# CPSC 535 <br> Importance Sampling Methods 

## AD

8th February 2007

- Importance Sampling
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- Normalized Importance Sampling.
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- Importance Sampling versus Rejection Sampling.
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$$
\widehat{\pi}_{N}(x)=\frac{1}{N} \sum_{i=1}^{N} \delta_{X^{(i)}}(x) \text { where } X \stackrel{(i) \stackrel{\text { i.i.d. }}{\sim} \pi \text {. } . \text {. }}{ }
$$

- For any $\varphi: \mathcal{X} \rightarrow \mathbb{R}$

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

- More precisely, we have

$$
\begin{aligned}
\mathbb{E}_{\left\{X^{(i)}\right\}}\left[\mathbb{E}_{\widehat{\pi}_{N}}(\varphi(X))\right] & =\mathbb{E}_{\pi}(\varphi(X)) \\
\operatorname{var}_{\left\{X^{(i)}\right\}}\left(\mathbb{E}_{\widehat{\pi}_{N}}(\varphi(X))\right) & =\frac{\operatorname{var}_{\pi}(\varphi(X))}{N} .
\end{aligned}
$$

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## Accept-Reject Procedure

- Direct methods feasible for standard distributions: inverse method, composition, etc.
- In case where $\pi \propto \pi^{*}$ does not admit any standard form, we can use a proposal distribution $q$ on $\mathcal{X}$ where $q \propto q^{*}$.
- We need $q$ to 'dominate' $\pi$; i.e.

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

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## Accept/Reject procedure

(1) Sample $Y \sim q$ and $U \sim \mathcal{U}(0,1)$.
(2) If $U<\frac{\pi^{*}(Y)}{C^{\prime} q^{*}(Y)}$ then return $Y$; otherwise return to step 1 .

- This is a simple generic algorithm but it requires coming up with a bound $C$.
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- You need to wait a random time to obtain some samples from $\pi$.
- 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 $\pi$.
- Is it possible to "recycle" these samples?


## Importance Sampling

- Consider again the target distribution $\pi$ and the proposal distribution q. We only require

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\pi(x)>0 \Rightarrow q(x)>0
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- In this case, the Importance Sampling (IS) identity is

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\pi(x)=w(x) q(x)
$$

where the so-called Importance Weight is given by

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

- It follows that

$$
\begin{aligned}
\mathbb{E}_{\pi}(\varphi(X)) & =\int_{\mathcal{X}} \varphi(x) \pi(x) d x=\int_{\mathcal{X}} \varphi(x) \frac{\pi(x)}{q(x)} q(x) d x \\
& =\mathbb{E}_{q}(w(X) \varphi(X))
\end{aligned}
$$

- Monte Carlo approximation of $q$ is

$$
\widehat{q}_{N}(x)=\frac{1}{N} \sum_{i=1}^{N} \delta_{X^{(i)}}(x) \text { where } X \stackrel{(i) \stackrel{\text { i.i.d. }}{\sim} q . ~}{q .}
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\widehat{\pi}_{N}(x)=\frac{1}{N} \sum_{i=1}^{N} w\left(X^{(i)}\right) \delta_{X^{(i)}}(x) .
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$$

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

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

- We have

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

and

$$
\begin{aligned}
\operatorname{var}_{\left\{X^{(i)}\right\}}\left(\mathbb{E}_{\widehat{q}_{N}}(\varphi(X))\right) & =\frac{\operatorname{var}_{q}(w(X) \varphi(X))}{N} \\
& =\frac{\mathbb{E}_{\pi}\left(w(X) \varphi^{2}(X)\right)-\mathbb{E}_{\pi}^{2}(\varphi(X))}{N}
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- In practice, it is recommended to ensure

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\mathbb{E}_{\pi}(w(X))=\int \frac{\pi^{2}(x)}{q(x)} d x<\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


Figure: IS approximation obtained using a Gaussian IS distribution


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

- We try to compute

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

where

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

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

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- We use $q_{1}(x)=\pi(x), q_{2}(x)=\frac{\Gamma(1)}{\sqrt{v \pi} \Gamma(1 / 2)}\left(1+\frac{x}{v \sigma}\right)^{-1}$ (Cauchy distribution) and $q_{3}(x)=\mathcal{N}\left(x ; 0, \frac{v}{v-2}\right)$ (variance chosen to match the variance of $\pi(x)$ )
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- It is easy to see that

$$
\frac{\pi(x)}{q_{2}(x)}<\infty \text { and } \int \frac{\pi(x)^{2}}{q_{3}(x)} d x=\infty, \frac{\pi(x)}{q_{3}(x)} \text { is unbounded }
$$



Figure: Performance for $v=12$ 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

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\int_{2.1}^{\infty} x^{5} \pi(x) d x
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- We now try to compute

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$$

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

$$
\begin{aligned}
\int_{2.1}^{\infty} x^{5} \pi(x) d x & =\int_{0}^{1 / 2.1} u^{-7} \pi(1 / u) d u \\
& =\frac{1}{2.1} \int_{0}^{1 / 2.1} 2.1 u^{-7} \pi(1 / u) d u
\end{aligned}
$$

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


Figure: Performance for $v=12$ 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

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q^{\mathrm{opt}}(x)=\frac{|\varphi(x)| \pi(x)}{\int_{\mathcal{X}}|\varphi(x)| \pi(x) d x}
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## Optimal Importance function

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- Proof:

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

and

$$
\begin{aligned}
\int q(x) \frac{\pi^{2}(x)}{q^{2}(x)} \varphi^{2}(x) d x & \geq\left(\int q(x) \frac{\pi(x)|\varphi(x)|}{q(x)} d x\right)^{2} \\
& =\left(\int \pi(x)|\varphi(x)| d x\right)^{2}
\end{aligned}
$$

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 $q(x) \propto q^{*}(x)$.


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- Normalized IS identity is based on

$$
\begin{aligned}
\pi(x) & =\frac{\pi^{*}(x)}{\int \pi^{*}(x) d x}=\frac{w^{*}(x) q^{*}(x)}{\int w^{*}(x) q^{*}(x) d x} \\
& =\frac{w^{*}(x) q(x)}{\int w^{*}(x) q(x) d x}=\frac{w(x) q(x)}{\int w(x) q(x) d x}
\end{aligned}
$$

where

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

- For any test function $\varphi$, we can also write

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

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

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

- 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 $\mathbb{E}(A)=\mu_{A}$ and $\mathbb{E}(B)=\mu_{B}$ then a two-dimensional Taylor expansion gives around $\mu=\left(\mu_{A}, \mu_{B}\right)$

$$
Z \approx g(\mu)+\left(A-\mu_{A}\right) \frac{\partial g}{\partial a}(\mu)+\left(B-\mu_{B}\right) \frac{\partial g}{\partial b}(\mu)
$$

It follows that

$$
\begin{gathered}
\mathbb{E}(Z) \approx g(\mu) \\
\operatorname{Var}(Z) \approx \sigma_{A}^{2} \frac{\partial g}{\partial a}^{2}(\mu)+\sigma_{B}^{2} \frac{\partial g^{2}}{\partial b}(\mu)+2 \frac{\partial g}{\partial a}(\mu) \frac{\partial g}{\partial b}(\mu) \sigma_{A, B}
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\end{gathered}
$$

- In our case

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

- We have

$$
\begin{gathered}
\frac{\partial g}{\partial a}(\mu) \frac{\partial g}{\partial b}(\mu)=-\frac{\mu_{A}}{\mu_{B}^{3}}, \frac{\partial g^{2}}{\partial a}(\mu)=\frac{1}{\mu_{B}^{2}}, \frac{\partial g^{2}}{\partial b}(\mu)=\frac{\mu_{A}^{2}}{\mu_{B}^{4}} \\
\mu_{A}=\mathbb{E}_{q}\left(w^{*}(X) \varphi(X)\right), \mu_{B}=\mathbb{E}_{q}\left(w^{*}(X)\right), \\
\sigma_{A}^{2}=\frac{\operatorname{var}_{q}\left(w^{*}(X) \varphi(X)\right)}{N}, \sigma_{B}^{2}=\frac{\operatorname{var}_{q}\left(w^{*}(X)\right)}{N} \\
\sigma_{A, B}=\frac{\mathbb{E}_{q}\left(w^{*}(X)^{2} \varphi(X)\right)-\mu_{A} \cdot \mu_{B}}{N} .
\end{gathered}
$$

- It follows that

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

- Asymptotically, we have a central limit theorem

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

where

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

- 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 .
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- There is some empirical evidence that Normalized IS performs better than standard IS in numerous cases.
- Using a second order Taylor expansion

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

gives

$$
\begin{aligned}
\mathbb{E}\left(\mathbb{E}_{\hat{\pi}_{N}}(\varphi(X))\right) \approx & g(\mu)+\frac{1}{2} \sigma_{A}^{2} \frac{\partial^{2} g}{\partial a^{2}}(\mu)+\frac{1}{2} \sigma_{B}^{2} \frac{\partial^{2} g}{\partial b^{2}}(\mu) \\
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\end{aligned}
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- It follows that asymptotically we have

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

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$$

- We have $B_{i a s}{ }^{2}$ 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

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

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

$$
\frac{\widehat{\sigma_{I S}^{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).


## Application to Bayesian Statistics

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- We can use the prior distribution as a candidate distribution $q(\theta)=q^{*}(\theta)=\pi(\theta)$.
- We also get an estimate of the marginal likelihood

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

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

$$
\left(\begin{array}{ll}
p_{1} & 1-p_{1} \\
1-p_{2} & p_{2}
\end{array}\right)
$$

that is $\operatorname{Pr}\left(X_{t+1}=1 \mid X_{t}=1\right)=1-\operatorname{Pr}\left(X_{t+1}=2 \mid X_{t}=1\right)=p_{1}$ and $\operatorname{Pr}\left(X_{t+1}=2 \mid X_{t}=2\right)=1-\operatorname{Pr}\left(X_{t+1}=1 \mid X_{t}=2\right)=p_{2}$. Physical constraints tell us that $p_{1}+p_{2}<1$.

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- Assume we observe $x_{1}, \ldots, x_{m}$ and the prior is

$$
\pi\left(p_{1}, p_{2}\right)=2 \mathbb{I}_{p_{1}+p_{2} \leq 1}
$$

then the posterior is

$$
\pi\left(p_{1}, p_{2} \mid 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} \leq 1}
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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.
- We are interested in estimating $\mathbb{E}\left[\varphi_{i}\left(p_{1}, p_{2}\right) \mid x_{1: m}\right]$ for $\varphi_{1}\left(p_{1}, p_{2}\right)=p_{1}, \varphi_{2}\left(p_{1}, p_{2}\right)=p_{2}, \varphi_{3}\left(p_{1}, p_{2}\right)=p_{1} /\left(1-p_{1}\right)$, $\varphi_{4}\left(p_{1}, p_{2}\right)=p_{2} /\left(1-p_{2}\right)$ and $\varphi_{5}\left(p_{1}, p_{2}\right)=\log \frac{p_{1}\left(1-p_{2}\right)}{p_{2}\left(1-p_{1}\right)}$ using Importance Sampling.
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- If there was no on $p_{1}+p_{2}<1$ and $\pi\left(p_{1}, p_{2}\right)$ was uniform on $[0,1] \times[0,1]$, then the posterior would be

$$
\begin{aligned}
\pi_{0}\left(p_{1}, p_{2} \mid x_{1: m}\right)= & \mathcal{B e}\left(p_{1} ; m_{1,1}+1, m_{1,2}+1\right) \\
& \mathcal{B e}\left(p_{2} ; m_{2,2}+1, m_{2,1}+1\right)
\end{aligned}
$$

but this is inefficient as for the given data ( $m_{1,1}, m_{1,2}, m_{2,2}, m_{2,1}$ ) we have $\pi_{0}\left(p_{1}+p_{2}<1 \mid x_{1: m}\right)=0.21$.

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

$$
\pi_{1}\left(p_{1}, p_{2} \mid x_{1: m}\right) \propto p_{1}^{m_{1,1}} p_{2}^{m_{2,2}}\left(1-p_{1}-p_{2}\right)^{m_{1,2}+m_{2,1}}
$$

but $\pi\left(p_{1}, p_{2} \mid x_{1: m}\right) / \pi_{1}\left(p_{1}, p_{2} \mid x_{1: m}\right)$ is unbounded.

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

$$
\begin{aligned}
\pi_{2}\left(p_{1}, p_{2} \mid x_{1: m}\right) & \propto \exp \left(-\left(m_{1,1}+m_{1,2}\right)\left(p_{1}-\widehat{p}_{1}\right)^{2} /\left(2 \widehat{p}_{1}\left(1-\widehat{p}_{1}\right)\right)\right) \\
& \times \exp \left(-\left(m_{2,1}+m_{2,2}\right)\left(p_{2}-\widehat{p}_{2}\right)^{2} /\left(2 \widehat{p}_{2}\left(1-\widehat{p}_{2}\right)\right)\right)
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$$

where $\widehat{p}_{1}=m_{1,1} /\left(m_{1,1}+m_{1,2}\right), \widehat{p}_{1}=m_{2,2} /\left(m_{2,2}+m_{2,1}\right)$. Then to simulate from this distribution, we simulate first $\pi_{2}\left(p_{1} \mid x_{1: m}\right)$ and then $\pi_{2}\left(p_{2} \mid x_{1: m}, p_{1}\right)$ which are univariate truncated Gaussian distribution which can be sampled using the inverse cdf method. The ratio $\pi\left(p_{1}, p_{2} \mid x_{1: m}\right) / \pi_{2}\left(p_{1}, p_{2} \mid x_{1: m}\right)$ is upper bounded.

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- A final one consists of using

$$
\pi_{3}\left(p_{1}, p_{2} \mid x_{1: m}\right)=\mathcal{B} e\left(p_{1} ; m_{1,1}+1, m_{1,2}+1\right) \pi_{3}\left(p_{2} \mid x_{1: m}, p_{1}\right)
$$

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

- Performance for $N=10,000$

| Distribution | $\varphi_{1}$ | $\varphi_{2}$ | $\varphi_{3}$ | $\varphi_{4}$ | $\varphi_{5}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\pi_{1}$ | 0.748 | 0.139 | 3.184 | 0.163 | 2.957 |
| $\pi_{2}$ | 0.689 | 0.210 | 2.319 | 0.283 | 2.211 |
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- Sampling from $\pi$ using rejection sampling works well but is computationally expensive. $\pi_{3}$ is computationally much cheaper whereas $\pi_{1}$ does extremely poorly as expected.


## Optimal Normalized Importance Sampling

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

$$
q^{\mathrm{opt}}(x)=\frac{\left|\varphi(x)-\mathbb{E}_{\pi}(\varphi)\right| \pi(x)}{\int_{\mathcal{X}}\left|\varphi(x)-\mathbb{E}_{\pi}(\varphi)\right| \pi(x) d x}
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- Proof:

$$
\begin{aligned}
& \int q(x) \frac{\pi^{2}(x)}{q^{2}(x)}\left(\varphi(x)-\mathbb{E}_{\pi}(\varphi)\right)^{2} d x \\
& \geq\left(\int q(x) \frac{\pi(x)\left|\varphi(x)-\mathbb{E}_{\pi}(\varphi)\right|}{q(x)} d x\right)^{2} \\
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and this lower bound is attained for $q^{\text {opt }}(x)$.

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


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- In statistics, we are usually not interested in a specific $\varphi$ but in several functions and we prefer having $q(x)$ as close as possible to $\pi(x)$.


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- Simple interpretation: The $N$ weighted samples are approximately equivalent to $M$ unweighted samples from $\pi$ where

$$
M=\frac{N}{1+\operatorname{var}_{q}(w(X))} \leq N
$$

## Computing Ratio of Normalizing Constant

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

$$
\frac{\int \pi^{*}(x) d x}{\int q^{*}(x) d x}=\int w^{*}(x) q(x) d x=\mathbb{E}_{q}\left[w^{*}(X)\right]
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- It is unbiased and has variance

$$
\operatorname{var}\left[\mathbb{E}_{\widehat{q}_{N}}\left[w^{*}(X)\right]\right]=\frac{\operatorname{var}_{q}\left(w^{*}(X)\right)}{N}
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- Open Question: How could you come up with a good estimate of $\int \pi^{*}(x) d x$ based on samples of $\pi$.
- IS is more powerful than you think.
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- Assume you have say to compute the importance weight

$$
w(\theta) \propto \int f(x, z \mid \theta) d z
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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 $\mathcal{X}=\mathbb{R}^{n}$

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

and

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q_{\sigma}(\theta)=\frac{1}{\left(2 \pi \sigma^{2}\right)^{n / 2}} \exp \left(-\frac{\sum_{i=1}^{n} \theta_{i}^{2}}{2 \sigma^{2}}\right)
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- We have for any $\sigma>1$

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w_{\sigma}(\theta)=\frac{\pi(\theta)}{q_{\sigma}(\theta)}=\sigma^{n} \exp \left(-\sum_{i=1}^{n} \frac{\theta_{i}^{2}}{2}\left(1-\frac{1}{\sigma^{2}}\right)\right) \leq \sigma^{n} \text { for any } \theta
$$

and

$$
\operatorname{var}_{q_{\sigma}}\left(\frac{\pi(\theta)}{q_{\sigma}(\theta)}\right)=\sigma^{n} \sigma^{\prime n}-1 \text { with } \sigma^{\prime 2}=\frac{\sigma^{2}}{\sigma^{2}-1 / 2}>1
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$$

- 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 $\mathbb{E}_{\pi}(\varphi(X))$ through IS

$$
\mathbb{E}_{\hat{\pi}_{N}}^{\text {SS }}(\varphi(X))=\frac{\sum_{i=1}^{N} w^{*}\left(X^{(i)}\right) \varphi\left(X^{(i)}\right)}{\sum_{i=1}^{N} w^{*}\left(X^{(i)}\right)}
$$

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

$$
\mathbb{E}_{\widehat{\pi}_{N}}^{\mathrm{RS}}(\varphi(X))=\frac{1}{K} \sum_{k=1}^{K} \varphi\left(X^{\left(i_{k}\right)}\right)
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where $K \leq N$ is a random variable corresponding to the number of samples accepted.

- We want to know which strategy performs the best.
- Define the artificial target $\bar{\pi}(x, y)$ on $\mathcal{X} \times[0,1]$ as

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

then

$$
\int \bar{\pi}(x, y) d y=\int_{0}^{\frac{\pi^{*}(x)}{C q^{*}(x)}} \frac{C q^{*}(x)}{\int \pi^{*}(x) d x} d y=\pi(x)
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$$
\int \bar{\pi}(x, y) d y=\int_{0}^{\frac{\pi^{*}(x)}{C q^{*}(x)}} \frac{C q^{*}(x)}{\int \pi^{*}(x) d x} d y=\pi(x)
$$

- Now let us consider the proposal distribution

$$
q(x, y)=q(x) \mathcal{U}_{[0,1]}(y) \text { for }(x, y) \in \mathcal{X} \times[0,1]
$$

- Then rejection sampling is nothing but IS on $\mathcal{X} \times[0,1]$ where

$$
w(x, y)=\frac{\bar{\pi}(x, y)}{q(x) \mathcal{U}_{[0,1]}(y)}= \begin{cases}\frac{C \int q^{*}(x) d x}{\int \pi^{*}(x) d x} & \text { for } y \in\left[0, \frac{\pi^{*}(x)}{C q^{*}(x)}\right] \\ 0, & \text { otherwise }\end{cases}
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$$
\mathbb{E}_{\hat{\pi}_{N}}^{\mathrm{RS}}(\varphi(X))=\frac{1}{K} \sum_{k=1}^{K} \varphi\left(X^{\left(i_{k}\right)}\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:

$$
\operatorname{var}_{q}[w(X, Y)] \geq \operatorname{var}_{q}[w(X)]
$$

More precisely, we have

$$
\begin{aligned}
\operatorname{var}[w(X, Y)] & =\operatorname{var}[\mathbb{E}[w(X, Y) \mid X]]+\mathbb{E}[\operatorname{var}[w(X, Y) \mid 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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- In both cases, the problem is to be able to design "clever" proposal distributions.
- Towards the end of this course, we will present advanced dynamic methods to address this problem.

