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)
- 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 $q(\cdot)$
- proposal distribution is denoted by $g(\cdot)$

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  - closest value to zero is $\approx 2.2 \cdot 10^{-308}$
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      $800 + \log(1 + exp(800 - 800)) \approx 800.69$
    - e.g. in Metropolis-algorithm compute the log of ratio of densities using the identity
      $\log(a/b) = \log(a) - \log(b)$

It’s all about expectations

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

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

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

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

It's all about expectations

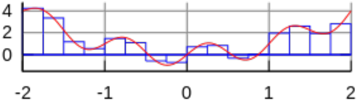
$$E_\theta[f(\theta)] = \int f(\theta)p(\theta|y)d\theta$$

- Conjugate priors and analytic solutions
- Grid integration and other quadrature rules
- Independent Monte Carlo, rejection and importance sampling
- Markov Chain Monte Carlo
- Distributional approximations (Laplace, VB, EP)

Quadrature integration

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

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



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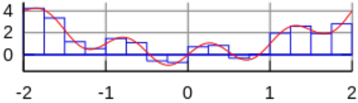

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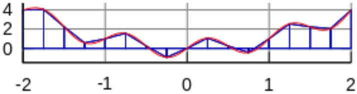
- In 1D further variations, e.g. trapezoid



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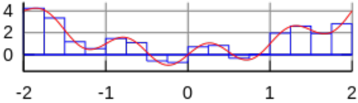

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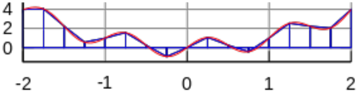

- In 2D and higher
  - nested quadrature
  - product rules

Monte Carlo - history

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

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- 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

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

$$\mathrm{E}(\theta) \approx \frac{1}{L}\sum_{l} \theta^{(l)}$$

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

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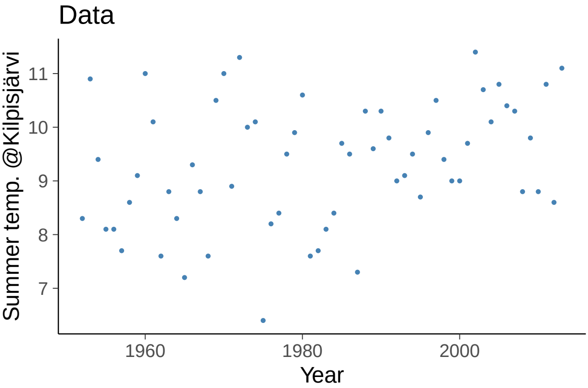
  - See Ch 4 for counter-examples for asymptotic normality

Example: Kilpisjärvi summer temperature

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



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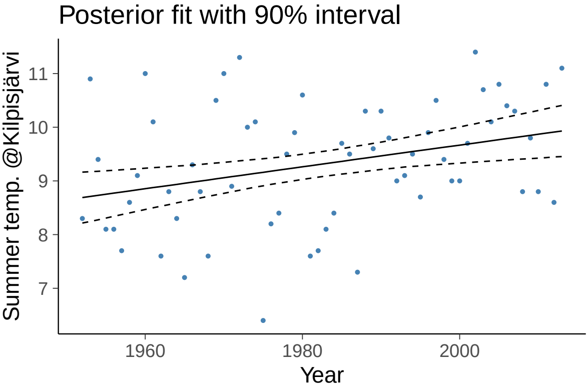

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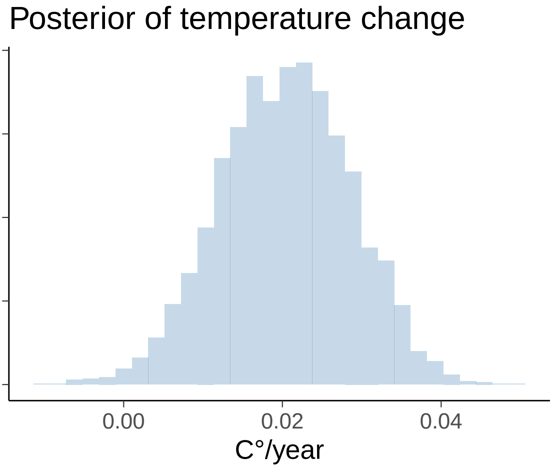

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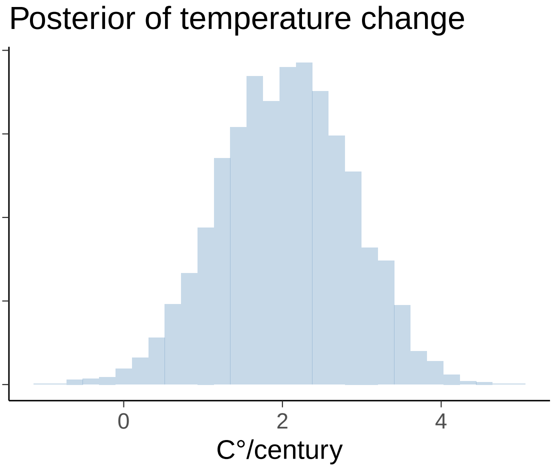

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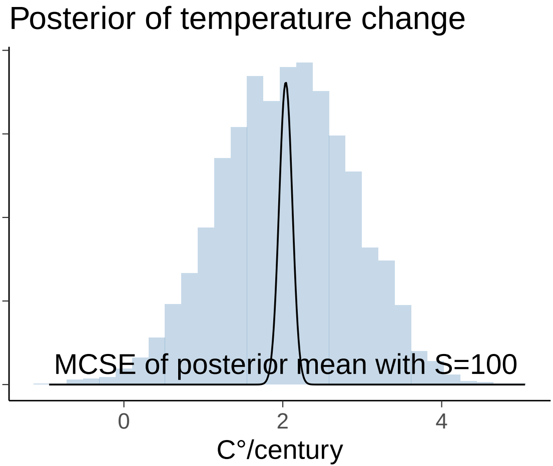

$\sigma_\theta \approx$ 0.827, MCSE $\approx$ 0.0827, total deviation $\approx$ 0.831

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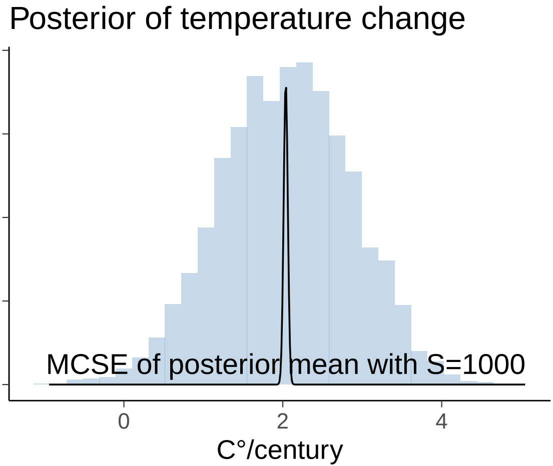

$\sigma_\theta \approx 0.827$, MCSE ≈ 0.0261, total deviation ≈ 0.827

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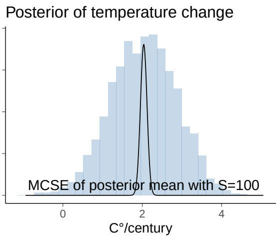

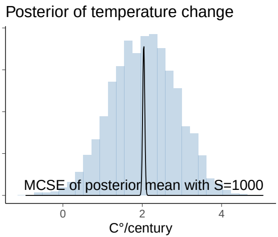

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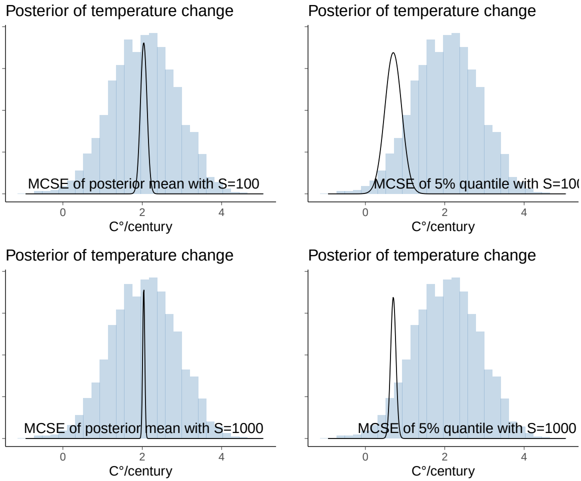

Posterior of temperature change

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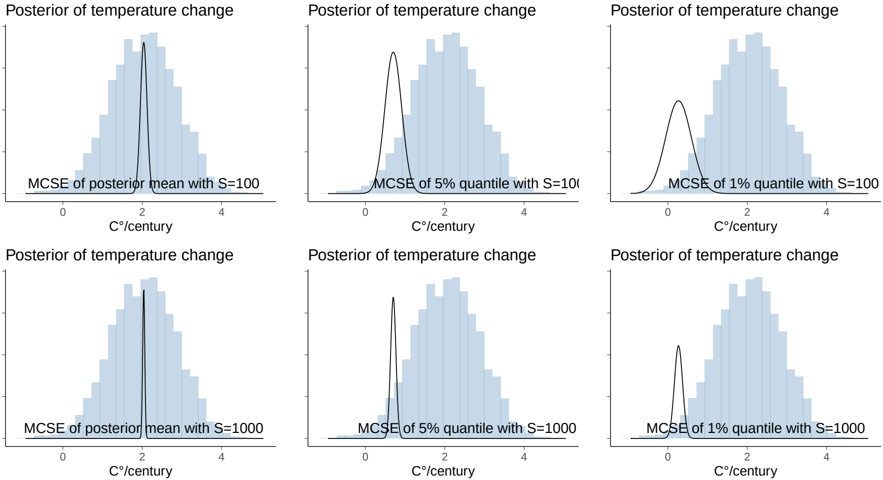

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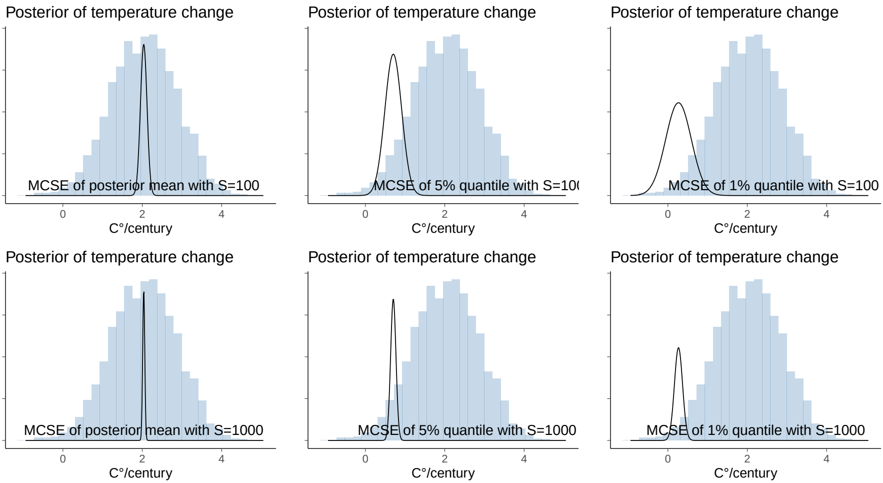

Tail quantiles are more difficult to estimate

How many simulation draws are needed?

- Posterior probability

$$p(\theta \in A) \approx \frac{1}{L} \sum_{l} I(\theta^{(l)} \in A)$$

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

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

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  ie. accuracy is about 5% units

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  - $L = 2500$ draws needed for 1% unit accuracy

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

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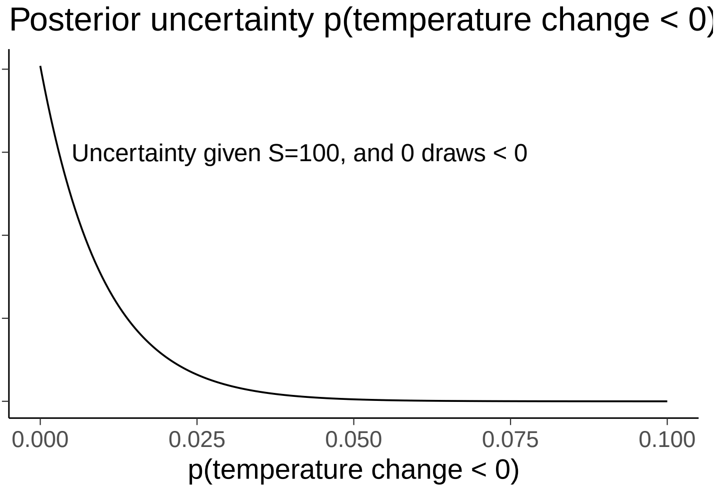

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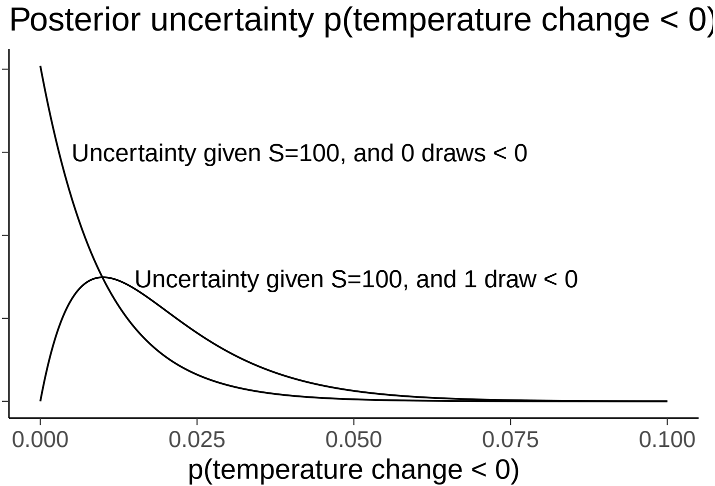

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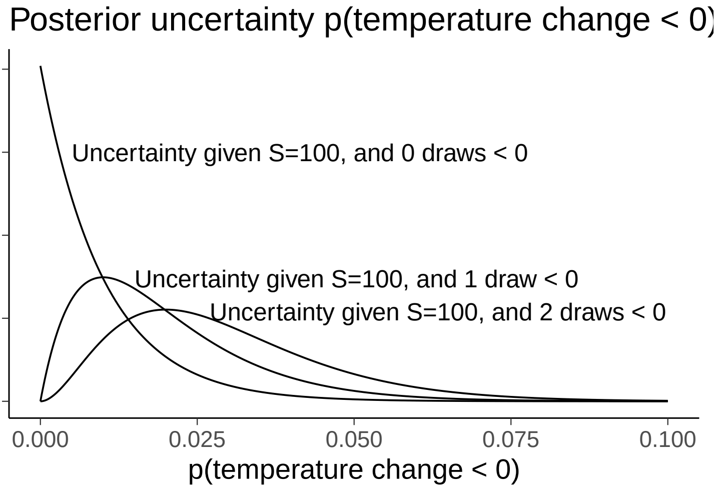

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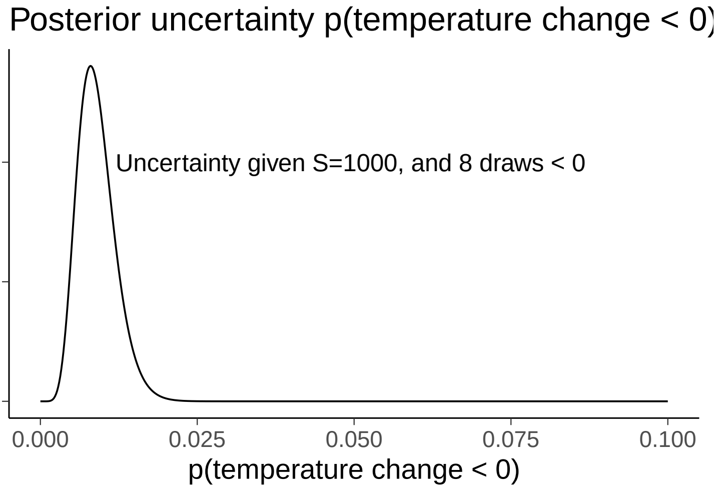

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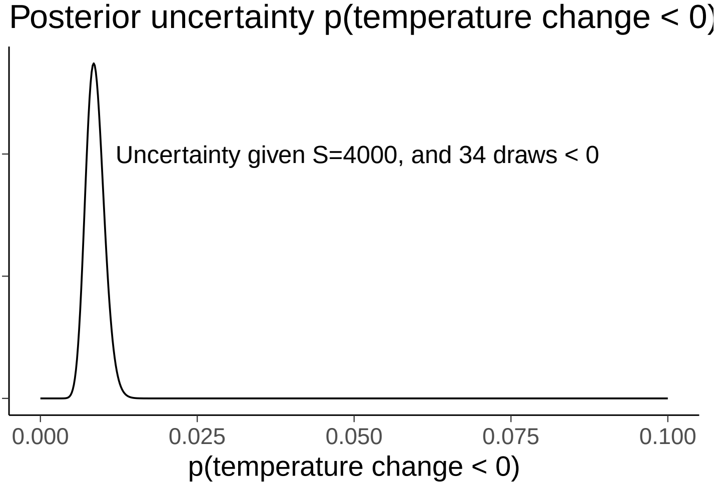

How many simulation draws are needed?

- 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 unifrom random numbers (eg. 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

  $$X_1 = \sqrt{-2\log(U_1)}\cos(2\pi U_2)$$
  $$X_2 = \sqrt{-2\log(U_1)}\sin(2\pi U_2)$$

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

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  $$X_1 = \sqrt{-2\log(U_1)}\cos(2\pi U_2)$$
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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 distrbution more than ten different methods
  - e.g. R uses inverse-CDF

Grid sampling and curse of dimensionality

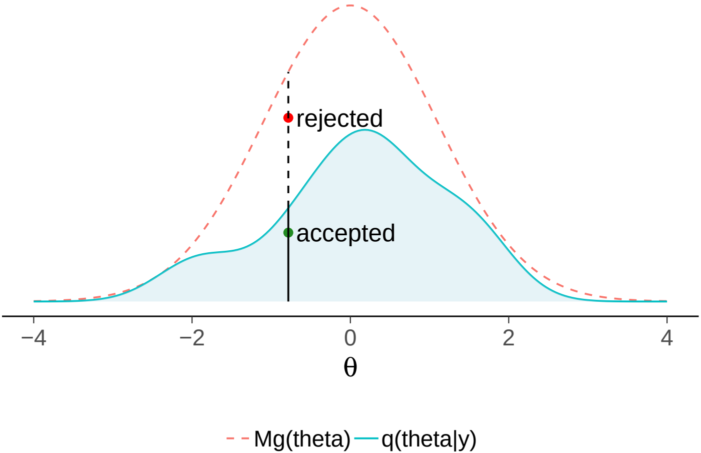
- 10 parameters
- if we don't know beforehand where the posterior mass is
  - need to choose wide box for the grid
  - need to have enough grid points to get some of them where essential mass is
- e.g. 50 or 1000 grid points per dimension
  - → $50^{10} \approx$ 1e17 grid points
  - → $1000^{10} \approx$ 1e30 grid points
- R and my current laptop can compute density of normal distribution about 20 million times per second
  - → evaluation in 1e17 grid points would take 150 years
  - → evaluation in 1e30 grid points would take 1 500 billion years

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 $Mg(\theta)/q(\theta|y)$



Rejection sampling

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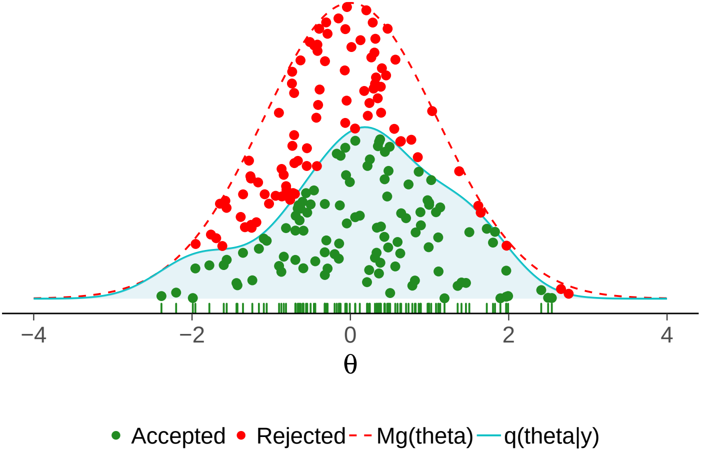
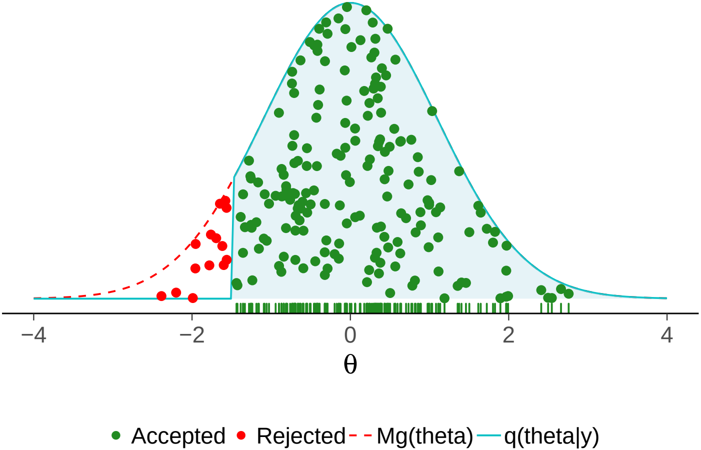


Rejection sampling

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

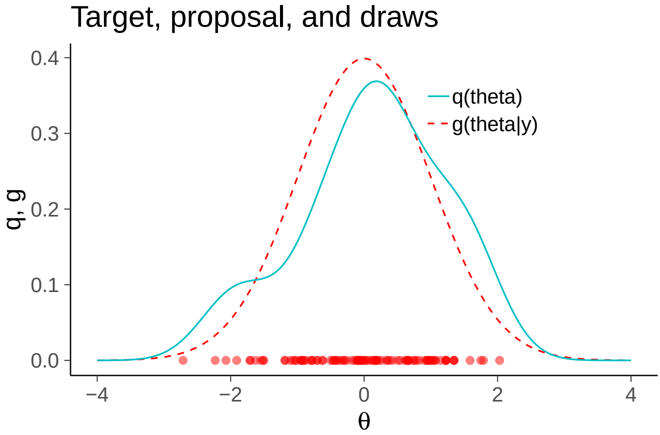


Rejection sampling

- 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

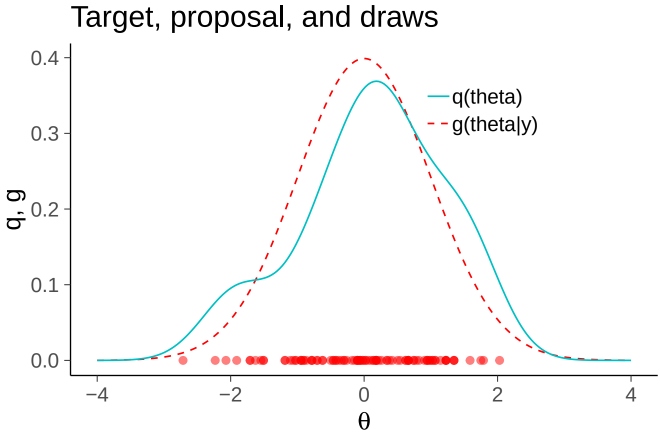
Importance sampling

- Proposal does not need to have a higher value everywhere



Importance sampling

- Proposal does not need to have a higher value everywhere



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

Importance sampling

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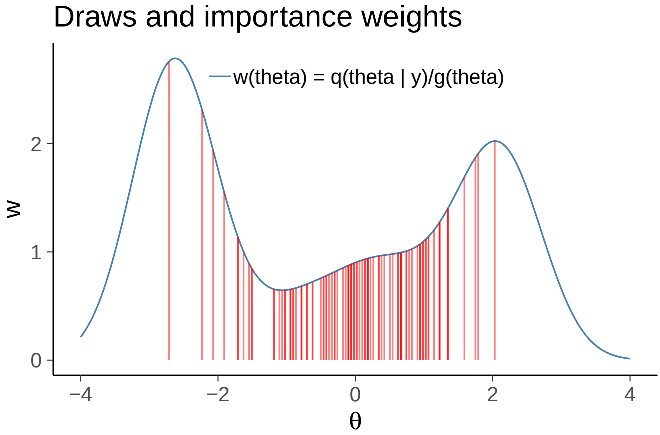


$$E[f(\theta)] \approx \frac{\sum_s w_s f(\theta^{(s)})}{\sum_s w_s}, \qquad \text{where} \quad w_s = \frac{q(\theta^{(s)})}{g(\theta^{(s)})}$$

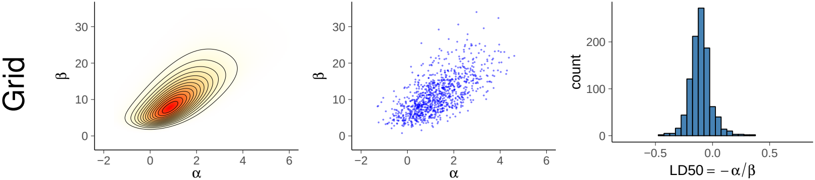
Importance sampling

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

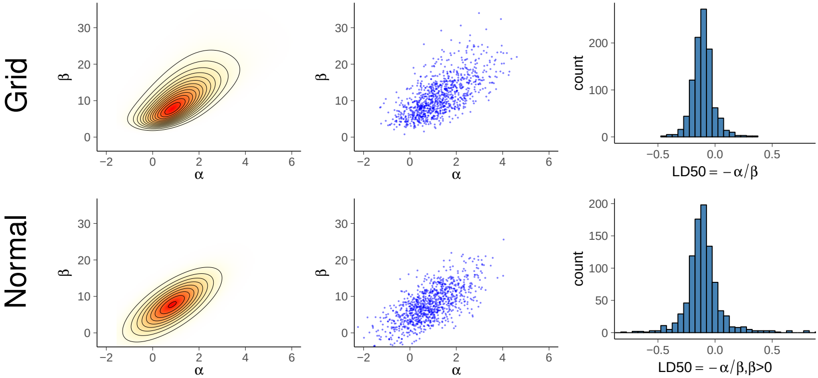
Importance sampling

- Variation of the weights affect the effective sample size
  - if single weight dominates, we have effectively one sample
  - if weights are equal, we have effectively S draws
- Central limit theorem holds only if variance of the weight distribution is finite
- See Vehtari, Gelman and Gabry (2017). Pareto smoothed importance sampling. arXiv preprint arXiv:1507.02646, https://arxiv.org/abs/1507.02646 for improved diagnostics and stability.

Example: Importance sampling in Bioassay

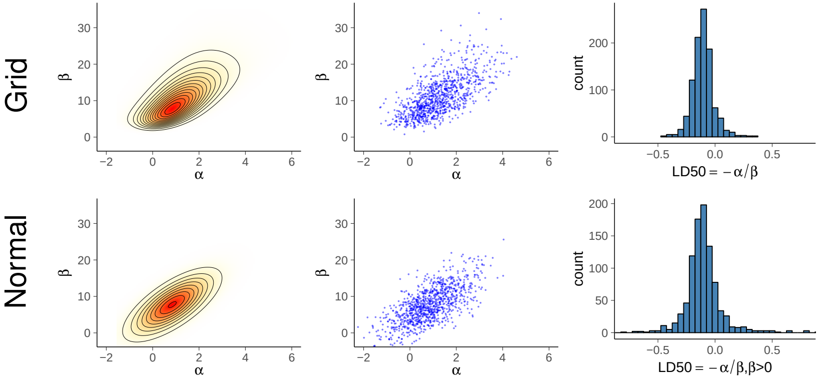


Example: Importance sampling in Bioassay



Normal approximation is discussed more in BDA3 Ch 4

Example: Importance sampling in Bioassay

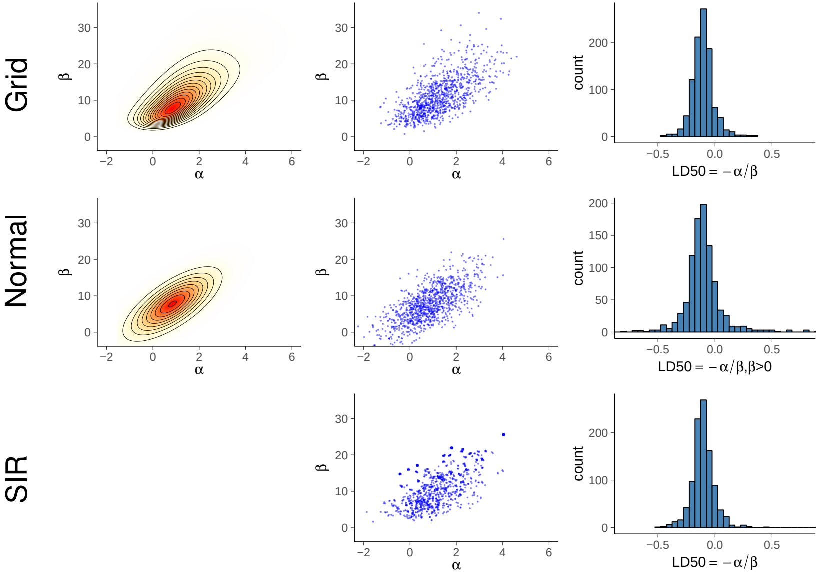


Normal approximation is discussed more in BDA3 Ch 4

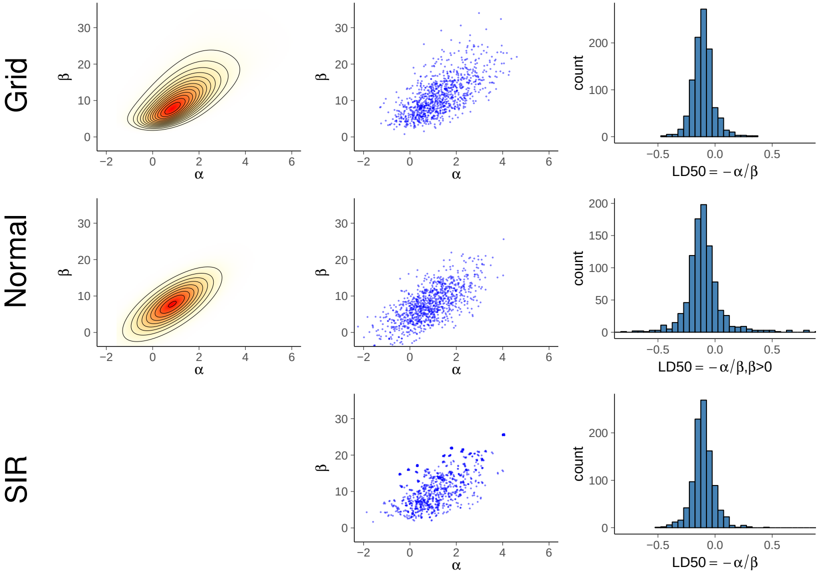
But the normal approximation is not that good here:

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

Example: Importance sampling in Bioassay

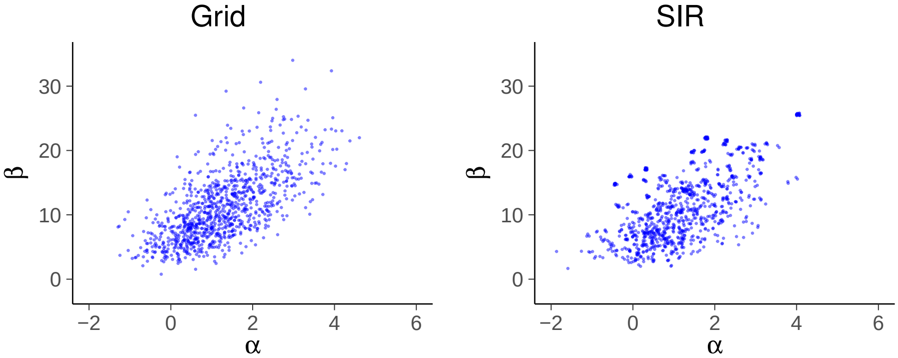


Example: Importance sampling in Bioassay



Grid sd(LD50) ≈ 0.1, SIR sd(LD50) ≈ 0.1

Example: Importance sampling in Bioassay



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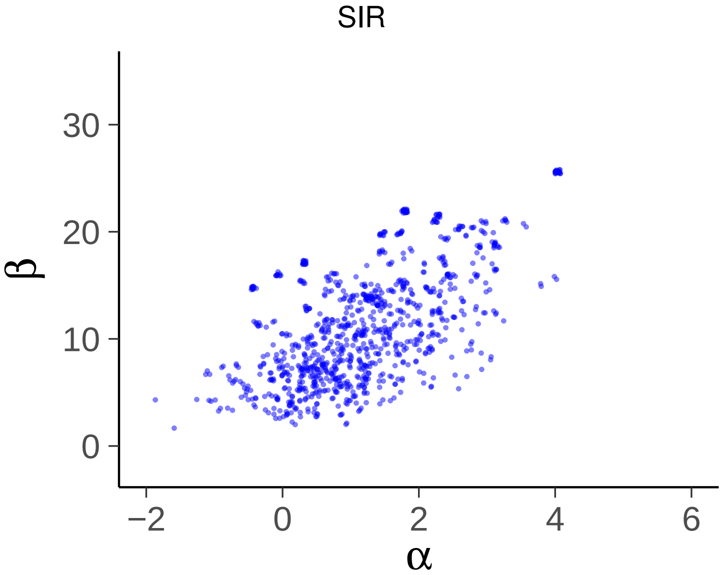

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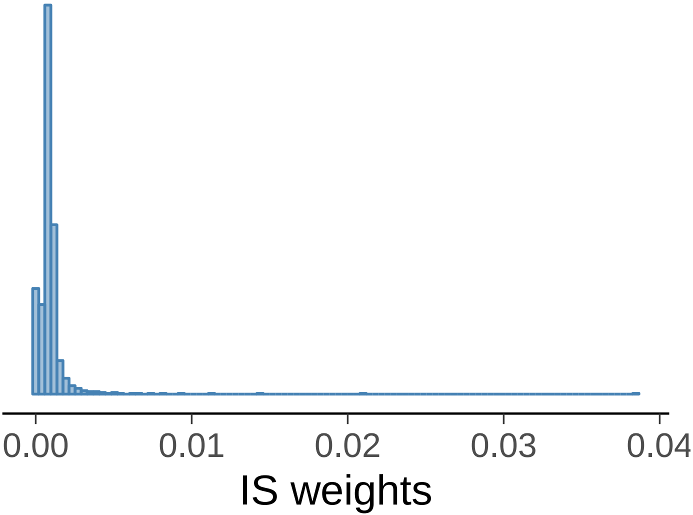

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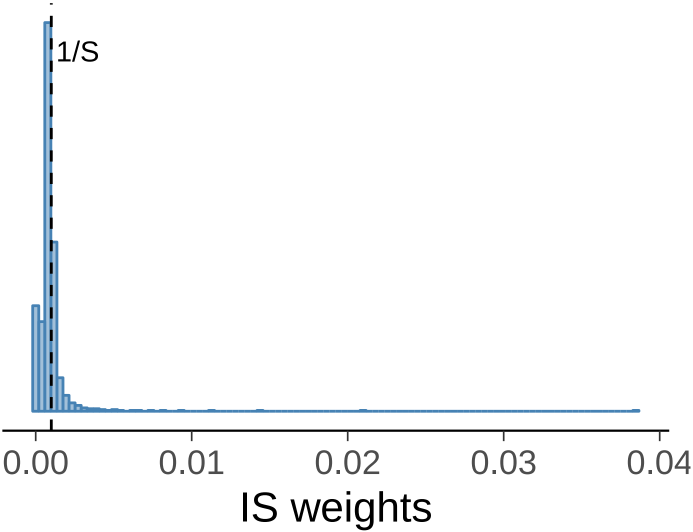

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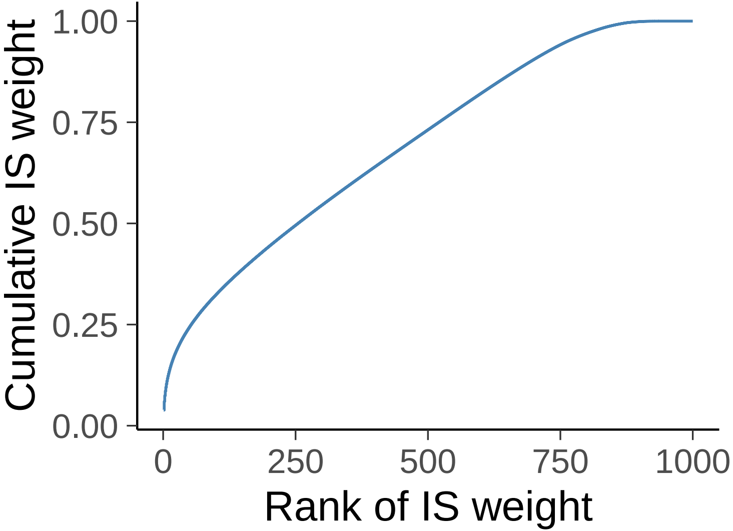
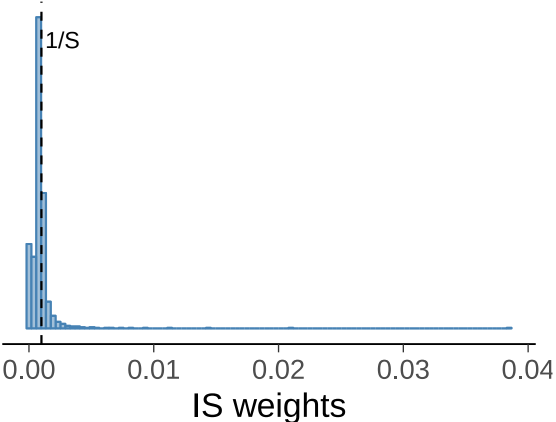
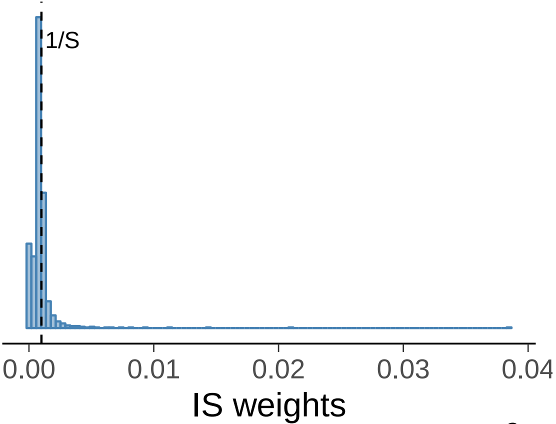


Example: Importance sampling in Bioassay



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

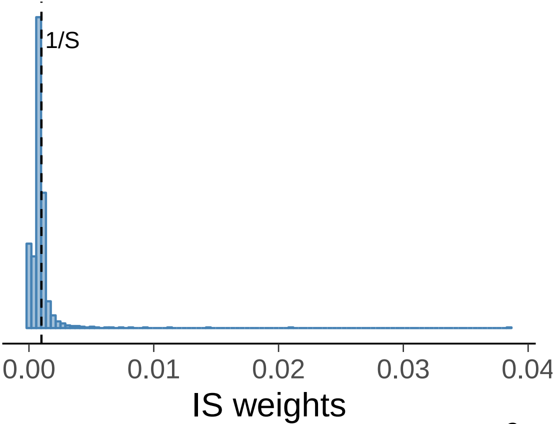
Example: Importance sampling in Bioassay



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

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

Example: Importance sampling in Bioassay



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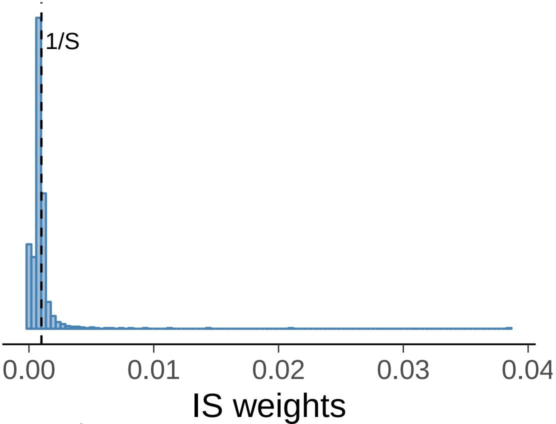
$S_{\text{eff}} \approx 270$

Example: Importance sampling in Bioassay



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

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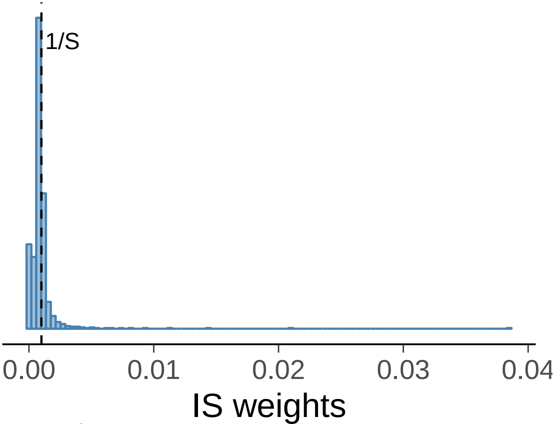
Example: Importance sampling in Bioassay



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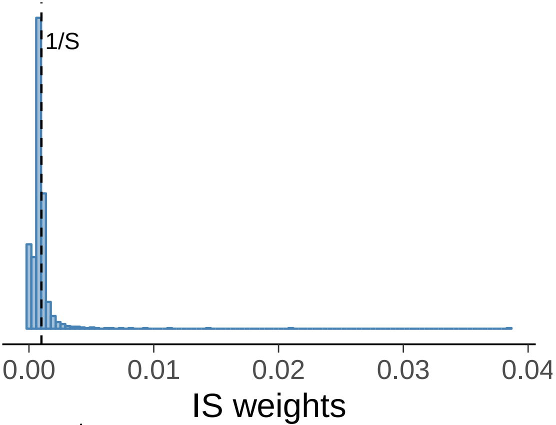
$S_{\text{eff}} \approx 270$

Pareto-k diagnostic preferably < 0.7:

Example: Importance sampling in Bioassay



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

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

Pareto-k diagnostic preferably < 0.7: $\hat{k} \approx 0.76$

Pareto smoothed importance sampling

- Pareto-k diagnostic estimate the number of existing moments ($\lfloor 1/k \rfloor$)
- Finite variance and central limit theorem for $k < 1/2$
- Finite mean and generalized central limit theorem for $k < 1$, but pre-asymptotic constant grows impractically large for $k > 0.7$
- See Vehtari, Gelman and Gabry (2017). Pareto smoothed importance sampling. arXiv preprint arXiv:1507.02646, https://arxiv.org/abs/1507.02646 for improved diagnostics and stability.

Importance sampling leave-one-out cross-validation

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

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

Curse of dimensionality

- Number of grid points increases exponentially
- Concentration of the measure, ie, 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 jow 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