

- Introduction
- Bayesian Computation
- Monte Carlo Methods
- · Direct sampling
- Indirect sampling
 - Rejection sampling
 - Importance sampling
 - Pareto-Smoothed
 Importance Sampling

Bayesian Statistics and Data Analysis Lecture 4

Måns Magnusson Department of Statistics, Uppsala University Thanks to Aki Vehtari, Aalto University



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Assignment 3

- Be more clear in the evaluation where is the problem.
- Example: "Some questions could be more clear"



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Notation

- In this chapter, generic $p(\theta)$ is used instead of $p(\theta|y)$
- Unnormalized distribution is denoted by $q(\cdot)$
 - $\int q(\theta)d\theta \neq 1$, but finite (i.e. $\int q(\theta)d\theta \leq \infty$
 - $q(\cdot) \propto p(\cdot)$
- Proposal distribution is denoted by $g(\cdot)$



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Numerical accuracy – floating point

- Floating point presentation of numbers. e.g. with 64bits
 - closest value to zero is $\approx 2.2 \cdot 10^{-308}$
 - generate sample of 600 from normal distribution: qr=rnorm(600)
 - calculate joint density given normal: prod(dnorm(qr)) → 0 (underflow)



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 - closest value to 1 is $pprox 1 \pm 2.2 \cdot 10^{-16}$
 - Laplace and ratio of girl and boy babies
 - pbeta $(0.5, 241945, 251527) \rightarrow 1$ (rounding)



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 - pbeta $(0.5, 241945, 251527) \rightarrow 1$ (rounding)
 - pbeta(0.5, 241945, 251527, lower.tail=FALSE) $\approx -1.2 \cdot 10^{-42}$

there is more accuracy near 0



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- Log densities
 - use log densities to avoid over- and underflows in floating point presentation
 - $prod(dnorm(qr)) \rightarrow 0$ (underflow)
 - $sum(dnorm(qr,log=TRUE)) \rightarrow -847.3$



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 - e.g. in Metropolis-algorithm (ex5) compute the log of ratio of densities using the identity log(a/b) = log(a) - log(b)



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 where
$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{\int p(y|\theta)p(\theta)d\theta}$$



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We can easily evaluate $p(y|\theta)p(\theta)$ for any θ , but the integral $\int p(y|\theta)p(\theta)d\theta$ is usually difficult.



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• Grid (equal spacing) evaluation with self-normalization

$$E_{p(\theta|y)}[f(\theta)] \approx \frac{\sum_{s=1}^{S} \left[f(\theta^{(s)}) q(\theta^{(s)}|y) \right]}{\sum_{s=1}^{S} q(\theta^{(s)}|y)}$$



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• Monte Carlo methods which can sample from $p(\theta^{(s)}|y)$ using only $q(\theta^{(s)}|y)$

$$E_{p(\theta|y)}[f(\theta)] \approx \frac{1}{S} \sum_{s=1}^{S} f(\theta^{(s)})$$



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$$E_{\theta}[f(\theta)] = \int f(\theta)p(\theta|y)d\theta$$

- Conjugate priors and analytic solutions (Ch 1-5)
- Grid integration and other quadrature rules (Ch 3, 10)
- Independent Monte Carlo, rejection and importance sampling (Ch 10)
- Markov Chain Monte Carlo (Ch 11-12)
- Distributional approximations (Laplace, VB, EP) (Ch 4, 13)



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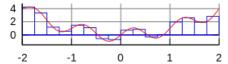
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Quadrature integration

- The simplest quadrature integration is grid integration
 - Evaluate function in a grid and compute

$$\mathrm{E}[-\alpha/\beta] \approx \sum_{t=1}^{T} w_{\mathrm{cell}}^{(t)} \frac{\alpha^{(t)}}{\beta^{(t)}},$$



where $w_{\text{cell}}^{(t)}$ is the normalized probability of a grid cell t, and $\alpha^{(t)}$ and $\beta^{(t)}$ are center locations of grid cells



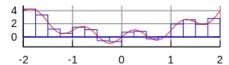
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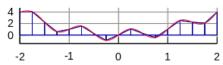
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• In 1D further variations with smaller error, e.g. trapezoid



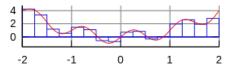


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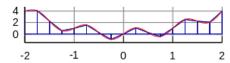
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- In 2D and higher
 - nested quadrature, product rules
 - but theres a curse of dimensionality...



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Monte Carlo integration/method

 Numerically (deterministic) compute an integral (midpoint) using S sample points

$$I_b^a(h) = \int_b^a h(\theta) d\theta \approx \sum_s^S h(\theta_s) \frac{w_s}{S}$$

where

$$w_s = b - a$$

and

$$\theta_i = a - (s + 0.5)\delta\theta$$



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• In Gelman et al (2013) notation and for a posteriors $p(\theta|y)$

$$E_{p(\theta|y)}(h(\theta)) = \int h(\theta)p(\theta|y)d\theta \approx \sum_{s}^{S} h(\theta_{s})p(\theta_{s}|y)\frac{w_{s}}{S}$$





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• If we have samples $\theta_s \sim p(\theta|y)$ we can approximate

$$E_{p(\theta|y)}(h(\theta)) = \int h(\theta)p(\theta|y)d\theta \approx \frac{1}{S} \sum_{s}^{S} h(\theta_{s})$$



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Monte Carlo - history

- Used already before computers
 - Buffon (18th century; needles)
 - De Forest, Darwin, Galton (19th century)
 - Pearson (19th century; roulette)
 - Gosset (Student, 1908; hat)



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 - they worked together in atomic bomb project
 - Metropolis and Ulam, "The Monte Carlo Method", 1949



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 - they worked together in atomic bomb project
 - Metropolis and Ulam, "The Monte Carlo Method", 1949
- Bayesians started to have enough cheap computation time in 1990s
 - BUGS project started 1989 (last OpenBUGS release 2014)
 - Gelfand & Smith, 1990
 - Stan initial release 2012



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Monte Carlo

- Simulate draws from the target distribution $p(\theta|y)$
 - these draws can be treated as any observations
 - a collection of draws is a sample of size S
- Use these draws, for example,
 - to compute means, deviations, quantiles
 - to draw histograms
 - to marginalize
 - etc.



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Monte Carlo vs. Deterministic Methods

- Monte Carlo (approximation) error is $\propto S^{-1/2}$
- Midpoint rule error is $\propto S^{-2}$
- Trapezoidal rule error is $\propto S^{-2}$
- Simpson rule error is $\propto S^{-4}$
- Monte Carlo is bad (even worse than midpoint approximation) Why use Monte Carlo integration?



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- Monte Carlo is bad (even worse than midpoint approximation)
- Monte Carlo has the same error irrespective of dimension D. i.e. $S_D = S$
- Numerical methods create a grid with $S_D = S^D$ When is Monte Carlo a better approach than Simpsons?



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$$(S_D^{\frac{1}{D}})^{-4} = S_D^{-\frac{1}{2}},$$

i.e. for d > 8 Monte Carlo is better.



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How many simulation draws are needed?

- How many draws or how big sample size S?
- If draws are independent
 - usual methods to estimate the uncertainty due to a finite number of observations (finite sample size)
- Markov chain Monte Carlo produces dependent draws (next week)
 - requires additional work to estimate the effective sample size



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How many simulation draws are needed?

Expectation of unknown quantity

$$E(\theta) \approx \frac{1}{S} \sum_{s=1}^{S} \theta^{(s)}$$

if S is big and $\theta^{(s)}$ are independent, way may assume that the distribution of the expectation approaches normal distribution (see Ch 4) with variance σ_{θ}^2/S (asymptotic normality)

• this variance is independent on dimensionality of θ (!)



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- this variance is independent on dimensionality of θ (!)
- total variance is sum of the epistemic uncertainty in the posterior and the uncertainty due to using finite number of Monte Carlo draws

$$\sigma_{\theta}^2 + \sigma_{\theta}^2 / S$$



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$$\sigma_{\theta}^2 + \sigma_{\theta}^2/S = \sigma_{\theta}^2(1+1/S)$$

• e.g. if S=100, deviation increases by $\sqrt{1+1/S}=1.005$ i.e. Monte Carlo error is very small (for the expectation)



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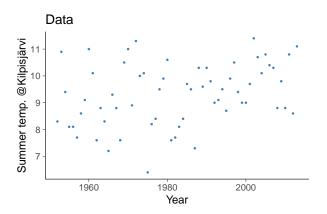
- e.g. if S=100, deviation increases by $\sqrt{1+1/S}=1.005$ i.e. Monte Carlo error is very small (for the expectation)
- See Ch 4 for counter-examples for asymptotic normality



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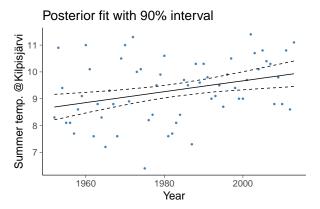
Average temperature in June, July, and August at Kilpisjärvi, Finland





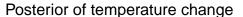
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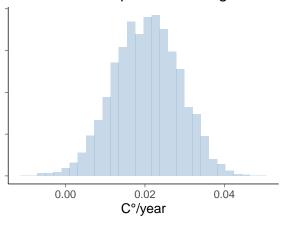
Average temperature in June, July, and August at Kilpisjärvi, Finland





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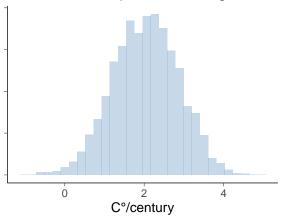






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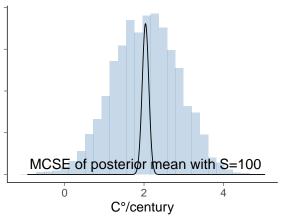






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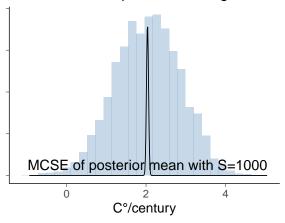


 $\sigma_{\theta} \approx 0.827$, MCSE ≈ 0.0827 , total deviation ≈ 0.831



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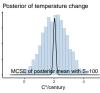
 $\sigma_{\theta} \approx 0.827$, MCSE ≈ 0.0261 , total deviation ≈ 0.827

total deviation² = $\sigma_{\theta}^2 + MCSE^2$



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Example: Kilpisjärvi summer temperature



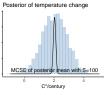
Posterior of temperature change

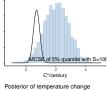




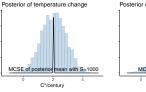
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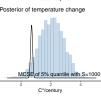
Example: Kilpisjärvi summer temperature





Posterior of temperature change

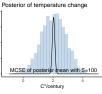


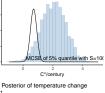




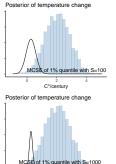
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Example: Kilpisjärvi summer temperature

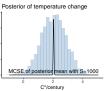


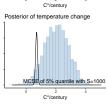


Posterior of temperature change



C°/century

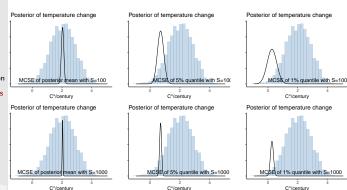








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Tail quantiles are more difficult to estimate



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$$p(\theta \in A) \approx \frac{1}{S} \sum_{l} I(\theta^{(s)} \in A)$$

where
$$I(\theta^{(s)} \in A) = 1$$
 if $\theta^{(s)} \in A$



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where
$$I(\theta^{(s)} \in A) = 1$$
 if $\theta^{(s)} \in A$

- $I(\cdot)$ is binomially distributed as $p(\theta \in A)$
 - $\rightarrow \operatorname{var}(I(\cdot)) = p(1-p)$ (Appendix A, p. 579)
 - \rightarrow standard deviation of p is $\approx \sqrt{p(1-p)/S}$



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- if S=100 and $p\approx 0.5$, $\sqrt{p(1-p)/S}=0.05$ i.e. accuracy is about 5% units



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- S = 2500 draws needed for 1% unit accuracy



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How many simulation draws are needed?

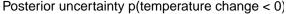
$$p(\theta \in A) \approx \frac{1}{5} \sum_{I} I(\theta^{(s)} \in A)$$

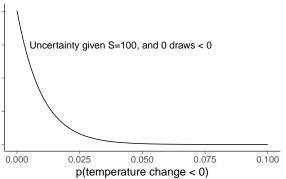
where
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- if S=100 and $p\approx 0.5$, $\sqrt{p(1-p)/S}=0.05$ i.e. accuracy is about 5% units
- S = 2500 draws needed for 1% unit accuracy
- To estimate small probabilities, a large number of draws is needed
 - to be able to estimate p, need to get draws with $\theta^{(l)} \in A$, which in expectation requires $S \gg 1/p$



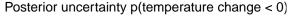
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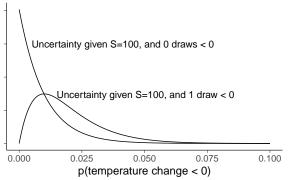






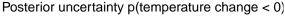
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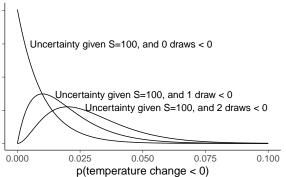






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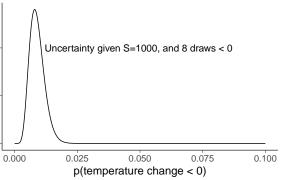






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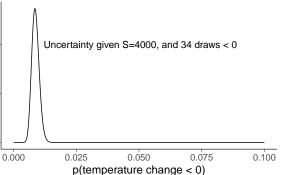






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 Too many digits make reading of the results slower and give false impression of the accuracy



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- Too many digits make reading of the results slower and give false impression of the accuracy
 - Don't show digits which are just random noise
 - check what is the Monte Carlo standard error



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 - 2.050774 and [0.7472868 3.3017524] (NO!)



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- Example: The probability that temp increase is positive



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 - 0.9960000 (NO!)



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 - 1.00 (depends on the context)



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- Example: The probability that temp increase is positive
 - 0.9960000 (NO!)
 - 1.00 (depends on the context)
 - With 4000 draws MCSE ≈ 0.002. We could report that probability is very likely larger than 0.99, or sample more to justify reporting three digits



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- Example: The probability that temp increase is positive
 - 0.9960000 (NO!)
 - 1.00 (depends on the context)
 - With 4000 draws MCSE ≈ 0.002. We could report that probability is very likely larger than 0.99, or sample more to justify reporting three digits
 - For probabilities close to 0 or 1, consider also when the model assumption justify certain accuracy
- For your project: Think for each reported value how many digits is sensible.



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- Less draws needed with
 - deterministic methods
 - marginalization (Rao-Blackwellization)
 - variance reduction methods, such, control variates



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How many simulation draws are needed?

- Number of independent draws needed doesn't depend on the number of dimensions
 - but it may be difficult to obtain independent draws in high dimensional case



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Direct sampling

- Direct simulation from known pdf/pmf, e.g. $p(\theta|y)$ in conjugate case
- Produces independent draws
 - Using analytic transformations of uniform random numbers (e.g. appendix A)
 - factorization
 - numerical inverse-CDF
- Problem: restricted to limited set of models



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Random number generators

How to sample from a pdf?



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Random number generators

- How to sample from a pdf?
- Good psuedo random number generators are sufficient for Bayesian inference
 - pseudo random generator uses deterministic algorithm to produce a sequence which is difficult to make difference from truly random sequence
 - modern software used for statistical analysis have good pseudo RNGs



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Direct simulation: Example

Box-Muller -method: If U_1 and U_2 are independent draws from distribution $\mathcal{U}(0,1)$, and

$$X_1 = \sqrt{-2\log(U_1)}\cos(2\pi U_2)$$

$$X_2 = \sqrt{-2\log(U_1)}\sin(2\pi U_2)$$

then X_1 and X_2 are independent draws from the distribution $\mathcal{N}(0,1)$



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$$X_2 = \sqrt{-2\log(U_1)}\sin(2\pi U_2)$$

then X_1 and X_2 are independent draws from the distribution $\mathcal{N}(0,1)$

- not the fastest method due to trigonometric computations
- for normal distribution more than ten different methods
 - e.g. R uses inverse-CDF



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Grid sampling and curse of dimensionality

- 10 parameters
- if we don't know beforehand where the posterior mass is
 - need to choose wide box for the grid
 - need to have enough grid points to get some of them where essential mass is

Can we do this?

- e.g. 50 or 1000 grid points per dimension
 - \rightarrow 50¹⁰ \approx 1e17 grid points
 - \rightarrow 1000¹⁰ \approx 1e30 grid points



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Grid sampling and curse of dimensionality

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 - need to choose wide box for the grid
 - need to have enough grid points to get some of them where essential mass is
- e.g. 50 or 1000 grid points per dimension
 - \rightarrow 50¹⁰ \approx 1e17 grid points
 - \rightarrow 1000¹⁰ \approx 1e30 grid points
- R and my current laptop can compute density of normal distribution about 20 million times per second
 - → evaluation in 1e17 grid points would take 150 years
 - ightarrow evaluation in 1e30 grid points would take 1 500 billion years



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Indirect sampling

- Rejection sampling
- Importance sampling
- Markov chain Monte Carlo (next week)



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Effective sampling size

- Efficient sampling size S_{eff} the number of samples using direct methods
- Common with weighted or correlated samples



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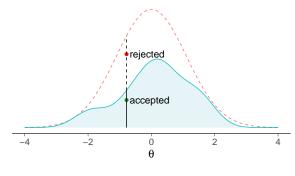
Effective sampling size

- Efficient sampling size S_{eff} the number of samples using direct methods
- Common with weighted or correlated samples
- Indirect methods usually have an $S_{\rm eff} < S$
- Informally an indication of performance of method



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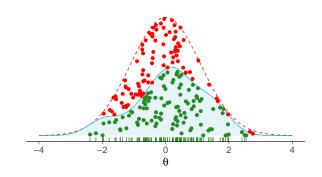
- Proposal $(g(\theta))$ forms envelope over the target distribution $q(\theta|y)/Mg(\theta) \leq 1$
- Draw from the proposal and accept with probability $q(\theta|y)/Mg(\theta)$





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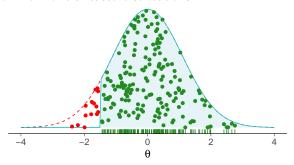


Accepted
 Rejected
 Mg(theta)
 g(thetaly)



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- Proposal $(g(\theta))$ forms envelope over the target distribution $q(\theta|y)/Mg(\theta) \leq 1$
- Draw from the proposal and accept with probability $q(\theta|y)/Mg(\theta)$
- Common for truncated distributions



Accepted
 Rejected
 Mg(theta)
 g(thetaly)



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• The number of accepted draws is the effective sample size S_{eff} When will this be work/not work (i.e. give high/low S_{eff})?



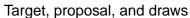
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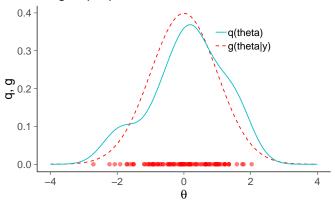
- The number of accepted draws is the effective sample size S_{eff}
 - with bad proposal distribution may require a lot of trials
 - selection of good proposal gets very difficult when the number of dimensions increase



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- Proposal does not need to have a higher value everywhere

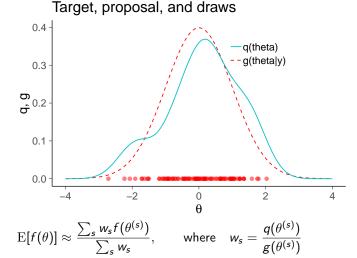






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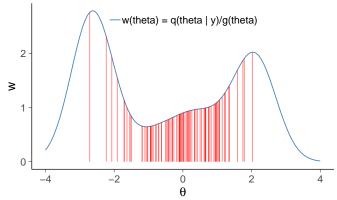
- Proposal does not need to have a higher value everywhere





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Proposal does not need to have a higher value everywhere
 Draws and importance weights



$$\mathrm{E}[f(heta)] pprox rac{\sum_s w_s f(heta^{(s)})}{\sum_s w_s}, \qquad ext{where} \quad w_s = rac{q(heta^{(s)})}{g(heta^{(s)})}$$



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 Resampling using normalized importance weights can be used to pick a smaller number of draws with uniform weights



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- Resampling using normalized importance weights can be used to pick a smaller number of draws with uniform weights
- Selection of good proposal gets more difficult when the number of dimensions increase
- Often used to correct distributional approximations and leave-one-out cross-validation



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- Variation of the weights affect the effective sample size
 - if single weight dominates, we have effectively one sample
 - if all weights are equal, we have effectively *S* draws

What does this mean? What is a good proposal $g(\theta)$?



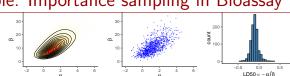
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- Variation of the weights affect the effective sample size
 - if single weight dominates, we have effectively one sample
 - if all weights are equal, we have effectively S draws
- Central limit theorem holds only if variance of the weight distribution is finite



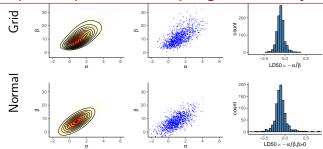
Grid

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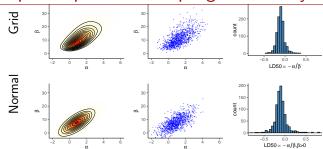
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Normal approximation is discussed more in BDA3 Ch 4



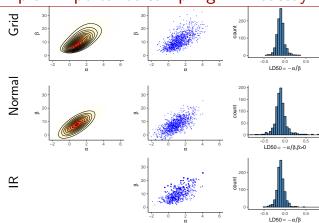
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Normal approximation is discussed more in BDA3 Ch 4 But the normal approximation is not that good here: Grid $sd(LD50) \approx 0.1$, Normal $sd(LD50) \approx .75!$

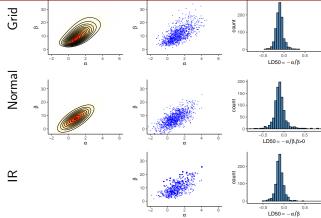


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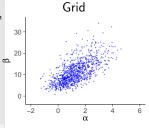
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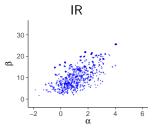


Grid sd(LD50) \approx 0.1, IR sd(LD50) \approx 0.1



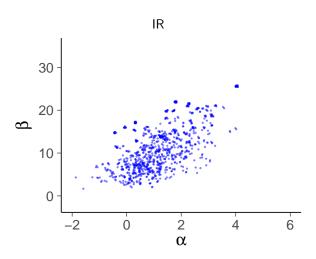
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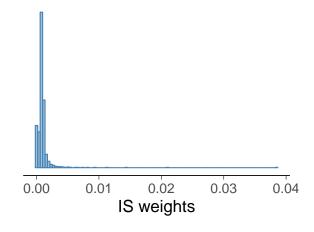


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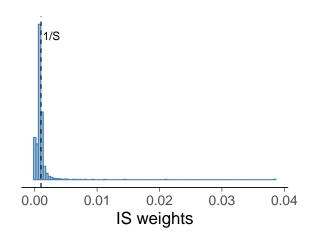


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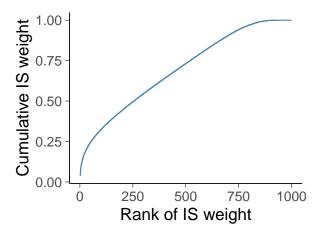


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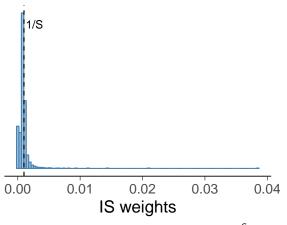


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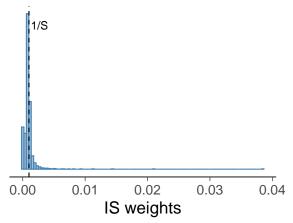
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$$\mathcal{S}_{ ext{eff}} = rac{1}{\sum_{s=1}^{\mathcal{S}} (ilde{w}(heta^s))^2}, \quad ext{where } ilde{w}(heta^s) = w(heta^s) / \sum_{s'=1}^{\mathcal{S}} w(heta^{s'})$$



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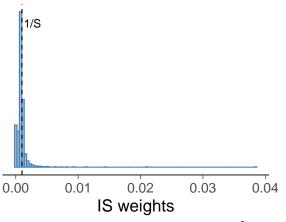
$$S_{ ext{eff}} = rac{1}{\sum_{s=1}^{S} (ilde{w}(heta^s))^2}, \quad ext{where } ilde{w}(heta^s) = w(heta^s) / \sum_{s'=1}^{S} w(heta^{s'})$$

BDA3 1st (2013) and 2nd (2014) printing have an error for $\tilde{w}(\theta^s)$. The normalized weights equation should not have the multiplier S (the normalized weights should sum to one). Errata for the book

http://www.stat.columbia.edu/~gelman/book/errata_bda3.txt



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$$S_{ ext{eff}} = rac{1}{\sum_{s=1}^{S} (\tilde{w}(heta^s))^2}, \quad ext{where } \tilde{w}(heta^s) = w(heta^s) / \sum_{s'=1}^{S} w(heta^{s'})$$

 $S_{\rm eff} \approx 270$



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Pareto smoothed importance sampling

- Pareto-Smoothed Importance sampling smooth the weights according to a Generalized Pareto(k) distribution
- Pareto-k diagnostic estimate the number of existing moments ([1/k])



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Pareto smoothed importance sampling

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- Pareto-k diagnostic estimate the number of existing moments (|1/k|)
- Finite variance and central limit theorem for k < 1/2



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Pareto smoothed importance sampling

- Pareto-Smoothed Importance sampling smooth the weights according to a Generalized Pareto(k) distribution
- Pareto-k diagnostic estimate the number of existing moments ([1/k])
- Finite variance and central limit theorem for k < 1/2
- Finite mean and generalized central limit theorem for k < 1, but pre-asymptotic constant grows impractically large for k > 0.7



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Importance sampling leave-one-out cross-validation

- Later in the course you will learn how $p(\theta|y)$ can be used as a proposal distribution for $p(\theta|y_{-i})$
 - which allows fast computation of leave-one-out cross-validation

$$p(y_i|y_{-i}) = \int p(y_i|\theta)p(\theta|y_{-i})d\theta$$



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Next week: Markov chain Monte Carlo (MCMC)

- Pros
 - Markov chain goes where most of the posterior mass is
 - Certain MCMC methods scale well to high dimensions
- Cons
 - Draws are dependent (affects how many draws are needed)
 - Convergence in practical time is not guaranteed



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 - Markov chain goes where most of the posterior mass is
 - Certain MCMC methods scale well to high dimensions
- Cons
 - Draws are dependent (affects how many draws are needed)
 - Convergence in practical time is not guaranteed
- MCMC methods in this course
 - Gibbs sampling: "iterative conditional sampling"
 - Metropolis: "random walk in joint distribution"
 - Dynamic Hamiltonian Monte Carlo: "state-of-the-art" used in Stan