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

Bayesian Statistics and Data Analysis

Lecture 4

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Thanks to Aki Vehtari, Aalto University



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



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



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 - calculate joint density given normal:
`prod(dnorm(qr))` → 0 (underflow)
 - see log densities in the next slide
 - closest value to 1 is $\approx 1 \pm 2.2 \cdot 10^{-16}$
 - Laplace and ratio of girl and boy babies
 - `pbeta(0.5, 241945, 251527)` → 1 (rounding)



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 - closest value to 1 is $\approx 1 \pm 2.2 \cdot 10^{-16}$
 - Laplace and ratio of girl and boy babies
 - `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



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



Numerical accuracy – log scale

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 - how many observations we can now handle?



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 - e.g. for $a > b$, compute
$$\log(\exp(a) + \exp(b)) = a + \log(1 + \exp(b - a))$$



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e.g. `log(exp(800) + exp(800))` $\rightarrow \text{Inf}$



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$$\log(\exp(a) + \exp(b)) = a + \log(1 + \exp(b - a))$$
 - e.g. $\log(\exp(800) + \exp(800)) \rightarrow \text{Inf}$
but $800 + \log(1 + \exp(800 - 800)) \approx 800.69$



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$$\log(\exp(a) + \exp(b)) = a + \log(1 + \exp(b - a))$$
e.g. $\log(\exp(800) + \exp(800)) \rightarrow \text{Inf}$ 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

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

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

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

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



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

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- 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)

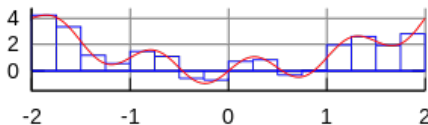


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Quadrature integration

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

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



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

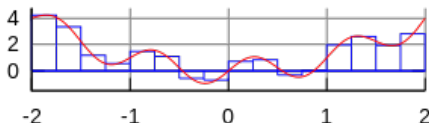


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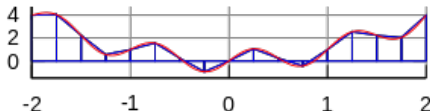
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- In 1D further variations with smaller error, e.g. trapezoid



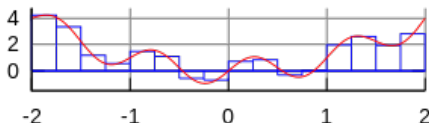


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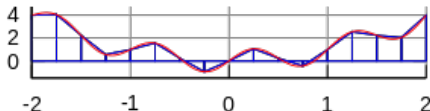
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- In 2D and higher
 - nested quadrature, product rules
 - but theres a curse of dimensionality...



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Monte Carlo - history

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



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



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



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- 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.



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Monte Carlo vs. deterministic

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- 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?

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- 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*



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How many simulation draws are needed?

- Expectation of unknown quantity

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

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

- this variance is independent on dimensionality of θ



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

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



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



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

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



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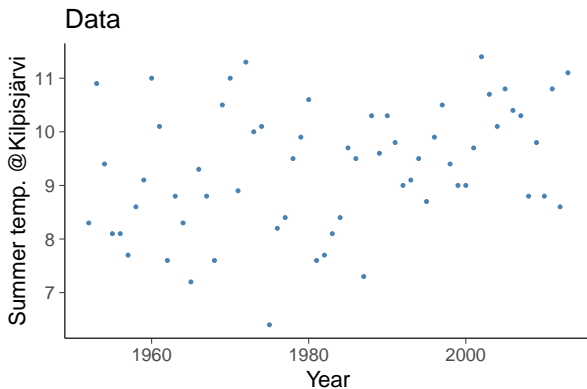
- e.g. if $S = 100$, deviation increases by $\sqrt{1 + 1/S} = 1.005$ i.e. Monte Carlo error is very small (for the expectation)
- See Ch 4 for counter-examples for asymptotic normality



Example: Kilpisjärvi summer temperature

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

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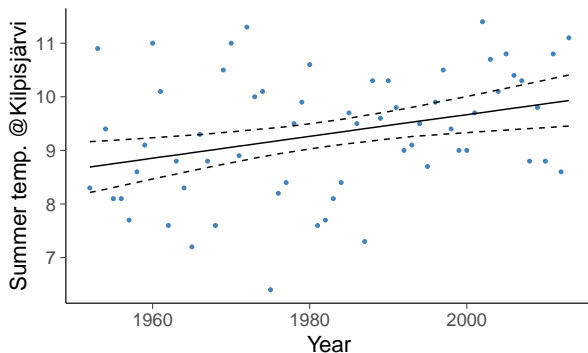




Example: Kilpisjärvi summer temperature

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

Posterior fit with 90% interval

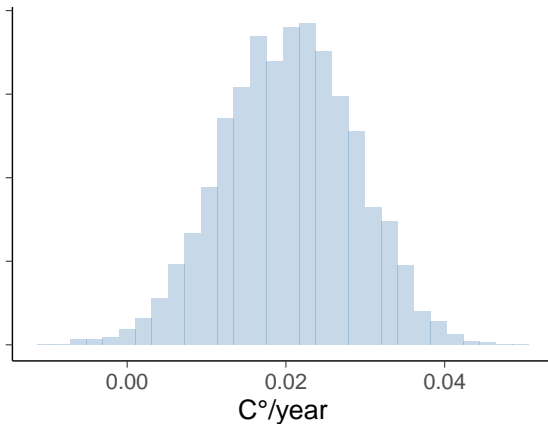




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Posterior of temperature change

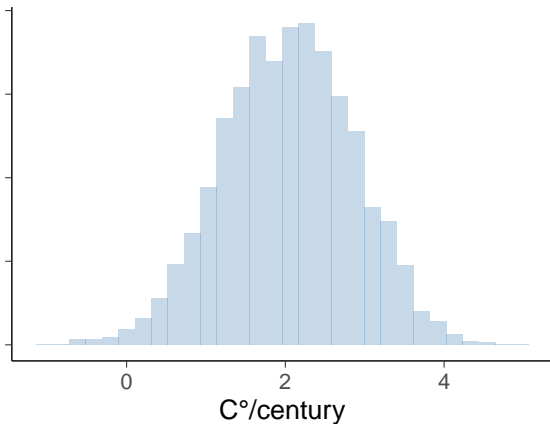




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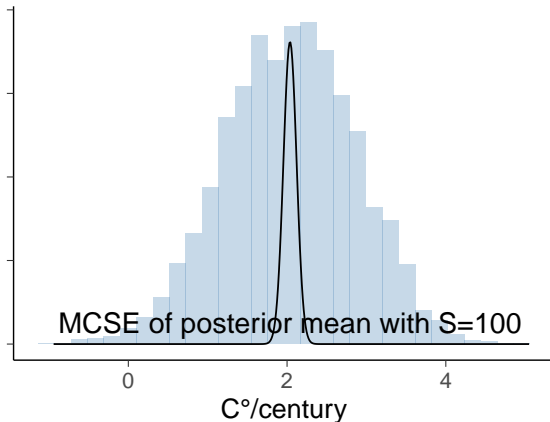




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Example: Kilpisjärvi summer temperature

Posterior of temperature change



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

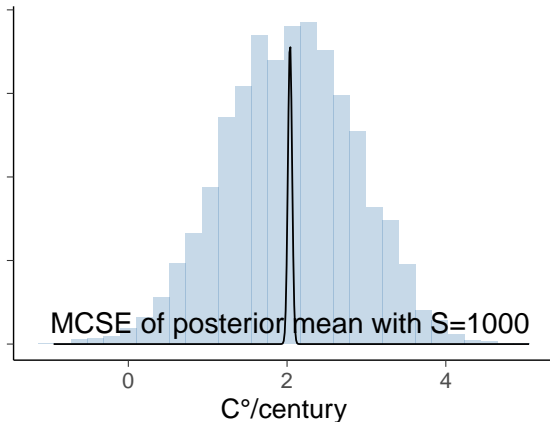
$$\text{total deviation}^2 = \sigma_\theta^2 + \text{MCSE}^2$$



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Example: Kilpisjärvi summer temperature

Posterior of temperature change



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

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

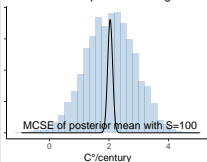


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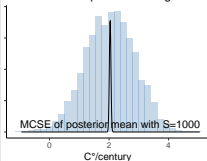
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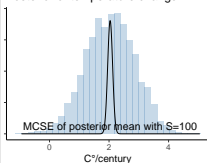




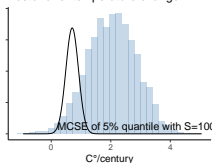
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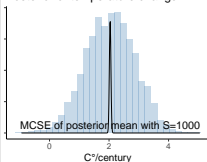
Posterior of temperature change



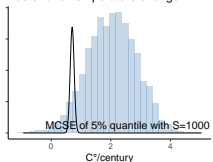
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Posterior of temperature change



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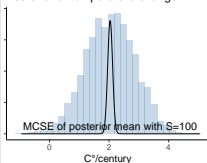




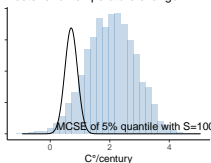
Example: Kilpisjärvi summer temperature

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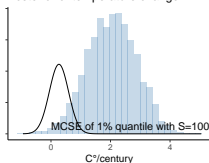
Posterior of temperature change



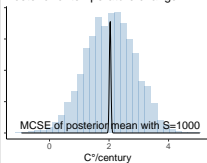
Posterior of temperature change



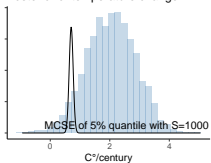
Posterior of temperature change



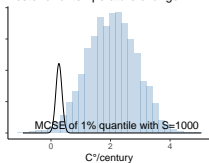
Posterior of temperature change



Posterior of temperature change



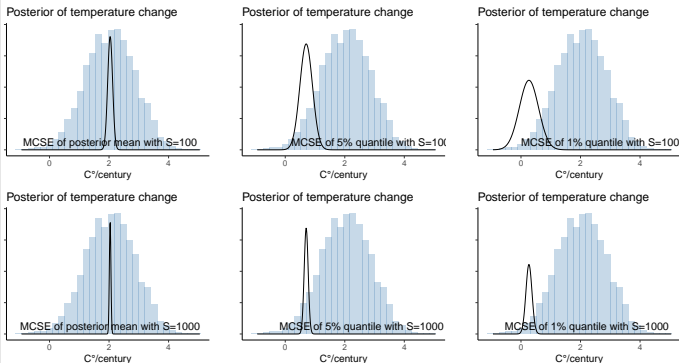
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Example: Kilpisjärvi summer temperature



Tail quantiles are more difficult to estimate



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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 $\theta^{(s)} \in A$



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



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



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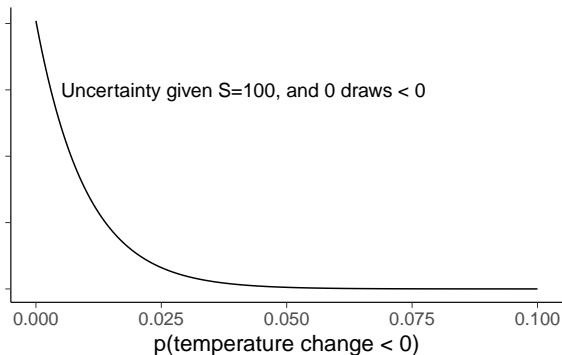
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i.e. accuracy is about 5% units
- $S = 2500$ draws needed for 1% unit accuracy
- To estimate small probabilities, a large number of draws is needed
 - to be able to estimate p , need to get draws with $\theta^{(l)} \in A$,
which in expectation requires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



Example: Kilpisjärvi summer temperature

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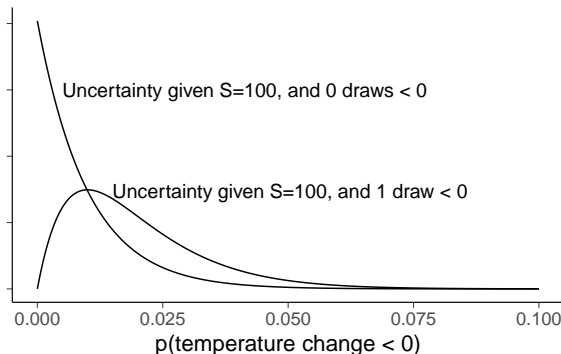
Posterior uncertainty $p(\text{temperature change} < 0)$





Example: Kilpisjärvi summer temperature

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

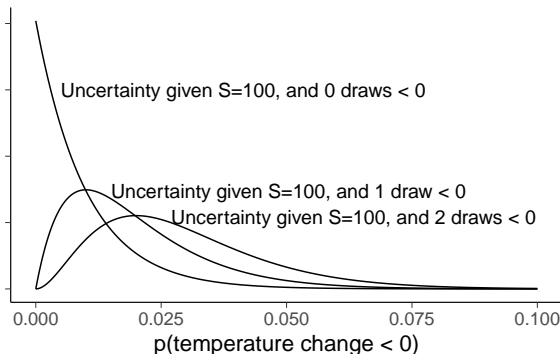


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Example: Kilpisjärvi summer temperature

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



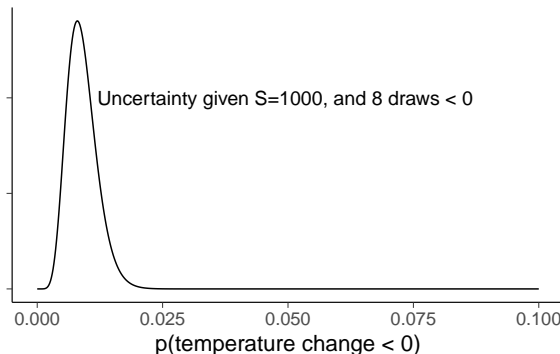
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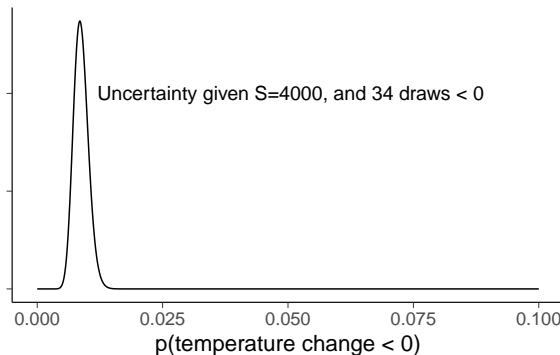




Example: Kilpisjärvi summer temperature

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





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How many digits to show in reports?

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

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How many digits to show in reports?

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- Don't show digits which are just random noise
 - check what is the Monte Carlo standard error

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 - 2.050774 and [0.7472868 3.3017524] (NO!)



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 - 0.9960000 (NO!)



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



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 - 0.9960000 (NO!)
 - 1.00 (depends on the context)
 - 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
- For your project: Think for each reported value how many digits is sensible.



How many simulation draws are needed?

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



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How many simulation draws are needed?

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



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- Produces independent draws
 - Using analytic transformations of uniform random numbers (e.g. appendix A)
 - factorization
 - numerical inverse-CDF
- Problem: restricted to limited set of models



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- 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



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- Box-Muller -method:

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

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

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

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



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Direct simulation: Example

- Box-Muller -method:

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

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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

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



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Indirect sampling

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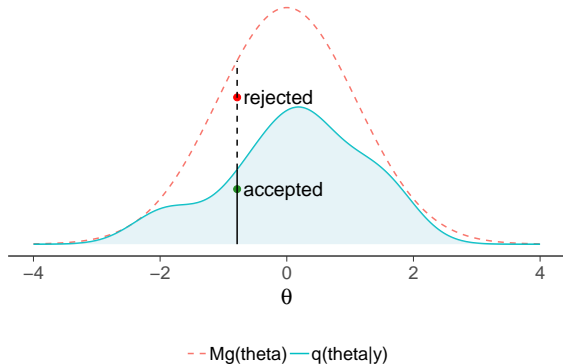
- Rejection sampling
- Importance sampling
- Markov chain Monte Carlo (next week)



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Rejection sampling

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

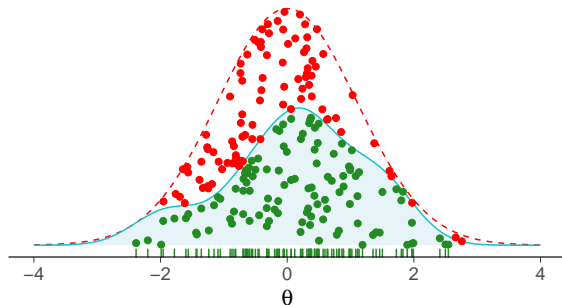




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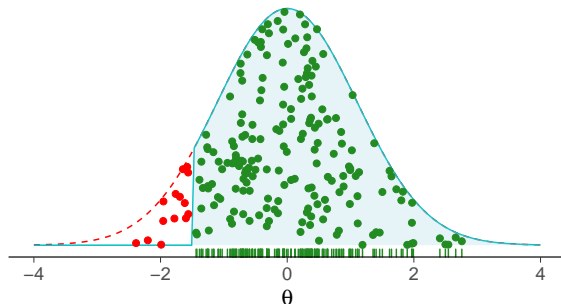
• Accepted • Rejected - - Mg(theta) — q(theta|y)



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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)



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- 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

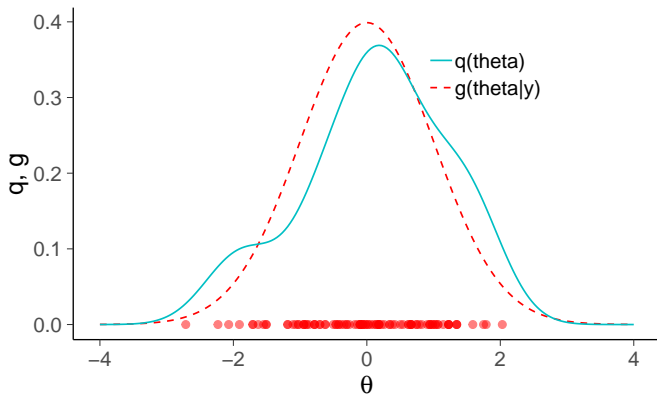


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Importance sampling

- Proposal does not need to have a higher value everywhere

Target, proposal, and draws



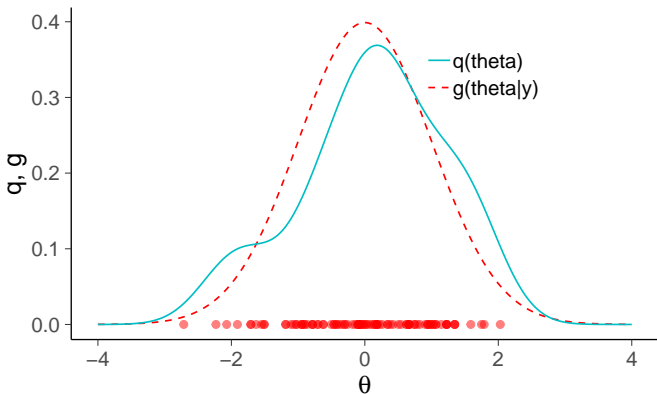


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Importance sampling

- Proposal does not need to have a higher value everywhere

Target, proposal, and draws



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

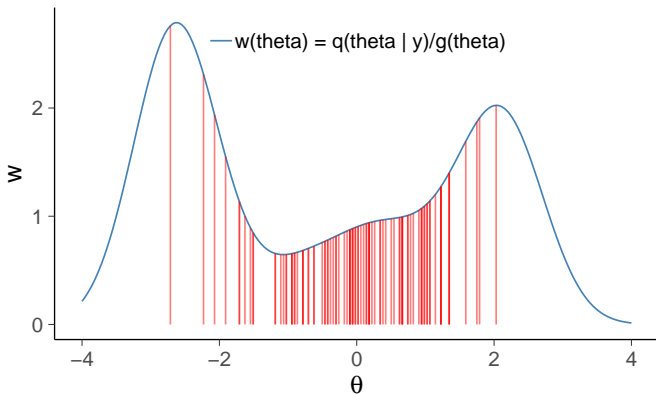


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Importance sampling

- Proposal does not need to have a higher value everywhere

Draws and importance weights



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



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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



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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



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



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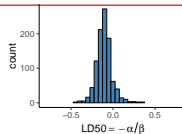
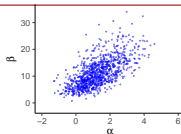
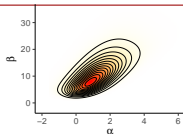
- Variation of the weights affect the **effective sample size**
 - if single weight dominates, we have effectively one sample
 - if weights are equal, we have effectively S draws
- Central limit theorem holds only if variance of the weight distribution is finite



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Example: Importance sampling in Bioassay

Grid



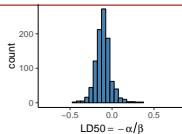
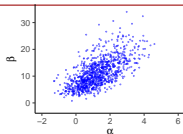
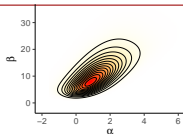
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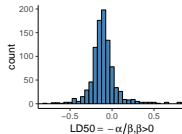
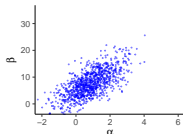
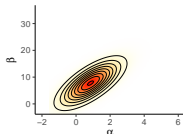
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Example: Importance sampling in Bioassay

Grid



Normal

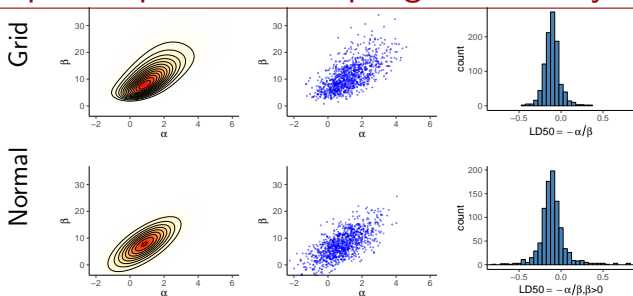


Normal approximation is discussed more in BDA3 Ch 4



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Example: Importance sampling in Bioassay



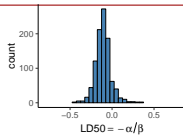
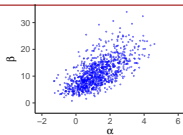
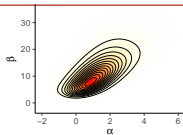
Normal approximation is discussed more in BDA3 Ch 4
But the normal approximation is not that good here:
Grid $\text{sd}(\text{LD50}) \approx 0.1$, Normal $\text{sd}(\text{LD50}) \approx .75!$



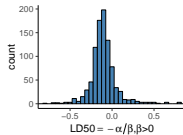
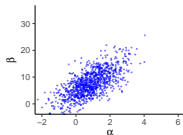
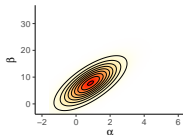
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Example: Importance sampling in Bioassay

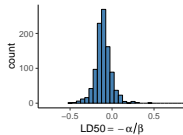
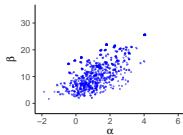
Grid



Normal



IR

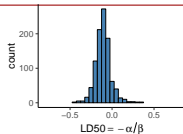
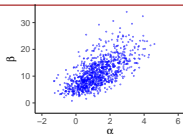
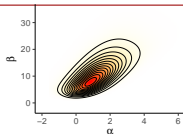




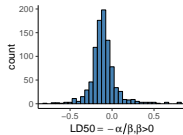
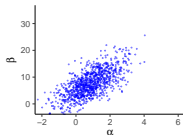
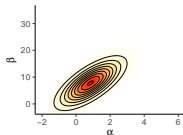
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Example: Importance sampling in Bioassay

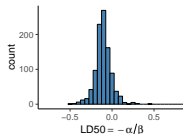
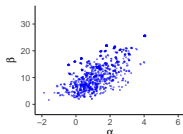
Grid



Normal



IR



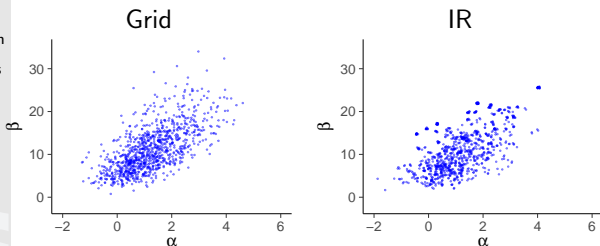
Grid $sd(LD50) \approx 0.1$, IR $sd(LD50) \approx 0.1$



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Example: Importance sampling in Bioassay

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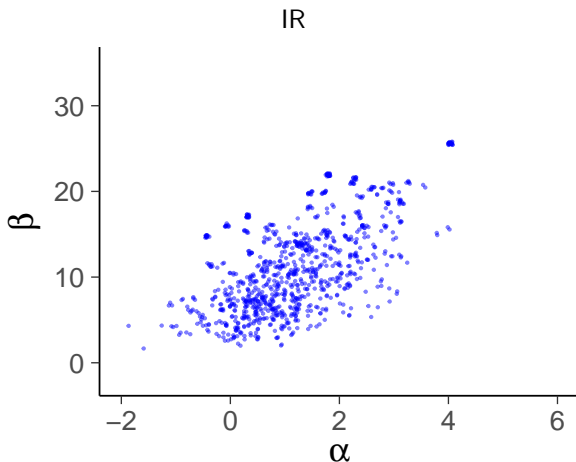




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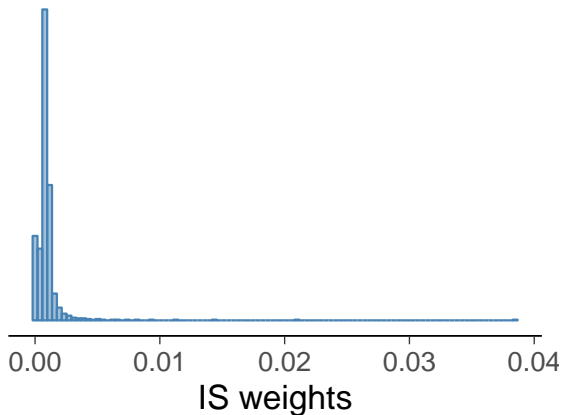




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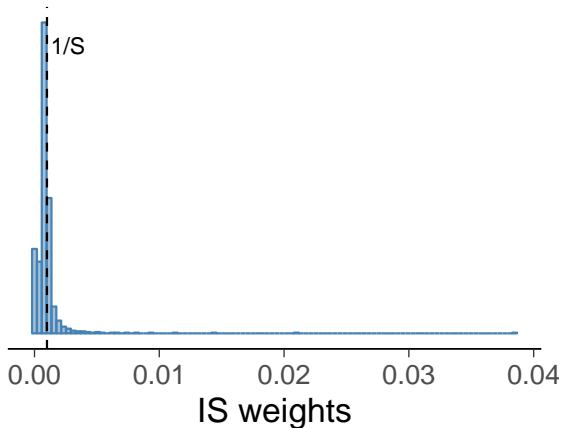




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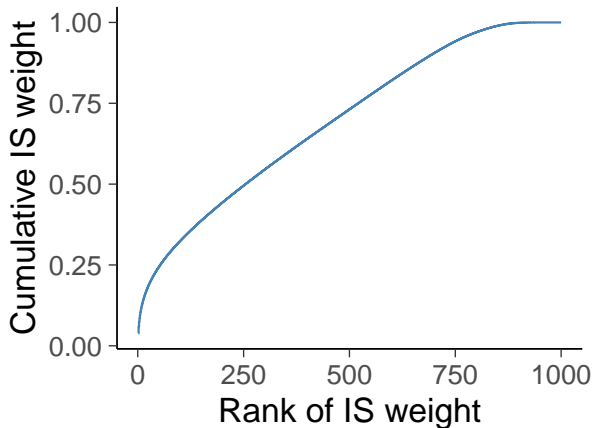




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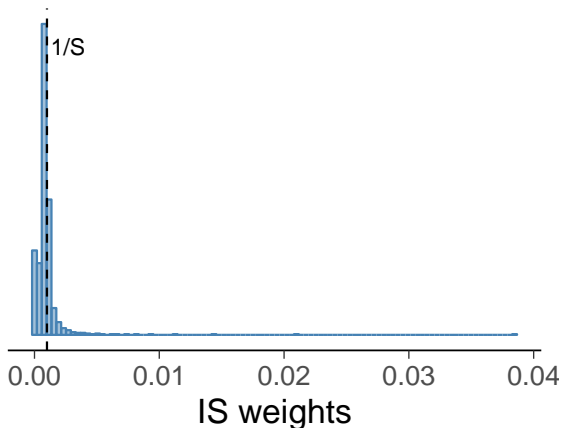
Example: Importance sampling in Bioassay





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Example: Importance sampling in Bioassay

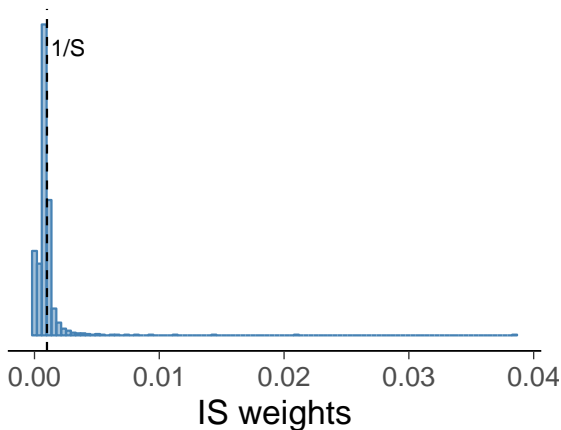


$$S_{\text{eff}} = \frac{1}{\sum_{s=1}^S (\tilde{w}(\theta^s))^2}, \quad \text{where } \tilde{w}(\theta^s) = w(\theta^s) / \sum_{s'=1}^S w(\theta^{s'})$$



- Introduction
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Example: Importance sampling in Bioassay



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

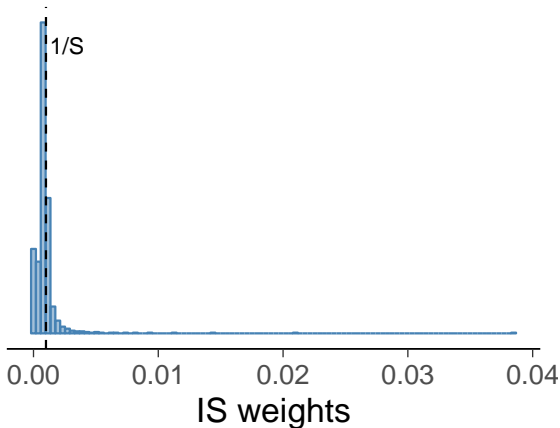
BDA3 1st (2013) and 2nd (2014) printing have an error for $\tilde{w}(\theta^s)$. The normalized weights equation should not have the multiplier S (the normalized weights should sum to one). Errata for the book

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



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Example: Importance sampling in Bioassay



$$S_{\text{eff}} = \frac{1}{\sum_{s=1}^S (\tilde{w}(\theta^s))^2}, \quad \text{where } \tilde{w}(\theta^s) = w(\theta^s) / \sum_{s'=1}^S w(\theta^{s'})$$
$$S_{\text{eff}} \approx 270$$



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Pareto smoothed importance sampling

- Introduction
- Bayesian Computation
- Monte Carlo Methods
 - Direct simulation
 - Rejection sampling
 - Importance sampling
 - Pareto-Smoothed Importance Sampling
- Pareto- k diagnostic estimate the number of existing moments ($\lfloor 1/k \rfloor$)



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Pareto smoothed importance sampling

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



- Introduction
- Bayesian Computation
- Monte Carlo Methods
 - Direct simulation
 - Rejection sampling
 - Importance sampling
 - Pareto-Smoothed Importance Sampling
- Pareto- k diagnostic estimate the number of existing moments ($\lfloor 1/k \rfloor$)
- Finite variance and central limit theorem for $k < 1/2$
- 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

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

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

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



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Curse of dimensionality

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

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



Next week: Markov chain Monte Carlo (MCMC)

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



Next week: Markov chain Monte Carlo (MCMC)

- Introduction
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- 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 sampling: “iterative conditional sampling”
 - Metropolis: “random walk in joint distribution”
 - Dynamic Hamiltonian Monte Carlo: “state-of-the-art” used in Stan