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Random Number Generation and Rejection Sampling

Computational Statistics

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March 31, 2026

Today

Leftovers From Last Lecture
Efficient computations of smoothing splines

Pseudo-Random Numbers
How do you simulate random numbers in R?

Rejection Sampling
General and useful method for sampling from a target distribution

Recall, that our smoothing spline estimate is

$$\boldsymbol{f} = \boldsymbol{\Phi}\beta$$

with $\boldsymbol{\Phi}_{ij} = \varphi_j(x_i)$, and

$$\begin{aligned} L(\boldsymbol{f}) &= (\boldsymbol{y} - \boldsymbol{f})^T(\boldsymbol{y} - \boldsymbol{f}) + \lambda \|f''\|_2^2 \\ &= (\boldsymbol{y} - \boldsymbol{\Phi}\beta)^T(\boldsymbol{y} - \boldsymbol{\Phi}\beta) + \lambda \beta^T \boldsymbol{\Omega}\beta \end{aligned}$$

with

$$\boldsymbol{\Omega}_{jk} = \int \varphi_j''(z)\varphi_k''(z)\mathrm{d}z.$$

Solution
The solution is

$$\hat{\beta} = (\boldsymbol{\Phi}^T\boldsymbol{\Phi} + \lambda\boldsymbol{\Omega})^{-1}\boldsymbol{\Phi}^T\boldsymbol{y}.$$

When n is large, computing $\boldsymbol{S}_\lambda \boldsymbol{y}$ directly is expensive.

In practice, we therefore often use fewer basis functions than data points, $p < n$.

Singular Value Decomposition

Using the singular value decomposition

$$\boldsymbol{\Phi} = \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T$$

we can rewrite the smoother matrix as

$$\boldsymbol{S}_\lambda = \widetilde{\boldsymbol{U}}(I + \lambda \operatorname{diag}(\boldsymbol{\gamma}))^{-1}\widetilde{\boldsymbol{U}}^T$$

where $\widetilde{\boldsymbol{U}} = \boldsymbol{U}\boldsymbol{W}$ and

$$\boldsymbol{D}^{-1}\boldsymbol{V}^T\boldsymbol{\Omega}\boldsymbol{V}\boldsymbol{D}^{-1} = \boldsymbol{W}\operatorname{diag}(\boldsymbol{\gamma})\boldsymbol{W}^T.$$

The columns of $\widetilde{\boldsymbol{U}}$ form the **Demmler-Reinsch basis**.

Interpretation

Project the data y onto the Demmler-Reinsch basis (columns of $\widetilde{\boldsymbol{U}}$) to get coefficients $\hat{\boldsymbol{\beta}} = \widetilde{\boldsymbol{U}}^T \boldsymbol{y}$.

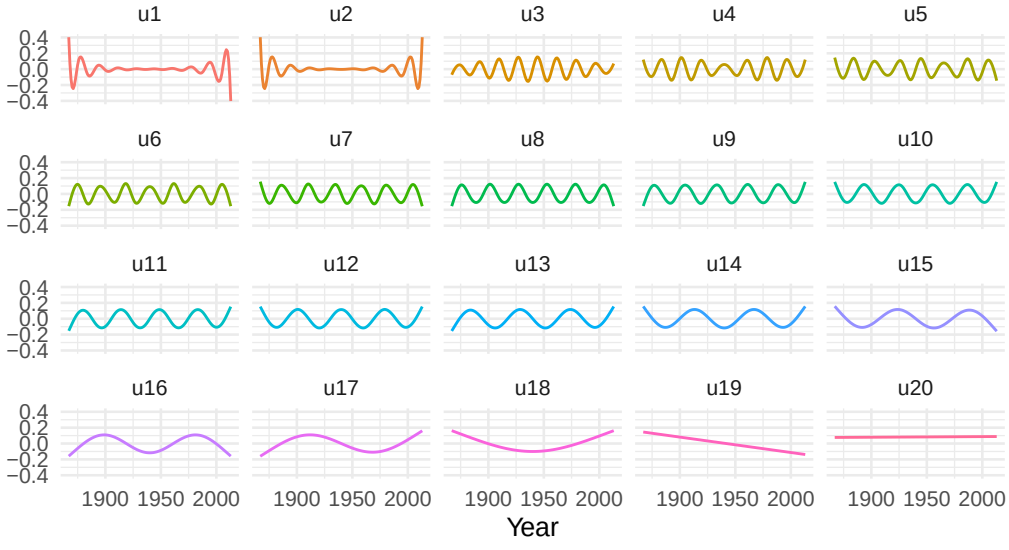
Each coefficient is shrunk according to the corresponding eigenvalue γ_i and smoothing parameter λ:

$$\hat{\boldsymbol{\beta}}_i(\lambda) = \frac{\hat{\beta}_i}{1 + \lambda\gamma_i}.$$

The final smoothed values are reconstructed by combining the shrunk coefficients with the basis functions.

$$\hat{\boldsymbol{f}} = \widetilde{\boldsymbol{U}}\hat{\boldsymbol{\beta}}(\lambda)$$

The Demmler-Reinsch Basis (Columns of $\widetilde{U}$)



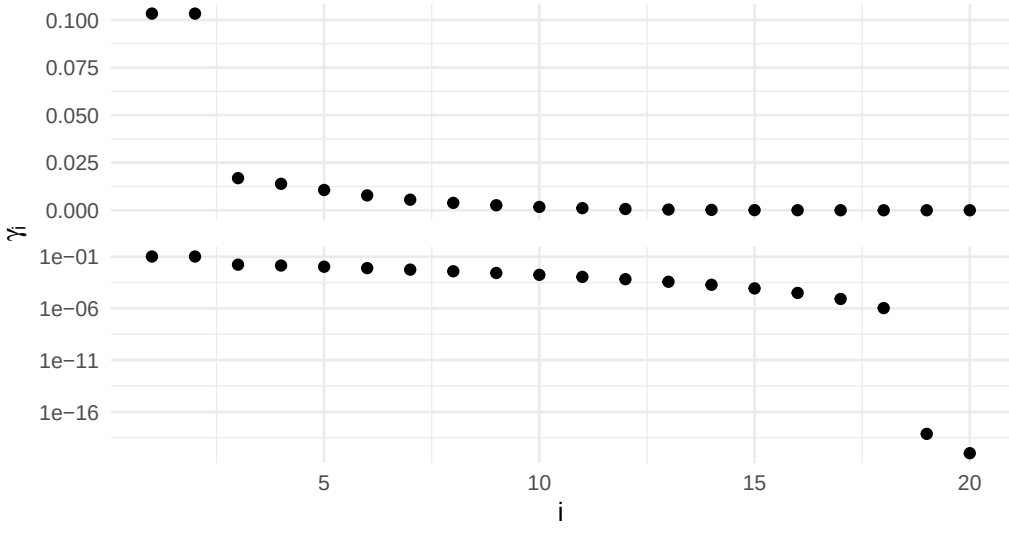


Figure 1: The eigenvalues γ_i of the penalty matrix in the Demmler-Reinsch basis.

Pseudo-Random Numbers

Computers have no concept of "true" randomness and instead generate **pseudo-random** numbers.

Not really random, but appear to be so.

A research field in itself, see `?RNG` in R for available algorithms.

Mersenne Twister
The default in R, which generates integers in the range

$$\{0, 1, \dots, 2^{32} - 1\}.$$

Long period: all combinations of consecutive integers up to dimension 623 occur equally often in a period.

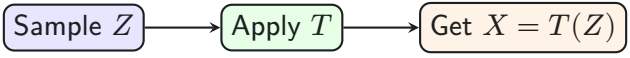
Uniform Random Variables i n R
`runif()` samples by just scaling these pseduo-random integers to the unit interval (with some tweaks to avoid division by 0).

Transformation Methods

What if we want to sample from a different distribution?

We could use **the transformation method**, which relies on the following fact:

If $T : \mathcal{Z} \to \mathbb{R}$ is a map and $Z \in \mathcal{Z}$ is a random variable we can sample, then we can sample $X = T(Z)$.



Transformation methods let us generate samples from complex distributions by applying a function to samples from a simpler distribution.

Example

To sample $X \sim \mathrm{Exp}(\lambda)$, use $X = -\log(U)/\lambda$ with $U \sim \mathrm{Uniform}(0, 1)$.

Inversion Sampling

A type of **transformation** sampling.

If $F^{-1} : (0, 1) \mapsto \mathbb{R}$ is the generalized inverse of a distribution function and U is uniformly distributed on $(0, 1)$ then

$$F^{-1}(U)$$

has distribution function F.

Computing F^{-1}: easy for discrete distributions, but hard for continuous ones.

Gaussian Random Variables

Box–Muller Method
A transformation of two independent uniforms into two independent Gaussian random variables (polar coordinates).

Inverse Transform
$X = \Phi^{-1}(U)$ where Φ is the distribution function for the Gaussian distribution.

Rejection Sampling
See Exercise 5.1 in CSwR or the Ziggurat algorithm.

Computing Φ^{-1}

Recall that

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-z^2/2} \mathrm{d}z.$$

But Φ^{-1} (the quantile function) does not have a closed-form expression.

We need to approximate Φ^{-1} numerically.

This, together with this technical approximation of Φ^{-1} is how R generates samples from $\mathcal{N}(0, 1)$.

Sampling in R

R has three basic options for customizing the behavior, set through `RNGkind()`.

```
RNGkind()
```

```
[1] "Mersenne-Twister" "Inversion"         "Rejection"
```

Options

- `kind`: type of pseudo-random number generator
- `normal.kind`: type of sampler for Normal samples
- `sample.kind`: type of sampler for `sample()`

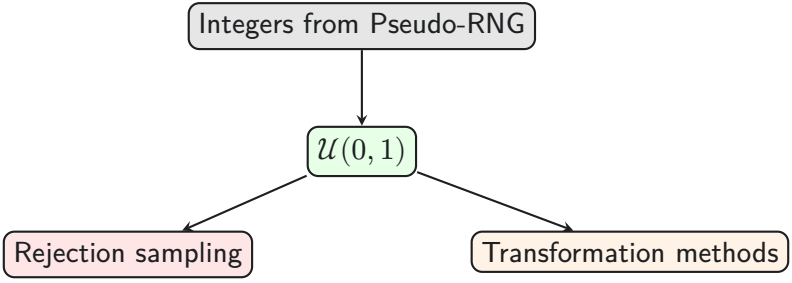


Figure 2: Main categories of sampling methods (in this course).

Example: Sampling from a t-Distribution

If we let

$$T(z, w) = \frac{z}{\sqrt{w/k}},$$

and take $Z \sim \mathcal{N}(0, 1)$ and $W \sim \chi^2_k$, then

$$X = T(Z, W) = \frac{Z}{\sqrt{W/k}} \sim t_k.$$

This transformation is used in R and other software to simulate t-distributed random variables.

Algorithm 1: Transformation sampling for the t-distribution

$z \leftarrow$ sample from $\mathcal{N}(0, 1)$;
$w \leftarrow$ sample from χ^2_k;
return $z/\sqrt{w/k}$;

Von Mises Distribution

The density on $(-\pi, \pi]$ is

$$f(x) = \frac{1}{2\pi I_0(\kappa)} \, e^{\kappa \cos(x-\mu)}$$

for $\kappa > 0$ and $\mu \in (-\pi, \pi]$ parameters and I_0 is the modified Bessel function.

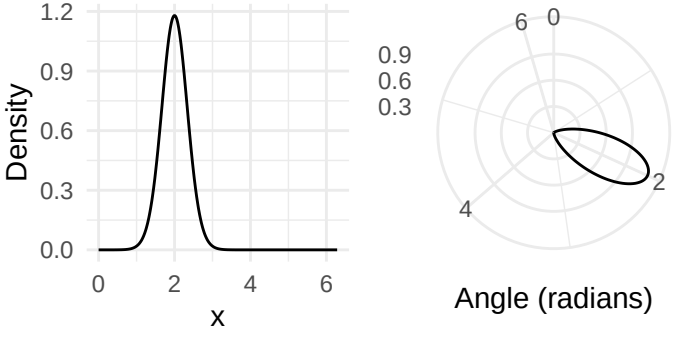


Figure 3: The von Mises density for $\mu = 2$ and $\kappa = 9$.

Using movMF

```r
library(movMF)
xy <- rmovMF(500, 0.5 * c(cos(-1.5), sin(-1.5)))

# rmovMF represents samples as elements on the unit circle
x <- acos(xy[, 1]) * sign(xy[, 2])
```

Problem

Can we sample via the transformation method? Yes, but not easily. There is no closed-form expression for the quantile function.

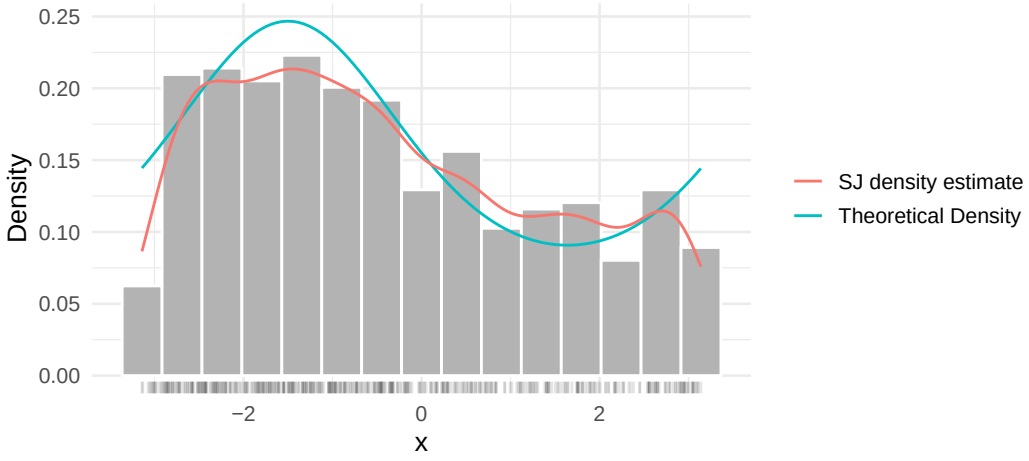


Figure 4: Histogram of samples from rmovMF()

Rejection Sampling

We want to sample from a target distribution $f(y)$ but have no readily available transform T for our proposal $g(y)$.

Let $Y_1, Y_2, ...$ be i.i.d. with density g on $\mathbb{R}$ and $U_1, U_2, ...$ be i.i.d. uniform and independent of Y_i for all i.

Define

$$k = \inf\left\{ n \geq 1 \mid U_n \leq \alpha \frac{f(Y_n)}{g(Y_n)} \right\},$$

for $\alpha \in (0, 1]$, where f is a density.

Theorem
If $f(y) \leq g(y)/\alpha$ for all $y \in \mathbb{R}$, then the distribution of Y_k has density f.

α is the **acceptance probability** and $g(y)/\alpha$ the **envelope** of f.

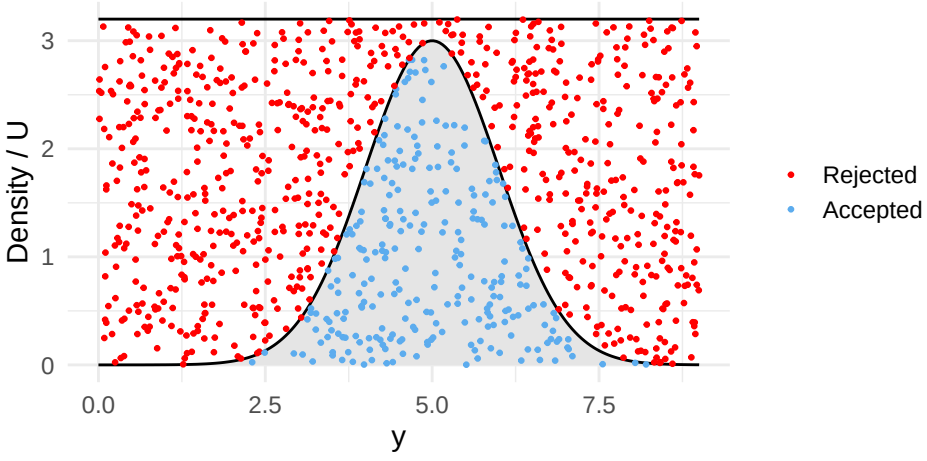


Figure 5: Illustration of rejection sampling for a normal target density, using a uniform proposal.

Normalizing Constants

Rejection sampling works with unnormalized densities!

Suppose:

- Target: $f(y) = cq(y)$ (unknown c)
- Proposal: $g(y) = dp(y)$ (unknown d)

Acceptance test:

$$U \leq \frac{\alpha f(y)}{g(y)} = \frac{\alpha c q(y)}{d p(y)}$$

If $\alpha = \frac{\alpha' d}{c}$, then

$$\frac{\alpha f(y)}{g(y)} = \frac{\alpha' q(y)}{p(y)}$$

Takeaway

You do not need to know c or d!

How to Find α'?

Given functions q and p, we need to find α' such that

$$\alpha' q(y) \leq p(y) \quad \text{for all } y.$$

How?
We can try to solve the problem

$$\alpha' = \inf_{y:q(y)>0} \frac{p(y)}{q(y)} > 0.$$

Optimally, find the minimum analytically.

Otherwise, numerically via optimization (e.g. `optimize()` in R).

Von Mises Rejection Sampling

Rejection sampling using the uniform proposal, $g(y) \propto 1$.

Since

$$e^{\kappa(\cos(y)-1)} = \alpha' e^{\kappa \cos(y)} \leq 1,$$

where $\alpha' = \exp(-\kappa)$, we reject if

$$U > e^{\kappa(\cos(Y)-1)}.$$

Algorithm 2: Rejection sampling for the von Mises distribution

repeat

  Generate $Y \sim \text{Uniform}(-\pi, \pi)$;

  Generate $U \sim \text{Uniform}(0, 1)$;

  if $U \leq e^{\kappa(\cos(Y)-1)}$ **then**

    Accept Y;

until *sample is accepted*;

Implementation

```
get_one_sample_vmises <- function(kappa) {
  repeat {
    Y <- runif(1, -pi, pi)
    U <- runif(1)
    if (U <= exp(kappa * (cos(Y) - 1))) {
      break
    }
  }
  Y
}
```

```
sample_vonmises_slow <- function(n, kappa) {
  replicate(n, get_one_sample_vmises(kappa))
}
```

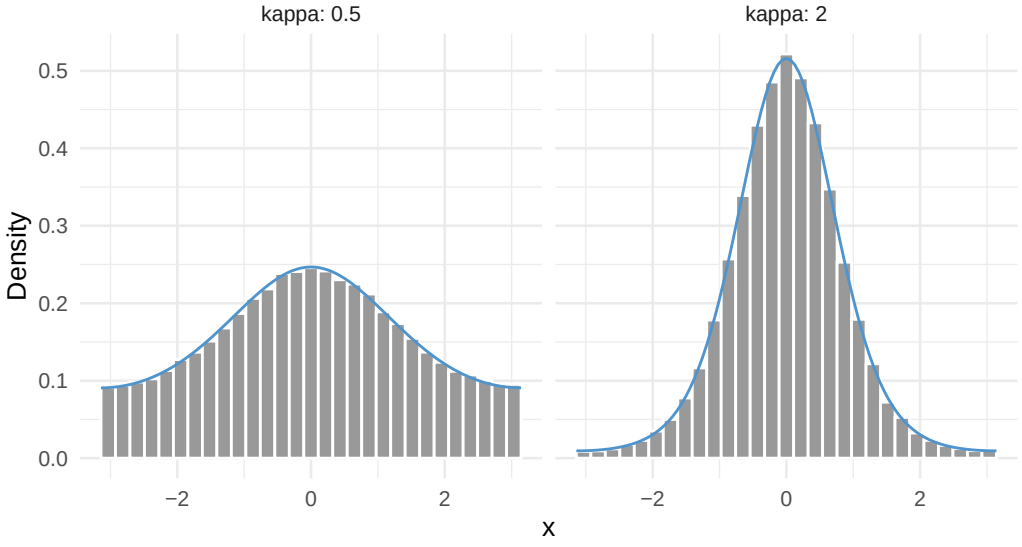


Figure 6: Histogram of samples from `sample_vonmises_slow()`, with theoretical density overlaid.

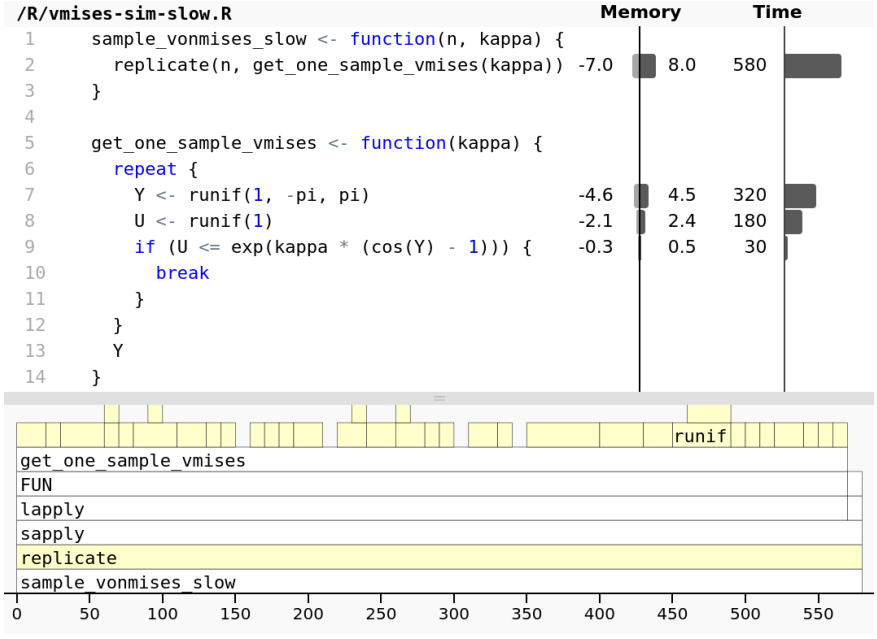


Figure 7: A line profile of the naive von Mises sampling implementation.

Findings from Profiling

The bottleneck is the repeated calls to `runif(1)`.

Both because of the for loop overhead, but also because calling the RNG for a single number is inefficient.

It is faster to generate all random numbers once and store them in a vector.

But how to do that for rejection sampling with an unknown number of rejections?

Vectorized (but Random Length) Rejection Sampler

We can speed up the rejection sampler by generating m proposal samples at once.

```
fixed_vonmises_sampler <- function(m, kappa) {
  Y <- runif(m, -pi, pi)
  u <- runif(m)
  accept <- u <= exp(kappa * (cos(Y) - 1))
  Y[accept]
}
```

Simple and fast, but returns a **random** number of samples!

We need a function that returns exactly n samples. But we don't know α in advance.

Algorithm 3: Sampling exactly n values via rejection sampling with unknown acceptance probability α.

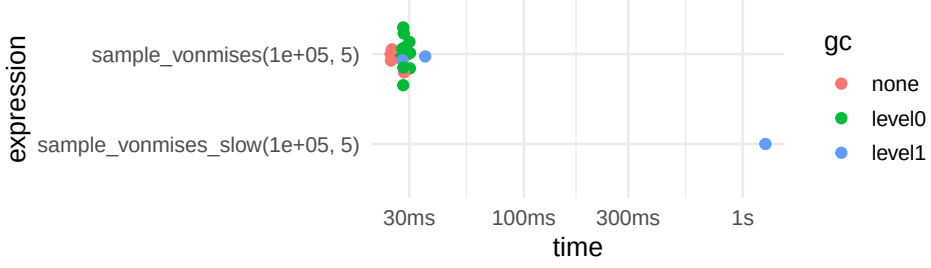
$\alpha \leftarrow 1$;
$\boldsymbol{y} \leftarrow$ empty vector;
$n_{\text{accepted}} \leftarrow 0$;
while $n_{accepted} < n$ **do**
  $m \leftarrow \lceil (n - n_{\text{accepted}})/\alpha \rceil$;
  $\boldsymbol{y}_{\text{new}} \leftarrow$ Generate m candidate samples $x_1, \ldots, x_m$;
  $n_{\text{accepted}} \leftarrow n_{\text{accepted}} +$ length$(\boldsymbol{y}_{\text{new}})$;
  if *first batch* **then**
    $\alpha \leftarrow (n_{\text{accepted}} + 1)/(m + 1)$ `// estimate acceptance probability`
  Append $\boldsymbol{y}_{\text{new}}$ to $\boldsymbol{y}$;
return $\boldsymbol{y}_{1:n}$

Function Factory for Rejection Sampling

```
new_rejection_sampler <- function(generator) {
  function(n, ...) {
    alpha <- 1
    y <- numeric(0)
    n_accepted <- 0
    while (n_accepted < n) {
      m <- ceiling((n - n_accepted) / alpha)
      y_new <- generator(m, ...)
      n_accepted <- n_accepted + length(y_new)
      if (length(y) == 0) {
        alpha <- (n_accepted + 1) / (m + 1)
      }
      y <- c(y, y_new)
    }
    list(x = y[seq_len(n)], alpha = alpha)
  }
}
```

```r
sample_vonmises <- new_rejection_sampler(fixed_vonmises_sampler)

bench::mark(
  sample_vonmises(1e5, 5),
  sample_vonmises_slow(1e5, 5),
  check = FALSE
) |>
  plot()
```



Adaptive Envelopes

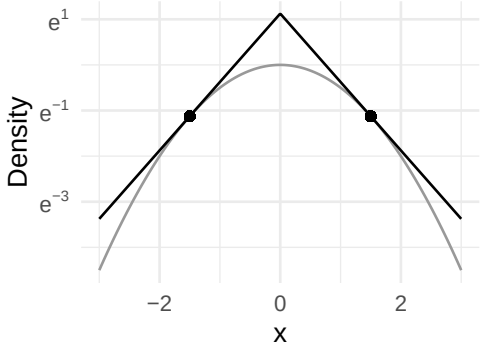
When f is *log-concave* on I we can construct bounds of the form

$$f(x) \leq e^{V(x)}$$

where

$$V(x) = \sum_{i=1}^{m} (a_i x + b_i) \mathbf{1}_{I_i}(x)$$

for intervals I_i forming a partition of I.



Typically, $a_i x + b_i$ is tangent to the graph of $\log(f)$ at $x_i \in I_i = (z_{i-1}, z_i]$ for

$$z_0 < x_1 < z_1 < x_2 < ... < z_{m-1} < x_m < z_m.$$

Beta Distribution

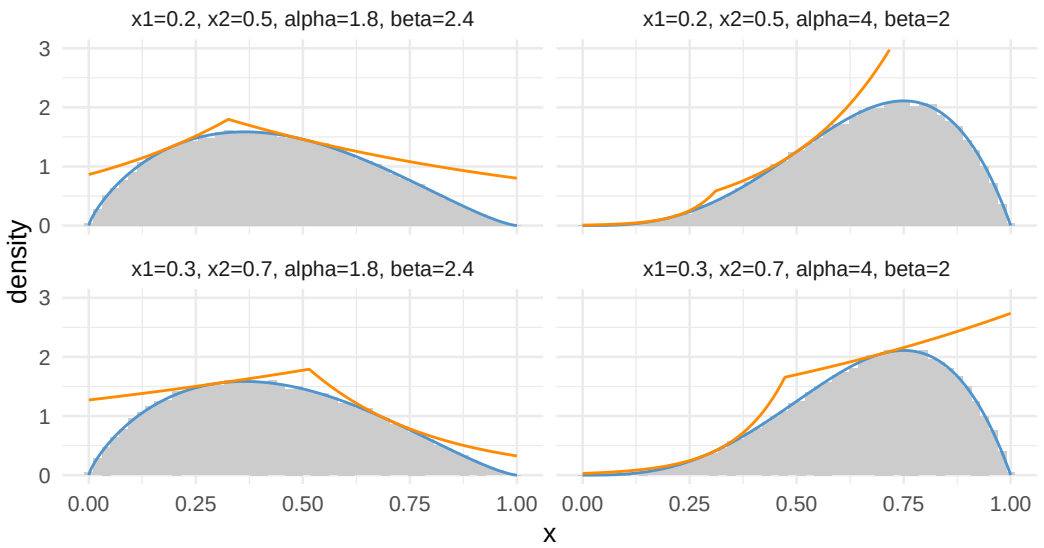


Figure 8: Histograms of samples from an adaptive envelope sampler with theoretical densities (blue) and envelopes (orange) overlaid.

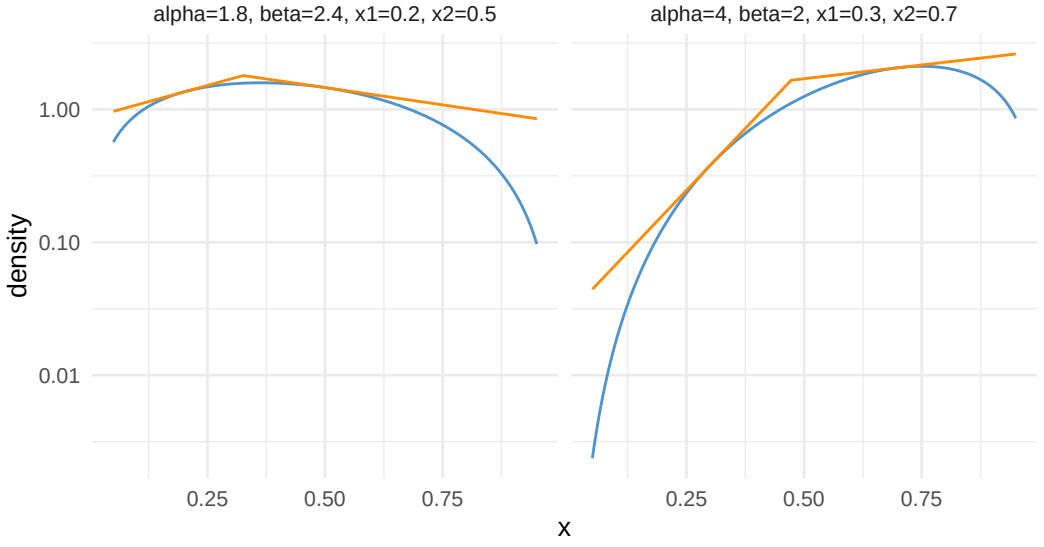


Figure 9: Theoretical densities (blue) and envelopes (orange) for different parameter values and choices of x_1 and x_2.

Von Mises Adaptive Envelopes

The von Mises density is unfortunately not globally log-concave.

But, it *is*

- log-concave on $(-\pi, \pi/2)$ and $(\pi/2, \pi)$ and
- log-convex on $(-\pi, -\pi/2)$ and $(-\pi/2, \pi/2)$.

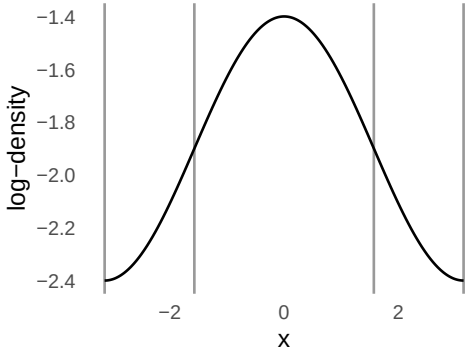


Figure 10: The von Mises density with $\kappa = 0.5$.

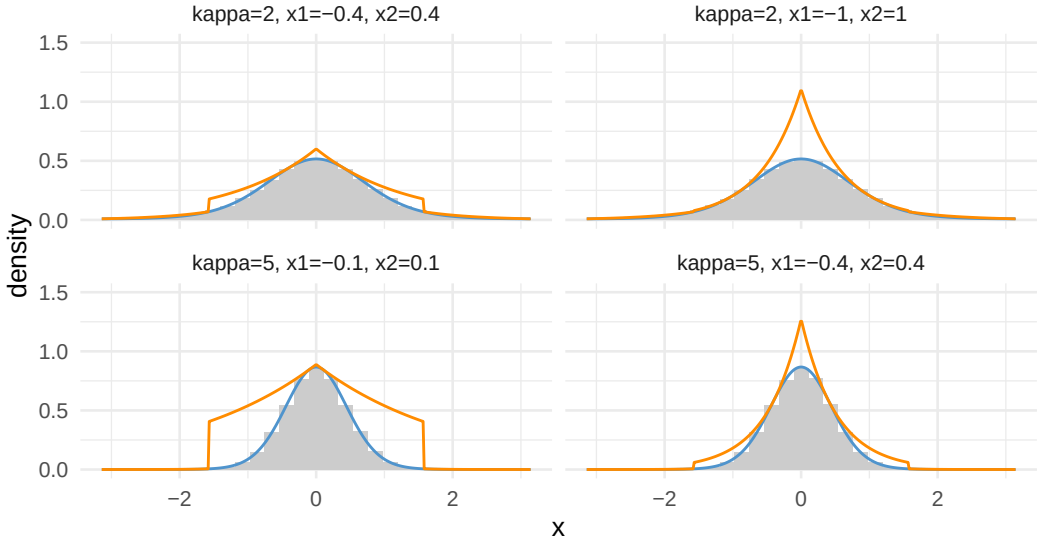


Figure 11: Histograms of samples from an adaptive envelope sampler for the von Mises distribution, with theoretical densities (blue) and envelopes (orange) overlaid.

Caveats about Adaptive Envelopes

Adaptive envelopes is a general and powerful technique, but tricky to implement!

Efficiency depends on number of rejections and also quality of implementation.

A good implementation should make use of new points to update envelope.

Transformation Methods vs. Rejection Sampling

Transformation Methods

Transform samples from a simple distribution to the target distribution.

Efficient if the transformation is available and cheap to compute.

But may not work for complex or unnormalized distributions!

Rejection Sampling

Uses a proposal distribution and accepts/rejects samples.

Works even if quantile function is unavailable or expensive.

Often less efficient, but very general.

Useful for complex, high-dimensional, or unnormalized distributions.

Takeaway

Use transformation methods when possible for efficiency; use rejection sampling when transformation is impractical or impossible.

Exercises

Step 1

Use the fact that

$$W = X_1^2 + ... + X_k^2 \sim \chi_k^2 \quad \text{for} \quad X_1, ..., X_k \sim_{\text{i.i.d.}} \mathcal{N}(0, 1)$$

to implement a function, `my_rchisq()`, such that `my_rchisq(n, k)` returns a sample of n i.i.d. observations from χ_k^2.

Step 2

Make another function `my_other_rchisq()` that uses inverse sampling.

Step 3

Benchmark your implementations against one another and `rchisq()`.