UiO : Matematisk institutt

Det matematisk-naturvitenskapelige fakultet

STK-4051/9051 Computational Statistics Spring 2022
Chapter 6 (and 5)

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Last time

- Stochastic gradient decent
  - What it is
  - Minibatch is one type of randomness
  - Proof of convergence
- Stochastic gradient decent
  - Neural nets, back propagation

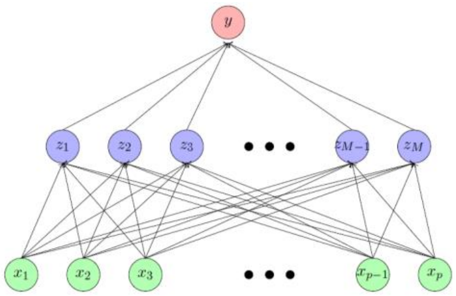


Figure 2: Visualisation of neural network with one hidden layer.

  - Spatial model $\widehat{KL}(f_\theta, g) = C - \frac{1}{\binom{n}{m}} \sum_{k=1}^{\binom{n}{m}} \log(f_\theta(y_k|s_k))$

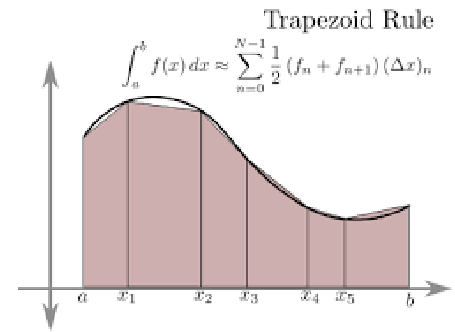
(https://www.researchgate.net/publication/259527954_A_Resampling-Based_Stochastic_Approximation_Method_for_Analysis_of_Large_Geostatistical_Data)

- Feed back
  - Hard to get the lecture

STK 4051/9051

- Optimization ~ Maximum likelihood
  - Continuous space (Newton-like methods, SGD,++)
  - Discrete/combinatorial
  - Missing/hidden variables (EM)
- Integration ~ Decision making - Bayesian inference
  - Direct methods low dimensions
  - Sequential Monte Carlo
  - Variance reduction methods
  - Markov chain Monte Carlo
- Additional topics for methods computation
  - Variational inference
  - STAN

Chapter 5, 1D integration



- Newton-Cotes Quadrature
  - Riemann rule
  - Trapezoidal rule
  - Simpsons rule
  - Random Sampling
  - **Efficient in 1D**

$$\left|\int_a^b f(x)\,dx - A_{\text{right}}\right| \le \frac{M_1(b-a)^2}{2n},$$

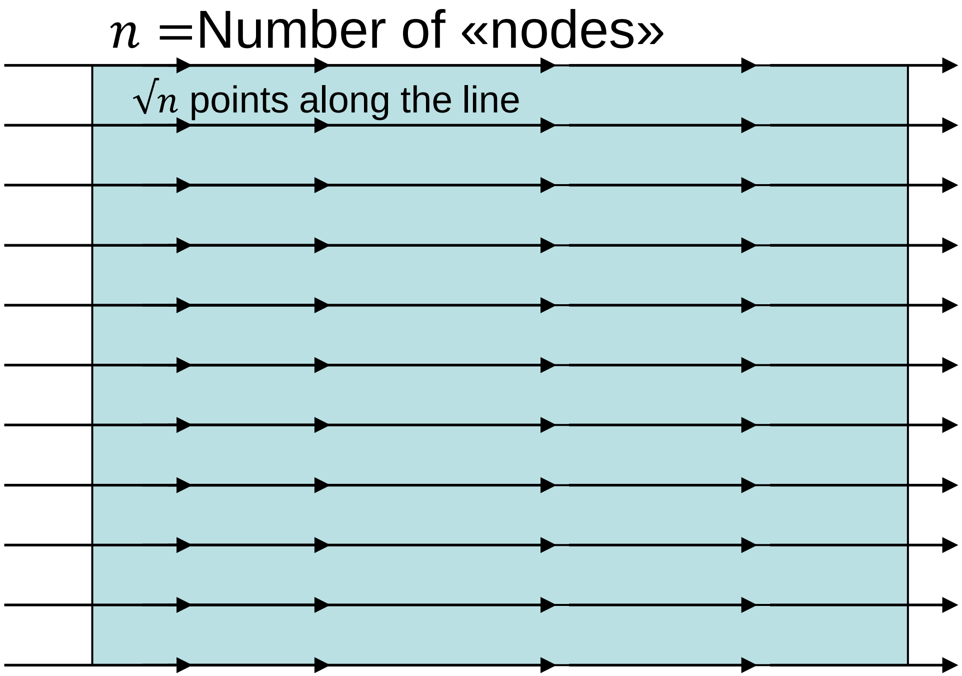
$$\left|\int_a^b f(x)\,dx - A_{\text{trap}}\right| \le \frac{M_2(b-a)^3}{12n^2},$$

$$\left|\int_a^b f(x)\,dx - A_{\text{S}}\right| \le \frac{M_4(b-a)^5}{180\,n^4}$$

$$\left|\int_a^b f(x)\,dx - A_{\text{r}}\right| \le \frac{M(b-a)}{\sqrt{n}}$$

- Romberg integration (stable)
- Gauss quadrature (popular)
- Higher order approximations is often bounded by the maximum of the derivative of the corresponding order
- Software for exact integration
  - Mathematica & Maple

Integration in R^d (Fubini-style)



$$I(S) = \iint_S f(x_1, x_2)\,dx_1 dx_2$$
$$= \int_c^d I(x_2)\,dx_2$$
$$I(x_2) = \int_a^b f(x_1, x_2)\,dx_1$$

$$\hat{I}(S) = \sum v_k \hat{I}(x_2^k) = \sum v_k \left(I(x_2^k) + E_1(x_2^k)\right)$$
$$= I(S) + E_2 + \sum v_k E_1(x_2^k)$$

The error is bounded by the integration error in each direction, but the number of nodes along each direction is $\sqrt{n}$

Curse of dimension for Quadrature formulas:

1D integral has convergence order:
$$O(n^{-r})$$
the Fubini integral in R^d has order:
$$O\left(n^{-r/d}\right)$$

Descision making under uncertainty

- In a project where the outcome is uncertain. How can we select the best solution?

- Quantify dominant uncertainty sources
- Propose different solutions «descisions»
- Simulate the outcome for all «solutions»
- Compare the distribution of outcomes for a quantity (e.g. NPV = net present value)

Buy or rent facilities for a project

- Buy and operate
  - CAPEX: 600 (50) MNOK
  - OPEX: 8 (4) MNOK/week
  - Revenue: 15 (5) MNOK/week in 2 years
- Rent
  - CAPEX: 0 MNOK
  - OPEX: 14 MNOK/week
  - Revenue: 15 (4) MNOK/week in 2 years

$$\text{Total Value} = \int \text{revenue}(t) - \text{OPEX}(t)dt \ - \text{CAPEX}$$

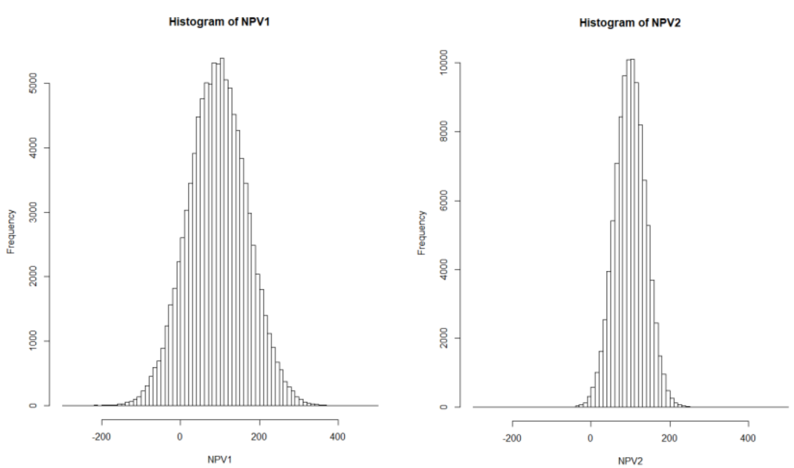
$$\text{Net Present Value} \ = \int [\text{revenue}(t) - \text{OPEX}(t)]e^{-t\nu}\, dt \ - \text{CAPEX}$$

- But income, CAPEX and OPEX are random variables
- How would you evaluate this?

Evaluation metrics?

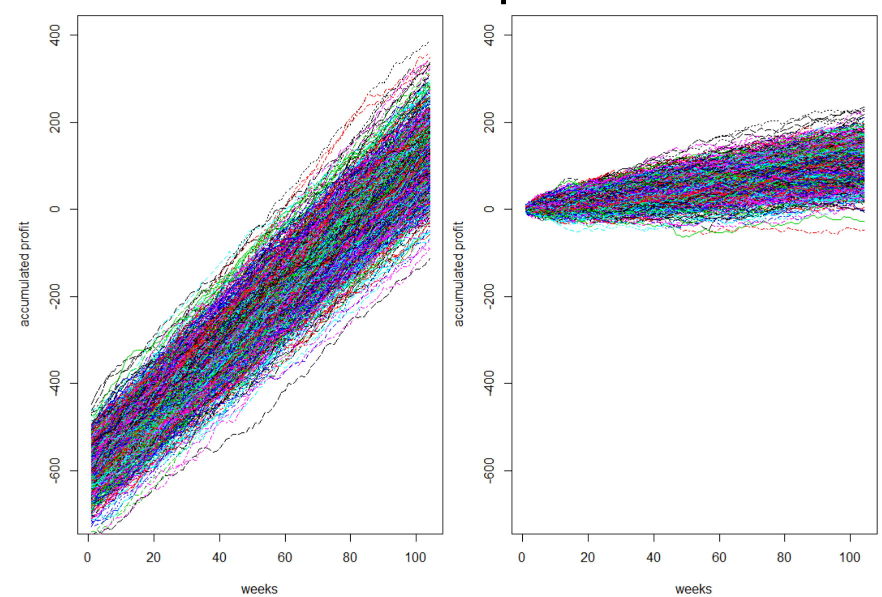
210 dimensional integral
Integral over time and
209 random variables
(104 weeks revenue & OPEX+ CAPEX)

- Expected NPV ? (93 vs 99)
- Expected Total Value? (128 vs 104)
- The probability not earning the CAPEX? (5%,0.5%)



Full distribution of NPV

Accumulated profit cases



Bayesian approach

- Likelihood $f(\mathbf{y}|\theta)$
- Introduce a prior $p(\theta)$ describing knowledge about θ prior to data
- Bayes theorem:

$$f(\theta|\mathbf{y}) = \frac{f(\theta)f(\mathbf{y}|\theta)}{f(\mathbf{y})}$$

$$f(\mathbf{y}) = \int_\theta f(\theta)f(\mathbf{y}|\theta)d\theta$$

- Bayesian paradigm: All relevant information about θ is contained in the posterior distribution $p(\theta|\mathbf{y})$
  - $\hat{\theta}_{post} = E[\theta|\mathbf{y}] = \int_\theta \theta p(\theta|\mathbf{y})d\theta$
  - Credibility interval (one-dimensional): $\alpha = \Pr(a < \theta < b|\mathbf{y}) = \int_a^b p(\theta|\mathbf{y})d\theta$
- Posterior: Updated knowledge based on both prior and data
- Numerical aspect: Bayesian approach change optimization to integration
- Many other integration problems both inside and outside statistics, will focus on

$$\mu = \int_\mathbf{x} h(\mathbf{x})f(\mathbf{x})d\mathbf{x}$$

- In many problems: $\mathbf{x}$ is high-dimensional

Image analysis – spatial structure

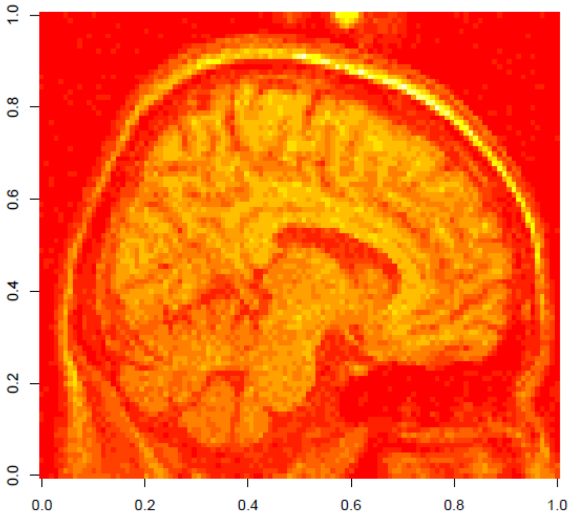
- Expect some smoothness in class-structure
- Markov Random field/Potts model:

$$\Pr(\mathbf{C}) = \Pr(C_{11}, \ldots, C_{n_1 n_2})$$
$$= \frac{1}{Z} e^{-\beta \sum_{||(i,j)-(i'j')||=1} I(C_{ij} \neq C_{i'j'})}$$

- Now interested in

$$\Pr(\mathbf{C}|\mathbf{y}) = \frac{\Pr(\mathbf{C}) \prod_{ij} f(y_{ij}|C_{ij})}{\sum_{\mathbf{C}'} \Pr(\mathbf{C}') \prod_{ij} f(y_{ij}|C'_{ij})}$$

- The sum in the denominator contains K^n terms,
  - $K =$ number of class
  - $n =$ number of pixels.
- Discrete type of "integration"



Monte Carlo method

- Aim (following notation from book):

$$\mu = E^{f(\mathbf{X})}[h(\mathbf{X})] = \begin{cases} \int_{\mathbf{x}} h(\mathbf{x})f(\mathbf{x}))d\mathbf{x} & \mathbf{x} \text{ continuous} \\ \sum_{\mathbf{x}} h(\mathbf{x})f(\mathbf{x}) & \mathbf{x} \text{ discrete} \end{cases}$$

- Monte Carlo:
  1. Simulate $\mathbf{X}_i \sim f(\mathbf{x}), i = 1, \ldots, n$
  2. Approximate μ by

$$\hat{\mu}_{MC} = \frac{1}{n}\sum_{i=1}^{n} h(\mathbf{x}_i)$$

- Properties:
  - Unbiased $E[\hat{\mu}_{MC}] = \mu$
  - If $X_1, \ldots, X_n$ are independent
    - Variance: $\text{var}[\hat{\mu}_{MC}] = \frac{1}{n}\text{var}[h(\mathbf{X})]$
    - Consistent: $\hat{\mu}_{MC} \to \mu$ as $n \to \infty$ if $\text{var}[h(\mathbf{X})] < \infty$
  - Estimate of variance:

$$\widehat{\text{var}}[\hat{\mu}_{MC}] = \frac{1}{n-1}\sum_{i=1}^{n}(h(\mathbf{x}_i) - \hat{\mu}_{MC})^2$$

- Main problem: How to simulate $\mathbf{X}_i \sim f(\cdot)$

The Fubini integral in R^d has order:

$$O\left(n^{-r/d}\right)$$

Monte Carlo method in R^d has order:

$$O\left(n^{-1/2}\right)$$

1) Independent of d
2) Does not depend on derivatives

Simulation techniques

- Exact methods
  - Inversion/transformation methods
  - Rejection sampling
- Approximate methods
  - Sampling importance resampling
  - Sequential Monte Carlo
  - Markov chain Monte Carlo (Chapter 7 and 8)
- Variance reduction methods
  - Importance sampling
  - Antithetic sampling
  - Control variates
  - Rao-blackwellization
  - Common random numbers

Random Number Generator (RNG) => uniform

- Physical methods (HRNG/TRNG) (Hardware-/True-)
  - based on microscopic phenomena,
    e.g. thermal noise, photoelectric effect
  - Still need to correct for bias/sequence correlation
- Computational methods, (PRNG, Pseudo-)
  - linear congruential generator
    - $X_{n+1} = (aX_n + b) \bmod m$
  - Initialize
    - Set seed (reproducible randomness)
    - Using the computer's real time clock
  - Mersenne Twister (Mersenne prime $2^{19937}-1$)
    - Default many programs
    - Good enough for our use
  - Cryptographically secure approaches (CSPRNG)

The inversion and the transformation methods

- Assume continuous distribution, density $f(x)$, CDF

$$F(x) = \int_{-\infty}^{x} f(u)du$$

- Assume $U \sim \text{Unif}[0,1]$
- Define $X = F^{-1}(U)$:

$$\begin{aligned} \Pr(X \leq x) &= \Pr(F^{-1}(U) \leq x) \\ &= \Pr(U \leq F(x)) = F(x) \end{aligned}$$

showing that $X \sim f(x)$!

- Assumes possible to generate U (good routines available)
- Assumes $F^{-1}(U)$ available
- Only applicable for univariate distributions
- Special case of transformation methods: $X = g(U)$
- Table 6.1: List of how to simulate most common distributions.

Table 6.1

TABLE 6.1 Some methods for generating a random variable X from familiar distributions.

Distribution	Method
Uniform	See [195, 227, 383, 538, 539, 557]. For $X \sim \text{Unif}(a, b)$; draw $U \sim \text{Unif}(0, 1)$; then let $X = a + (b - a)U$.
Normal(μ, σ^2) and Lognormal(μ, σ^2)	Draw $U_1, U_2 \sim$ i.i.d. Unif(0, 1); then $X_1 = \mu + \sigma\sqrt{-2\log U_1}\cos\{2\pi U_2\}$ and $X_2 = \mu + \sigma\sqrt{-2\log U_1}\sin\{2\pi U_2\}$ are independent $N(\mu, \sigma^2)$. If $X \sim N(\mu, \sigma^2)$ then $\exp\{X\} \sim \text{Lognormal}(\mu, \sigma^2)$.
Multivariate $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$	Generate standard multivariate normal vector, $\mathbf{Y}$, coordinatewise; then $\mathbf{X} = \boldsymbol{\Sigma}^{-1/2}\mathbf{Y} + \boldsymbol{\mu}$.
Cauchy(α, β)	Draw $U \sim \text{Unif}(0, 1)$; then $X = \alpha + \beta\tan\{\pi(U - \frac{1}{2})\}$.
Exponential(λ)	Draw $U \sim \text{Unif}(0, 1)$; then $X = -(\log U)/\lambda$.
Poisson(λ)	Draw $U_1, U_2, \ldots \sim$ i.i.d. Unif(0, 1); then $X = j - 1$, where j is the lowest index for which $\prod_{i=1}^{j} U_i < e^{-\lambda}$.
Gamma(r, λ)	See Example 6.1, references, or for integer r, $X = -(1/\lambda)\sum_{i=1}^{r}\log U_i$ for $U_1, \ldots, U_r \sim$ i.i.d. Unif(0, 1).
Chi-square (df $= k$)	Draw $Y_1, \ldots, Y_k \sim$ i.i.d. $N(0, 1)$, then $X = \sum_{i=1}^{k} Y_i^2$; or draw $X \sim \text{Gamma}(k/2, \frac{1}{2})$.
Student's t (df $= k$) and $F_{k,m}$ distribution	Draw $Y \sim N(0, 1)$, $Z \sim \chi^2_k$, $W \sim \chi^2_m$ independently, then $X = Y/\sqrt{Z/k}$ has the t distribution and $F = (Z/k)/(W/m)$ has the F distribution.
Beta(a, b)	Draw $Y \sim \text{Gamma}(a, 1)$ and $Z \sim \text{Gamma}(b, 1)$ independently; then $X = Y/(Y + Z)$.
Bernoulli(p) and Binomial(n, p)	Draw $U \sim \text{Unif}(0, 1)$; then $X = 1_{\{U<p\}}$ is Bernoulli(p). The sum of n independent Bernoulli(p) draws has a Binomial(n, p) distribution.
Negative Binomial(r, p)	Draw $U_1, \ldots, U_r \sim$ i.i.d. Unif(0, 1); then $X = \sum_{i=1}^{r}\lfloor(\log U_i)/\log\{1-p\}\rfloor$, and $\lfloor\cdot\rfloor$ means greatest integer.
Multinomial($1, (p_1, \ldots, p_k)$)	Partition [0, 1] into k segments so the ith segment has length p_i. Draw $U \sim \text{Unif}(0, 1)$; then let X equal the index of the segment into which U falls. Tally such draws for Multinomial($n, (p_1, \ldots, p_k)$).
Dirichlet($\alpha_1, \ldots, \alpha_k$)	Draw independent $Y_i \sim \text{Gamma}(\alpha_i, 1)$ for $i = 1, \ldots, k$; then $\mathbf{X}^{\mathrm{T}} = \left(Y_1/\sum_{i=1}^{k} Y_i, \ldots, Y_k/\sum_{i=1}^{k} Y_i\right)$.

Rejection sampling

Common «set up»

- Difficult to simulate from $f(x)$ directly
- Easy to simulate from $g(x) \approx f(x)$.
- Assume $\exists \alpha \leq 1$ such that for all x: $f(x) \leq \underbrace{g(x)/\alpha \equiv e(x)}$ (the envelope)
- Algorithm:
  1. Sample $Y \sim g(\cdot)$.
  2. Sample $U \sim \text{Unif}(0, 1)$.
  3. If $U \leq f(Y)/e(Y)$, put $X = Y$, otherwise return to step 1
- Distribution of X:

$$\Pr(X \leq x) = \Pr(Y \leq x | U \leq \tfrac{f(Y)}{e(Y)}) = \frac{\Pr(Y \leq x, U \leq \frac{f(Y)}{e(Y)})}{\Pr(U \leq \frac{f(Y)}{e(Y)})}$$

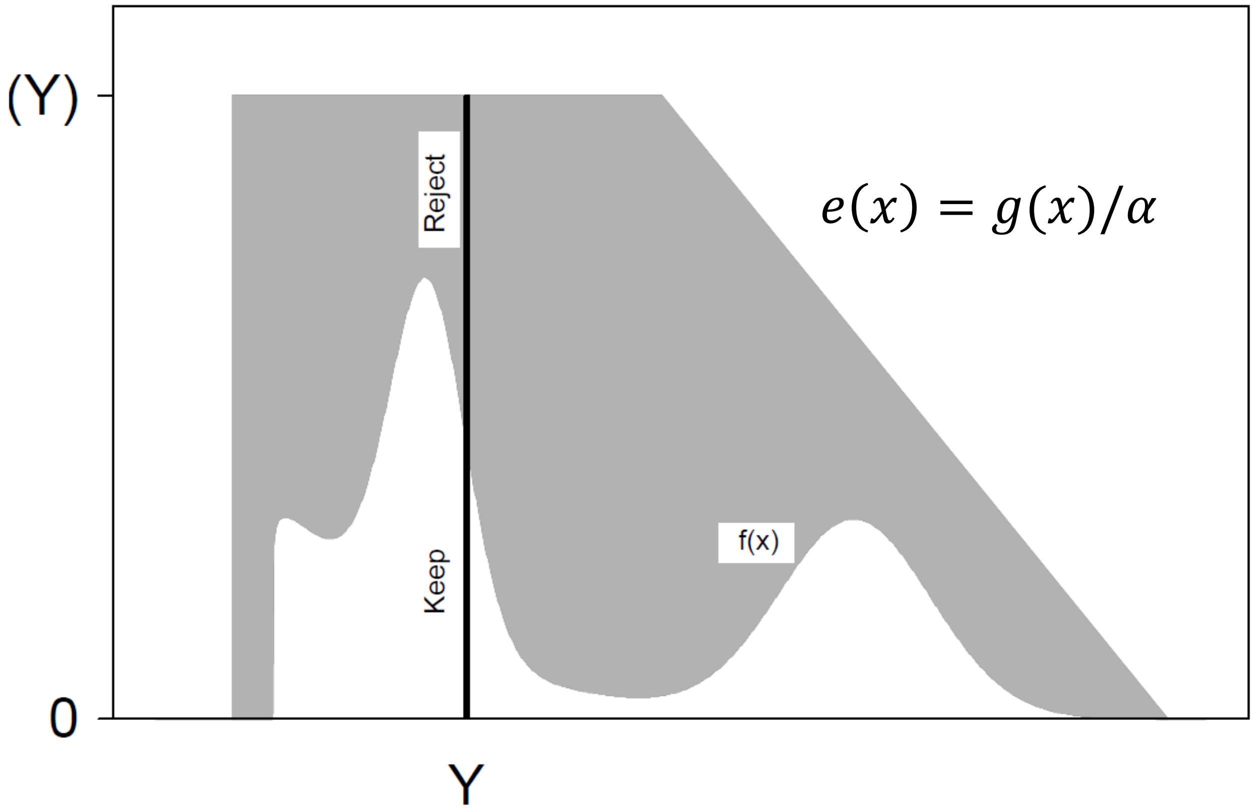
$$= \frac{\int_{-\infty}^{x} \int_{0}^{f(y)/e(y)} du g(y) dy}{\int_{-\infty}^{\infty} \int_{0}^{f(y)/e(y)} du g(y) dy} = \frac{\int_{-\infty}^{x} \frac{f(y)}{e(y)} g(y) dy}{\int_{-\infty}^{\infty} \frac{f(y)}{e(y)} g(y) dy}$$

$$= \int_{-\infty}^{x} f(y) dy = F(x)$$

- $\alpha = \Pr(U \leq \frac{f(Y)}{e(Y)})$ is the probability for acceptance
- α^{-1} is the expected number of iterations.

Rejection sampling using an envelope

1. $U \sim \text{Unif}(0,1)$ and accept if $U \leq f(Y)/e(Y)$ is equivalent to
2. $U \sim \text{Unif}(0, e(Y))$ and accept if $U \leq f(Y)$



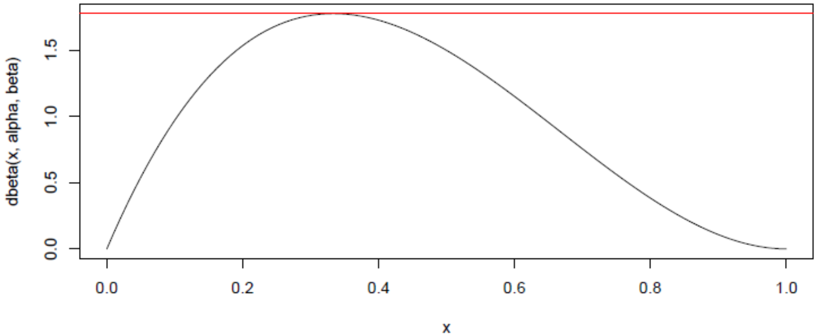
3. $U \sim Unif(0,1)$ and accept *if* $U \leq \alpha f(Y)/g(Y)$

Example rejection sampling

1. Aim: Simulate from Beta distribution:

$$f(x) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} x^{\alpha-1}(1-x)^{\beta-1}$$

2. $\arg\max_x f(x) = \frac{\alpha-1}{\alpha+\beta-2} = x^*$
3. Define $g(x) = 1; 0 < x < 1$. Then $g(x) \geq f(x)/f(x^*)$



4. Accept if $U \leq f(x)/f(x^*)$
5. `beta_rej.R`

What if the normalizing constant is unknown

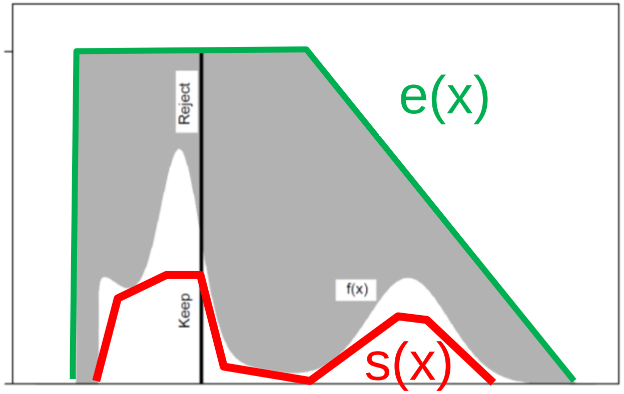
- Assume $f(x) = c \cdot q(x),\ c -$ unknown
- If we can find, $\tilde{\alpha}$ such that:
  - $g(x) \geq \tilde{\alpha} q(x) \quad = \frac{\tilde{\alpha}}{c} f(x) = \alpha f(x)$ $\quad \boxed{\alpha = \frac{\tilde{\alpha}}{c}}$
- Then:

$$U \leq \frac{\alpha f(Y)}{g(Y)} \Leftrightarrow U \leq \frac{\tilde{\alpha} q(Y)}{g(Y)}$$

- We need not know *c !*
- True acceptance rate is unknown: $\frac{\tilde{\alpha}}{c}$
- If we can estimate acceptance rate, we can estimate c

Squeezed rejection sampling

- Assume
  - $\exists \alpha \leq 1$ and $g(\cdot)$ such that for all x: $f(x) \leq g(x)/\alpha \equiv e(x)$
  - $\exists s(x) \leq f(x)$ which is easy to evaluate
- Note: $U \leq s(Y)/e(Y)$ imply $U \leq f(Y)/e(Y)$

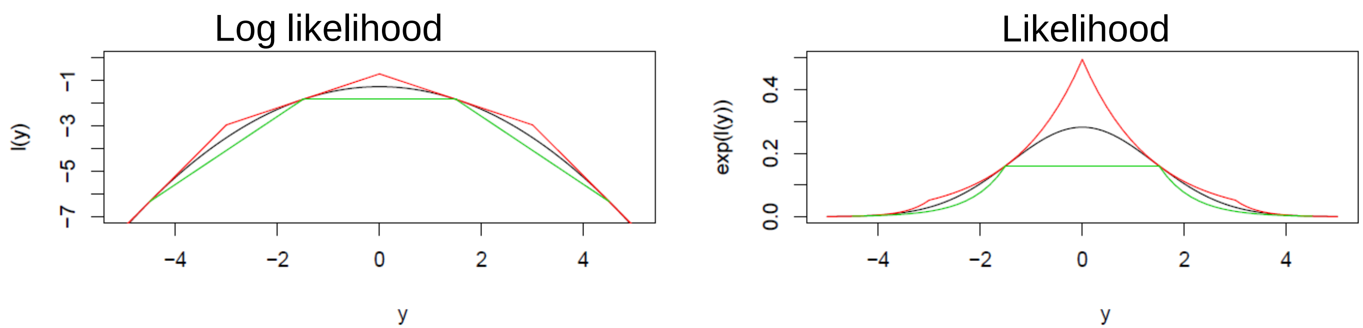


- Algorithm:
  1. Sample $Y \sim g(\cdot)$.
  2. Sample $U \sim \text{Unif}(0, 1)$.
  3. If $U \leq s(Y)/e(Y)$, accept $X = Y$
  4. If $U > s(Y)/e(Y)$, but $U \leq f(Y)/e(Y)$, accept $X = Y$
  5. If $U > f(Y)/e(Y)$, go to step 1

Adaptive rejection sampling

- Main challenge: Construct suitable envelope
- Assume now $l(x) = \log f(x)$ is concave and differentiable
- Choose initial points $x_1, x_2, \dots, x_k$ such that $l'(x_1) > 0$, $l'(x_k) < 0$
- $e_k^*(x)$: Piecewise linear upper hull of $l(x)$

concave:
1) Never above the tangent in any point (super-gradient)
2) Never below the line connecting two points



- Proposal distribution:

$$g(x) = c \exp\{\ell(x_i) + \ell'(x_i)(x - x_i)\} \qquad \text{for } x \in [z_{i-1}, z_i]$$

$$z_i = \frac{\ell(x_{i+1}) - \ell(x_i) - x_{i+1}\ell'(x_{i+1}) + x_i\ell'(x_i)}{\ell'(x_i) - \ell'(x_{i+1})}$$

Possible to calculate c and also easily find $G(x)$ and $G^{-1}(x)$

- Also possible to define squeezing function

$$s_k^*(x) = \frac{(x_{i+1} - x)\ell(x_i) + (x - x_i)\ell(x_{i+1})}{x_{i+1} - x_i}$$

Adaptive rejection sampling

1. Start with $x_1, \ldots, x_k$ and calculate $e_k(x), s_k(x), g_k(x)$
2. Generate $x \sim g(x)$
3. If $U \leq s_k(Y)/e_k(Y)$, accept $X = Y$, goto step 6
4. If $U > s_k(Y)/e_k(Y)$, but $U \leq f(Y)/e_k(Y)$
   1. accept $X = Y$
   2. Add X to $\{x_1, \ldots, x_k\}$ and update to $e_{k+1}(x), s_{k+1}(x), g_{k+1}(x)$ and go to step 6
5. If $U > f(Y)/e(Y)$, reject and go to step 2
6. If not enough samples, return to step 2

Example: `ars.R`

```
library(ars)
```

Importance sampling (approximate)

- Rewriting

$$\mu = \int h(\mathbf{x})f(\mathbf{x})d\mathbf{x} = \int \frac{h(\mathbf{x})f(\mathbf{x})}{g(\mathbf{x})}g(\mathbf{x})d\mathbf{x} = \frac{\int \frac{h(\mathbf{x})f(\mathbf{x})}{g(\mathbf{x})}g(\mathbf{x})d\mathbf{x}}{\int \frac{f(\mathbf{x})}{g(\mathbf{x})}g(\mathbf{x})d\mathbf{x}}$$

- Assume $X_1, \ldots, X_n$ iid from $g(\mathbf{x})$. (We know how to sample from g(**x**))

- Two alternative estimates

$$\hat{\mu}_{IS}^* = \frac{1}{n}\sum_{i=1}^n h(\mathbf{X}_i)w^*(\mathbf{X}_i), \quad w^*(X_i) = \frac{f(\mathbf{X}_i)}{g(\mathbf{X}_i)}$$

$$\hat{\mu}_{IS} = \sum_{i=1}^n h(\mathbf{X}_i)w(\mathbf{X}_i), \quad w(\mathbf{X}_i) = \frac{w^*(\mathbf{X}_i)}{\sum_{j=1}^n w^*(\mathbf{X}_j)}$$

- $w^*(\mathbf{X}_i)$ called importance weights
- $w(\mathbf{X}_i)$ called the normalized importance weights

What can go wrong???

- Monte Carlo integration:
  - $E_f\left(h(X)\right) < \infty$ (this is the number we want)
  - $E_f(h(X)^2) < \infty$ (this is additional requirement)
- Importance sampling:
  - $E_g\left(h(X)w^*(X)\right) = E_f\,(h(X)) < \infty$ (ok ☺)
  - $E_g\left(\left(h(X)w^*(X)\right)^2\right) = E_f\left(h(X)^2w^*(X)\right) < \infty$ (??)

$w^*(X) = \frac{f(X)}{g(X)}$ in rejection sampling this is bounded by α^{-1}

Importance sampling version 1

$$\hat{\mu}_{IS}^* = \frac{1}{n}\sum_{i=1}^n h(\mathbf{X}_i)w(\mathbf{X}_i), \quad w^*(\mathbf{X}_i) = \frac{f(\mathbf{X}_i)}{g(\mathbf{X}_i)}$$

$$E[w^*(\boldsymbol{X}_i)] = \int \frac{f(\boldsymbol{x})}{g(\boldsymbol{x})}g(\boldsymbol{x})d\boldsymbol{x} = \int f(\boldsymbol{x})d\boldsymbol{x} = 1$$

$$E[\hat{\mu}_{IS}^*] = \int h(\boldsymbol{x})\frac{f(\boldsymbol{x})}{g(\boldsymbol{x})}g(\boldsymbol{x})d\boldsymbol{x} = \int h(\boldsymbol{x})f(\boldsymbol{x})d\boldsymbol{x} = \mu$$

$$\text{Var}[\hat{\mu}_{IS}^*] = \frac{1}{n}\text{Var}^g[h(\mathbf{X})w^*(\mathbf{X})]$$

- Can be unstable if $g(\mathbf{x})$ small when $f(\mathbf{x})$ large
- $g(\mathbf{x})$ should have heavier tails than $f(\mathbf{x})$.
- If only one $h(\mathbf{X})$ of interest, should choose

$$g(\mathbf{x}) \propto |h(\mathbf{x})|f(\mathbf{x})$$

- Often interested in many functions, focus on making variability of $w^*(\mathbf{X})$ small

Importance sampling version 2

$$\hat{\mu}_{IS} = \sum_{i=1}^{n} h(\mathbf{X}_i)w(\mathbf{X}_i), \quad w(\mathbf{X}_i) = \frac{w^*(\mathbf{X}_i)}{\sum_{j=1}^{n} w^*(\mathbf{X}_j)}$$

- Based on

$$\mu = \frac{\int \frac{h(\mathbf{x})f(\mathbf{x})}{g(\mathbf{x})} g(\mathbf{x})d\mathbf{x}}{\int \frac{f(\mathbf{x})}{g(\mathbf{x})} g(\mathbf{x})d\mathbf{x}} = \frac{\mu}{1} \approx \frac{\hat{\mu}_{IS}^*}{\hat{1}_{IS}^*} = \hat{\mu}_{IS}$$

$$\hat{\mu}_{IS}^* = \bar{t}, \quad t_i = t(\mathbf{X}_i) = h(\mathbf{X}_i)w^*(\mathbf{X}_i)$$

$$\hat{1}_{IS}^* = \bar{w}^*$$

- Why also estimate denominator?
  - What would be best if   h(x) = c (constant)?
  - Correlations between nominator and denominator

Impact of normalization

$$\frac{\hat{\mu}^*_{IS}}{\hat{1}^*_{IS}} = \hat{\mu}_{IS} \qquad \hat{1}^*_{IS} = \bar{w}^*$$

- Taylor approximation of $1/\bar{w}^*$ around 1:

$$\frac{1}{\bar{w}^*} \approx 1 - (\bar{w}^* - 1) + (\bar{w}^* - 1)^2$$

giving

$$\begin{aligned}\hat{\mu}_{IS} &\approx \bar{t}\,[1 - (\overline{w}^* - 1) + (\overline{w}^* - 1)^2] \\ &= \bar{t} - (\bar{t} - \mu)(\overline{w}^* - 1) - \mu(\overline{w}^* - 1) + \bar{t}\,(\overline{w}^* - 1)^2\end{aligned}$$

$$\begin{aligned}E[\hat{\mu}_{IS}] &= E\{\bar{t} - (\bar{t} - \mu)(\overline{w}^* - 1) - \mu(\overline{w}^* - 1) + \bar{t}\,(\overline{w}^* - 1)^2\} + \mathcal{O}(n^{-2}) \\ &= \mu - \frac{1}{n}\mathrm{cov}[t(\boldsymbol{X}), w(\boldsymbol{X})] - 0 + \frac{\mu}{n}\mathrm{var}(w(\boldsymbol{X})) + \mathcal{O}(n^{-2})\end{aligned}$$

$$\begin{aligned}\mathrm{var}[\hat{\mu}_{IS}] &= E\left\{\left((\bar{t} - \mu) - \mu(\overline{w}^* - 1)\right)^2\right\} + \mathcal{O}(n^{-2}) \\ &= \frac{1}{n}\left[\mathrm{var}\big(t(\boldsymbol{X})\big) + \mu^2\mathrm{var}\big(w^*(\boldsymbol{X})\big) - 2\mu\cdot\mathrm{cov}[t(X), w^*(X)]\right] + \mathcal{O}(n^{-2})\end{aligned}$$

$$\boxed{\mathrm{MSE}[\hat{\mu}_{IS}] - \mathrm{MSE}[\hat{\mu}^*_{IS}] = \frac{1}{n}\left(\mu^2\mathrm{var}[w^*(\mathbf{X})] - 2\mu\mathrm{cov}[t(\mathbf{X}), w^*(\mathbf{X})]\right) + \mathcal{O}(n^{-2})}$$

When is normalization better?

$$\boxed{\mathrm{MSE}[\hat{\mu}_{IS}] - \mathrm{MSE}[\hat{\mu}^*_{IS}] = \frac{1}{n}\left(\mu^2 \mathrm{var}[w^*(\mathbf{X})] - 2\mu \mathrm{cov}[t(\mathbf{X}), w^*(\mathbf{X})]\right) + \mathcal{O}(n^{-2})}$$

- Gain if

$$\mathrm{cov}[t(\mathbf{X}), w^*(\mathbf{X})] > \frac{\mu \mathrm{var}[w^*(\mathbf{X})]}{2}$$

$$\Updownarrow$$

$$\mathrm{cor}[t(\mathbf{X}), w^*(\mathbf{X})] > \frac{\sqrt{\mathrm{var}[w^*(\mathbf{X})]}}{2\sqrt{\mathrm{var}[t(\mathbf{X})]}/\mu} = \frac{\mathrm{cv}[w^*(\mathbf{X})]}{2\mathrm{cv}[t(\mathbf{X})]}$$

- Example: `imp_samp_beta.R`

Coefficient of variation:
cv(X)=std(X)/E(X)

Effective sample size

- Assume $w_i = w(\mathbf{X}_i)$, $i = 1, \ldots, n$ are normalized weights
- Define effective sample size by

$$\boxed{\widehat{N}_{eff} = \frac{1}{\sum_{i=1}^{n} w_i^2}}$$

Ex 1:	if $w_i = \frac{1}{n}$ for all i	$\widehat{N}_{eff} = n$
Ex 2:	if $w_i = 0, i \leq z, w_i = \frac{1}{n-z}, i > z$	$\widehat{N}_{eff} = n - z$
Ex 3:	if $w_i = 0, i \neq j, w_j = 1$	$\widehat{N}_{eff} = 1$

Sampling importance resampling

- Assume now we want to sample from $f(\mathbf{x})$, difficult
- Easy to sample from $g(\mathbf{x})$.
- Sampling importance resampling
  1. Sample $\mathbf{Y}_1, ..., \mathbf{Y}_m$ iid from g
  2. Calculate standardized importance weights

$$w(\mathbf{Y}_i) = \frac{f(\mathbf{Y}_i)/g(\mathbf{Y}_i)}{\sum_{j=1}^m f(\mathbf{Y}_j)/g(\mathbf{Y}_j)}, i = 1, ..., m$$

  3. Resample $\mathbf{X}_1, ..., \mathbf{X}_n$ from $\{\mathbf{Y}_1, ..., \mathbf{Y}_m\}$ with probabilities $w(\mathbf{Y}_1), ..., w(\mathbf{Y}_m)$
- Properties: As $m \to \infty$
  - X_i converges in distribution to $f(\mathbf{x})$
  - Correlations between X_i's decreases to zero
- For finite m: Correlation between samples

Sampling importance resampling

- Assume
  - $Y_1, \ldots, Y_m$ iid from g
  - $X_1, \ldots, X_n$ resampled from $\{Y_1, \ldots, Y_m\}$, $w(Y_i) = \frac{f(Y_i}{g(Y_i)}$
- Two possible estimates of $\mu = E^f[X]$:

$$\hat{\mu}_{SIR} = \frac{1}{m}\sum_{i=1}^{m} X_i$$

$$\hat{\mu}_{IS} = \sum_{i=1}^{m} w(Y_i)Y_i$$

Can show

$$E[(\hat{\mu}_{IS} - \mu)^2] \leq E[(\hat{\mu}_{SIR} - \mu)^2]$$

Why consider SIR?

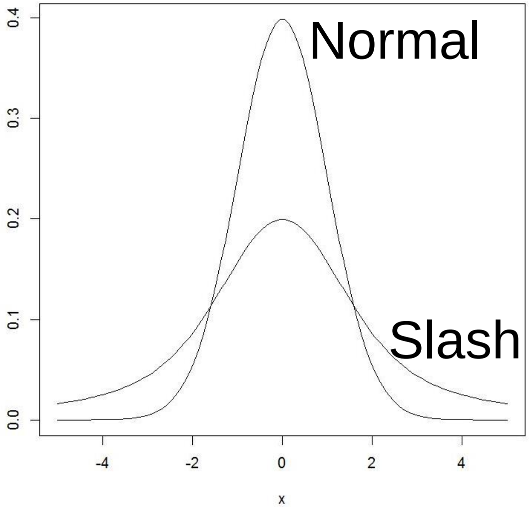
- Sometimes beneficial to have **equally weighted** samples
- May be beneficial at a later stage of analysis process
- If we want to evaluate E(*h(x)*) where *h(x)* is hard to evaluate
- Usually n < m

Example: slash distribution

- Controlled example (we know the truth)
- Y has slash distribution when $Y = \frac{X}{U}$
  $X \sim N(0,1), U \sim \mathrm{Unif}(0,1)$

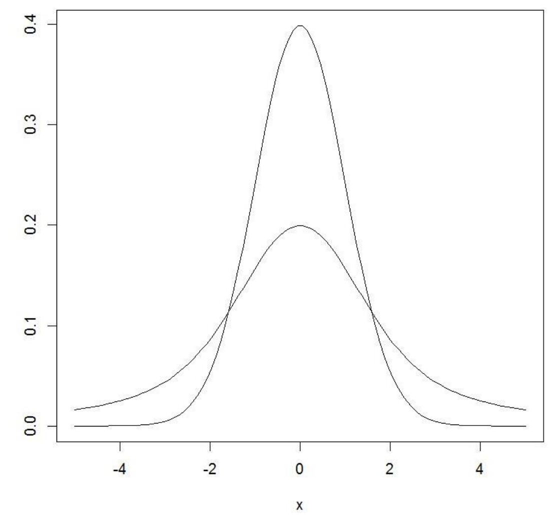
$$f(y) = \begin{cases} \frac{1-\exp\{-y^2/2\}}{y^2\sqrt{2\pi}}, & y \neq 0, \\ \frac{1}{2\sqrt{2\pi}}, & y = 0. \end{cases}$$

- Sampling Experiments
  1. X from Y
  2. Y from X
- Methods
  1. Rejection sampling
  2. Importance sampling
  3. Sampling importance resampling



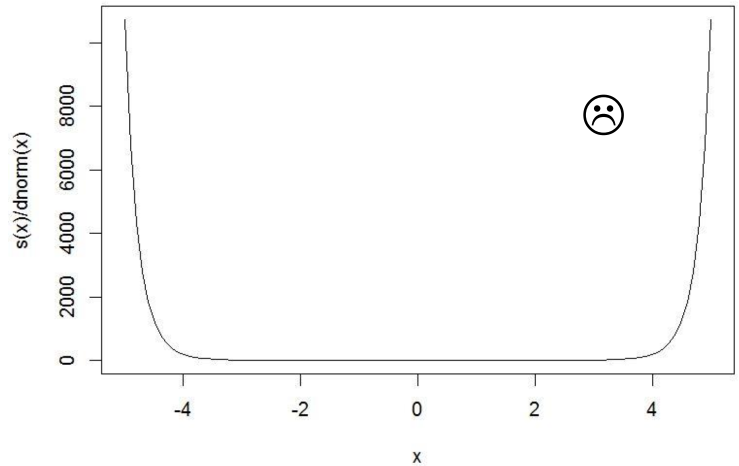
Two test functions

- Ex1: x
- Ex2: h(x)= sin(x)+0.2cos(2*pi*x)

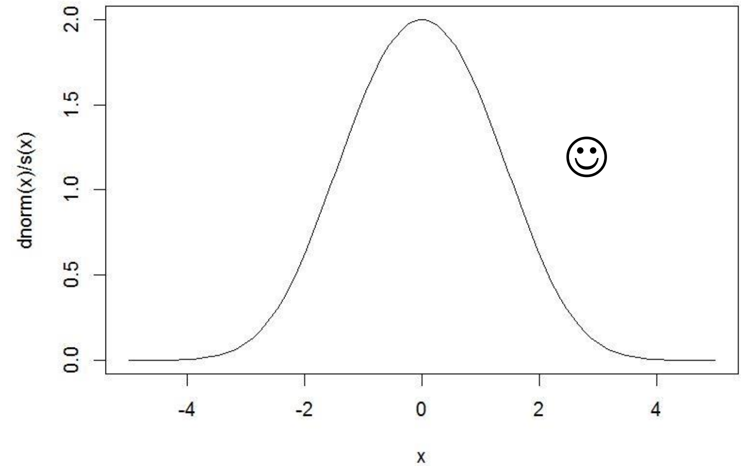


- Ratios:

Slash /normal



Normal/slash



- Ex1: x
- Ex2: h(x)= sin(x)+0.2cos(2*pi*x)

```
> m = 1000
> x=rnorm(m)
> y =rnorm(m)/runif(m)
> show(c(mean(x), mean(h(x)), mean(y), mean(h(y))))
[1] -0.04743281 -0.02314847 -0.71528509  0.01710263
>
>
>
> m = 100000
> x=rnorm(m)
> y =rnorm(m)/runif(m)
> show(c(mean(x), mean(h(x)), mean(y), mean(h(y))))
[1]  0.001369078  0.001019647  0.542154961 -0.004230678
>
>
>
> m = 10000000
> x=rnorm(m)
> y =rnorm(m)/runif(m)
> show(c(mean(x), mean(h(x)), mean(y), mean(h(y))))
[1]  3.115531e-05  4.417861e-05 -8.361942e-01 -2.532640e-05
```

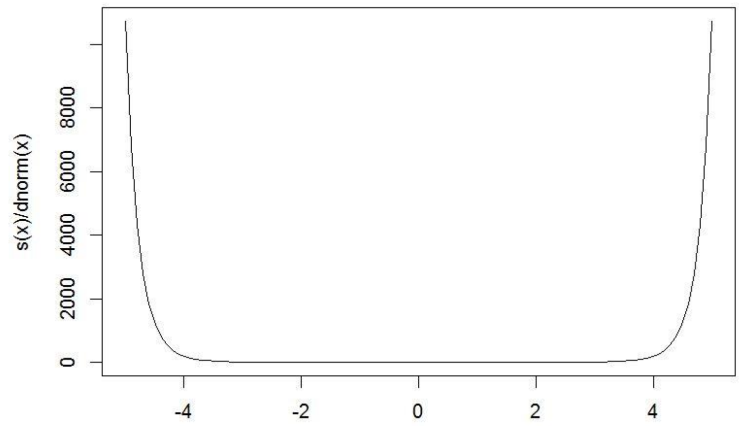
Slash distribution does not have a mean
=> The average does not converge

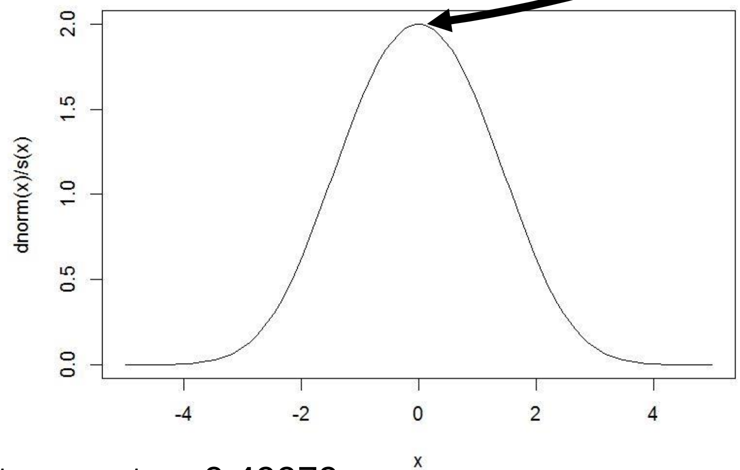
```
> m = 1000
> x=rnorm(m)
> y =rnorm(m)/runif(m)
> show(c(sd(x), sd(h(x)), sd(y), sd(h(y))))
[1]  0.9951861  0.6712401 65.3199546  0.7001361
>
>
> m = 100000
> x=rnorm(m)
> y =rnorm(m)/runif(m)
> show(c(sd(x), sd(h(x)), sd(y), sd(h(y))))
[1]    0.9956829    0.6726304 1328.0501683    0.7122169
>
>
>
> m = 10000000
> x=rnorm(m)
> y =rnorm(m)/runif(m)
> show(c(sd(x), sd(h(x)), sd(y), sd(h(y))))
[1] 9.997296e-01 6.724661e-01 1.110357e+04 7.138005e-01
>
```

Slash distribution does not have a variance
=> The sd(y) increase with sample size

Rejection sampling

- Normal from slash bounded by 2
- Slash from Normal unbounded
  (no rejection sampling possibel)



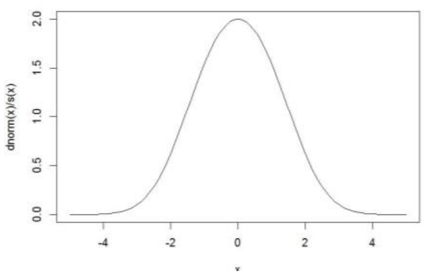


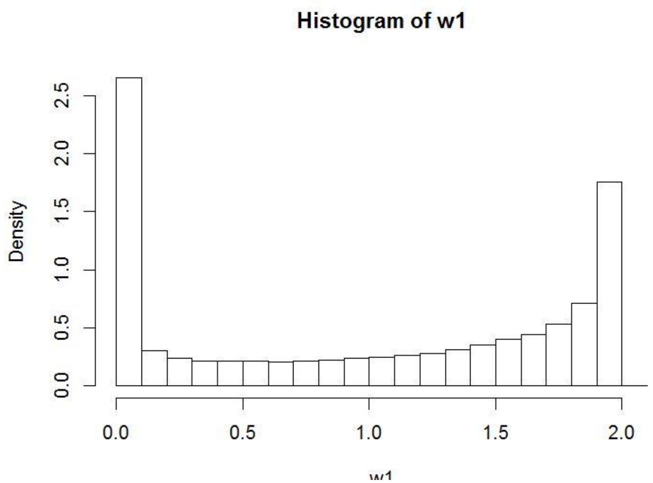

```
> y =rnorm(m)/runif(m)
> U=runif(m)
> accept = dnorm(y)/(s(y)*2)
> sample = y[U<accept]
>
> length(sample)
[1] 49979
> max(accept)
[1] 1
> min(accept)
[1] 0
```

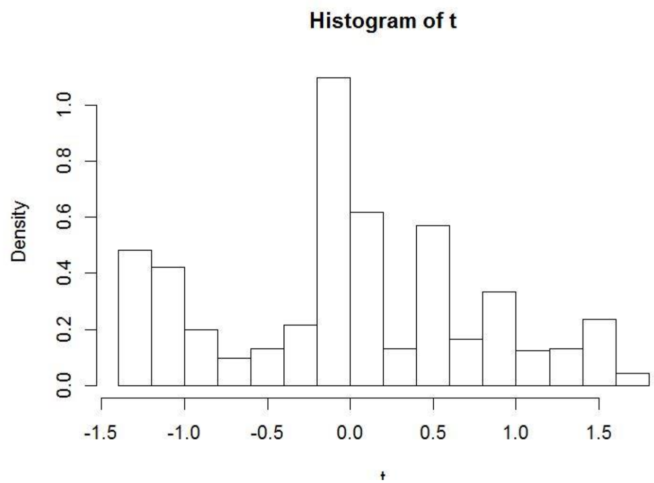
Observed acceptance rate: 0.49979
Theoretical acceptance rate: 0.50000

Sample from slash, estimate propeties of normal distribution

$f(x)/g(x)$



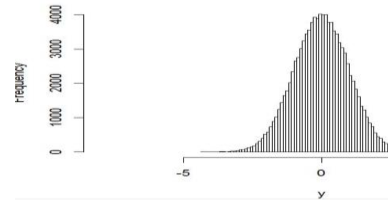




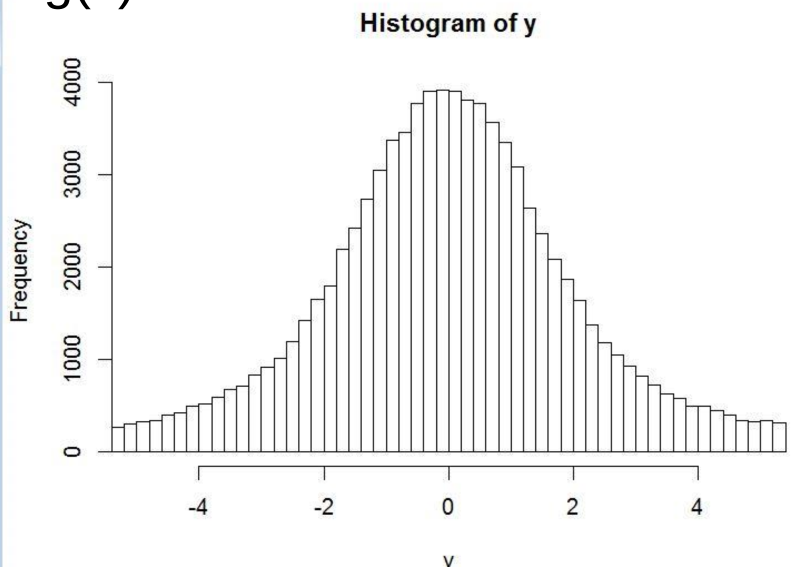

```
> m=100000
> ## importance sampling
> y =rnorm(m)/runif(m)
> w1 = dnorm(y)/s(y)
> wn1 = w1/sum(w1)
> mean(w1)
[1] 1.002287
>
>
> neff = 1/sum(wn1^2)
> show(neff/m)
[1] 0.6213973
```

```
>
> t=h(y)*w1
> mean(t)
[1] -0.0007471106
```

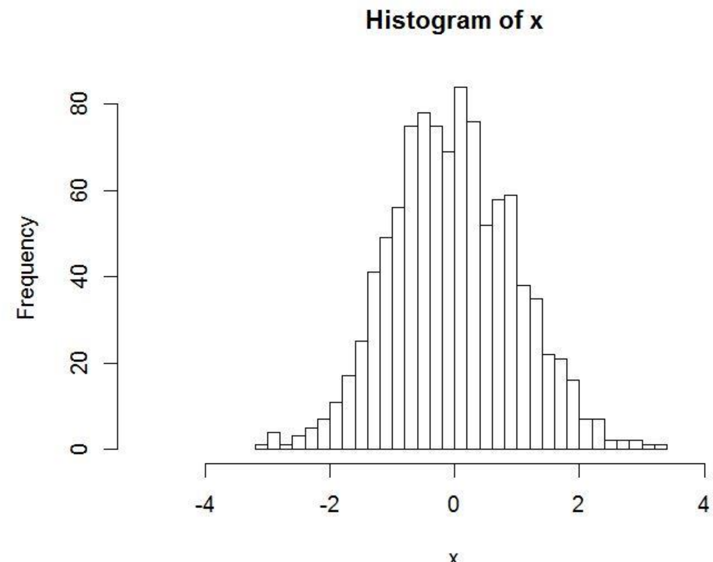
SIR normal from slash



Sample from g(x)

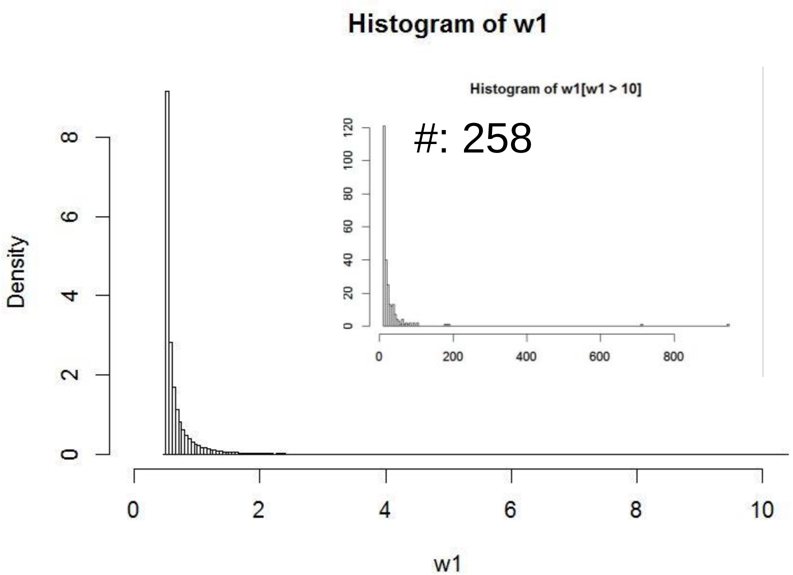


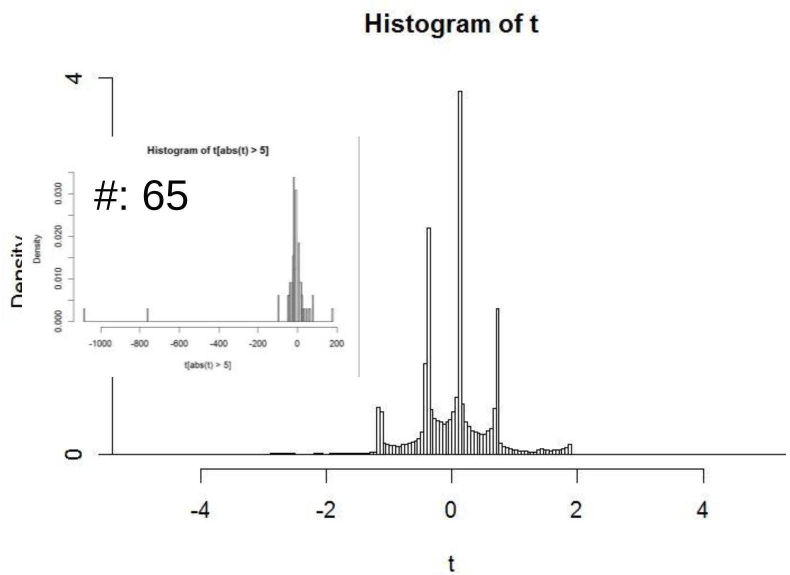
Approximate sample from f(x)




```
n = 1000
x = sample(y,n,replace=T,prob=wn1)
par(mfrow=c(1,2))
hist(y,1000000,xlim=c(-5 ,5))
hist(x,40,xlim=c(-5 ,5))
```

Sample from normal, estimate in slash

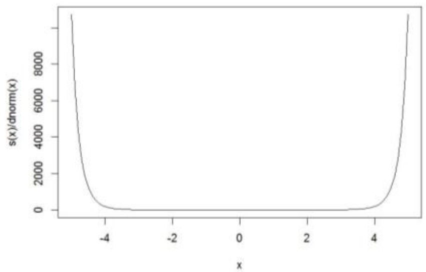




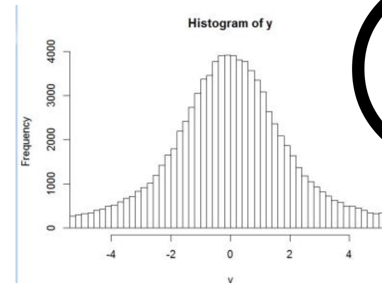

```
>
> m=100000
> ## importance sampling
> y =rnorm(m)
> w1 = s(y)/dnorm(y)
> wn1 = w1/sum(w1)
> mean(w1)
[1] 0.8170563
>
>
> neff = 1/sum(wn1^2)
> show(neff/m)
[1] 0.03708686
```

Some weigths are very large!
Gives low «effective number samples»

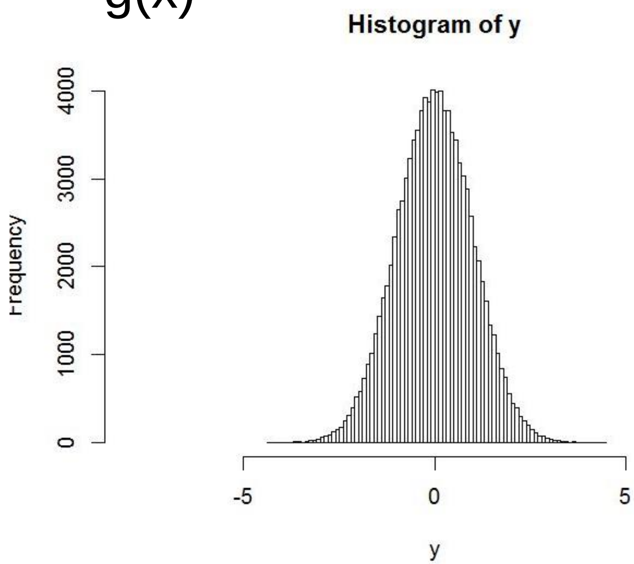
$f(x)/g(x)$



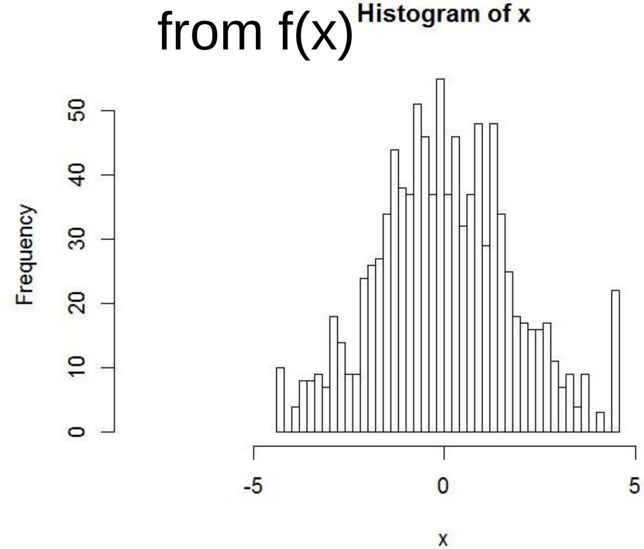
SIR slash from normal



Sample from g(x)

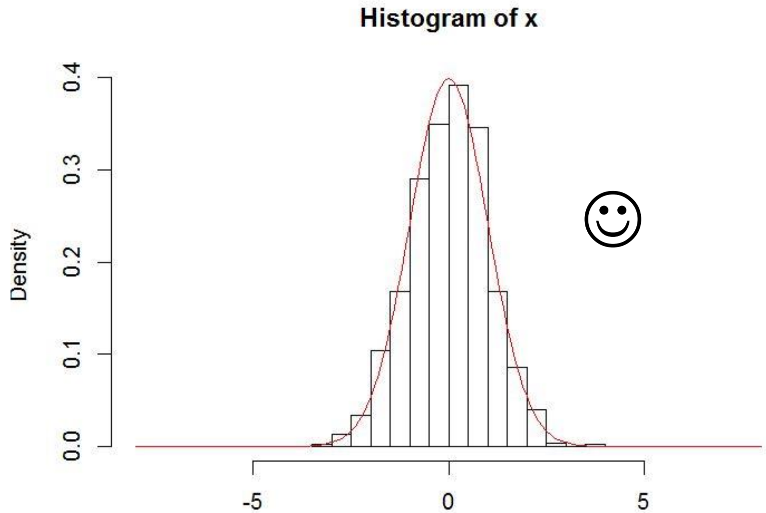


Approximate sample from f(x)

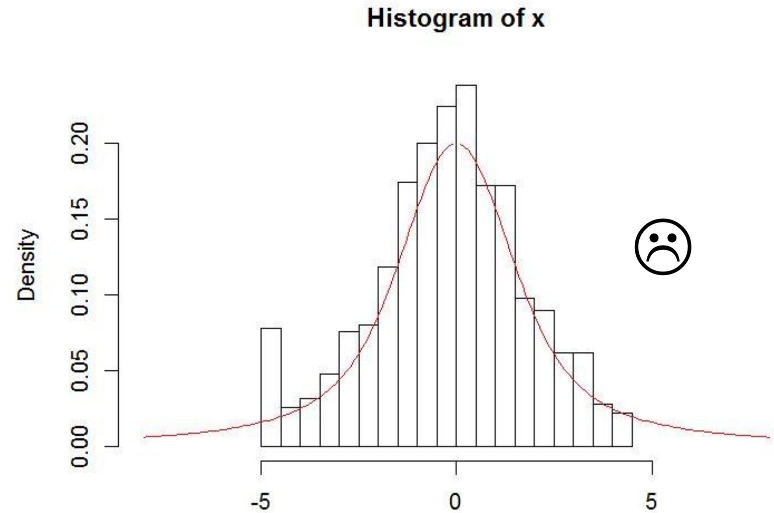



```
> ## SIR resample
> y =rnorm(m)
> w1 = s(y)/dnorm(y)
> wn1 = w1/sum(w1)
> n = 1000
> x = sample(y,n,replace=T,prob=wn1)
> par(mfrow=c(1,2))
> hist(y,1000,xlim=c(-8 ,8))
> hist(x,40,xlim=c(-8 ,8))
```

SIR:
normal from slash and slash from normal




```
> y =rnorm(m)/runif(m)
> w = dnorm(y)/s(y)
> x = sample(y,n,replace=T,prob=w)
> x = sort(x)
> hist(x,20,freq=F,xlim=c(-8,8))
> xp=seq(-8,8,by=0.1)
> lines(xp,dnorm(xp),col=2)
```




```
> y = rnorm(m)
> w = s(y)/dnorm(y)
> x = sample(y,n,replace=T,prob=w)
> x = sort(x)
> hist(x,20,freq=F,xlim=c(-8,8))
> lines(xp,s(xp),col=2)
```