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)) $\rightarrow$ 0 (underflow)

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    - Laplace and ratio of girl and boy babies
    - pbeta(0.5, 241945, 251527) $\rightarrow$ 1 (rounding)

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    - pbeta(0.5, 241945, 251527, lower.tail=FALSE) $\approx -1.2 \cdot 10^{-42}$
      there is more accuracy near 0

Numerical accuracy – log scale

- Log densities
  - use log densities to avoid over- and underflows in floating point presentation
    - prod(dnorm(qr)) $\rightarrow$ 0 (underflow)
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      but $800 + \log(1 + \exp(800 - 800)) \approx 800.69$
    - 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

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

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- Grid (equal spacing) evaluation with self-normalization

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

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

It's all about expectations

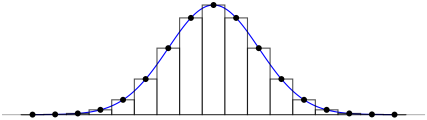
$$E_\theta[f(\theta)] = \int f(\theta)p(\theta|y)d\theta$$

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

Quadrature integration

- The simplest quadrature integration is grid integration

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



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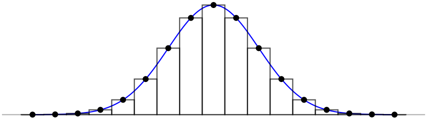

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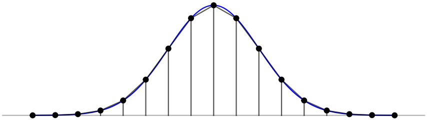

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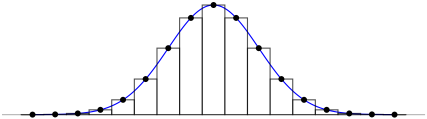

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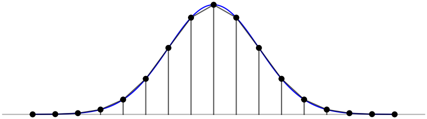

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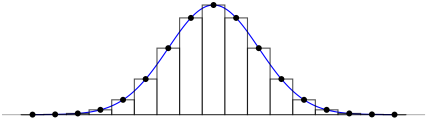

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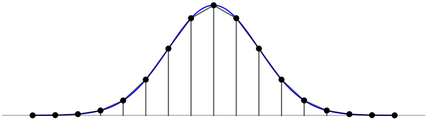

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- In 2D and higher
  - nested quadrature
  - product rules

Monte Carlo - history

- Used already before computers
  - Buffon (18th century; needles)
  - De Forest, Darwin, Galton (19th century)
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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

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

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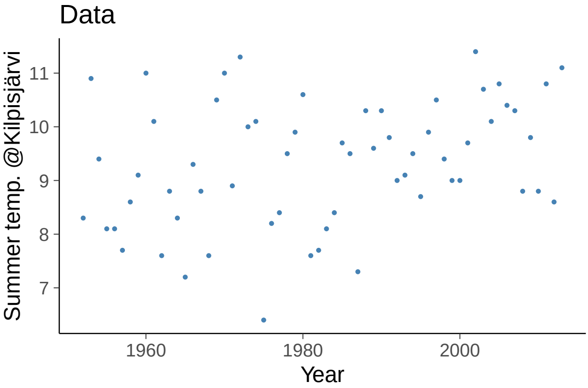
  - See BDA3 Ch 4 for counter-examples for asymptotic normality

Example: Kilpisjärvi summer temperature

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



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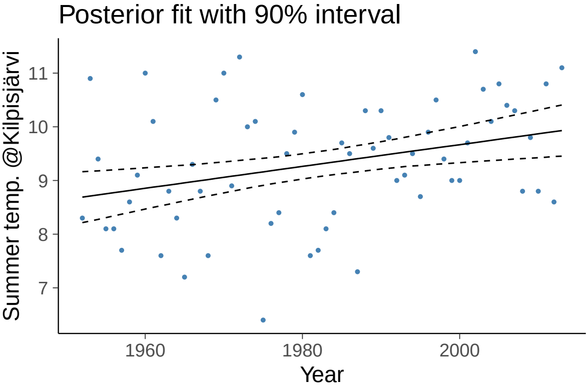

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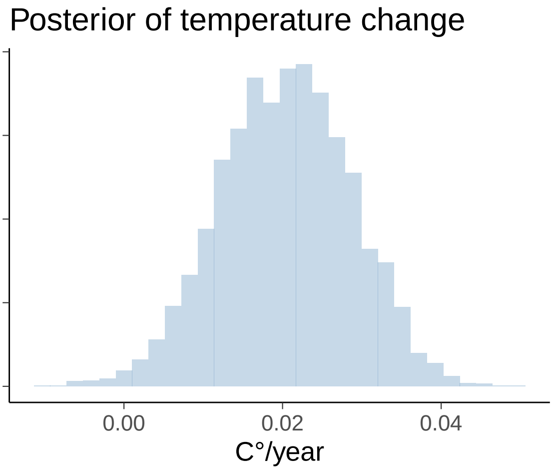

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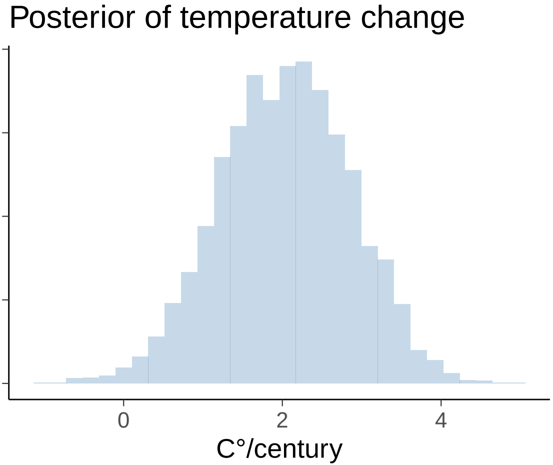

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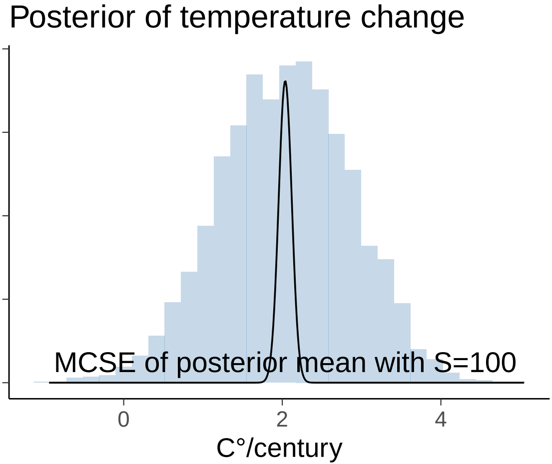

$\sigma_\theta \approx 0.827$, MCSE ≈ 0.0827, total deviation ≈ 0.831

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

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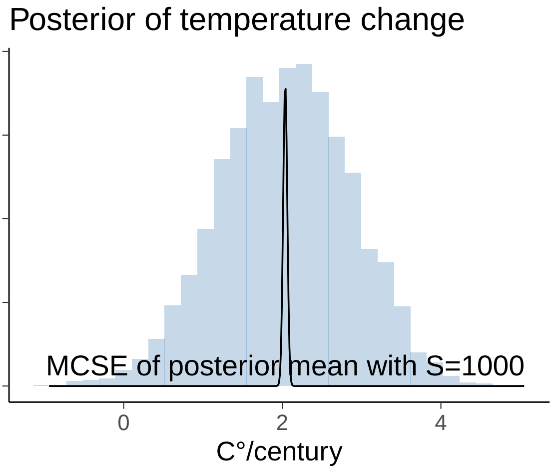

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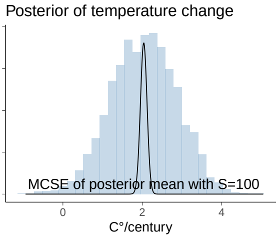

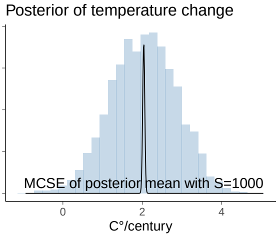

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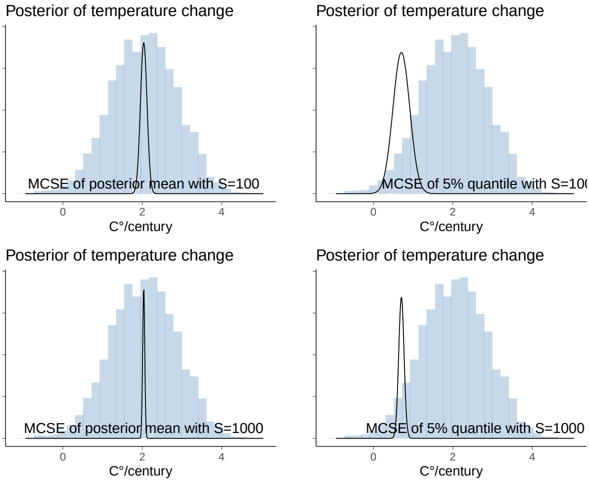

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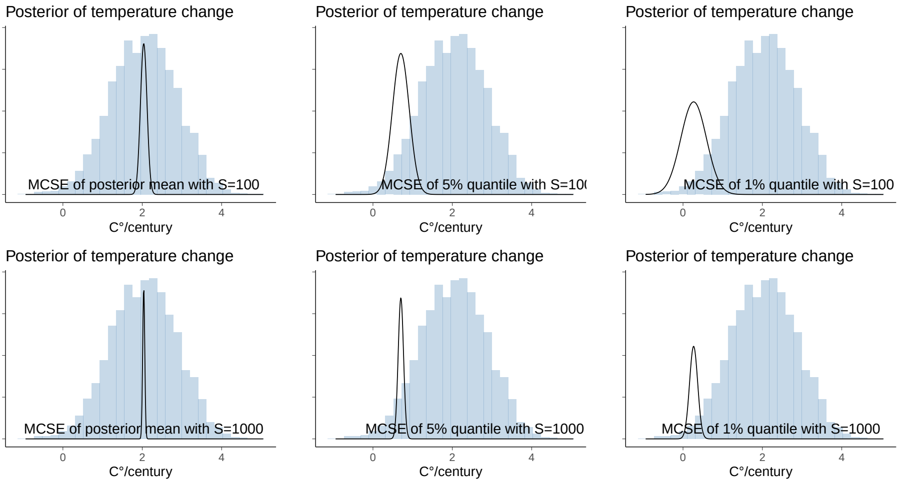

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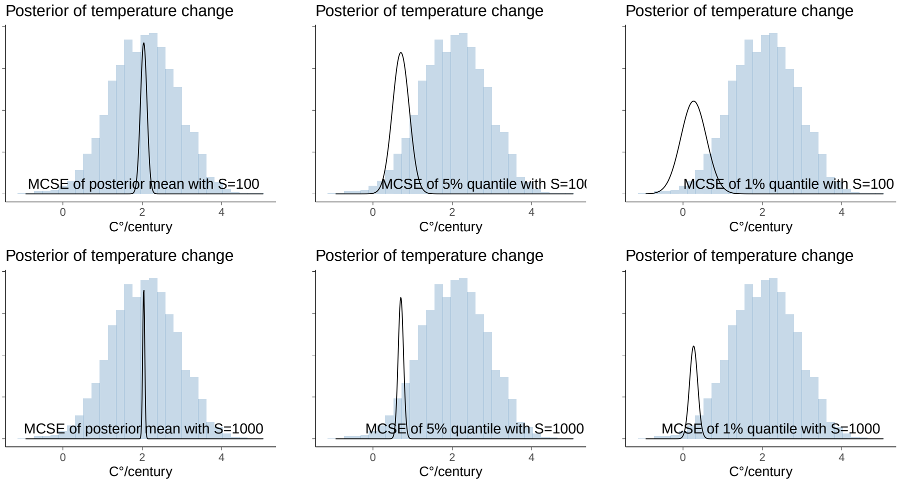

Tail quantiles are more difficult to estimate

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 $p(\theta \in A)$
  - $\rightarrow$ $\mathrm{var}(I(\cdot)) = p(1-p)$ (Appendix A, p. 579)
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- 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 $S \gg 1/p$

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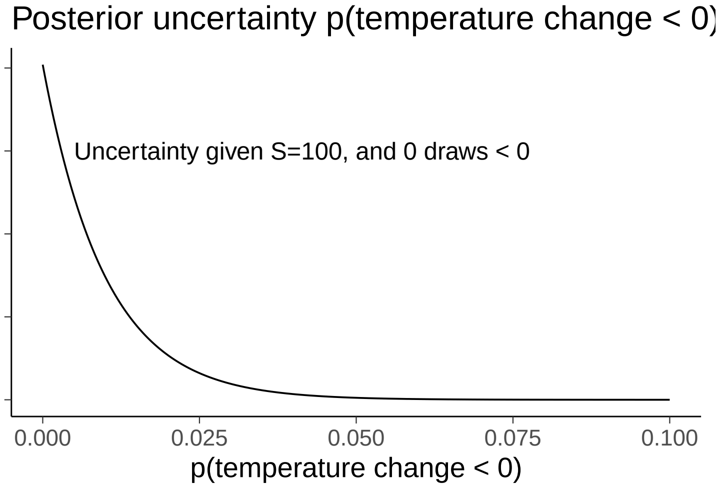

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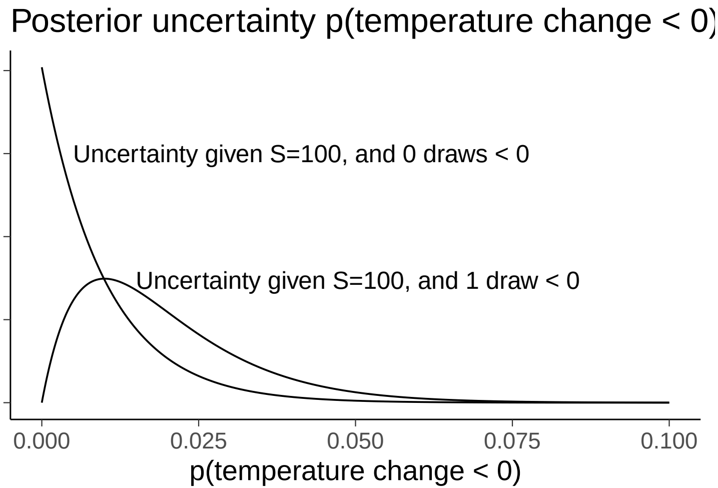

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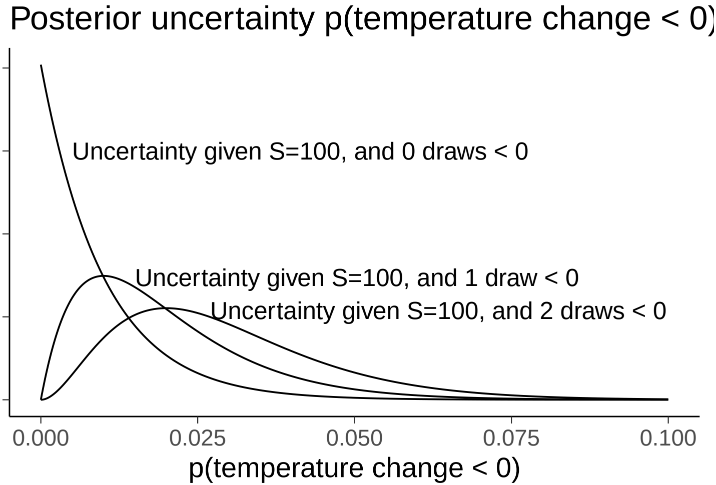

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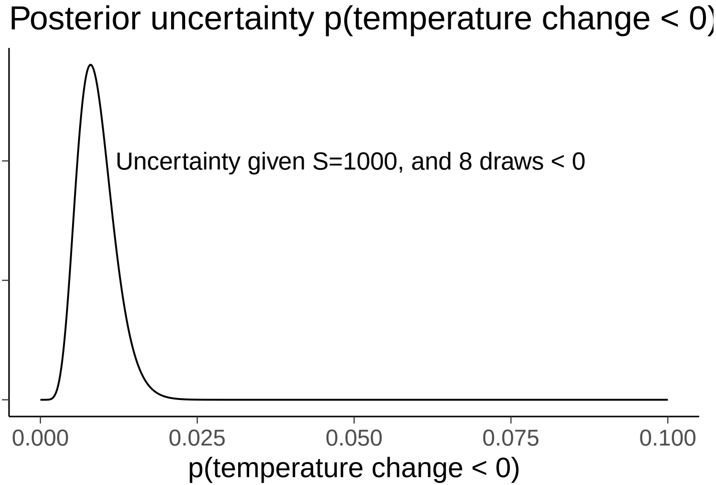

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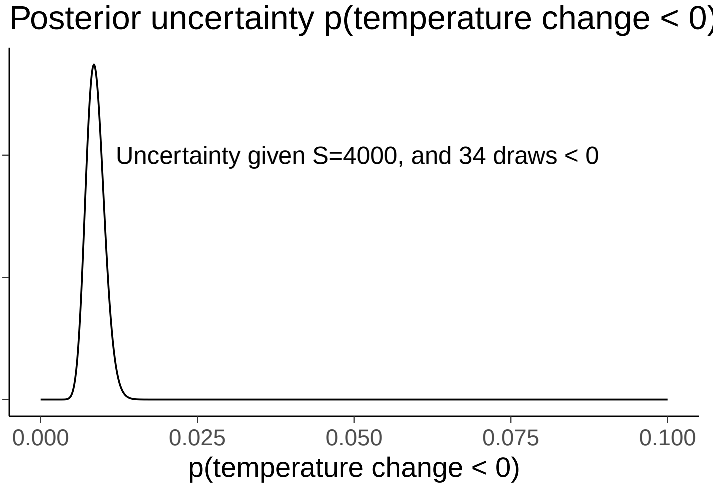

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See also https://avehtari.github.io/casestudies/Digits/digits.html

More data

- The analysis I just showed used data from 1952–2013

More data

- The analysis I just showed used data from 1952–2013
- With data data from 1952–2022
    - The probability that temp increase is positive:
      0.9995 ± 0.000353,
      which can be reported as more than 99.9% probability
    - With data from other locations we would be even more certain

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 $\mathrm{U}(0, 1)$, 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 $\mathrm{N}(0, 1)$
    - 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

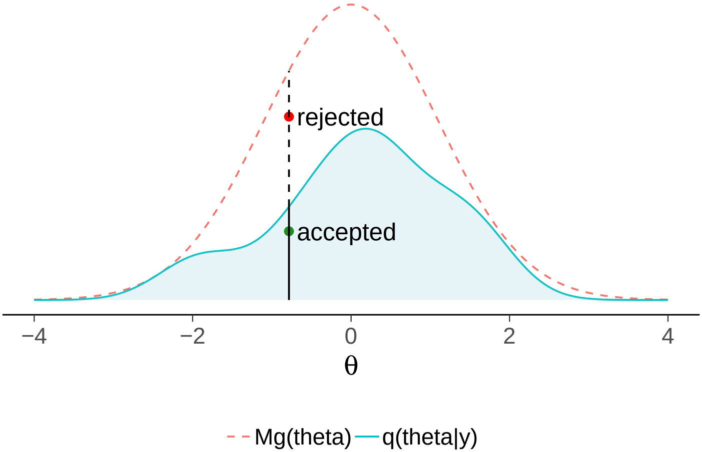
- 10 parameters
- if we don't know beforehand where the posterior mass is
  - need to choose wide box for the grid
  - need to have enough grid points to get some of them where essential mass is
- e.g. 50 or 1000 grid points per dimension
  - $\rightarrow$ $50^{10} \approx$ 1e17 grid points
  - $\rightarrow$ $1000^{10} \approx$ 1e30 grid points
- R and my current laptop can compute density of normal distribution about 50 million times per second
  - $\rightarrow$ evaluation in 1e17 grid points would take 60 years
  - $\rightarrow$ evaluation in 1e30 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 $q(\theta|y)/Mg(\theta)$



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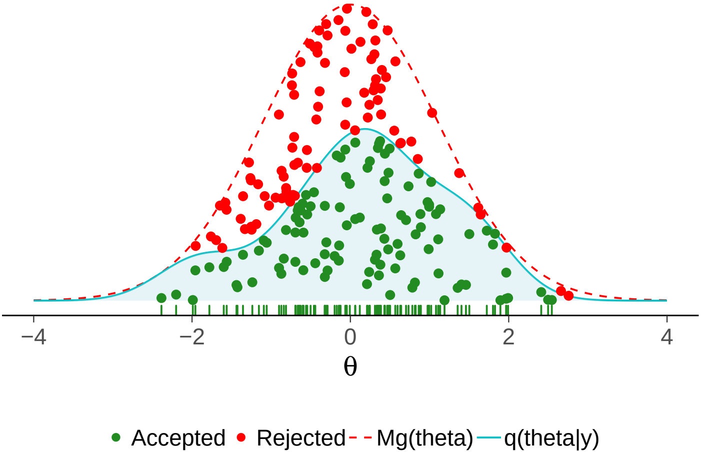
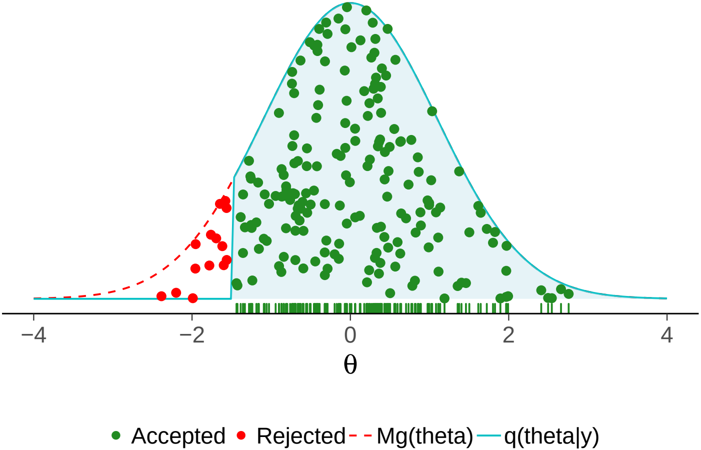


Rejection sampling

- 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

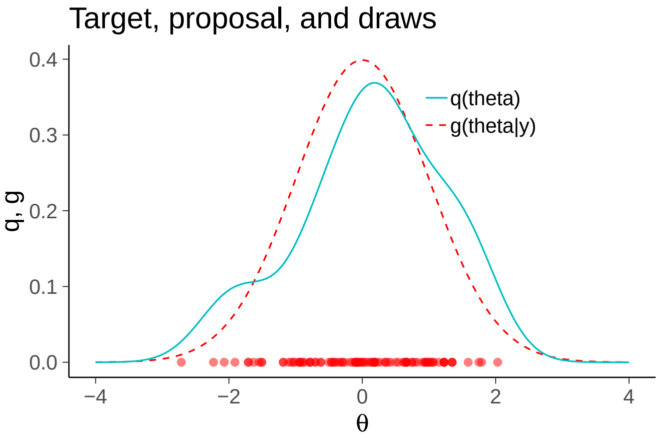


Rejection sampling

- 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



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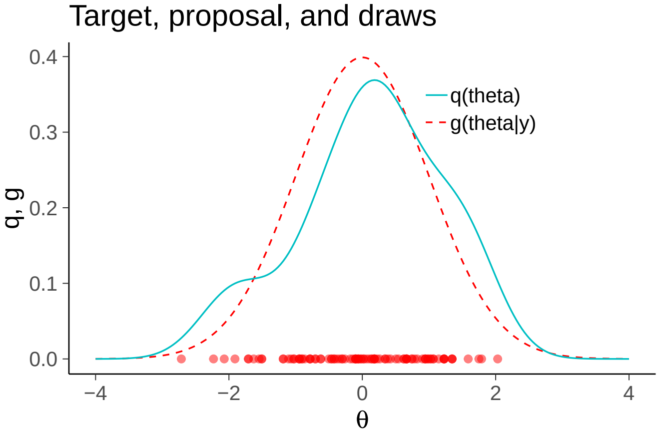

$$E[f(\theta)] \approx \frac{\sum_s w_s f(\theta^{(s)})}{\sum_s w_s}, \qquad \text{where} \quad w_s = \frac{q(\theta^{(s)})}{g(\theta^{(s)})}$$

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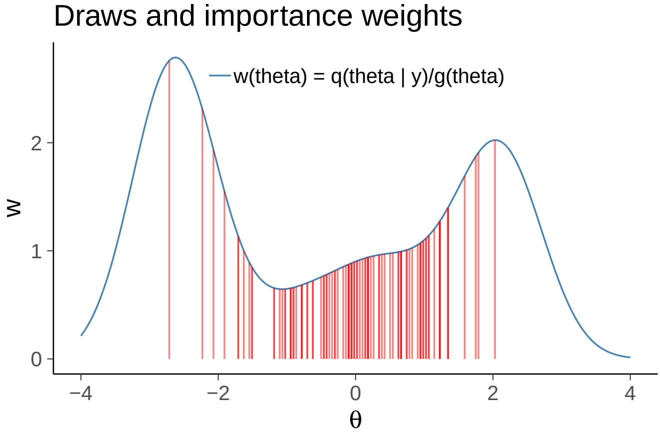

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Some uses of importance sampling

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In general selection of good proposal gets more difficult when the number of dimensions increase, but there are many use case

- 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

- If $h(\theta)w$ and w have finite variance $\rightarrow$ CLT
  - variance goes down as $1/S$
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- If variance is infinite, but mean is finite
  $\rightarrow$ *generalized CLT and asymptotic consistency*
- Pre-asymptotic and asymptotic behavior can be really different!

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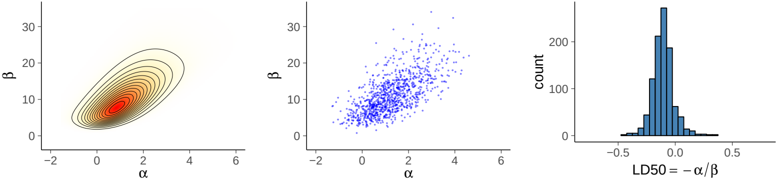
- But it can be convenient to obtain draws with equal weights
  - resample the draws according to the weights
  - some original draws may be included more than once
  - loses some information, but now the weights are equal

Example: Importance sampling in Bioassay

Grid



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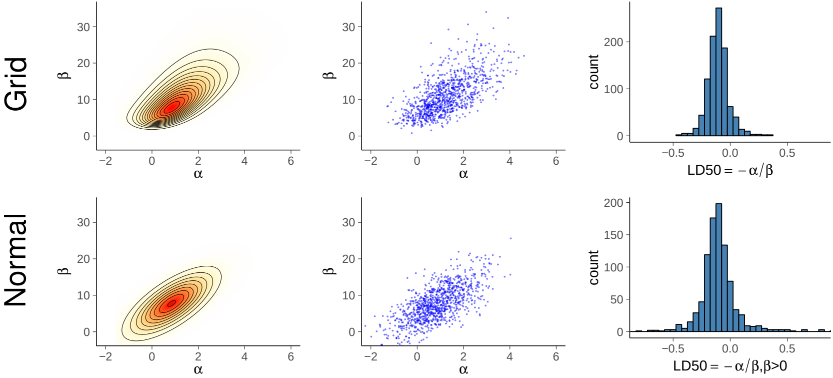

Normal approximation is discussed more in BDA3 Ch 4

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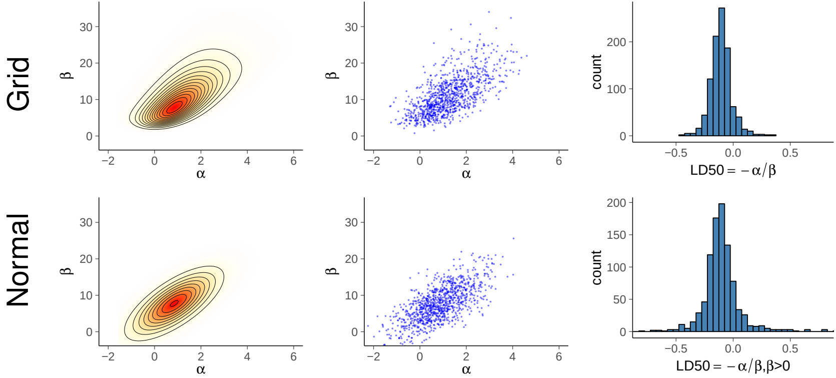

Normal approximation is discussed more in BDA3 Ch 4
But the normal approximation is not that good here:
Grid sd(LD50) $\approx$ 0.1, Normal sd(LD50) $\approx$ .75!

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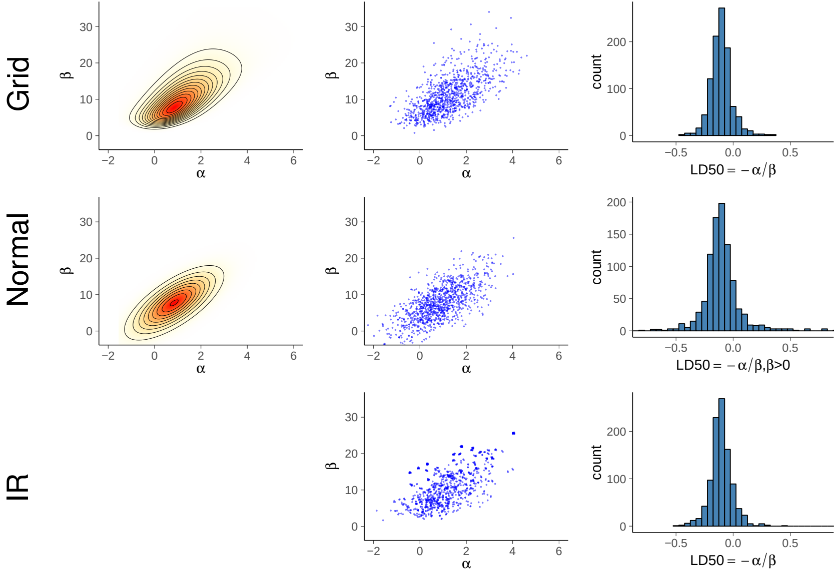

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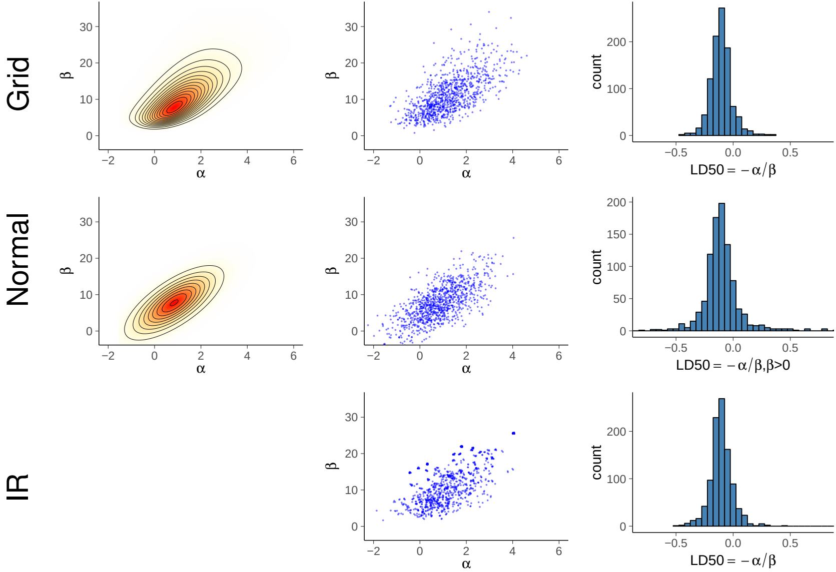

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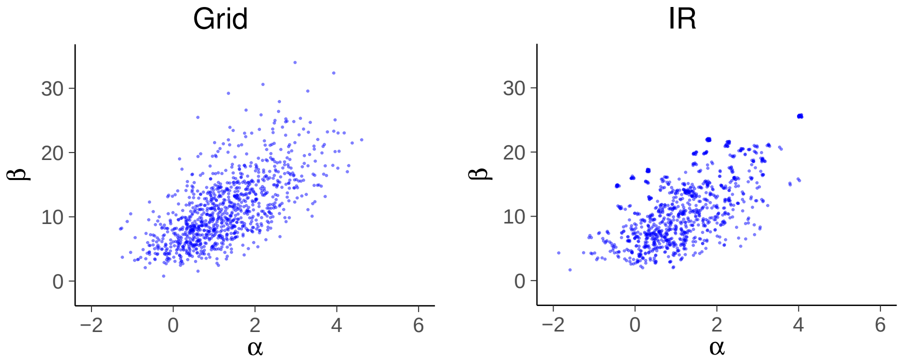

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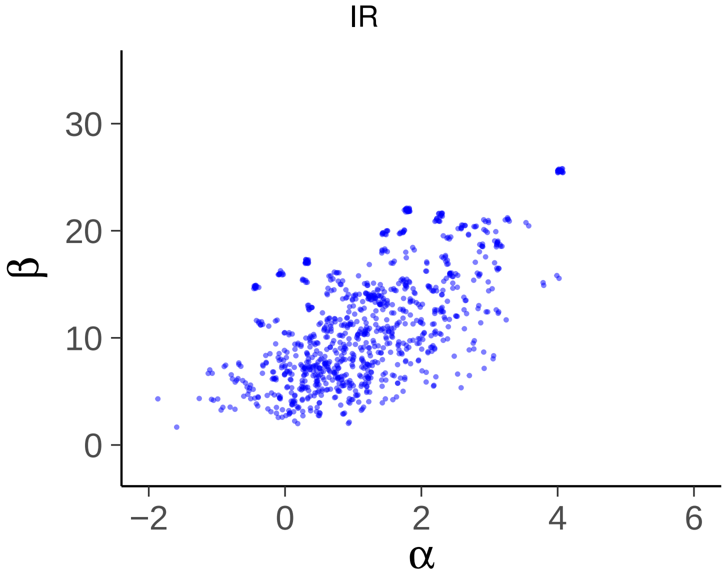

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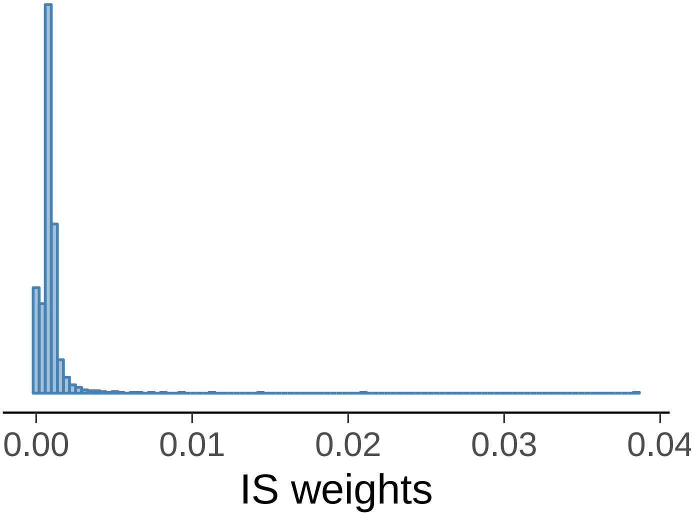

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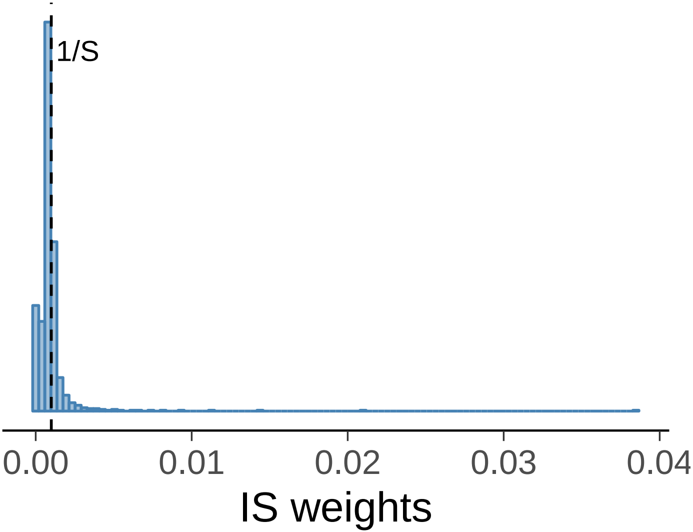

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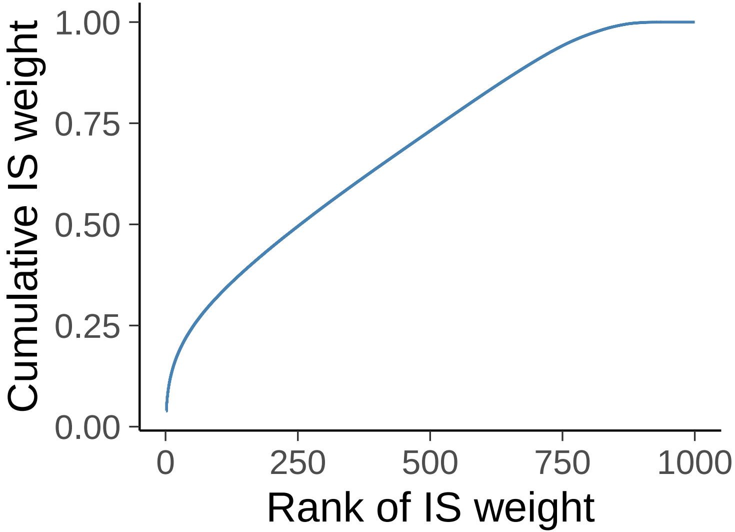

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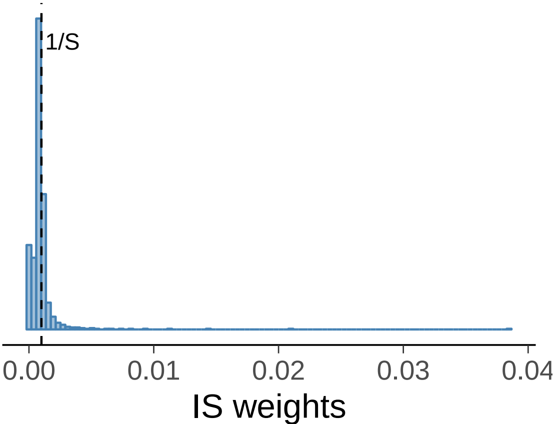

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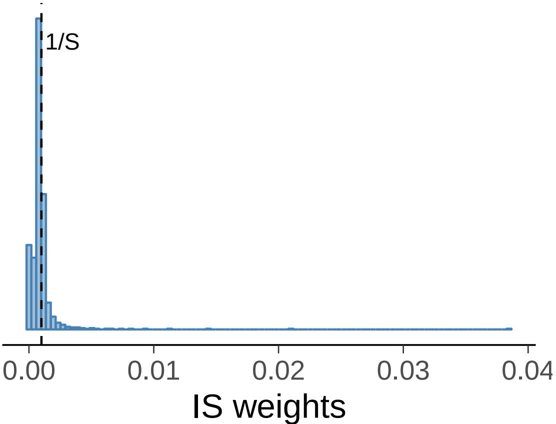

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BDA3 1st (2013) and 2nd (2014) printing have an error for $\tilde{w}(\theta^s)$. The equation should not have the multiplier S (the normalized weights should sum to one). Online version is correct. Errata for the book http://www.stat.columbia.edu/~gelman/book/errata_bda3.txt

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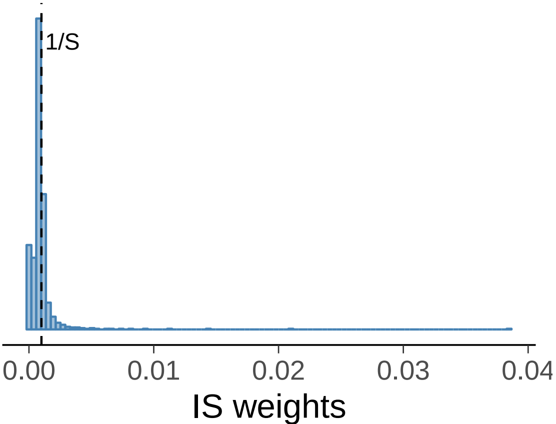

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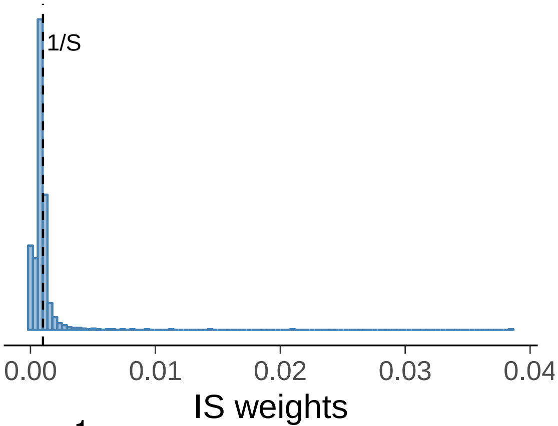

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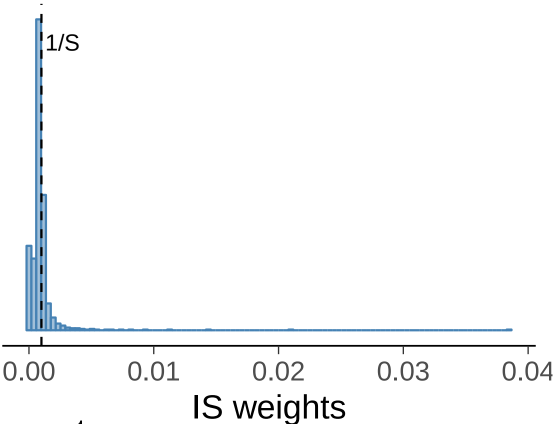

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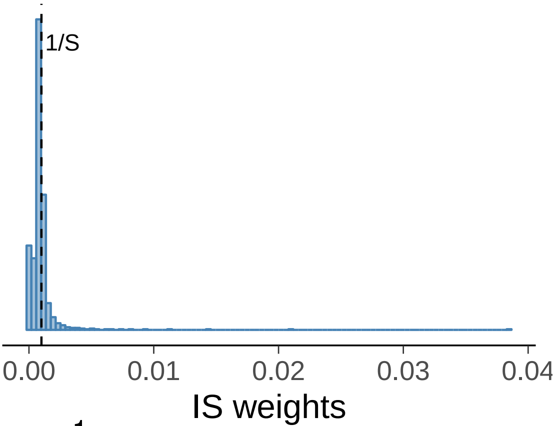

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If one $\tilde{w}(\theta^s) = 1$, and others 0, then $S_{\mathrm{eff}} = 1/1 = 1$

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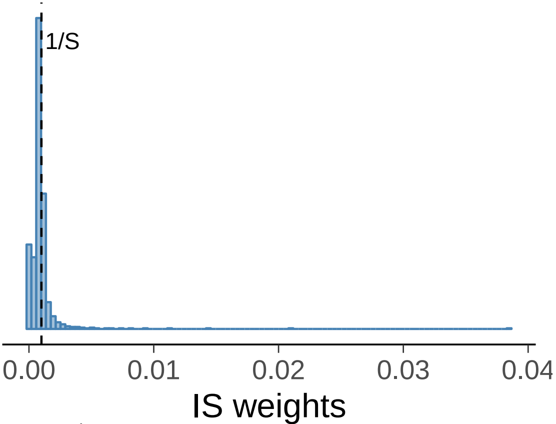

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Pareto-k diagnostic preferably < 0.7:

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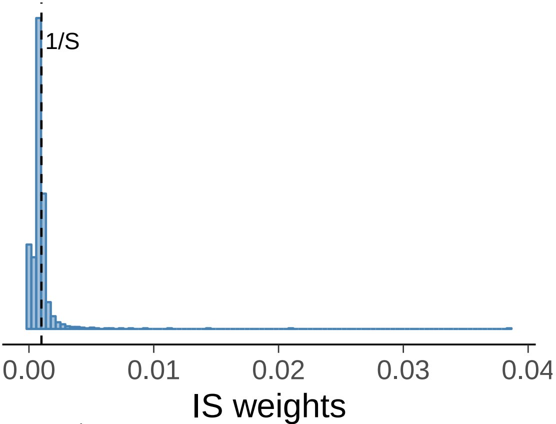

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Pareto-k diagnostic preferably < 0.7: $\hat{k} \approx 0.65$

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.

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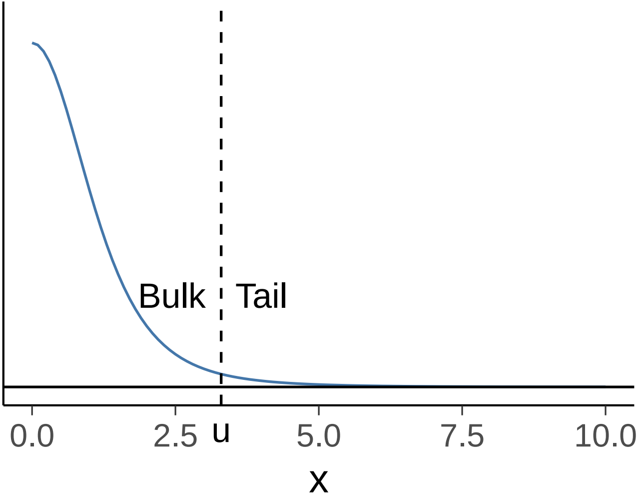
  - shape parameter k tells the number of *fractional moments* as $1/k$
  - estimate $\hat{k}$ from finite data
  - the statistical behavior of distribution of mean can be predicted by generalized CLT
    - minimum sample size and convergence rate given $\hat{k}$

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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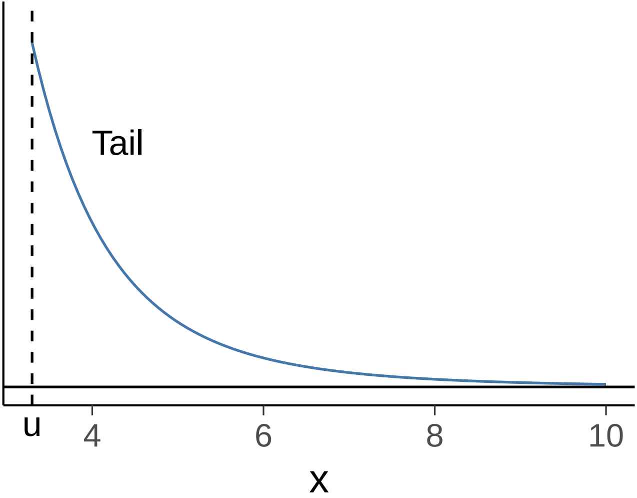

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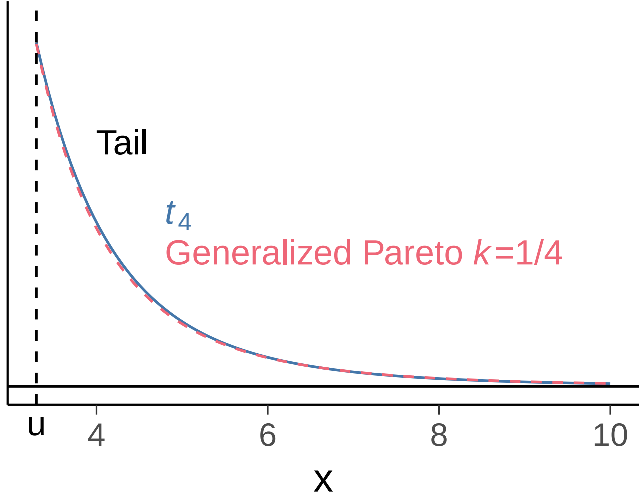

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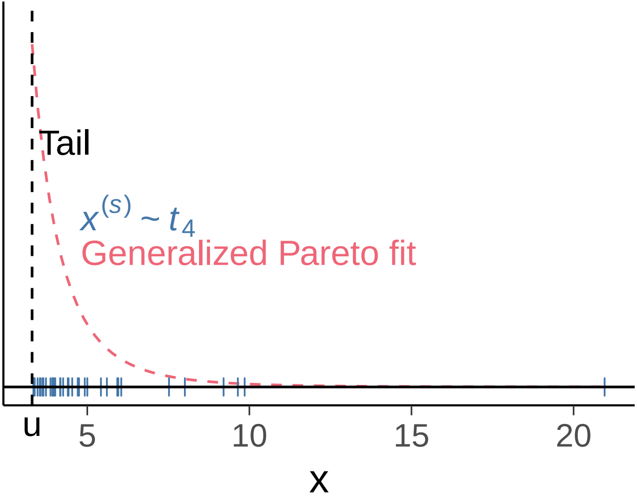
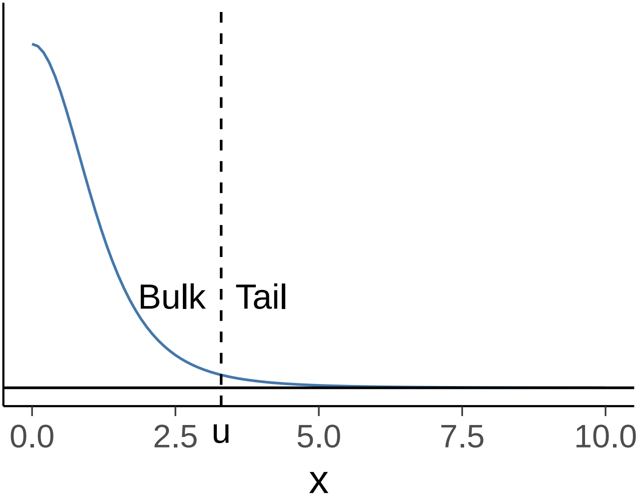
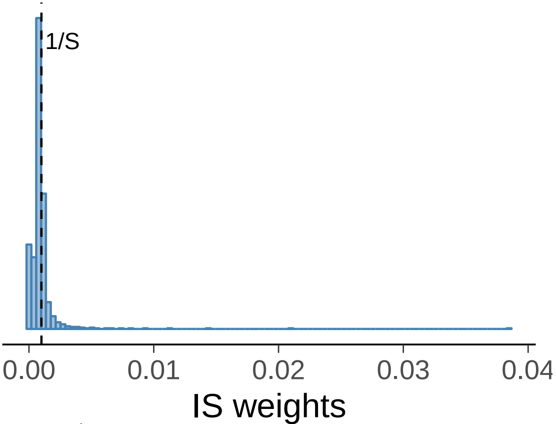


Pareto-$\hat{k}$ diagnostic

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



Example: Importance sampling in Bioassay



$$S_{\text{eff}} = \frac{1}{\sum_{s=1}^{S}(\tilde{w}(\theta^s))^2}, \quad \text{is based on variance of } \tilde{w}(\theta^s)$$

$S_{\text{eff}} \approx 396$

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

Pareto-$\hat{k}$ and convergence rate

- CLT says that to half the MCSE, need 4 times bigger S

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- 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 at 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