

# Chapter 10

- 10.1 Numerical integration (overview)
- 10.2 Distributional approximations (overview, more in Chapter 4 and 13)
- 10.3 Direct simulation and rejection sampling (overview)
- 10.4 Importance sampling (used in PSIS-LOO discussed later)
- 10.5 How many simulation draws are needed? (Ex 10.1 and 10.2)
  - see chapter notes and extra slides for how many significant digits to report
- 10.6 Software (can be skipped)
- 10.7 Debugging (can be skipped)

# 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
  - $q(\cdot) \propto p(\cdot)$
- 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:  
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    - Laplace and ratio of girl and boy babies
    - `pbeta(0.5, 241945, 251527)` → 1 (rounding)

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    - `pbeta(0.5, 241945, 251527)` → 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))` → 0 (underflow)
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but `800 + log(1 + exp(800 - 800))` ≈ 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

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

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

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- Grid (equal spacing) evaluation with self-normalization

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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

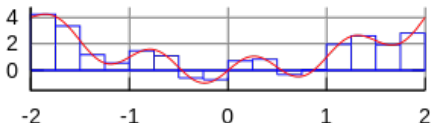
$$E_{\theta}[f(\theta)] = \int f(\theta)p(\theta|y)d\theta$$

- 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)

# Quadrature integration

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

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

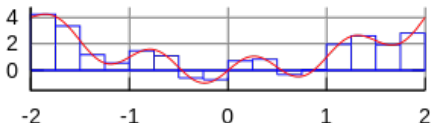


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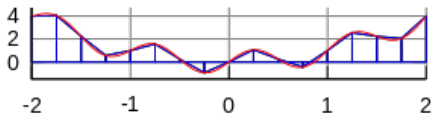
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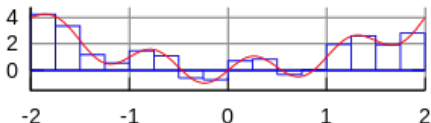
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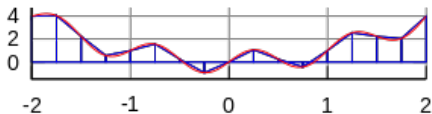
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- In 2D and higher
  - nested quadrature
  - product rules

# 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
  - these draws can be treated as any observations
  - a collection of draws is sample
- Use these draws, for example,
  - to compute means, deviations, quantiles
  - to draw histograms
  - to marginalize
  - etc.

# Monte Carlo vs. deterministic

- Monte Carlo = simulation methods
  - evaluation points are selected stochastically (randomly)
- Deterministic methods (e.g. grid)
  - evaluation points are selected by some deterministic rule
  - good deterministic methods converge faster (need less function evaluations)

# How many simulation draws are needed?

- How many draws or how big sample size?
- 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
  - requires additional work to estimate the **effective sample size**

# 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)

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

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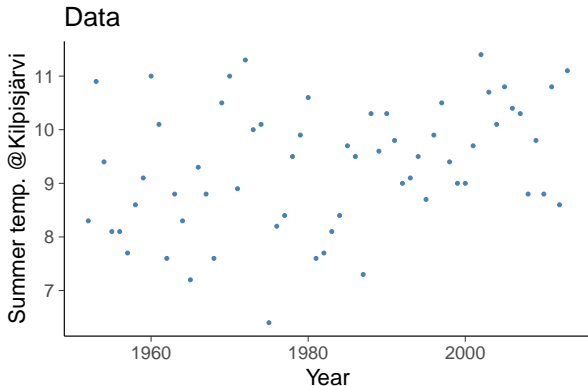
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- See Ch 4 for counter-examples for asymptotic normality

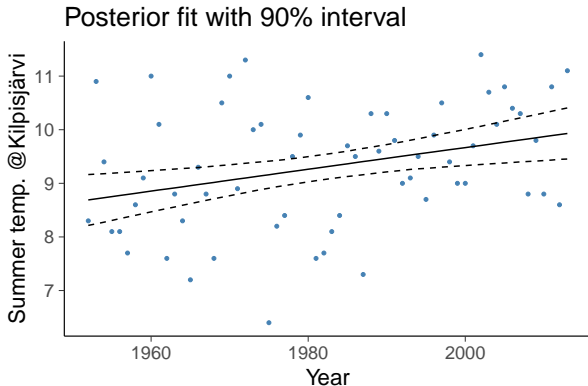
# Example: Kilpisjärvi summer temperature

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



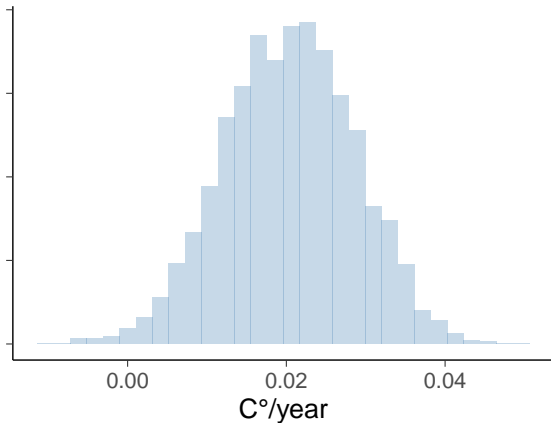
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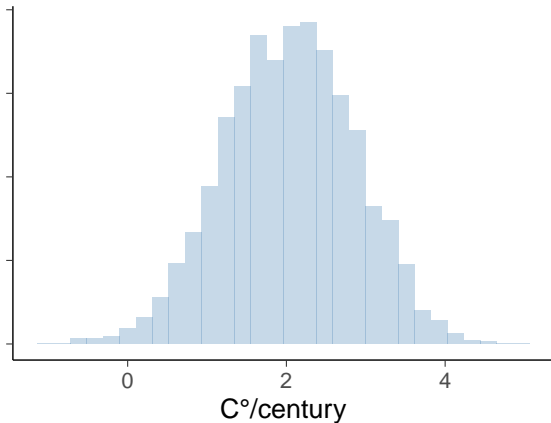
## Example: Kilpisjärvi summer temperature

Posterior of temperature change



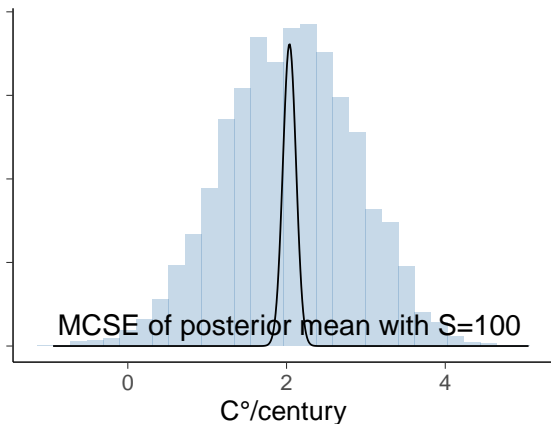
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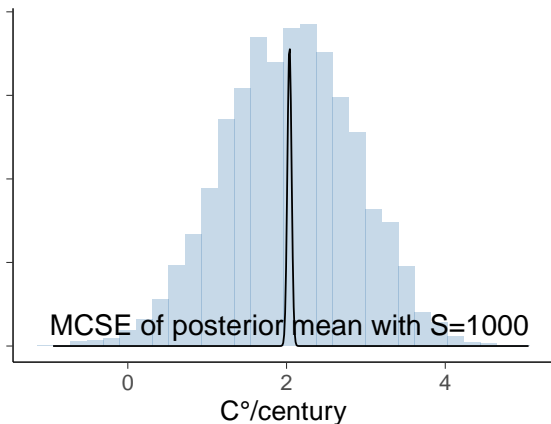


$\sigma_{\theta} \approx 0.827$ ,  $\text{MCSE} \approx 0.0827$ , total deviation  $\approx 0.831$

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

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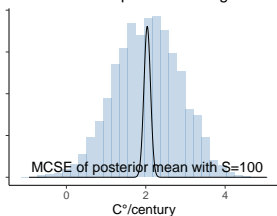


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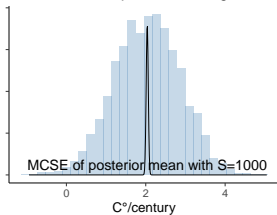
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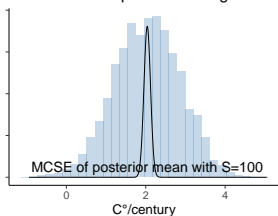
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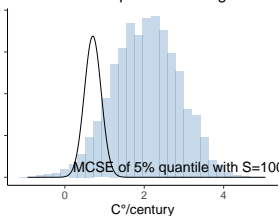


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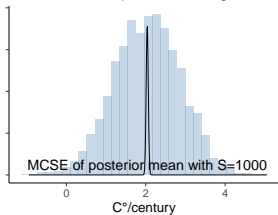
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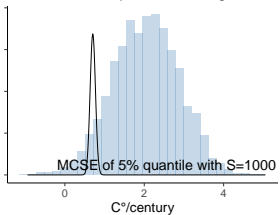
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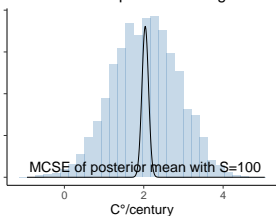


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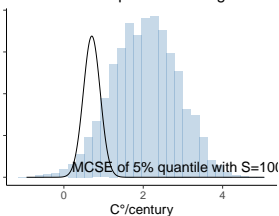


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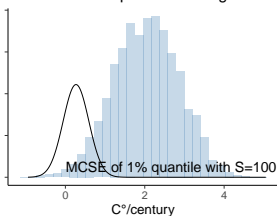
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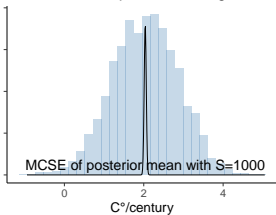
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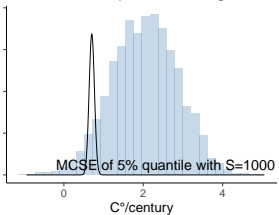
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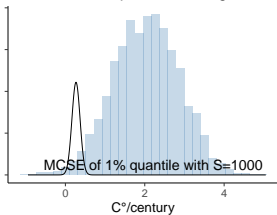
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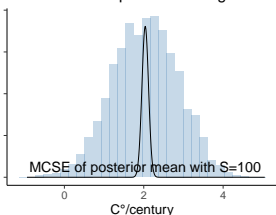


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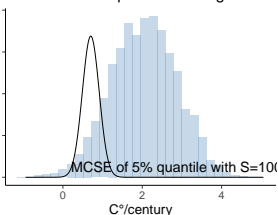


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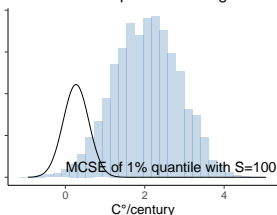
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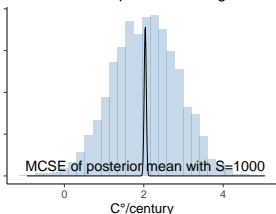
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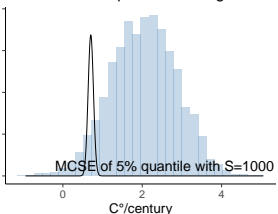
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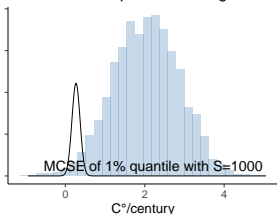
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Tail quantiles are more difficult to estimate

# How many simulation draws are needed?

- Posterior probability

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

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

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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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- Posterior probability

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

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

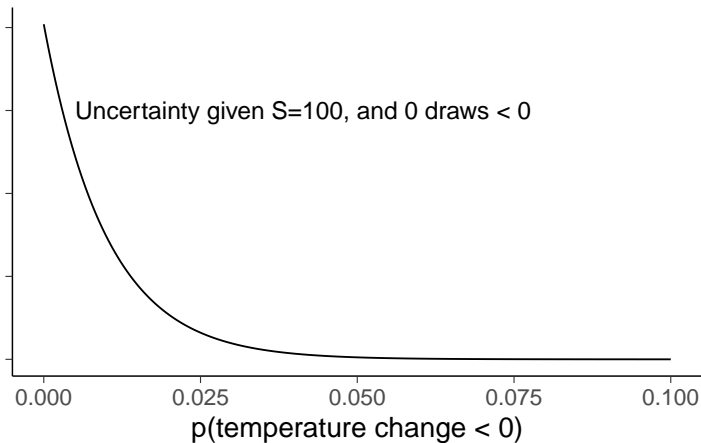
$$p(\theta \in A) \approx \frac{1}{S} \sum_l I(\theta^{(s)} \in A)$$

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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  $S \gg 1/p$

## Example: Kilpisjärvi summer temperature

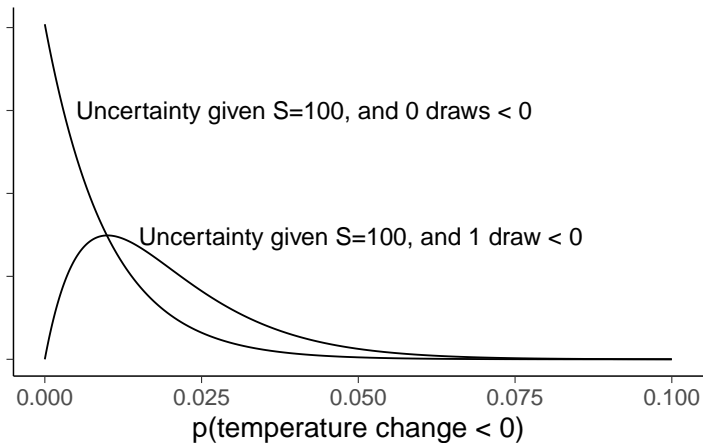
Posterior uncertainty  $p(\text{temperature change} < 0)$





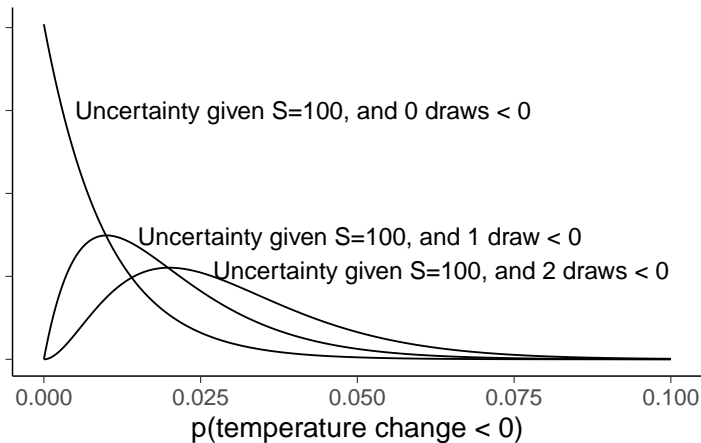
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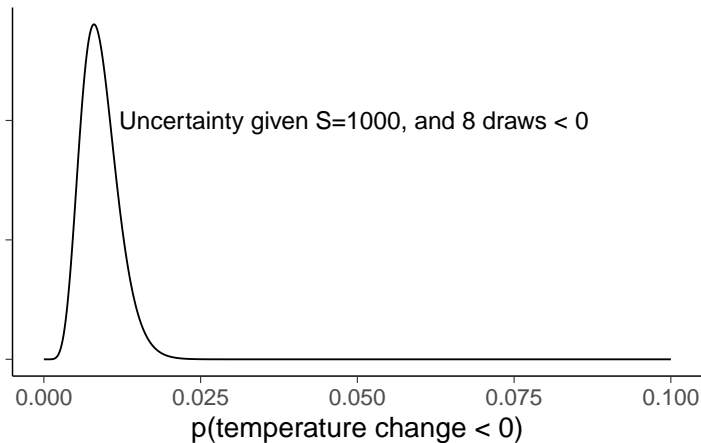
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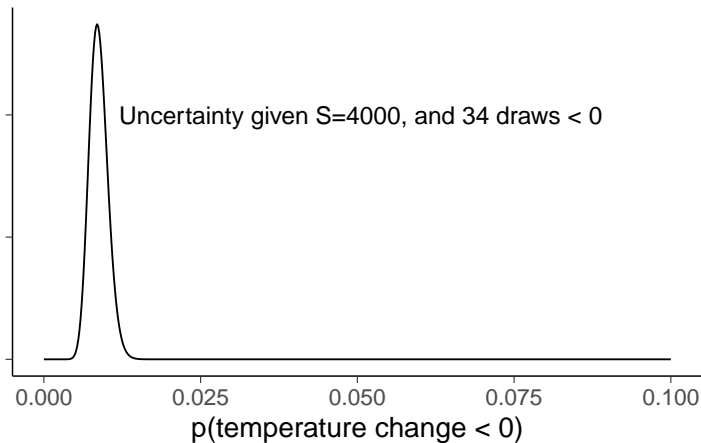
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  - With 4000 draws  $\text{MCSE} \approx 0.002$ . We could report that probability is **very likely larger than 0.99**, or sample more to justify reporting three digits
  - For probabilities close to 0 or 1, consider also when the model assumption justify certain accuracy



# 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 simulation

- 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

- Good pseudo 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

## Direct simulation: Example

- Box-Muller -method:

If  $U_1$  and  $U_2$  are independent draws from distribution  $U(0, 1)$ , 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  $N(0, 1)$

- 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
- e.g. 50 or 1000 grid points per dimension
  - $50^{10} \approx 1\text{e}17$  grid points
  - $1000^{10} \approx 1\text{e}30$  grid points
- R and my current laptop can compute density of normal distribution about 20 million times per second
  - evaluation in  $1\text{e}17$  grid points would take 150 years
  - evaluation in  $1\text{e}30$  grid points would take 1 500 billion years

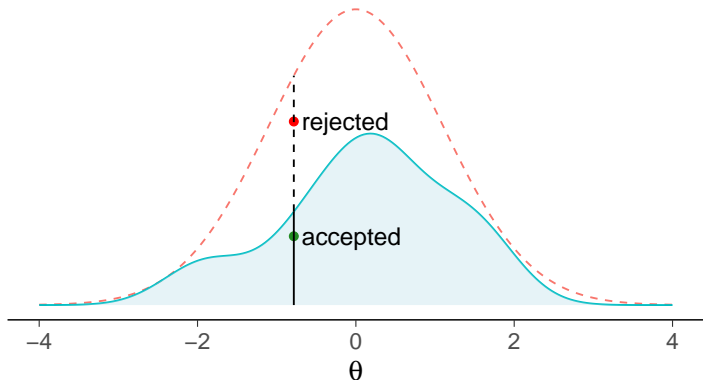
# Indirect sampling

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



# Rejection sampling

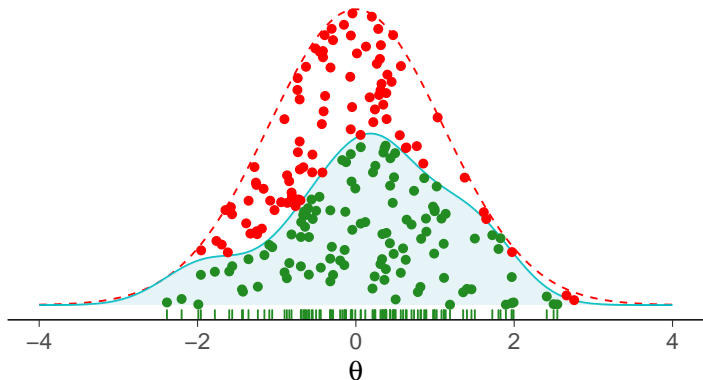
- Proposal forms envelope over the target distribution  
 $q(\theta|y)/Mg(\theta) \leq 1$
- Draw from the proposal and accept with probability  
 $q(\theta|y)/Mg(\theta)$



--  $Mg(\theta)$  —  $q(\theta|y)$

# Rejection sampling

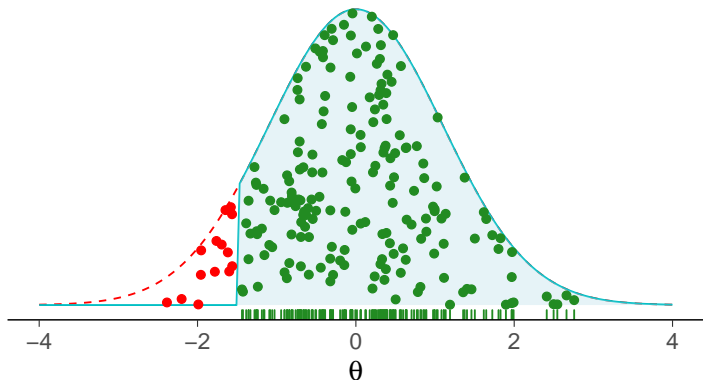
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● Accepted ● Rejected - -  $Mg(\theta)$  —  $q(\theta|y)$

# Rejection sampling

- Proposal 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) — q(theta|y)

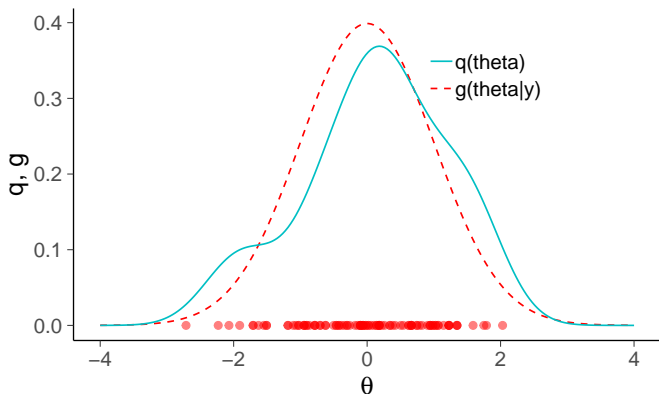
# Rejection sampling

- The number of accepted draws is the effective sample size
  - with bad proposal distribution may require a lot of trials
  - selection of good proposal gets very difficult when the number of dimensions increase
  - reliable diagnostics and thus can be a useful part

# Importance sampling

- Proposal does not need to have a higher value everywhere

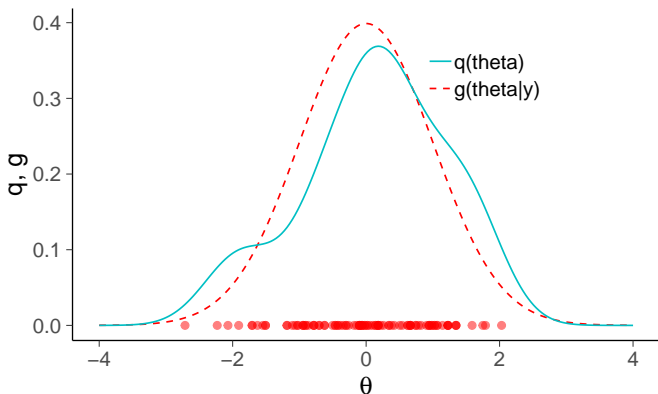
Target, proposal, and draws



# Importance sampling

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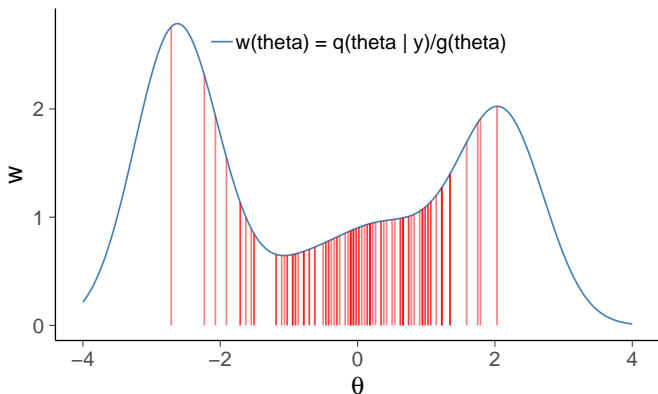


$$E[f(\theta)] \approx \frac{\sum_s w_s f(\theta^{(s)})}{\sum_s w_s}, \quad \text{where} \quad w_s = \frac{q(\theta^{(s)})}{g(\theta^{(s)})}$$

# Importance sampling

- Proposal does not need to have a higher value everywhere

Draws and importance weights



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

# Importance sampling

- 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

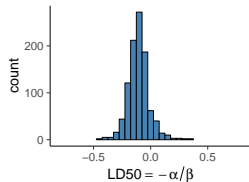
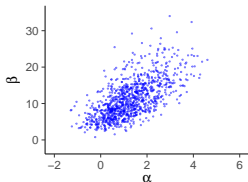
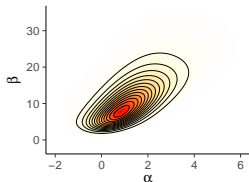


# Importance sampling

- Variation of the weights affect the effective sample size
  - if single weight dominates, we have effectively one sample
  - if weights are equal, we have effectively  $S$  draws
- Central limit theorem holds only if variance of the weight distribution is finite
- See Vehtari, Simpson, Gelman, Yuling and Gabry (2019). Pareto smoothed importance sampling. arXiv preprint arXiv:1507.02646, <https://arxiv.org/abs/1507.02646> for improved diagnostics and stability.

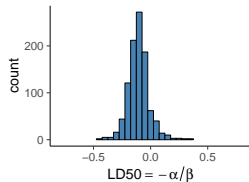
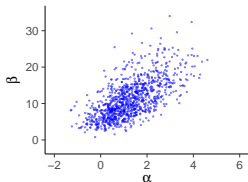
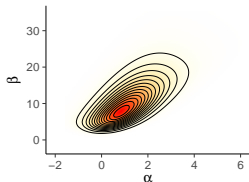
# Example: Importance sampling in Bioassay

Grid

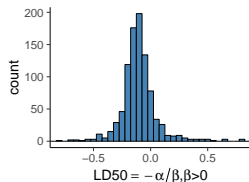
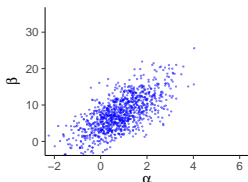
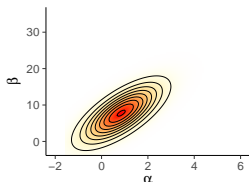


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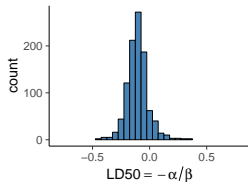
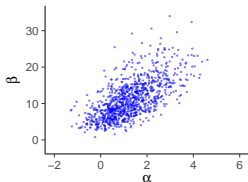
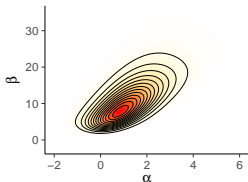
Normal



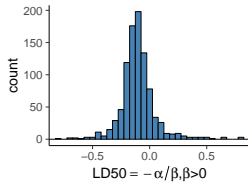
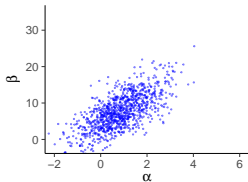
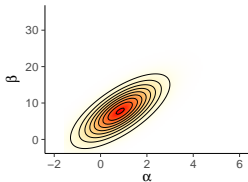
Normal approximation is discussed more in BDA3 Ch 4

# Example: Importance sampling in Bioassay

Grid



Normal



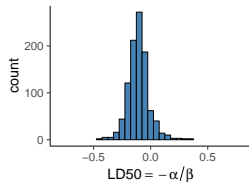
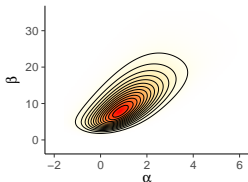
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But the normal approximation is not that good here:

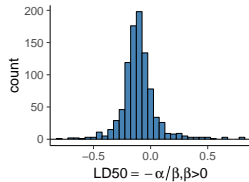
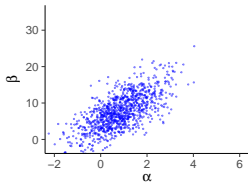
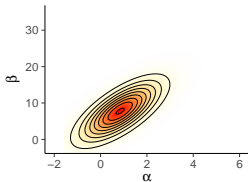
Grid  $sd(LD50) \approx 0.1$ , Normal  $sd(LD50) \approx .75$ !

# Example: Importance sampling in Bioassay

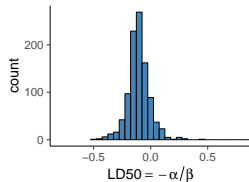
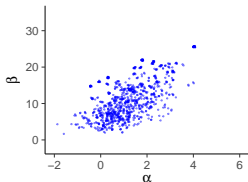
Grid



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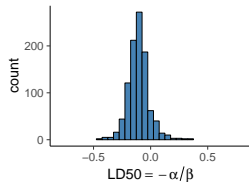
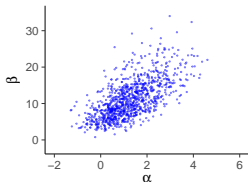
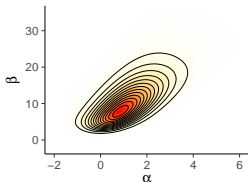


IR

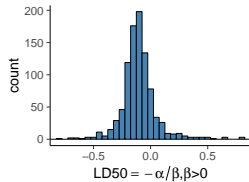
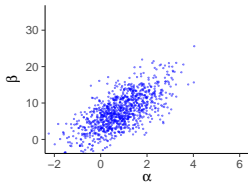
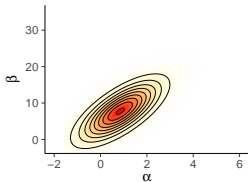


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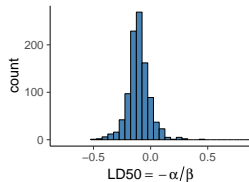
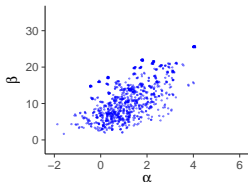
Grid



Normal



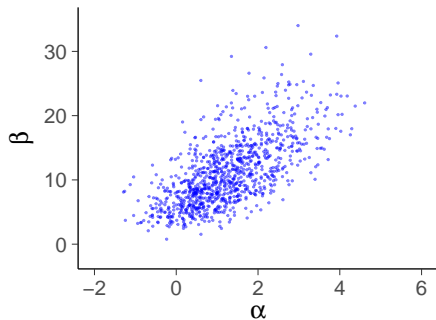
IR



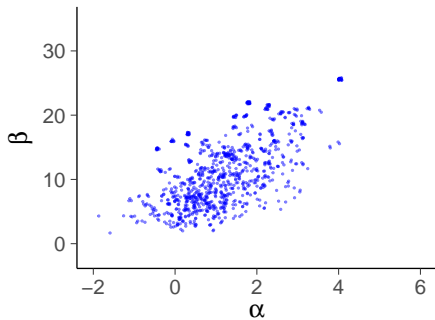
Grid  $sd(LD50) \approx 0.1$ , IR  $sd(LD50) \approx 0.1$

## Example: Importance sampling in Bioassay

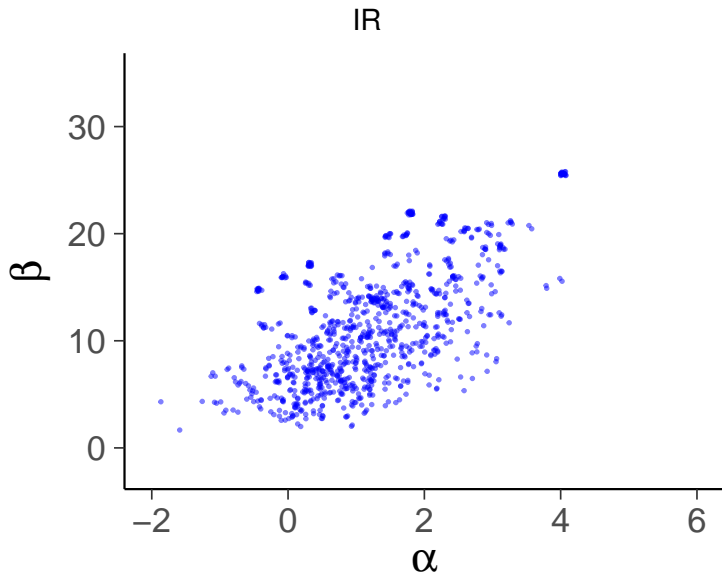
Grid



IR

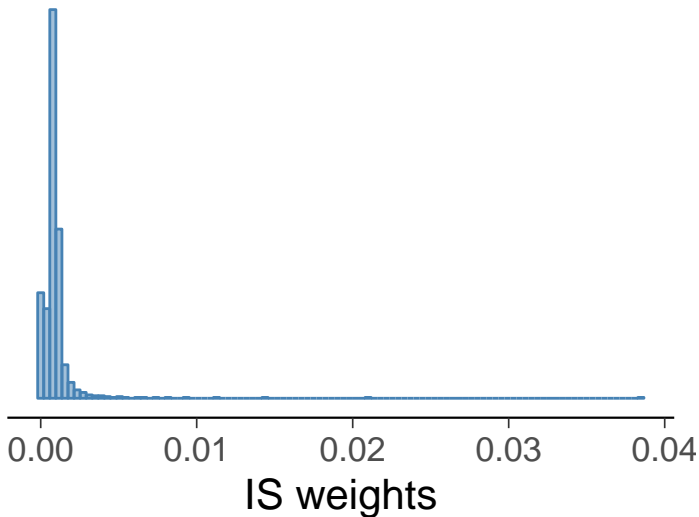


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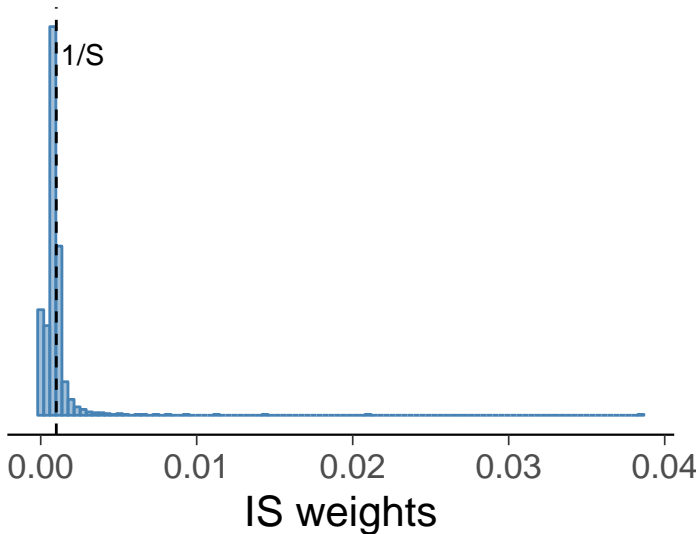




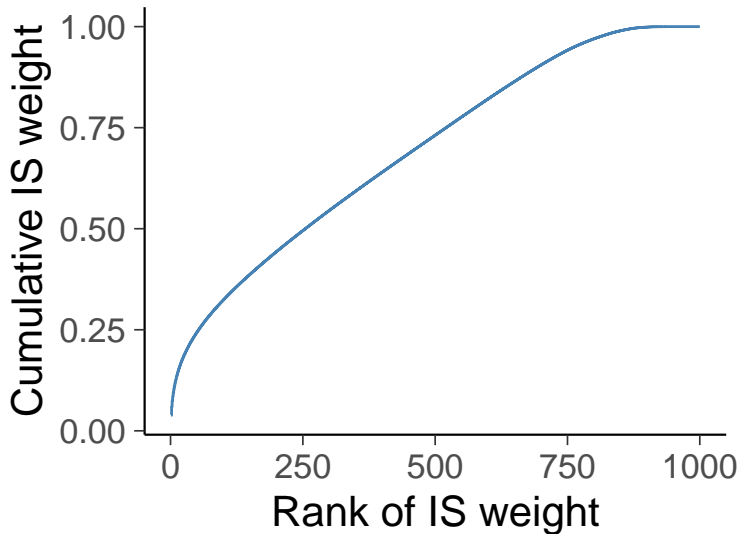
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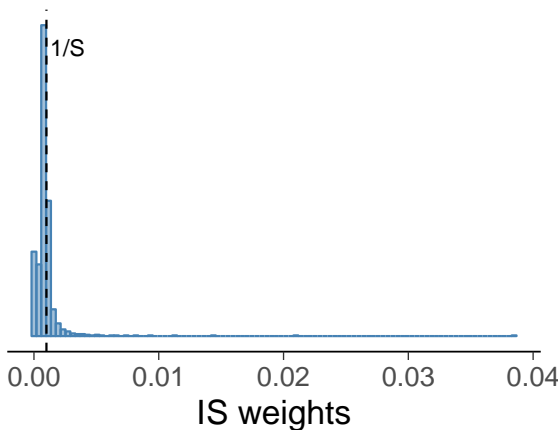
## Example: Importance sampling in Bioassay



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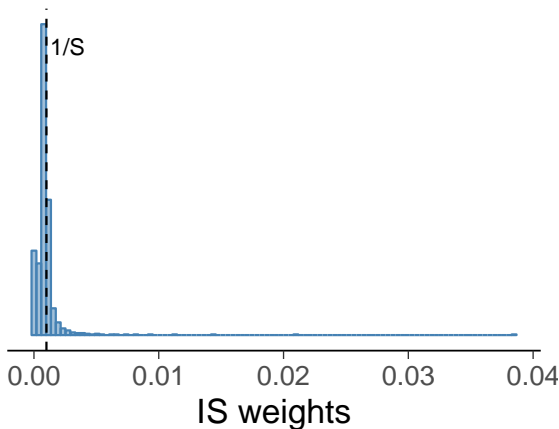


## Example: Importance sampling in Bioassay



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

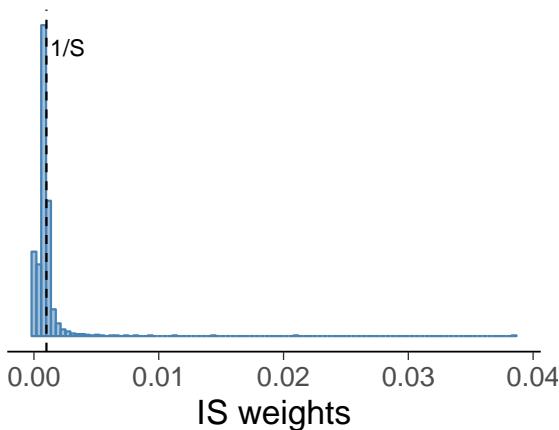
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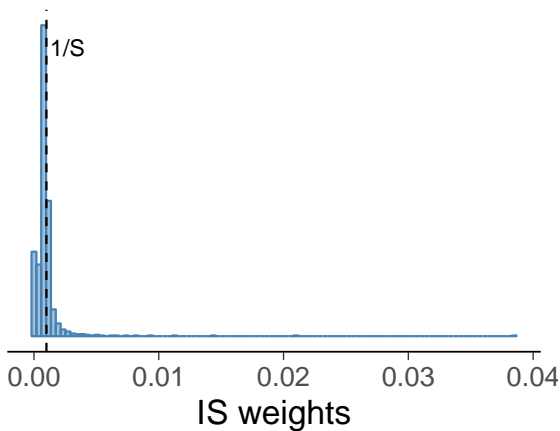
BDA3 1st (2013) and 2nd (2014) printing have an error for  $\tilde{w}(\theta^s)$ . The normalized weights equation should not have the multiplier S (the normalized weights should sum to one). Errata for the book [http://www.stat.columbia.edu/~gelman/book/errata\\_bda3.txt](http://www.stat.columbia.edu/~gelman/book/errata_bda3.txt)

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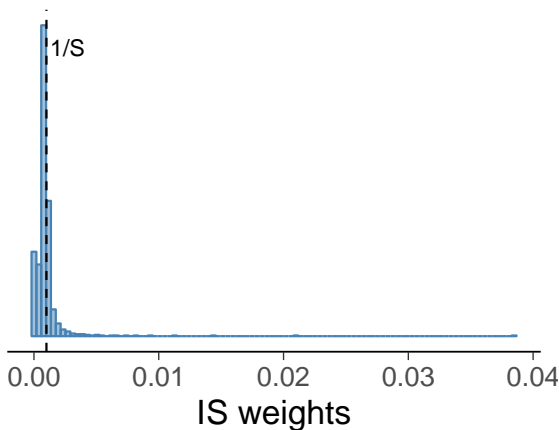
## Example: Importance sampling in Bioassay



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## Example: Importance sampling in Bioassay



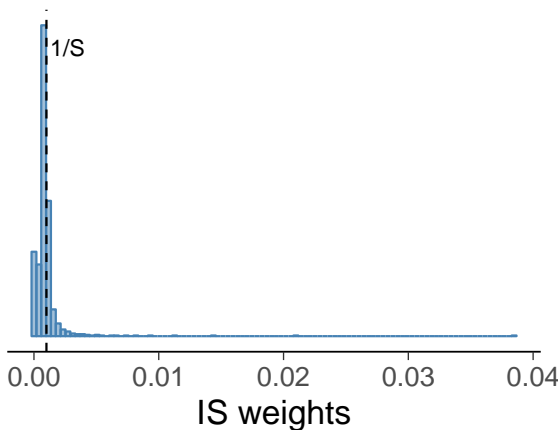
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Pareto- $k$  diagnostic preferably  $< 0.7$ :



## Example: Importance sampling in Bioassay



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Pareto- $k$  diagnostic preferably  $< 0.7$ :  $\hat{k} \approx 0.76$

# Pareto smoothed importance sampling

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- See Vehtari, Simpson, Gelman, Yuling and Gabry (2019). Pareto smoothed importance sampling. arXiv preprint arXiv:1507.02646, <https://arxiv.org/abs/1507.02646> for improved diagnostics and stability.

# 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

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

# Curse of dimensionality

- Number of grid points increases exponentially
- Concentration of the measure, i.e., where is the most of the mass?

# 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
- MCMC methods in this course
  - Gibbs: “iterative conditional sampling”
  - Metropolis: “random walk in joint distribution”
  - Dynamic Hamiltonian Monte Carlo: “state-of-the-art” used in Stan