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Bayesian Statistics and Data Analysis
Lecture 4

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Thanks to Aki Vehtari, Aalto University

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 $g(\cdot)$

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)) $\rightarrow$ 0 (underflow)

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    - 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

Numerical accuracy – log scale

- Log densities
  - use log densities to avoid over- and underflows in floating point presentation
    - prod(dnorm(qr)) $\rightarrow$ 0 (underflow)
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      e.g. $\log(\exp(800) + \exp(800)) \to$ Inf

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      but $800 + \log(1 + \exp(800 - 800)) \approx 800.69$

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      but $800 + \log(1 + \exp(800 - 800)) \approx 800.69$
    - e.g. in Metropolis-algorithm (ex5) compute the log of ratio of densities using the identity
      $\log(a/b) = \log(a) - \log(b)$

It's all about expectations

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

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

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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 $q(\theta^{(s)}|y)$

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

It's all about expectations

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

- 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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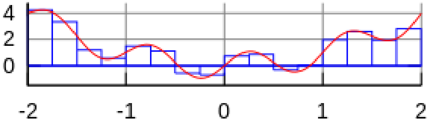
Quadrature integration

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

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



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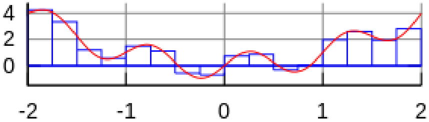

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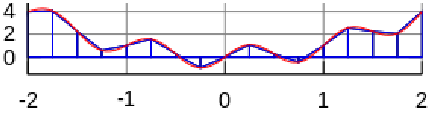
- In 1D further variations with smaller error, e.g. trapezoid



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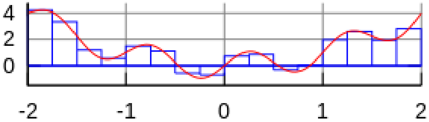

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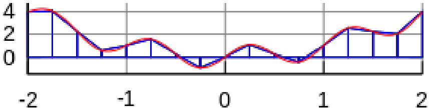

- In 2D and higher
  - nested quadrature, product rules
  - but theres a curse of dimensionality...

Monte Carlo integration/method

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

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

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 $p(\theta|y)$

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

$$E_{p(\theta|y)}(h(\theta)) \approx \int f(\theta)p(\theta|y)d\theta = \frac{1}{S}\sum_s^S f(\theta_s)$$

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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  - 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

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.

Monte Carlo vs. Deterministic Methods

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- 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 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.

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*

How many simulation draws are needed?

- Expectation of unknown quantity

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

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

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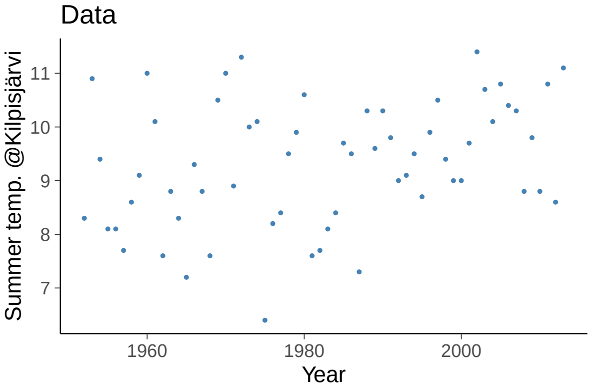
  - See Ch 4 for counter-examples for asymptotic normality

Example: Kilpisjärvi summer temperature

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



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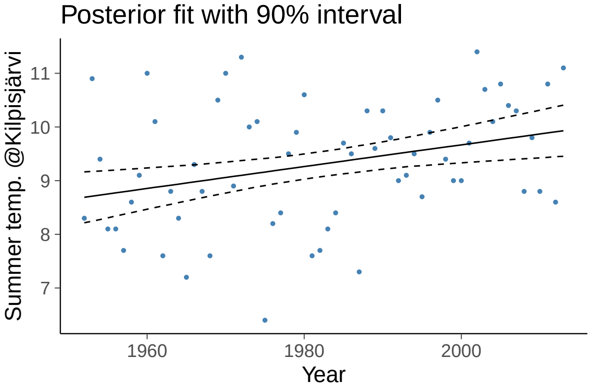

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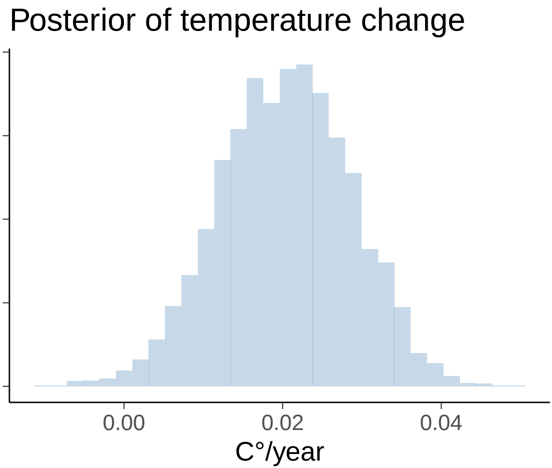

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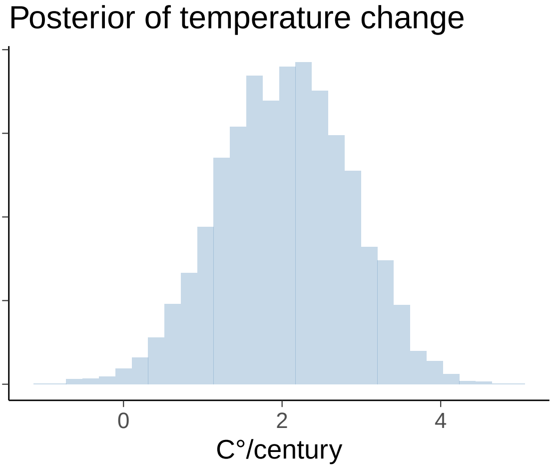

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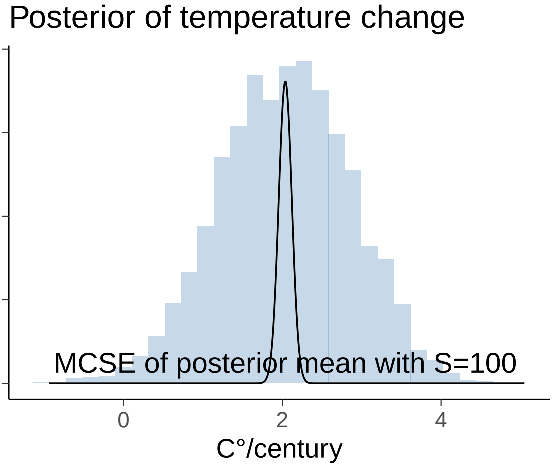

$\sigma_\theta \approx 0.827$, MCSE ≈ 0.0827, total deviation ≈ 0.831

total deviation$^2 = \sigma_\theta^2 +$ MCSE^2

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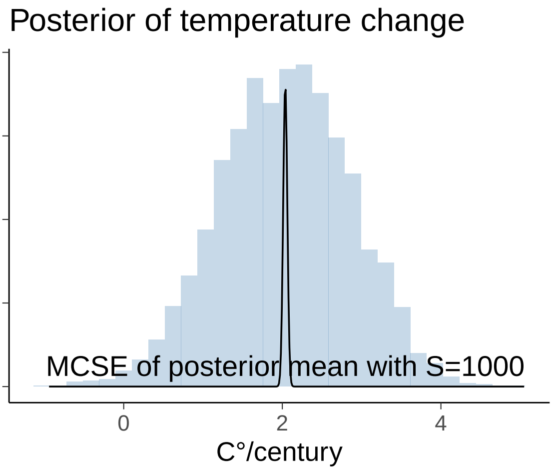

$\sigma_\theta \approx 0.827$, MCSE ≈ 0.0261, total deviation ≈ 0.827

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

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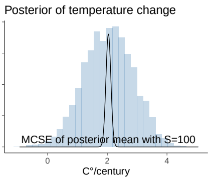

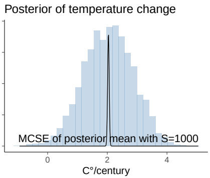

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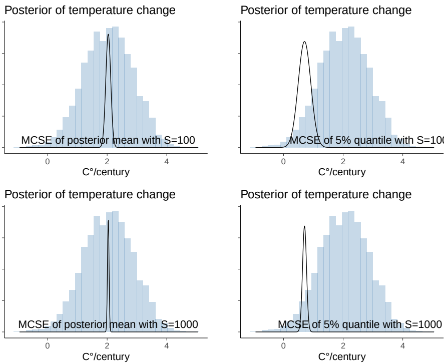

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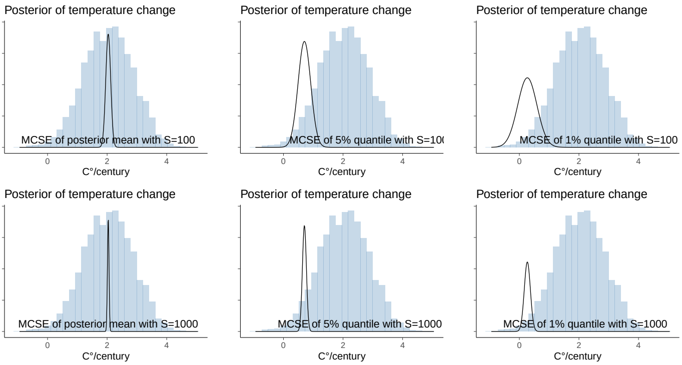

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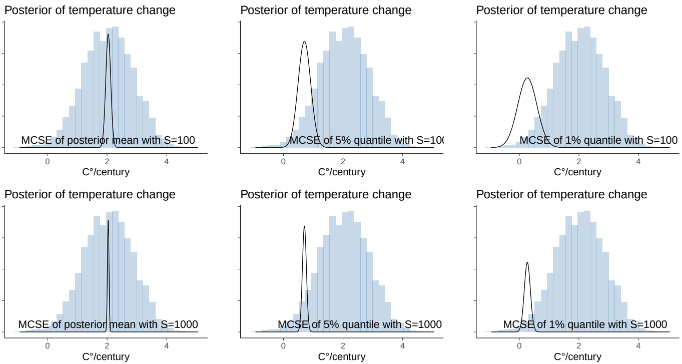

Tail quantiles are more difficult to estimate

How many simulation draws are needed?

- Posterior probability

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

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  - $\rightarrow$ $\mathrm{var}(I(\cdot)) = p(1-p)$ (Appendix A, p. 579)
  - $\rightarrow$ standard deviation of p is $\approx \sqrt{p(1-p)/S}$

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  - $\rightarrow$ standard deviation of p is $\approx \sqrt{p(1-p)/S}$
- 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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  - $\rightarrow$ $\mathrm{var}(I(\cdot)) = p(1-p)$ (Appendix A, p. 579)
  - $\rightarrow$ standard deviation of p is $\approx \sqrt{p(1-p)/S}$
- 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

How many simulation draws are needed?

- Posterior probability

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

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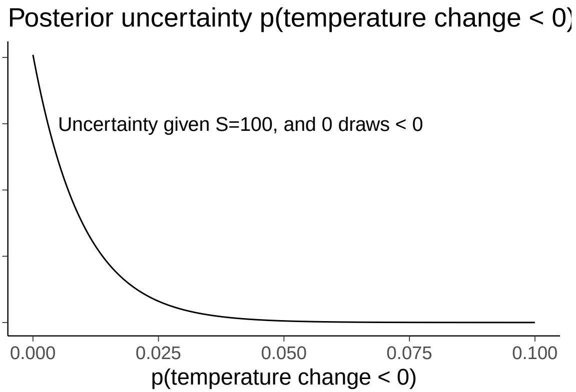
  - $S = 2500$ draws needed for 1% unit accuracy
- To estimate small probabilities, a large number of draws is needed
  - to be able to estimate p, need to get draws with $\theta^{(l)} \in A$, which in expectation requires $S \gg 1/p$

Example: Kilpisjärvi summer temperature



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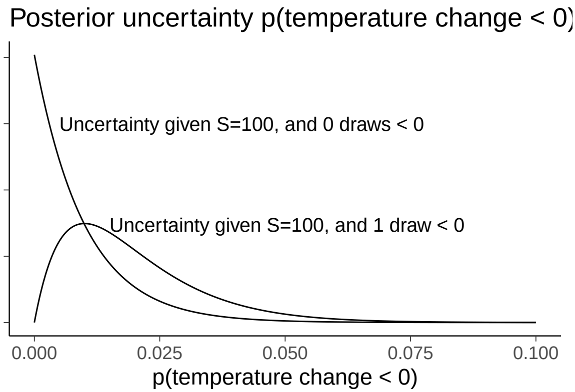

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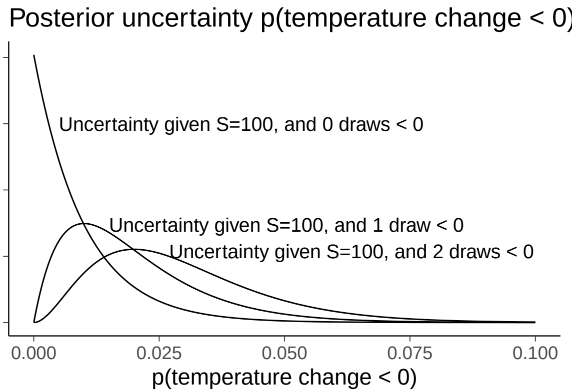

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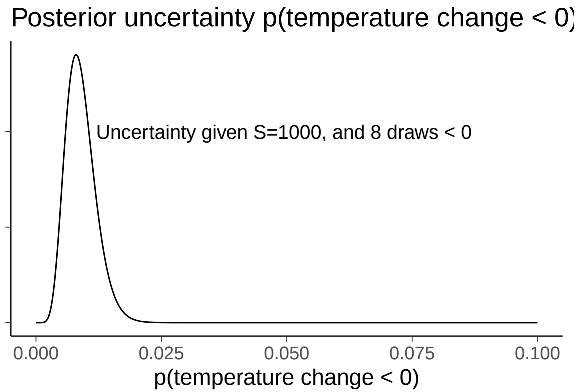

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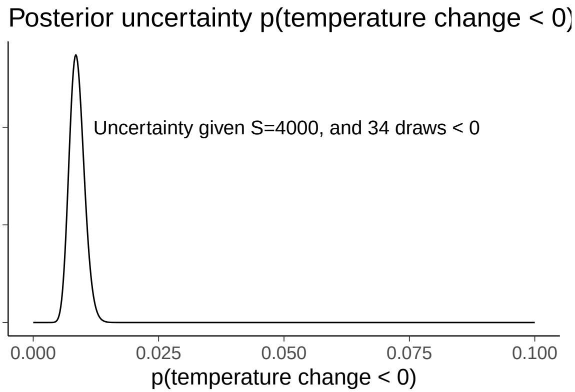

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  - With 4000 draws MCSE $\approx$ 0.002. We could report that probability is very likely larger than 0.99, or sample more to justify reporting three digits
  - For probabilities close to 0 or 1, consider also when the model assumption justify certain accuracy
- For your project: Think for each reported value how many digits is sensible.

How many simulation draws are needed?

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

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

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

Random number generators

- How to sample from a pdf?

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

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

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  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

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

  $\rightarrow$ $50^{10} \approx$ 1e17 grid points

  $\rightarrow$ $1000^{10} \approx$ 1e30 grid points

Grid sampling and curse of dimensionality

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- 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
- e.g. 50 or 1000 grid points per dimension
  - $\rightarrow$ $50^{10} \approx$ 1e17 grid points
  - $\rightarrow$ $1000^{10} \approx$ 1e30 grid points
- R and my current laptop can compute density of normal distribution about 20 million times per second
  - $\rightarrow$ evaluation in 1e17 grid points would take 150 years
  - $\rightarrow$ evaluation in 1e30 grid points would take 1 500 billion years

Indirect sampling

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

Effective sampling size

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

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 $S_{\text{eff}} < S$
- Informally an indication of performance of method

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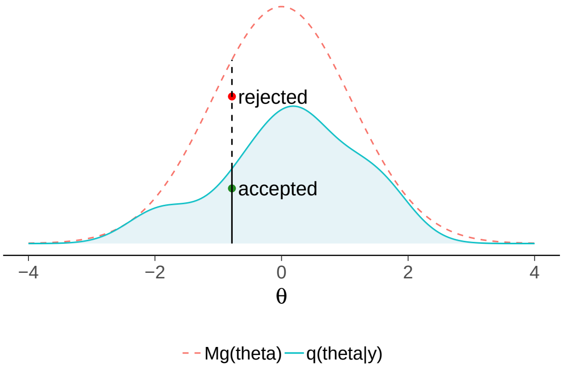
Rejection sampling

- 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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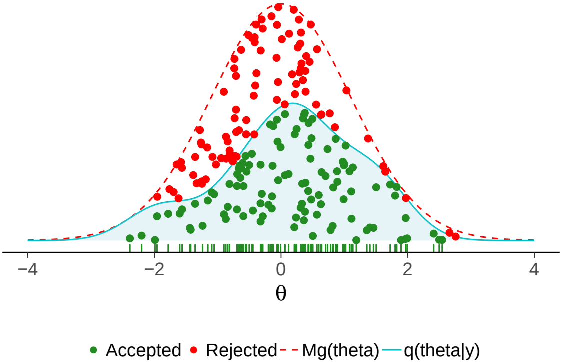
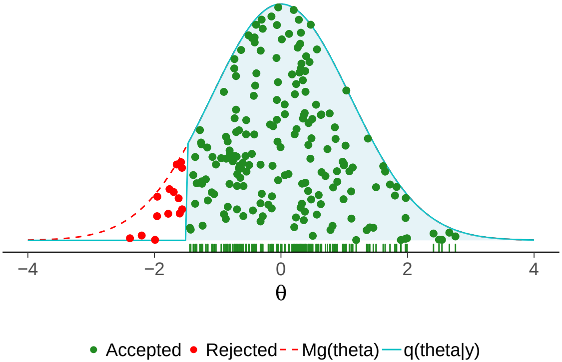


Rejection sampling

- 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



Rejection sampling

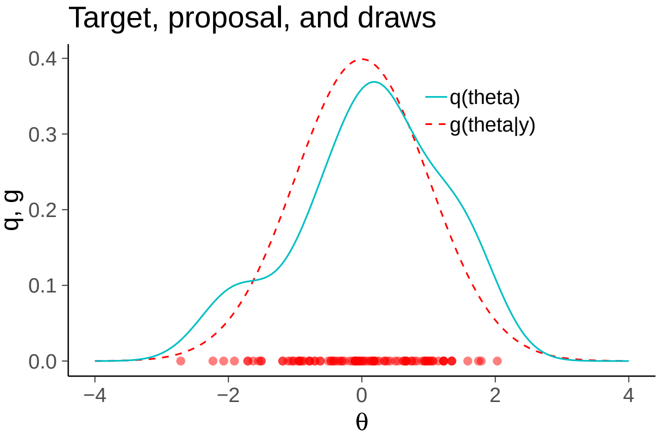
- The number of accepted draws is the effective sample size S_{eff}
  When will this be work/not work (i.e. give high/low S_{eff}?

Rejection sampling

- 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

Importance sampling

- Proposal does not need to have a higher value everywhere



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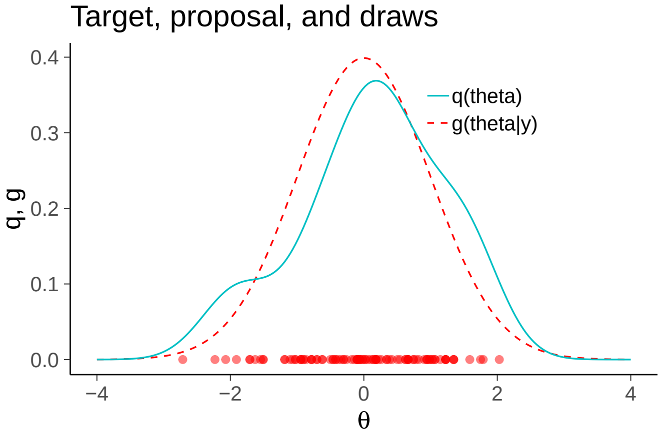

$$\mathrm{E}[f(\theta)] \approx \frac{\sum_s w_s f(\theta^{(s)})}{\sum_s w_s}, \qquad \text{where} \quad w_s = \frac{q(\theta^{(s)})}{g(\theta^{(s)})}$$

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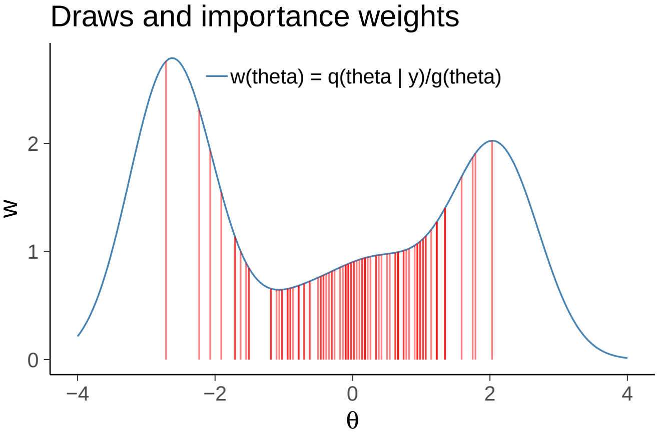

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Importance sampling

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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

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

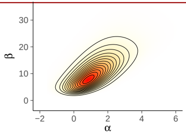
What does this mean? What is a good proposal $g(\theta)$?

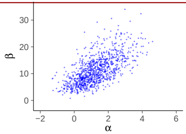
Importance sampling

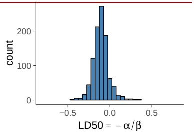
- Variation of the weights affect the effective sample size
  - if single weight dominates, we have effectively one sample
  - if all weights are equal, we have effectively S draws
- Central limit theorem holds only if variance of the weight distribution is finite

Example: Importance sampling in Bioassay

Grid







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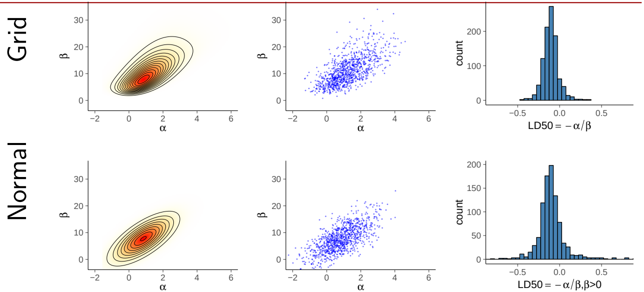

Normal approximation is discussed more in BDA3 Ch 4

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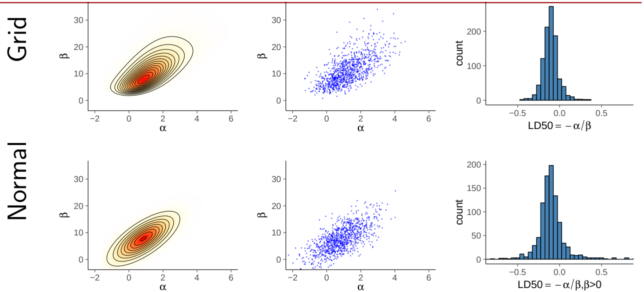
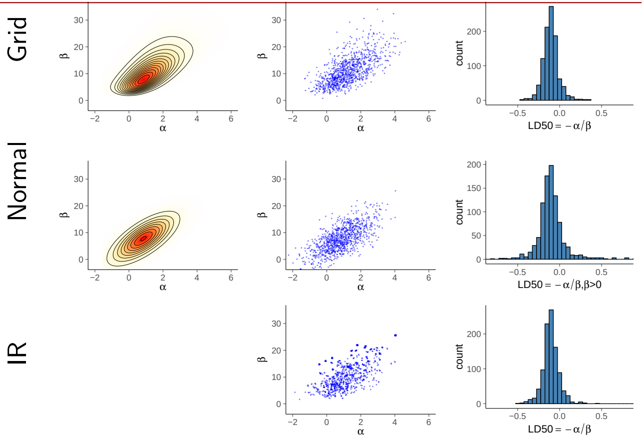


Normal approximation is discussed more in BDA3 Ch 4

But the normal approximation is not that good here:

Grid sd(LD50) $\approx$ 0.1, Normal sd(LD50) $\approx$ .75!

Example: Importance sampling in Bioassay



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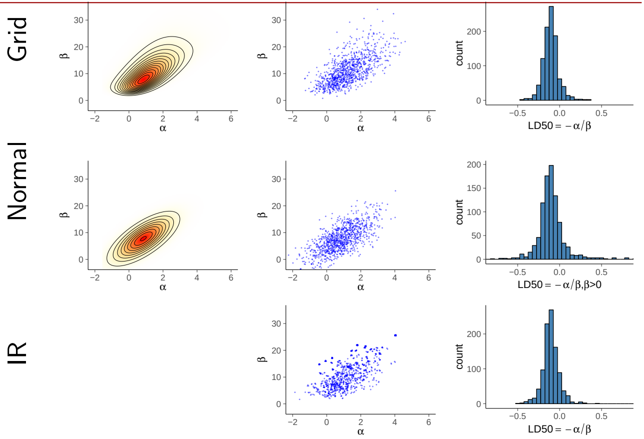

Grid sd(LD50) ≈ 0.1, IR sd(LD50) ≈ 0.1

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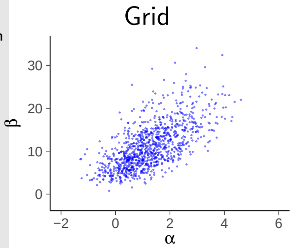

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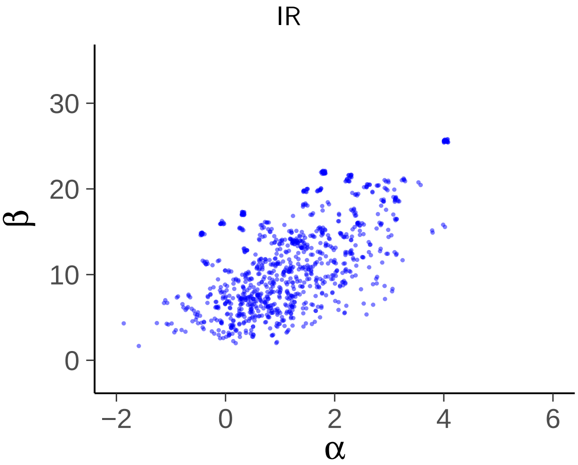

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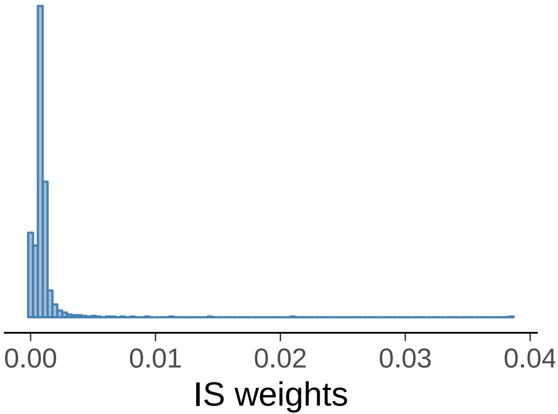

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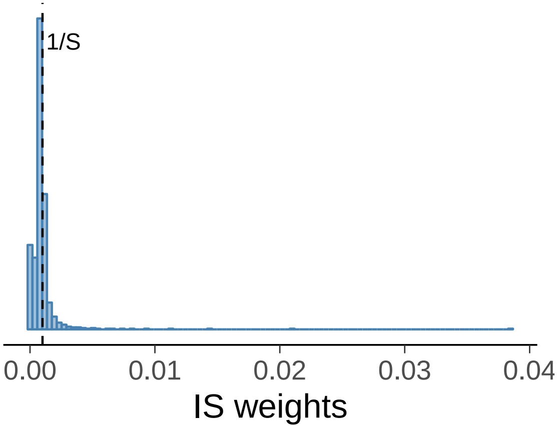

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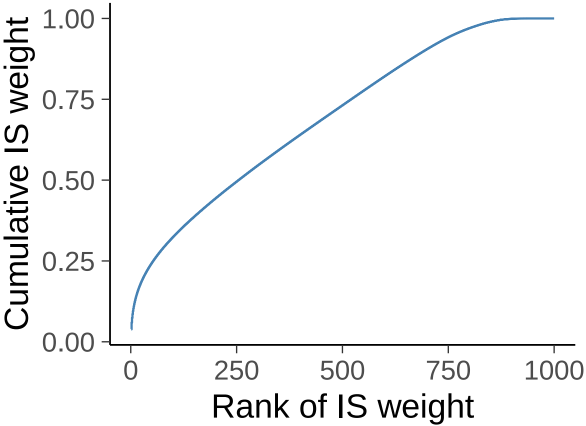

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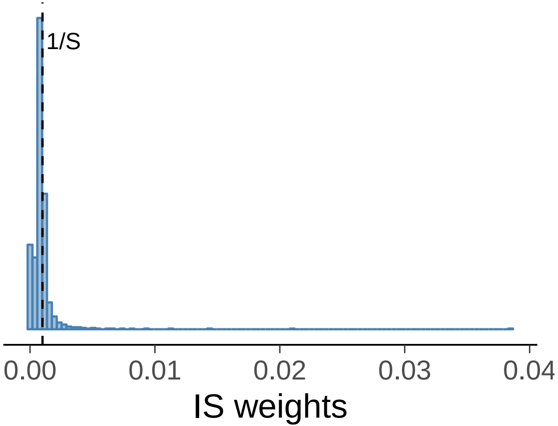

$$S_{\text{eff}} = \frac{1}{\sum_{s=1}^{S} (\tilde{w}(\theta^s))^2}, \quad \text{where } \tilde{w}(\theta^s) = w(\theta^s) / \sum_{s'=1}^{S} w(\theta^{s'})$$

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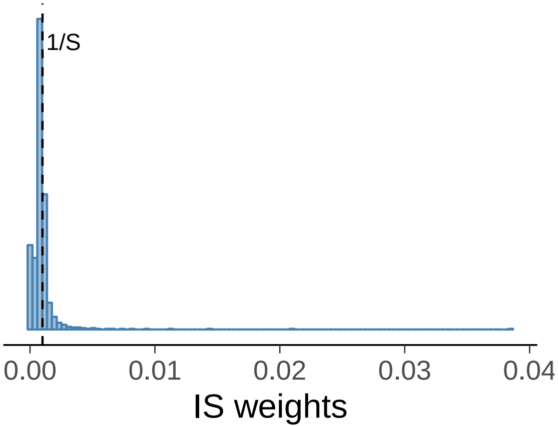

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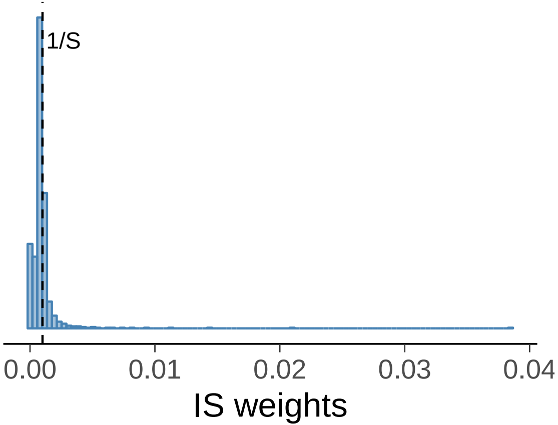
BDA3 1st (2013) and 2nd (2014) printing have an error for $\tilde{w}(\theta^s)$. The normalized weights equation should not have the multiplier S (the normalized weights should sum to one). Errata for the book http://www.stat.columbia.edu/~gelman/book/errata_bda3.txt

Example: Importance sampling in Bioassay



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$$S_{\text{eff}} \approx 270$$

Pareto smoothed importance sampling

- Pareto-k diagnostic estimate the number of existing moments ($\lfloor 1/k \rfloor$)

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- Pareto-k diagnostic estimate the number of existing moments ($\lfloor 1/k \rfloor$)
- 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 $k > 0.7$

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

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

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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  - 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