### 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, Lecture 9)
- 10.5 How many simulation draws are needed?
  - see chapter notes for how many significant digits to report
  - this week focus on independent draws and importance sampling, next week necessary adjustments needed for Markov chain Monte Carlo
- 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  $g(\cdot)$

- Floating point presentation of numbers. e.g. with 64bits
  - closest value to zero is  $\approx 2.2 \cdot 10^{-308}$ 
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    - pbeta(0.5, 241945, 251527, lower.tail=FALSE)  $\approx -1.2 \cdot 10^{-42}$  there is more accuracy near 0

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    - e.g. in Metropolis-algorithm (Assignment 5) compute the log of ratio of densities using the identity log(a/b) = log(a) - log(b)

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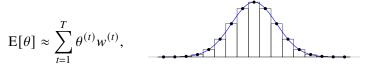
 Monte Carlo methods which can sample from p(θ<sup>(s)</sup>|y) using only q(θ<sup>(s)</sup>|y) (each draw has weight 1/S)

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

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

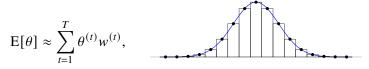
- Conjugate priors and analytic solutions (Ch 1-5, Lec 2–3)
- Grid integration and other quadrature rules (Ch 3, 10, Lec 3–4)
- Independent Monte Carlo, rejection and importance sampling (Ch 10, Lec 4)
- Markov Chain Monte Carlo (Ch 11-12, Lec 5–6)
- Distributional approximations (Laplace, VB, EP) (Ch 4, 13)

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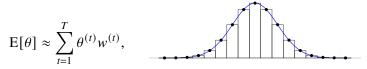


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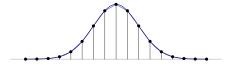


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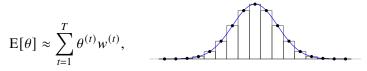
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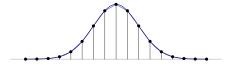
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- Adaptive quadrature methods add evaluation points where needed, e.g., R function integrate()
- In 2D and higher
  - nested quadrature
  - product rules

### Monte Carlo - history

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

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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)

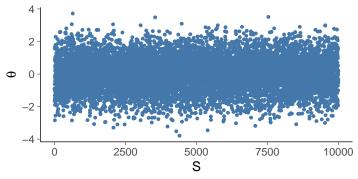
- How many draws or how big sample size?
- If draws are independent
  - usual methods to estimate the uncertainty due to a finite number of observations (finite sample size)
- Markov chain Monte Carlo produces dependent draws
  - requires additional work to estimate the effective sample size
  - next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

- Expectation of unknown quantity  $E(\theta) \approx \frac{1}{S} \sum_{s=1}^{S} \theta^{(s)}$ 
  - If *S* is big,
  - $\theta^{(s)}$  are independent, and
  - $p(\theta)$  has finite variance,

then the central limit theorem (CLT) states that the distribution of the expectation approaches normal distribution (see BDA3 Ch 4) with variance  $\sigma_a^2/S$  (asymptotic normality)

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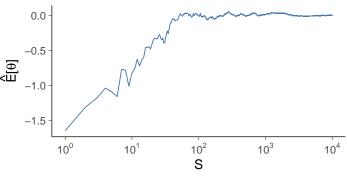
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rnorm(n=10000, mean=0, sd=1)

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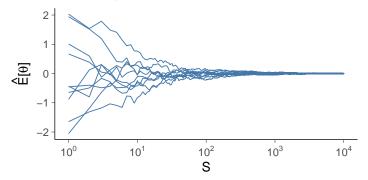
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cummean(rnorm(n=10000, mean=0, sd=1))

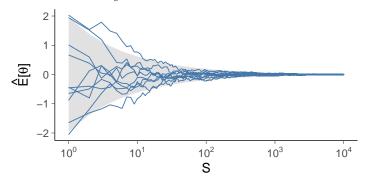
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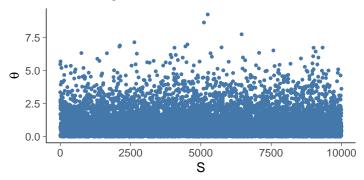
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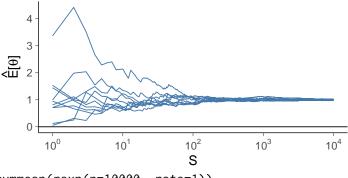
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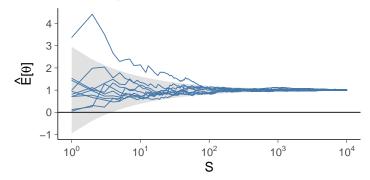
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- $\sigma_{\theta}/\sqrt{S}$  is called Monte Carlo standard error (MCSE)

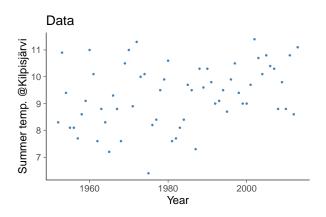
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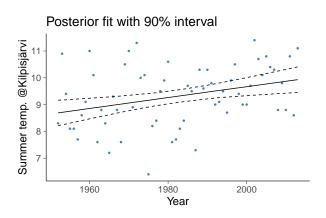
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- In practice,  $\sigma_{\theta}$  will be estimated by

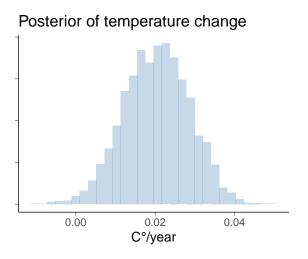
$$\sqrt{1/(S-1)\sum_{s=1}^{S}(\theta^{(s)}-E(\theta))^2}$$

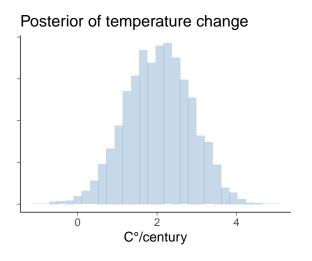
Average temperature in June, July, and August at Kilpisjärvi, Finland in 1952–2013

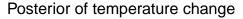


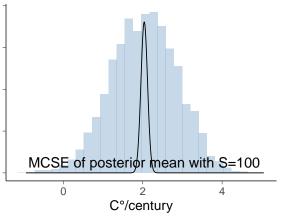
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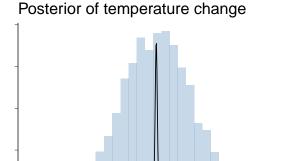








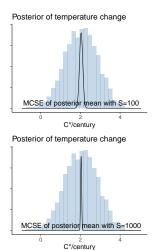
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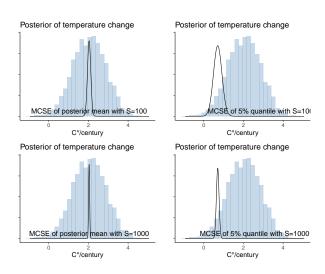


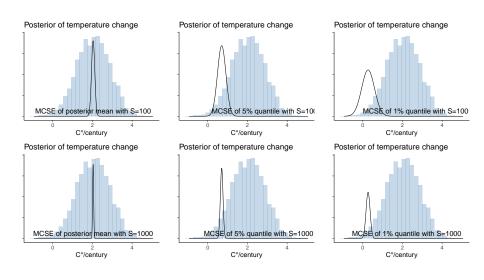
MCSE of posterior mean with S=1000

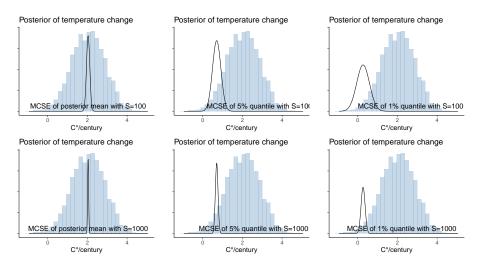
C°/century

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









Tail quantiles are more difficult to estimate

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

Posterior probability

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

- $I(\cdot)$  is binomially distributed as  $p(\theta \in A)$ 
  - use beta CDF, or normal approximation
  - $\rightarrow$  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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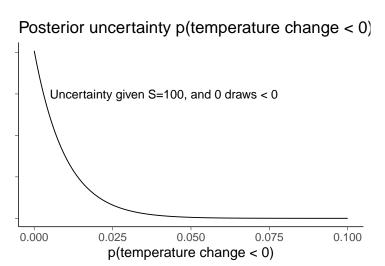
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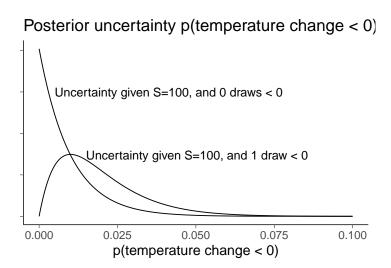
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- S = 2000 draws needed for 1% unit accuracy

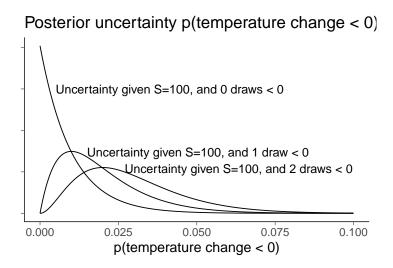
Posterior probability

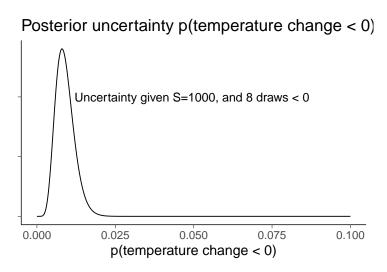
$$p(\theta \in A) \approx \frac{1}{S} \sum_{I} I(\theta^{(s)} \in A)$$

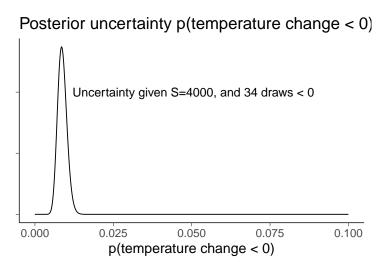
- $I(\cdot)$  is binomially distributed as  $p(\theta \in A)$ 
  - use beta CDF, or normal approximation
  - $\rightarrow$  var $(I(\cdot)) = p(1-p)S$  (Appendix A, p. 579)
  - $\rightarrow$  standard deviation of p is  $\sqrt{p(1-p)/S}$
- if S=100 and we observe  $\frac{1}{S}\sum_{l}I(\theta^{(s)}\in A)=0.05$ , 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  $S \gg 1/p$











# From probabilities to quantiles

- Probability:  $p(\theta < A) \approx \frac{1}{S} \sum_{l} I(\theta^{(s)} < A)$
- 5%-quantile: Find *A* so that  $p(\theta < A) = 0.05$

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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.

Posterior mean and 5% and 95% quantiles:

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#### The corresponding MCSE estimates:

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The corresponding MCSE estimates:

These \_mcse functions are for MCMC draws, but if the number of draws is big ( $\geq 1000$ ), then these are accurate enough for independent MC draws, too

Posterior probability and the corresponding MCSE estimate:

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See also https://users.aalto.fi/~ave/casestudies/Digits/digits.html

#### More data

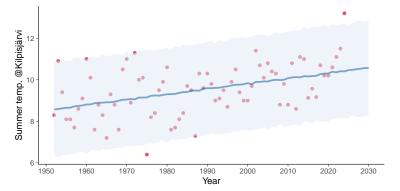
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- Summer 2023 was the second hottest in the recorded history
- Summer 2024 was the hottest in the recorded history



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

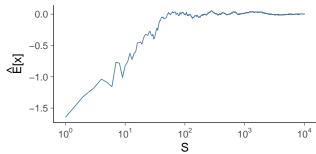
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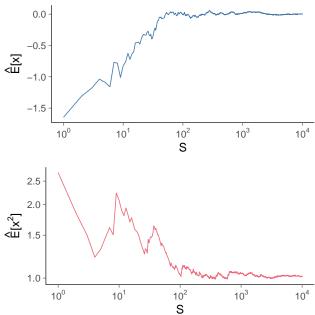
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- How to check if a distribution has finite mean and variance?
  - Pareto-k diagnostic

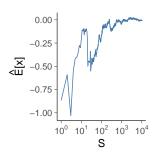
- N has all moments finite
- $t_{\nu}$  has less than  $\nu$  fractional moments

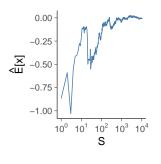
# Simple example: $x \sim N$

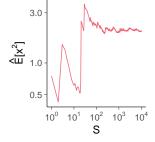


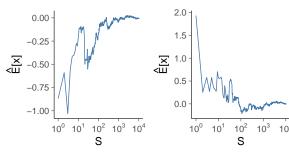
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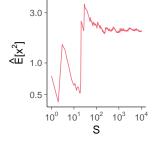


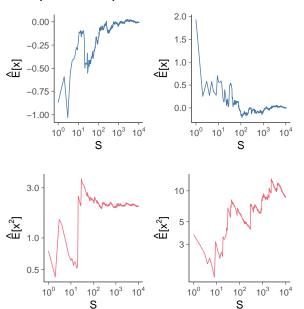




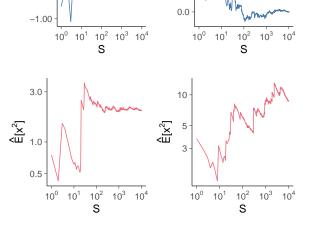








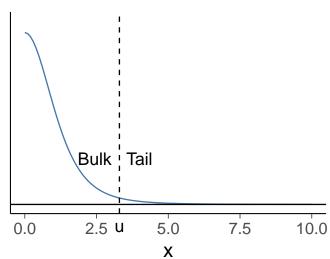
10<sup>1</sup> 10<sup>2</sup>

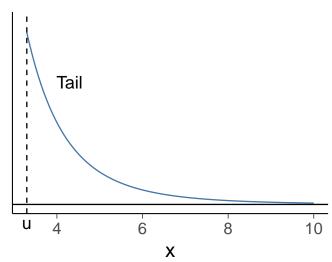


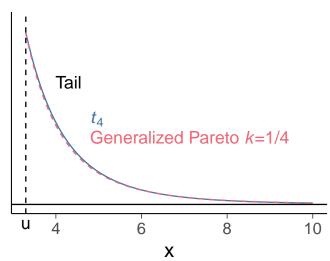
#### Simple example: $x \sim t_4$ , $t_{1/2}$ $t_2$ 2.5 -0.00 1.5 -0.250.0 1.0 0.5 -0.75 -5.00.0 -1.0010<sup>0</sup> 10<sup>1</sup> 10<sup>2</sup> 10<sup>3</sup> 10<sup>4</sup> 10<sup>1</sup> 10<sup>2</sup> 10<sup>0</sup> 10<sup>1</sup> 10000 3.0 10 100 $\hat{E}[x^2]$ 5 3 0.5 -

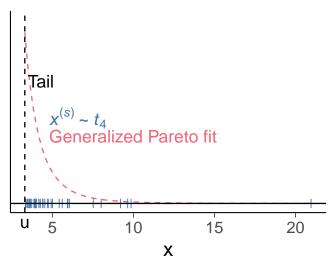
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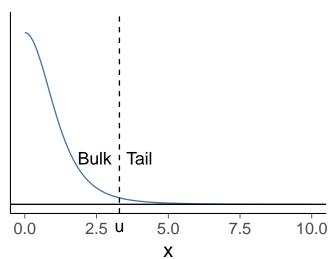




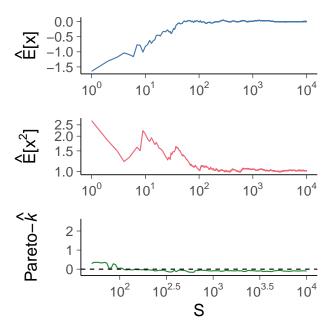




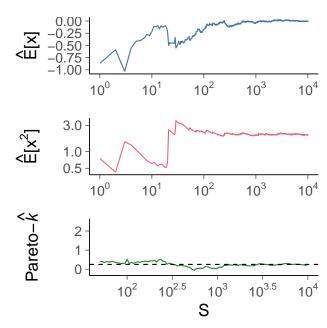
GPD has a shape parameter k, and 1/k finite fractional moments



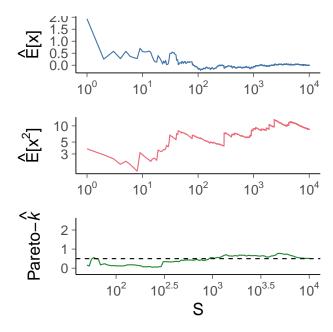
# Pareto- $\hat{k}$ diagnostic: $x \sim N$



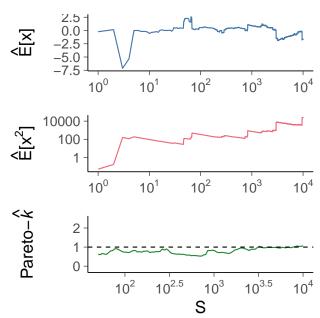
# Pareto- $\hat{k}$ diagnostic: $x \sim t_4$



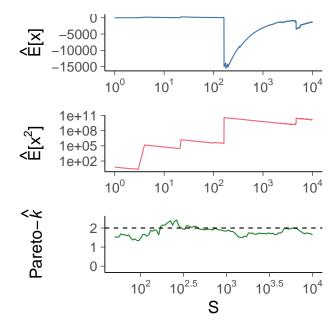
# Pareto- $\hat{k}$ diagnostic: $x \sim t_2$



# Pareto- $\hat{k}$ diagnostic: $x \sim t_1$



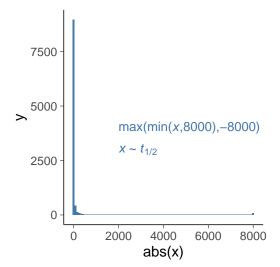
# Pareto- $\hat{k}$ diagnostic: $x \sim t_{1/2}$



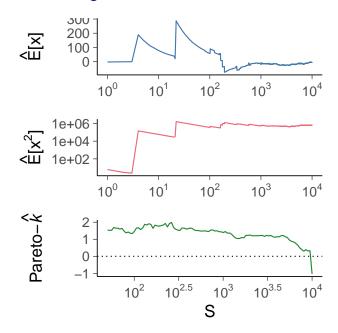
# Pareto- $\hat{k}$ diagnostic is pre-asymptotic diagnostic

Thick tailed but truncated distribution

We can make estimates only based on what we have observed.



## Pareto- $\hat{k}$ diagnostic: thick-tailed bounded distribution



#### Thick-tailed bounded distributions in practice

 Thick-tailed distributions are common in importance sampling and variational divergence estimation

## Pareto- $\hat{k}$ in posterior package

> drt |> summarise\_draws(mean, mcse\_mean)

```
variablemeanmcse_meanxn0.0100.021xt30.0250.033xt2_50.0310.039xt20.0460.054xt1_50.0920.13xt10.331.5
```

## Pareto- $\hat{k}$ in posterior package

> drt |> summarise\_draws(mean, mcse\_mean, pareto\_khat)

```
variable
                     khat
       mean mcse_mean
      0.010
              0.021
                   -0.072
xn
xt3
      0.025
              0.033 0.33
xt2_5 0.031
              0.039 0.41
xt2 0.046 0.054 0.52
xt1_5 0.092 0.13 0.69
xt1
      0.33
              1.5
                    1.0
```

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- $\hat{k}$  estimate has it's own variation given finite sample size
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- Pareto-smoothing improves the mean estimate
  - reliable mean and MCSE estimates when Pareto-k < 0.7
  - required minimum sample size and convergence rate estimates for different values of k
  - more on lecture 9

#### 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

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

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

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

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- not the fastest method due to trigonometric computations
- for normal distribution more than ten different methods
- e.g. R uses inverse-CDF

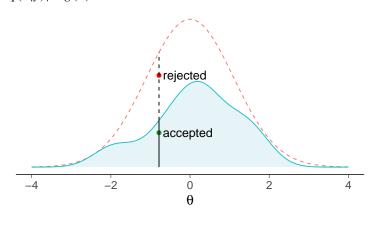
### Grid sampling and curse of dimensionality

- 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
  - →  $50^{10} \approx 1e17$  grid points
  - $\rightarrow$  1000<sup>10</sup>  $\approx$  1e30 grid points
- R and my current laptop can compute density of normal distribution about 50 million times per second
  - → evaluation in 1e17 grid points would take 60 years
  - ightarrow evaluation in 1e30 grid points would take 600 billion years

### Indirect sampling

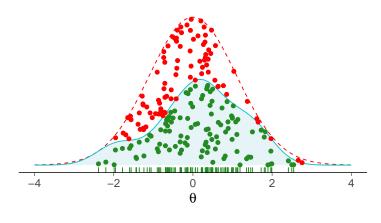
- Rejection sampling
- Importance sampling
- Markov chain Monte Carlo (next week)

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



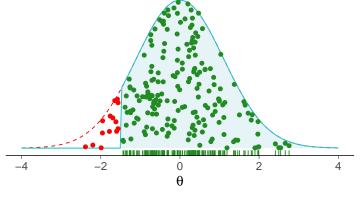
Mg(theta) — q(theta|y)

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Accepted • Rejected - - Mg(theta) - - q(thetaly)

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- Common for truncated distributions

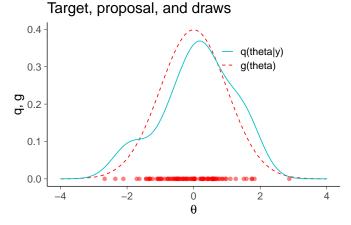


Accepted • Rejected - - Mg(theta) — q(theta|y)

- 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

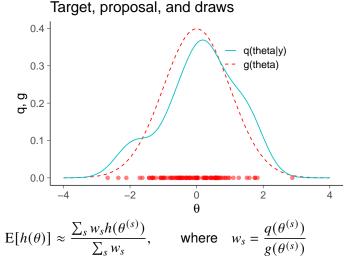
#### Importance sampling

- Proposal does not need to have a higher value everywhere



### Importance sampling

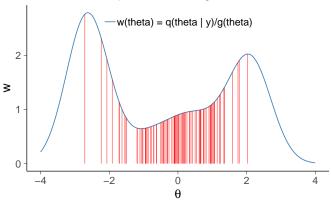
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### Importance sampling

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#### Draws and importance weights



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

### 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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- 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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  - variance goes down as 1/S
  - Effective sample size (ESS) takes into account the variability in the weights

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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

Using the weighted draws is good

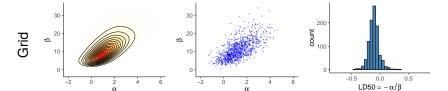
$$E[h(\theta)] \approx \frac{\sum_{s} w_{s} h(\theta^{(s)})}{\sum_{s} w_{s}}$$

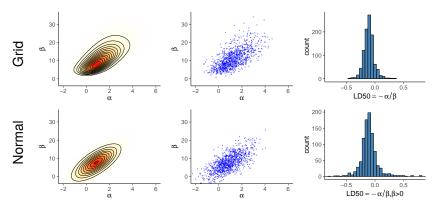
#### Importance re-sampling

Using the weighted draws is good

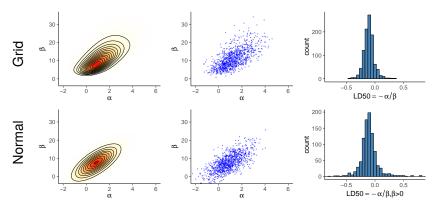
$$E[h(\theta)] \approx \frac{\sum_{s} w_{s} h(\theta^{(s)})}{\sum_{s} w_{s}}$$

- 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

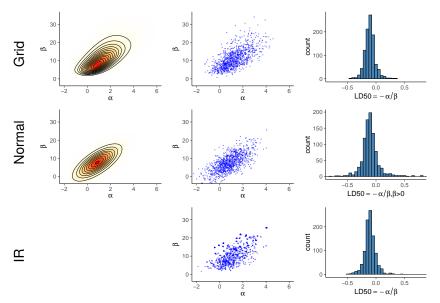


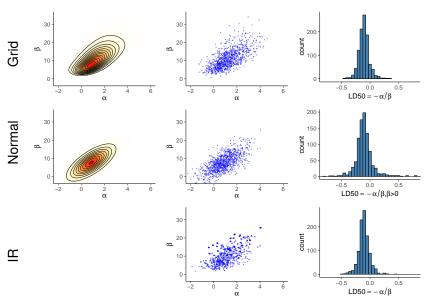


Normal approximation is discussed more in BDA3 Ch 4

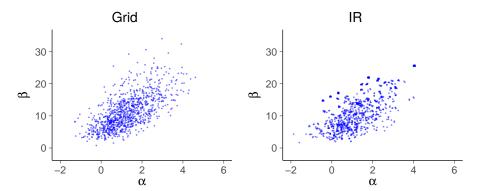


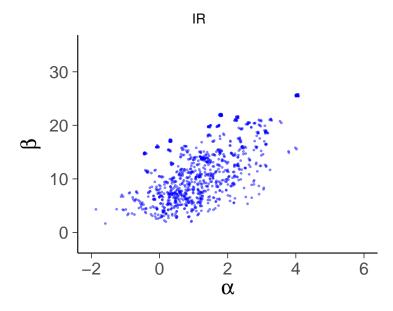
Normal approximation is discussed more in BDA3 Ch 4 But the normal approximation is not that good here: Grid sd(LD50)  $\approx$  0.1, Normal sd(LD50)  $\approx$  .75!

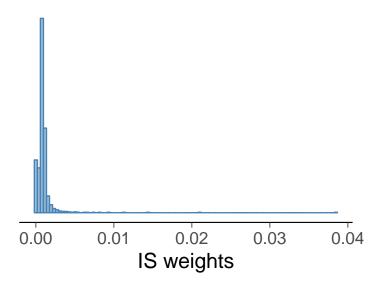


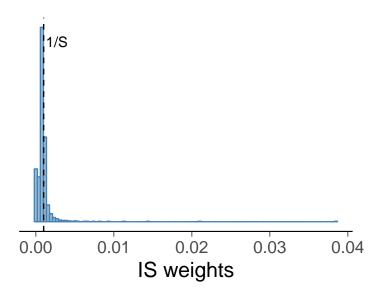


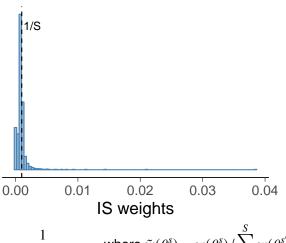
Grid sd(LD50)  $\approx$  0.1, IR sd(LD50)  $\approx$  0.1



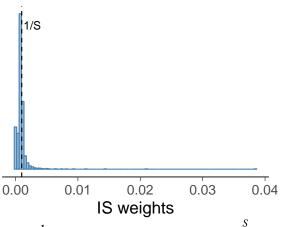






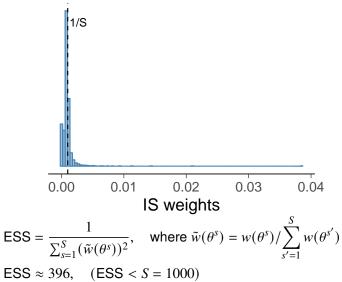


$$\mathsf{ESS} = \frac{1}{\sum_{s=1}^{S} (\tilde{w}(\theta^s))^2}, \quad \mathsf{where} \ \tilde{w}(\theta^s) = w(\theta^s) / \sum_{s'=1}^{S} w(\theta^{s'})$$

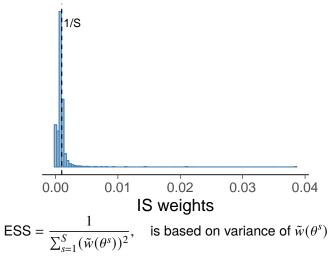


$$\mathsf{ESS} = \frac{1}{\sum_{s=1}^{S} (\tilde{w}(\theta^s))^2}, \quad \mathsf{where} \ \tilde{w}(\theta^s) = w(\theta^s) / \sum_{s'=1}^{S} w(\theta^{s'})$$

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

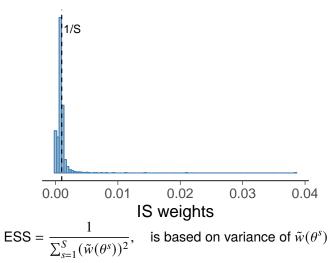


ESS  $\approx 396$ , (ESS < S = 1000)



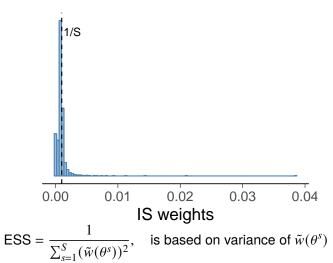
$$ESS = \frac{1}{\sum^{S} (\tilde{w}(\theta^{s}))^{2}}, \text{ is based on variance of } \tilde{w}(\theta^{s})$$

ESS ≈ 396

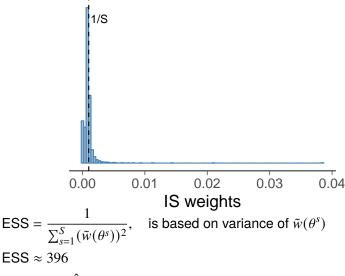


$$\mathsf{ESS} \approx 396$$

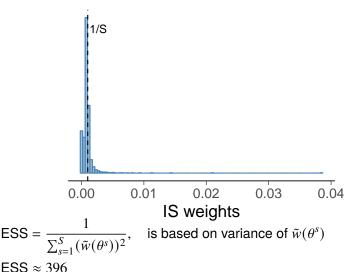
If all 
$$\tilde{w}(\theta^s) = 1/S$$
, then ESS =  $1/(SS^{-2}) = S$ 



If all 
$$\tilde{w}(\theta^s) = 1/S$$
, then ESS =  $1/(SS^{-2}) = S$   
If one  $\tilde{w}(\theta^s) = 1$ , and others 0, then ESS =  $1/1 = 1$ 



Pareto- $\hat{k} \approx 0.65$ , CLT does not hold



Pareto- $\hat{k} \approx 0.65$ , CLT does not hold

with Pareto-smoothing the estimate would be fine if  $\hat{k} < 0.7$ 

#### 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

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

#### 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)

#### Curse of dimensionality

- Number of grid points increases exponentially
- Concentration of the measure, that is, 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