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) → 1 (rounding)

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    - pbeta(0.5, 241945, 251527) $\rightarrow$ 1 (rounding)
    - pbeta(0.5, 241945, 251527, lower.tail=FALSE) $\approx -1.2 \cdot 10^{-42}$
      there is more accuracy near 0

Numerical accuracy – log scale

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

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

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

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- Grid (equal spacing) evaluation with self-normalization

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

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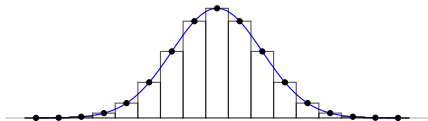
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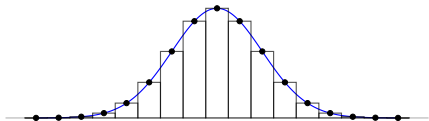
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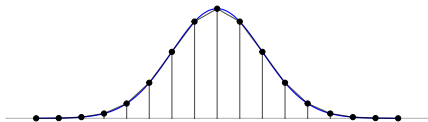
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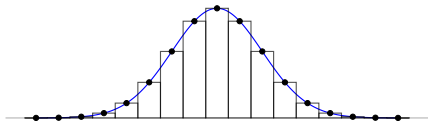
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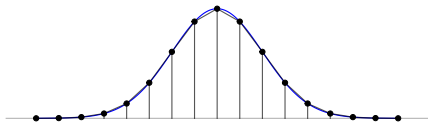
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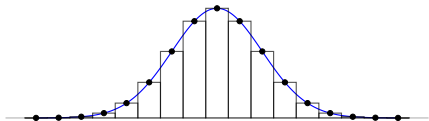
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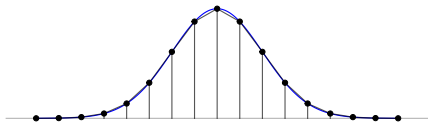
- Adaptive quadrature methods add evaluation points where needed, e.g., R function `integrate()`
- In 2D and higher
  - nested quadrature
  - product rules

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

Monte Carlo

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

Monte Carlo vs. deterministic

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

How many simulation draws are needed?

- How many draws or how big sample size?
- If draws are independent
  - usual methods to estimate the uncertainty due to a finite number of observations (finite sample size)
- Markov chain Monte Carlo produces dependent draws
  - requires additional work to estimate the effective sample size

How many simulation draws are needed?

- Expectation of unknown quantity

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

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)

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  - $\sigma_\theta/\sqrt{S}$ is called Monte Carlo standard error (MCSE)

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- $\sigma_\theta/\sqrt{S}$ is called Monte Carlo standard error (MCSE)
- In practice, σ_θ will be estimated by
  $\sqrt{1/(S-1) \sum_{s=1}^{S} (\theta^{(s)} - \mathrm{E}(\theta))^2}$

Example: Kilpisjärvi summer temperature

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

Data
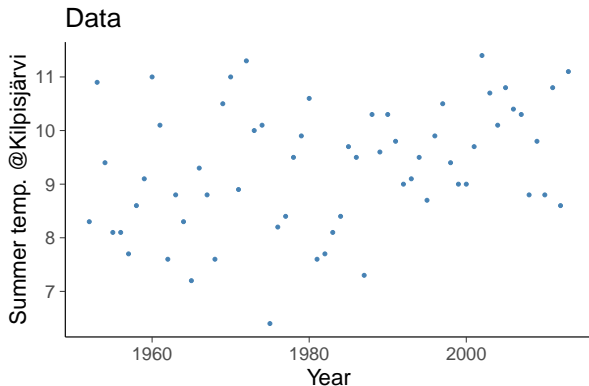
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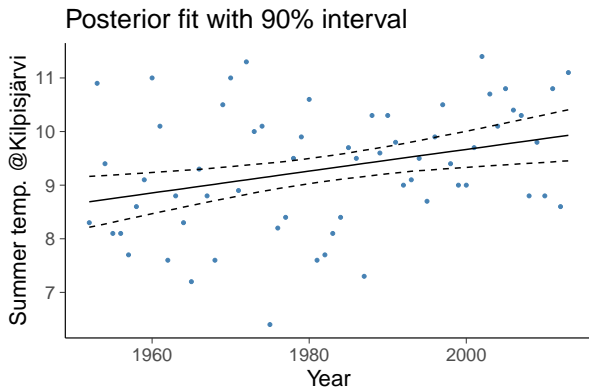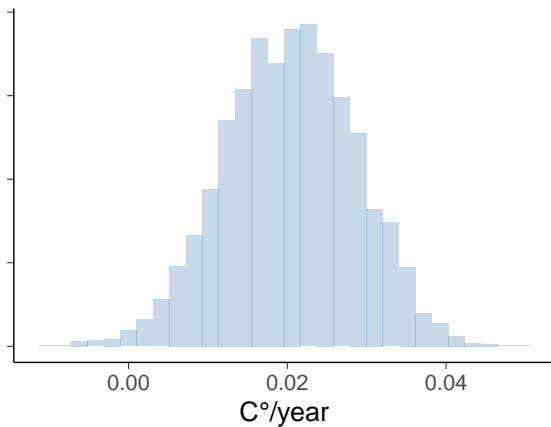
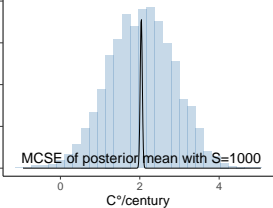Posterior of temperature change

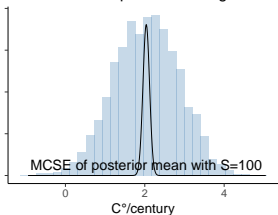# Example: Kilpisjärvi summer temperature

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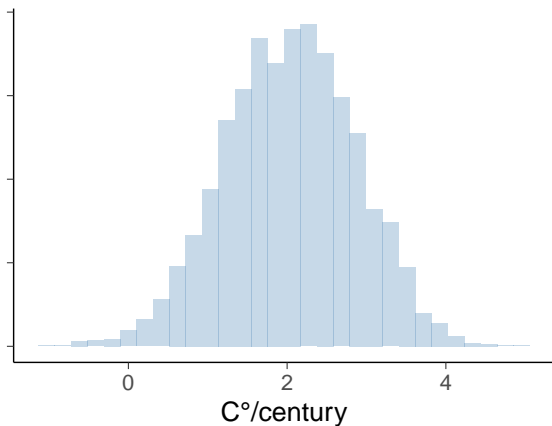
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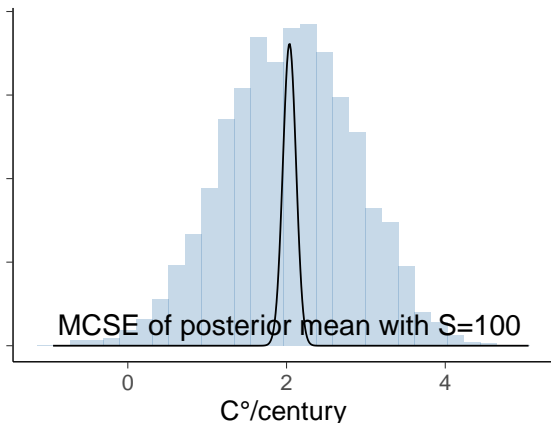
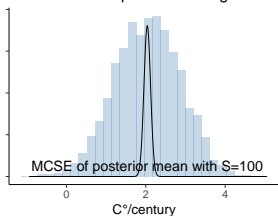$\sigma_\theta \approx 0.83$, MCSE $= \sigma_\theta/\sqrt{S} \approx 0.083$,
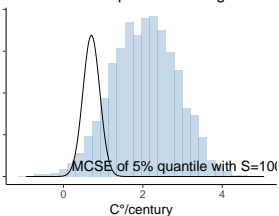in repeated sampling we may expect mean estimate to vary within
(1.8, 2.1) (90% interval)

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Posterior of temperature change

MCSE of posterior mean with S=1000

0   2   4
C°/century
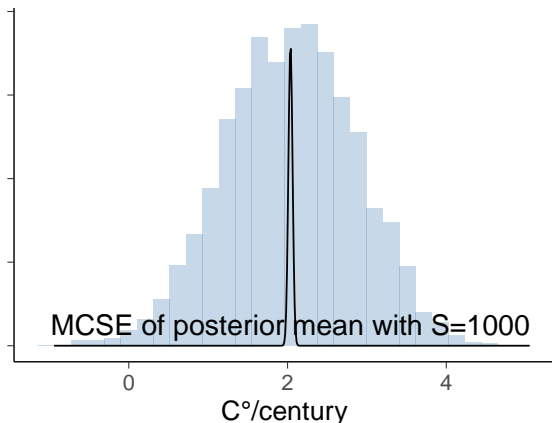
$\sigma_\theta \approx 0.83$, MCSE ≈ 0.026,
in repeated sampling we may expect mean estimate to vary within
(1.9, 2.0) (90% interval)

Example: Kilpisjärvi summer temperature

Posterior of temperature change

MCSE of posterior mean with S=100

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C°/century

Posterior of temperature change

MCSE of posterior mean with S=1000

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C°/century

Example: Kilpisjärvi summer temperature

Posterior of temperature change — MCSE of posterior mean with S=100
C°/century

Posterior of temperature change — MCSE of 5% quantile with S=100
C°/century

Posterior of temperature change — MCSE of posterior mean with S=1000
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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
  - $\rightarrow \ \mathrm{var}(I(\cdot)) = p(1 - p)S$ (Appendix A, p. 579)
  - $\rightarrow$ 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 $\sqrt{p(1-p)/S} \approx 0.02$
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  or from quantiles of beta distribution the range is $(0.02, 0.1)$

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- 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 $S \gg 1/p$
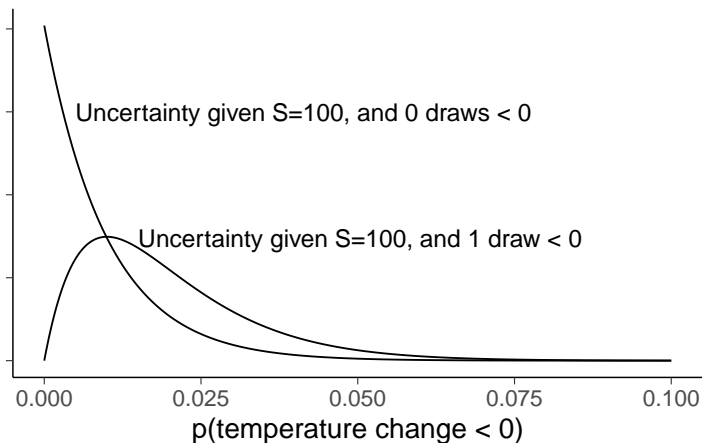
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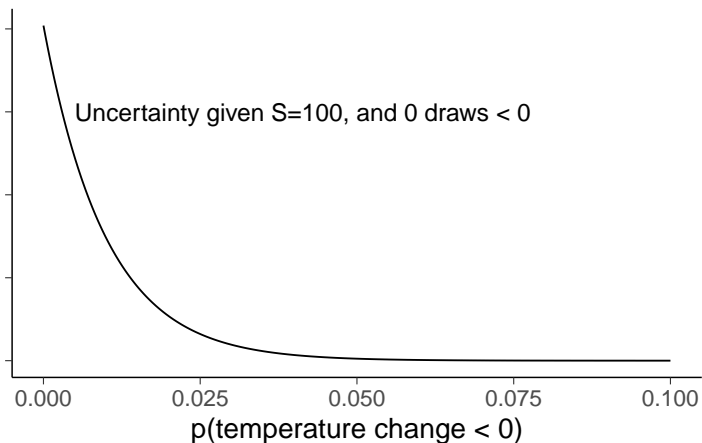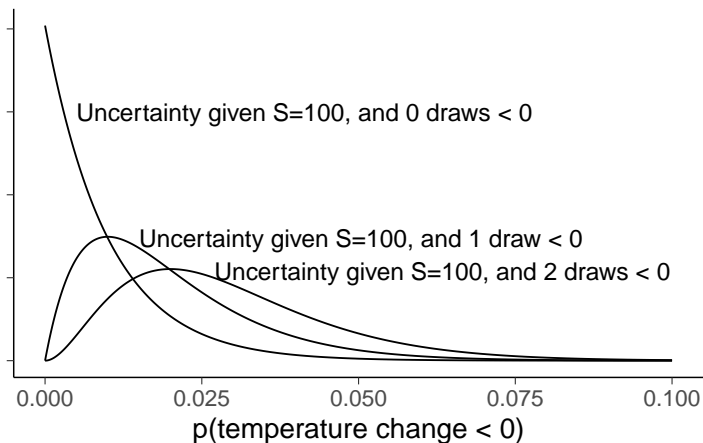
Posterior uncertainty p(temperature change < 0)

Uncertainty given S=100, and 0 draws < 0

p(temperature change < 0)

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Posterior uncertainty p(temperature change < 0)

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Uncertainty given S=100, and 1 draw < 0

Uncertainty given S=100, and 2 draws < 0

p(temperature change < 0)

Example: Kilpisjärvi summer temperature

Posterior uncertainty p(temperature change < 0)

Uncertainty given S=1000, and 8 draws < 0

Example: Kilpisjärvi summer temperature

Posterior uncertainty p(temperature change < 0)

Uncertainty given S=4000, and 34 draws < 0
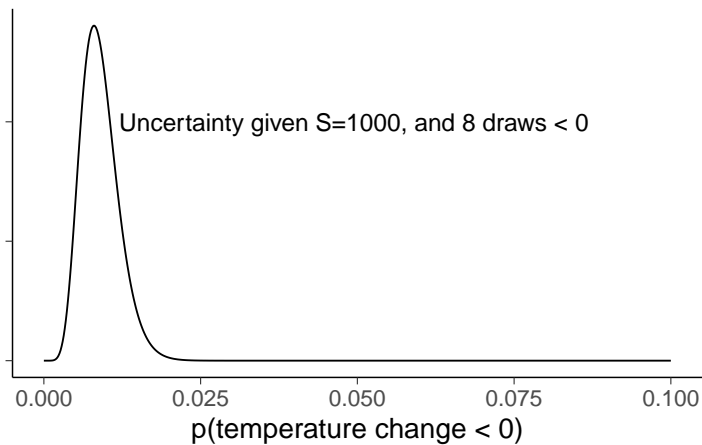
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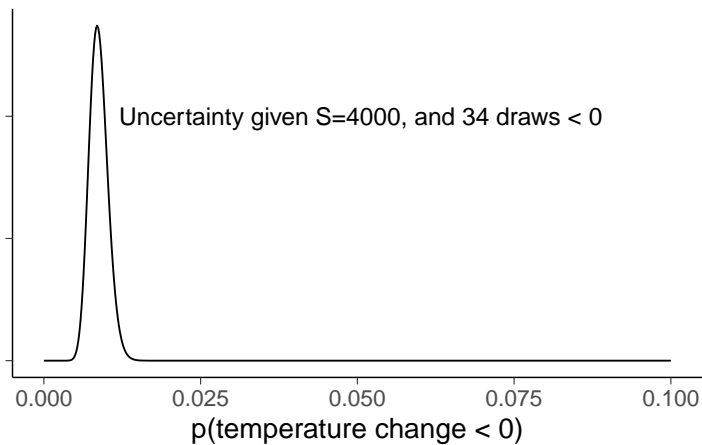
From probabilities to quantiles

- Probability: $p(\theta < A) \approx \frac{1}{S} \sum_l I(\theta^{(s)} < A)$
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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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See also https://avehtari.github.io/casestudies/Digits/digits.html

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    which can be reported as more than 99.9% probability
  - 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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- 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
  - $\rightarrow$ $50^{10} \approx$ 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 $q(\theta|y)/Mg(\theta)$
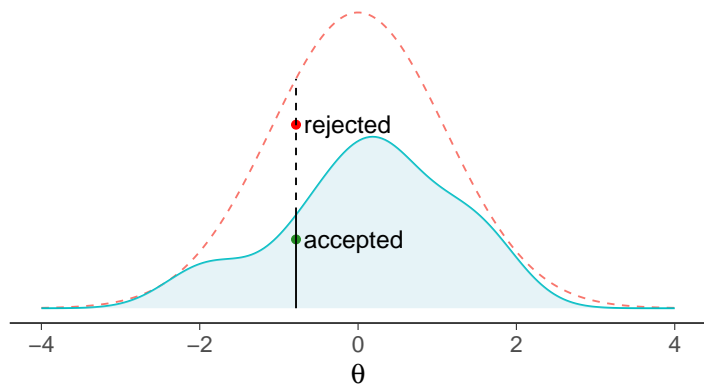
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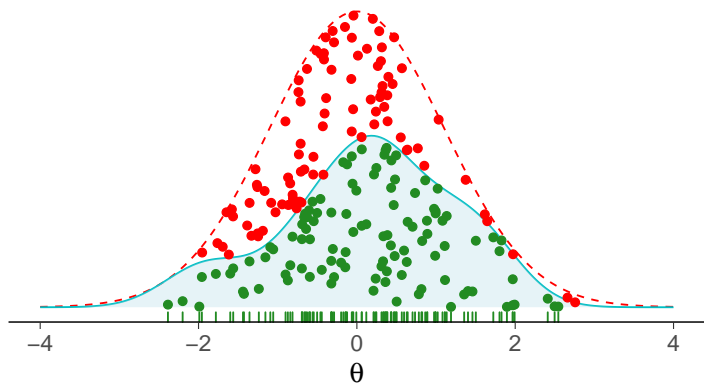
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Rejection sampling

- 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
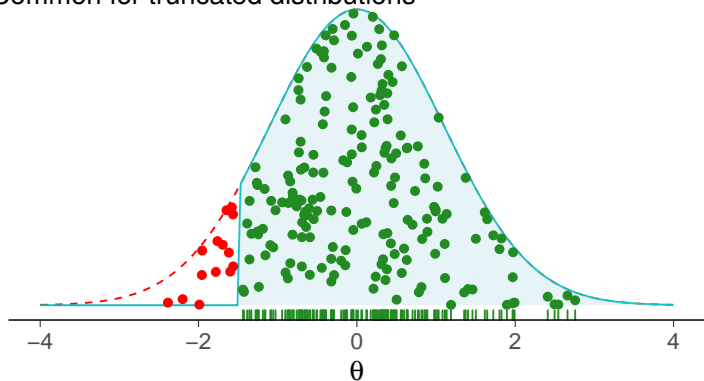
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Rejection sampling

- 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

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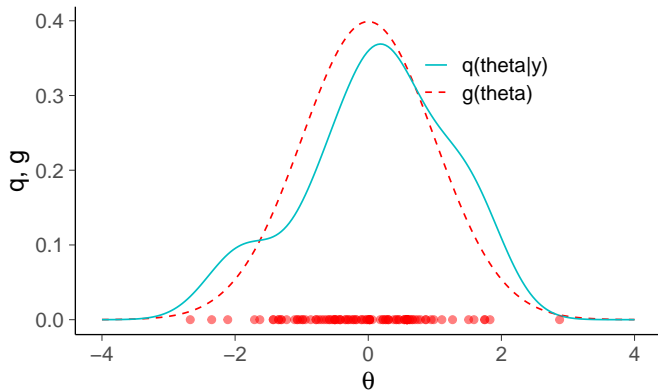
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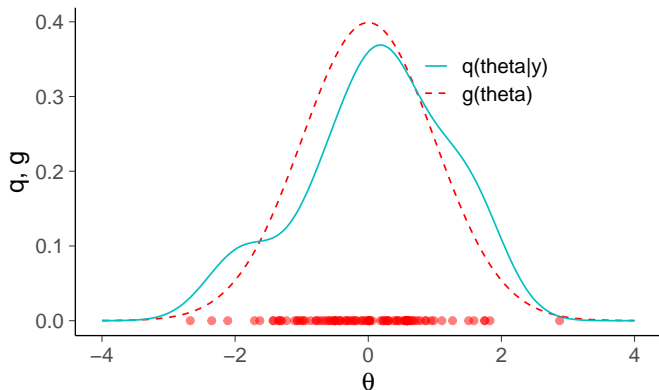
$$E[h(\theta)] \approx \frac{\sum_s w_s h(\theta^{(s)})}{\sum_s w_s}, \qquad \text{where} \quad w_s = \frac{q(\theta^{(s)})}{g(\theta^{(s)})}$$

Importance sampling

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Draws and importance weights
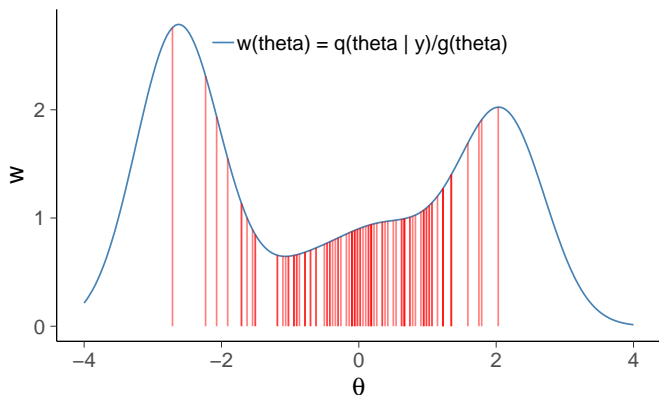
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Some uses of importance sampling

In general selection of good proposal gets more difficult when the number of dimensions increase, but there are many special use case which scale well (e.g. I've used IS up to 10k dimensions)

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In general selection of good proposal gets more difficult when the number of dimensions increase, but there are many special use case which scale well (e.g. I've used IS up to 10k dimensions)

- 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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  - generally not trivial
- Pre-asymptotic and asymptotic behavior can be really different!

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
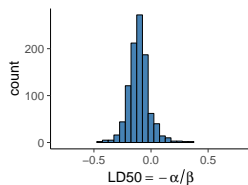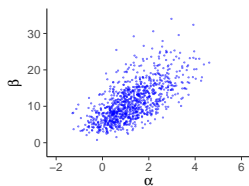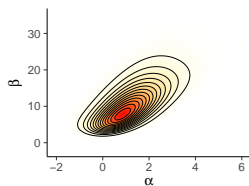
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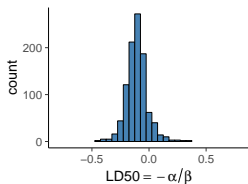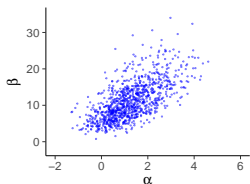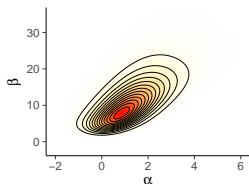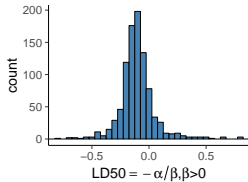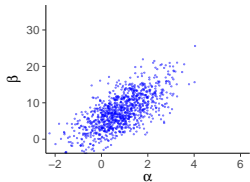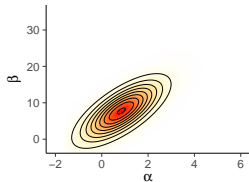
Normal approximation is discussed more in BDA3 Ch 4

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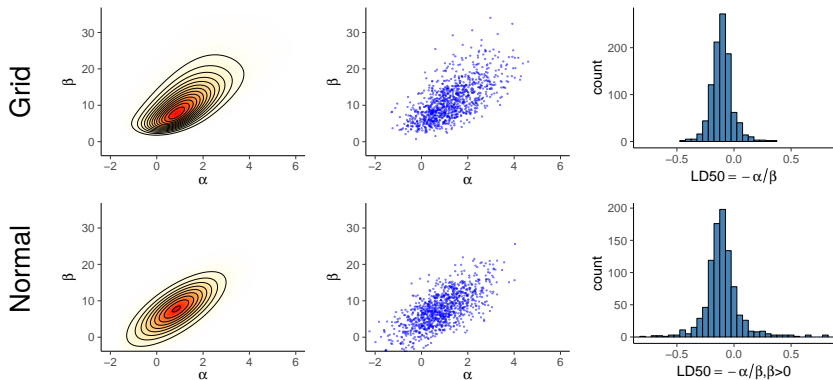
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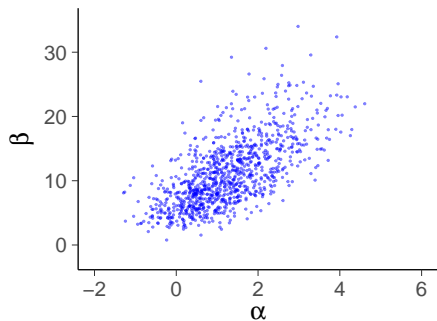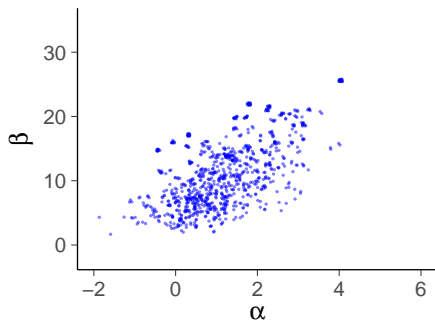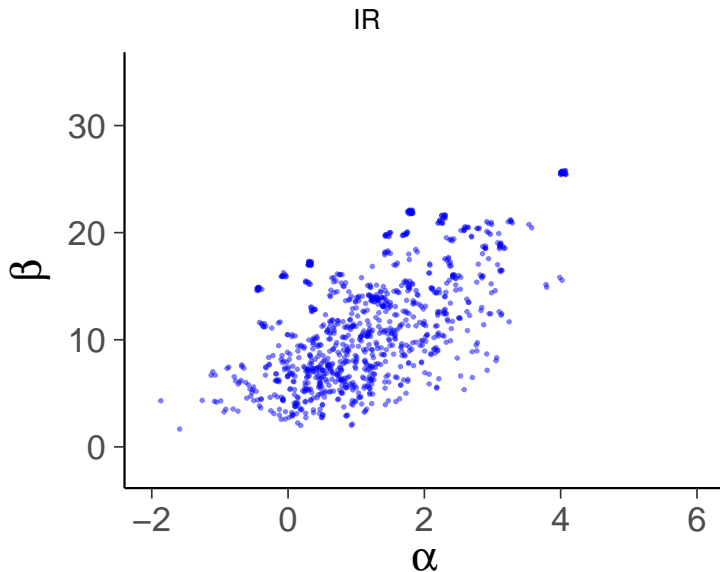But the normal approximation is not that good here:
Grid sd(LD50) $\approx$ 0.1, Normal sd(LD50) $\approx$ .75!

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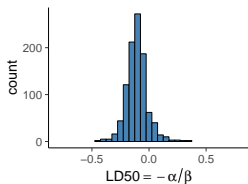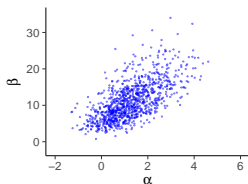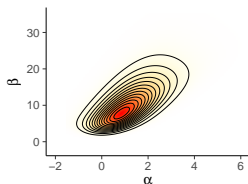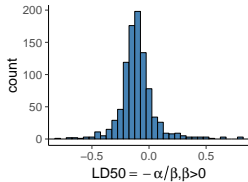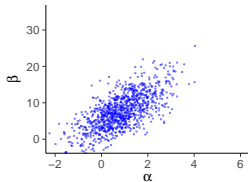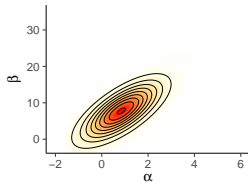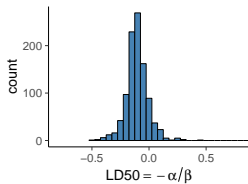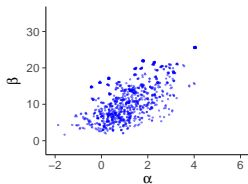
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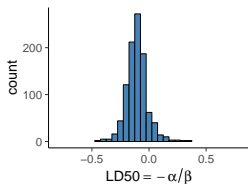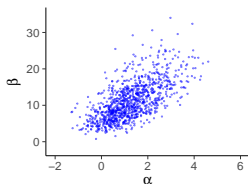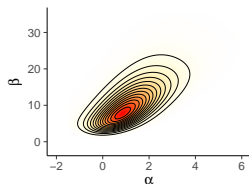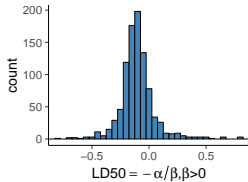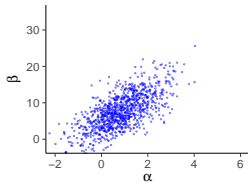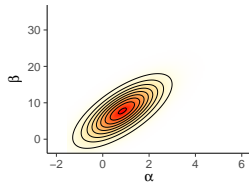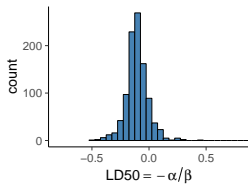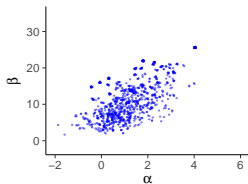
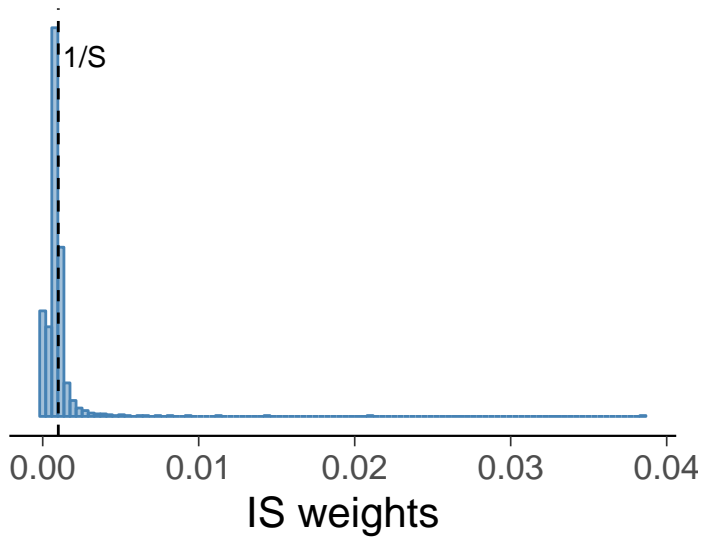Grid sd(LD50) $\approx$ 0.1, IR sd(LD50) $\approx$ 0.1

Example: Importance sampling in Bioassay

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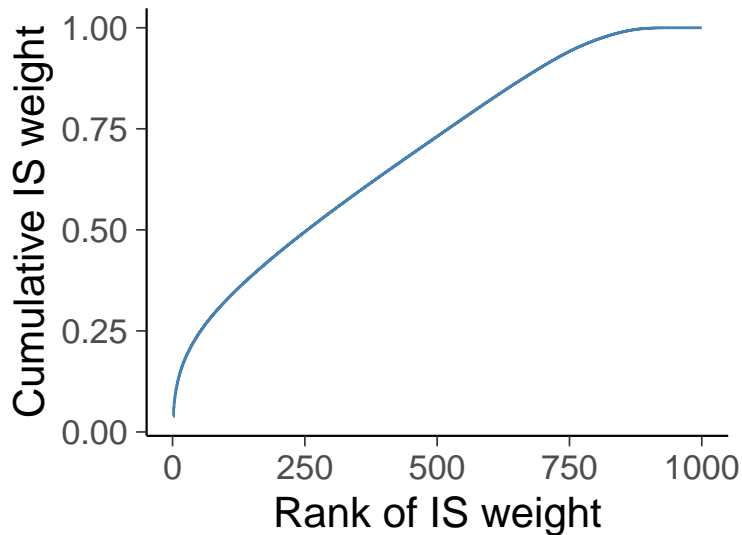# Example: Importance sampling in Bioassay

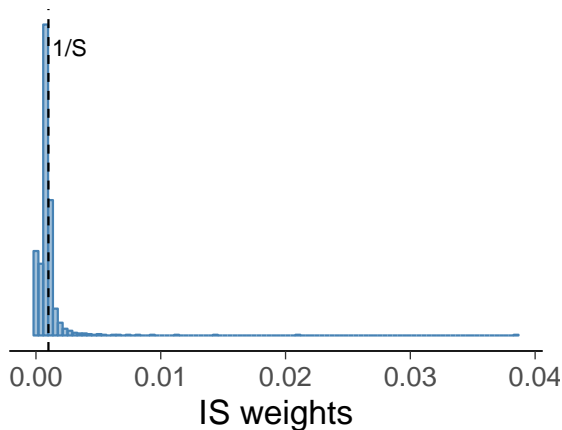IS weights
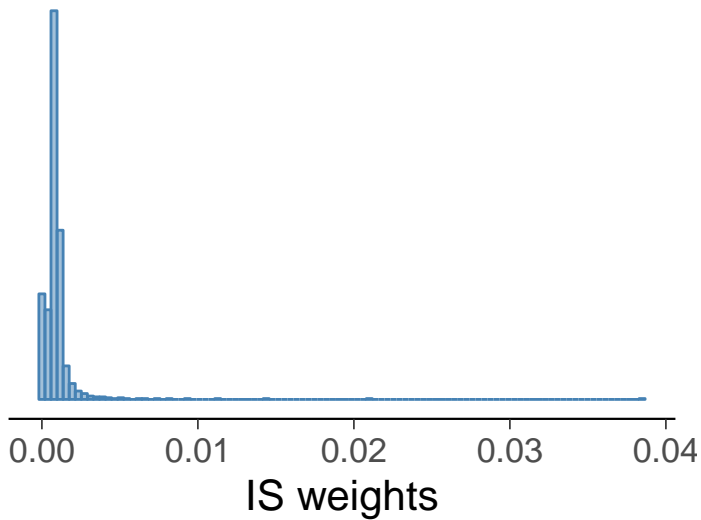
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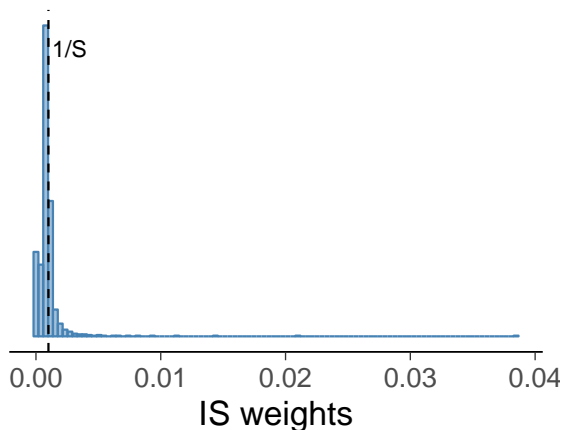# Example: Importance sampling in Bioassay

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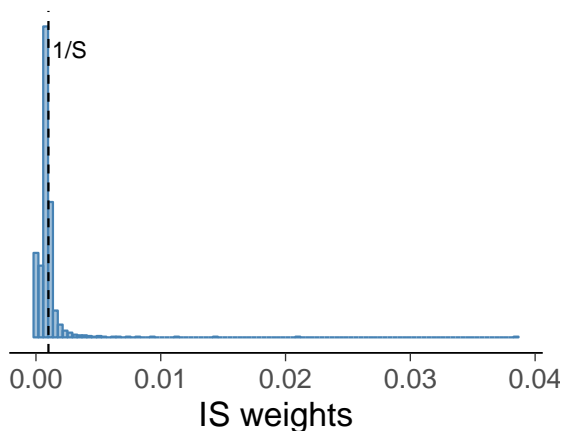
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$$\text{ESS} = \frac{1}{\sum_{s=1}^{S} (\tilde{w}(\theta^s))^2}, \quad \text{where } \tilde{w}(\theta^s) = w(\theta^s) / \sum_{s'=1}^{S} w(\theta^{s'})$$

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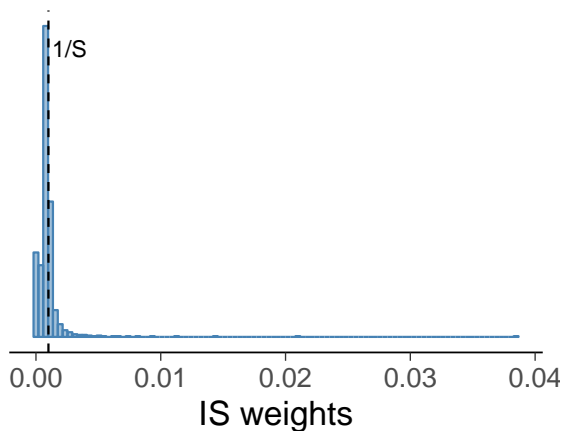http://www.stat.columbia.edu/~gelman/book/errata_bda3.txt

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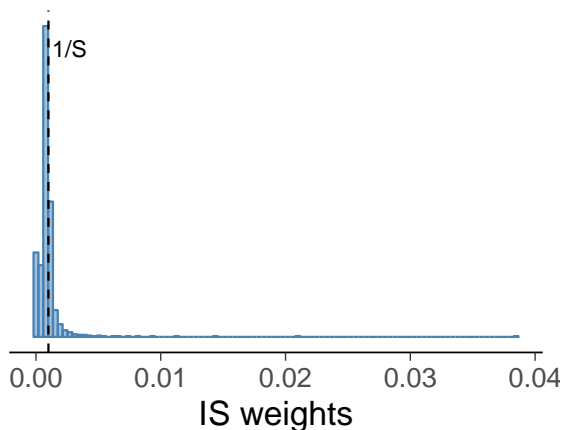
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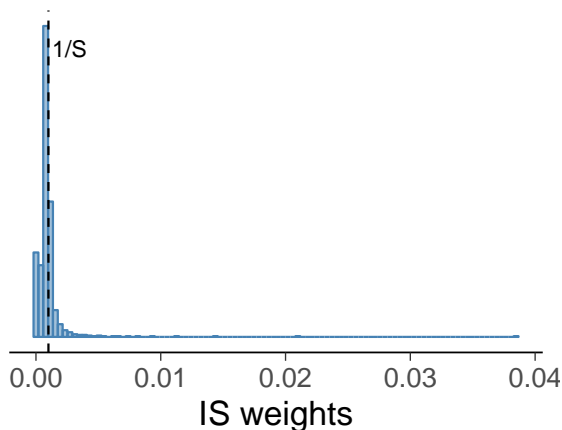

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If one $\tilde{w}(\theta^s) = 1$, and others 0, then $\text{ESS} = 1/1 = 1$
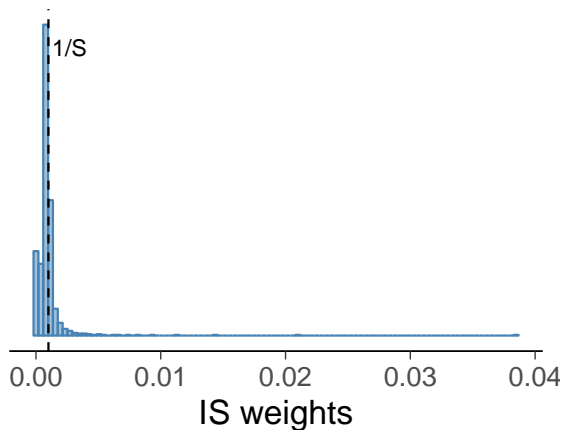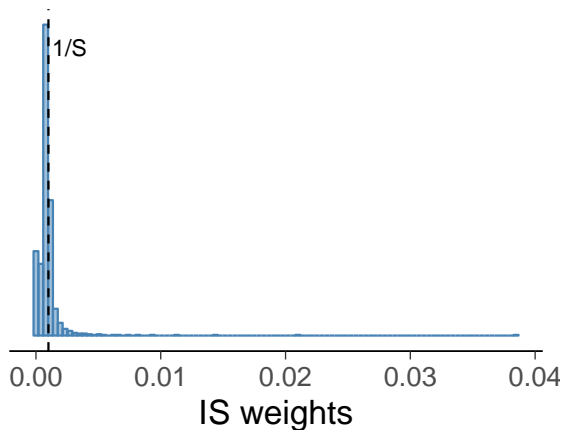
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Pareto-k diagnostic preferably < 0.7:

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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.

Pareto-$\hat{k}$ diagnostic

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  - we can estimate tail of a distribution with a Pareto distribution

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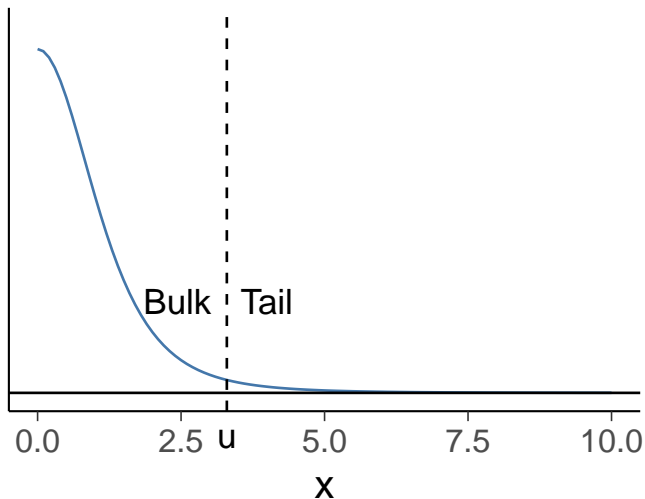
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  - estimate $\hat{k}$ from finite data
  - the statistical behavior of distribution of mean can be predicted by generalized CLT
    - minimum sample size and convergence rate given $\hat{k}$

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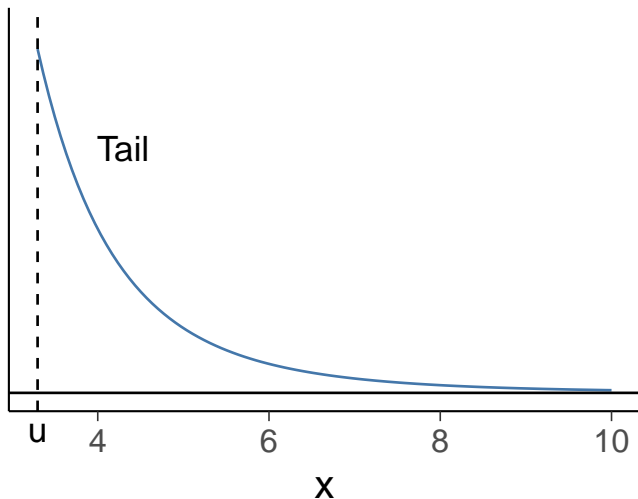
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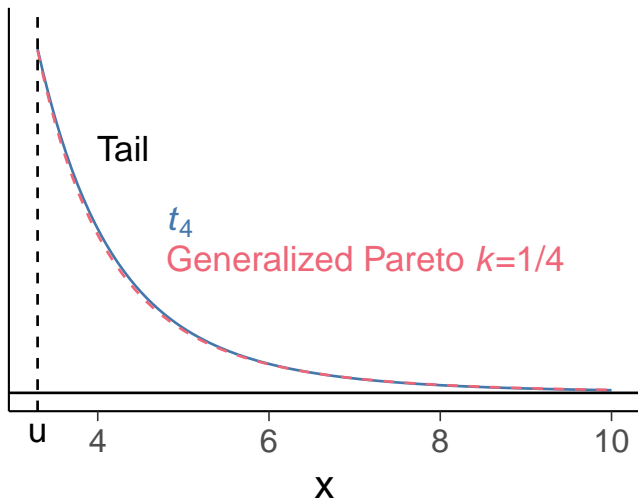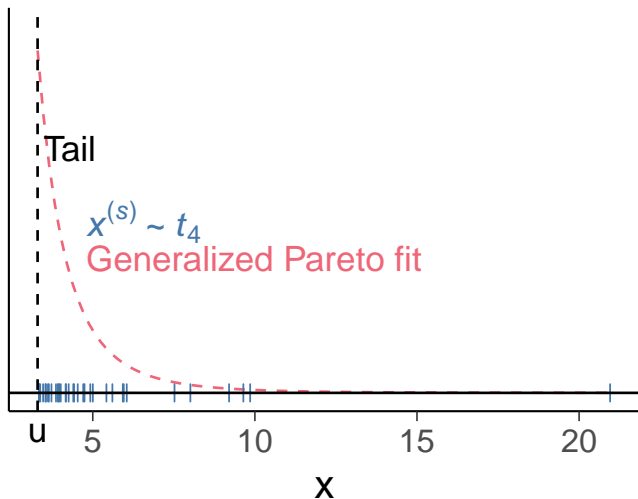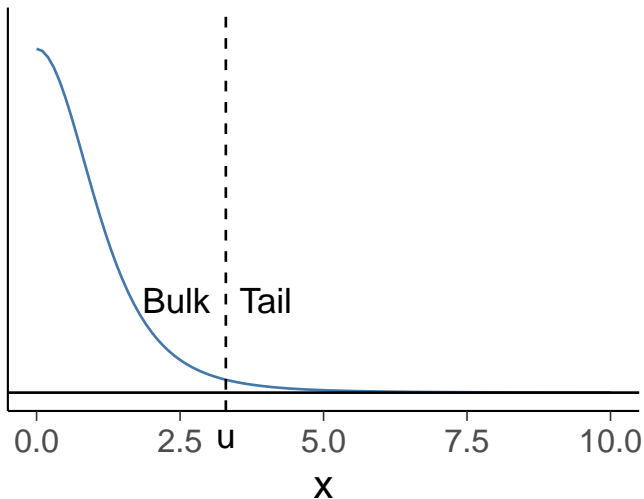
Pareto-$\hat{k}$ diagnostic

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

Example: Importance sampling in Bioassay
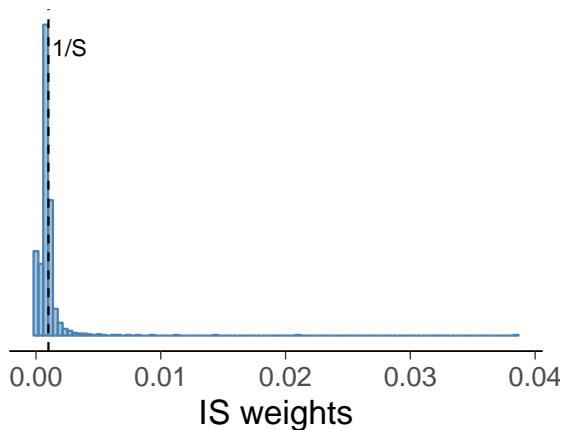
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Pareto-$\hat{k}$ and convergence rate of PSIS

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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