Supplementary material for the transformed density rejection algorithm

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Abstract

This document aims to provide an understandable guide to the transformed density rejection algorithm and explain all choices made for the mir implementation.

1 Intro to random sampling

The implementation is available at `mir.random.flex`.
Two introductory blog posts explain the basics of non-uniform random sampling and describe the implementation of the transformed density rejection sampling method.
Additionally the report *Transformed Density Rejection with Inflection Points* should be considered.
All code listings can be browsed online at `https://github.com/wilzbach/flex-paper`.

2 Area A_h

For the sampling we want to be able to compute the inverse CDF for any x in a choosen interval.
The area below a constructed hat function (and thus respectively for the squeeze function) within the interval $[\ell, r]$ can be calculated by its definite integral. F_{T_c} is the antiderivative (aka primitive integral) of the inverse transformation T^{-1} as $h(x) = T^{-1}(\tilde{h}(x))$ and $F_{T_c}(x) = \int_{-\infty}^{x} T^{-1}(t)dt$. Note that $\tilde{h}(x)' = \beta$.

$$
\begin{aligned}
A_h &= \int_\ell^r h(x)dx \\
&= \int_\ell^r T^{-1}(\tilde{h}(x)) * \frac{\tilde{h}'(x)}{\tilde{h}'(x)} dx \\
&= \int_\ell^r (F_T(\tilde{h}(x))' * \frac{1}{\tilde{h}'(x)} dx \\
&= \frac{1}{\beta}\big(F_{T_c}(\tilde{h}(r)) - F_{T_c}(\tilde{h}(\ell))\big)
\end{aligned}
$$

The CDF $H_i(x)$ with $x \in [l_i, r_i]$ is thus:

$$
\frac{1}{\beta}\big(F_{T_c}(\tilde{h}(x)) - F_{T_c}(\tilde{h}(\ell))\big)
$$

with $H_i(r_i) = A_h$.
Note that $H_(x)$ is only defined if $\beta \neq 0$.

2.1 c = 1

From $T^{-1} = x$ follows trivially its integral $F_{T_1} = \frac{1}{2} * x^{\frac{2}{1}}$ and then we can simplify the above equation to:

$$
\begin{aligned}
A_h &= \frac{1}{\beta}\big(F_{T_1}(h(r)) - F_{T_1}(h(\ell))\big) \\
&= \frac{1}{\beta}\left(0.5 * (\alpha + \beta * (r - x_0))^2 - 0.5 * (\alpha + \beta * (\ell - x_0))^2\right)
\end{aligned}
$$

2.1.1 Z-Trick

Z-Trick, x_0 can only be either r or ℓ, thus either $r - x_0$ or $\ell - x_0$ is zero.

$I) \quad x_0 = \ell$

$$
\begin{aligned}
A_h &= \frac{0.5}{\beta}\left((\alpha + \beta * (r - \ell))^2 - \alpha^2\right) \\
&= \frac{0.5}{\beta}\left(\alpha^2 + 2 * \alpha * \beta * (r - \ell) + (\beta * (r - \ell))^2 - \alpha^2\right) \\
&= \frac{0.5}{\beta}\left(2 * \alpha * \beta * (r - \ell) + (\beta * (r - \ell))^2\right) \\
&= 0.5 * \left(2 * \alpha * (r - \ell) + \beta * (r - \ell)^2\right) \\
&= 0.5 * (r - \ell) * (2 * \alpha + \beta * (r - \ell)) \\
&= (r - \ell) * (\alpha + 0.5 * \beta * (r - \ell))
\end{aligned}
$$

$II) \quad x_0 = r$

$$
\begin{aligned}
A_h &= \frac{0.5}{\beta}\left(\alpha^2 - (\alpha + \beta * (\ell - r))^2\right) \\
&= \frac{0.5}{\beta}\left(\alpha^2 - \alpha^2 - 2 * \alpha * \beta * (\ell - r) - (\beta * (\ell - r))^2\right) \\
&= \frac{0.5}{\beta}\left(-2 * \alpha * \beta * (\ell - r) - (\beta * (\ell - r))^2\right) \\
&= -0.5 * \left(2 * \alpha * (\ell - r) + \beta * (\ell - r)^2\right) \\
&= -0.5 * (\ell - r) * (2 * \alpha + \beta * (\ell - r)) \\
&= -(\ell - r) * (\alpha + 0.5 * \beta * (\ell - r)) \\
&= (r - \ell) * (\alpha + 0.5 * \beta * (\ell - r))
\end{aligned}
$$

this means with a helper function $\sigma(x)$ which is

$$
\sigma(x) = \begin{cases} 1 & \text{for } x = \ell \\ -1 & \text{for } x = r \end{cases}
$$

we can summarize this in one equation:

$$
A_{h_1} = (r - \ell) * (\alpha + 0.5 * \beta * \sigma(x) * (r - \ell))
$$

2.2 c = 0

$F_{T_0} = e^x$

$$
A_{h_0} = \frac{1}{\beta}\left(e^{h(r)} - e^{h(\ell)}\right)
$$

First we simplify the equation a bit:

$$
\begin{aligned}
A_{h_0} &= \frac{1}{\beta}\left(e^{h(r)} - e^{h(\ell)}\right) \\
&= \frac{1}{\beta}\left(e^{\alpha+\beta(r-x_0)} - e^{\alpha+\beta(l-x_0)}\right) \\
&= \frac{1}{\beta}\left(e^{\alpha+\beta r-\beta x_0} - e^{\alpha+\beta l-\beta x_0}\right) \\
&= \frac{1}{\beta}\left(e^{\alpha} * e^{\beta r} * e^{-\beta x_0} - e^{\alpha} * e^{\beta l} * e^{-\beta * x_0}\right) \\
&= \frac{1}{\beta}\left(e^{\alpha-\beta x_0} * \left(e^{\beta r} - e^{\beta \ell}\right)\right)
\end{aligned}
$$

Again we use the z-trick to distinguish between both cases.
I) $x_0 = \ell$:

$$
\begin{aligned}
A_{h_0} &= \frac{1}{\beta}\left(e^{\alpha-\beta * x_0} * \left(e^{\beta r} - e^{\beta \ell}\right)\right) \\
&= \frac{1}{\beta}\left(e^{\alpha-\beta * \ell} * \left(e^{\beta r} - e^{\beta \ell}\right)\right) \\
&= \frac{1}{\beta}\left(e^{\alpha-\beta\ell-\beta r} - e^{\alpha-\beta\ell+\beta\ell}\right) \\
&= \frac{1}{\beta}\left(e^{\alpha-\beta\ell-\beta r} - e^{\alpha}\right) \\
&= \frac{e^{\alpha}}{\beta}\left(e^{-\beta\ell-\beta r} - 1)\right) \\
&= \frac{e^{\alpha}}{\beta}\left(e^{\beta(r-\ell)} - 1\right)
\end{aligned}
$$

With Taylor-Series of $n = 4$ with $k = \beta(r-\ell)$ and $e^{\alpha} = g(x)$ we can approximate this arbitrarily, e.g. for $n = 3$,

$$
A_{h_0} = \frac{e^{\alpha}}{\beta}\left(1 + k + \frac{k^2}{2} + \frac{k^3}{6} - 1\right)
$$

and for more precision we can increase n to 4.

$$
A_{h_0} = \frac{e^{\alpha}}{\beta}\left(1 + k + \frac{k^2}{2} + \frac{k^3}{6} + \frac{k^4}{24} - 1\right)
$$

II) $x_0 = r$:

$$
\begin{aligned}
A_{h_0} &= \frac{1}{\beta}\left(e^{\alpha-\beta*x_0} * \left(e^{\beta r} - e^{\beta \ell}\right)\right) \\
&= \frac{1}{\beta}\left(e^{\alpha-\beta*r} * \left(e^{\beta r} - e^{\beta \ell}\right)\right) \\
&= \frac{1}{\beta}\left(e^{\alpha-\beta r-\beta r} - e^{\alpha-\beta r+\beta \ell}\right) \\
&= \frac{1}{\beta}\left(e^{\alpha} - e^{\alpha-\beta r+\beta \ell}\right) \\
&= \frac{e^{\alpha}}{\beta}\left(1 - e^{-\beta r+\beta \ell})\right) \\
&= \frac{e^{\alpha}}{\beta}\left(1 - e^{\beta(\ell-r)}\right)
\end{aligned}
$$

hence in general

$$
\frac{e^{\alpha} * \sigma(x)}{\beta}\left(e^{\beta*\sigma(x)(r-\ell)} - 1\right)
$$

and thus:

$$
A_{h_0} = \frac{e^{\alpha}}{\beta} * \sigma(x) * \left(e^{\beta*\sigma(x)(\ell-r)} - 1\right)
$$

and with Taylor-series:

$$
A_{h_0} = \frac{e^{\alpha} * \sigma(x)}{\beta}\left(1 + k + \frac{k^2}{2} + \frac{k^3}{6} + \frac{k^4}{24} - 1\right)
$$

where $k = \beta * \sigma(x) * (r - l)$

2.3 c = -0.5

$T_{-0.5}^{-1} = \frac{1}{x^2}$, hence $F_{T_{-0.5}} = -\frac{1}{x}$

2.3.1 Z-trick

$$
\begin{aligned}
A_h &= \frac{1}{\beta}\left(\frac{-1}{\tilde{h}(r)} - \frac{-1}{\tilde{h}(\ell)}\right) \\
&= \frac{1}{\beta}\left(-\frac{1}{\tilde{h}(r)} + \frac{1}{\tilde{h}(\ell)}\right) \\
&= \frac{1}{\beta}\left(\frac{1}{\tilde{h}(l)} - \frac{1}{\tilde{h}(r)}\right)
\end{aligned}
$$

2.3.2 Z-trick

I) $x_0 = \ell$

$$
\begin{aligned}
A_{h_{-0.5}} &= \frac{0}{\beta}\left(\frac{1}{\alpha} - \frac{1}{\alpha - (\beta * (\ell - r)}\right) \\
&= \frac{1}{\alpha\beta} - \frac{1}{\alpha\beta - (\beta^2 * (\ell - r)} \\
&= \frac{\alpha\beta - (\beta^2 * (\ell - r)}{(\alpha\beta) * (\alpha\beta - (\beta^2 * (\ell - r))} - \frac{\alpha\beta}{\alpha\beta * (\alpha\beta - (\beta^2 * (\ell - r))} \\
&= \frac{-\beta^2 * (\ell - r)}{\alpha\beta * \alpha\beta - \alpha\beta(\beta^2 * (\ell - r))} \\
&= \frac{-(\ell - r)}{\alpha^2 - \alpha\beta(\ell - r)} \\
&= \frac{r - \ell}{\alpha^2 + \alpha\beta(r - \ell)}
\end{aligned}
$$

II) $x_0 = r$

$$
A_{h_{-0.5}} = \frac{1}{\beta}\left(\frac{1}{\alpha - (\beta * (r - \ell)} - \frac{1}{\alpha}\right)
$$

and thus in general:

$$
A_{h_{-0.5}} = \frac{r - \ell}{\alpha^2 + \alpha\beta * \sigma(x) * (r - \ell)}
$$

2.4 c = -1

$T_{-1} = -\frac{1}{x}$, thus its integral $F_{T_{-1}} = -log(-x)$

$$
\begin{aligned}
A_{h_{-1}} &= \frac{1}{\beta}\left(-log(-\tilde{h}(r)) + log(-\tilde{h}(l))\right) \\
&= \frac{1}{\beta}\left(-log(-\alpha - (\beta * (r - \ell))) + log(-\alpha)\right)
\end{aligned}
$$

we use the Z-trick again:
I) $x_0 = \ell$

$$
\begin{aligned}
A_{h_{-1}} &= \frac{1}{\beta}\left(-log(-\tilde{h}(r)) + log(-\tilde{h}(l))\right) \\
&= \frac{1}{\beta}\left(-log(-\alpha - (\beta * (r - \ell))) + log(-\alpha)\right)
\end{aligned}
$$

II) $x_0 = r$

$$
A_{h_{-1}} = \frac{1}{\beta}\left(-log(-\alpha) + log(-\alpha - (\beta * (\ell - r)))\right)
$$

and in general:

$$
A_{h_{-1}} = \frac{\sigma(x)}{\beta}\left(-log(-\alpha - (\beta * \sigma(x) * (r - \ell))) + log(-\alpha)\right)
$$

Please note that if $\beta \sim 0$, this gets undefined. Thus this special case needs to be covered separately.

2.5 $c > 0$

$T_c^{-1} = x^{1/c}$, thus it's integral is $F_T = \frac{c}{c+1} * x^{\frac{c+1}{c}}$

$$
\begin{aligned}
A_h &= \frac{1}{\beta}\left(\frac{c}{c+1}h(r)^{\frac{c+1}{c}} - \frac{c}{c+1}h(\ell)^{\frac{c+1}{c}}\right) \\
A_h &= \frac{c}{\beta * (c+1)}\left(h(r)^{\frac{c+1}{c}} - h(\ell)^{\frac{c+1}{c}}\right)
\end{aligned}
$$

we use the z-trick again:
I) $x_0 = \ell$

$$
A_h = \frac{c}{\beta * (c+1)}\left((\alpha + \beta * (r - \ell))^{\frac{c+1}{c}} - \alpha^{\frac{c+1}{c}}\right)
$$

II) $x_0 = r$

$$
A_h = \frac{c}{\beta * (c+1)}\left(\alpha^{\frac{c+1}{c}} - (\alpha + \beta * (\ell - r))^{\frac{c+1}{c}}\right)
$$

thus in general:

$$
A_h = \frac{c * \sigma(x)}{\beta * (c+1)}\left((\alpha + \beta * \sigma(x) * (r - \ell))^{\frac{c+1}{c}} - \alpha^{\frac{c+1}{c}}\right)
$$

2.6 $c < 0$

$T_c^{-1} = (-x)^{1/c}$ and thus the integral is $F_T = -\frac{c}{c+1} * (-x)^{\frac{c+1}{c}}$

$$A_h = \frac{1}{\beta}\left(-\frac{c}{c+1}(-\tilde{h}(r))^{\frac{c+1}{c}} + \frac{c}{c+1}(-\tilde{h}(\ell))^{\frac{c+1}{c}}\right)$$
$$A_h = \frac{c}{\beta * (c+1)}\left(-(-\tilde{h}(r))^{\frac{c+1}{c}} + (-\tilde{h}(\ell))^{\frac{c+1}{c}}\right)$$

we use the z-trick again:
I) $x_0 = \ell$

$$A_h = \frac{c}{\beta * (c+1)}\left(-(-\alpha - \beta * (r-\ell))^{\frac{c+1}{c}} + (-\alpha)^{\frac{c+1}{c}}\right)$$

II) $x_0 = r$

$$A_h = \frac{c}{\beta * (c+1)}\left(-(-\alpha)^{\frac{c+1}{c}} + (-\alpha - \beta * (r-\ell))^{\frac{c+1}{c}}\right)$$

and thus in general:

$$A_h = \frac{c * \sigma(x)}{\beta * (c+1)}\left(-(-\alpha - \beta * \sigma(x)(r-\ell))^{\frac{c+1}{c}} + (-\alpha)^{\frac{c+1}{c}}\right)$$

and for any c:

$$A_h = \frac{c * \sigma(x) * sgn(c)}{\beta * (c+1)}\left((sgn(c) * (\alpha + \beta * \sigma(x) * (r-\ell)))^{\frac{c+1}{c}} - (sgn(c) * \alpha)^{\frac{c+1}{c}}\right)$$

Be aware that here in both cases if $\beta \sim 0$ the results may get undefined.

3 Inversion

Moreover with $H_i(x)$ can now define the inverse CDF $H_i(x)^{-1}$. Note that $H_i(x) = A_i$ if $x = r$.

$$H(x) = \frac{1}{\beta}\big(F_T(h(x)) - F_T(h(\ell))\big)$$

then if $H(x) = U$:

$$
\begin{aligned}
U &= \frac{1}{\beta}\big(F_T(h(x)) - F_T(h(\ell))\big) \\
U * \beta &= \big(F_T(h(x)) - F_T(h(\ell))\big) \\
(U * \beta) + F_T(h(\ell)) &= F_T(h(x)) \\
F_T^{-1}((U * \beta) + F_T(h(\ell))) &= F_T^{-1}(F_T(h(x))) \\
&= h(x) \\
h^{-1}\left(F_T^{-1}((U * \beta) + F_T(h(\ell)))\right) &= x
\end{aligned}
$$

the inverse of $h(x) = \alpha + \beta * (x - x_0)$ is as follows:

$$
\begin{aligned}
y &= \alpha + \beta * (x - x_0) \\
y - \alpha &= (x - x_0) \\
\frac{y - \alpha}{\beta} &= (x - x_0) \\
x_0 + \frac{y - \alpha}{\beta} &= x
\end{aligned}
$$

and thus with $h^{-1}(c)$ we can write:

$$
x = x_0 + \frac{1}{\beta}\left(F_T^{-1}((U * \beta) + F_T(h(\ell))) - \alpha\right)
$$

We can simplify the equation even more for the special cases given:

3.1 c = 0

$F_T = e^x$, $F_T^{-1} = log(x)$

$$
\begin{aligned}
H^{-1}(U) &= h^{-1}\left(log\left(U\beta + e^{h(\ell)}\right)\right) \\
&= x_0 + \frac{1}{\beta}\left(log\left(U\beta + e^{h(\ell)}\right) - \alpha\right)
\end{aligned}
$$

3.2 c = 1

$F_T = 0.5 * x^2$, $F_T^{-1} = (2x)^{0.5}$

$$
\begin{aligned}
H^{-1}(U) &= h^{-1}\left(2*\left(U\beta+(0.5*h(\ell))^2\right)\right)^{0.5} \\
&= h^{-1}\left(2*\left(U\beta+(0.25*(\alpha+\beta*(\ell-x_0))^2)\right)\right)^{0.5} \\
&= h^{-1}\left(2*\left(U\beta+(0.25*(\alpha^2+2*\alpha*\beta*(\ell-x_0)+\beta^2*(\ell-x_0)^2))\right)\right)^{0.5}
\end{aligned}
$$

3.3 c = -0.5

$F_T = -\frac{1}{x}$, $F_T^{-1} = -\frac{1}{x}$

$$
H^{-1}(U) = h^{-1}\left(-\frac{1}{U\beta - \frac{1}{h(\ell)}}\right)
$$

3.4 c = -1

$F_T = -log(-x)$, $F_T^{-1} = -exp(-x)$

$$
H^{-1}(U) = h^{-1}\left(-exp\left(U\beta - log(-h(\ell))\right)\right)
$$

3.5 $c > 0$

$F_T = \frac{c}{c+1} * x^{\frac{c+1}{c}}$, $F_T^{-1} = \frac{c+1}{c} * x^{\frac{c}{c+1}}$

$$
H^{-1}(U) = h^{-1} * \frac{c+1}{c} * \left(U\beta + \frac{c}{c+1} * (h(\ell))^{\frac{c+1}{c}}\right)^{\frac{c}{c+1}}
$$

3.6 $c < 0$

$F_T = -\frac{c}{c+1} * (-x)^{\frac{c+1}{c}}$, $F_T^{-1} = -\frac{c+1}{c} * (-x)^{\frac{c}{c+1}}$

$$
\begin{aligned}
H^{-1}(U) &= h^{-1} * -\frac{c+1}{c} * \left(-U\beta - \frac{c}{c+1} * -(-h(\ell))^{\frac{c+1}{c}}\right)^{\frac{c}{c+1}} \\
&= h^{-1} * -\frac{c+1}{c} * \left(-U\beta + \frac{c}{c+1}(-h(\ell))^{\frac{c+1}{c}}\right)^{\frac{c}{c+1}}
\end{aligned}
$$