Normal Inverse Gaussian Approximation for Molecular Communications

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***Abstract*—The inverse Gaussian (IG) distribution is a well-established distribution for the first hitting time in flow-induced diffusion molecular communications. However, the distribution of the difference between two independent IG-distributed random variables has not been derived yet, although it is very important for the analysis of many molecular communication systems. For example, for deriving crossover probabilities or characterizing the noise in time between release modulation. In this letter, we propose an approximation by a normal inverse Gaussian (NIG) distribution and derive an asymptotic tail approximation. Numerical evaluations showed that the NIG approximation matches very well with the solution obtained through numerical integration, in particular for the tails. Moreover, the asymptotic tail approximation converges very quickly to the actual probability and outperforms state-of-the-art tail approximations.**

***Index Terms*—Molecular communications, flow-induced diffusion channel, normal inverse Gaussian distribution, inverse Gaussian distribution,**

I. Introduction

Mcommunication broadly defines information transmission using chemical signals [1]. It is a promising candidate for communications at nano-scale due to its ultra-high efficiency [2] and bio-compatibility. The main envisioned applications are in the area of nano-medicine [3] (e.g., targeted drug delivery). Currently, molecular communication research can be split into three areas: 1) *Living system modelling* aims at gaining more insights into molecular communication processes occurring in biological live system using techniques originating from communications engineering (e.g., quantifying information in protein structures [4]) 2) *Living systems interface* aims to control the behavior of biological systems (e.g., connecting synthetic biology to electronics using redox modality [5]) 3) *Artificial molecular communication* focuses on the design, fabrication and testing of human-made molecular communication systems (e.g., artificial chemical communication between gated nanoparticles [6]).

In molecular communications the information can be encoded using molecule's concentration [7], number [8], release time [9], type [10] or a combination of the aforementioned methods. The information molecules can be transported from the transmitter to the receiver through pure diffusion, diffusion with flow, active transport (e.g., molecular motors [11]) and bacteria [12]. Most molecular communication research is devoted to diffusion-based molecular communication. In this case the receiver can be classified as either passive or active [13]. Typically a passive receiver only observes the molecules in the environment, but does not react with the information molecules. In contrast, for active receiver a chemical reaction between receiver and molecules takes place and the molecules is recognized by the receiver due to the reaction. The first hitting time in pure diffusion and flow-induced diffusion channels with an active (absorbing) receiver [14] can be modelled by a Lévy [15] and inverse Gaussian (IG) [9] distribution, respectively. The difference between two independent Lévy-distributed random variables follows a stable distribution [15]. This distribution is very important in order to characterize crossover probabilities [8], [16], [17] and noise in time between release modulation [15] for pure diffusion channels. However, to the best of our knowledge the distribution of the difference between two IG-distributed random variables has not been derived yet. So far, only an asymptotic tail approximation was proposed in [16].

In this letter, we present an approximation of the distribution of the difference between two IG-distributed random variables by a normal inverse Gaussian (NIG) distribution. Through moment matching we derive closed-form expressions for the four parameters of the NIG distribution. Moreover, we derive an asymptotic tail approximation. Numerical evaluations showed that the NIG approximation matches very well with the results obtained through numerical integration, in particular for the tails. The tail approximation converges much faster than the state-of-the-art approximation proposed in [16].

II. Inverse Gaussian Distribution

In this section, we briefly discuss the main properties of the inverse Gaussian (IG) distribution[1]. The probability density function (PDF) of an IG-distributed random variable X is given by [18]

$$f_X(x) = \frac{a}{\sqrt{2\pi}} \exp(ab) x^{-3/2} \exp\left(-\frac{1}{2}\left(a^2 x^{-1} + b^2 x\right)\right), \; x > 0, \tag{1}$$

with the parameters $a > 0$ and $b > 0$. We indicate an IG-distributed random variable with the parameters (a, b) by $X \sim \mathrm{IG}(a, b)$. The cumulative distribution function (CDF) can be expressed as

$$\begin{aligned} F_X(x) =& \phi\left((bx)^{1/2} - ax^{-1/2}\right) + \exp\left(2ab\right) \\ &+ \phi\left(-(bx)^{1/2} - ax^{-1/2}\right), \quad x > 0, \end{aligned} \tag{2}$$

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[1]Please refer to [18] for more details.

with the CDF of the standard normal distribution $\phi(x) = 1/\sqrt{2\pi}\int_{-\infty}^{x}\exp(-t^2/2)\mathrm{d}t$. Moreover, the tail probability is given by $\bar{F}_X(x) = 1 - F_X(x)$. The moment-generating function of X can be expressed as

$$M_X(t) = \exp\left(ab - a\sqrt{b^2 - 2t}\right). \tag{3}$$

It is important to note that the IG distribution is only closed under convolution, i.e. the linear combination of IG-distributed random variables is also IG-distributed, if certain conditions are fulfilled [18]. Suppose $V = \sum_{i=1}^{N} c_i X_i$, with $X_i = IG(a_i, b_i)$, $c_i > 0$ and all X_i are independent. The random variable V is only IG-distributed, iff $b_i/\sqrt{c_i} = c$ for all i. Then the moment-generating function of V is given by

$$\begin{aligned} M_V(t) &= \prod_{i=1}^{N} M_{X_i}(c_i t) \\ &= \prod_{i=1}^{N} \exp\left(a_i\left(b_i - \sqrt{b_i^2 - 2c_i t}\right)\right) \\ &= \exp\left(\sum_{i=1}^{N} a_i\sqrt{c_i}\left(c - \sqrt{c^2 - 2t}\right)\right). \end{aligned} \tag{4}$$

Thus, $V \sim \mathrm{IG}\left(\sum_{i=1}^{N} a_i\sqrt{c_i}, c\right)$. The constancy of $b_i/\sqrt{c_i}$ is a necessary condition for V to be IG-distributed.

III. Normale Inverse Gaussian Approximation

Let's consider a random variable $Z = X_1 - X_2$, with $X_1 \sim \mathrm{IG}(a_1, b_1)$ and $X_2 \sim \mathrm{IG}(a_2, b_2)$. Assuming X_1 and X_2 are independent the PDF of Z can be expressed as

$$f_Z(z) = \left(f_{X_1} * f_{X_2}^{-}\right)(z) = \int_{-\infty}^{\infty} f_{X_1}(u) f_{X_2}(u - z)\mathrm{d}u, \tag{5}$$

with $f_{X_2}^{-} = f_{X_2}(-x)$. The moment-generating function of Z is given by

$$\begin{aligned} M_Z(t) &= M_{X_1}(t) M_{X_2}(-t) \\ &= \exp\left(a_1 b_1 + a_2 b_2 - \left(a_1\sqrt{b_1^2 - 2t} + a_2\sqrt{b_2^2 + 2t}\right)\right). \end{aligned} \tag{6}$$

Since $b_1 \neq b_2$ the random variable Z is not IG-distributed (cf. Sec. II). Although the moment-generating function of Z can easily be derived, the PDF of Z is difficult to analyze. Moreover, to the best of our knowledge, neither a closed-form expression nor an approximation has been derived so far. In the following we propose the normal inverse Gaussian (NIG) distribution as an appropriate approximation for Z, since the NIG distribution is a flexible system of distributions, including heavy-tailed and skewness distributions. The NIG approximation was introduced in [19] and it was shown through numerical results that NIG approximation has a smaller approximation error compared to Gram-Charlier expansion [20] and Edgeworth expansion [21].

The PDF of a NIG-distributed random variable Y is defined by [19]

$$\begin{aligned} f_Y(y) = &\frac{\alpha\delta}{\pi}\exp\left(\delta\sqrt{\alpha^2 - \beta^2} - \beta(y - \mu)\right) \\ &\times \frac{K_1\left(\alpha\sqrt{\delta^2 + (y-\mu)^2}\right)}{\sqrt{\delta^2 + (y-\mu)^2}}, \end{aligned} \tag{7}$$

with the parameters $\alpha > 0$, $\delta > 0$, $\mu \in \mathbb{R}$ and $0 \leq |\beta| < \alpha$ and $K_1(\cdot)$ denotes the modified Bessel function of the third kind with index 1. The parameters α, β, μ and δ determine the tail heaviness, asymmetry, location and scaling of the distribution. The Gaussian distribution arises as a special case of the NIG distribution by setting $\alpha \to \infty$, $\beta = 0$ and $\delta = \sigma^2\alpha$, where σ^2 denotes the variance of the Gaussian distribution. The relation between mean $\mathcal{M}$, variance $\mathcal{V}$, skewness $\mathcal{S}$ and excess kurtosis $\mathcal{K}$ of Y is given by [19]

$$\begin{aligned} \alpha &= 3\rho^{1/2}(\rho - 1)^{-1}\mathcal{V}^{-1/2}|\mathcal{S}|^{-1} \\ \beta &= 3(\rho - 1)^{-1}\mathcal{V}^{-1/2}\mathcal{S}^{-1} \\ \mu &= \mathcal{M} - 3\rho^{-1}\mathcal{V}^{1/2}\mathcal{S}^{-1} \\ \delta &= 3\rho^{-1}(\rho - 1)^{1/2}\mathcal{V}^{-1/2}|\mathcal{S}|^{-1}, \end{aligned} \tag{8}$$

where $\rho = 3\mathcal{K}\mathcal{S}^{-2} - 4 > 1$.

We approximate the unknown distribution of Z by matching the mean, variance, skewness and excess kurtosis of Z with the NIG distribution, which is known as moment matching method [22]. The moments are then used to derive the parameters α, β, μ and δ according to (8). The mean, variance, skewness and excess kurtosis of Z can be expressed in terms cumulants

$$\begin{aligned} \hat{\mathcal{M}} &= \kappa_1, & \hat{\mathcal{V}} &= \kappa_2, \\ \hat{\mathcal{S}} &= \frac{\kappa_3}{\kappa_2^{3/2}}, & \hat{\mathcal{K}} &= \frac{\kappa_4}{\kappa_2^2}. \end{aligned} \tag{9}$$

where κ_n, $n = 1\ldots,4$, denotes the nth cumulant of Z. The cumulants can be derived using the moment-generating function of Z defined in (6)

$$\kappa_n = \left.\frac{\partial^n}{\partial t^n}\ln M_Z(t)\right|_{t=0}. \tag{10}$$

In the following we present the analytical expressions for the parameters α, β, μ and δ for two important cases in molecular communications.

A. Case 1: $a_1 = a_2 = a$ and $b_1 = b_2 = b$

In this case the moment-generating function of Z can be written as

$$\begin{aligned} M_Z(t) &= M_{X_1}(t) M_{X_2}(-t) \\ &= \exp\left(ab + ab - \left(a\sqrt{b^2 - 2t} + a\sqrt{b^2 + 2t}\right)\right). \end{aligned} \tag{11}$$

The moments are obtained by applying (10) and (9)

$$\begin{aligned} \hat{\mathcal{M}} &= 0, & \hat{\mathcal{V}} &= \frac{2a}{b^3}, \\ \hat{\mathcal{S}} &= 0, & \hat{\mathcal{K}} &= \frac{15}{2ab}. \end{aligned} \tag{12}$$

The parameters of the corresponding NIG distribution can be derived using the relation in (8) and can be expressed as

$$\begin{aligned} \alpha &= \frac{b^2}{\sqrt{5}}, & \beta &= 0, \\ \mu &= 0, & \delta &= \frac{2}{\sqrt{5}}\frac{a}{b}. \end{aligned} \tag{13}$$

The resulting NIG distribution is symmetric, since $\beta = 0$.

B. Case 2: $b_1/a_1 = b_2/a_2 = c$

In this case the moment-generating function of Z can be written as

$$\begin{aligned} M_Z(t) &= M_{X_1}(t)M_{X_2}(-t) \\ &= \exp\left(\left(a_1^2 + a_2^2\right)c - \left(a_1\sqrt{a_1^2c^2 - 2t} + a_2\sqrt{a_2^2c^2 + 2t}\right)\right). \end{aligned} \tag{14}$$

Similar to case 1, the moments can be calculated using (10) and (9)

$$\begin{aligned} \hat{\mathcal{M}} &= 0, & \hat{\mathcal{V}} &= \frac{a_1^{-2} + a_1^{-2}}{c^3}, \\ \hat{\mathcal{S}} &= \frac{3\left(a_1^{-2} + a_1^{-2}\right)}{\sqrt{c\left(a_1^{-2} + a_1^{-2}\right)^3}}, & \hat{\mathcal{K}} &= \frac{15\left(a_1^{-6} + a_1^{-6}\right)}{c\left(a_1^{-2} + a_1^{-2}\right)^2}. \end{aligned} \tag{15}$$

The parameters of the corresponding NIG distribution can be expressed as

$$\begin{aligned} \alpha &= \frac{\left(a_1^2 - a_2^2\right)^2\sqrt{\left(a_1^4 + 3a_1^2a_2^2 + a_2^4\right)\left(a_1^2 - a_2^2\right)^{-2}|\tau|}}{5a_1^2a_2^2\sqrt{\left(a_1^{-2} + a_2^{-2}\right)c^{-3}}}, \\ \beta &= \frac{\left(-a_1^2 + a_2^2\right)c^2}{5}, \\ \mu &= \frac{a_1^4 - a_2^4}{\left(a_1^4 + 3a_1^2a_2^2 + a_2^4\right)c}, \\ \delta &= \frac{\sqrt{5}a_1^2a_2^2\sqrt{\left(a_1^{-2} + a_2^{-2}\right)c^{-3}}\,|\tau|}{\sqrt{a_1^2a_2^2\left(a_1^2 - a_2^2\right)^{-2}(a_1^4 + 3a_1^2a_2^2 + a_2^4)}}, \end{aligned} \tag{16}$$

with

$$\tau = \frac{\left(a_1^{-2} + a_2^{-2}\right)^{3/2}\sqrt{c}}{a_1^{-4} - a_2^{-4}}.$$

The NIG distribution is asymmetric, since $\beta \neq 0$.

IV. Tail Approximation

The tail probability of the random variable Z, defined in (5), is given by

$$\begin{aligned} \bar{F}_Z(z) = \Pr(Z > z) &= \int_z^\infty f_Z(t)\mathrm{d}t \\ &= \int_z^\infty \int_{-\infty}^\infty f_{X_1}(u)f_{X_2}(u-t)\mathrm{d}u\mathrm{d}t \\ &= \int_z^\infty \int_{-\infty}^\infty f_{X_1}(v+t)f_{X_2}(v)\mathrm{d}v\mathrm{d}t \\ &= \int_{-\infty}^\infty f_{X_2}(v)\int_z^\infty f_{X_1}(v+t)\mathrm{d}t\mathrm{d}v \\ &= \int_{-\infty}^\infty f_{X_2}(v)\bar{F}_{X_1}(v+z)\mathrm{d}v. \end{aligned} \tag{17}$$

The asymptotic tail behavior can be derived as follows

$$\begin{aligned} \lim_{z\to\infty}\frac{\bar{F}_Z(z)}{\bar{F}_{X_1}(z)} &= \lim_{z\to\infty}\int_{-\infty}^\infty \frac{f_{X_2}(v)\bar{F}_{X_1}(z+v)}{\bar{F}_{X_1}(z)}\mathrm{d}v \\ &= \int_{-\infty}^\infty \lim_{z\to\infty}\frac{\bar{F}_{X_1}(z+v)}{\bar{F}_{X_1}(z)}f_{X_2}(v)\mathrm{d}v \\ &= \int_{-\infty}^\infty \exp\left(-b_1^2/2v\right)f_{X_2}(v)\mathrm{d}v, \end{aligned} \tag{18}$$

where we used $\lim_{z\to\infty}\bar{F}_{X_1}(z+v)/\bar{F}_{X_1}(z) = \exp(-b_1^2/2v)$ for all v real [23]. Thus, the asymptotic tail behavior of Z is given by

$$\begin{aligned} \lim_{z\to\infty}\bar{F}_Z(z) &= \bar{F}_{X_1}(z)\int_{-\infty}^\infty \exp\left(-b_1^2/2v\right)f_{X_2}(v)\mathrm{d}v \\ &= \bar{F}_{X_1}(z)M_{X_2}(-b_1^2/2), \end{aligned} \tag{19}$$

where $M_{X_1}(x)$ denotes the moment-generating function of the inverse Gaussian distribution defined in (3).

V. Applications in Molecular Communications

For molecular communications in flow-induced diffusion channels, the random time between the release of molecules until the first arrival at an absorbing receiver [14] can be modelled as IG-distributed random variable – so-called first hitting time. In the following, we discuss two applications showing the importance of knowing the distribution of the difference between two independent IG-distributed random variables.

A. Timing Channels

We consider timing channels where the information is encoded in the time duration between two consecutive release of molecules [15]. The arrival time of a single molecule released

TABLE I
KL DIVERGENCE PERFORMANCE OF THE NIG APPROXIMATION

v [μm/s]	d [m]	D_1 [μm^2/s]	D_2 [μm^2/s]	$D(f_Z \| \hat{f}_Z)$
Case 1 - Symmetric PDF (cf. Figs. 1 and 2)				
1	1	0.5	0.5	1.3×10^{-2}
2	1	0.5	0.5	4×10^{-3}
1	2	0.5	0.5	3×10^{-3}
Case 2 - Asymmetric PDF (cf. Figs. 3 and 4)				
1	2	0.5	0.1	1.2×10^{-3}
1	2	0.5	2.5	3.2×10^{-2}

at time S is given by $Y = S + X$, where X denotes the first hitting time and follows an IG distribution. If the information is encoded in $Z_s = S_2 - S_1$, where S_1 and S_2 denote the release time of the individual molecules, the channel model is given by [15]

$$\begin{aligned} Y_2 - Y_1 &= S_2 - S_1 + X_2 - X_1 \\ Z_y &= Z_s + Z_x, \end{aligned} \tag{20}$$

with the noise term $Z_x = X_2 - X_1$ and X_1 and X_2 are IG-distributed random variables. In order to analyze such timing channels the distribution of Z_x is of interest. Since the exact distribution of Z_x is hard to determine, it can be approximated by a NIG distribution (Sec. III).

B. Crossover Probability

Let's assume that two molecules of different type, representing bit 0 and bit 1, are released a time interval T apart. The first hitting time of the first and second transmitted molecules is given by X_1 and X_2, respectively, and follow an IG distribution. The probability for the released molecules to arrive out-of-order can be expressed as

$$\Pr(X_1 - X_2 > T) = \Pr(Z_x > T), \tag{21}$$

which is referred to as crossover probability. In order to evaluate the crossover probability in (21) the distribution of Z_x is of interest. Since the exact distribution of Z_x is hard to determine, a possible solution is to approximate Z_x by a NIG distribution (cf. Sec. III). It is important to note that the crossover probability in (21) is frequently used for the theoretical analysis of molecular molecular communication systems. For example, based on the crossover probability an approximated error performance for different channel coding techniques was presented in [16] and the channel capacity for binary molecule shift keying was derived in [17].

VI. NUMERICAL EVALUATION

For the numerical evaluation we consider molecular communications in a semi-infinite one-dimensional (1D) fluidic environment (e.g., blood vessel) between a receiver and a transmitter that are placed at a distance d. Moreover, we assume a positive flow with velocity v from transmitter to receiver. For such a flow-induced diffusion channels the first hitting time of a released molecule at an absorbing receiver [14] follows an IG distribution.

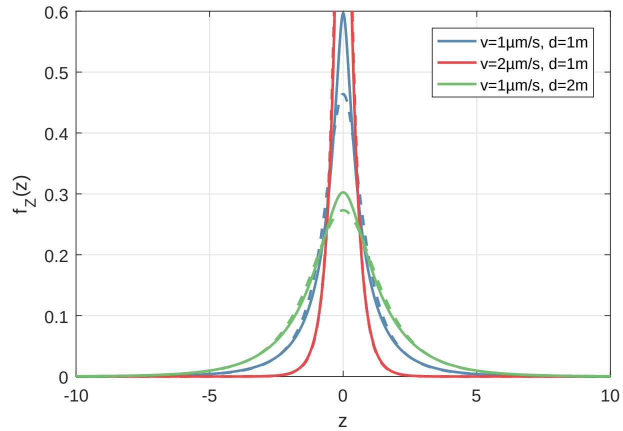

Fig. 1. Probability density function of $Z = X_1 - X_2$ for case 1 (cf. Sec. III-A). The solid lines indicate the PDF obtained through numerical integration of (5) and the dashed lines correspond to the NIG approximation with the parameters in (13).

Figs. 1 – 4 show the PDF and the tail probability of the random variable $Z = X_1 - X_2$, where X_1 and X_2 are IG-distributed random variables with the parameters

$$\begin{aligned} a_1 &= \frac{d}{\sqrt{2D_1}}, \qquad a_2 = \frac{d}{\sqrt{2D_2}}, \\ b_1 &= \frac{v}{\sqrt{2D_1}}, \qquad b_2 = \frac{v}{\sqrt{2D_2}}, \end{aligned} \tag{22}$$

where D_1 and D_2 denote the diffusion coefficients of the released molecules. In Figs. 1 – 4 the solid lines indicate the results obtained through numerically integration of (5) and the dashed lines correspond to the NIG approximation. Moreover, the dotted lines in Figs. 2 and 4 represent the asymptotic tail behavior. Moreover, we use the Kullback-Leibler (KL) divergence to evaluate the performance of the NIG approximation. The KL divergence between the actual distribution $f_Z(z)$, obtained through numerical integration of (5), and the NIG approximation $\hat{f}_Z(z)$ can be calculated by [24]

$$D\left(f_Z \| \hat{f}_Z\right) = \int_{-\infty}^{\infty} f_Z(z) \ln \frac{f_Z(z)}{\hat{f}_Z(z)} \mathrm{d}z. \tag{23}$$

The KL divergence of different scenarios is summarized in Tab. I.

In Figs. 1 and 2 the PDF and tail probability for case 1 (cf. Sec. III-A) are shown. In this case $a_1 = a_2 = d/\sqrt{2D_1}$ and $b_1 = b_2 = v/\sqrt{2D_1}$, with $D_1 = 0.5 \times 10^{-12}\,\mu$m^2/s. The PDF is symmetric and we observe that increasing the distance broadens the peak of the PDF and results in a longer tail, whereas an increase in the velocity results in a narrow peak and a shorter tail. We observe a very good match between the numerical results and the NIG approximation, in particular for the tails. Moreover, it can be seen that the asymptotic approximation of the tail probability quickly converges to the actual probability.

Figs. 3 and 4 shows the PDF and tail probability for case 2 (cf. Sec. III-B). In this case $b_1/a_1 = b_2/a_2 = v/d$, with $v = 1\,\mu m/s$ and $d = 2\,$m. The PDF is asymmetric and we

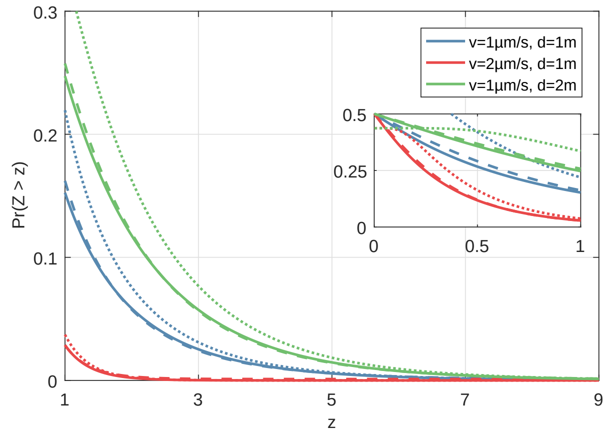

Fig. 2. Tail probability of $Z = X_1 - X_2$ for case 1 (cf. Sec. III-A). The solid lines indicate the tail obtained through numerical integration of (17), the dashed lines correspond to the tail probability of the NIG approximation with the parameters in (13) and the dotted lines represent the asymptotic tail behavior derived in (19).

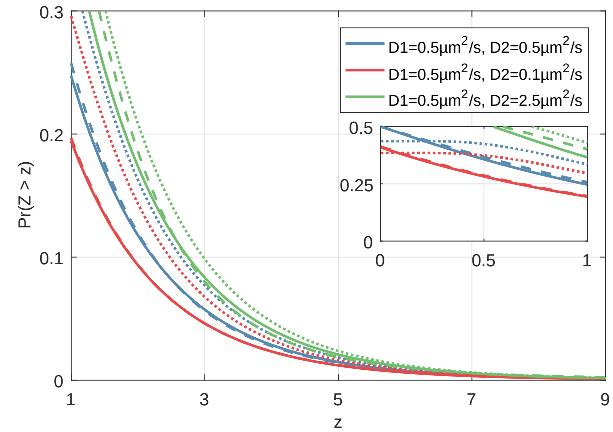

Fig. 4. Tail probability of $Z = X_1 - X_2$ for case 2 (cf. Sec. III-B). The solid lines indicate the tail obtained through numerical integration of (17), the dashed lines correspond to the tail probability of the NIG approximation with the parameters in (16) and the dotted lines represent the asymptotic tail behavior derived in (19).

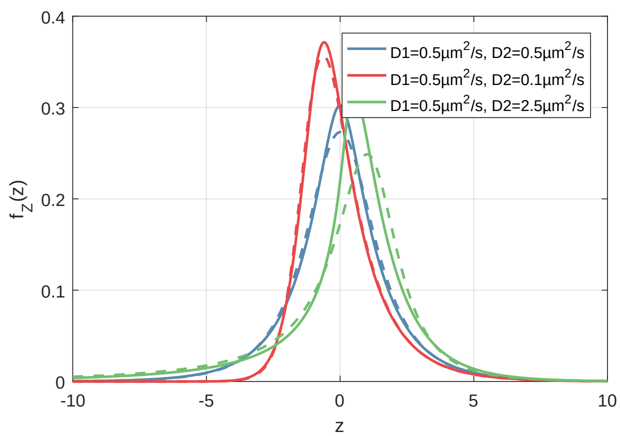

Fig. 3. Probability density function of $Z = X_1 - X_2$ for case 2 (cf. Sec. III-A). The solid lines indicate the PDF obtained through numerical integration of (5) and the dashed lines correspond to the NIG approximation with the parameters in (16).

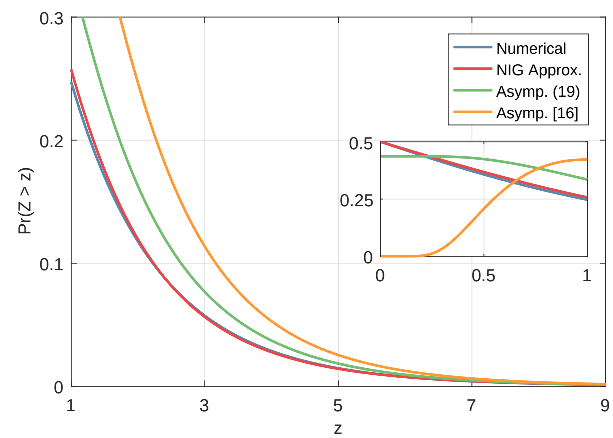

Fig. 5. Tail probability comparison for case 1 (cf. Sec. III-A), with $v = 1\,\mu$m/s, $d = 2\,\mu$m and $D_1 = 0.5 \times 10^{-12}\,\mu$m²/s.

observe a positive skew (right tail is longer) if D_2 becomes smaller compared to D_1 and a negative skew (left tail is longer) if D_2 becomes larger compared to D_1. We observe a very good match between the numerical solution and the NIG approximation, in particular for the tails, and the asymptotic tail approximation quickly converges to the actual probability.

In Fig. 5 we compare the asymptotic tail approximation in (19) with a recently proposed tail approximation given by [16]

$$\bar{F}_Z(z) = \frac{4D_1}{v^2} \exp\left(\frac{\left(\sqrt{2}-1\right) dv}{2D_1}\right) f_{X_1}(x), \tag{24}$$

where $f_{X_1}(x)$ denotes the PDF of an IG distribution defined in (1). We observe that asymptotic tail approximation in (19) converges much faster than the approximation in (24). Moreover, the approximation in (24) is only valid if the PDF is symmetric, whereas the approximation in (19) can also be applied to asymmetric PDFs.

VII. Conclusions

In this letter, we have proposed an approximation for the distribution of the difference between two independent IG-distributed random variables. We derived the four parameters of the NIG distribution through the moment matching method. Moreover, we have presented an asymptotic tail approximation. We have shown numerically that the NIG approximation matches very well with the results obtained through numerically integration and the asymptotic tail approximation converges quickly to the actual probability. It is important to note that the proposed approximations are very important for the analysis of flow-induced diffusive molecular communications. For example, for deriving crossover probabilities or characterizing the noise in time between release modulation.

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