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  - Computational aspects
- Bayesian Computation
   Numerical integration
- 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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#### Notation

• In this chapter, generic  $p(\theta)$  is used instead of  $p(\theta|y)$ 



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- 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.  $\int q(\theta)d\theta \leq \infty$
  - $q(\cdot) \propto p(\cdot)$



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- Proposal distribution is denoted by  $g(\cdot)$



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- 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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    - the smallest distinguishable difference from 1 is about  $\approx 1 + 2.2 \cdot 10^{-16}$ 
      - Ratio of girl and boy babies
      - pbeta(0.5, 241945, 251527) → 1 (rounding)



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    - pbeta $(0.5, 241945, 251527) \rightarrow 1$  (rounding)
    - pbeta(0.5, 241945, 251527, lower.tail=FALSE) $\approx 1.15 \cdot 10^{-42}$

there is more accuracy near 0



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- DFMO in R!



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  - use log densities to avoid over- and underflows in floating point presentation
    - $prod(dnorm(qr)) \rightarrow 0$  (underflow)
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    - e.g. in Metropolis-algorithm (next week) compute the log of ratio of densities using the identity log(a/b) = log(a) - log(b)



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#### Section 2

# Bayesian Computation



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$$E_{p(\theta|y)}[f(\theta)] = \int f(\theta)p(\theta|y)d\theta,$$
 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  $\theta$ , 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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  - Conjugate priors and analytic solutions (Ch 1-5)



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  - (Distributional approximations, Ch 4, 13)



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#### Subsection 1

Numerical integration



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#### Riemann recap

Remember the Riemann sum (where  $x_s^*$ :

$$I_a^b = \sum_{s=1}^S f(x_s^*) \, \Delta x_s \,,$$

where

$$\Delta x = \frac{b-a}{S}$$
 and  $x_s^* \in [x_{i-s}, x_s]$ 



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where

$$\Delta x = \frac{b-a}{S}$$
 and  $x_s^* \in [x_{i-s}, x_s]$ 

And the Riemann integral:

$$\int_a^b f(x) dx = \lim_{\|\Delta x\| \to 0} \sum_{i=1}^S f(x_i^*) \Delta x_i,$$



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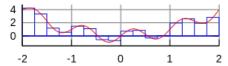
Now lets use the Riemann sum to approximate the Riemann integral!



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- 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

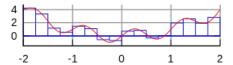


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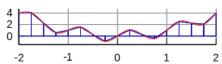
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In 1D further variations with smaller error, e.g. trapezoid

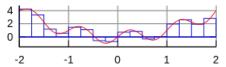




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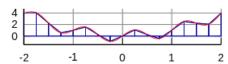
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• In 1D further variations with smaller error, e.g. trapezoid



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



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#### Monte Carlo Methods



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# Monte Carlo integration/method

• 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

$$E_{p(\theta|y)}(h(\theta)) = \int h(\theta)p(\theta|y)d\theta \approx \frac{1}{5}\sum_{s}^{5}h(\theta_{s})$$



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

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

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



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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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- "Monte Carlo method" term was proposed by Metropolis, von Neumann or Ulam in the end of 1940s
  - they worked together in atomic bomb project
  - Metropolis and Ulam, "The Monte Carlo Method", 1949



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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)
- "Monte Carlo method" term was proposed by Metropolis, von Neumann or Ulam in the end of 1940s
  - 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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## 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
  - ightarrow 50<sup>10</sup> pprox 1e17 grid points
  - $\rightarrow$  1000<sup>10</sup>  $\approx$  1e30 grid points



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  - ightarrow 50<sup>10</sup> pprox 1e17 grid points
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- 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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- 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  $\sigma_{\theta}^2/S$  (asymptotic normality)

• this variance is independent on dimensionality of  $\theta$  (!)



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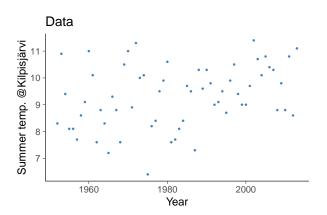
$$\sigma_{\theta}^2 + \sigma_{\theta}^2 / S = \sigma_{\theta}^2 (1 + 1/S)$$

- 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)
- See Ch 4 for counter-examples for asymptotic normality



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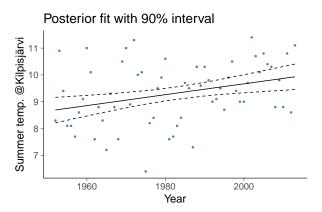
Average temperature in June, July, and August at Kilpisjärvi, Finland





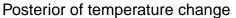
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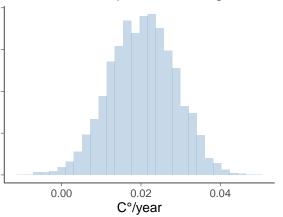
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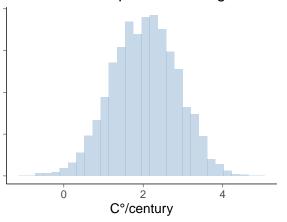




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#### Importance sampling Pareto-Smoothed Importance Sampling





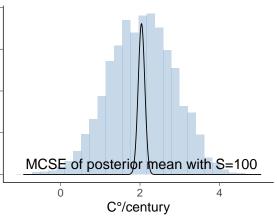


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### Example: Kilpisjärvi summer temperature



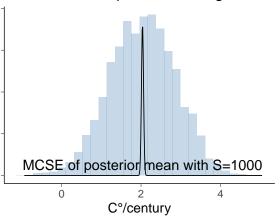


 $\sigma_{\theta} \approx 0.827$ , MCSE  $\approx 0.0827$ , total deviation  $\approx 0.831$ total deviation<sup>2</sup> =  $\sigma_{\theta}^2 + MCSE^2$ 



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## Example: Kilpisjärvi summer temperature



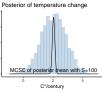


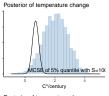
Posterior of temperature change

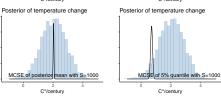




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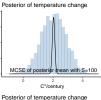


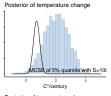


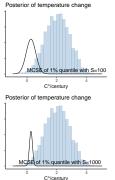


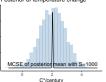
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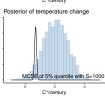
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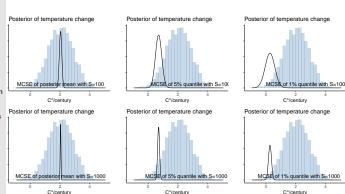








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Tail quantiles are more difficult to estimate



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Posterior probability

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

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



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Posterior probability

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

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?

Posterior probability

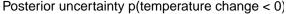
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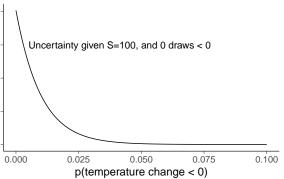
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- if S=100 and  $p\approx 0.5$ ,  $\sqrt{p(1-p)/S}=0.05$  i.e. accuracy is about 5% units
- S = 2500 draws needed for 1% unit accuracy
- To estimate small probabilities, a large number of draws is needed
  - to be able to estimate p, need to get draws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



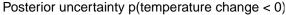
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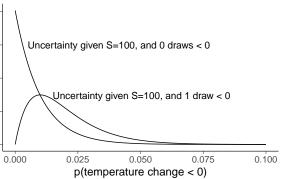






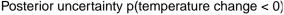
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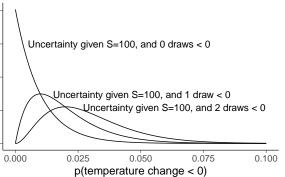






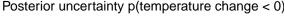
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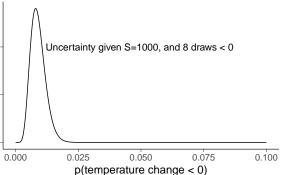






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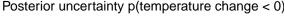


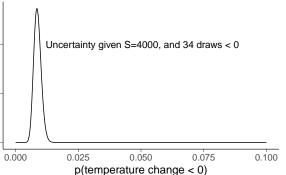




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### Example: Kilpisjärvi summer temperature







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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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- Don't show digits which are just random noise
  - check what is the Monte Carlo standard error
- Show meaningful digits given the posterior uncertainty



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- Example: The mean and 90% central posterior interval for temperature increase C°/century based on posterior draws



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  - 2.050774 and [0.7472868 3.3017524] (NO!)



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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
- Show meaningful digits given the posterior uncertainty
- Example: The mean and 90% central posterior interval for temperature increase C°/century based on posterior draws
  - 2.050774 and [0.7472868 3.3017524] (NO!)
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  - 0.9960000 (NO!)



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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  $\approx$  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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### How many simulation draws are needed?

- 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



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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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$$X_1 = \sqrt{-2\log(U_1)}\cos(2\pi U_2)$$
  
 $X_2 = \sqrt{-2\log(U_1)}\sin(2\pi U_2)$ 

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

- 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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# Indirect sampling



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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<sub>eff</sub> the number of samples using direct methods
- Common with weighted or correlated samples



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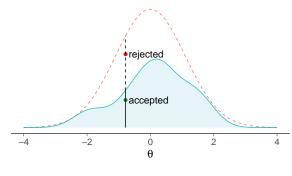
### Effective sampling size

- Efficient sampling size S<sub>eff</sub> 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  $q(\theta|y)/Mg(\theta)$

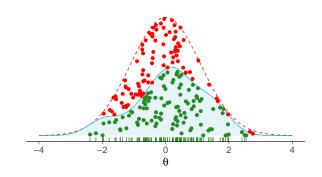


-- Mg(theta) -- q(theta|y)



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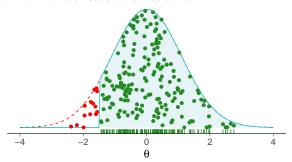


Accepted
 Rejected
 Mg(theta)
 g(thetaly)



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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<sub>eff</sub>
 When will this be work/not work (i.e. give high/low S<sub>eff</sub>)?



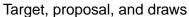
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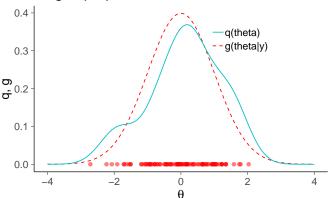
- The number of accepted draws is the effective sample size  $S_{\mathrm{eff}}$ 
  - with bad proposal distribution may require a lot of trials
  - selection of good proposal gets very difficult when the number of dimensions increase



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- Proposal does not need to have a higher value everywhere

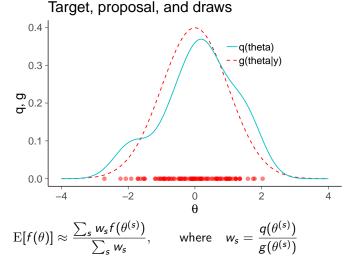






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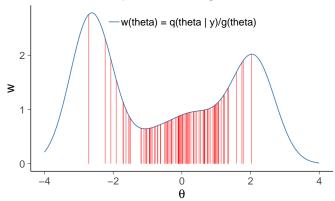
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Proposal does not need to have a higher value everywhere
 Draws and importance weights



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



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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



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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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#### Importance sampling

- 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  $g(\theta)$ ?



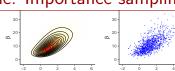
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#### Importance sampling

- 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



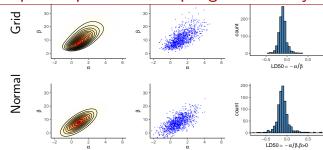
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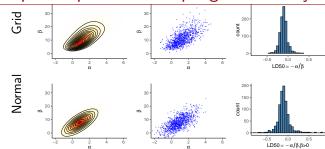
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Normal approximation is discussed more in BDA3 Ch 4



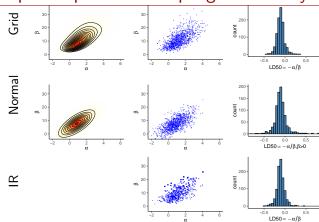
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Normal approximation is discussed more in BDA3 Ch 4 But the normal approximation is not that good here: Grid  $sd(LD50) \approx 0.1$ , Normal  $sd(LD50) \approx .75!$ 



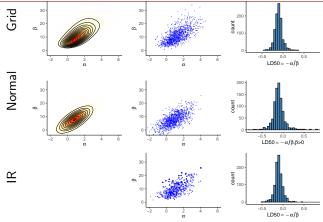
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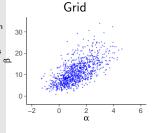


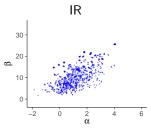
Grid sd(LD50)  $\approx$  0.1, IR sd(LD50)  $\approx$  0.1





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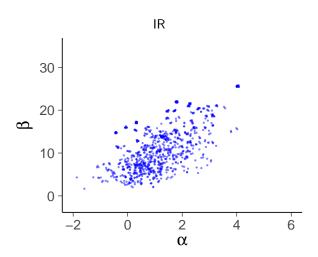






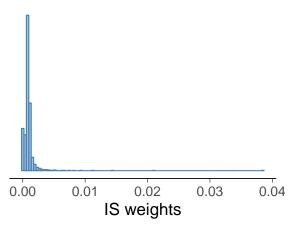
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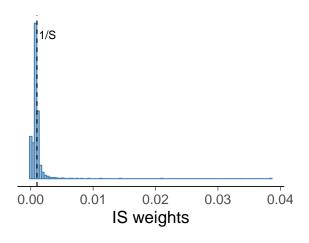


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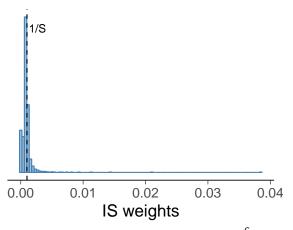
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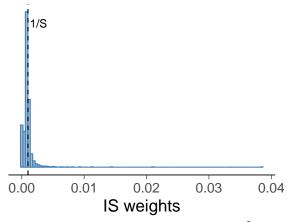
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$$\mathcal{S}_{ ext{eff}} = rac{1}{\sum_{s=1}^{S} ( ilde{w}( heta^s))^2}, \quad ext{where } ilde{w}( heta^s) = w( heta^s) / \sum_{s'=1}^{S} w( heta^{s'})$$



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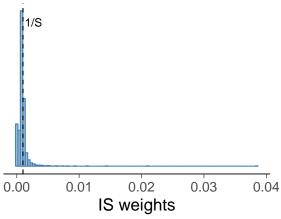
$$S_{ ext{eff}} = rac{1}{\sum_{s=1}^{S} (\tilde{w}( heta^s))^2}, \quad ext{where } \tilde{w}( heta^s) = w( heta^s) / \sum_{s'=1}^{S} w( heta^{s'})$$

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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  $S_{ ext{eff}} pprox 270$ 



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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

- 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



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     Importance Sampling

#### 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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- Indirect sampling
  - Rejection sampling
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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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  - Certain MCMC methods scale well to high dimensions
- Cons
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- 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