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First passage time distribution for anomalous diffusion

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Abstract

We study the first passage time (FPT) problem in Levy type of anomalous diffusion. Using the recently formulated fractional Fokker–Planck equation, we obtain an analytic expression for the FPT distribution which, in the large passage time limit, is characterized by a universal power law. Contrasting this power law with the asymptotic FPT distribution from another type of anomalous diffusion exemplified by the fractional Brownian motion, we show that the two types of anomalous diffusions give rise to two distinct scaling behavior. © 2000 Published by Elsevier Science B.V.

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1. Introduction

For a stochastic process, the first passage time (FPT) is defined as the time T when the process, starting from a given point, reaches a predetermined level for the first time, and is a random variable [1]. Escape times from a random potential, intervals between neural spikes, and fatigue failure times of engineering structures are all examples of FPTs, arising in physics [2], biology [3], and engineering [4], respectively. Thus, knowledge of the FPT distribution, $f(t)$, is essential for the effective application of probabilistic analysis. (As a convention we use capital letters to denote random variables and lower case letters to denote their values.) Unfortunately, only in very few cases does one have explicit analytical expressions for $f(t)$. One such case is the ordinary Brownian motion, an example of ordinary diffusion, in which the FPT is described by the famous inverse Gaussian law [5]. The main contribution of this work is the derivation of the exact solution of $f(t)$ for a much broader class of stochastic processes, namely, the Levy type of anomalous diffusion [6–18] in which the mean square displacement of the diffusive variable $X(t)$ scales with time as $\langle X^2(t) \rangle \sim t^\gamma$ with $0 < \gamma < 2$. Specifically, using a recently formulated framework of fractional Fokker–Planck equation (FFPE) [19], we express $f(t)$ in terms of Fox or H-functions [20,21], which is shown to contain the inverse Gaussian distribution as a special case. Furthermore, we show that in the asymptotic limit of large t , $f(t)$ scales with t as $f(t) \sim t^{-1-\gamma/2}$. Our

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next result concerns the comparison with a different type of anomalous diffusion, represented by fractional Brownian motion (fBm) [22,23], where again $\langle X^2(t) \rangle \sim t^\gamma$ with $0 < \gamma < 2$. For this type, we argue that $f(t) \sim t^{\gamma/2-2}$ for large t , a result that has been conjectured earlier [24]. Finally, we present numerical simulations which verify the analytical results.

2. FFPE and derivation of FPT distribution

The Levy type of anomalous diffusion considered in this work is a class of non Gaussian and non Markovian processes founded on the continuous time random walk (CTRW) where the waiting time obeys certain power law distribution [6,7]. Let $\phi(y,u)$ denote the joint probability density between the waiting time U and the jump size Y . It can be shown that, depending on the specific form of $\phi(y,u)$, the CTRW can produce both subdiffusive ($0 < \gamma < 1$) and superdiffusive processes ($1 < \gamma < 2$) as well as ordinary diffusion ($\gamma = 1$) [6,7,25]. For example, consider

$$\phi(y,u) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp[-y^2/2\sigma^2] \frac{(\alpha-1)/\tau}{(1+u/\tau)^\alpha}, \quad (1)$$

where Y and U are decoupled with Y being a Gaussian variable. (We note that, strictly speaking, the distribution of U is not a Levy stable distribution, but belongs to the domain of attraction [23] of a one-sided stable Levy law. We call U a ‘‘Levy type of variable’’ for want of a better name.) For $1 < \alpha < 2$, the corresponding CTRW is characterized by a subdiffusive process with $\gamma = \alpha - 1$, and for $\alpha \geq 2$, one gets ordinary diffusion with $\gamma = 1$. If, on the other hand, Y and U are coupled through

$$\phi(y,u) = \frac{1}{2} \delta(u/\tau - |y|/\sigma) \frac{(\beta-1)/\tau}{(1+u/\tau)^\beta}, \quad (2)$$

where $2 < \beta < 3$ and $\delta(\cdot)$ is the Dirac delta function, the CTRW describes a superdiffusive process with $\gamma = 4 - \beta$.

Let $W(x,t)$ be the probability density function for a CTRW $X(t)$ with $X(0) = 0$. Consider the generalized diffusion limit where σ and τ are scaling parameters for the space and time variables. For the subdiffusive case, this means taking the limit $\sigma^2 \rightarrow 0$ and $\tau \rightarrow 0$ with $K = \sigma^2/2\Gamma(1-\gamma)\tau^\gamma$ kept a constant, and for the superdiffusive process, this means taking the same limit with $K = (3-\gamma)(2-\gamma)\Gamma(\gamma-1)\sigma^2/2(5-2\gamma)\tau^\gamma$ kept a constant. In this limit it can be shown [6,7] that the evolution of $W(x,t)$ is determined by the following FFPE [19]:

$$W(x,t) - W(x,0) = {}_0D_t^{-\gamma} K \frac{\partial^2}{\partial x^2} W(x,t), \quad 0 < \gamma < 2, \quad (3)$$

where the Riemann-Liouville fractional integral operator ${}_0D_t^{-\gamma}$ is defined as [26,27]

$${}_0D_t^{-\gamma} W(x,t) = \frac{1}{\Gamma(\gamma)} \int_0^t dt' (t-t')^{\gamma-1} W(x,t'), \quad \gamma > 0, \quad (4)$$

with $\Gamma(z)$ being the gamma function [28]. The constant K is the generalized diffusion constant defined in the above generalized diffusion limit. From Eq. (3) it is easily shown that $\langle X^2(t) \rangle = 2Kt^\gamma/\Gamma(1+\gamma)$.

In the framework of the Fokker-Planck equation, the first passage time problem is defined in terms of having absorbing boundaries at $x = -\infty$ and $x = a$, where a is the predetermined level of crossing, with the initial condition $W(x,0) = \delta(x)$ [1]. An equivalent formulation, due to symmetry, is to solve Eq. (3) with the following boundary and initial conditions: $W(0,t) = 0$, $W(\infty,t) = 0$, $W(x,0) = \delta(x-a)$, where $x = a$ is the new starting point of the process, containing the initial concentration of the distribution. (This latter formulation makes the

subsequent derivation less cumbersome.) Once we solve for $W(x,t)$, the first passage time distribution $f(T)$ is given by [1]

$$f(t) = -\frac{d}{dt} \int_0^\infty dx W(x,t). \quad (5)$$

Taking into account of the boundary and initial conditions we are led to the following expansion for $W(x,t)$ [29]

$$W(x,t) = \frac{2}{\pi} \int_0^\infty dk \sin kx \sin ka A(k,t), \quad (6)$$

with $A(k,0) = 1$. To determine the unknown function $A(k,t)$, we substitute the above expansion for $W(x,t)$ in Eq. (3) and, after straightforward algebra, obtain $A(k,t) - 1 = -Kk^2 {}_0D_t^{-\gamma} A(k,t)$. Taking the Laplace transform with respect to t , we have

$$A(k,p) = \frac{1}{p + k^2 K p^{1-\gamma}}, \quad (7)$$

where $A(k,p)$ is the Laplace transform of $A(k,t)$. Here we have applied the result [27] that the Laplace transform of ${}_0D_t^{-\gamma} A(k,t)$ is $A(k,p)/p^\gamma$. Inverse Laplace transform of Eq. (7) yields [30]

$$A(k,t) = E_\gamma(-k^2 K t^\gamma), \quad (8)$$

where $E_\gamma(z)$ is the Mittag–Leffler function [30]. Substituting Eq. (8) into Eq. (6) we get

$$W(x,t) = \frac{2}{\pi} \int_0^\infty dk \sin kx \sin ka E_\gamma(-k^2 K t^\gamma). \quad (9)$$

To proceed further, we introduce the Fox or H-function [20,21] which has the following alternating power series expansion:

$$H_{p,q}^{m,n} \left(z \left| \begin{array}{l} (a_j, A_j)_{j=1,\dots,p} \\ (b_j, B_j)_{j=1,\dots,q} \end{array} \right. \right) = \sum_{l=1}^m \sum_{k=0}^{\infty} \frac{(-1)^k z^{s_{lk}}}{k! B_l} \times \frac{\prod_{j=1, j \neq l}^m \Gamma(b_j - B_j s_{lk}) \prod_{r=1}^n \Gamma(1 - a_r + A_r s_{lk})}{\prod_{u=m+1}^q \Gamma(1 - b_u + B_u s_{lk}) \prod_{v=n+1}^p \Gamma(a_v - A_v s_{lk})}, \quad (10)$$

where $s_{lk} = (b_l + k)/B_l$ and an empty product is interpreted as unity. Further, m, n, p, q are nonnegative integers such that $0 \leq n \leq p$, $1 \leq m \leq q$; A_j, B_j are positive numbers; a_j, b_j can be complex numbers. The H-function has several remarkable properties [21] which are listed in Appendix A.

By comparing the series expansion [30] of the Mittag–Leffler function $E_\gamma(z)$ with that of the H-function [cf. Eq. (10)], Eq. (9) can be rewritten as

$$W(x,t) = \frac{2}{\pi} \int_0^\infty dk \sin kx \sin ka H_{1,2}^{1,1} \left(k^2 K t^\gamma \left| \begin{array}{l} (0,1) \\ (0,1), (0,\gamma) \end{array} \right. \right). \quad (11)$$

Letting $k' = k(Kt^\gamma)^{1/2}$ and using Property 5 [Eq. (A.3)] of H-functions, the above equation becomes

$$W(x,t) = \frac{1}{2\pi (Kt^\gamma)^{1/2}} \int_0^\infty dk' [\cos k'(x-a) - \cos k'(x+a)] H_{1,2}^{1,1} \left(k' \left| \begin{array}{l} (0,1/2) \\ (0,1/2), (0,\gamma/2) \end{array} \right. \right). \quad (12)$$

The Fourier cosine transforms can be solved by successive applications of a Laplace and an inverse Laplace transform (a technique pioneered by Fox [31] for solving a wide variety of integral transforms) to give [32]

$$W(x,t) = \frac{1}{2|x-a|} H_{3,3}^{2,1} \left(\frac{|x-a|}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1,1/2), & (1,\gamma/2), & (1,1/2) \\ (1,1), & (1,1/2), & (1,1/2) \end{matrix} \right. \right) - \frac{1}{2(x+a)} H_{3,3}^{2,1} \left(\frac{x+a}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1,1/2), & (1,\gamma/2), & (1,1/2) \\ (1,1), & (1,1/2), & (1,1/2) \end{matrix} \right. \right). \quad (13)$$

Now, applying Properties 2, 1, 3 and 6 of the H-functions (listed in Appendix A) in the given order, we finally get

$$W(x,t) = \frac{1}{2(Kt^\gamma)^{1/2}} \left[H_{1,1}^{1,0} \left(\frac{|x-a|}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1-\gamma/2, \gamma/2) \\ (0,1) \end{matrix} \right. \right) - H_{1,1}^{1,0} \left(\frac{x+a}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1-\gamma/2, \gamma/2) \\ (0,1) \end{matrix} \right. \right) \right]. \quad (14)$$

Substituting Eq. (14) into Eq. (5) we have

$$f(t) = -\frac{d}{dt} \left[\frac{1}{2(Kt^\gamma)^{1/2}} \int_0^\infty dx H_{1,1}^{1,0} \left(\frac{|x-a|}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1-\gamma/2, \gamma/2) \\ (0,1) \end{matrix} \right. \right) \right] + \frac{d}{dt} \left[\frac{1}{2(Kt^\gamma)^{1/2}} \int_0^\infty dx H_{1,1}^{1,0} \left(\frac{x+a}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1-\gamma/2, \gamma/2) \\ (0,1) \end{matrix} \right. \right) \right]. \quad (15)$$

Removing the explicit time dependence in the integrands by rewriting the integrals in terms of $z = (x-a)/(Kt^\gamma)^{1/2}$, $z' = (x+a)/(Kt^\gamma)^{1/2}$, the above integrals can be explicitly evaluated to give:

$$f(t) = \frac{a\gamma}{2K^{1/2}t^{(2+\gamma)/2}} H_{1,1}^{1,0} \left(\frac{a}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1-\gamma/2, \gamma/2) \\ (0,1) \end{matrix} \right. \right), \quad (16)$$

which is the main result of this Letter. It should be noted that H-functions were first used in the context of probability distributions by Schneider [33]. They have also been used to express solutions of fractional diffusion equations [34]. In addition, the FPT problem in the context of Levy processes has been considered in Ref. [35].

The series expansion of the H-function in Eq. (16) [cf. Eq. (10)] is

$$f(t) = \frac{a\gamma}{2K^{1/2}t^{(2+\gamma)/2}} \sum_{k=0}^{\infty} \frac{(-a/(Kt^\gamma)^{1/2})^k}{k! \Gamma(1-\gamma/2-k\gamma/2)}. \quad (17)$$

This turns out to be also the series expansion of the Maitland's generalized hypergeometric function or the Wright function ${}_0\psi_1$ [30]. Thus, an alternative expression for $f(t)$ is

$$f(t) = \frac{a\gamma}{2K^{1/2}t^{(2+\gamma)/2}} {}_0\psi_1 \left(-; \begin{matrix} - \\ (1-\gamma/2, -\gamma/2) \end{matrix}; -\frac{a}{(Kt^\gamma)^{1/2}} \right). \quad (18)$$

For $\gamma = 1$ (ordinary Brownian motion), the Wright function reduces to the following simple formula

$$f(t) = \frac{a}{(4\pi Kt^3)^{1/2}} e^{-a^2/4Kt}. \quad (19)$$

This is the expected inverse Gaussian distribution for the FPT distribution of the ordinary Brownian motion [5].

Next, we consider the asymptotic behavior of the FPT distribution for large values of t . Refer to Eq. (16). Let $z = a/(Kt^\gamma)^{1/2}$. It is known that [21,36], for small z , $H_{1,1}^{1,0}(z) \sim |z|^{b_1/B_1} = 1$, since $b_1 = 0$ and $B_1 = 1$. Therefore, the FPT distribution $f(t)$, for large t , is characterized by the power law relation

$$f(t) \sim t^{-1-\gamma/2}, \quad (20)$$

which becomes the well known $-3/2$ scaling law for the ordinary Brownian motion. This power law behavior has been observed earlier by Balakrishnan [37] for subdiffusive processes ($0 < \gamma < 1$) using a different method. Using our method the same scaling law is shown to be applicable also to superdiffusive processes. After some manipulation, we can also determine the location t_{\max} of the maximum of the FPT distribution:

$$t_{\max} = \left(\frac{2d\gamma}{4-\gamma} \right)^{(2-\gamma)/\gamma}, \quad (21)$$

where $d = (1 - \gamma/2)(\gamma/2)^{\gamma/(2-\gamma)}(a/\sqrt{K})^{2/(2-\gamma)}$. From Eq. (20), we see that the mean first passage time and all higher moments of the FPT distribution are undefined for $0 < \gamma < 2$.

The theoretical prediction for the full FPT distribution given in Eq. (16) is verified by numerically simulating the underlying CTRW process characterized by the probability density function $\phi(y,u)$ [cf. Eq. (1)]. For the sake of numerical efficiency, we replace the waiting time distribution in $\phi(y,u)$ by the Pareto distribution [38] which is well justified for small values of τ . Ten million realizations of the CTRW process are used to generate the numerical FPT distribution. The results are shown in Fig. 1 for $\gamma = 0.5$, $a = 1.0$, $\tau = 10^{-4}$ and $K = 0.1$. We note that the numerical simulation is in excellent agreement with the theoretical prediction. The agreement would get even better as the generalized diffusion limit is approached (that is, as $\tau \rightarrow 0$ and $\sigma^2 \rightarrow 0$ with K held a constant).

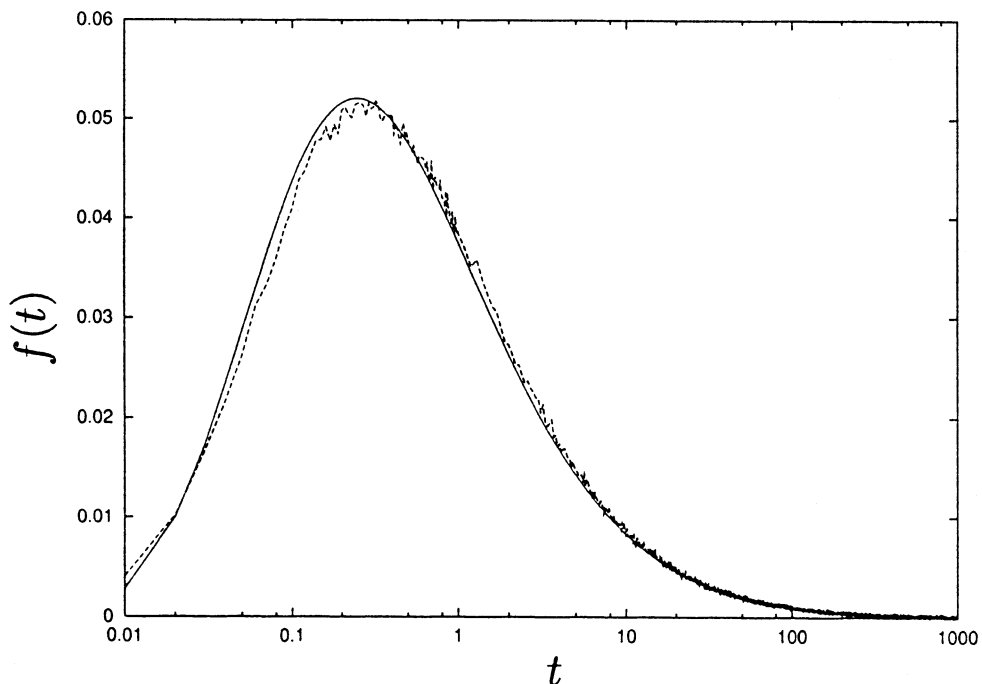


Fig. 1. Comparison of the theoretical FPT distribution (solid line) with the distribution (dashed line) obtained by numerically simulating the underlying CTRW process for a Levy type anomalous diffusion with $\gamma = 0.5$.

3. Anomalous diffusion of the fBm type

Fractional Brownian motion $X(t)$ [22,23] is a Gaussian process with $X(0) = 0$, $\langle X(t) \rangle = 0$ and $\langle [X(t) - X(s)]^2 \rangle = |t - s|^\gamma$ ($0 < \gamma < 2$). By definition it provides us with another type of anomalous diffusion. The exact FPT distribution of this process is not known. It was conjectured [24], based on scaling argument and numerical evidence, that for large t , $f(t)$ scales with t as

$$f(t) \sim t^{\gamma/2-2}. \quad (22)$$

Notice that this power law behavior is different from that in Eq. (20) even though the mean square displacement $\langle X(t)^2 \rangle$ has the same power law behavior ($\langle X(t)^2 \rangle \sim t^\gamma$) for both types of anomalous diffusion. Below we give a heuristic argument for this power law using a recent result [39] concerning the distribution of the maximum of a fBm over a given interval.

Without loss of generality we set the threshold at $a = 1$. Let the probability that the maximum M_t of the fBm $X(t)$ with $X(0) = 0$ is less than 1 in the time interval $[0, t]$ be denoted by $P(t)$:

$$P(t) = \text{Prob}(M_t < 1) \quad (23)$$

Clearly, $P(t)$ is also the probability that the first passage time T of the fBm is greater than t :

$$\text{Prob}(T > t) = P(t). \quad (24)$$

This implies that the first passage time distribution $f(t)$ is given by

$$f(t) = \frac{d}{dt} \text{Prob}(T \leq t) = -\frac{d}{dt} \text{Prob}(T \geq t) = -\frac{d}{dt} P(t). \quad (25)$$

Recent work by Molchan [39] shows that, in the large t limit, $P(t)$ scales with t as

$$P(t) \sim t^{\gamma/2-1}, \quad t \rightarrow \infty. \quad (26)$$

Substituting this in Eq. (25) we obtain Eq. (22).

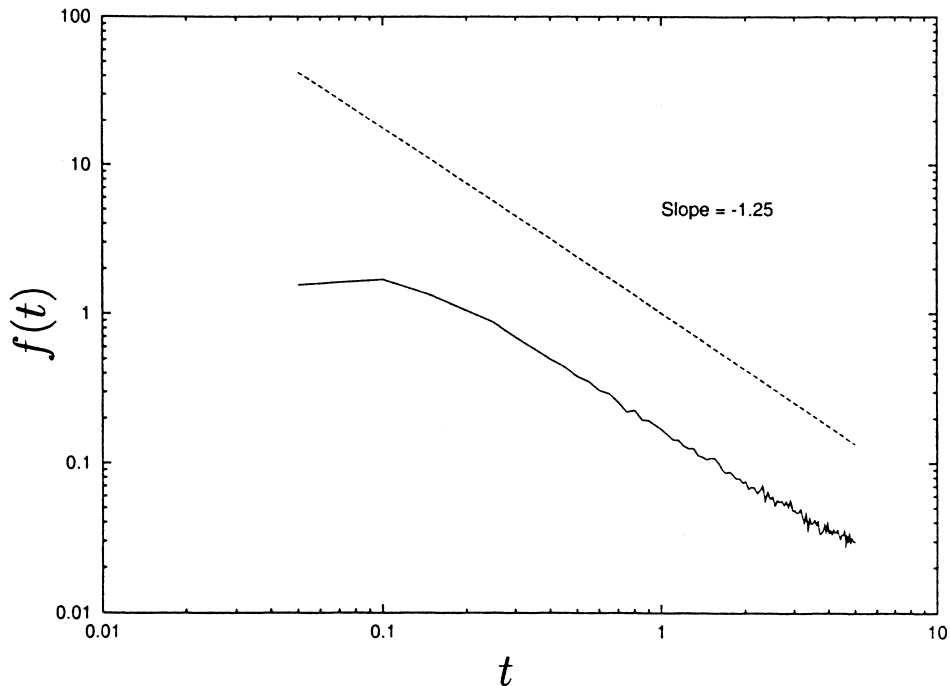


Fig. 2. Comparison of the theoretically predicted power law behavior of the FPT distribution for a fBm with $\gamma = 1.5$ (dashed line) with the numerical simulation (solid line).

We present numerical results to verify Eq. (22). Sinai's formula [40] for the power spectrum of the fractional Gaussian noise (fGn) is used to generate the fBm. The log-log plot of the FPT distribution is shown in Fig. 2 ($\gamma = 1.5$). It is clear that the predicted slope of $\gamma/2 - 2 = -1.25$ is in excellent agreement with the numerical simulation.

4. Conclusions

The two types of anomalous diffusions considered in this work lead to two distinct scaling behavior, Eq. (20) and Eq. (22), for the respective FPT distributions in the asymptotic limit, despite the fact that they are both described by the same mean square displacement. Eq. (20) is expected to be applicable to all CTRW types of processes, regardless of the specific forms of $\phi(y, u)$, for which the generalized diffusion limit leads to Eq. (3). On the other hand, we expect Eq. (22) to hold for Gaussian processes where $\langle [X(t) - X(s)]^2 \rangle \sim |t - s|^\gamma$ for large $|t - s|$.

In this work we considered only processes with $\langle X(t) \rangle = 0$ where the asymptotic limits of the FPT distributions are described by power laws. For a fBm, little is known about its FPT distribution when $\langle X(t) \rangle \neq 0$. For a Levy type of diffusion process, some exact results can be derived for the Laplace transform of the FPT distribution when $\langle X(t) \rangle \neq 0$. We will present these results in other publications.

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Appendix A. Properties of H-functions

The H-function has the following properties [21] which have used in the main text.

Property 1. The H-function is symmetric in the pairs $(a_1, A_1), \dots, (a_n, A_n)$, likewise $(a_{n+1}, A_{n+1}), \dots, (a_p, A_p)$; in $(b_1, B_1), \dots, (b_m, B_m)$ and in $(b_{m+1}, B_{m+1}), \dots, (b_q, B_q)$.

Property 2. Provided $n \geq 1$ and $q > m$,

$$\begin{aligned} H_{p,q}^{m,n} \left(z \left| \begin{array}{cccc} (a_1, A_1), & (a_2, A_2), & \cdots, & (a_p, A_p) \\ (b_1, B_1), & \cdots, & (b_{q-1}, B_{q-1}), & (a_1, A_1) \end{array} \right. \right) \\ = H_{p-1, q-1}^{m, n-1} \left(z \left| \begin{array}{ccc} (a_2, A_2), & \cdots, & (a_p, A_p) \\ (b_1, B_1), & \cdots, & (b_{q-1}, B_{q-1}) \end{array} \right. \right). \end{aligned} \quad (\text{A.1})$$

Property 3. Provided $m \geq 2$ and $p > n$,

$$\begin{aligned} H_{p,q}^{m,n} \left(z \left| \begin{array}{cccc} (a_1, A_1), & \cdots, & (a_{p-1}, A_{p-1}), & (b_1, B_1) \\ (b_1, B_1), & (b_2, B_2), & \cdots, & (b_q, B_q) \end{array} \right. \right) \\ = H_{p-1, q-1}^{m-1, n} \left(z \left| \begin{array}{ccc} (a_1, A_1), & \cdots, & (a_{p-1}, A_{p-1}) \\ (b_2, B_2), & \cdots, & (b_q, B_q) \end{array} \right. \right). \end{aligned} \quad (\text{A.2})$$

Property 4.

$$H_{p,q}^{m,n} \left(z \left| \begin{array}{c} (a_j, A_j)_{j=1, \dots, p} \\ (b_j, B_j)_{j=1, \dots, q} \end{array} \right. \right) = H_{q,p}^{n,m} \left(\frac{1}{z} \left| \begin{array}{c} (1 - b_j, B_j)_{j=1, \dots, q} \\ (1 - a_j, A_j)_{j=1, \dots, p} \end{array} \right. \right). \quad (\text{A.3})$$

Property 5. For $k > 0$,

$$\frac{1}{k} H_{p,q}^{m,n} \left(z \left| \begin{array}{c} (a_j, A_j)_{j=1, \dots, p} \\ (b_j, B_j)_{j=1, \dots, q} \end{array} \right. \right) = H_{p,q}^{m,n} \left(z^k \left| \begin{array}{c} (a_j, kA_j)_{j=1, \dots, p} \\ (b_j, kB_j)_{j=1, \dots, q} \end{array} \right. \right). \quad (\text{A.4})$$

Property 6.

$$z^\rho H_{p,q}^{m,n} \left(z \left| \begin{array}{c} (a_j, A_j)_{j=1, \dots, p} \\ (b_j, B_j)_{j=1, \dots, q} \end{array} \right. \right) = H_{p,q}^{m,n} \left(z \left| \begin{array}{c} (a_j + \rho A_j, A_j)_{j=1, \dots, p} \\ (b_j + \rho B_j, B_j)_{j=1, \dots, q} \end{array} \right. \right). \quad (\text{A.5})$$

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