Sampling Pólya-Gamma random variates: alternate and approximate techniques

Jesse Windle, Nicholas G. Polson, James G. Scott

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Abstract

Efficiently sampling from the Pólya-Gamma distribution, PG(b, z), is an essential element of Pólya-Gamma data augmentation. [Polson et al., 2013] show how to efficiently sample from the PG(1, z) distribution. We build two new samplers that offer improved performance when sampling from the PG(b, z) distribution and b is not unity.

Contents

1 Introduction

2 The Pólya-Gamma distribution

3 A \( J^* (n, z) \) sampler for \( n \in \mathbb{N} \)
   3.1 Sampling from \( J^* (1, z) \) ............................................. 7
   3.2 Sampling \( J^* (n, z) \) .................................................. 9

4 An Alternate \( J^* (h, z) \) Sampler
   4.1 An Alternate \( J^* (h) \) sampler ........................................ 9
   4.2 An Alternate \( J^* (h, z) \) Sampler ................................. 13
   4.3 Recapitulation ............................................................ 15

5 An Approximate \( J^* (b, z) \) Sampler
   5.1 The Saddle Point Approximation ................................. 15
   5.2 Sampling the saddlepoint approximation ....................... 16
   5.3 Recapitulation ............................................................ 23

6 Comparing the Samplers ................................................... 24

1 Introduction

Efficiently sampling Pólya-Gamma random variates is an essential element of the eponymously named data augmentation technique [Polson et al., 2013]. The technique
is applicable whenever one encounters a posterior distribution of the form

\[ p(\beta | y) \propto p(\beta) \prod_{i=1}^{n} \frac{(e^{\psi_i})^{a_i}}{(1 + e^{\psi_i})^{b_i}} \]

where \( \psi_i = x_i \beta \) and \( a_i \) and \( b_i \) are some functions of the data \( y \) and other parameters.

Introducing the auxiliary variables \( \omega = (\omega_i)_{i=1}^{N} \), independently distributed according to \( (\omega_i | \beta, y) \sim \text{PG}(b_i, \psi_i) \)

where \( \text{PG}(b_i, \psi_i) \) is a Pólya-Gamma random variate, yields the joint density

\[ p(\beta, \omega | y) \propto p(\omega | \beta, y) p(\beta | y) \]

whose complete conditional \( p(\beta | \omega, y) \) is Gaussian. Thus, one may approximate the joint density by iteratively sampling from \( p(\beta | \omega, y) \) and \( p(\omega | \beta, y) = \prod_{i=1}^{N} p(\omega_i | \psi_i, y) \). Clearly, the effective sampling rate of this Markov Chain depends upon how quickly one can sample Pólya-Gamma random variates. (The effective sampling rate is the rate at which a Markov Chain can produce approximately independent samples.) Polson et al. [2013] showed how to efficiently sample from the PG(1, z) distribution. Here we consider alternative techniques for sampling from the Pólya-Gamma distribution which are useful for other portions of its parameter space. We will construct an alternative sampler that is useful for drawing PG(1, z) when \( b \in \mathbb{R}^n \) is greater than unity, though not too large, and an approximate sampler for drawing PG(1, z) when \( b \) is large. (This manuscript is a revised version of a chapter in the first author’s dissertation [Windle, 2013].)

2 The Pólya-Gamma distribution

**Definition 1** (The Pólya-Gamma Distribution). Suppose \( b > 0 \) and \( z \geq 0 \). The Pólya-Gamma distribution \( \text{PG}(b) \) is defined by the density \( p_{\text{PG}}(x|b) \) on \( \mathbb{R}^+ \) with respect to Lebesgue measure that has the Laplace transform

\[ \cosh^{-b}(\sqrt{2t/2}) = \int_{0}^{\infty} \exp(-tx)p_{\text{PG}}(x|b)dx. \]

A random variable \( X \sim \text{PG}(b, z) \) for \( z > 0 \) is defined by exponentially tilting the \( \text{PG}(b) \) family:

\[ p_{\text{PG}}(x|b, z) = \cosh^{b}(z/2) \exp(-xz^{2}/2)p_{\text{PG}}(x|b). \]

We need to verify that this is, indeed, a valid Laplace transform. Biane et al. [2001] essentially show this and many other properties in their survey of laws that connect analytic number theory and Brownian excursions. One of the laws surveyed, which we denote by \( J^*(b) \), has a Laplace transform given by

\[ \mathbb{E}[e^{-tJ^*(b)}] = \cosh^{-b}(\sqrt{2t}). \]

Biane et al. [2001] show that this distribution has a density and derive one of its representations. Thus, the existence of \( \text{PG}(b) = J^*(b)/4 \) is verified and the definition of \( \text{PG}(b, z) \) is valid. When devising samplers, we find it convenient to work with the \( J^*(b) \) distribution since there is then a trove of prior work to reference directly, instead
of obliquely by a re-scaling. Similar to the definition of \( PG(b, z) \), we define \( J^*(b, z) \) by exponential tilting:

\[
p_{J^*}(x|z, b) = \cosh^b(z) e^{-xz^2/2} p_{J^*}(x|b).
\]

Equivalently:

**Definition 2.** \( J^*(b, z) \) is the distribution with Laplace transform

\[
\cosh^b(z) \cosh^{-b}(\sqrt{2t + z^2}).
\]

**Fact 3.** The following aspects of the \( J^*(b, z) \) distribution are useful.

1. \( PG(b, z) = \frac{1}{4} J^*(b, z/2) \).
2. \( J^*(b) \) has a density and it may be written as

\[
p_{J^*}(x|b) = \frac{2^b}{\Gamma(b)} \sum_{n=0}^{\infty} (-1)^n \frac{\Gamma(n+b)}{\Gamma(n+1)} \frac{2n+b}{\sqrt{2\pi x^3}} \exp\left(-\frac{(2n+b)^2}{2x}\right).
\]

Thus, the density of \( J^*(b, z) \) is

\[
p_{J^*}(x|b, z) = \cosh^b(z) e^{-xz^2/2} p_{J^*}(x|b).
\]

3. The \( J^*(b, z) \) distribution is infinitely divisible. Thus, if \( X \sim J^*(nb, z) \) where \( b > 0 \) and \( n \in \mathbb{N} \), and \( X_i \ i.i.d. \sim J^*(b, z) \) for \( i = 1, \ldots, n \), then

\[
X \overset{D}{=} \sum_{i=1}^{n} X_i.
\]

4. The moment generating function of \( J^*(b, z) \) is

\[
M(t; b, z) = \cosh^b(z) \cos^b(\sqrt{2t - z^2})
\]

and may be written as an infinite product

\[
\prod_{n=0}^{\infty} \left(1 - \frac{t}{d_n}\right)^{-b}, \quad d_n = \frac{\pi^2}{2} \left(n + \frac{1}{2}\right)^2 + \frac{z^2}{2}.
\]

5. Hence, \( J^*(b, z) \) is an infinite convolution of gammas and can be represented as

\[
J^*(b, z) \sim \sum_{n=0}^{\infty} \frac{g_n}{d_n}, \quad g_n \ i.i.d \sim Ga(b, 1).
\]

**Proof.** Biane et al. [2001] provide justification for items (2), (3), and essentially (5). Justification for items (1) and (4) are in Polson et al. [2013], though we present the arguments here. For item (1), let \( X = J^*(b, z/2) \) and \( Y = X/4 \) transform

\[
p_{J^*}(x|b, z/2)dx = \cosh^b(z/2) \exp\left(-\frac{xz^2}{4}\right) p_{J^*}(x|b)dx
\]

to

\[
cosh^b(z/2) \exp\left(-\frac{y^2}{2}\right) p_{J^*}(4y|b)dy = \cosh^b(z/2) \exp(-yz^2/2) p_{PG}(y|b)dy.
\]
The last expression is by definition $Y \sim PG(b, z)$. Regarding (4), recall the Laplace transform of $J^*(b, z)$ (Definition 2) is 

$$
\varphi(t|b, z) = \cosh^b(z) \cosh^{-b}(\sqrt{2t + z^2}).
$$

By the Weierstrass factorization theorem [Pennisi 1976], $\cosh(\sqrt{2t})$ can be written as

$$
\cosh(\sqrt{2t}) = \prod_{n=0}^{\infty} \left(1 + \frac{t}{c_n}\right), \quad c_n = \frac{\pi^2}{2}(n + 1/2)^2.
$$

Taking the reciprocal of $\varphi(t|1, z)$ yields

$$
\frac{\cosh(\sqrt{2t} + z^2)}{\cosh(z)} = \frac{\prod_{n=0}^{\infty} \left(1 + \frac{t + z^2/2}{c_n}\right)}{\prod_{n=0}^{\infty} \left(1 + \frac{z^2/2}{c_n}\right)} = \prod_{i=0}^{\infty} \left(1 + \frac{t}{c_n + z^2/2}\right);
$$

thus,

$$
\varphi(t|b, z) = \prod_{n=0}^{\infty} \left(1 + \frac{t}{d_n}\right)^{-b}, \quad d_n = \frac{\pi^2}{2}(n + 1/2)^2 + z^2.
$$

Since $\varphi(-t; b, z) = M(t; b, z)$ we have

$$
M(t; b, z) = \prod_{n=0}^{\infty} \left(1 - \frac{t}{d_n}\right)^{-b}
$$

and

$$
\frac{M(t; b, z)}{\cosh^b(z)} = \cosh^{-b}(\sqrt{-2t + z^2}) = \cos^{-b}(\sqrt{2t - z^2}).
$$

Regarding item (5), one may invert the infinite product representation of Laplace transform to show that

$$
J^*(b, z) \sim \sum_{n=0}^{\infty} \frac{g_n}{d_n}, \quad g_n \overset{iid}{\sim} Ga(b, 1).
$$

Below we describe Polson et al. [2013]'s $J^*(1, z)$ sampler, which is motivated by Devroye [2009] and which relies on a reciprocal relationship noticed by Ciesielski and Taylor [1962], who show that in addition to Fact (3.2) one may represent the density of a $J^*(1)$ random variable as

$$
\sum_{n=0}^{\infty} (-1)^n \pi \left(n + \frac{1}{2}\right) e^{-(n+1/2)^2 \pi^2 x/2}. \quad (2)
$$

By pasting these two densities together, one can construct an extremely efficient sampler. Unfortunately, there is no known general reciprocal relationship that would extend this approach to $J^*(n)$ for general $n$; however, Biane et al. [2001] provide an alternate density for the $J^*(2)$ distribution based upon a reciprocal relationship with another random variable.
While there may not be an obvious reciprocal relationship to use, one may find other alternate representations for the density of $J^*(b)$ random variables when $b$ is a positive integer. Exploiting an idea from Kent [1980] for infinite convolutions of exponential random variables, one may invert the moment generating function using partial fractions. Consider the moment generating function of $J^*(h)$:

$$M(t) = \prod_{n=0}^{\infty} \left(1 - \frac{t}{c_n}\right)^{-h}, \quad c_n = \frac{\pi^2}{2}(n + 1/2)^2$$  \hspace{1cm} (3)

This can be expanded by partial fractions so that

$$M(t) = \sum_{n=0}^{\infty} \sum_{m=1}^{h} \frac{A_{nm}}{(t - c_n)^m}. \hspace{1cm} (4)$$

Inverting this sum term by term we find that one can represent the density as

$$f(x|\nu) = \sum_{n=0}^{\infty} \sum_{m=1}^{h} A_{nm} x^{m-1} e^{-(c_n x)/(m-1)!},$$

and infinite sum of gamma kernels.

To find formulas for the $\{A_{nm}\}_{nm}$ coefficients, consider the Laurent series expansion of $M(t)$ about $c_i$.

$$M(t) = \sum_{n=0}^{\infty} a_n^{(i)} (t - c_i)^n + \sum_{m=1}^{h} b_m^{(i)} (t - c_i)^m. \hspace{1cm} (5)$$

Such an expansions is valid since $c_n$ is an isolated singular point. Since the coefficients at the pole are unique, comparing coefficients in (4) and (5) shows that $A_{im} = b_m^{(i)}$. Further, one may calculate $b_m^{(i)}$ by considering the function

$$\nu_h(t) = (t - c_i)^h M(t)$$

and then computing

$$b_m^{(i)} = \nu_h^{(h-m)}(c_i)/(h-m)!. \hspace{1cm} (6)$$

(See Churchill and Brown [1984].) Writing the MGF in product form, as in (3), we see that

$$\nu_h(t) = (-c_i)^h \prod_{n \neq i} \left(1 - \frac{t}{c_n}\right)^{-h}. \hspace{1cm} (7)$$

Define

$$\psi_h(t) = h \log(-c_i) - h \sum_{n \neq i} \left(1 - \frac{t}{c_n}\right).$$

Then $\nu_h(t) = \exp \psi_h(t)$ and the derivatives of $\psi$ can then be expressed as

$$\nu'_h = e^{\psi_h} \psi'_h,$$

$$\nu''_h = e^{\psi_h} (\psi'_h)^2 + e^{\psi_h} \psi''_h,$$

$$\nu'''_h = e^{\psi_h} (\psi'_h)^3 + 3e^{\psi_h} \psi'_h \psi''_h + e^{\psi_h} \psi'''_h$$

... = ...
where

$$\psi^{(k)}_h(t) = (k-1)! \sum_{m \neq i} (c_n - t)^{-k}.$$ 

Thus, one may calculate $b^{(i)}_m$ numerically using $\psi^{(k)}_h$, though the convergence may be slow.

However, the most important coefficient, $b^{(i)}_h$, is already known. Make the dependence of $b^{(i)}_m$ on $h$ explicit by writing $b^{(i)}_m(h)$. From the formulas above we know that $b^{(i)}_h(c_i) = \exp(h(c_i))^h$ and that $\nu_h(c_i) = \exp(\psi_1(c_i))^h$. But $\exp(\psi_1(c_i)) = \nu_1(c_i) = b^{(i)}_1(1)$. From the reciprocal relationship provided at the start of the section, we know that $b^{(i)}_1(1) = (-1)^i \sqrt{2\pi}$. Thus,

$$A_{ih} = b^{(i)}_h(h) = (-1)^i h^{2c_i/2}.$$ 

For $h \in \mathbb{N}$, the density for $J^*(h)$ takes the form

$$f(x|h) = \sum_{n=0}^{\infty} \left[ \sum_{m=1}^{h} \frac{A_{nm}(h-1)!}{A_{nh}(m-1)!} \frac{1}{x^{h-m}} \right] A_{nh} x^{h-1} e^{-c_i x} \frac{e^{-c_0 x}}{(h-1)!}$$

so the $A_{nh}$ terms dominate for large $x$. Further, among those terms, the first,

$$\frac{A_{0h} x^{h-1} e^{-c_0 x}}{(h-1)!} = \frac{(\pi/2)^{h} x^{h-1} e^{-c_0 x}}{(h-1)!},$$

should dominate as $x \to \infty$.

**Remark 4.** This provides insight into the tail behavior of the $J^*(h)$ distribution. For the right tail, we expect the density to decay as a $Ga(h,c_0)$ distribution. Examining the representation (6.2), we expect the left tail to decay like $IGa(1/2, h^2/2)$. These two observations will prove useful when finding an approximation of the $J^*(h)$ density. We may multiply each of these densities by $e^{-x^2/2}$ to determine the tail behavior of $J^*(h,z)$: the right tail should look like $Ga(h,c_0 + z^2/2)$ while the left tail should look like $IG(\mu = h/z, h^2)$.

### 3 A $J^*(n, z)$ sampler for $n \in \mathbb{N}$

Polson et al. [2013] show how to efficiently sample from the $J^*(1, z)$ distribution. Their approach is motivated by Devroye [2009]. This section recaps that work, since it will help clarify the provenance of the other samplers in this paper.

The $J^*(1, z)$ sampler employs von Neumann’s alternating sum method [Devroye, 1986], which is an accept/reject algorithm for densities that may be represented as infinite, alternating sums. To remind the reader about accept/reject samplers, one generates a random variable $Y$ with density $f$ by repeatedly generating a proposal $X$ from density $g$ and $U$ from $U(0, c g(X))$ where $c \geq \|f/g\|_{\infty}$ until

$$U \leq f(X); \text{ then set } Y \leftarrow X.$$ 

(See Robert and Casella [2005] for more details.) The von Neumann alternating sum method requires that the density be expressed as an infinite, alternating sum

$$f(x) = \lim_{n \to \infty} S_n(x), \quad S_n(x) = \sum_{i=0}^{n} (-1)^i a_i(x)$$
for which the partial sums $S_i$ satisfy the partial sum criterion

$$\forall x, S_0(x) > S_1(x) > \ldots > f(x) > \ldots > S_3(x) > S_1(x),$$

(7)

which is equivalent to the sequence $\{a_i(x)\}_{i=1}^\infty$ decreasing in $i$ for all $x$. In that case, we have that $u < f(x)$ if and only if there is some odd $i$ such that $u \leq S_i(x)$ and $u > f(x)$ if and only if there is some even $i$ such that $u \geq S_i(x)$. Thus one need not calculate the infinite sum to see if $u < f(x)$, one only needs to calculate as many terms as necessary to find that $u \leq S_i(x)$ or $u \geq S_i(x)$ for even $i$. (We must be careful when $x = 0$.) One rarely needs to calculate a partial sum past $S_1(x)$ before deciding to accept or reject [Polson et al., 2013].

3.1 Sampling from $J^*(1, z)$

The $J^*(1)$ density may be represented in two different ways

$$f(x) = \sum_{i=0}^{n} (-1)^n a^L_n(x) = \sum_{i=0}^{n} (-1)^n a^R_n(x),$$

corresponding to Fact (3.2) and (2), where

$$a^L_n(x) = \pi (n + \frac{1}{2}) \left(\frac{2}{\pi x}\right)^{3/2} \exp\left(- \frac{2(n + 1/2)^2}{x}\right)$$

(8)

and

$$a^R_n(x) = \pi (n + \frac{1}{2}) \exp\left(- \frac{(n + 1/2)^2 \pi^2 x}{2}\right).$$

(9)

Neither $\{a^L_n(x)\}_{n=0}^\infty$ or $\{a^R_n(x)\}_{n=0}^\infty$ are decreasing for all $x$, thus neither satisfy the partial sum criterion. However, Devroye shows that $a^R_n(x)$ is decreasing on $I_R = [(\log 3)/\pi^2, \infty)$ and that $a^L_n(x)$ is decreasing for $I_L = [0, 4/\log 3]$. These intervals overlap and hence one may pick $t$ in the intersection of these two intervals to define the piecewise coefficient

$$a_n(x) = \begin{cases} a^L_n(x), & x \leq t \\ a^R_n(x), & x > t \end{cases}$$

so that $a_n(x) \geq a_{n+1}(x)$ for all $n$ and all $x \geq 0$. Devroye finds that $t = 2/\pi$ is the best choice of $t$ for his $J^*(1, 0)$ sampler, which is where $a^L_n(x) = a^R_n(x)$. Below we show that this still holds for $J^*(1, z)$. Thus the density $f$ may be written as

$$f(x) = \sum_{i=0}^{\infty} (-1)^n a_n(x)$$

and this representation does satisfy the partial sum criterion [7]. The density of $J^*(1, z)$ is then

$$f(x|z) = \cosh(z) \exp(-xz^2/2) f(x)$$

according to our construction of $J^*(1, z)$, in which case it also has an infinite sum representation

$$f(x|z) = \sum_{i=0}^{\infty} (-1)a_n(x|z), a_n(x|z) = \cosh(z) \exp(-xz^2/2)a_n(x)$$
that satisfies (7) for the partial sums \( S_n(x) = \sum_{i=0}^{n}(-1)^{i}a_i(x) \), as
\[
a_n(x) \geq a_{n+1}(x) \implies a_n(x|z) \geq a_{n+1}(x|z).
\]

Following our initial discussion of the von Neumann alternating sum method, all that remains is to find a suitable proposal distribution \( g \). One would like to find a distribution \( g \) for which \( \|f/g\|_{\infty} \) is small, since this controls the rejection rate. A natural candidate for \( g \) is the density defined by the kernel \( S_0(x|z) = a_0(x|z) \) as \( S_0(x|z) \geq f(x|z) \) for all \( x \). In that case, we sample \( X \sim g \) until \( U \sim U(0, a_0(x|z)) \) has \( U \leq f(X) \).

The proposal \( g \) is thus defined from (8) and (9) by
\[
g(x|z) \propto a_0(x|z) = \cosh(z) \begin{cases} \left( \frac{2}{\pi x^3} \right)^{1/2} \exp \left( \frac{-1}{2x} - \frac{z^2}{2} \right) & x < t \\ \pi/2 \exp \left( - \left[ \frac{\pi^2}{8} + \frac{z^2}{2} \right] x \right) & x \geq t. \end{cases}
\]
Let \( a_0^L(x|z) = a_0(x|z)1\{x < t\} \) be the left-hand kernel and define the right-hand kernel \( a_0^R(x|z) \) similarly. Rewriting the exponent in the left-hand kernel yields
\[
\frac{-1}{2x} - \frac{z^2}{2} = \frac{-z^2}{2x} (x^2 - 2x|z|^{-1} + 2x|z|^{-1} + z^{-2}) = \frac{-z^2}{2x} (x - |z|^{-1})^2 - |z|;
\]
hence
\[
a_0^L(x|z) = (1 + e^{-2|z|}) IG(x|\mu = |z|^{-1}, \lambda = 1)
\]
where \( IG(x|\mu, \lambda) \) is the density of the inverse Gaussian distribution,
\[
IG(x|\mu, \lambda) = \left( \frac{\lambda}{2\pi x^3} \right)^{1/2} \exp \left( -\frac{\lambda(x - \mu)^2}{2\mu^2x} \right).
\]
The normalizing constants
\[
p = \int_0^t a_0^L(x|z)dx \quad \text{and} \quad q = \int_t^\infty a_0^R(x|z)dx \quad (10)
\]
let us express \( g \) as the mixture
\[
g(x|z) = \frac{p}{p+q} a_0^L(x|z) + \frac{q}{p+q} a_0^R(x|z)
\]
and shows that (suppressing the dependence on \( t \))
\[
c(z)g(x|z) = a_0(x|z) \quad \text{where} \quad c(z) = p(z) + q(z).
\]
Thus, one may draw \( X \sim g(x|z) \) as
\[
X \sim \begin{cases} IG(\mu = |z|^{-1}, \lambda = 1)1\{x < t\}, & \text{with prob. } p/(p+q) \\
\mathcal{E} \left( \text{rate } = \frac{\pi^2}{8} + \frac{z^2}{2} \right)1\{x \geq t\}, & \text{with prob. } q/(p+q).
\end{cases}
\]
One may sample from the truncated exponential by taking \( X \sim Ex \left( \text{rate } = \frac{\pi^2}{8} + \frac{z^2}{2} \right) \) and returning \( X + t \). Sampling from the truncated inverse Gaussian requires a bit more work (see Appendix 2 in [Windle 2013]). To recapitulate, to draw \( J^*(1, z) \):
1. Sample $X \sim g(x \mid z)$.
2. Generate $U \sim \mathcal{U}(0, a_0(X \mid z))$.
3. Iteratively calculate $S_n(X \mid z)$, starting at $S_1(X \mid z)$, until $U \leq S_n(X \mid z)$ for an odd $n$ or $U > S_n(X \mid z)$ for an even $n$.
4. Accept if $n$ is odd; return to step 1 if $n$ is even.

### 3.2 Sampling $J^*(n, z)$

One can use the $J^*(1, z)$ sampler to generate draws from the $J^*(n, z)$ distribution when $n$ is a positive integer. As shown by Fact 3.3, sample $X \sim J^*(1, z)$ for $i = 1, \ldots, n$ and then return $Y = \sum_{i=1}^n X_i$.

### 4 An Alternate $J^*(h, z)$ Sampler

Here we show how to sample $J^*(h, z)$ when $h$ is not a positive integer.

#### 4.1 An Alternate $J^*(h)$ sampler

The basic strategy will be the same as in §3 find two functions $\ell$ and $r$ such that the density $f$ is dominated by $\ell$ on $(0, t]$ and $r$ on $(t, \infty)$. Truncated versions of $\ell$ and $r$ can then be used to generate a proposal. Previously, these proposals came from the density of $f$, which when $h = 1$, has two infinite, alternating sum representations. Pasting together these two representations together one may immediately appeal to the von Neumann alternating sum technique to accept or reject a proposal; but this only works when $h = 1$. For $h \neq 1$, the density in Fact 3.2 is still valid:

$$f(x \mid h) = \frac{q^h}{\Gamma(h)} \sum_{n=0}^{\infty} (-1)^n \frac{\Gamma(n + h)}{\Gamma(n + 1)} \frac{(2n + h)}{\sqrt{2\pi x^3}} \exp \left( - \frac{(2n + h)^2}{2x} \right).$$  \hspace{1cm} (11)

We know that the coefficients of this alternating sum, which we call $a_n^L$, are not decreasing in $n \in \mathbb{N}_0$ for all $x > 0$; they are only decreasing in $n \in \mathbb{N}_0$ for $x$ in some interval $I_L$. However, it is the case that $a_n^L(x \mid h)$ is decreasing for sufficiently large $n$ for all $x > 0$. Thus, we may still appeal to a von Neumann-like procedure, but only once we know that we have reached an $n^*(x)$ so that $a_n^L(x \mid h)$ is decreasing for $n \geq n^*$. The following proposition shows that we can identify when this is the case.

**Proposition 5.** Fix $h \geq 1$ and $x > 0$. The coefficients $\{a_n^L(x)\}_{n=0}^{\infty}$ in (11) are decreasing, or they are increasing and then decreasing. Further, if $a_n^L(x)$ is decreasing for $n \geq n^*$, then $a_n^L(x)$ is decreasing for $n \geq n^*$ for $x \leq x^*$.

**Proof.** Fix $h \geq 1$ and $x > 0$; calculate $a_{n+1}^L(x \mid h)/a_n^L(x \mid h)$. It is

\[
\begin{align*}
\frac{\Gamma(n + 1) \Gamma(n + 1 + h)}{\Gamma(n + 2) \Gamma(n + h)} & \frac{2n + 2 + h}{2n + h} \exp \left\{ - \frac{1}{2x} \left[ (2n + 2 + h)^2 - (2n + h)^2 \right] \right\} \\
& = \frac{n + h}{n + 1} \frac{2n + h + 2}{2n + h} \exp \left\{ - \frac{1}{2x} \left[ 4(2n + h) + 4 \right] \right\} \\
& = \left(1 + \frac{h}{n + 1}\right) \left(1 + \frac{2}{2n + h}\right) \exp \left\{ - \frac{2}{x} \left[ (2n + h) + 1 \right] \right\}.
\end{align*}
\]
Since \( x > 0 \), the exponential term decays to zero as \( n \) diverges and there is smallest \( n^* \in \mathbb{N}_0 \) for which this quantity is less than unity. Further, it is less than unity for all such \( n \geq n^* \) as all three terms in the product are decreasing in \( n \). The ratio also decreases as \( x \) decreases, thus \( a_n^L(y) \) is decreasing for \( n \geq n^* \) when \( y \leq x \).

**Corollary 6.** Suppose \( h \geq 1 \) and \( x > 0 \) and let \( S_n^L(x|h) = \sum_{i=0}^n (-1)^i a_n^L(x|h) \). There is an \( n^* \in \mathbb{N}_0 \) for which \( f(y|h) < S_n^L(y|h) \) for all even \( n \geq n^* \) and \( f(y|h) > S_n^L(y|h) \) for all odd \( n \geq n^* \) for \( y \leq x \).

**Corollary 7.** There is an \( x^*(h) \),

\[
x^*(h) = \sup \left\{ x : \{ a_n^L(x|h)\}_{n=0}^\infty \text{ is decreasing} \right\},
\]

so that \( \{ a_n^L(x|h)\}_{n=0}^\infty \) is decreasing for all \( x < x^* \). Thus \( \ell(x|h) = a_0^L(x|h) \) satisfies

\[
S_n(x|h) \leq \ell(x|h), \quad \forall n \in \mathbb{N}_0, \forall x < x^*(h).
\]

When \( h = 1 \), we have another representation of \( f(x|h) \) as an infinite alternating sum. This is not the case when \( h \neq 1 \); however, revisiting \([6] \), when \( h \in \mathbb{N} \), we may also write \( f(x|h) \) as

\[
f(x|h) = \sum_{n=0}^{\infty} \sum_{m=1}^{h} \frac{A_{nm}(h-1)!}{A_{nh}(m-1)! x^{h-m}} A_{nh} x^{h-1} e^{-cnx} (h-1)! , \quad c_n = \frac{\pi^2}{2} (n + 1/2)^2.
\]

When \( x \) is large, the term with \( m = h \) will dominate, leaving

\[
\sum_{n=0}^{\infty} A_{nh} x^{h-1} e^{-cnx} (h-1)! , \quad A_{nh} = (-1)^n h (2cn)^{h/2}.
\]

Again, since \( e^{-cnx} \) decays rapidly in \( n \) the first term of this sum should be the most important. Hence, for sufficiently large \( x \), \( f(x|h) \) should look like

\[
r(x|h) = \frac{A_0 x^{h-1} e^{-cnx}}{(h-1)!} = \frac{\pi/2^{h/2} x^{h-1} e^{-cnx}}{(h-1)!}.
\]

This will be the right hand side proposal.

**Conjecture 8.** The functions \( \ell(x|h) \) and \( r(x|h) \) dominate \( f(x|h) \) on overlapping intervals that contain a point \( t(h) \).

For \( h \geq 1 \), we know that \( \ell(x|h) \) will dominate \( f(x|h) \) on some interval \([0, x^*(h)]\) from Corollary \([7] \). We have not proved that \( r(x|h) \) dominates \( f(x|h) \) on an overlapping interval; however, we do have numerical evidence that this is the case. Let \( \rho_L(x|h) = f(x|h)/\ell(x|h) \) and \( \rho_R(x|h) = f(x|h)/r(x|h) \). If both \( \rho_L(x|h) \) and \( \rho_R(x|h) \) are less than unity on overlapping intervals, then \( \ell \) and \( r \) dominate \( f \) on overlapping intervals. As seen in Figure \([1] \) this appears to be the case for both \( \rho_L \) and \( \rho_R \) on the entire real line. In that case, \( \ell \) and \( r \) are both valid bounding kernels and the proposal density

\[
g(x|h) \propto k(x|h) = \begin{cases} \ell(x|h), & x < t \\ r(x|h), & x \geq t. \end{cases}
\]
has
\[ f(x|h) \leq k(x|h) \text{ for all } x > 0; \]
further, \( g(x|h) \) is a mixture
\[ g(x|h) = \frac{p}{p+q} \ell(x|h) + \frac{q}{p+q} r(x|h) \]
where
\[ p(t|h) = \int_0^t \ell(x|h)dx \text{ and } q(t|h) = \int_t^\infty r(x|h)dx \]
and the normalizing constant of \( k(x|h) \) is \( c(t|h)^{-1} \) where
\[ c(t|h) = p(t|h) + q(t|h). \]
Thus, Corollary [6] and Conjecture [8] lead to the following sampler:
1. Sample \( X \sim g(x|h) \)
2. Sample \( U \sim \mathcal{U}(0, k(X|h)) \).
3. Iteratively calculate the partial sums \( S_n^L(x|h) \) until
   - \( S_n^L(X|h) \) has decreased from \( n-1 \) to \( n \), and
   - \( U < S_n^L(X|h) \) for odd \( n \) or \( S_n^L(X|h) < U \) for even \( n \).

Both \( \ell(x|h) \) and \( r(x|h) \) are kernels of known densities. In particular,
\[ \ell(x|h) = \frac{2^h}{\Gamma(1)} \frac{h}{\sqrt{2\pi}} x^{-3/2} \exp \left( - \frac{h^2}{2x} \right), \]
is the kernel of an inverse Gamma distribution, IGa(1/2, \( h^2/2 \)), and
\[ r(x|h) = \frac{(\pi/2)^{h/2} x^{h-1} e^{-\frac{\pi^2}{8} x}}{(h-1)!} \]
is the kernel of gamma distribution, Ga(\( h, \pi^2/8 \)). We can rewrite
\[ \ell(x|h) = 2^h \text{IGa}(x|h, 1/2, h^2/2) \]
to find
\[ p(t|h) = 2^h \frac{\Gamma(1/2, (h^2/2)/t)}{\Gamma(1/2)} \]
where \( \Gamma(a, b) \) is the upper incomplete gamma function, and we can rewrite
\[ r(x|h) = (4/\pi)^h \text{Ga}(x|h, \text{rate} = \pi^2/8) \]
to find
\[ q(t|h) = \left( \frac{4}{\pi} \right)^h \frac{\Gamma(h, (\pi^2/8)t)}{\Gamma(h)}. \]
Note that this provides a way to calculate \( t(h) \), since we want to minimize \( c(t|h) = p(t|h) + q(t|h) \). This is identical to choosing the truncation point \( t(h) \) to be the point at which \( \rho^L(x|h) \) and \( \rho^R(x|h) \) intersect.
Figure 1: A plot of the $f(x|h)/\ell(x|h)$ and $f(x|h)/r(x|h)$ for $h = 1.0$ to $h = 4.0$ by 0.1. The dark lines correspond to $h = 1$. The curve corresponding to $\ell$ increases monotonically while the curve corresponding to $r$ decreases monotonically. The black line plots the point of intersection between the two curves as $h$ changes.
4.2 An Alternate $J^*(h, z)$ Sampler

Recall Fact 3.2 which says the density of $J^*(h, z)$ is

$$f(x|h, z) = \cosh^h(z)e^{-x^2/2}f(x|h)$$

where $f(x|h)$ is given in (11). Following the general path put forth in the previous section, one finds that almost nothing changes. In particular, if we let $a_n^L(x|h, z) = \cosh^h(z)e^{-xz^2/2}a_n^L(x|h)$ and let $S_n^L(x|h, z) = \sum_{i=0}^n(-1)^ia_n^L(x|h, z)$, then the analogous propositions, corollaries, and conjectures from the previous section still hold. In particular,

$$\frac{a_{n+1}^L(x|h)}{a_n^L(x|h)} = \frac{a_{n+1}^L(x|h, z)}{a_n^L(x|h, z)}$$

so Proposition 5, Corollary 6, and Corollary 7 hold with $a_n^L(x|h)$ replaced by $a_n^L(x|h, z)$, $S_n^L(x|h)$ replaced by $S_n^L(x|h, z)$, and $\ell(x|h)$ replaced by $\ell(x|h, z) = a_n^L(x|h, z)$. Additionally, nothing changes with regards the bounding kernel since

$$f(x|h) \leq k(x|h) \iff f(x|h, z) \leq k(x|h, z)$$

where

$$k(x|h, z) = \cosh^h(z)e^{-xz^2/2}k(x|h).$$

Hence the only major change is the form of the proposal density and the corresponding mixture representation. After adjusting, the left bounding kernel becomes

$$\ell(x|h, z) = \cosh^h(z)2^h\frac{h}{\sqrt{2\pi}x^{-3/2}}\exp\left(-\frac{h^2}{2x} - \frac{xz^2}{2}\right),$$

and the right bounding kernel becomes

$$r(x|h, z) = \cosh^h(z)\frac{(\pi/2)^{h/2}x^{-h-1}}{(h-1)!}\exp\left[-\left(\frac{\pi^2}{8} + \frac{z^2}{2}\right)x\right].$$

Let

$$g(x|h, z) \propto k(x|h, z) = \begin{cases} \ell(x|h, z), & x < t(h) \\ r(x|h, z), & x \geq t(h), \end{cases}$$

and

$$p(t|h, z) = \int_0^t \ell(x|h, z)dx \text{ and } q(t|h, z) = \int_t^\infty r(x|h, z)dx.$$ 

Then one can represent $g(x|h, z)$ as the mixture

$$g(x|h, z) = \frac{p}{p+q} \ell(x|h, z) + \frac{q}{p+q} r(x|h, z)$$

and the normalizing constant of $k(x|h, z)$ is (suppressing the dependence on $t$)

$$c(h, z) = p(h, z) + q(h, z)$$

Thus, one can sample $J^*(h, z)$ by

1. Sample $X \sim g(x|h, z)$
2. Sample $U \sim U(0, k(x|h))$.

3. Iteratively calculate the partial sums $S_n^L(x|h)$ until

- $S_n^L(X|h)$ has decreased from $n - 1$ to $n$, and
- $U < S_n^L(X|h)$ for odd $n$ or $S_n^L(X|h) < U$ for even $n$.

Note that the above procedure uses $k(x|h)$ and $S_n(x|h)$ instead of $k(x|h,z)$ and $S_n(x|h,z)$. This is because

\[
\tilde{f}(x|h)/\tilde{g}(x|h) = \tilde{f}(x|h,z)/\tilde{g}(x|h,z)
\]

and

\[
\tilde{f}(x|h)/S_n^L(x|h) = \tilde{f}(x|h,z)/S_n^L(x|h,z).
\]

Again, the kernels $\ell(x|h, z)$ and $r(x|h)$ are recognizable. The exponential term of $\ell(x|h, z)$ is

\[
-\frac{z^2}{2x}\left[\left(\frac{h}{z}\right)^2 + x^2\right].
\]

Completing the square yields

\[
-\frac{(z/h)^2 h^2}{2x}[(x - h/z)^2] - zh;
\]

so

\[
\ell(x|h, z) = (1 + e^{-2|z|})h \cdot \frac{h}{\sqrt{2\pi x^3}} \exp\left(-\frac{(z/h)^2 h^2}{2x}[(x - h/z)^2]\right),
\]

which is the kernel of an inverse Gaussian distribution with parameters $\mu = h/z$ and $\lambda = h^2$. The right kernel is a gamma distribution with shape parameter $h$ and rate parameter $\lambda_z = \pi^2/8 + z^2/2$. Thus, the left hand is

\[
\ell(x|h, z) = (1 + e^{-2|z|})h IG(x|\mu = h/z, \lambda = h^2) \quad \text{for } z > 0
\]

and

\[
\ell(x|h, 0) = 2h IGa(x|1/2, h^2/2);
\]

the right hand kernel is

\[
r(x|h, z) = \left(\frac{\pi/2}{\lambda_z}\right)^h \text{Ga}(x|h, \text{rate} = \lambda_z), \; \lambda_z = \pi^2/8 + z^2/2;
\]

and the respective weights are

\[
p(t|h, z) = (2^h e^{-zh}) \Phi_{IG}(t|h/z, h^2),
\]

\[
p(t|h, 0) = 2^h \frac{\Gamma(1/2, (h^2/2)(1/t))}{\Gamma(1/2)},
\]

and

\[
q(t|h, z) = \left(\frac{\pi/2}{\lambda_z}\right)^h \frac{\Gamma(h, \lambda_z t)}{\Gamma(h)}.
\]
Truncation Point

The normalizing constant $c(t|h,z)$ is

$$c(t|h,z) = \int_0^t \cosh^h(z)e^{-xz^2/2}\ell(x|h)dx + \int_t^\infty \cosh^h(z)e^{-xz^2/2}r(x|h)dx.$$ 

To minimize $c(t|h,z)$ over $t$, note that the critical points, which satisfy

$$\cosh^h(z)e^{-xz^2/2}\left[\ell(x|h) - r(x|h)\right] = 0,$$

are independent of $z$. Hence we only need to calculate the best $t = t(h)$ as a function of $h$.

4.3 Recapitulation

The method put forth in this section can produce draws from $J^*(h,z)$ for $h \geq 1$ if Conjecture 8 holds. We numerically verify this is the case for $h \in [1,4]$. In practice, to draw $J^*(h,z)$ when $h > 4$, we take sums independent $J^*$ random variates like before. The new sampler is limited in two ways. First, the best truncation point $t$ is a function of $h$, and must be calculated numerically. Second, the normalizing constant $c(h,z)$ grows as $h$ increases. The former is not too troubling as one may precompute many $t(h)$ and then interpolate between values of $h$ not specified. However, the latter is disturbing as $1/c(h,z)$ is the probability of accepting a proposal. Thus, as $h$ increases the probability of accepting a proposal decreases. To address this deficiency, we devise yet another sampler.

5 An Approximate $J^*(b,z)$ Sampler

Daniels [1954] provides a method to construct approximations to the density of the mean of $n$ independent and identically distributed random variables. More generally, Daniels procedure produces approximations to the density of $X(n)/n$ where $X(h)$ is an infinitely divisible family [Sato, 1999]. The approximation improves as $n$ increases. This is precisely the scenario we are interested in addressing, as $J^*(n,z)$ is infinitely divisible and the two previously proposed samplers do not perform well when sampling $J^*(n,z)$, or equivalently $J^*(n,z)/n$, for large $n$.

5.1 The Saddle Point Approximation

The method of Daniels [1954] and variants thereof are known as saddlepoint approximations or the method of steepest decent. In addition to Daniels [1954], Murray [1974] provides an accessible explanation of the asymptotic expansion and approximation, including numerous helpful graphics. A more technical analysis may be found in the paper by Barndorff-Nielsen and Cox [1979] and the books by Butler [2007] and Jensen [1995]. McLeish [2010] provides several examples of simulating random variates following the approach of Lugannani and Rice [1980]. Below, we briefly summarize the basic idea behind the approximation following Daniels [1954].
Let $X(h)$ be an infinitely divisible family. Let $M(t)$ denote the moment generating function of $X(1)$, and let $K(t)$ denote its cumulant generating function:

$$M(t) = e^{K(t)} = \int_{-\infty}^{\infty} e^{tx} f(x) \, dx.$$ 

where $f(x)$ is the density of the random variable $X(1)$. Let $\bar{x}$ denote $X(n)/n$, which can be thought of as the sample mean of $n$ independent $X(1)$ random variables when $n$ is an integer. The MGF of $\bar{x}$ is $M_n(t/n)$ and its Fourier inversion is

$$f_n(\bar{x}) = \frac{n}{2\pi} \int_{-\infty}^{\infty} e^{n[K(T) - T\bar{x}]} \, dT.$$ 

One can concentrate mass at $T_0 + 0i$ where $T_0$ is chosen to minimize

$$K(T) - T\bar{x} \text{ over } T \in \mathbb{R},$$

which will be a saddle point. Consequently, one may descend quickly in the directions perpendicular to the real axis at $T_0 + 0i$, which leads to an integral like

$$f_n(\bar{x}) = \frac{n}{2\pi i} \int_{T_0 - \infty i}^{T_0 + \infty i} e^{n[K(T) - T\bar{x}]} \, dT,$$

though some care must be taken with the path of integration near $T_0 + 0i$. Performing an asymptotic expansion of $K(T)$ at $T_0$ and integrating yields the approximation of Daniels:

$$sp_n(\bar{x}) = (\frac{n}{2\pi})^{1/2} K''(T_0)^{-1/2} e^{n[K(T_0) - T_0\bar{x}]};$$

note $T_0(x)$ solves

$$K'(T_0) - \bar{x} = 0. \quad (12)$$

Daniels [1954] (p. 639) provides conditions that ensure the approximation will hold, which in the case of the $J^*(1, z)$ distribution are

$$\lim_{u \to (\pi^2/8)^{-}} K_0'(u) = \infty \text{ and } \lim_{u \to -\infty} K_0'(u) = 0$$

where $K_0(u) = \log \cos \sqrt{2u}$ is the cumulant generating function of $J^*(1)$. As seen in Fact [11] this is indeed the case.

### 5.2 Sampling the saddlepoint approximation

The saddlepoint approximation provides a good point-wise approximation of the density of $J^*(n, z)/n$. To make this useful for Pólya-Gamma data augmentation, we need
to sample from the density proportional to $sp_n(x)$. (Henceforth we drop the bar notation for $\bar{x}$.) One general approach is to bound $\log sp_n(x)$ from above by piecewise linear functions, in which case the approximation will consist of a mixture of truncated exponentials. When the log-density is a concave function, one is assured that such an approximation exists. Devroye provides several examples of how this may be used in practice, even for the case of arbitrary log-concave densities [Devroye, 1986, 2012]. Figure 2 shows an example of a piecewise linear envelope that bounds a log-concave density. One can construct such an envelope by picking points $\{x_i\}$ on the graph of the density $f$, finding the tangent lines $L_i$ at each point, and then constructing the function $e(x) = \min_i L_i(x)$, which corresponds to a piecewise linear function.

We follow the piecewise linear envelope approach, though with a few modifications. In particular, we will bound the term $K(t) - tx$ found in the exponent of $sp_n(x)$ rather than the kernel itself using functions more complex than affine transforms. It will require some care to make sure that the subsequent envelope does not supersede $\log sp_n(x)$ too much. However, by working with $K(t) - tx$ directly, we avoid having to deal with the $K''(t)$ term in $sp_n(x)$, which will cause the mode of $sp_n(x)$ to shift as $n$ changes.

Recall that $t$ is implicitly a function of $x$ that arises via the minimization of $K(t) - tx$ over $t$. This may be phrased in terms of convex duality via

$$\phi(x) = \min_{s \in \mathbb{R}} \{K(s) - sx\}$$

where $K(t)$ is the cumulant generating function: $K(t)$ is strictly convex on $\text{dom } K = \{t : K(t) < \infty\}$ as $J^*(1, z)$ has a second moment [Jensen, 1995]. Using this notation, we may write

$$sp_n(x) = \left(\frac{n}{2\pi}\right)^{1/2} K''(t(x))^{-1/2} e^{n\phi(x)}.$$ 

When needed, we will write $K_z(t)$ to denote the explicit dependence on $z$, though usually we will suppress the dependence on $z$. The connection to duality will help us find a good bound for $\phi(x)$; the following facts will be useful.
Fact 9. Let $K$ be the cumulant generating function of $J^*(1, z)$. Let $\phi(x)$ be the concave dual of $K$ as in \cite{13}. Let

$$t(x) = \arg\min_{s \in \mathbb{R}} \left\{ K(s) - sx \right\}.$$ 

Assume that when we write $t$ we are implicitly evaluating it at $x$. Then

1. $K(t)$ is strictly convex.
2. $K(t)$ is smooth.
3. $K'(t) = x$;
4. $\phi(x) = K(t) - tx$;
5. $\phi'(x) = -t$;
6. $\frac{dt}{dx}(x) = [K''(t)]^{-1}$;
7. As seen by item (3), $\phi'(x)$ is maximized when $t(x) = 0$. Thus,

$$m = \arg\max_x \phi(x) \text{ is attained when } m = K'(0).$$

Proof. Barndorff-Nielsen \cite{1978} shows that (1) holds so long as $J^*(1, z)$ has a second moment, which it does. The cumulant generating function $K(t) = -\log \cos \sqrt{2t}$ is smooth by composition of smooth functions so long as

$$\cos \sqrt{2t} = \begin{cases} \cos \sqrt{2t}, & t \geq 0 \\ \cosh \sqrt{2|t|}, & t < 0 \end{cases}$$

is smooth. For $t \neq 0$ this holds since $\cos$ and $\cosh$ are smooth and $\sqrt{2t}$ is smooth for $t \neq 0$. For $t = 0$, this follows from the Taylor expansion of $\cos$ and $\cosh$. Items (3)-(7) are consequences of (1) and (2).

Remark 10. Sometimes it will be helpful to work with a shifted version of $t$: $u = t - z^2/2$. To reiterate, we will go between three different variables: $x$, $t$, and $u$ characterized by the bijections

1. $x = K'(t)$ and
2. $u = t - z^2/2$.

It will also be helpful to have the derivatives of $K$ on hand and a few facts about $x$ and $u$.

Fact 11. Recall that $K(t) = \log \cosh(z) - \log \cos \sqrt{2u}$ is the cumulant generating function of $J^*(1, z)$. Its derivatives, with respect to $t$, are:

1. $K'(t) = \frac{\tan \sqrt{2u}}{\sqrt{2u}}$;
2. $K''(t) = \frac{\tan^2(\sqrt{2u})}{2u} + \frac{1}{2u} \left( 1 - \frac{\tan \sqrt{2u}}{\sqrt{2u}} \right)$.
Note that we are implicitly evaluating $u$ at $t$ as described in Remark 10. As shown above, $K'(t) = x$. Evaluating $K''$ at $t(x)$ yields

$$K''(t) = x^2 + \frac{1}{2u} (1 - x).$$

We may write $\frac{\tan \sqrt{s}}{\sqrt{s}}$ piecewise as

$$\frac{\tan \sqrt{s}}{\sqrt{s}} = \begin{cases} 
\tan \sqrt{s}, & s > 0 \\
\tanh \frac{\sqrt{|s|}}{|s|}, & s < 0 \\
1, & s = 0.
\end{cases}$$

The last fact can be seen by taking the Taylor expansion around $s = 0$. Thus, $u < 0 \iff x < 1$, $u > 0 \iff x > 1$, and $u = 0 \iff x = 1$.

This leads to the following two claims, which will help us bound the saddlepoint approximation. Notice that in each case, we adjust $\phi(x)$ to match the shape of the tails as suggested by Remark 10.

**Lemma 12.** The function $\eta_r(x) = \phi(x) - (\log(x) - \log(x_c))$ is strictly concave for $x > 0$.

**Proof.** Taking derivatives:

$$\eta'_r(x) = \phi'(x) - \frac{1}{x}$$

and

$$\eta''_r(x) = -\frac{dt}{dx}(x) + \frac{1}{x^2}.$$ 

Using Fact 9 this is negative if and only if

$$[K''(t)]^{-1} \geq \frac{1}{x^2} \iff x^2 \geq K''(t) \iff 0 \geq \frac{(1 - x)}{2u}.$$

When $x > 1$, $u(x) > 0$, and $\eta''_r(x) < 0$. When $x < 1$, $u(x) < 0$, and $\eta''_r(x) < 0$. Continuity of $K''$ ensures that $\eta''_r(1) \leq 0$.

**Lemma 13.** The function $\eta_l(x) = \phi(x) - \frac{1}{2} \left( \frac{1}{x_c} - \frac{1}{x} \right)$ is strictly concave for $x > 0$.

**Proof.** Taking derivatives:

$$\eta'_l(x) = \phi'(x) - \frac{1}{2x^2}$$

and

$$\eta''_l(x) = -\frac{dt}{dx}(x) + \frac{1}{x^3}.$$ 

Using Fact 9 this is negative if and only if

$$[K''(t)]^{-1} \geq \frac{1}{x^3} \iff x^3 \geq K''(t) \iff (x^2 + \frac{1}{2u})(x - 1) \geq 0.$$ 

Again, we know that when $x > 1$, $u > 0$, and hence $\eta_l(x) < 0$. When $x < 1$ we need to show that $x^2 + 1/(2u) < 0$. This is equivalent to showing that

$$x^2 < -\frac{1}{2u} \iff 2ux^2 < -1, u < 0.$$
That is
\[
\tan^2 \sqrt{2u} > -1 \iff \tanh \sqrt{|2u|} > -1, \text{ for } u < 0,
\]
which indeed holds. Thus, when \( x < 1 \), \( \eta_l(x) < 0 \). Again, continuity of \( K'' \) then ensures that \( \eta''_l(1) \leq 0 \).

These two lemmas ensure the following claim.

**Lemma 14.** Let
\[
\delta(x) = \begin{cases} 
\frac{1}{2} \left( \frac{1}{x} - \frac{1}{x^3} \right), & x \leq x_c, \\
\log(x) - \log(x_c), & x > x_c.
\end{cases}
\]
Then \( \eta(x) = \phi(x) - \delta(x) \), is continuous on \( \mathbb{R} \) and concave on the intervals \((0, x_c)\) and \((x_c, \infty)\).

We may create an envelope enclosing \( \phi \) in the following way. See Figure 3 for a graphical interpretation.

1. Pick three points \( x_\ell < x_c < x_r \) corresponding to left, center, and right.
2. Find the tangent lines \( L_\ell \) and \( L_r \) that touch the graph of \( \eta \) at \( x_\ell \) and \( x_r \).
3. Construct an envelope of \( \eta \) using those two lines, that is
\[
e(x) = \begin{cases} 
L_\ell(x), & x < x_c, \\
L_r(x), & x \geq x_c.
\end{cases}
\]
Then an envelope for \( \phi(x) \) is
\[
\phi(x) \leq e(x) + \delta(x).
\]

**Conjecture 15.** \( K''(t)/x^2 \) is increasing on \( x > 0 \) with \( \lim_{x \to 0^+} K''(t)/x^2 = 0 \) and \( \lim_{x \to 0^+} K''(t)/x^3 = 1 \) and \( K''(t)/x^3 \) is decreasing on \( x > 0 \) with \( \lim_{x \to 0^+} K''(t)/x^3 = 1 \) and \( \lim_{x \to \infty} K''(t)/x^3 = 0 \).

This can be seen by plotting these functions; however, we do not have a complete proof currently. Instead, we employ the following lemma.

**Lemma 16.** Given \( x_c \in (0, \infty) \), there are constants \( \alpha_\ell, \alpha_r > 0 \) such that \( K''(t) \) satisfies
\[
1 \geq \frac{K''(t)}{x^3} \geq \alpha_\ell \text{ for } x < x_c
\]
and
\[
1 \geq \frac{K''(t)}{x^2} \geq \alpha_r \text{ for } x > x_c.
\]

**Proof.** The upper bounds are verified in the proofs of Lemmas 13 and 12. For the lower bounds, recall that \( K''(t(x)) > 0 \) for \( x \in I_M := [1/M, M] \) for any \( M > 1 \). Thus, \( K''(t(x)) \) is bounded from below on \( I_M \). In addition, \( x^2 \) and \( x^3 \) are bounded on the same interval from above. Hence the ratios \( K''(t)/x^3 \) and \( K''(t)/x^2 \) are bounded from below on \( I_M \) and we only need to consider the tail behavior of these ratios.

Let \( v(x) = 2u(x) \). When \( x < 1 \), \( v < 0 \), and \( x^2|v| = \tanh^2 \sqrt{|v|} \) the ratio
\[
\frac{K''(t)/x^3}{\frac{1}{x} - \frac{1-x}{x(x^2|v|)}} = \frac{1}{x} - \frac{1-x}{x \tanh^2 \sqrt{|v|}}.
\]
Employing the trigonometric identity \(-\sinh^2 x = 1 - \coth^2 x\) and writing out \(x(v)\) yields

\[
\frac{1}{\tanh^2 \sqrt{|v|}} + \frac{1}{x} \left(1 - \coth^2 \sqrt{|v|}\right) = \frac{1}{\tanh^2 \sqrt{|v|}} - \frac{\sqrt{|v|} \cosh \sqrt{|v|}}{\sinh^3 \sqrt{|v|}}.
\]

As \(v \to -\infty\) the first term converges to unity while the second term vanishes. Since \(v\) is an increasing function of \(x\) that diverges to \(-\infty\) as \(x \to 0^+\), for any \(1 > \alpha_\ell > 0\), there is an \(M > 1\) such that \(K''(t)/x^3 > \alpha_\ell\) for \(x < 1/M\).

Similarly, when \(x > 1\), \(v > 0\), and \(x^2v = \tan^2 \sqrt{x}\) the ratio

\[
K''(t)/x^2 = 1 + \frac{1-x}{x^2v} = 1 + \frac{1-x}{\tan^2 \sqrt{v}}.
\]

The last term can be rewritten as

\[
\frac{1-x}{\tan^2 \sqrt{v}} = \frac{1}{\tan \sqrt{v}} \left(\frac{1}{\tan \sqrt{v}} - 1\right),
\]

which converges to zero as \(v \to (\pi/2)^2\). Since \(v\) is increasing in \(x\) and converges to \((\pi/2)^2\) as \(x \to \infty\), for any \(1 > \alpha_r > 0\), there is an \(M > 1\) such that \(K''(t)/x^2 > \alpha_r\) for \(x > M\).

\[\square\]

Lemma \[14\] and Lemma \[16\] give us the following proposition.

**Proposition 17.** There exists constants \(1 > \alpha_\ell, \alpha_r > 0\) such that the saddle point approximation of \(J^*(n,z)/n\) is bounded by the envelope

\[
k(x|h,z) = \left(\frac{n}{2\pi}\right)^{1/2} \left\{\begin{array}{ll}
\alpha_\ell^{-1/2} e^{n \frac{z^2}{2x}} x^{-3/2} \exp\left(-\frac{n}{2x} + nL_\ell(x|z)\right), & x < x_c \\
\alpha_r^{-1/2} x_c^{n} x^{-n-1} \exp\left(nL_r(x|z)\right), & x > x_c,
\end{array}\right.
\]

where \(L_\ell\) is the line touching \(\eta\) at \(x_\ell\) and \(L_r\) is the line touching \(\eta\) at \(x_r\). Further, \(L_\ell'\) and \(L_r'\) are negative when \(x_{\ell} \geq m = \arg\max_x \phi(x)\).

**Proof.** Lemma \[14\] and Lemma \[16\] provide the envelope. It only remains to show that the slopes of \(L_\ell\) and \(L_r\) are negative when \(x_{\ell} \geq m\). Note that the concavity of \(\phi\) ensures that \(\phi'(x) \leq 0\) when \(x \geq m\). Thus, in the left case, \(L_\ell'(x_{\ell}) = \phi'(x_{\ell}) - \frac{1}{2x_{\ell}^2} < 0\). Similarly, in the right case, \(L_r'(x_r) = \phi'(x_r) - \frac{1}{x_r} < 0\). \(\square\)

Given the stipulation that \(x_{\ell} \geq \arg\max_x \phi(x)\), the left hand kernel, \(k_\ell(x|h,z)\), is an inverse Gaussian kernel while the right hand kernel, \(k_r(x|h,z)\), is a gamma kernel. To see this let \(\rho_\ell = -2L_\ell'(x)\) and \(b_\ell = L_\ell(0)\); then the exponent of the left hand kernel is

\[
nb_\ell - \frac{n \rho_\ell x}{2} - \frac{n}{2x} = -\frac{n \rho_\ell}{2x} \left(\frac{1}{\rho_\ell} + x^2\right) + nb_\ell.
\]

Taking the first term and completing the square yields

\[
\frac{-n \rho_\ell}{2x}\left(x - \frac{1}{\sqrt{\rho_\ell}}\right)^2 - n\sqrt{\rho_\ell}.
\]
Thus
\[ k_k(x|h, z) = \kappa_{k}(\frac{n}{2\pi^2x^2})^{1/2} \exp \left\{ -\frac{n\rho_k}{2} (x - \frac{1}{\sqrt{\rho_k}})^2 \right\} \]
where
\[ \kappa_{k} = \alpha_{k}^{-1/2} e^{\frac{n}{2x^2} + nb_{k} - n\sqrt{\rho_k}} \]
so \( k_k \) is the kernel of an inverse Gaussian distribution with parameters \( \mu = 1/\sqrt{\rho_k} \) and \( \lambda = n \). For the right hand kernel let \( \rho_r = -L_r'(x) \) and \( b_r = L_r(0) \), which yields
\[ k_r(x|h, z) = \kappa_{r}(n\rho_r)^{n-1} \frac{n}{\Gamma(n)} \exp(-n\rho_r x) \]
where
\[ \kappa_{r} = \left( \frac{n}{2\pi\alpha_r} \right)^{1/2} e^{\frac{nb_r}{n\rho_r}} \frac{\Gamma(n)}{(n\rho_r)^n} \]
so \( k_r \) is the kernel of a Gamma distribution with shape \( n \) and rate \( n\rho_r \). These two observations show that \( g(x|h, z) \propto k(x|h, z) \) is a mixture, which can be sampled in a manner similar to the previous two algorithms.

We have yet to specify the points \( x_k, x_m, \) or \( x_r \). As mentioned at the outset, it is important to choose these points carefully so that the envelope does not exceed the target density by too much. Currently, we set \( x_k \) to be the mode of \( \phi \). By picking \( x_k \) to match the maximum of \( \phi \) we guarantee that the mode of \( sp_n(x) \) matches the mode of \( k(x|h, z) \) as \( n \to \infty \). We could set \( x_r = 1.2x_k \) and then chose \( x_m \) so that \( L_{r}(x_m) = L_{r}(x_c) \), in which case the envelope \( e \) is continuous. When that is the case the following proposition holds. However, this requires a non-linear solve, so in practice we simply set \( x_c = 1.1x_k \).

**Proposition 18.** Suppose \( e \) is continuous. Let \( m \) be the maximum of \( \phi(x) \). If \( x_k = m \), then the envelope \( e(x) + \delta(x) \) takes on its maximum at \( m \) as well. Further, as \( n \to \infty \), the mode of the saddlepoint approximation converges to the mode of \( k(x|h, z) \).

**Proof.** Suppose \( m \) maximizes \( \phi \) and \( x_k = m \). Then
\[ e'(x_k) + \delta'(x_k) = \phi'(x_k) = 0. \]
Since \( e'(x_k) + \delta'(x_k) \) is strictly concave on \((0, x_c]\), \( x_k \) must be the maximum of the left-hand portion of the envelope for \( \phi \). We will show that this is the only maximum by contradiction. Suppose the right-hand portion of the envelope of \( \phi \) has a maximum at \( y > x_c \). Since that portion is also strictly concave, we must have \( \phi'(y) - \delta'(y) = 0 \implies \phi'(y) = \delta'(y) \). But \( \phi'(y) < 0 \) since \( y > m \) and \( \delta'(y) = 1/y > 0 \), a contradiction.

To see that the modes of \( sp_n \) and \( k(x|h, z) \) converge as \( n \to \infty \), take the log of each. The log of the saddlepoint approximation is like
\[ \phi(x) - \frac{1}{2n} \log K''(t(x)) \]
while the log of the left hand kernel, where the maximum is, is like
\[ e(x) + \delta(x) - \frac{3}{2n} \log x. \]
Since \( \delta \) and \( \phi \) are concave and decay faster than \( \log x \) as \( x \to 0^+ \) and \( \log x \) is increasing, we know that the argmax of each converges to \( m \).
Figure 3: The saddlepoint approximation. The saddle point approximation is proportional to $[K''(t(x))]^{-0.5} \exp(n\phi(x))$. In the left plot, $\eta(x)$ is a solid black curve, which is bounded from above by an envelope of the dotted blue line on the left and the dotted cyan line on the right. The green line is $-\delta(x)$. On the right, the saddlepoint approximation in black, and the left and right envelopes are in blue and cyan respectively. This bound is a bit exaggerated since $n = 4$, which is rather small. The bounding envelope improves as $n$ increases.

Collecting all of the above lemmas leads to the following approximate sampler of $J^*(n,z)$. Some preliminary notation: let $\phi_z(x)$ be the concave dual of $K_z(t)$; let $sp_n(x|z)$ be the saddle point approximation; and let $m$ be the mode of $\phi_z$: $m = (\tanh z)/z$.

- **Preprocess.**
  1. Let $x_\ell = m$, $x_c = 1.1x_\ell$, and $x_r = 1.2x_\ell$.
  2. Calculate the tangent lines of $\eta$ at $x_\ell$ and $x_r$; $L_\ell(x|z)$ and $L_r(x|z)$ respectively.
  3. Construct the proposal $g(x|n,z) \propto k(x|n,z)$.

- **Accept/reject.**
  1. Draw $X \sim g(x|n,z)$.
  2. Draw $U \sim U(0,k(X|n,z))$.
  3. If $U > sp_n(X|z)$, return to 1.
  4. Return $nX$.

### 5.3 Recapitulation

The saddlepoint approximation sampler generates approximate $J^*(n,z)$ random variates when $n$ is large, a regime that the previous two samplers handled poorly. The saddlepoint approximation sampler is similar to the previous two samplers in that the proposal is a mixture of an inverse Gaussian kernel and a gamma kernel. Hence the basic framework to simulate the approximation requires routines already developed in §3 and §4. We have identified that a good choice of $x_\ell$ is the mode of $\phi$; however, we have not yet identified the optimal choices of $x_c$ and $x_r$. The values of $x_\ell$, $x_c$, and $x_r$ depend on the tilting parameter $z$, but not the shape parameter $n$ in $J^*(n,z)$. Thus, one could preprocess $x_\ell$, $x_r$, and $x_c$ for various values of $z$ and then interpolate.
6 Comparing the Samplers

We have a total of four $J^*(n,z)$ samplers available: the method from §3, which we call the Devroye approach, based upon sampling $J^*(1,z)$ random variates; the method from §4, which we call the alternate approach, that lets one directly draw $J^*(n,z)$ for $n \in \{1,4\}$; the method from §5 using the saddlepoint approximation; and the method based upon Fact 3.5, where one simply truncates the infinite sum after, for instance, drawing 200 gamma random variables. Recall that to sample $J^*(n,z)$ using the $J^*(1,z)$ sampler, one sums $n$ independent copies of $J^*(1,z)$. Similarly, to sample $J^*(n,z)$ when $n > 4$ using the alternate method, we sum an appropriate number of $J^*(b_i,z), b_i \in (1,4)$ so that $\sum_{i=1}^{m} b_i = n$.

We compare these methods empirically on a MacBook Pro with 2 GHz Intel Core i7 CPU and 8GB 1333 MHz DDR3 RAM. For a variety of $(n,z)$ pairs, we record the time taken to sample 10,000 $J^*(n,z)$ random variates. Table 1 reports the best method for each $(n,z)$ pair, along with the speed up over the Devroye approach as measured by the ratio of the time taken to draw samples using the Devroye method to the time taken to draw samples using the best method. The Devroye approach works well for $n = 1, 2$ while the alternate method works well for $n = 3, \ldots, 10$. The saddlepoint approximation works well for moderate to large $n$. These general observations do not change drastically across different $z$, though changing $z$ can change the best sampler for fixed $n$. Based upon these observations, we may generate a hybrid sampler, which uses the Devroye method when $n = 1, 2$, the alternate method for $n \in (1,13) \backslash \{1,2\}$, the saddlepoint method when $13 \leq n \leq 170$, and a normal approximation for $n \geq 170$. The normal approximation is not strictly necessary for large $n$, but the pre-built routines used to calculate the gamma function break down for $n \geq 170$. In this case, a simple fix is to calculate the mean and variance of the PG($n,z$) distribution using the moment generating function from Fact 3, and then sample from a normal distribution by matching moments. The central limit theorem suggests that this is a reasonable approximation when $n$ is sufficiently large.

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Table 1: $J^*(n, z)$ benchmarks. For each method and each $(n, z)$ pair the time taken to draw 10,000 samples was recorded and compared. The left portion of the table lists the best method for each $(n, z)$ pair. The methods benchmarked include DV, the method from §3; AL, the method from §4; SP, the method from §5; and GA, an approximate draw using a truncated sum of 200 gamma random variates based upon Fact 3.5. Notice that the truncated sum method never wins. The DV method wins for small $n$; the AL method wins for modest $n$, and the SP method wins for medium and large $n$. The right hand portion of the table shows the ratio of the time taken to sample each $(n, z)$ pair using DV to the time taken to sample using the best method.
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