A transformed density rejection based algorithm for densities with poles and inflection points

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Non-Uniform Random Number Generation

Given:

- sequence $U_1, U_2, \ldots$ of "truly" IID uniform random numbers.

Task:

- transform into sequence $X_1, X_2, \ldots$ of random variates with **given distribution**

$$U_1, U_2, U_3, U_4, \ldots \quad \longrightarrow \quad X_1, X_2, X_3, \ldots$$

Most popular methods:

- Inversion method
- **Acceptance-Rejection** method

Automatic Algorithm

Idea:

One algorithm works for a large class of distributions.

- Works for non-standard distributions.
- Generators with known structural properties.
- Can be used by “non-experts” for special problems.

Required:

- PDF, CDF, ... of the distribution.
- Location of mode, “main part”, ... of the distribution.
- ...

Automatic Algorithm – Wishlist

- **Fast**.
- **Exact** (at least in $\mathbb{R}$).
- We can control the properties (accuracy, efficiency, ...) of the algorithm.
- Uses as **few** information as possible about distribution.
- User interface for a library implementation should be as **simple** as possible.

  (Complexity of algorithm should be hidden from user.)

Here: We assume that only the (log-)PDF f and its derivative are given.

Inversion Method

If $U \sim \mathcal{U}(0,1)$, then

$$X = F^{-1}(U) = \text{inf}\,\{x\colon F(x) \geq U\} \sim F$$

1. Generate $U \sim U(0,1)$.
2. Compute $X = F^{-1}(U)$. $\Leftarrow$ **Problem (?)**
3. Return X.

Inversion Method

Advantages:

- Most general method for generating non-uniform random variates.
- Get **one** random variate X for each uniform U.
- **Preserves** the structural properties of the underlying uniform PRNG.

Disadvantages:

- CDF and/or its inverse often not given in closed form.
- Numerical methods may be slow and/or require large tables.
- Numerical methods are **not exact**.
- There are issues with poles.

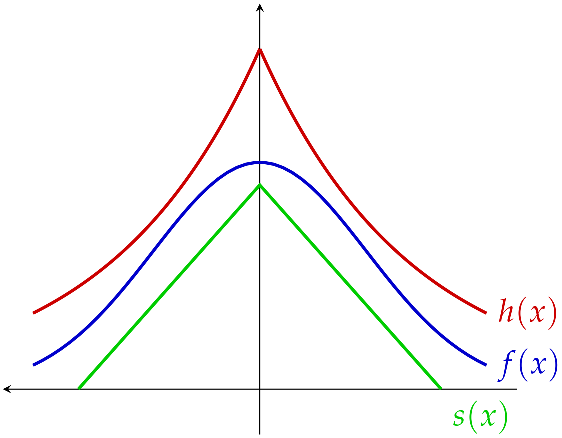
Derflinger et al. (2010) propose an inversion algorithm, when only the PDF is known.

Acceptance-Rejection Method

Need **hat** h and **squeeze** s, s.t.

$$s(x) \leq f(x) \leq h(x)$$

1. Generate $X \sim h$.
2. Generate $U \sim U(0,1)$.
3. If $U \cdot h(X) \leq s(X)$
4. Return X.
5. If $U \cdot h(X) \leq f(X)$,
6. Return X.
7. Else try again.



Acceptance-Rejection

Requirements:

- Hat function h must be a multiple of some PDF.

Properties:

- Works for unnormalized PDFs.
- Performance parameter: rejection constant.

Wishlist:

- $h \approx f$
- Sampling $X \sim h$ should be fast and simple (ideally by inversion).
- Evaluation of squeeze s should be cheap.

Acceptance-Rejection – Rejection Constant

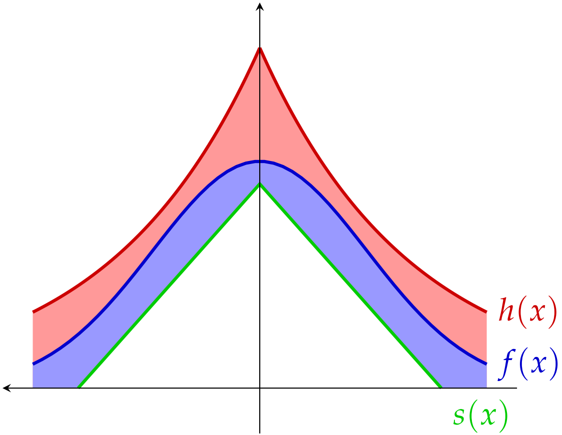
Rejection constant:

$$\alpha = \frac{\int_{\mathbb{R}} h(x)\,dx}{\int_{\mathbb{R}} f(x)\,dx}$$

Ratio hat-squeeze:

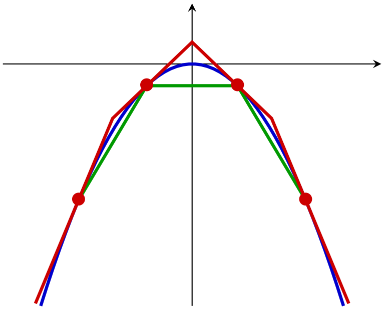
$$\rho = \frac{\int_{\mathbb{R}} h(x)\,dx}{\int_{\mathbb{R}} s(x)\,dx}$$

$$\rho \geq \alpha \geq 1$$

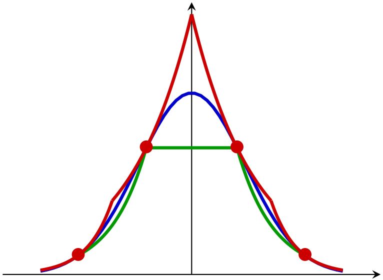


Transformed Density Rejection

Devroye (1984): tangents and secants to construct hat $h(x)$ and squeeze $s(x)$ for **log-concave** PDFs.



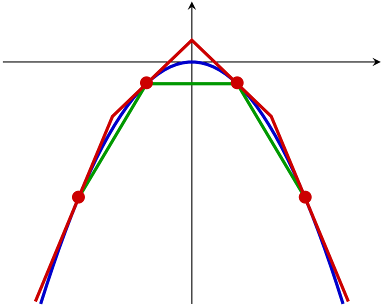
log-scale



original scale

Transformed Density Rejection

Gilks and Wild (1992): adaptive rejection sampling



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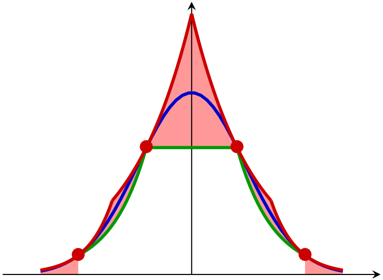

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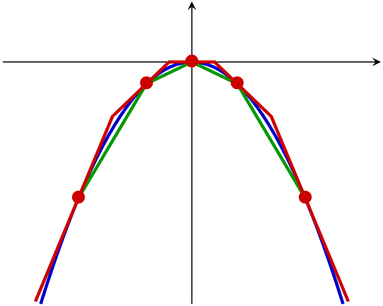

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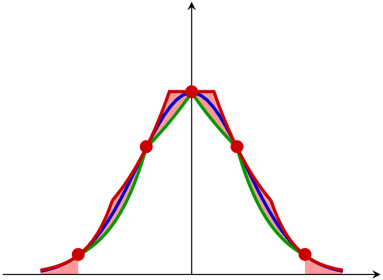

original scale

$$\rho \to 1 \quad \text{for} \quad N \to \infty$$

Transformed Density Rejection – Algorithm

1. Start with an initial partition.
2. Repeat:
3. Compute $h(x)$ and $s(x)$ for each subinterval.
4. Split every subinterval I where the $\int_I (h(x) - s(x))dx$ is too large.
5. Until ρ is as small as desired.
6. Run acceptance-rejection loop.

Transformed Density Rejection – Properties

- Requires PDF f and derivative f'.
- Performance can be controlled by input parameter ρ.

For $\rho \approx 1$ we find:

- Possibly expensive setup.
- (Very) fast marginal generation time (hardly depends on f.)
- Generation from hat is $\mathcal{O}(1)$
  (by guide table or alias method.)
- Algorithm close to inversion.

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Disadvantage: Restricted to **log-concave** distributions!

T-concave Distributions

Hörmann (1995): Generalizes to T_c-concave distribution, i.e., $T_c \circ f$ is concave.

$$T_c(x) = \begin{cases} \log(x) & \text{for } c = 0 \\ \operatorname{sgn}(c)x^c & \text{for } c \neq 0 \end{cases}$$

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- If f is T_{c_1}-concave, then it T_{c_2}-concave for all $c_2 \leq c_1$.
- Hat and squeeze are piecewise exponential or power functions.
- In transformed scale and $c \neq 0$: hat and squeeze must not intersect x-axis.
- For unbounded intervals: $c > -1$.
- For unbounded f (pole): $c < -1$.

T-convex

Obviously the idea also works for T_c-convex distributions with the roles of tangents and secants exchanged (Evans and Swartz, 1998).

Idea: Split domain into intervals where f is either T_c-concave or T_c-convex.

Issues:

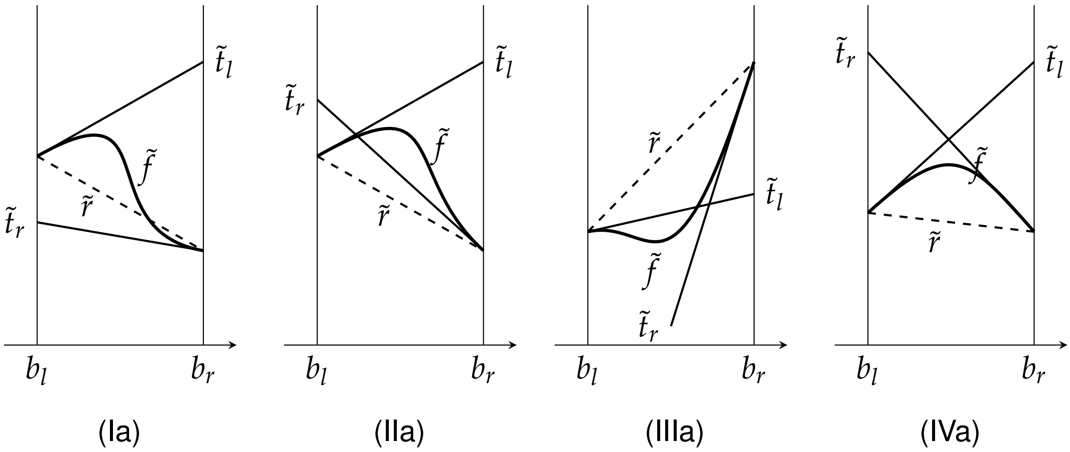
- Need f''.
- Have to compute inflection points of transformed density $T_c \circ f$.
- Is the API still simple?
- Is the algorithm still exact when we have to apply root finding algorithms?
- Can be replace the exact position of inflection points by a **rough** estimate?

A Rough Estimate

Botts, Hörmann, and L (2012):

- Suppose we have a subdivision into intervals.
- Assume that there is **at most one** inflection point of the $T_c \circ f$ in each subinterval $[b_l, b_r]$.
- Then only the four cases below are possible (plus their symmetric analogs).

Possible Cases



Possible Cases

Botts et al. (2012):

- Each interval belongs to (at most) one of these 4+4 types.
- In all cases we can use tangents and secants
  for constructing **hat** and **squeeze**.
- The type can be determined by the inequalities below.

Detect Cases I

Type	$\tilde{f}'$ and R	$\tilde{f}''$	squeeze and hat
Ia	$\tilde{f}'(b_l), \tilde{f}'(b_r) \geq R$	$\tilde{f}''(b_l) \leq 0 \leq \tilde{f}''(b_r)$	$\tilde{t}_r(x) \leq \tilde{f}(x) \leq \tilde{t}_l(x)$
IIa	$\tilde{f}'(b_l) \geq R \geq \tilde{f}'(b_r)$	$\tilde{f}''(b_l) \leq 0 \leq \tilde{f}''(b_r)$	$\tilde{r}(x) \leq \tilde{f}(x) \leq \tilde{t}_l(x)$
IIIa	$\tilde{f}'(b_l) \leq R \leq \tilde{f}'(b_r)$	$\tilde{f}''(b_l) \leq 0 \leq \tilde{f}''(b_r)$	$\tilde{t}_r(x) \leq \tilde{f}(x) \leq \tilde{r}(x)$
IVa	$\tilde{f}'(b_l) \geq R \geq \tilde{f}'(b_r)$	$\tilde{f}''(b_l), \tilde{f}''(b_r) \leq 0$	$\tilde{r}(x) \leq \tilde{f}(x) \leq \tilde{t}_l(x), \tilde{t}_r(x)$

Observe: We need the slope of the secant:

$$R = \frac{\tilde{f}(b_r) - \tilde{f}(b_l)}{b_r - b_l}$$

Detect Cases II

Type	$\tilde{f}'$ and R	$\tilde{f}''$	squeeze and hat
Ib	$\tilde{f}'(b_l), \tilde{f}'(b_r) \leq R$	$\tilde{f}''(b_l) \geq 0 \geq \tilde{f}''(b_r)$	$\tilde{t}_l(x) \leq \tilde{f}(x) \leq \tilde{t}_r(x)$
IIb	$\tilde{f}'(b_l) \geq R \geq \tilde{f}'(b_r)$	$\tilde{f}''(b_l) \geq 0 \geq \tilde{f}''(b_r)$	$\tilde{r}(x) \leq \tilde{f}(x) \leq \tilde{t}_r(x)$
IIIb	$\tilde{f}'(b_l) \leq R \leq \tilde{f}'(b_r)$	$\tilde{f}''(b_l) \geq 0 \geq \tilde{f}''(b_r)$	$\tilde{t}_l(x) \leq \tilde{f}(x) \leq \tilde{r}(x)$
IVb	$\tilde{f}'(b_l) \leq R \leq \tilde{f}'(b_r)$	$\tilde{f}''(b_l), \tilde{f}''(b_r) \geq 0$	$\tilde{t}_l(x), \tilde{t}_r(x) \leq \tilde{f}(x) \leq \tilde{r}(x)$

Observe: **We still need f''!** Can we avoid this?

Avoid 2nd Derivative I

Some cases are unique:

Case	$\tilde{f}'$ and R	Type
(1)	$\tilde{f}'(b_l), \tilde{f}'(b_r) \geq R$	(Ia)
(2)	$\tilde{f}'(b_l), \tilde{f}'(b_r) \leq R$	(Ib)

If neither (1) nor (2) holds we need an **additional** test point $p \in (b_l, b_r)$.

Avoid 2nd Derivative II

Case	$\tilde{f}'$ and R	$\tilde{f}(p)$	Type
(3)	$\tilde{f}'(b_l) \geq R \geq \tilde{f}'(b_r)$		—
(3.1)	$\tilde{f}'(p) \leq \tilde{f}'(b_r)$		(IIa)
(3.2)	$\tilde{f}'(p) \geq \tilde{f}'(b_l)$		(IIb)
(3.3)	$\tilde{f}'(b_l) \geq \tilde{f}'(p) \geq \tilde{f}'(b_r)$		—
(3.3.1)		$\tilde{f}(p) > \tilde{t}_l(p)$	(IIb)
(3.3.2)		$\tilde{f}(p) > \tilde{t}_r(p)$	(IIa)
(3.3.3)		$\tilde{f}(p) \leq \tilde{t}_l(p), \tilde{t}_r(p)$	(IIb $\mid$ IVa) + (IIa $\mid$ IVa)

Avoid 2nd Derivative III

Case	$\tilde{f}'$ and R	$\tilde{f}(p)$	Type
(4)	$\tilde{f}'(b_l) \le R \le \tilde{f}'(b_r)$		—
⋮			
(4.3)		$\tilde{f}'(b_l) \le \tilde{f}'(p) \le \tilde{f}'(b_r)$	—
⋮			
(4.3.3)		$\tilde{f}(p) \ge \tilde{t}_l(p), \tilde{t}_r(p)$	(IIIa $\mid$ IVb) + (IIIb $\mid$ IVb)

"(IIIa $\mid$ IVb) + (IIIb $\mid$ IVb)" means that we have to split $[b_l, b_r]$ into two subintervals of the respective types.

Combined Types

We now cannot decide between some case:

Type	$\tilde{f}'$ and R	$\tilde{f}''$	squeeze and hat
IIa | IVa	$\tilde{f}'(b_l) \geq R \geq \tilde{f}'(b_r)$	$\tilde{f}''(b_l) \leq 0$	$\tilde{r}(x) \leq \tilde{f}(x) \leq \tilde{t}_l(x)$
IIb | IVa	$\tilde{f}'(b_l) \geq R \geq \tilde{f}'(b_r)$	$\tilde{f}''(b_r) \leq 0$	$\tilde{r}(x) \leq \tilde{f}(x) \leq \tilde{t}_r(x)$
IIIa | IVb	$\tilde{f}'(b_l) \leq R \leq \tilde{f}'(b_r)$	$\tilde{f}''(b_r) \geq 0$	$\tilde{t}_r(x) \leq \tilde{f}(x) \leq \tilde{r}(x)$
IIIb | IVb	$\tilde{f}'(b_l) \leq R \leq \tilde{f}'(b_r)$	$\tilde{f}''(b_l) \geq 0$	$\tilde{t}_l(x) \leq \tilde{f}(x) \leq \tilde{r}(x)$

Nevertheless we still can construct hat and squeeze.

Sign of 2nd Derivative

- Once the type of the interval is known, we can use the above tables to determine the **sign** of $f''(b_l)$ and/or $f''(b_r)$.
- Then for any two points $c, c+\delta$ in (b_l, b_r),
  the sign can be determined for at least one of $f''(c)$ and $f''(c+\delta)$.
- This allows to determine the type when an interval is splitted at c or $c+\delta$ during the setup.
- In particular we thus get rid of the combined types.

Poles

Let p be a pole of f.
Then the secant of $T_c \circ f$ on a small interval $[p, b_r]$ can be used for constructing a hat function whenever

$$-1 > c > \limsup_{x \to p} \mathrm{lc}_f(x)$$

where

$$\mathrm{lc}_f(x) = 1 - \frac{f''(x)\, f(x)}{f'(x)^2}$$

(local concavity).

Work in progress. We test whether the method from Hörmann, L, and Derflinger (2007) can be used to find an appropriate c.

Examples

Generalized Hyperbolic distribution has PDF

$$f(x) = e^{\beta(x-\mu)} \frac{\mathrm{K}_{\lambda-1/2}\left(\alpha\sqrt{\delta^2 + (x-\mu)^2}\right)}{\left(\sqrt{\delta^2 + (x-\mu)^2}/\alpha\right)^{1/2-\lambda}},$$

where $\mathrm{K}_\nu(.)$ denotes the modified Bessel function of the third kind.

For $c = -1/2$,
$T_{-1/2} \circ f$ may have a single convex interval on one or both sides of the mode.

Examples

Watson distribution has PDF

$$f(\mathbf{x}) \propto \exp\left(\kappa \boldsymbol{\mu}' \mathbf{x}\right) \qquad \text{on} \quad S^d = \{\mathbf{x} \colon \|\mathbf{x}\|_2 = 1\}$$

It can be decomposed as $\mathbf{X} = \left(\sqrt{1 - W^2}\mathbf{Y}, W\right)$, where $\mathbf{Y}$ is uniformly distributed on the hypersphere orthogonal to $\boldsymbol{\mu}$ and W has log-density

$$g(w) = \kappa w^2 + \frac{d-3}{2} \log\left(1 - w^2\right)$$

on domain $[0, 1]$.
It can be easily shown that $\log \circ g$ has at most one inflection point.

Examples

... and of course it works for all truncated distributions
whenever it works on its entire domain.

Tinflex

The method is implemented in **R** package `Tinflex`:

`https://CRAN.R-project.org/package=Tinflex`

Conclusion

- We have created an automatic algorithm based on the acceptance-rejection method for quite general continuous univariate distributions.
- Requirements: (log-)PDF, its derivative, a partition of the domain s.t. each subinterval contains at most one inflection point of the transformed density.
- We avoid the computation of inflection points and f''.
- Simpler interface for user ...
- ... but higher complexity for the implementation (mostly look-ups in tables of satisfied inequalities).

Thank You

for your attention!

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