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M. B., Flegg and P. K., Pollett (2007) First passage time density for the ehrenfest model.

Applied Probability Trust (February 26, 2007)

FIRST PASSAGE TIME DENSITY FOR THE EHRENFEST MODEL

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Abstract

We derive an explicit expression for the probability density of the first passage time to state 0 for the Ehrenfest diffusion model in continuous time.

Keywords: Urn models; hitting times.

AMS 2000 SUBJECT CLASSIFICATION: PRIMARY 60J27
SECONDARY 60K40

1. Introduction

The Ehrenfest model was introduced by Paul and Tatyana Ehrenfest [7] as a model for gas diffusion, to help explain why the entropy of a closed system must increase. Mathematical treatments were later given by Kac [12] and Feller [8], and since then the model has appeared in variety of contexts: where a closed system comprises units of two types and transmutation occurs from one to the other. The particular application that motivated the present work comes from the study of thermal fragmentation of aerosols [9, 10, 11]. Particles are suspended in a gas and weakly interacting (*dispersion forces*) molecules bond pairs of particles. For any given pair, there are K bonding sites. It is assumed, as part of the model, that fragmentation/evaporation of existing bonds occurs at rate μ for each bond and rebonding/condensation occurs at rate λ for each vacant site. We assume that μ and λ are both strictly positive. If $X(t)$ is the number of bonds at time t, then $(X(t),\, t \geq 0)$ is assumed to be a continuous-time Markov chain taking values in $S = \{0, 1, \ldots, K\}$ with transition rates $q_{n,n+1} = \lambda(K-n)$ and $q_{n,n-1} = \mu n$ for $n = 1, 2, \ldots, K$. However, in our model $q_{0n} = \delta_{0n}$, because once there are no bonds present, the two particles dissociate and rebonding does not occur. Thus, our model differs from the usual Ehrenfest model in that 0 is an absorbing state. We are interested in the time T it takes for the particles to dissociate starting with $X(0) = N$ bonds. T is therefore the first passage time to state 0 in the standard Ehrenfest model. We derive an explicit analytical expression for the probability density function of T.

If K were large, as it would be in the classical context, T would have an approximate exponential distribution (see for example [14]), but in the aerosols application K is usually small ($K \lesssim 10$), and thus it is useful to have an explicit expression. This would also be true in other modelling contexts, for example in animal population networks (metapopulations),

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where the state is the number of occupied habitat patches and the "per-capita" upward and downward rates are the rates of colonisation and local extinction; here the total number of patches would be moderate.

The theory of hitting times is well developed (see the books of Syski [17] and Kemperman [15]), but there are few explicit formulae available for specific models. Exceptions to this are in the recent work of Di Crescenzo and colleagues [3, 4, 5, 16, 6], where special structure in a wide range of continuous-time models has been exploited. The property of "central symmetry" exploited in [5, 6] would, in the present context, require $\lambda = \mu$, and thus is far too restrictive for our purposes. Di Crescenzo studied the Ehrenfest model with $\lambda = \mu$ and K even in Section 4.1 of [5], and obtained an explicit expression for the probability density of the first passage time to the "symmetry state" $K/2$ starting from any state N.

Comprehensive early treatments of the Ehrenfest model in continuous-time were given by Karlin and McGregor [13] and Bellman and Harris [2]. In Section 4 of [13] an expression is given for the transition probabilities $P_{ij}(t) = \Pr(X(t) = j|X(0) = i)$, both in terms of generating functions and explicitly in terms Krawtchouk (orthogonal) polynomials. It is therefore not surprising that the first passage time density can be evaluated explicitly, because its Laplace transform is the ratio of the Laplace transforms of $P_{i0}(t)$ and $P_{00}(t)$. However, we will find it convenient to work directly from the Kolmogorov forward equations.

2. First passage time denisty

For the Ehrenfest model with absorption at 0 the forward equations are

$$\frac{dP_0}{dt} = \mu P_1 \qquad \frac{dP_1}{dt} = -(\lambda(K-1)+\mu)P_1 + 2\mu P_2$$
$$\frac{dP_i}{dt} = \lambda(K-(i-1))P_{i-1} - (\lambda(K-i)+\mu i)P_i + \mu(i+1)P_{i+1} \quad (i = 2, \dots, K-1)$$
$$\frac{dP_K}{dt} = \lambda P_{K-1} - \mu K P_K.$$

with $P_0(0) = \delta_{N0}$, where $P_i(t) = P_{Ni}(t)$. In terms of the probability generating function $H(z,t) = \sum_{i=0}^{K} P_i(t) z^i$, they are summarised by the partial differential equation

$$\frac{\partial H}{\partial t} + (\lambda z + \mu)(z-1)\frac{\partial H}{\partial z} - \lambda K(z-1)H = -\lambda K(z-1)P_0(t),$$

with the boundary conditions $H(0,t) = P_0(t)$, $H(1,t) = 1$ and $H(z,0) = z^N$. In order to make the boundary conditions homogeneous, it will be convenient to work in terms of $G = H + 1$:

$$\frac{\partial G}{\partial t} + (\lambda z + \mu)(z-1)\frac{\partial G}{\partial z} - \lambda K(z-1)G = -\lambda K(z-1)Q(t), \tag{1}$$

where $Q(t) = P_0(t) - 1$, with $G(0,t) = Q(t)$, $G(1,t) = 0$ and $G(z,0) = z^N - 1$. Our immediate aim is to evaluate $Q(t)$ and thus determine $P_0(t) = \Pr(T \le t|X(0) = N)$.

By considering the homogeneous form of (1), a separation of variables argument suggests that we should look for a solution of the form

$$G(z,t) = \sum_{i=1}^{K} A_i(t)\,(\lambda z + \mu)^{K-i}\,(z-1)^i, \tag{2}$$

for suitable functions $(A_i(t))$ that do not depend on z. Notice that G given by (2) satisfies the boundary condition $G(1,t) = 0$. On substituting (2) into (1) we obtain

$$\sum_{i=1}^{K} \left(A_i'(t) + (\lambda+\mu) i A_i(t)\right)(\lambda z + \mu)^{K-i}\,(z-1)^i = -\lambda K\,(z-1)\,Q(t).$$

Thus, if we can find constants (C_i) such that $\sum_{i=1}^{K} C_i\,(\lambda z + \mu)^{K-i}\,(z-1)^i = -\lambda K\,(z-1)$, then it is clear that (A_i) will satisfy

$$A_i'(t) + i\,(\lambda+\mu)\,A_i(t) = C_i Q(t) \qquad (i = 1, 2, \ldots, K). \tag{3}$$

The following lemma shows that this is possible, and at the same time establishes the existence of functions $(A_i(t))$ satisfying (2).

Lemma 1. *Let $K \geq 1$, and let f be a polynomial with real coefficients that satisfies $f(1) = 0$ and has degree no greater than K. Then, $\forall\ a, b > 0$, $\exists$ uniquely, constants (B_i) such that*

$$f(z) = \sum_{i=1}^{K} B_i\,(az+b)^{K-i}\,(z-1)^i. \tag{4}$$

They are given by $B_i = g_i(1)$, where

$$g_i(z) = \frac{1}{i!}\,\frac{d^{i-1}}{dz^{i-1}}\,(az+b)^{i-K}\left(\frac{d}{dz} - \frac{aK}{az+b}\right) f(z). \tag{5}$$

Proof. First observe that

$$(az+b)^{i-K}\left(\frac{d}{dz} - \frac{aK}{az+b}\right) f(z) = \sum_{j=1}^{K} B_j (a+b) j (az+b)^{i-j-1} (z-1)^{j-1}.$$

Then, by Leibniz Theorem,

$$\begin{aligned} g_i(z) &= \frac{1}{i!}\,\frac{d^{i-1}}{dz^{i-1}}(az+b)^{i-K}\left(\frac{d}{dz} - \frac{aK}{az+b}\right) f(z) \\ &= \sum_{k=0}^{i-1}\sum_{j=1}^{K} B_j \frac{j}{i!}(a+b)\binom{i-1}{k}\frac{d^{i-k-1}}{dz^{i-k-1}}(az+b)^{i-j-1}\frac{d^k}{dz^k}(z-1)^{j-1}. \end{aligned}$$

Now, since for $j \geq 1$, $(d^k/dz^k)(z-1)^{j-1}\big|_{z=1} = (j-1)!\delta_{k,j-1}$, we get

$$g_i(1) = \sum_{j=1}^{i} B_j \frac{j!}{i!}(a+b)\binom{i-1}{j-1}\frac{d^{i-j}}{dz^{i-j}}(az+b)^{i-j-1}\Bigg|_{z=1} = B_i,$$

because $(d^{i-j}/dz^{i-j})\,(az+b)^{i-j-1}\big|_{z=1} = (a+b)^{-1}\delta_{ij}$. □

Indeed we can evaluate (C_i) explicitly. Putting $a=\lambda$ and $b=\mu$, setting $f(z)=-\lambda K\,(z-1)$, and evaluating the derivatives in (5), we find that

$$C_i=-\lambda K\binom{K-1}{i-1}\frac{(-\lambda)^{i-1}}{(\lambda+\mu)^{K-1}}\qquad(i=1,\dots,K).\tag{6}$$

(This can be established more simply by direct substitution in the right-hand side of (4).)

Next, we take Laplace transforms in (3), writing $\widetilde{F}(s)$ for the Laplace transform of $F(t)$. We find that $s\widetilde{A}_i(s)-A_i(0)+i\,(\lambda+\mu)\,\widetilde{A}_i(s)=C_i\widetilde{Q}(s)$, and hence that

$$\widetilde{A}_i(s)=\frac{C_i\widetilde{Q}(s)+A_i(0)}{s+i\,(\lambda+\mu)}.$$

Since we require $G(0,t)=Q(t)$, (2) yields $\widetilde{Q}(s)=\sum_{i=1}^{K}\widetilde{A}_i(s)\mu^{K-i}(-1)^i$. Therefore,

$$\widetilde{Q}(s)=\left(1-\sum_{i=1}^{K}\frac{C_i(-1)^i\mu^{K-i}}{s+i\,(\lambda+\mu)}\right)^{-1}\sum_{i=1}^{K}\frac{A_i(0)(-1)^i\mu^{K-i}}{s+i\,(\lambda+\mu)}.\tag{7}$$

The condition $G(z,0)=z^N-1$ entails $z^N-1=\sum_{i=1}^{K}A_i(0)\,(\lambda z+\mu)^{K-i}\,(z-1)^i$, and so the constants $(A_j(0))$ can be determined from Lemma 1. Putting $a=\lambda$ and $b=\mu$ and setting $f(z)=z^N-1$, we find that

$$A_i(0)=\sum_{j=1}^{\min\{i,N\}}\binom{N}{j}\binom{K-j}{i-j}\frac{(-\lambda)^{i-j}}{(\lambda+\mu)^{K-j}}\qquad(i=1,\dots,K).\tag{8}$$

We therefore have an explicit expression for $\widetilde{Q}(s)$, and it remains for us to invert the Laplace transform. The change of variable $s\to s/(\lambda+\mu)$ makes the calculations more manageable. If $\widetilde{R}(s)=(\lambda+\mu)\widetilde{Q}((\lambda+\mu)s)$, then $\widetilde{R}(s)$ will be the Laplace transform of $R(t)=Q(t/(\lambda+\mu))$.

Set $\rho=\mu/(\lambda+\mu)$ and $\alpha=\lambda/\mu$. Then, on substituting (6) and (8) into (7) we find that $\widetilde{R}(s)=\sum_{i=1}^{K}a_iU_i(s)$, where

$$a_i=\rho^K\alpha^i\sum_{j=1}^{\min\{i,N\}}\binom{N}{j}\binom{K-j}{i-j}(-1)^j(1-\rho)^{-j}$$

and

$$U_i(s)=\frac{1}{(s+i)\left(1-\rho^K\sum_{j=1}^{K}\binom{K}{j}\alpha^j\left(\frac{j}{s+j}\right)\right)}.$$

Notice that there is no singularity in $U_i(s)$ at $s=-i$. But, we shall prove that $U_i(s)$ has precisely K (first-order) singularities, $r_1,\dots,r_K$, which satisfy $r_i\in(-i,-i+1)$ $(i=1,2,\dots,K)$. Observe that

$$1-\rho^K\sum_{j=1}^{K}\binom{K}{j}\alpha^j\left(\frac{j}{s+j}\right)=\rho^K\sum_{j=0}^{K}\binom{K}{j}\alpha^j\left(\frac{s}{s+j}\right)=\frac{\phi(s)}{\prod_{k=1}^{K}(s+k)},$$

where

$$\phi(s) = \rho^K \sum_{j=0}^{K} \binom{K}{j} \alpha^j \prod_{\substack{k=0\\k\neq j}}^{K} (s+k)$$

is a degree K polynomial. Its K zeros, $r_1, \ldots, r_K$, are distinct and satisfy $r_i \in (-i, -i+1)$ because $\phi(-j) = K!\rho^K(-\alpha)^j$ $(j = 0, 1, \ldots, K)$ are $K+1$ distinct values of ϕ that alternate in sign, and, since the leading term of $\phi(s)$ is s^K, we may write $\phi(s) = \prod_{m=1}^{K}(s - r_m)$. Therefore, $U_i(s) = V_i(s)/\prod_{m=1}^{K}(s - r_m)$, where $V_i(s) = \prod_{k=1,\,k\neq i}^{K}(s+k)$ is a degree $K-1$ polynomial that does not vanish at any of $r_1, \ldots, r_K$ (and hence $r_1, \ldots, r_K$ are all the singularities of $U_i(s)$). Using partial fractions we get

$$U_i(s) = \sum_{m=1}^{K} \left(\frac{1}{s - r_m}\right) \frac{V_i(r_m)}{\prod_{k\neq m}(r_m - r_k)},$$

and so the inversion of $\widetilde{R}(s)$ is straightforward:

$$R(t) = \sum_{m=1}^{K} e^{r_m t} \sum_{i=1}^{K} a_i \frac{V_i(r_m)}{\prod_{k\neq m}(r_m - r_k)} = \sum_{m=1}^{K} e^{r_m t} \frac{1}{\prod_{k\neq m}(r_m - r_k)} \sum_{i=1}^{K} a_i \prod_{k\neq i}(r_m + k).$$

(Both products are over $k = 1, 2, \ldots, K$.) Finally, since $R(t) = Q((\lambda+\mu)t)$, we obtain

$$P_0(t) = 1 + Q(t) = 1 + \sum_{m=1}^{K} e^{r_m(\lambda+\mu)t} \frac{1}{\prod_{k\neq m}(r_m - r_k)} \sum_{i=1}^{K} a_i \prod_{k\neq i}(r_m + k).$$

On substituting for a_i, putting $s_i = -r_i$ to have $s_i > 0\ \forall\ i$, and differentiating with respect to t, we arrive at our main result.

Theorem 1. *The probability density function f of the first passage time to 0 starting in N is given by*

$$f(t) = \sum_{m=1}^{K} \frac{s_m(\lambda+\mu)e^{-s_m(\lambda+\mu)t}}{\prod_{k\neq m}(s_k - s_m)} \sum_{i=1}^{K} \rho^{K-i} \prod_{k\neq i}(k - s_m) \sum_{j=1}^{\min\{i,N\}} \binom{N}{j}\binom{K-j}{i-j}(-1)^{j-1}(1-\rho)^{i-j},$$

where $\rho = \mu/(\lambda+\mu)$ and $s_1, \ldots, s_K$ are the roots of

$$\sum_{j=0}^{K} \binom{K}{j} \left(\frac{\lambda}{\mu}\right)^j \prod_{\substack{k=0\\k\neq j}}^{K} (s-k) = 0,$$

arranged so that $s_m \in (m-1, m)$ $(m = 1, 2, \ldots, K)$.

Remarks (1) Notice that in the limit as $\lambda \to 0$, $r_m \to m$ and $P_0(t) \to (1 - e^{-\mu t})^N$. By reworking our arguments, this can be obtained as an exact result, $P_0(t) = (1 - e^{-\mu t})^N$, when

$\lambda = 0$. It is obviously true because when $\lambda = 0$ the N bonds fragment independently at the same rate μ, each bond lasting for an exponentially distributed amount of time, and thus T is the maximum of these times.

(2) From more elementary considerations (see for example Section 8.1 of [1]), the expected first-passage time from N to 0 is

$$\mathbb{E}(T) = \sum_{n=1}^{N} \frac{1}{\mu_n \pi_n} \sum_{m=n}^{K} \pi_m,$$

where $\mu_n = \mu n$ and $\pi_n = \binom{K}{n}(1-\rho)^n \rho^{K-n}$ $(n = 0, 1, \ldots, K)$, which leads to the explicit expression

$$\mathbb{E}(T) = \frac{1}{\mu} \sum_{j=1}^{N} \sum_{i=j}^{K} \binom{K-j}{i-j} \binom{i}{j}^{-1} \left(\frac{\lambda}{\mu}\right)^{i-j}.$$

This can be shown to be consistent with Theorem 1 by evaluating $\mathbb{E}(T)$ either as $\int_0^\infty Q(t)dt$ or as $-\widetilde{Q}(0)$.

Acknowledgements

The work of Phil Pollett is supported by the Australian Research Council Centre of Excellence for Mathematics and Statistics of Complex Systems.

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