \\ \mathbb{E}_{\widehat{\pi}_{N}}\left(\varphi\left(X\right)\right) &= \sum_{i=1}^{N} W^{(i)} \varphi\left(X^{(i)}\right). \end{aligned}$$

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• The estimates are a ratio of estimates.

• Contrary to standard IS, this estimate is biased but by the LLN it is asymptotically consistent.

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- Derivation of the asymptotic bias and variance based on the delta method.

Asymptotic Bias and Variance

 Assume you have Z = g (A, B) with E (A) = µ_A and E (B) = µ_B then a two-dimensional Taylor expansion gives around µ = (µ_A, µ_B)

$$Z \approx g(\mu) + (A - \mu_A) \frac{\partial g}{\partial a}(\mu) + (B - \mu_B) \frac{\partial g}{\partial b}(\mu).$$

It follows that

$$\mathbb{E}(Z) \approx g(\mu),$$

$$Var(Z) \approx \sigma_{A}^{2} \frac{\partial g}{\partial a}^{2}(\mu) + \sigma_{B}^{2} \frac{\partial g}{\partial b}^{2}(\mu) + 2 \frac{\partial g}{\partial a}(\mu) \frac{\partial g}{\partial b}(\mu) \sigma_{A,B}.$$

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In our case

$$Z = \mathbb{E}_{\widehat{\pi}_{N}}\left(\varphi\left(X\right)\right) = \frac{\mathbb{E}_{\widehat{q}_{N}}\left(w^{*}\left(X\right)\varphi\left(X\right)\right)}{\mathbb{E}_{\widehat{q}_{N}}\left(w^{*}\left(X\right)\right)} = \frac{A}{B}$$

• We have

$$\frac{\partial g}{\partial a}(\mu) \frac{\partial g}{\partial b}(\mu) = -\frac{\mu_A}{\mu_B^3}, \ \frac{\partial g}{\partial a}(\mu) = \frac{1}{\mu_B^2}, \ \frac{\partial g}{\partial b}(\mu) = \frac{\mu_A^2}{\mu_B^4},$$

$$\mu_{A} = \mathbb{E}_{q} \left(w^{*} \left(X \right) \varphi \left(X \right) \right), \ \mu_{B} = \mathbb{E}_{q} \left(w^{*} \left(X \right) \right),$$

$$\sigma_{A}^{2} = \frac{\operatorname{var}_{q} \left(w^{*} \left(X \right) \varphi \left(X \right) \right)}{N}, \ \sigma_{B}^{2} = \frac{\operatorname{var}_{q} \left(w^{*} \left(X \right) \right)}{N}$$

$$\sigma_{A,B} = \frac{\mathbb{E}_{q} \left(w^{*} \left(X \right)^{2} \varphi \left(X \right) \right) - \mu_{A} \cdot \mu_{B}}{N}.$$

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• It follows that

$$\begin{aligned} & \operatorname{var}\left(\mathbb{E}_{\widehat{\pi}_{N}}\left(\varphi\left(X\right)\right)\right) \\ \approx & \sigma_{A}^{2} \frac{\partial g}{\partial a}^{2}\left(\mu\right) + \sigma_{B}^{2} \frac{\partial g}{\partial b}^{2}\left(\mu\right) + 2\frac{\partial g}{\partial a}\left(\mu\right) \frac{\partial g}{\partial b}\left(\mu\right) \sigma_{A,B} \\ = & \frac{\sigma_{A}^{2}}{\mu_{B}^{2}} + \frac{\sigma_{B}^{2} \mu_{A}^{2}}{\mu_{B}^{4}} - 2\frac{\mu_{A} \sigma_{A,B}}{\mu_{B}^{3}} \end{aligned}$$

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• Asymptotically, we have a central limit theorem

$$\sqrt{N}\left(\mathbb{E}_{\widehat{\pi}_{N}}\left(\varphi\left(X\right)\right)-\mathbb{E}_{\pi}\left(\varphi\left(X\right)\right)\right)\Rightarrow\mathcal{N}\left(0,\sigma_{IS}^{2}\left(\varphi\right)\right)$$

where

$$\sigma_{IS}^{2}\left(\varphi\right) = \int \frac{\pi^{2}\left(x\right)}{q\left(x\right)} \left(\varphi\left(x\right) - \mathbb{E}_{\pi}\left(\varphi\right)\right)^{2} dx$$

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• In practice, it is now necessary but highly recommended to select the proposal q such that

$$\sup_{x \in \mathcal{X}} w(x) < \infty \text{ or equivalently } \sup_{x \in \mathcal{X}} w^*(x) < \infty.$$

• In practice, it is now necessary but highly recommended to select the proposal *q* such that

$$\sup_{x \in \mathcal{X}} w(x) < \infty \text{ or equivalently } \sup_{x \in \mathcal{X}} w^*(x) < \infty.$$

• There is some empirical evidence that Normalized IS performs better than standard IS in numerous cases.

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• Using a second order Taylor expansion

$$\begin{split} & Z \approx g\left(\mu\right) + \left(A - \mu_{A}\right) \frac{\partial g}{\partial a}\left(\mu\right) + \left(B - \mu_{B}\right) \frac{\partial g}{\partial b}\left(\mu\right) \\ & + \frac{1}{2} \left(A - \mu_{A}\right)^{2} \frac{\partial^{2} g}{\partial a^{2}}\left(\mu\right) + \frac{1}{2} \left(B - \mu_{B}\right)^{2} \frac{\partial^{2} g}{\partial b^{2}}\left(\mu\right) \\ & + \left(A - \mu_{A}\right) \left(B - \mu_{B}\right) \frac{\partial^{2} g}{\partial a \partial b}\left(\mu\right) \end{split}$$

gives

$$\mathbb{E}\left(\mathbb{E}_{\widehat{\pi}_{N}}\left(\varphi\left(X\right)\right)\right) \approx g\left(\mu\right) + \frac{1}{2}\sigma_{A}^{2}\frac{\partial^{2}g}{\partial a^{2}}\left(\mu\right) + \frac{1}{2}\sigma_{B}^{2}\frac{\partial^{2}g}{\partial b^{2}}\left(\mu\right) \\ + \sigma_{A,B}\frac{\partial^{2}g}{\partial a\partial b}\left(\mu\right).$$

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• It follows that asymptotically we have

$$N\left(\mathbb{E}_{\widehat{\pi}_{N}}\left(\varphi\left(X\right)\right)-\mathbb{E}_{\pi}\left(\varphi\left(X\right)\right)\right)\rightarrow-\int\frac{\pi^{2}\left(x\right)}{q\left(x\right)}\left(\varphi\left(x\right)-\mathbb{E}_{\pi}\left(\varphi\right)\right)dx.$$

• Using a second order Taylor expansion

$$\begin{split} & Z \approx g\left(\mu\right) + \left(A - \mu_{A}\right) \frac{\partial g}{\partial a}\left(\mu\right) + \left(B - \mu_{B}\right) \frac{\partial g}{\partial b}\left(\mu\right) \\ & + \frac{1}{2} \left(A - \mu_{A}\right)^{2} \frac{\partial^{2} g}{\partial a^{2}}\left(\mu\right) + \frac{1}{2} \left(B - \mu_{B}\right)^{2} \frac{\partial^{2} g}{\partial b^{2}}\left(\mu\right) \\ & + \left(A - \mu_{A}\right) \left(B - \mu_{B}\right) \frac{\partial^{2} g}{\partial a \partial b}\left(\mu\right) \end{split}$$

gives

$$\mathbb{E}\left(\mathbb{E}_{\widehat{\pi}_{N}}\left(\varphi\left(X\right)\right)\right) \approx g\left(\mu\right) + \frac{1}{2}\sigma_{A}^{2}\frac{\partial^{2}g}{\partial a^{2}}\left(\mu\right) + \frac{1}{2}\sigma_{B}^{2}\frac{\partial^{2}g}{\partial b^{2}}\left(\mu\right) \\ + \sigma_{A,B}\frac{\partial^{2}g}{\partial a\partial b}\left(\mu\right).$$

• It follows that asymptotically we have

$$N\left(\mathbb{E}_{\widehat{\pi}_{N}}\left(\varphi\left(X\right)\right)-\mathbb{E}_{\pi}\left(\varphi\left(X\right)\right)\right)\rightarrow-\int\frac{\pi^{2}\left(x\right)}{q\left(x\right)}\left(\varphi\left(x\right)-\mathbb{E}_{\pi}\left(\varphi\right)\right)dx.$$

• We have $Bias^2$ of order $1/N^2$ and Variance of order 1/N.

• The asymptotic variance (and also the asymptotic bias) can be consistently estimated from the data using

$$\frac{\widehat{\sigma_{IS}^2(\varphi)}}{N} = \frac{\widehat{\sigma}_A^2}{\widehat{\mu}_B^2} + \frac{\widehat{\sigma}_B^2 \widehat{\mu}_A^2}{\widehat{\mu}_B^4} - 2\frac{\widehat{\mu}_A \widehat{\sigma}_{A,B}}{\widehat{\mu}_B^3}$$

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• You can also compute the variance of the variance estimate; see Geweke (1989).

• Consider a Bayesian model: prior $\pi(\theta)$ and likelihood $f(x|\theta)$.

Application to Bayesian Statistics

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- The posterior distribution is given by

$$\begin{aligned} \pi\left(\left.\theta\right|x\right) &= \frac{\pi(\theta)f(x|\theta)}{\int_{\Theta}\pi(\theta)f(x|\theta)d\theta} \propto \pi^{*}\left(\left.\theta\right|x\right) \\ \text{where } \pi^{*}\left(\left.\theta\right|x\right) &= \pi\left(\theta\right)f\left(\left.x\right|\theta\right). \end{aligned}$$

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where $\pi^* \left(\left. \theta \right| x \right) = \pi \left(\theta \right) f(x|\theta)$.

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$$\int_{\Theta} \pi(\theta) f(x|\theta) d\theta.$$

• *Example*: Application to Bayesian analysis of Markov chain. Consider a two state Markov chain with transition matrix F

$$\left(egin{array}{cc} p_1 & 1-p_1 \ 1-p_2 & p_2 \end{array}
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that is $\Pr(X_{t+1} = 1 | X_t = 1) = 1 - \Pr(X_{t+1} = 2 | X_t = 1) = p_1$ and $\Pr(X_{t+1} = 2 | X_t = 2) = 1 - \Pr(X_{t+1} = 1 | X_t = 2) = p_2$. Physical constraints tell us that $p_1 + p_2 < 1$. • *Example*: Application to Bayesian analysis of Markov chain. Consider a two state Markov chain with transition matrix F

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• Assume we observe *x*₁, ..., *x_m* and the prior is

$$\pi\left(\mathbf{p}_{1},\mathbf{p}_{2}
ight)=2\mathbb{I}_{p_{1}+p_{2}\leq1}$$

then the posterior is

$$\pi \left(\left. p_{1}, p_{2} \right| x_{1:m} \right) \propto p_{1}^{m_{1,1}} \left(1 - p_{1} \right)^{m_{1,2}} \left(1 - p_{2} \right)^{m_{2,1}} p_{2}^{m_{2,2}} \mathbb{I}_{p_{1} + p_{2} \le 1}$$

where

$$m_{i,j} = \sum_{t=1}^{m-1} \mathbb{I}_{x_t=i} \mathbb{I}_{x_{t+1}=i}$$

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 The posterior does not admit a standard expression and its normalizing constant is unnknown. We can sample from it using rejection sampling.
 AD () • We are interested in estimating $\mathbb{E} \left[\varphi_i (p_1, p_2) | x_{1:m} \right]$ for $\varphi_1 (p_1, p_2) = p_1$, $\varphi_2 (p_1, p_2) = p_2$, $\varphi_3 (p_1, p_2) = p_1 / (1 - p_1)$, $\varphi_4 (p_1, p_2) = p_2 / (1 - p_2)$ and $\varphi_5 (p_1, p_2) = \log \frac{p_1(1 - p_2)}{p_2(1 - p_1)}$ using Importance Sampling.

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- If there was no on $p_1 + p_2 < 1$ and $\pi(p_1, p_2)$ was uniform on $[0, 1] \times [0, 1]$, then the posterior would be

$$\pi_0(p_1, p_2 | x_{1:m}) = \mathcal{B}e(p_1; m_{1,1} + 1, m_{1,2} + 1)$$
$$\mathcal{B}e(p_2; m_{2,2} + 1, m_{2,1} + 1)$$

but this is inefficient as for the given data $(m_{1,1}, m_{1,2}, m_{2,2}, m_{2,1})$ we have $\pi_0 (p_1 + p_2 < 1 | x_{1:m}) = 0.21$.

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but this is inefficient as for the given data $(m_{1,1}, m_{1,2}, m_{2,2}, m_{2,1})$ we have $\pi_0 (p_1 + p_2 < 1 | x_{1:m}) = 0.21$.

 The form of the posterior suggests using a Dirichlet distribution with density

$$\pi_1(p_1, p_2|x_{1:m}) \propto p_1^{m_{1,1}} p_2^{m_{2,2}} (1-p_1-p_2)^{m_{1,2}+m_{2,1}}$$

but $\pi(p_1, p_2 | x_{1:m}) / \pi_1(p_1, p_2 | x_{1:m})$ is unbounded.

• (Geweke, 1989) proposed using the normal approximation to the binomial distribution

$$\pi_{2}(p_{1}, p_{2}|x_{1:m}) \propto \exp\left(-(m_{1,1} + m_{1,2})(p_{1} - \hat{p}_{1})^{2} / (2\hat{p}_{1}(1 - \hat{p}_{1}))\right) \times \exp\left(-(m_{2,1} + m_{2,2})(p_{2} - \hat{p}_{2})^{2} / (2\hat{p}_{2}(1 - \hat{p}_{2}))\right)$$

where $\hat{p}_1 = m_{1,1}/(m_{1,1} + m_{1,2})$, $\hat{p}_1 = m_{2,2}/(m_{2,2} + m_{2,1})$. Then to simulate from this distribution, we simulate first $\pi_2(p_1|x_{1:m})$ and then $\pi_2(p_2|x_{1:m}, p_1)$ which are univariate truncated Gaussian distribution which can be sampled using the inverse cdf method. The ratio $\pi(p_1, p_2|x_{1:m})/\pi_2(p_1, p_2|x_{1:m})$ is upper bounded.

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 $\pi_{3}(p_{1}, p_{2} | x_{1:m}) = \mathcal{B}e(p_{1}; m_{1,1} + 1, m_{1,2} + 1) \pi_{3}(p_{2} | x_{1:m}, p_{1})$ where $\pi(p_{2} | x_{1:m}, p_{1}) \propto (1 - p_{2})^{m_{2,1}} p_{2}^{m_{2,2}} \mathbb{I}_{p_{2} \leq 1 - p_{1}}$ is badly approximated through $\pi_{3}(p_{2} | x_{1:m}, p_{1}) = \frac{2}{(1 - p_{1})^{2}} p_{2} \mathbb{I}_{p_{2} \leq 1 - p_{1}}$. It is straightforward to check that $\pi(p_{1}, p_{2} | x_{1:m}) / \pi_{3}(p_{1}, p_{2} | x_{1:m}) \propto (1 - p_{2})^{m_{2,1}} p_{2}^{m_{2,2}} / \frac{2}{(1 - p_{1})^{2}} p_{2} < \infty.$

Distribution	φ_1	φ_2	φ_3	φ_4	φ_5
π_1	0.748	0.139	3.184	0.163	2.957
π_2	0.689	0.210	2.319	0.283	2.211
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• Performance for N = 10,000

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• Sampling from π using rejection sampling works well but is computationally expensive. π_3 is computationally much cheaper whereas π_1 does extremely poorly as expected.
Optimal Normalized Importance Sampling

 For a given test function, one can minimize the normalized IS asymptotic variance using

$$q^{\text{opt}}(x) = \frac{|\varphi(x) - \mathbb{E}_{\pi}(\varphi)| \pi(x)}{\int_{\mathcal{X}} |\varphi(x) - \mathbb{E}_{\pi}(\varphi)| \pi(x) \, dx}$$

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Proof.

$$\int q(x) \frac{\pi^{2}(x)}{q^{2}(x)} \left(\varphi(x) - \mathbb{E}_{\pi}(\varphi)\right)^{2} dx$$

$$\geq \left(\int q(x) \frac{\pi(x)|\varphi(x) - \mathbb{E}_{\pi}(\varphi)|}{q(x)} dx\right)^{2}$$

$$= \left(\int \pi(x) |\varphi(x) - \mathbb{E}_{\pi}(\varphi)| dx\right)^{2}$$

and this lower bound is attained for $q^{\text{opt}}(x)$.

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Proof:

$$\int q(x) \frac{\pi^{2}(x)}{q^{2}(x)} \left(\varphi(x) - \mathbb{E}_{\pi}(\varphi)\right)^{2} dx \geq \left(\int q(x) \frac{\pi(x)|\varphi(x) - \mathbb{E}_{\pi}(\varphi)|}{q(x)} dx\right)^{2} = \left(\int \pi(x) |\varphi(x) - \mathbb{E}_{\pi}(\varphi)| dx\right)^{2}$$

and this lower bound is attained for $q^{\text{opt}}(x)$.

• This result is practically useless because it requires knowing $\mathbb{E}_{\pi}(\varphi)$ but it suggests approximations.

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- For flat functions, one can approximate the variance by

$$\mathsf{var}\left(\mathbb{E}_{\widehat{\pi}_{N}}\left(\varphi\left(X\right)\right)\right)\approx\left(1+\mathsf{var}_{q}\left(w\left(X\right)\right)\right)\frac{\mathsf{var}\left(\mathbb{E}_{\pi}\left(\varphi\left(X\right)\right)\right)}{N}.$$

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• Simple interpretation: The N weighted samples are approximately equivalent to M unweighted samples from π where

$$M = rac{N}{1 + \operatorname{var}_q\left(w\left(X
ight)
ight)} \leq N.$$

Computing Ratio of Normalizing Constant

 However, we are often interested in estimating the ratio of normalizing constants

$$\frac{\int \pi^{*}\left(x\right) dx}{\int q^{*}\left(x\right) dx} = \int w^{*}\left(x\right) q\left(x\right) dx = \mathbb{E}_{q}\left[w^{*}\left(X\right)\right].$$

using

$$\mathbb{E}_{\widehat{q}_{N}}\left[w^{*}\left(X\right)\right] = \frac{1}{N}\sum_{i=1}^{N}w^{*}\left(X^{(i)}\right)$$

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using

$$\mathbb{E}_{\widehat{q}_{N}}\left[w^{*}\left(X\right)\right] = \frac{1}{N}\sum_{i=1}^{N}w^{*}\left(X^{(i)}\right)$$

• It is unbiased and has variance

$$extsf{var}\left[\mathbb{E}_{\widehat{q}_{\mathcal{N}}}\left[w^{*}\left(X
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• Clearly if you have $q\left(x
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Image: A matrix

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 Open Question: How could you come up with a good estimate of ∫ π^{*} (x) dx based on samples of π.
 • IS is more powerful than you think.

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- IS is more powerful than you think.
- Assume you have say to compute the importance weight

$$w(\theta) \propto \int f(x, z | \theta) dz$$

i.e. the likelihood is very complex and might not admit a closed-form expression.

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i.e. the likelihood is very complex and might not admit a closed-form expression.

• You do NOT need to compute $w\left(\theta^{(i)}\right)$ exactly, an unbiased estimate of it is sufficient.

Limitations of Importance Sampling

• Consider the case where $\mathcal{X} = \mathbb{R}^n$

$$\pi\left(\theta\right) = \frac{1}{\left(2\pi\right)^{n/2}} \exp\left(-\frac{\sum_{i=1}^{n} \theta_{i}^{2}}{2}\right)$$

and

$$q_{\sigma}\left(heta
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 ${\scriptstyle \bullet }$ We have for any $\sigma >1$

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 Despites having a very good proposal then the variance of the weights increases exponentially fast with the dimension of the problem.

Normalized Importance Sampling versus Rejection Sampling

• Given N samples from q, we estimate $\mathbb{E}_{\pi}\left(\varphi\left(X
ight)
ight)$ through IS

$$\mathbb{E}_{\widehat{\pi}_{N}}^{\mathsf{IS}}\left(\varphi\left(X\right)\right) = \frac{\sum_{i=1}^{N} w^{*}\left(X^{(i)}\right) \varphi\left(X^{(i)}\right)}{\sum_{i=1}^{N} w^{*}\left(X^{(i)}\right)}$$

or we "filter" the samples through rejection and propose instead

$$\mathbb{E}_{\widehat{\pi}_{\mathcal{N}}}^{\mathsf{RS}}\left(\varphi\left(X\right)\right) = \frac{1}{\mathcal{K}}\sum_{k=1}^{\mathcal{K}}\varphi\left(X^{\left(i_{k}\right)}\right)$$

where $K \leq N$ is a random variable corresponding to the number of samples accepted.

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• We want to know which strategy performs the best.

• Define the artificial target $\overline{\pi}(x,y)$ on $\mathcal{X} \times [0,1]$ as

$$\overline{\pi}(x,y) = \begin{cases} \frac{Cq^*(x)}{\int \pi^*(x)dx}, & \text{for } \left\{ (x,y) : x \in \mathcal{X} \text{ and } y \in \left[0, \frac{\pi^*(x)}{Cq^*(x)} \right] \\ 0 & \text{otherwise} \end{cases}$$

then

$$\int \overline{\pi}(x,y) \, dy = \int_{0}^{\frac{\pi^{*}(x)}{Cq^{*}(x)}} \frac{Cq^{*}(x)}{\int \pi^{*}(x) \, dx} dy = \pi(x) \, .$$

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• Now let us consider the proposal distribution

$$q\left(x,y
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ight]}\left(y
ight) ext{ for }\left(x,y
ight)\in\mathcal{X} imes\left[0,1
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 \bullet Then rejection sampling is nothing but IS on $\mathcal{X} \times [0,1]$ where

$$w(x,y) = \frac{\overline{\pi}(x,y)}{q(x)\mathcal{U}_{[0,1]}(y)} = \begin{cases} \frac{C\int q^*(x)dx}{\int \pi^*(x)dx} & \text{for } y \in \left[0, \frac{\pi^*(x)}{Cq^*(x)}\right]\\ 0, & \text{otherwise.} \end{cases}$$

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• We have

$$\mathbb{E}_{\widehat{\pi}_{N}}^{\mathsf{RS}}\left(\varphi\left(X\right)\right) = \frac{1}{K}\sum_{k=1}^{K}\varphi\left(X^{(i_{k})}\right) = \frac{\sum_{i=1}^{N}w\left(X^{(i)}, Y^{(i)}\right)\varphi\left(X^{(i)}\right)}{\sum_{i=1}^{N}w\left(X^{(i)}, Y^{(i)}\right)}.$$

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• Compared to standard IS, RS performs IS on an enlarged space.

• The variance of the importance weights from RS is higher than for standard IS:

$$\operatorname{var}_{q}\left[w\left(X,Y
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More precisely, we have

$$var[w(X, Y)] = var[\mathbb{E}[w(X, Y)|X]] + \mathbb{E}[var[w(X, Y)|X]]$$

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 To compute integrals, Rejection sampling is inefficient and you should simply use IS. • Like Rejection, IS is useful for small non-standard distributions but collapses for most "interesting" problems.

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- Towards the end of this course, we will present advanced dynamic methods to address this problem.