

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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but `800 + log(1 + exp(800 - 800))` ≈ 800.69
 - e.g. in Metropolis-algorithm (Assignment 5) compute the log of ratio of densities using the identity
$$\log(a/b) = \log(a) - \log(b)$$

It's all about expectations

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

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

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

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- Monte Carlo methods which can sample from $p(\theta^{(s)}|y)$ using only $q(\theta^{(s)}|y)$ (each draw has weight $1/S$)

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

It's all about expectations

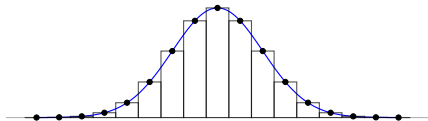
$$E_{\theta}[h(\theta)] = \int h(\theta)p(\theta|y)d\theta$$

- 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

$$E[\theta] \approx \sum_{t=1}^T \theta^{(t)} w^{(t)},$$

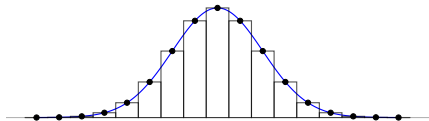


where $w^{(t)}$ is the normalized probability of a grid cell t , and $\alpha^{(t)}$ and $\beta^{(t)}$ are center locations of grid cells

Quadrature integration

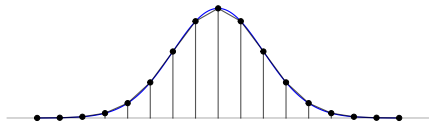
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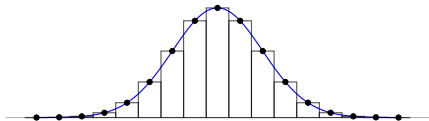
- In 1D further variations with better accuracy, e.g. trapezoid



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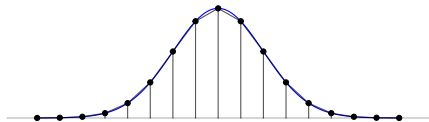
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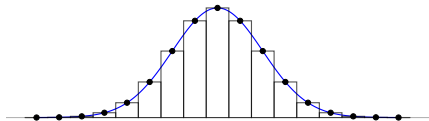


- Adaptive quadrature methods add evaluation points where needed, e.g., R function `integrate()`

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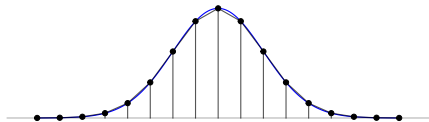
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- Adaptive quadrature methods add evaluation points where needed, e.g., R function `integrate()`
- In 2D and higher
 - nested quadrature
 - product rules

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
 - Metropolis and Ulam, "The Monte Carlo Method", 1949

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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 BDA3 Ch 4) with variance σ_{θ}^2 / S (asymptotic normality)

- this variance is independent on dimensionality of θ

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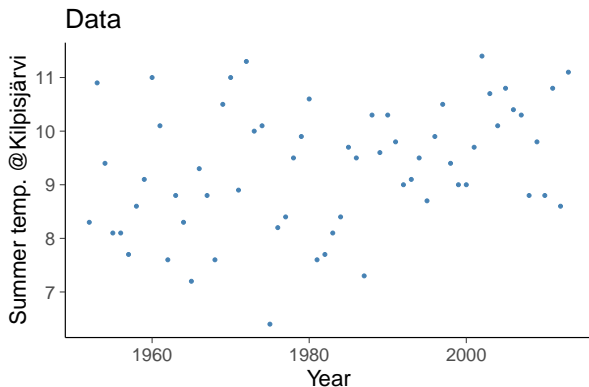
if S is big and $\theta^{(s)}$ are independent, way may assume that the distribution of the expectation approaches normal distribution (see BDA3 Ch 4) with variance σ_θ^2/S (asymptotic normality)

- this variance is independent on dimensionality of θ
- See BDA3 Ch 4 for counter-examples for asymptotic normality
- σ_θ/\sqrt{S} is called Monte Carlo standard error (MCSE)
- In practice, σ_θ will be estimated by

$$\sqrt{1/(S-1) \sum_{s=1}^S (\theta^{(s)} - E(\theta))^2}$$

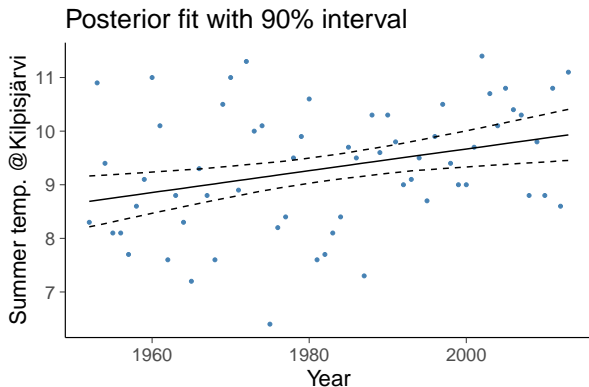
Example: Kilpisjärvi summer temperature

Average temperature in June, July, and August at Kilpisjärvi, Finland in 1952–2013



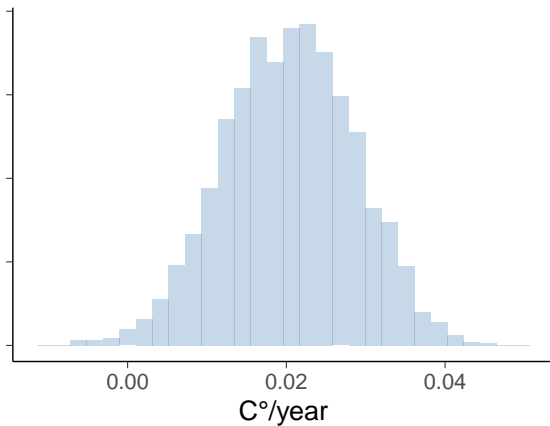
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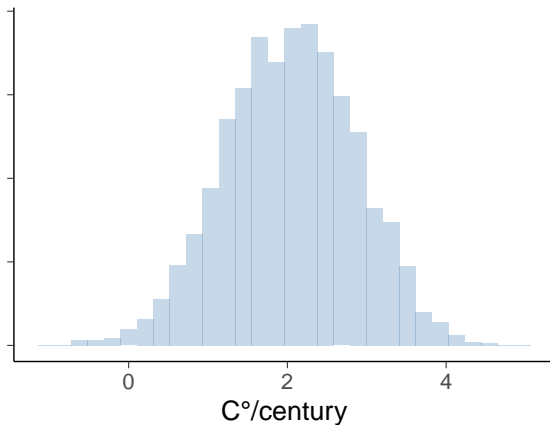
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Posterior of temperature change



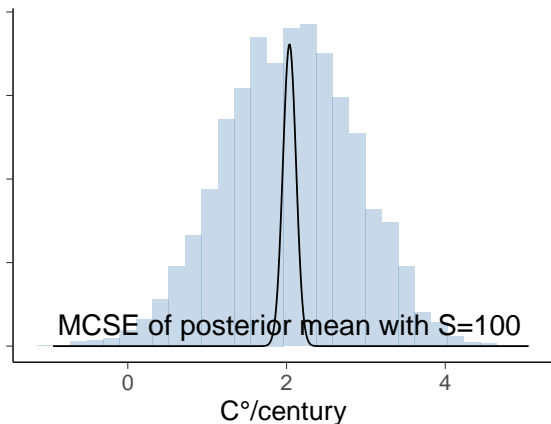
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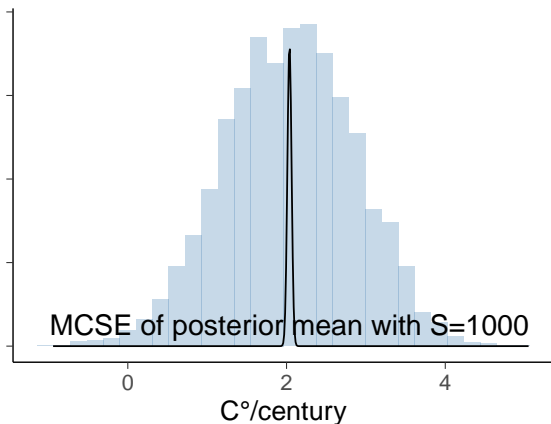
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$\sigma_{\theta} \approx 0.83$, $\text{MCSE} = \sigma_{\theta} / \sqrt{S} \approx 0.083$,
in repeated sampling we may expect mean estimate to vary
within (1.8, 2.1) (90% interval)

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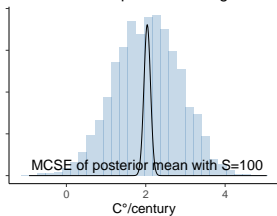
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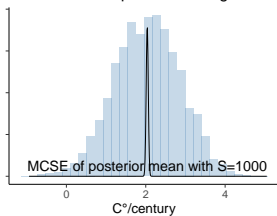
$\sigma_{\theta} \approx 0.83$, $\text{MCSE} \approx 0.026$,
in repeated sampling we may expect mean estimate to vary
within (1.9, 2.0) (90% interval)

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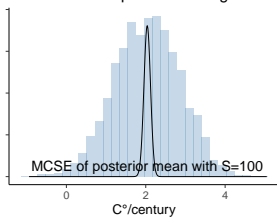


Posterior of temperature change

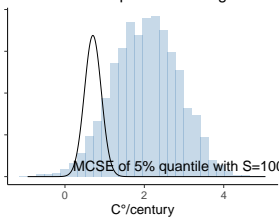


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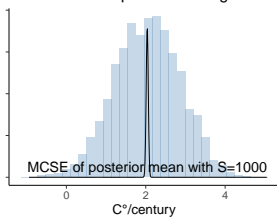
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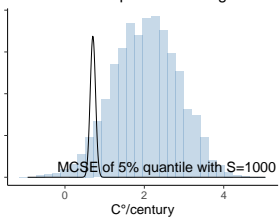
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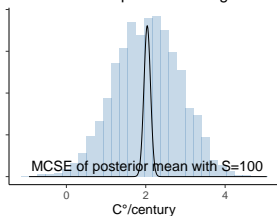


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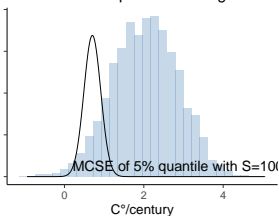


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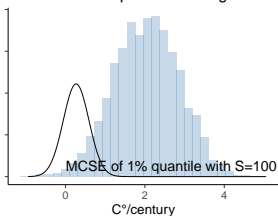
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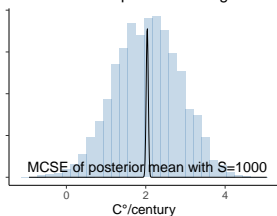
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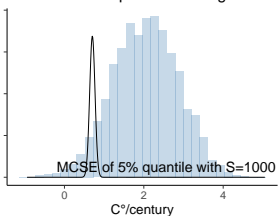
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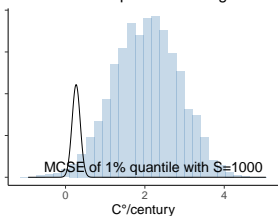
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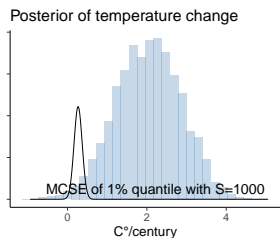
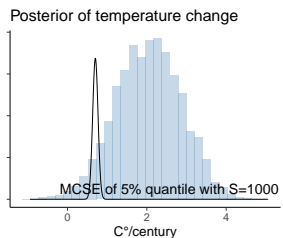
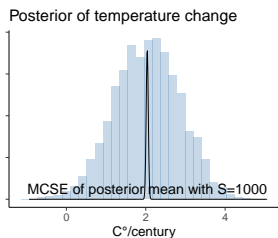
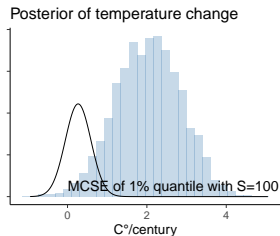
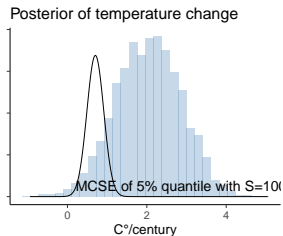
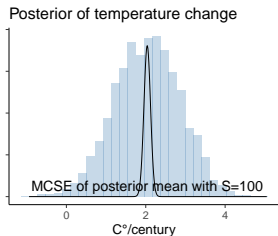
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Tail quantiles are more difficult to estimate

See Vehtari, Gelman, Simpson, Carpenter, & Bürkner (2021) for quantile MCSE computation.

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 $p(\theta \in A)$
 - use beta CDF, or normal approximation
 - $\text{var}(I(\cdot)) = p(1 - p)S$ (Appendix A, p. 579)
 - standard deviation of p is $\sqrt{p(1 - p)/S}$

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- if $S = 100$ and we observe $\frac{1}{S} \sum_l I(\theta^{(s)} \in A) = 0.05$,
then $\sqrt{p(1 - p)/S} \approx 0.02$
i.e. accuracy is about 4% units
or from quantiles of beta distribution the range is (0.02, 0.1)

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- $S = 2000$ draws needed for 1% unit accuracy

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- Posterior probability

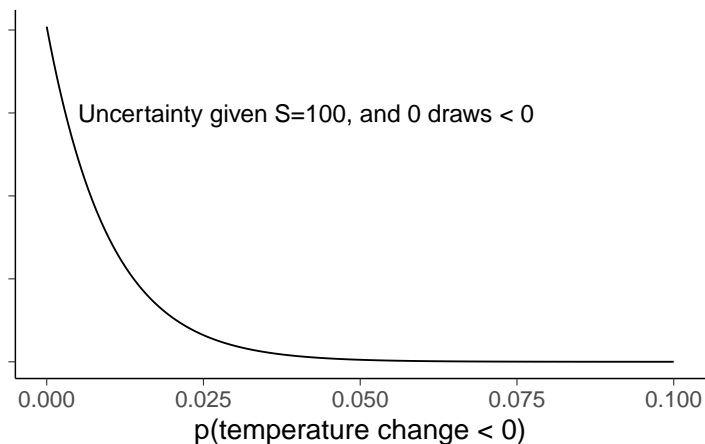
$$p(\theta \in A) \approx \frac{1}{S} \sum_l I(\theta^{(s)} \in A)$$

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

- $I(\cdot)$ is binomially distributed as $p(\theta \in A)$
 - use beta CDF, or normal approximation
 - $\text{var}(I(\cdot)) = p(1 - p)S$ (Appendix A, p. 579)
 - standard deviation of p is $\sqrt{p(1 - p)/S}$
- if $S = 100$ and we observe $\frac{1}{S} \sum_l I(\theta^{(s)} \in A) = 0.05$,
then $\sqrt{p(1 - p)/S} \approx 0.02$
i.e. accuracy is about 4% units
or from quantiles of beta distribution the range is (0.02, 0.1)
- $S = 2000$ draws needed for 1% unit accuracy
- To estimate small probabilities, a large number of draws is needed
 - to be able to estimate small p , need to get draws with $\theta^{(l)} \in A$, which in expectation requires $S \gg 1/p$

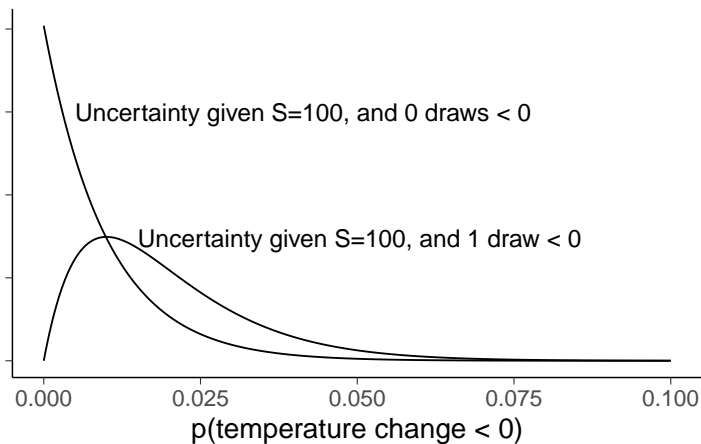
Example: Kilpisjärvi summer temperature

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



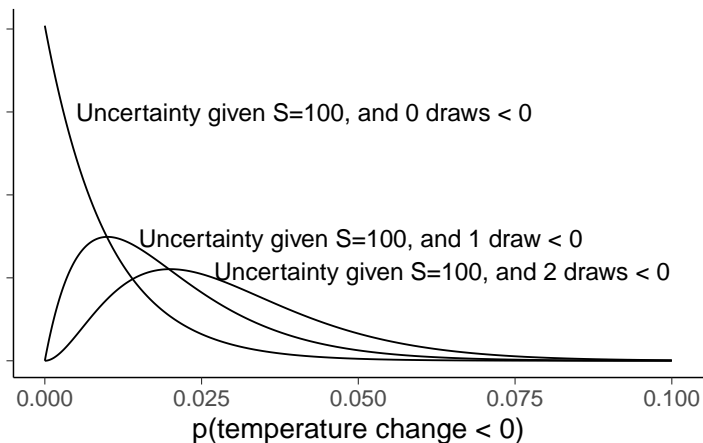
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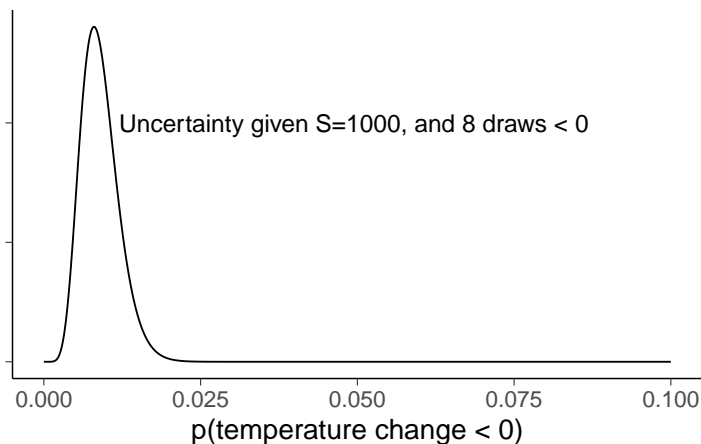
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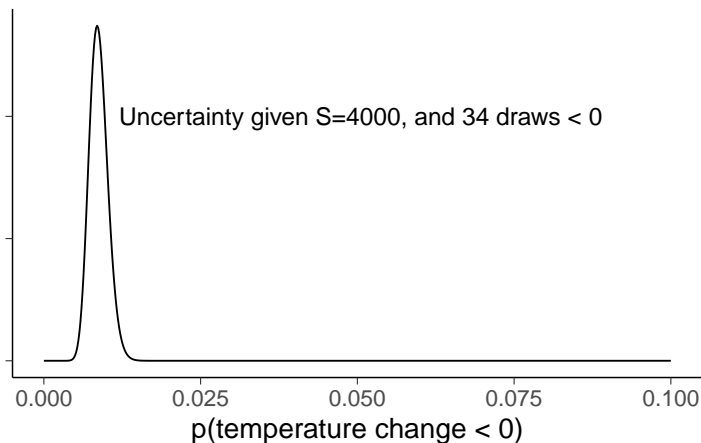
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- If $S = 1000$ and uncertainty interval for 5% probability is $(0.04, 0.06)$ (see earlier slide), we can find uncertainty interval (A^-, A^+) , so that $p(\theta < A^-) = 0.04$, and $p(\theta < A^+) = 0.06$

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 - we can summarise this interval by transforming it to MCSE
 - see examples in <https://avehtari.github.io/casestudies/Digits/digits.html>
 - if interested, see algorithm details in Vehtari, Gelman, Simpson, Carpenter, & Bürkner (2021), doi.org/10.1214/20-BA1221.

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 - The probability that temp increase is positive:
 0.9995 ± 0.0006 (90% interval),
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 - With data from other locations we would be even more certain
- Summer 2023 was the hottest in the recorded history

How many simulation draws are needed?

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 - deterministic methods
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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
- Some algorithms are less efficient
 - Compute MCSE using *effective sample size (ESS)* instead of the number of draws S
 - Usually $ESS < S$

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

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

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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

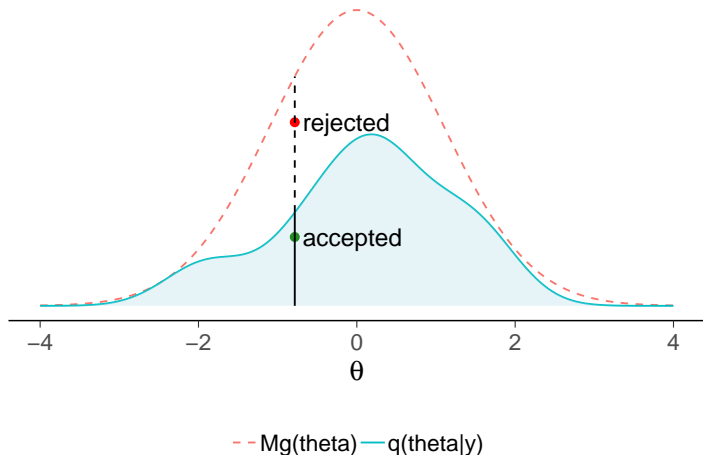
- 10 parameters
- if we don't know beforehand where the posterior mass is
 - need to choose wide box for the grid
 - need to have enough grid points to get some of them where essential mass is
- e.g. 50 or 1000 grid points per dimension
 - $50^{10} \approx 1\text{e}17$ grid points
 - $1000^{10} \approx 1\text{e}30$ grid points
- R and my current laptop can compute density of normal distribution about 50 million times per second
 - evaluation in $1\text{e}17$ grid points would take 60 years
 - evaluation in $1\text{e}30$ grid points would take 600 billion years

Indirect sampling

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

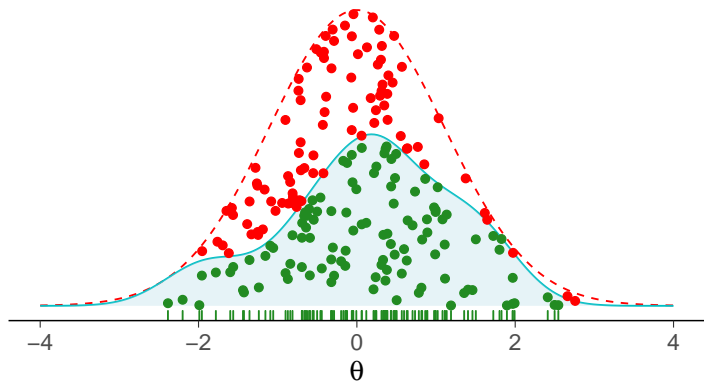
Rejection sampling

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

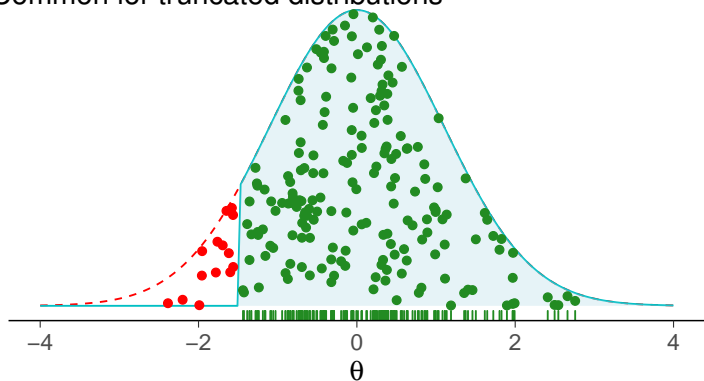
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Rejection sampling

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 $q(\theta|y)/Mg(\theta)$
- Common for truncated distributions



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

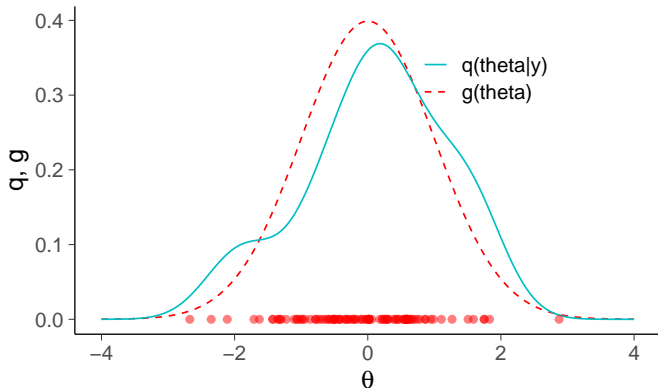
Rejection sampling

- The effective sample size (ESS) is the number of accepted draws
 - 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

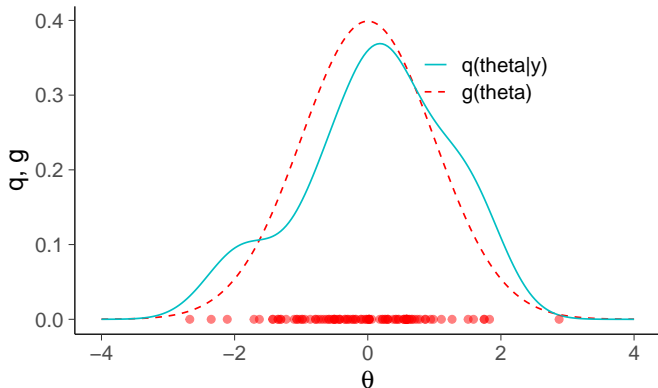
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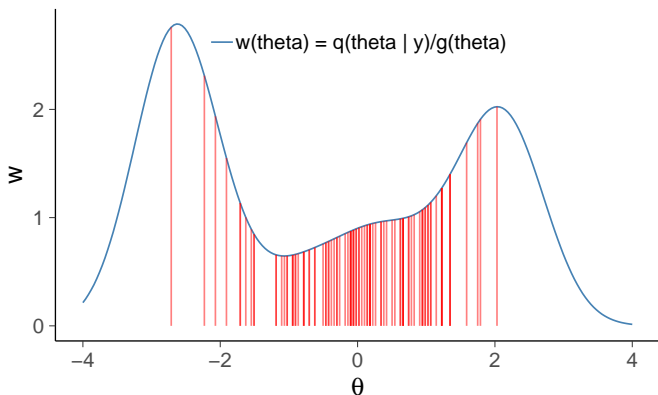


$$E[h(\theta)] \approx \frac{\sum_s w_s h(\theta^{(s)})}{\sum_s w_s}, \quad \text{where} \quad w_s = \frac{q(\theta^{(s)})}{g(\theta^{(s)})}$$

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Draws and importance weights



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- Fast leave-one-out cross-validation
- Fast bootstrapping
- Fast prior and likelihood sensitivity analysis
- Conformal Bayesian computation
- Particle filtering
- Improving distributional approximations (e.g Laplace, VI)

IS finite variance and central limit theorem

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 - sometimes these can be guaranteed by construction, e.g., by choosing $g(\theta)$ so that $w(\theta)$ is bounded
 - generally not trivial
- Pre-asymptotic and asymptotic behavior can be really different!

Importance re-sampling

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Importance re-sampling

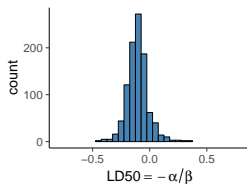
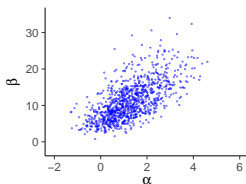
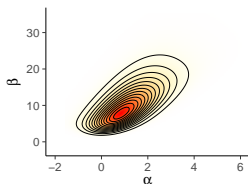
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- But it can be convenient to obtain draws with equal weights
 - resample the draws according to the weights
 - some original draws may be included more than once
 - loses some information, but now the weights are equal

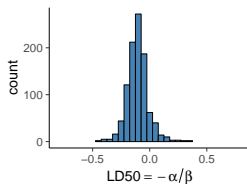
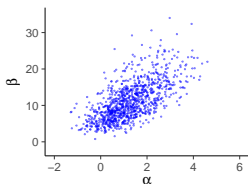
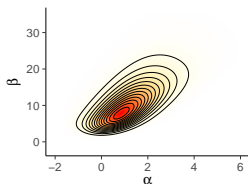
Example: Importance sampling in Bioassay

Grid

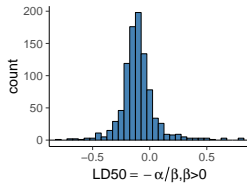
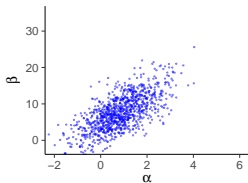
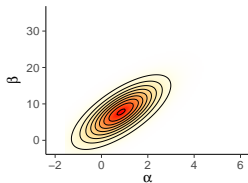


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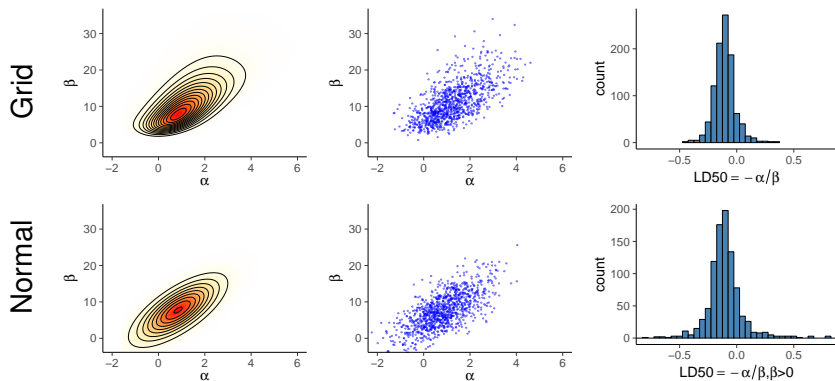


Normal



Normal approximation is discussed more in BDA3 Ch 4

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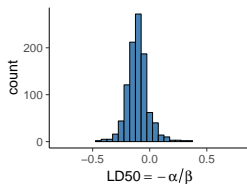
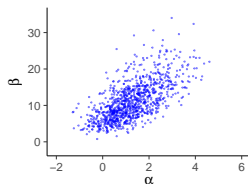
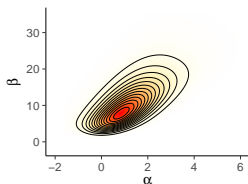
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But the normal approximation is not that good here:

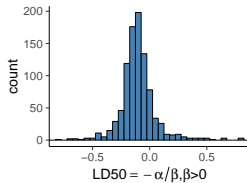
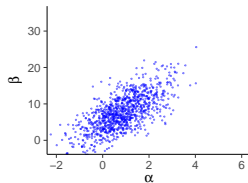
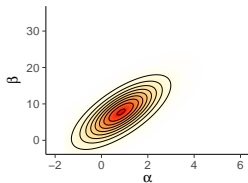
Grid $\text{sd}(\text{LD50}) \approx 0.1$, Normal $\text{sd}(\text{LD50}) \approx .75!$

Example: Importance sampling in Bioassay

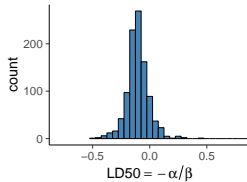
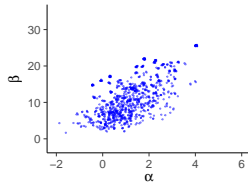
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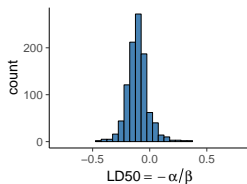
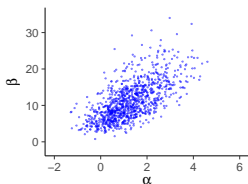
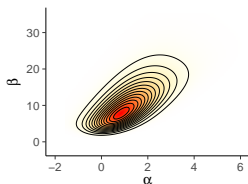


IR

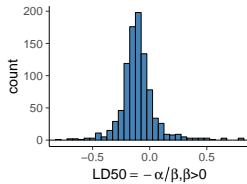
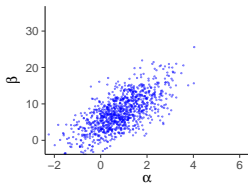
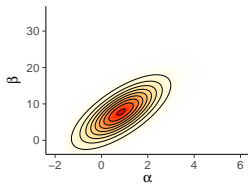


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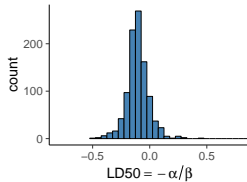
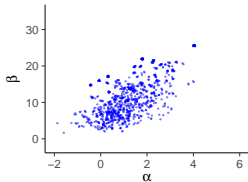
Grid



Normal



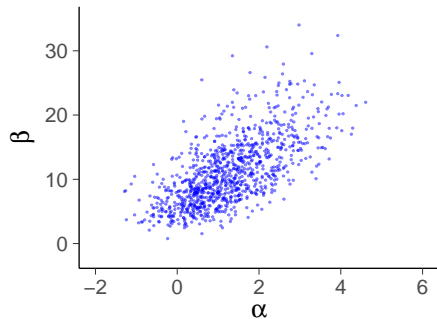
IR



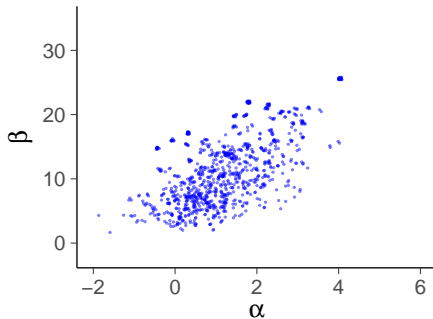
Grid $sd(LD50) \approx 0.1$, IR $sd(LD50) \approx 0.1$

Example: Importance sampling in Bioassay

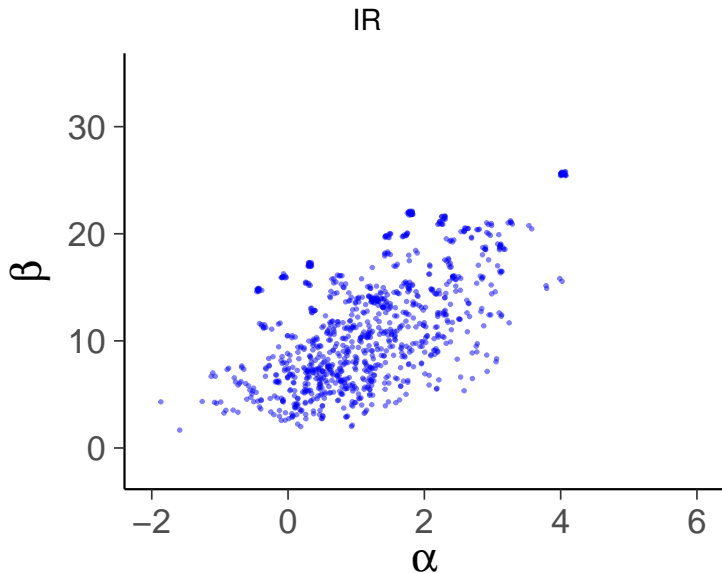
Grid



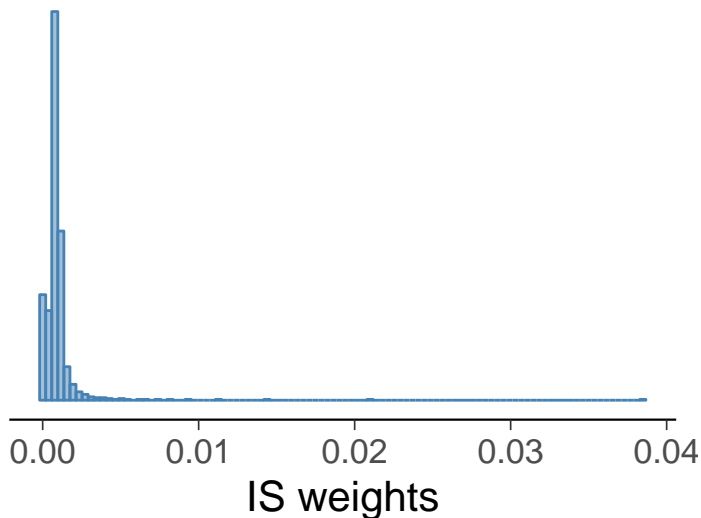
IR



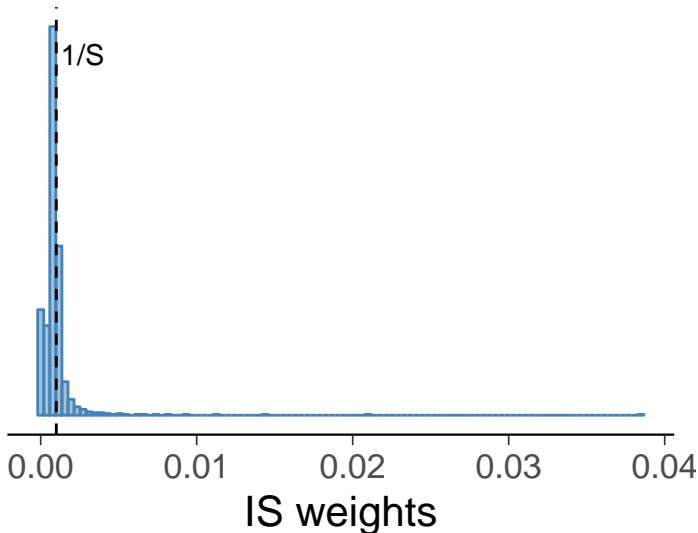
Example: Importance sampling in Bioassay



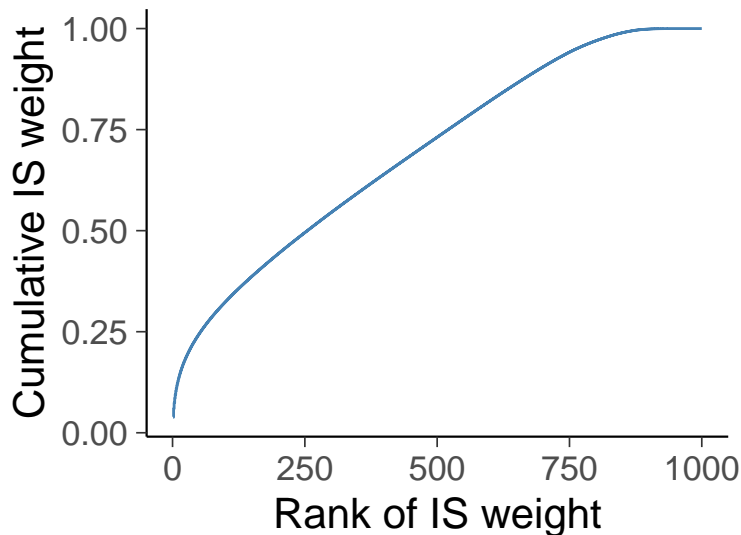
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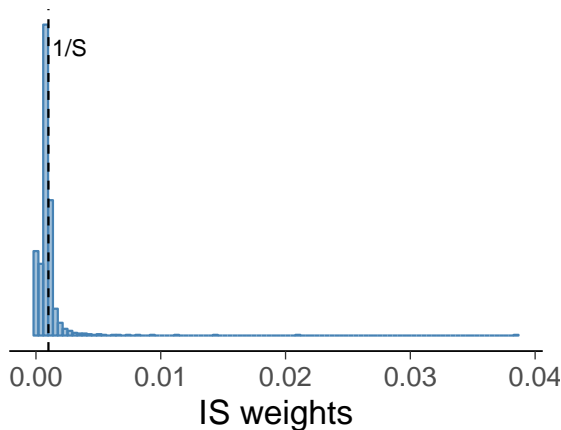
Example: Importance sampling in Bioassay



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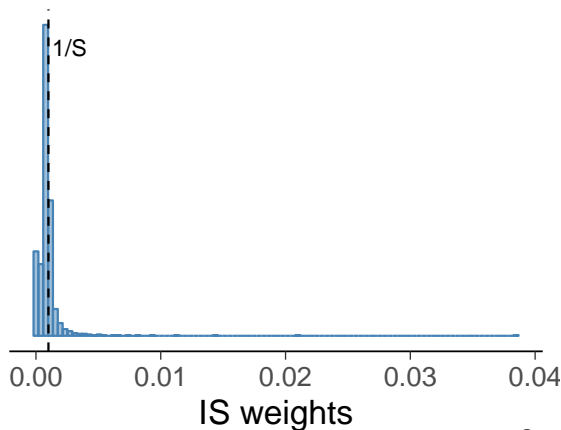


Example: Importance sampling in Bioassay



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

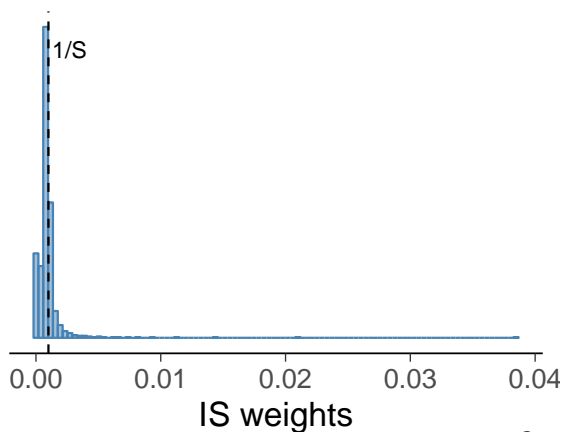
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BDA3 1st (2013) and 2nd (2014) printing have an error for $\tilde{w}(\theta^s)$. The equation should not have the multiplier S (the normalized weights should sum to one). Online version is correct. Errata for the book http://www.stat.columbia.edu/~gelman/book/errata_bda3.txt

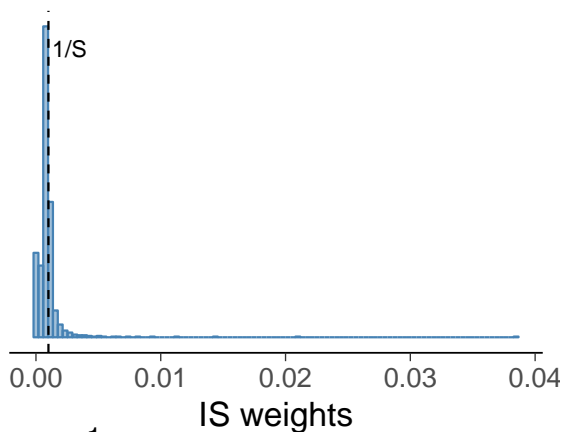
Example: Importance sampling in Bioassay



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$$\text{ESS} \approx 396, \quad (\text{ESS} < S = 1000)$$

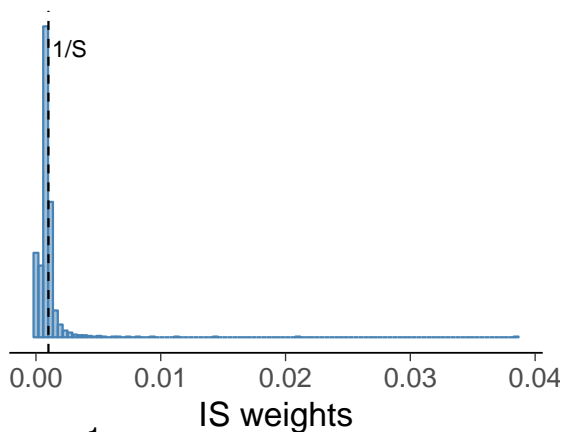
Example: Importance sampling in Bioassay



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Example: Importance sampling in Bioassay

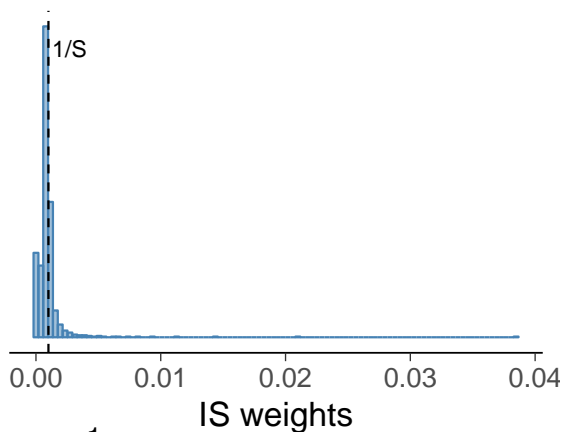


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If all $\tilde{w}(\theta^s) = 1/S$, then $\text{ESS} = 1/(SS^{-2}) = S$

Example: Importance sampling in Bioassay



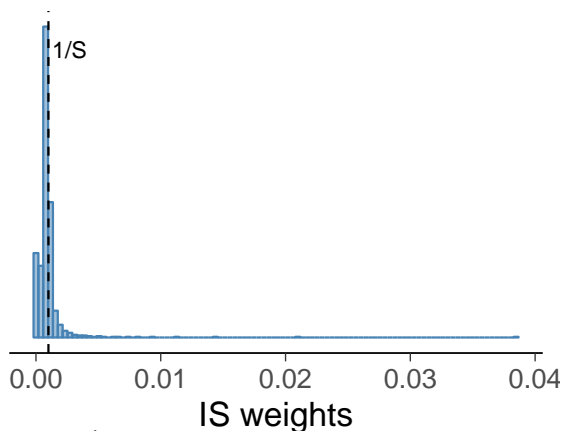
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If all $\tilde{w}(\theta^s) = 1/S$, then $\text{ESS} = 1/(SS^{-2}) = S$

If one $\tilde{w}(\theta^s) = 1$, and others 0, then $\text{ESS} = 1/1 = 1$

Example: Importance sampling in Bioassay

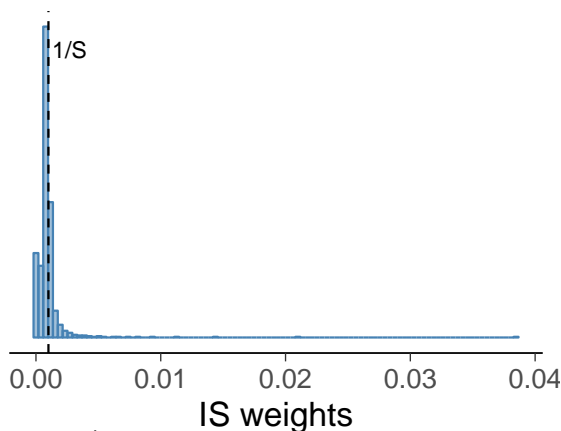


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Example: Importance sampling in Bioassay



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Pareto- k diagnostic preferably < 0.7 : $\hat{k} \approx 0.65$

Pareto- \hat{k} diagnostic

- Based on extreme value analysis and generalized central limit theorem

See more in Vehtari, Simpson, Gelman, Yao, and Gabry (2022). Pareto smoothed importance sampling. [arXiv:1507.02646](https://arxiv.org/abs/1507.02646).

Pareto- \hat{k} diagnostic

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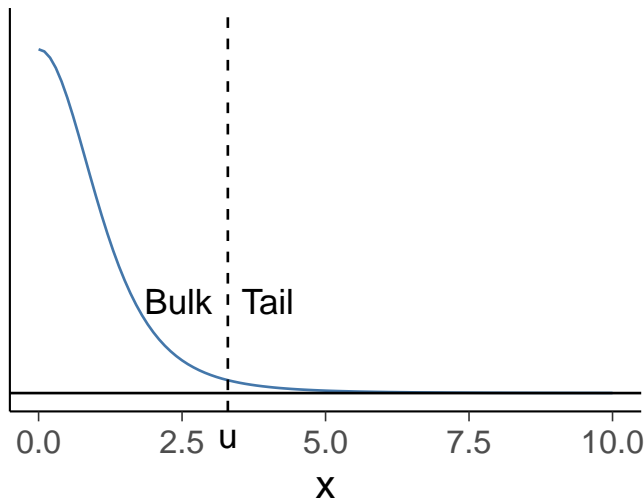
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 - shape parameter k tells the number of *fractional moments* as $1/k$
 - estimate \hat{k} from finite data
 - the statistical behavior of distribution of mean can be predicted by generalized CLT
 - minimum sample size and convergence rate given \hat{k}

See more in Vehtari, Simpson, Gelman, Yao, and Gabry (2022). Pareto smoothed importance sampling. arXiv:1507.02646.

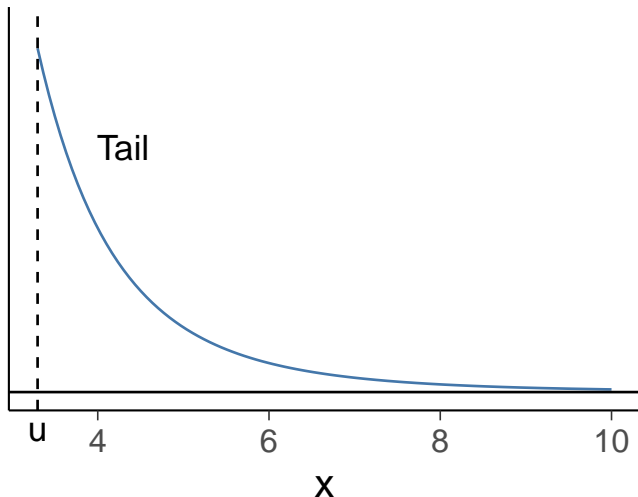
Pareto- \hat{k} diagnostic

Pickands (1975): many distributions have tail ($x > u$) that is well approximated with Generalized Pareto distribution (GPD)



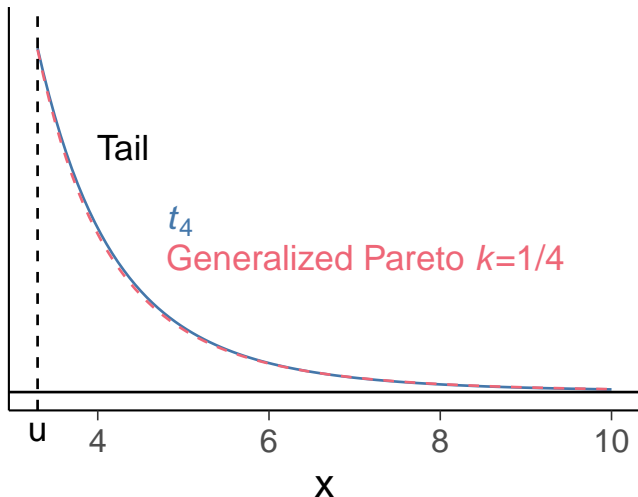
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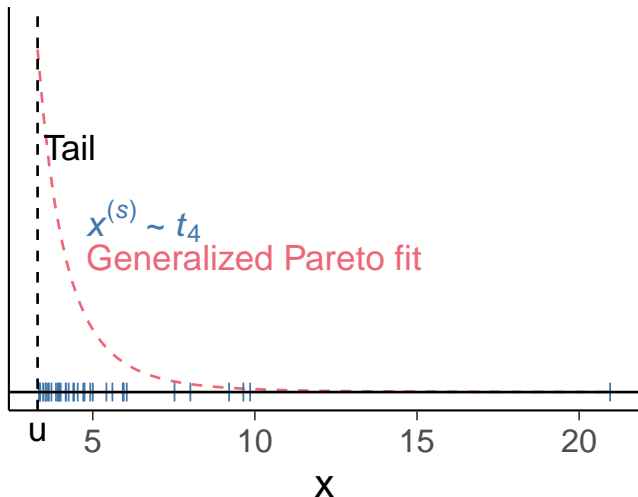
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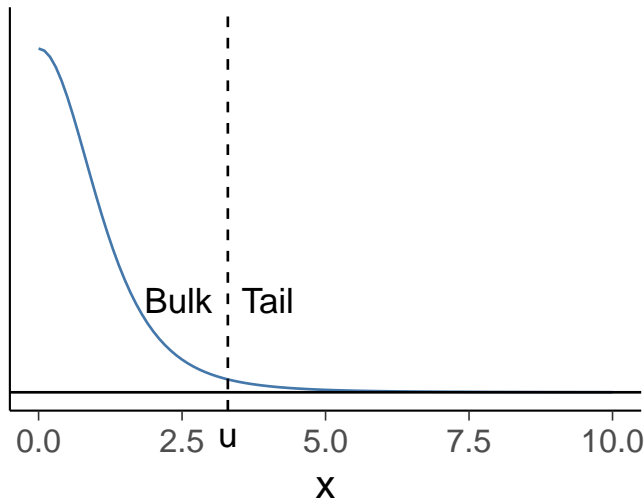
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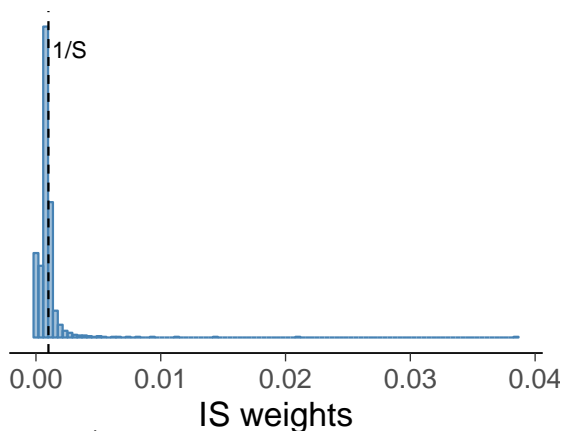


Pareto- \hat{k} diagnostic

GPD has a shape parameter k ,
and $1/k$ finite fractional moments



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Pareto- \hat{k} and convergence rate

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Pareto- \hat{k} and convergence rate

- CLT says that to half the MCSE, need 4 times bigger S
- If Pareto- $\hat{k} \approx 0.7$, to half the MCSE, need 10 times bigger S
- If Pareto- $\hat{k} > 1$, to half the MCSE, nothing helps

Pareto smoothed importance sampling (PSIS)

- Replace the largest observed ratios with expected ordered statistics of the fitted Pareto distribution
 - corresponds to modeling of the tail, and as usual, modeling reduces the noise

Estimating Pareto- \hat{k}

- Fast empirical profile Bayes quadrature estimate by Zhang and Stephens (2009)
 - excellent accuracy compared to exact Bayesian inference
 - see more in Vehtari, Simpson, Gelman, Yao & Gabry (2022)

Pareto- \hat{k} diagnostic use cases

- Importance sampling
 - leave-one-out cross-validation (Vehtari et al., 2016, 2017; Bürkner et al., 2020)
 - Bayesian stacking (Yao et al., 2018, 2021, 2022)
 - leave-future-out cross-validation (Bürkner et al., 2020)
 - Bayesian bootstrap (Paananen et al., 2021, online appendix)
 - prior and likelihood sensitivity analysis (Kallioinen et al., 2021)
 - improving distributional approximations (Yao et al., 2018; Zhang et al., 2021; Dhaka et al., 2021)
 - implicitly adaptive importance sampling (Paananen et al., 2021)
- Stochastic optimization (Dhaka et al., 2020)
- Divergences and gradients in VI (Dhaka et al., 2021)
- MCMC (Paananen et al., 2021)

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