

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:
`prod(dnorm(qr))` → 0 (underflow)

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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)
 - `sum(dnorm(qr,log=TRUE))` → -847.3

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e.g. `log(exp(800) + exp(800))` → Inf
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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We can easily evaluate $p(y|\theta)p(\theta)$ for any θ , but the integral $\int p(y|\theta)p(\theta)d\theta$ is usually difficult.

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- Grid (equal spacing) evaluation with self-normalization

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

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

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

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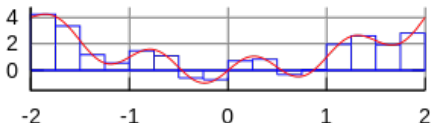
$$E_{\theta}[f(\theta)] = \int f(\theta)p(\theta|y)d\theta$$

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

Quadrature integration

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

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

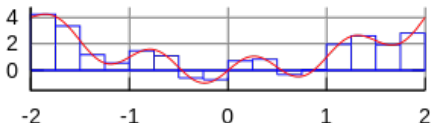


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Quadrature integration

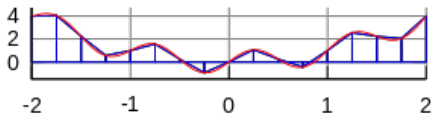
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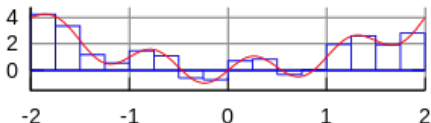
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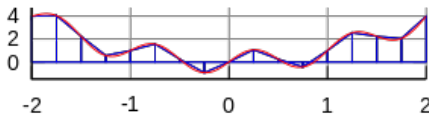
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- In 2D and higher
 - nested quadrature
 - product rules

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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 - they worked together in atomic bomb project
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- 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 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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i.e. Monte Carlo error is very small (for the expectation)

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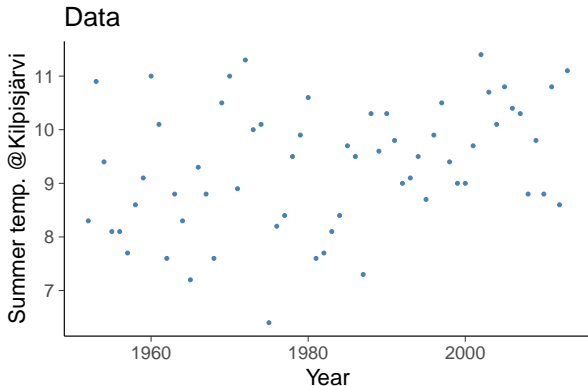
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- See Ch 4 for counter-examples for asymptotic normality

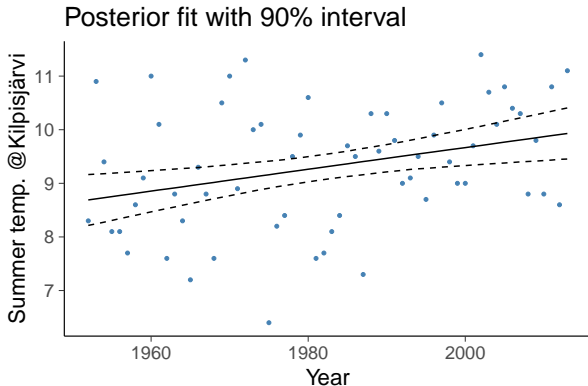
Example: Kilpisjärvi summer temperature

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



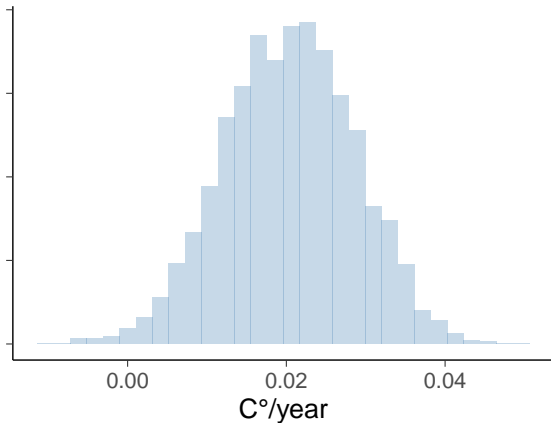
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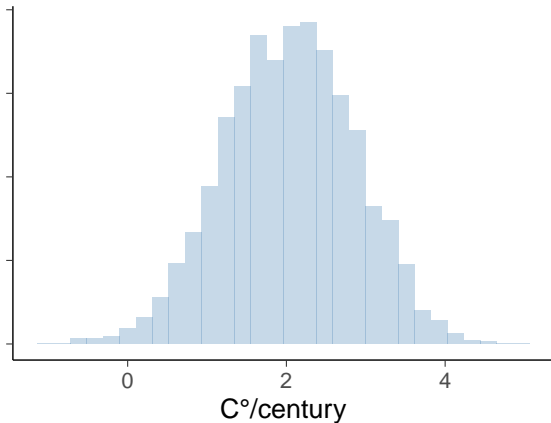
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Posterior of temperature change



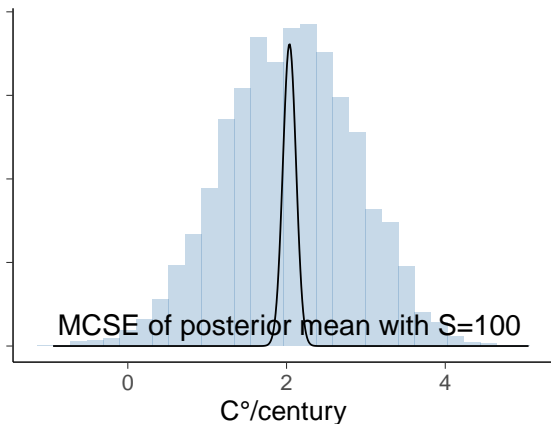
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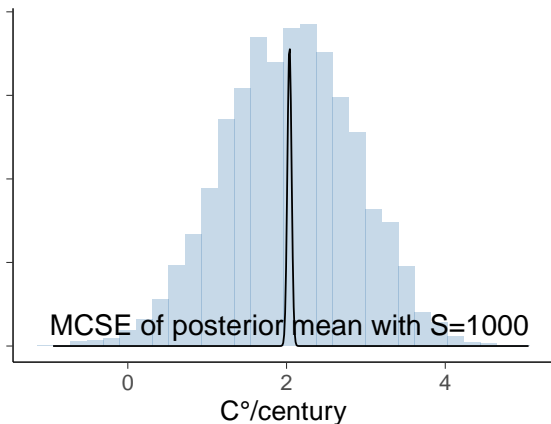


$\sigma_{\theta} \approx 0.827$, $\text{MCSE} \approx 0.0827$, total deviation ≈ 0.831

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

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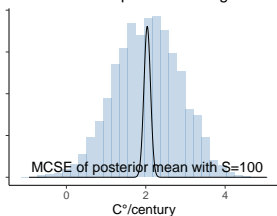


$\sigma_{\theta} \approx 0.827$, $\text{MCSE} \approx 0.0261$, total deviation ≈ 0.827

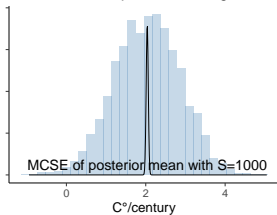
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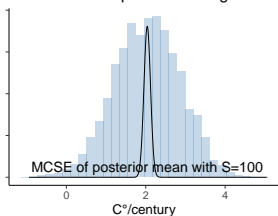


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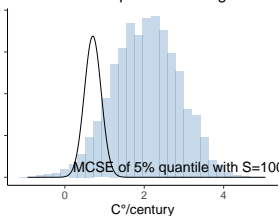


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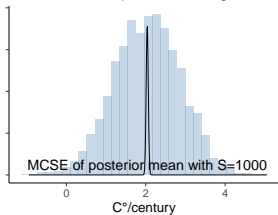
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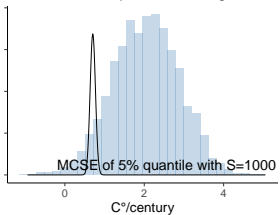
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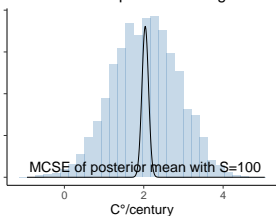


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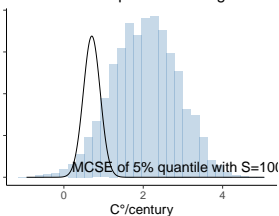


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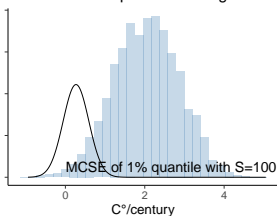
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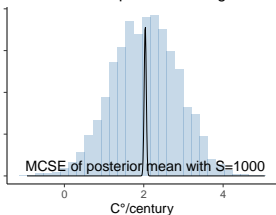
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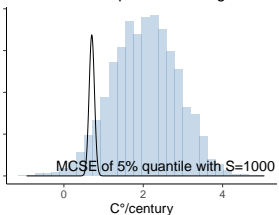
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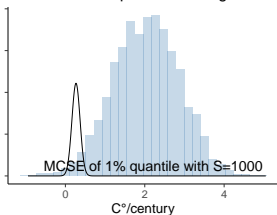
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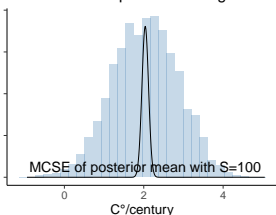


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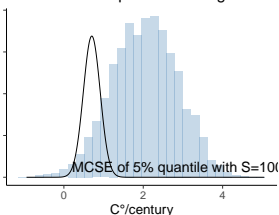


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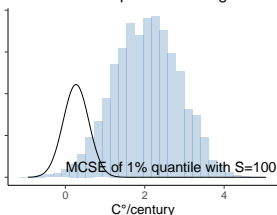
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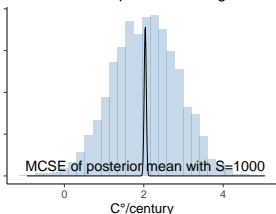
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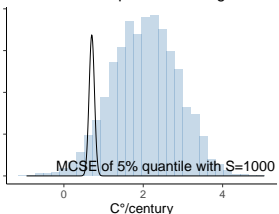
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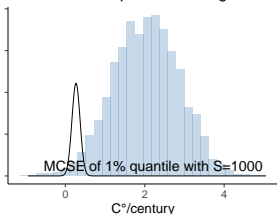
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Tail quantiles are more difficult to estimate

How many simulation draws are needed?

- Posterior probability

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

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

- $I(\cdot)$ is binomially distributed as $p(\theta \in A)$
 - $\text{var}(I(\cdot)) = p(1 - p)$ (Appendix A, p. 579)
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- $S = 2500$ draws needed for 1% unit accuracy

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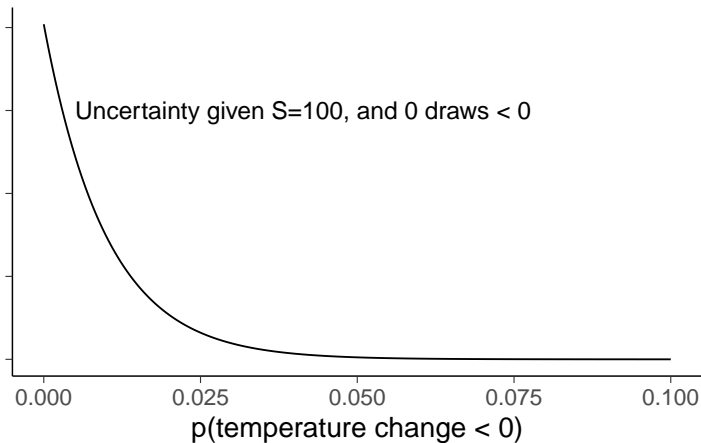
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 - standard deviation of p is $\sqrt{p(1 - p)/S}$
- if $S = 100$ and $p \approx 0.5$, $\sqrt{p(1 - p)/S} = 0.05$
i.e. accuracy is about 5% units
- $S = 2500$ draws needed for 1% unit accuracy
- To estimate small probabilities, a large number of draws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

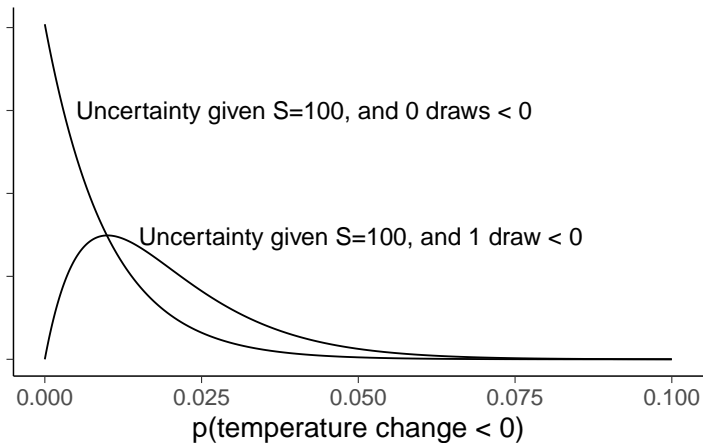
Example: Kilpisjärvi summer temperature

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



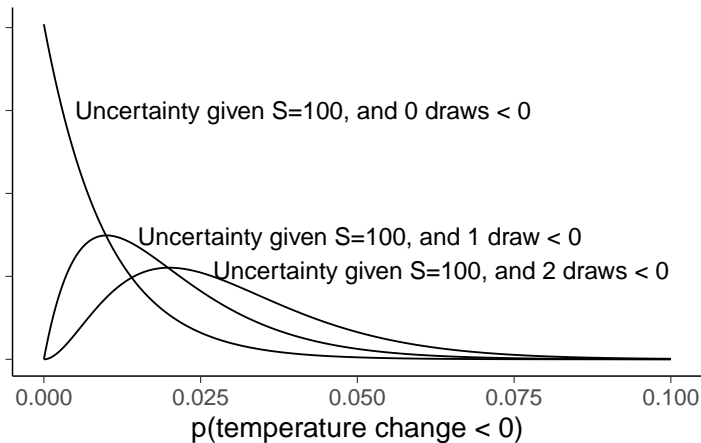
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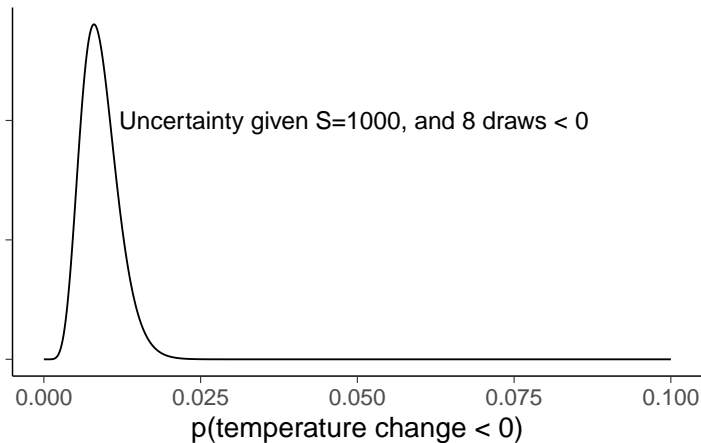
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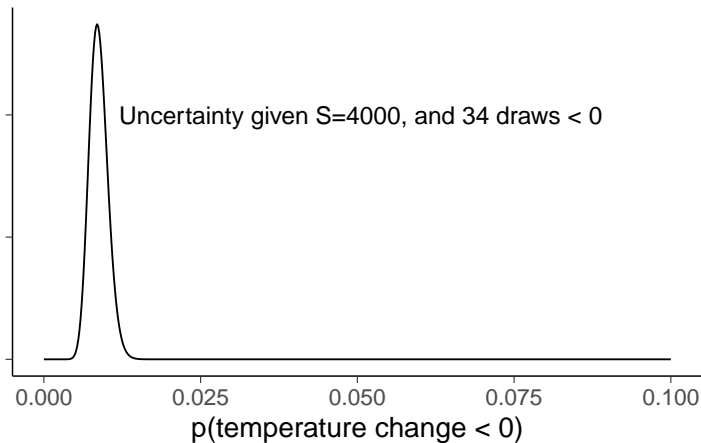
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 - With 4000 draws MCSE ≈ 0.002 . We could report that probability is very likely larger than 0.99, or sample more to justify reporting three digits
 - For probabilities close to 0 or 1, consider also when the model assumption justify certain accuracy

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

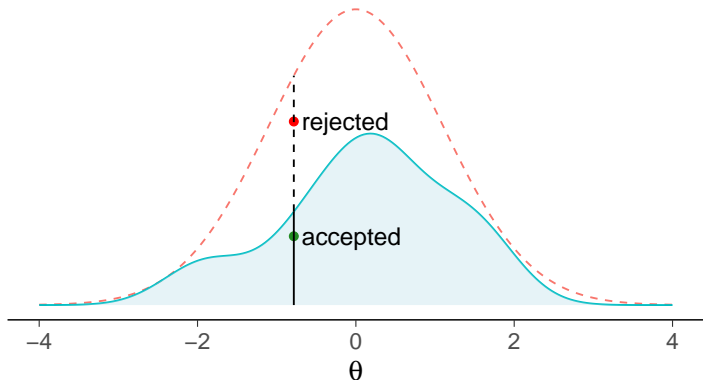
- 10 parameters
- if we don't know beforehand where the posterior mass is
 - need to choose wide box for the grid
 - need to have enough grid points to get some of them where essential mass is
- e.g. 50 or 1000 grid points per dimension
 - $50^{10} \approx 1\text{e}17$ grid points
 - $1000^{10} \approx 1\text{e}30$ 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

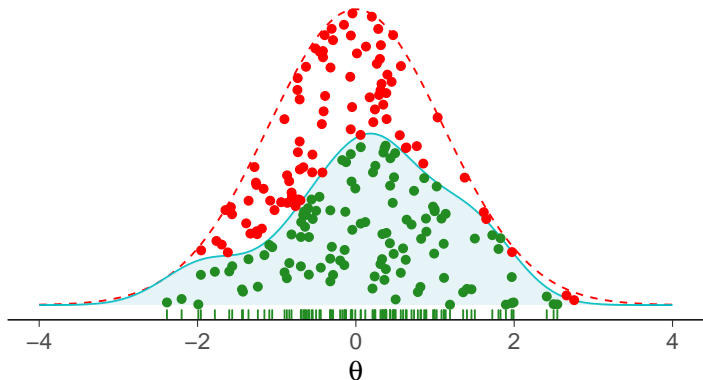
- Proposal forms envelope over the target distribution
 $q(\theta|y)/Mg(\theta) \leq 1$
- Draw from the proposal and accept with probability
 $q(\theta|y)/Mg(\theta)$



-- $Mg(\theta)$ — $q(\theta|y)$

Rejection sampling

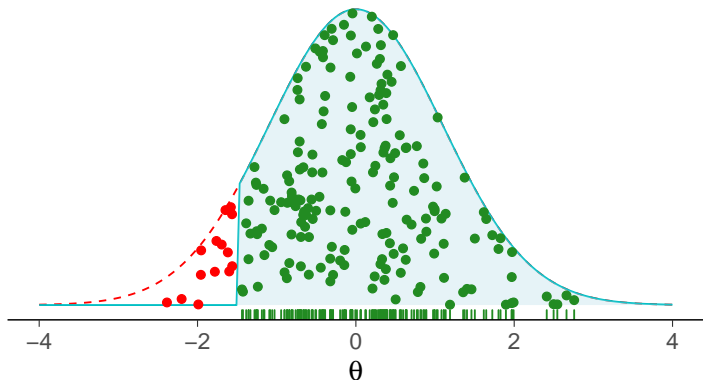
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● Accepted ● Rejected - - Mg(theta) — q(theta|y)

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)

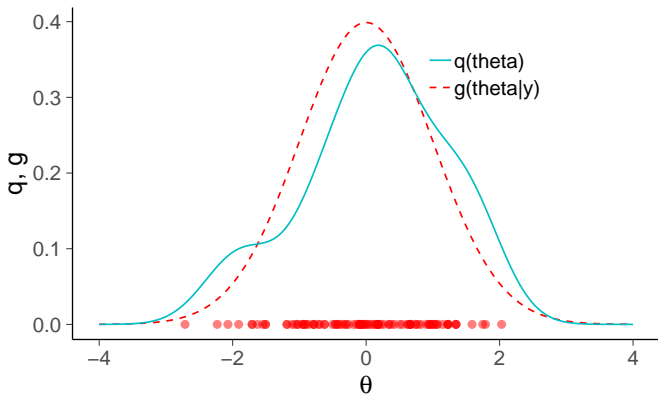
Rejection sampling

- 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

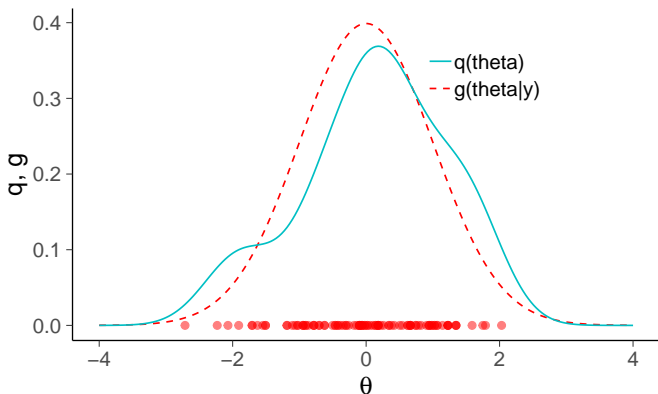
Target, proposal, and draws



Importance sampling

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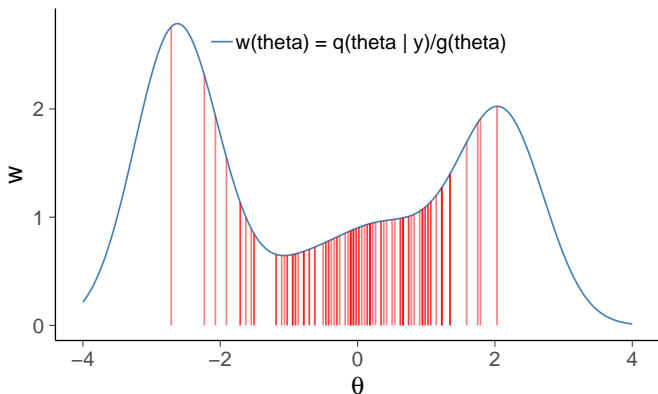


$$E[f(\theta)] \approx \frac{\sum_s w_s f(\theta^{(s)})}{\sum_s w_s}, \quad \text{where} \quad w_s = \frac{q(\theta^{(s)})}{g(\theta^{(s)})}$$

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

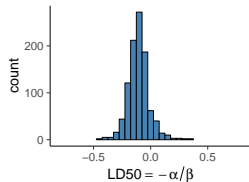
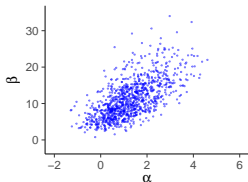
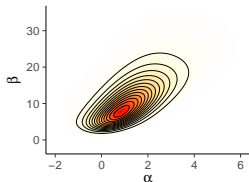
- Resampling using normalized importance weights can be used to pick a smaller number of draws with uniform weights
- Selection of good proposal gets more difficult when the number of dimensions increase
- Often used to correct distributional approximations

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.

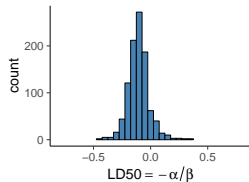
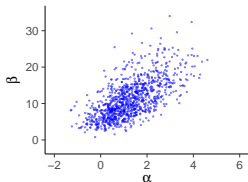
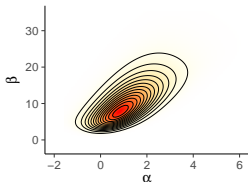
Example: Importance sampling in Bioassay

Grid

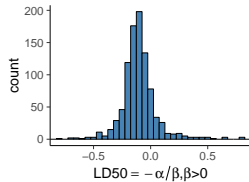
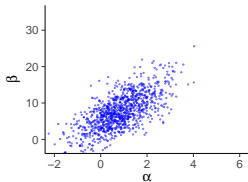
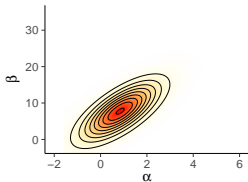


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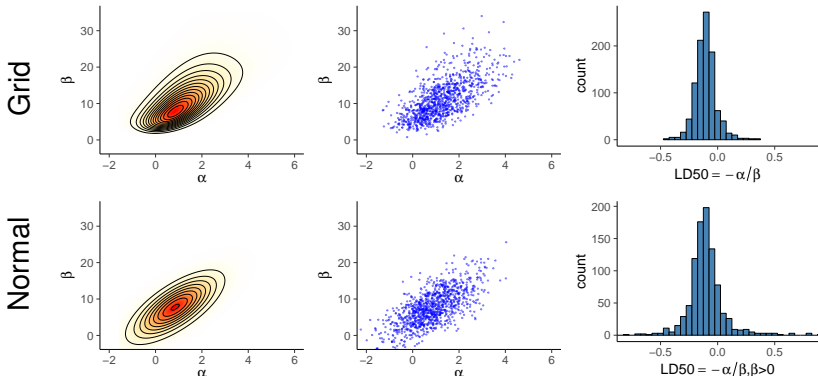


Normal



Normal approximation is discussed more in BDA3 Ch 4

Example: Importance sampling in Bioassay



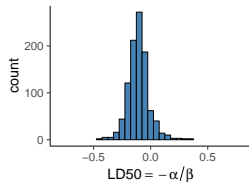
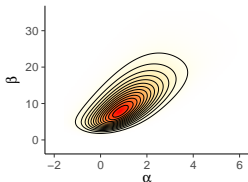
Normal approximation is discussed more in BDA3 Ch 4

But the normal approximation is not that good here:

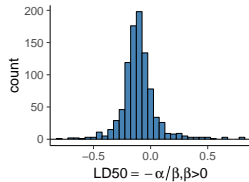
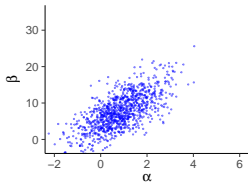
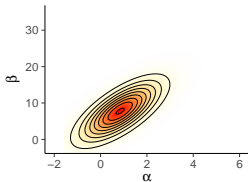
Grid $\text{sd}(\text{LD50}) \approx 0.1$, Normal $\text{sd}(\text{LD50}) \approx .75$!

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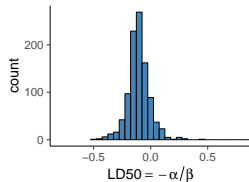
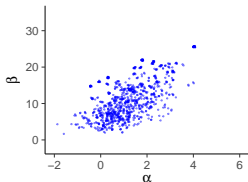
Grid



Normal

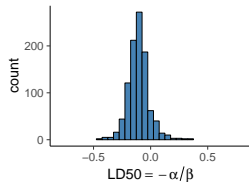
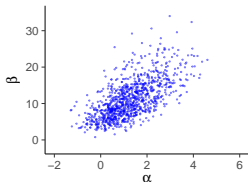
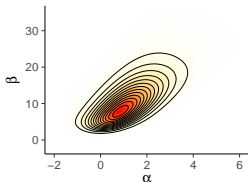


IR

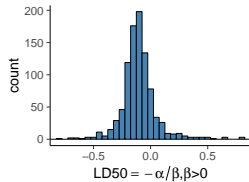
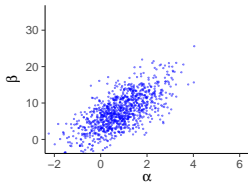
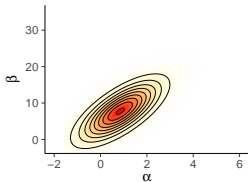


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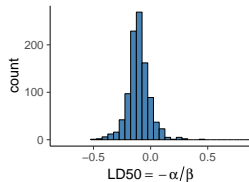
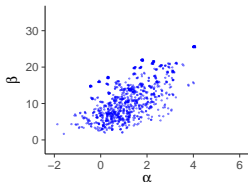
Grid



Normal



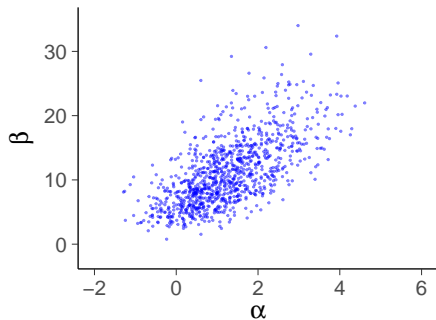
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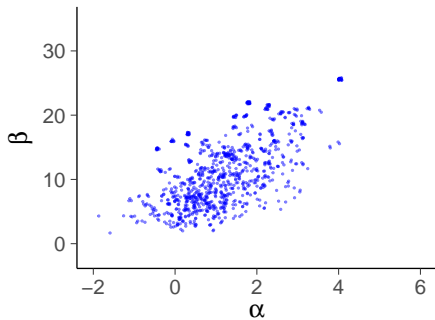
Grid $sd(LD50) \approx 0.1$, IR $sd(LD50) \approx 0.1$

Example: Importance sampling in Bioassay

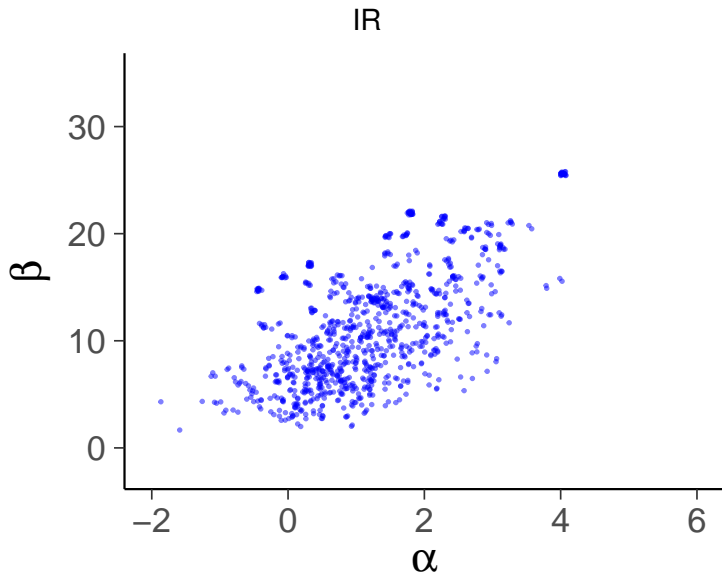
Grid



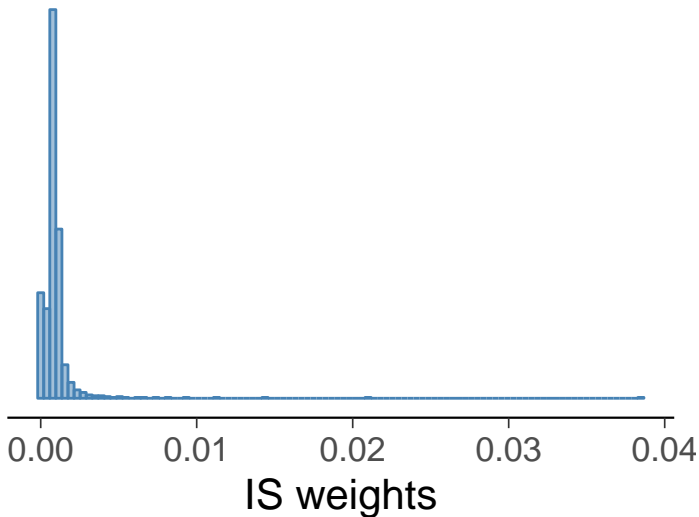
IR



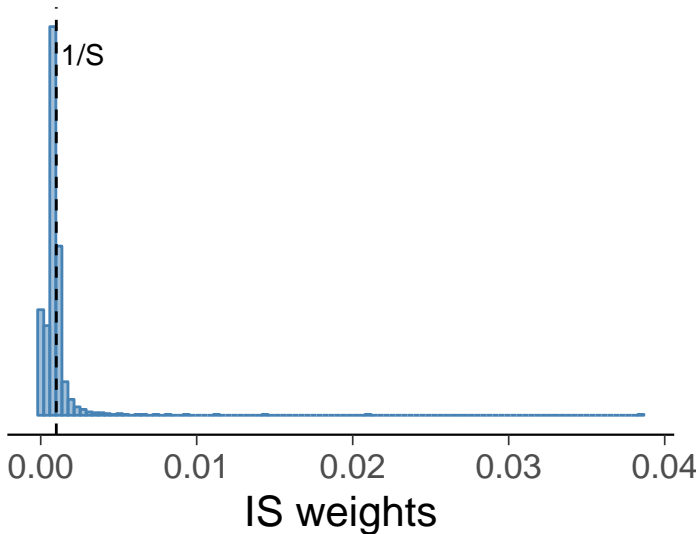
Example: Importance sampling in Bioassay



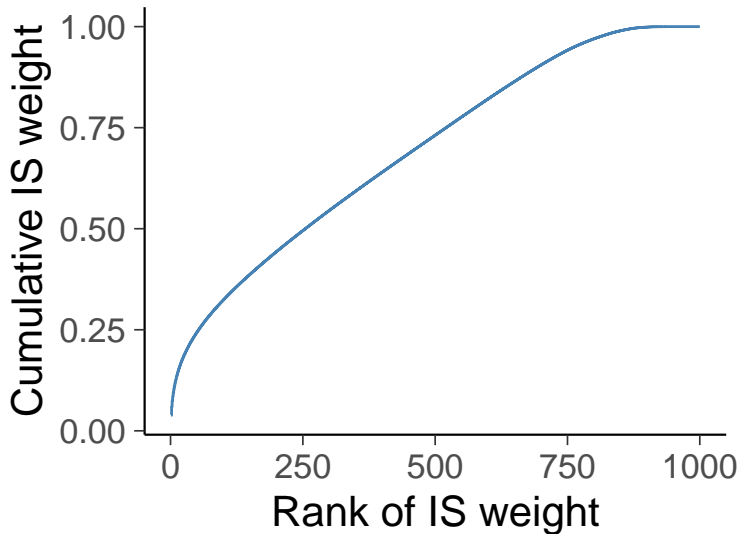
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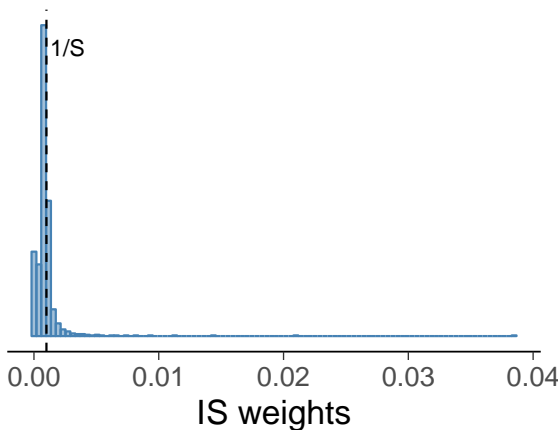
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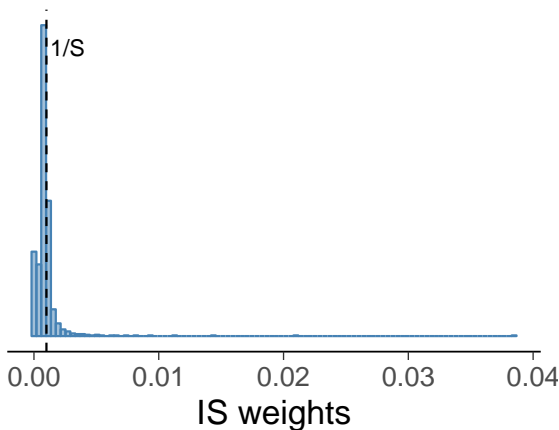


Example: Importance sampling in Bioassay



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

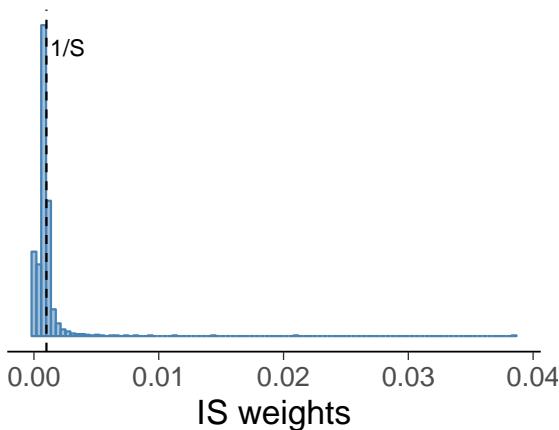
Example: Importance sampling in Bioassay



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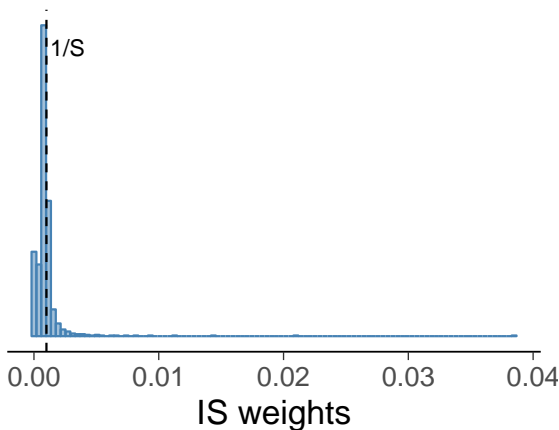
BDA3 1st (2013) and 2nd (2014) printing have an error for $\tilde{w}(\theta^s)$. The normalized weights equation should not have the multiplier S (the normalized weights should sum to one). Errata for the book http://www.stat.columbia.edu/~gelman/book/errata_bda3.txt

Example: Importance sampling in Bioassay



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

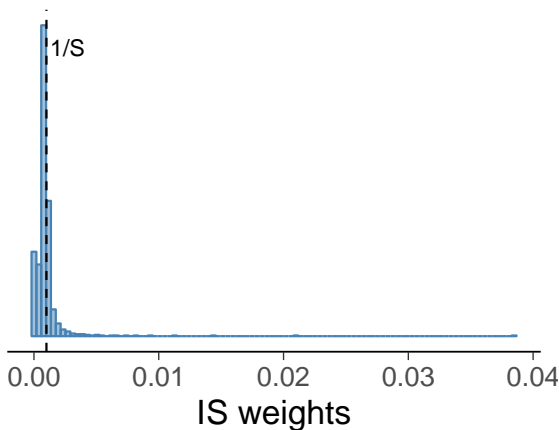
Example: Importance sampling in Bioassay



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Example: Importance sampling in Bioassay

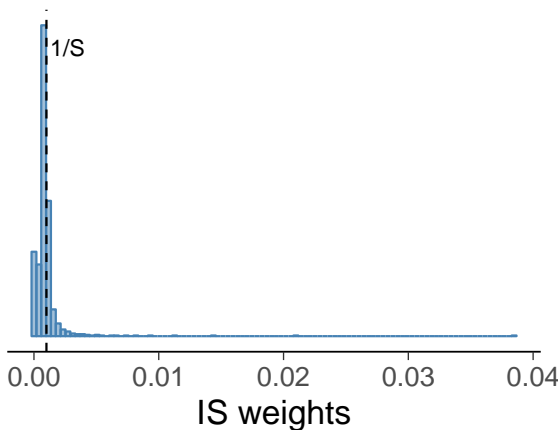


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Pareto- k diagnostic preferably < 0.7 :

Example: Importance sampling in Bioassay



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

Pareto- k diagnostic preferably < 0.7 : $\hat{k} \approx 0.57$

Pareto smoothed importance sampling

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

Pareto smoothed importance sampling

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

Pareto smoothed importance sampling

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- Finite variance and central limit theorem for $k < 1/2$
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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