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Stationary distributions in the atom-on-demand problem

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Abstract

In this note a probability model for the number of atoms in a magneto-optical trap is suggested. We study an ergodic Markov chain for the number of atoms in the trap under a feedback regime for different load distributions. Formulas for the stationary distribution of the process are derived in several cases. They can be used to adjust the loading rate of atoms to maximize the probability of a single atom in the trap. Approximate optimal regimes are found.

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Keywords: Binomial distribution; Geometric distribution; Geometric ergodicity; Poisson distribution; Stationary distribution

1. Introduction

The ability to control individual atoms is crucial in quantum information processing (quantum computational schemes) and nanotechnology (control over dopants and the atom-by-atom construction). Atom-on-demand technology represents a fundamental step towards this goal. Bettermann et al. (1996) have suggested a birth–death process model in continuous time for an uncontrolled number of atoms present in a magneto-optical trap (MOT), while Hill and McClelland (2003) employed a deterministic model by suppressing random nature of load and loss processes.

In this paper we suggest and study a stochastic recursive model for the number of atoms in a MOT, designed to isolate single atoms. According to this model, X_n, the number of atoms in the trap at step n, is a Markov chain. Under mild conditions we prove its geometric ergodicity. For several pairs of load and loss distributions the probability of isolating exactly one atom in the stationary regime is determined. To attain the highest likelihood of a single atom in the trap, this probability is to be maximized, and approximately optimal parameters for that are found. For uniform loss we prove the existence of a stationary distribution and determine it for general load. Similar results are obtained for geometric load. Assuming that the load distribution has a finite second moment, the stationary distribution for the binomial loss is derived.

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2. The atom-on-demand Markov chain model

Because of physical limitations, the number of atoms in the MOT cannot be monitored continuously, the trap can only be checked every T seconds. During that period more than one atom can get inside the trap before the door is closed. Let R_n be a random variable representing the load (number of atoms entering the trap at step n), and let X_n be the number of atoms in the MOT at step n. Denote by Y_n the random loss (the number of atoms which escaped the trap between steps $n-1$ and n).

A simple recursive model for the number X_n of atoms present in the MOT at step n under a feedback regime is

$$X_n = \begin{cases} R_n & \text{if } X_{n-1} \leqslant Y_{n-1}, \\ X_{n-1} - Y_{n-1} & \text{if } X_{n-1} > Y_{n-1}, \end{cases} \tag{2.1}$$

with independent R_n and (X_i, Y_i), $1 \leqslant i \leqslant n-1$. At step $n-1$ there is a random number X_{n-1} atoms in the MOT. With Y_{n-1} atoms removed, $(X_{n-1} - Y_{n-1})_+$ atoms are left in the MOT. If this number is zero, the load is applied and X_n is determined by this load; otherwise, no atoms are added to the MOT, and $X_n = X_{n-1} - Y_{n-1}$. Clearly, X_n, $n = 1, 2, \ldots$ forms a countable state Markov chain in discrete time. One cannot observe the number of atoms in the trap, but an empty MOT is recognized. The chain is run until it reaches the stationary regime. It is of interest to study the steady-state distribution and to determine the parameters which maximize π_1, the probability of having exactly one atom under this distribution.

2.1. *A sufficient condition for the stationary distribution*

The transition probabilities of the Markov chain X_n are

$$\begin{aligned} P(y|x) &= P(X_n = y | X_{n-1} = x) \\ &= P(X_n = y, Y_{n-1} \geqslant x | X_{n-1} = x) + P(X_{n-1} - Y_{n-1} = y, Y_{n-1} < x | X_{n-1} = x) \\ &= P(R_n = y) P(Y_{n-1} \geqslant x | X_{n-1} = x) + P(Y_{n-1} = x - y | X_{n-1} = x) \mathbf{1}_{\{1 \leqslant y \leqslant x\}} \\ &= r(y) \cdot \sum_{k=x}^{\infty} f(k|x) + f(x-y|x) \mathbf{1}_{\{1 \leqslant y \leqslant x\}}. \end{aligned} \tag{2.2}$$

For a fixed $X_n = x$, denote by $f(\cdot|x)$ the discrete density of the conditional distribution of Y_n. It is assumed that it does not depend on n and $f(0|x) < 1$ (with a positive probability at least one atom is lost). Clearly $f(y|x) = 0$ for $y > x$, so that (2.2) can be rewritten as

$$P(y|x) = r(y) f(x|x) + f(x-y|x) \mathbf{1}_{\{1 \leqslant y \leqslant x\}}. \tag{2.3}$$

Here $0 < r(k) = P(R_n = k) < 1$ assuming that the probability of loading no atoms or at least one atom are both positive. Note that if for $k \geqslant x$ one has $f(x|k) > 0$, and if the support of R_n is of the form $\{0, 1, \ldots, M\}$ possibly with $M = \infty$, then the chain is irreducible.

Assuming that a stationary distribution with $\pi_0 > 0$ exists, define for $n \geqslant 1$,

$$v_n = \frac{\pi_n}{\pi_0}.$$

Then $v = (v_1, v_2, \ldots) \in l_1$, since $\sum_{i \geqslant 1} v_i = \|v\|_1 = (1 - \pi_0)/\pi_0$. Clearly π can be recovered from v,

$$\pi_0 = \frac{1}{1 + \|v\|_1}, \quad \pi_n = \frac{v_n}{1 + \|v\|_1}, \quad n = 1, 2, \ldots . \tag{2.4}$$

One has

$$P(x|0) = r(0) \cdot f(x|x) = r(0) d_x,$$

where $d_0 = 1$, and

$$\sum_{n=0}^{\infty} \pi_n P(n|0) = r(0) \sum_{n=0}^{\infty} \pi_n d_n = \pi_0, \tag{2.5}$$

so that with the superscript T denoting the transpose,

$$\sum_{k \geqslant 1} d_k v_k = v^{\mathrm{T}} d = \frac{1}{r(0)} - 1.$$

Also $P(y|0) = r(y)$.

The reduced transition probabilities matrix P formed by elements $\{P(y|x), x \geqslant 1, y \geqslant 1\}$ can be written in the form

$$P = B + d\tilde{r}^{\mathrm{T}}, \tag{2.6}$$

where $\tilde{r} = (r(1), r(2), \ldots)^{\mathrm{T}}$ and

$$B = \begin{pmatrix} f(0|1) & 0 & 0 & \ldots \\ f(1|2) & f(0|2) & 0 & \ldots \\ f(2|3) & f(1|3) & f(0|3) & \ldots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

From the stationarity of π we get $v^{\mathrm{T}} P = v^{\mathrm{T}} - \tilde{r}^{\mathrm{T}}$, and (2.6) implies that

$$v^{\mathrm{T}} P = v^{\mathrm{T}} B + v^{\mathrm{T}} d\tilde{r}^{\mathrm{T}} = v^{\mathrm{T}} B + \left(\frac{1}{r(0)} - 1\right)\tilde{r}^{\mathrm{T}}.$$

Thus with $C = B^{\mathrm{T}}$,

$$(I - C)v = \frac{1}{r(0)}\,\tilde{r}. \tag{2.7}$$

Under general conditions, $\pi_0 > 0$ (for example if $f(x|\,x) > 0$ for all x). If (2.7) has a unique solution in l_1, then by Theorem 6.9 in Kemeny et al. (1976, p. 135) the Markov chain with the transition probabilities (2.3) is ergodic.

Assuming that the Markov chain X_n is irreducible, one can prove its geometric ergodicity under general conditions using a result from Nummelin (1984, p. 90). These conditions hold in all cases considered in Section 3, and then the nth step transition probability $P^n(x, A)$ tends uniformly to the stationary limit $\pi(A)$ with a common geometric rate over any $A \subset \{0, 1, \ldots\}$.

Theorem 1. *If* $\limsup_{x\to\infty} f(0|x) < 1$ *and* $E(\beta^R) < \infty$ *for some* $\beta > 1$, *then* $\{X_n\}$ *is geometrically ergodic, i.e. for some* c *and* $\rho < 1$

$$|P^n(x|y) - \pi_x| \leqslant c\rho^n, \quad n = 1, 2, \ldots \,. \tag{2.8}$$

Proof. We show that for some $0 < \zeta < 1$, $b > 0$ and a finite set of states F

$$\sum_y P(x|y)\beta^y \leqslant \zeta\beta^x + b\mathbf{1}_F(x). \tag{2.9}$$

Using (2.3), one gets

$$\begin{aligned}\sum_y P(x|y)\beta^y &= \sum_y [f(x|x)r(y) + f(x-y|x)\mathbf{1}_{[y,\infty)}(x)]\beta^y \\ &= \left(\sum_y \beta^y r(y)\right) f(x|x) + \beta^x \sum_{1\leqslant y\leqslant x} \beta^{y-x} f(x-y|x) \\ &\leqslant E(\beta^R)P(Y_n = x|X_n = x) + \beta^x E(\beta^{-Y_n}|X_n = x) \\ &= \beta^x[\beta^{-x}E(\beta^R)P(Y_n = x|X_n = x) + E(\beta^{-Y_n}|X_n = x)].\end{aligned}$$

For any ζ, $1-(1-\beta^{-1})[1-\limsup_{x\to\infty} f(0|x)] < \zeta < 1$, so that there is an x_ζ such that for $x > x_\zeta$,

$$\beta^{-x}E(\beta^R)P(Y_n = x|X_n = x) + E(\beta^{-Y_n}|X_n = x) < \zeta,$$

and the conclusion easily follows with $F = \{0, 1, \ldots, x_\zeta\}$. □

A result in Meyn and Tweedie (1994) can be used to relate the convergence rate in (2.8) to the parameters used in the drift inequality (2.9).

3. Two approaches

We give two approaches for solving (2.7). The first consists in directly solving (2.7) and is exemplified by the uniform loss and a general load or by the geometric load and a general loss distribution. The second approach uses an expansion of $(I-C)^{-1}$ and is illustrated by a binomial loss and a general load.

3.1. Uniform loss

In the uniform loss case, $f(y|x) = 1/(x+1)$, $y = 0, \ldots, x$ and (2.7) has a unique solution in l_1 since the homogeneous equation obtained by replacing the right-hand side by 0 has a unique solution in l_1, namely the null solution. Indeed,

$$nv_n - (n+1)v_{n+1} = 0,$$

so that $v_n = (1/n)v_1$, which corresponds to an element in l_1 if and only if $v_1 = 0$, i.e. $v = 0$.

Next, we solve (2.7) in l_1. One has

$$nv_n - (n+1)v_{n+1} = (n+1)(r_n - r_{n+1})/r_0$$

and

$$v_1 - nv_n = (2r_1 + r_2 + \cdots + r_{n-1} - nr_n)/r_0.$$

Since $v, r \in l_1$, one has $v_1 = (1 - r_0 + r_1)/r_0$. Therefore,

$$v_n = \frac{1 - r_0 - r_1 - \cdots - r_{n-1} + nr_n}{nr_0} \geqslant 0 \tag{3.1}$$

and

$$v_1 = \frac{1 - r_0 + r_1}{r_0}, \ldots, v_{n+1} = \frac{n}{n+1} v_n - \frac{r_n - r_{n+1}}{r_0}. \tag{3.2}$$

Thus,

$$\|v\|_1 = \frac{1}{r_0} \sum_{n\geqslant 1} \left(1 + \sum_{i=1}^{n} \frac{1}{i}\right) r_n$$

and $v \in l_1$ if $E(\log R) < \infty$.

Introduce now g, the moment generating function of the stationary distribution, and m, the moment generating function of the load distribution. Notice from (2.7) that

$$\sum_{n\geqslant 1}\frac{1}{n+1}\,v_n=v_1-\frac{r_1}{r_0}.$$

According to (2.4), $\sum_{n\geqslant 0}\pi_n(n+1)^{-1}=\pi_0/r_0$, so that

$$E\left(\frac{1}{X+1}\right)=\frac{\pi_0}{r_0}.$$

We have

$$E(\mathrm{e}^{tX_{n+1}}|X_n)=\frac{m(t)}{X_n+1}+\sum_{k=1}^{X_n}\frac{\mathrm{e}^{tk}}{X_n+1}=\frac{1}{X_n+1}\left[m(t)-\frac{\mathrm{e}^t}{\mathrm{e}^t-1}\right]+\frac{\mathrm{e}^{t(X_n+1)}}{X_n+1}.$$

Therefore, for the stationary distribution

$$E\mathrm{e}^{tX}=h(t)+E\left(\frac{1}{X+1}\,\mathrm{e}^{t(X+1)}\right),$$

where

$$h(t)=\frac{\pi_0}{r_0}\left[m(t)-\frac{\mathrm{e}^t}{\mathrm{e}^t-1}\right].$$

Differentiating with respect to t gives a linear differential equation for g,

$$g'(t)=h'(t)+\mathrm{e}^t g(t),$$

with the solution

$$g(t)=1+\int_0^t h'(z)\mathrm{e}^{-\mathrm{e}^z}\,\mathrm{d}z\cdot\mathrm{e}^{\mathrm{e}^t}=1+\frac{\pi_0}{r_0}\int_0^t\left[m'(z)-\frac{\mathrm{e}^z}{(\mathrm{e}^z-1)^2}\right]\mathrm{e}^{-\mathrm{e}^z}\,\mathrm{d}z\cdot\mathrm{e}^{\mathrm{e}^t}.$$

The expected value of the number of atoms in the trap under stationary regime can be derived either from the moment generating function or directly as above,

$$E(X_{n+1}|X_n)=\frac{ER}{X_n+1}+\sum_{k=1}^{X_n}\frac{k}{X_n+1},$$

which gives

$$EX=\frac{2\pi_0 ER}{r_0}.$$

Further moments of this distribution can be found using the same argument. For example,

$$EX^2=\frac{\pi_0}{2r_0}[3ER^2+ER].$$

3.2. Poisson load and uniform loss

When the load R is Poisson(λ), exact formulas for the stationary distribution can be obtained. Rewrite (3.1) as

$$v_n=\frac{1}{n}\,\mathrm{e}^{\lambda}P(R\geqslant n)+\frac{\lambda^n}{n!}=\frac{1}{n}\mathrm{e}^{\lambda}\int_0^1\frac{t^{n-1}\mathrm{e}^{-\lambda t}\lambda^n}{(n-1)!}\,\mathrm{d}t+\frac{\lambda^n}{n!},$$

so that

$$\|v\|_1 = \sum_{n\geqslant 1}\left(\mathrm{e}^{\lambda}\int_0^1 \frac{t^{n-1}\mathrm{e}^{-\lambda t}\lambda^n}{n!}\,\mathrm{d}t + \frac{\lambda^n}{n!}\right)$$

$$= \mathrm{e}^{\lambda}\int_0^1 \frac{\mathrm{e}^{-\lambda t}}{t}\sum_{n\geqslant 1}\frac{(\lambda t)^n}{n!}\,\mathrm{d}t + \mathrm{e}^{\lambda} - 1 = \mathrm{e}^{\lambda}\int_0^1 \frac{1-\mathrm{e}^{-\lambda t}}{t}\,\mathrm{d}t + \mathrm{e}^{\lambda} - 1.$$

Note that

$$\int_0^1 \frac{1-\mathrm{e}^{-\lambda t}}{t}\,\mathrm{d}t = \gamma + \ln(\lambda) + \mathrm{Ei}(1,\lambda),$$

where $\mathrm{Ei}(\cdot,\cdot)$ is the exponential integral function. Substituting in (2.4), we obtain exact formulas for the stationary probabilities. For example,

$$\pi_1 = \frac{v_1}{1+\|v\|_1} = \frac{1-\mathrm{e}^{-\lambda}+\lambda\mathrm{e}^{-\lambda}}{\int_0^1((1-\mathrm{e}^{-\lambda t})/t)\,\mathrm{d}t + 1}. \tag{3.3}$$

The probability of exactly one atom in the trap, π_1 is maximized when $\hat{\lambda} = 1.027767647$. One has

$$EX = \frac{2\lambda}{\int_0^1((1-\mathrm{e}^{\lambda t})/t)\,\mathrm{d}t + 1},$$

$$EX^2 = \frac{3\lambda^2 + 4\lambda}{2(\int_0^1((1-\mathrm{e}^{\lambda t})/t)\,\mathrm{d}t + 1)},$$

and one can prove by induction that $EX^k \sim \lambda^k$. According to the Carleman Theorem (Shohat and Tamarkin, 1943), these moments uniquely determine the distribution of X.

3.3. Binomial loss

Suppose the loss distribution is binomial(X_n, p), $0<p<1$, and the load distribution has the finite second moment. We denote $D = \mathrm{diag}(1,2,\ldots)$.

Eq. (2.7) can be rewritten as

$$(I - DCD^{-1})u = l, \tag{3.4}$$

with $u = Dv$ and $l = D\tilde{r}/r(0)$. The upper triangular matrix $G = DCD^{-1}$ is given by elements

$$g_{ij} = \frac{i(j-1)!}{i!(j-i)!}\,p^{j-i}(1-p)^i,$$

for $j \geqslant i \geqslant 1$. We have

$$\sum_{i\geqslant 1} g_{ij} = \sum_{i=1}^{j} \frac{(j-1)!}{(i-1)!(j-i)!}\,p^{j-i}(1-p)^i = 1-p$$

and

$$\sum_{j\geqslant 1} g_{ij} = \sum_{j\geqslant i} \frac{(j-1)!}{(i-1)!(j-i)!}\,p^{j-i}(1-p)^i = 1.$$

Using a theorem by Schur (Halmos, 1982, Problem 37 with $p_i \equiv 1$), we see that the operator defined by the matrix G has norm in $\mathbb{L}_2$ less than $\sqrt{1-p}<1$ (as $g_{11} = 1-p$, $\|G\|_2 \geqslant 1-p$). Therefore, $I-G$ is invertible in $\mathbb{L}_2$ and the solution of (3.4) is

$$u = \sum_{k\geqslant 0} G^k l. \tag{3.5}$$

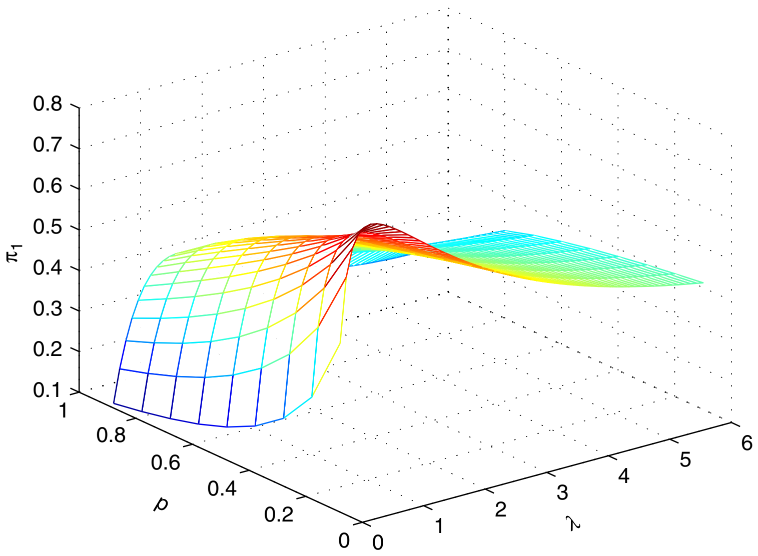

Fig. 1. The stationary probability π_1 for Poisson(λ) load and binomial(p) loss.

Since $l \in l_2$, Dv is in l_2 and by the Cauchy–Schwartz inequality, $v \in l_1$. Denote by α_{ij} the elements of $(I-G)^{-1}$, and put $\alpha_j = \sum_{k \leqslant j} \alpha_{kj}/k$. Notice that $\alpha_{11} = \alpha_1 = 1/p$.

One can prove the recurrence formulas,

$$\alpha_{ij} = \delta_{ij} + \sum_{k=i}^{j} \alpha_{ik} g_{kj}, \quad \alpha_j = \frac{1}{j} + \sum_{k=1}^{j} \alpha_k g_{kj},$$

which show that $\alpha_j \leqslant \alpha_1$ and

$$\alpha_{1j} \leqslant \frac{\alpha_{11}}{j} = \frac{1}{jp}.$$

Substituting (3.5) into (2.4), we get

$$\pi_1 = \frac{\sum_{j=1}^{\infty} j\alpha_{1j} r(j)}{r(0) + \sum_{j=1}^{\infty} j\alpha_j r(j)}. \tag{3.6}$$

Fig. 1 shows the stationary probability π_1 for Poisson(λ) load and binomial(p) loss. Define the truncation π_1^n of π_1 as

$$\pi_1^n = \frac{\sum_{j=1}^{n} j\alpha_{1j} r(j)}{r(0) + \sum_{j=1}^{n} j\alpha_j r(j)}.$$

Using the upper bound for α_{1j} and α_j, one obtains

$$|\pi_1 - \pi_1^n| \leqslant \frac{1}{p} \sum_{k=n}^{\infty} r(k) + \frac{1-r(0)}{p^2} \sum_{k=n}^{\infty} kr(k) \tag{3.7}$$

and

$$\lim_{n\to\infty} |\pi_1 - \pi_1^n| = 0.$$

Given a margin of error ε, (3.7) can be used to obtain a level of truncation n_ε for which $|\pi_1 - \pi_1^n| < \varepsilon$ for any $n \geqslant n_\varepsilon$. For Poisson($\lambda$) load, the upper bound in (3.7) takes the form, $e^{-\lambda}(p + \lambda - \lambda e^{-\lambda})\gamma(\lambda, n-1)p^{-2}$ where γ is the incomplete gamma function.

A formula similar to (3.6) holds for Poisson loss and Poisson load distributions.

3.4. Geometric loss

Assume that for a fixed $X_n = x$, the loss distribution is that of $\min[Z, x]$, where Z is a geometric random variable, $P(Z = k) = p(1-p)^k \; k = 0, 1, \ldots$.

In this case, the inverse of $I - C$ in (2.7) takes a simple form,

$$(I-C)^{-1} = \begin{pmatrix} \frac{1}{1-p} & \frac{p}{1-p} & \frac{p}{1-p} & \cdots \\ 0 & \frac{1}{1-p} & \frac{p}{1-p} & \cdots \\ 0 & 0 & \frac{1}{1-p} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

so that

$$v_n = \frac{1}{r_0(1-p)}\left[r_n + p\sum_{k\geqslant n+1} r_k\right].$$

Therefore,

$$\|v\|_1 = \frac{(1-p)(1-r_0) + pER}{r_0(1-p)}.$$

The stationary distribution is

$$\pi_n = \frac{r_n + p\sum_{k\geqslant n} r_k}{1-p+pER}. \tag{3.8}$$

In particular,

$$\pi_1 = \frac{r_1 + p(1-r_0-r_1)}{1+p(ER-1)}, \tag{3.9}$$

which is an increasing function in p if

$$1 - r_0 \geqslant r_1 ER. \tag{3.10}$$

Thus $p \uparrow 1$ is optimal, regardless of the load distribution satisfying (3.10). This condition holds for the Poisson(λ) load. It is straightforward to check that for $\lambda \approx 0$, $\pi_1 \approx 1$.

Using (3.8), the expected value for the stationary distribution can be evaluated for general load

$$EX = \frac{(p+2)ER + pER^2}{2+2p[ER-1]}.$$

3.5. Geometric load

Let the load be geometric(p) and the loss Y_n, given $X_n = x$, is $\min[Y, x]$ with distribution of Y independent of n. Then the matrix $I - C$ has the form

$$\begin{pmatrix} 1-f(0) & -f(1) & -f(2) & \cdots \\ 0 & 1-f(0) & -f(1) & \cdots \\ 0 & 0 & 1-f(0) & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

The inverse $(I-C)^{-1}=h_{ij}$ is an upper triangular matrix with $h_{ii}=(1-f(0))^{-1}$, for $0\leqslant i<k, h_{i,i+k}=c(k)$, where $c(k)$ is the first row of H. As in the uniform loss case, since the homogeneous version of (2.7) only has the null solution, (2.7) has a unique solution v in l_1.

Employing the Laplace transforms of the sequences $f(i)$ and $c(k)$, we obtain $(1-\mathscr{L}_f(s))\mathscr{L}_c(s)=1$, so that

$$\mathscr{L}_c(s)=\frac{1}{1-\mathscr{L}_f(s)}.$$

Note that the solution for (2.7) is given by

$$v_k=\sum_{i\geqslant 0} c_i\tilde{r}_{i+k}, \quad k\geqslant 1.$$

If the load is geometric(p), then

$$v_k=\sum_{i\geqslant 0} c_i(1-p)^{i+k}=(1-p)^k\mathscr{L}_c(1-p)=\frac{(1-p)^k}{1-\mathscr{L}_f(1-p)}$$

and $\|v\|_1=(1-p)/[p(1-\mathscr{L}_f(1-p))]$. Substituting in (2.4), one derives exact formulas for the stationary probabilities,

$$\pi_k=\frac{p(1-p)^k}{1-p\mathscr{L}_f(1-p)}, \quad k\geqslant 1. \tag{3.11}$$

4. Conclusions

The table below with rows corresponding to combinations of loss and load distributions gives formulas for π_1 and the optimal parameter values (when available).

Load	Loss	π_1	Optimal parameter(s)
General	Geometric(p)	(3.9)	
Geometric(p)	General	(3.11)	
Geometric(q)	Geometric(p)	(3.9)	$p,q\sim 1$
Poisson(λ)	Geometric(p)	(3.9)	$\lambda\sim 0,\ p\sim 1$
Poisson(λ)	Uniform	(3.3)	$\lambda=1.027767647$
Poisson(λ)	Poisson(μ)	(3.6)	$\lambda,\mu\sim 0,\mu/\lambda\sim 0$
Poisson(λ)	Binomial(p)	(3.6)	same as above

Additional information about Poisson load entries in the table can be found in Rukhin and Bebu (2006).

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