The Multiple-Urn Ehrenfest Model

A Look into Eigenanalysis and Hitting Times

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Willamette Mathematics Consortium REU

July 30, 2016

What will we cover today?

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(1) Markov chains

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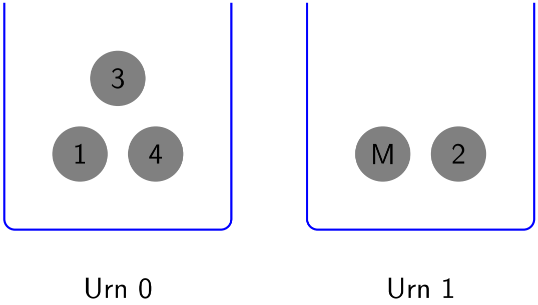
(6) Summary

The Ehrenfest urn model example



What is a Markov chain?

A **Markov chain** is a sequence of random variables $X_0, X_1, X_2, ...$ such that $\Pr[X_{n+1} = s_{n+1} \mid X_0 = s_0, X_1 = s_1, ..., X_n = s_n] = \Pr[X_{n+1} = s_{n+1} \mid X_n = s_n]$ where $s_0, s_1, ..., s_n, s_{n+1}$ are elements in the state space of the Markov chain.

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Let X_n denote the number of balls in Urn 1 at time $n = 0, 1, 2....$ Then $(X_0, X_1, ...)$ forms a Markov chain with the state space $S = \{0, 1, ..., M\}$.

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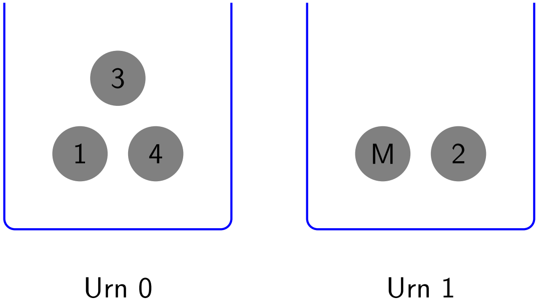

Transition matrix

A $k \times k$ matrix $\mathbb{P}$ is said to be a **transition matrix** of a Markov chain $(X_0, X_1, ...)$ with state space $S = \{s_1, ..., s_k\}$ if

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For the Ehrenfest urn model with M=5 balls, the transition matrix is:

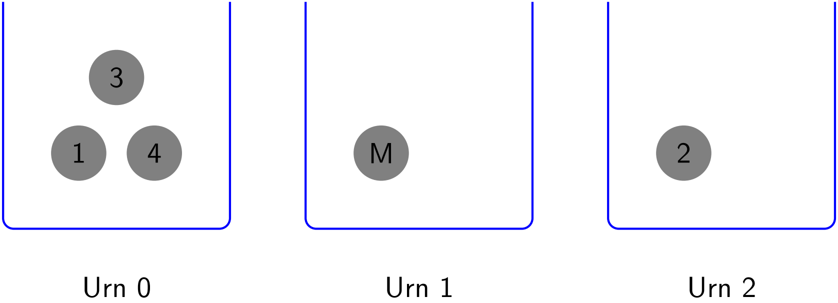
$$\begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \begin{array}{c} \begin{array}{cccccc} 0 & 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1/5 & 0 & 4/5 & 0 & 0 & 0 \\ 0 & 2/5 & 0 & 3/5 & 0 & 0 \\ 0 & 0 & 3/5 & 0 & 2/5 & 0 \\ 0 & 0 & 0 & 4/5 & 0 & 1/5 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \end{array}$$

Stationary distribution

Let $(X_0, X_1, ...)$ be a Markov chain with state space $S = \{s_1, ..., s_k\}$ and transition matrix $\mathbb{P}$. A row vector $\boldsymbol{\pi}$=$(\pi_1, ..., \pi_k)$ is said to be a **stationary distribution** for the Markov chain, if it satisfies

(i)$\pi_i \geq 0$ for $i = 1, ..., k$, and $\sum_{i=1}^{k} \pi_i = 1$, and
(ii)$\boldsymbol{\pi}\mathbb{P}$=$\boldsymbol{\pi}$, meaning that $\sum_{i=1}^{k} \pi_i \mathbb{P}_{i,j} = \pi_j$ for $j = 1, ..., k$.

The 3-urn Ehrenfest model



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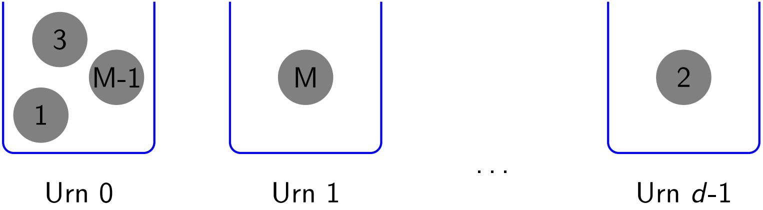

Motivation for studying the multiple-urn Ehrenfest model

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For example, a finite Markov chain converges to a stationary distribution if and only if its transition matrix has eigenvalue 1 with multiplicity 1 and all other eigenvalues are of modulus less than 1.

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That is, we can find an invertible matrix $\mathbb{A}$ such that

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This helps us compute $\mathbb{P}^n$:

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Our observation:
For the 3-urn model with M balls, the transition matrix has $(M + 1)$ distinct eigenvalues equally distanced between 1 and $\frac{-1}{2}$, and the kth largest eigenvalue has multiplicity k.

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Our observation:
For the 3-urn model with M balls, the transition matrix has $(M+1)$ distinct eigenvalues equally distanced between 1 and $\frac{-1}{2}$, and the kth largest eigenvalue has multiplicity k. Let $\alpha = \frac{3}{2M}$. Then the eigenvalues are given by

$$1, (1-\alpha)_2, (1-2\alpha)_3, ..., \left(\frac{-1}{2}\right)_{M+1}.$$

Mark Kac's results

In 1947, mathematician Mark Kac examined the Ehrenfest urn model with 2 urns and found that the eigenvectors and eigenvalues of the transition matrix are determined by a system of linear equations using the generating function

$$f(z) = \sum_{k=0}^{\infty} x_k z^k$$

where x_k is the kth component of the eigenvector $\mathbf{x}$.

Mark Kac's results

Using Kac's function as a model, we define the following polynomial to generate the row eigenvectors for the 3-urn model:

$$f^M(z_1, z_2) = \sum_{s_1=0}^{M} \sum_{s_2=0}^{M-s_1} a_{(s_1,s_2)} z_1^{s_1} z_2^{s_2}$$

where $a_{(s_1,s_2)}$ is the (s_1, s_2)th component of the eigenvector $\mathbf{a}$ from the transition matrix $\mathbb{P}$.

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Derived partial differential equation

Using the fact that $\mathbf{a}\mathbb{P} = \lambda\mathbf{a}$ for any eigenvector $\mathbf{a}$ with eigenvalue λ, we are able to substitute in our transition probabilities, multiply each term by $z_1^{s_1} z_2^{s_2}$, and sum over all of s_1 and s_2.

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After collecting like terms and simplifying, we obtain the partial differential equation

$$(1 - z_1)(1 + z_1 + z_2)\frac{\partial f^M}{\partial z_1} + (1 - z_2)(1 + z_1 + z_2)\frac{\partial f^M}{\partial z_2} + M(z_1 + z_2 - 2\lambda)f^M(z_1, z_2) = 0.$$

Generating function and eigenvalues for $d = 3$ urns

Theorem

The coefficients of the functions

$$f^M_{(r_1,r_2)}(z_1, z_2) = (1 - z_1)^{r_1}(1 - z_2)^{r_2}(1 + z_1 + z_2)^{r_3},$$

where r_1, r_2, *and* r_3 *are nonnegative integers and* $r_1 + r_2 + r_3 = M$, *define a set of linearly independent eigenvectors of the 3-urn M-ball transition matrix.*

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Corollary

The eigenvalues of the 3-urn M-ball transition matrix are $\lambda = \frac{3}{2M} r_3 - \frac{1}{2}$ for $r_3 \in \{0, \cdots, M\}$. Eigenvalue λ has multiplicity $\frac{2M}{3}(1 - \lambda) + 1$.

Example: The row eigenvector matrix $\mathbb{A}$ for $M = 3$ balls

Consider the function $f^{3}_{(r_1,r_2)}(z_1, z_2) = (1 - z_1)^{r_1}(1 - z_2)^{r_2}(1 + z_1 + z_2)^{r_3}$.
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$$\begin{aligned} f^3_{(1,0)}(z_1, z_2) &= (1 - z_1)(1 + z_1 + z_2)^2 \\ &= 1 + z_1 + 2z_2 - z_1^2 + 0z_1z_2 + z_2^2 - z_1^3 - 2z_1^2z_2 - z_1z_2^2 + 0z_2^3 \end{aligned}$$

and

$$\begin{aligned} f^3_{(0,1)}(z_1, z_2) &= (1 - z_2)(1 + z_1 + z_2)^2 \\ &= 1 + 2z_1 + z_2 + z_1^2 + 0z_1z_2 - z_2^2 + 0z_1^3 - z_1^2z_2 - 2z_1z_2^2 - z_2^3. \end{aligned}$$

The row eigenvectors corresponding to each of these polynomials are

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Example: The row eigenvector matrix $\mathbb{A}$ for $M = 3$ balls

So for $f^3_{(r_1,r_2)}(z_1, z_2)$, we have the row eigenvector matrix

	1	z_1	z_2	z_1^2	$z_1 z_2$	z_2^2	z_1^3	$z_1^2 z_2$	$z_1 z_2^2$	z_2^3
$(0,0)$	1	3	3	3	6	3	1	3	3	1
$(1,0)$	1	1	2	−1	0	1	−1	−2	−1	0
$(0,1)$	1	2	1	1	0	−1	0	−1	−2	−1
$(2,0)$	1	−1	1	−1	−2	0	1	1	0	0
$(1,1)$	1	0	0	−1	−1	−1	0	1	1	0
$(0,2)$	1	1	−1	0	−2	−1	0	0	1	1
$(3,0)$	1	−3	0	3	0	0	−1	0	0	0
$(2,1)$	1	−2	−1	1	2	0	0	−1	0	0
$(1,2)$	1	−1	−2	0	2	1	0	0	−1	0
$(0,3)$	1	0	−3	0	0	3	0	0	0	−1

$= \mathbb{A}$.

Generating function and eigenvalues for d urns

Theorem

The coefficients of the functions

$$f_{\mathbf{r}}^M(\mathbf{z}) = \left(\prod_{k=1}^{d-1}(1 - z_k)^{r_k}\right)\left(1 + \sum_{k=1}^{d-1} z_k\right)^{r_d},$$

where all the components of $\mathbf{r}$ *are nonnegative integers and* $\sum_{k=1}^{d} r_k = M$, *define a set of linearly independent eigenvectors of the* M*-ball* d*-urn transition matrix.*

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Corollary

The eigenvalues of the d*-urn* M*-ball transition matrix are* $\lambda = \frac{d}{M(d-1)} r_d - \frac{1}{d-1}$ *for* $r_d \in \{0, \cdots, M\}$*. Eigenvalue* λ *has multiplicity* $\binom{\frac{M(d-1)}{d}(1-\lambda)+d-2}{d-2}$.

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$d = 3$, $M = 1$:

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 0 \\ 1 & 0 & -1 \end{bmatrix}^{-1} = \frac{1}{3}\begin{bmatrix} 1 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{bmatrix}$$

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Finding the inverse matrix $\mathbb{A}^{-1}$ for $d = 3$ urns

This pattern suggests that the rows of the inverse matrix $\mathbb{A}^{-1}$ are generated by

$$\tilde{f}^M_{(s_1,s_2)}(z_1, z_2) = \frac{1}{3^M}(1 - 2z_1 + z_2)^{s_1}(1 + z_1 - 2z_2)^{s_2}(1 + z_1 + z_2)^{s_3},$$

where s_1, s_2, s_3 are nonnegative integers such that $s_1 + s_2 + s_3 = M$. s_1, s_2, s_3 are the same as the r_1, r_2, r_3 used to generate the corresponding row of the original eigenvector matrix $\mathbb{A}$.

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This function is also a valid solution to our partial differential equation.

The d-urn inverse matrix

Theorem

The rows of the matrix $\mathbb{A}^{-1}$ are the coefficients of

$$\tilde{f}_{\mathbf{s}}^{M}(\mathbf{z}) = \frac{1}{d^M}\left(\prod_{k=1}^{d-1}(1-(d-1)z_k+\sum_{i\neq k} z_i)^{s_k}\right)\left(1+\sum_{k=1}^{d-1} z_k\right)^{M-\sum_{k=1}^{d-1} s_k},$$

where the row corresponding to the vector $\mathbf{s}$ *in* $\tilde{f}_{\mathbf{s}}^{M}(\mathbf{z})$ *is in the same position as the row corresponding to* $\mathbf{r}$ *in* $f_{\mathbf{r}}^{M}(\mathbf{z})$.

Proof: $\tilde{f}_{\mathbf{s}}^{M}(\mathbf{z})$ generates $\mathbb{A}^{-1}$

To prove that $\tilde{f}_{\mathbf{s}}^{M}(\mathbf{z})$ generates $\mathbb{A}^{-1}$, let the coefficients of $f_{\mathbf{r}}^{M}(\mathbf{z})$ and $\tilde{f}_{\mathbf{s}}^{M}(\mathbf{z})$ be $a_{\mathbf{r},\mathbf{s}}^{(M)}$ and $\frac{1}{d^M} b_{\mathbf{s},\mathbf{t}}^{(M)}$, respectively, so that $\frac{1}{d^M}\mathbb{B}$ is the matrix generated by $\tilde{f}_{\mathbf{s}}^{M}(\mathbf{z})$.

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It is sufficient to prove that:

$$\frac{1}{d^M}\sum_{\mathbf{s}} a_{\mathbf{r},\mathbf{s}}^{(M)} b_{\mathbf{s},\mathbf{t}}^{(M)} = \begin{cases} 1 & \text{if } \mathbf{r} = \mathbf{t}, \\ 0 & \text{otherwise.} \end{cases}$$

This condition can be proved by induction on M.

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Using diagonalization, we can compute the n-step transition matrix $\mathbb{P}^n$ more efficiently. Assuming $d << M$,

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		Steps		
		100	200	400
Balls	10	0.637	0.786	0.806
	20	26.861	29.771	34.201

(Ordinary matrix multiplication)

		Steps		
		100	200	400
Balls	10	0.215	0.229	0.234
	20	9.017	9.453	9.655

(Diagonalization)

Mixing times

Mixing times

The **total variation distance** between a probability distribution $\mathbf{p}$ and the stationary distribution $\boldsymbol{\pi}$ is given by

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$$d_{TV}(\mathbf{p}, \boldsymbol{\pi}) = \frac{1}{2} \sum_i |p_i - \pi_i|.$$

The **mixing time** of a Markov chain is the minimum number of steps it takes for the total variation distance to be less than a given ϵ:

$$t_{mix}(\epsilon) = min\{n : d_{TV}(\mathbb{P}^n, \boldsymbol{\pi}) \leq \epsilon\}$$

Mixing time bounds

We can bound the mixing time of the Ehrenfest urn model as follows:

$$ln(\frac{1}{2\epsilon})(\frac{1}{1-\lambda_*} - 1) \leq t_{mix}(\epsilon) \leq -ln(\epsilon \boldsymbol{\pi}_{min})(\frac{1}{1-\lambda_*})$$

where

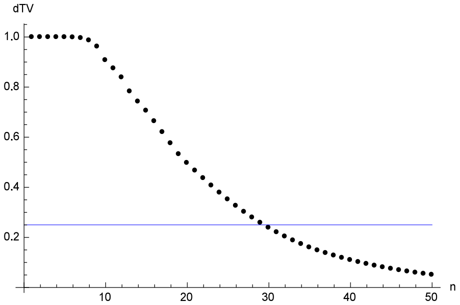
$$\lambda_* = 1 - \frac{d}{(d-1)M}$$

is the second-largest eigenvalue of $\mathbb{P}$ and

$$\boldsymbol{\pi}_{min} = \frac{1}{d^M}.$$

Mixing times: example

Consider $d = 3$ urns, $M = 20$ balls, $\epsilon = 0.25$. If we start with all the balls in one urn, $t_{mix} = 30$.



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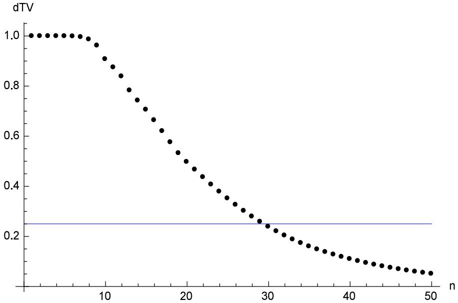

The bounds on the mixing time are approximately

$$8 \le t_{mix} \le 312.$$

Mixing times for the multiple-urn Ehrenfest model

Using the eigenanalysis, we can precisely quantify the mixing times for the multiple urn Ehrenfest model.

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Beginning with all balls in an urn, and with the choice of $\epsilon = 0.25$, we have

M	$t_{\text{mix}}(\epsilon)$	$d_{TV}(\mathbb{P}^n, \boldsymbol{\pi})$
5	5	0.2305
10	13	0.2177
20	30	0.239
40	70	0.2407
80	158	0.2476

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When $M = 80$, the dimensions of the transition matrix $\mathbb{P}$ are $\binom{82}{2} \times \binom{82}{2}$, or 3321×3321. Even equipped with the eigenanalysis, it took R more than 5 hours to compute the total variation distance.

Hitting times

For a Markov chain X_n, $n \geq 0$, the **hitting time** (or *first passage time*) from state $\mathbf{r}$ to state $\mathbf{s}$ is the minimum number of steps the chain takes to reach state $\mathbf{s}$ for the first time when the chain initially starts at state $\mathbf{r}$. The expected value of such a hitting time is denoted by $\mathbb{E}_r\left[T_s\right]$, where

$$T_{\mathbf{s}} = min\{n \geq 0 : X_n = \mathbf{s}, X_i \neq \mathbf{s}, \text{for all } i < n\}.$$

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(1) How long does it take to empty a full urn?

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(3) How long does it take to transfer all balls in a full urn to an empty urn?

Computing expected hitting times

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$$\mathbb{E}_{\mathbf{r}}\left[T_{\mathbf{s}}\right] \quad = \quad \mathbb{E}[T_{\mathbf{s}} \,|\, X_0 = \mathbf{r}]$$

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$$\begin{aligned} \mathbb{E}_{\mathbf{r}}\left[T_{\mathbf{s}}\right] &= \mathbb{E}[T_{\mathbf{s}} \,|\, X_0 = \mathbf{r}] \\ &= 1 + \sum_{\mathbf{k}} \mathbb{E}[T_{\mathbf{s}} \,|\, X_1 = \mathbf{k}] \times \mathbb{P}_{\mathbf{r},\mathbf{k}} \end{aligned}$$

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If we label $\tau_{\mathbf{r},\mathbf{s}} = \mathbb{E}_{\mathbf{r}}\left[T_{\mathbf{s}}\right]$, it amounts to solve the linear system

$$\tau_{\mathbf{r},\mathbf{s}} = 1 + \sum_{\mathbf{k}} \tau_{\mathbf{k},\mathbf{s}} \times \mathbb{P}_{\mathbf{r},\mathbf{k}},$$

and the number of unknowns $\tau_{\mathbf{r},\mathbf{s}}$ equals the square of the size of the state space of the Markov chain.

Emptying a full urn, our method

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$$T_k = \begin{cases} 1 & \text{with probability } \frac{M-k}{M}, \\ 1 + T'_k & \text{with probability } \frac{k(d-2)}{M(d-1)}, \\ 1 + T_{k-1} + T'_k & \text{with probability } \frac{k}{M(d-1)}, \end{cases}$$

where T'_k is a random variable with the same distribution as T_k.

Emptying a full urn

We find that

$$\mathbb{E}[T_k] = \frac{1}{\binom{M-1}{k}} \sum_{j=0}^{k} \frac{\binom{M}{j}}{(d-1)^{k-j}}$$

Emptying a full urn

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Filling an empty urn

Redefining T_k as the time to have $k+1$ balls in an urn initially containing k balls,

$$\mathbb{E}[T_k] = \frac{d-1}{\binom{M-1}{k}} \sum_{j=0}^{k} \binom{M}{j} (d-1)^{k-j}.$$

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Using the same method, we find that the expected time to fill a specific empty urn is

$$\mathbb{E}_{empty}\left[T_{full}\right] = M(d-1) \sum_{k=0}^{M-1} \frac{d^k}{k+1}.$$

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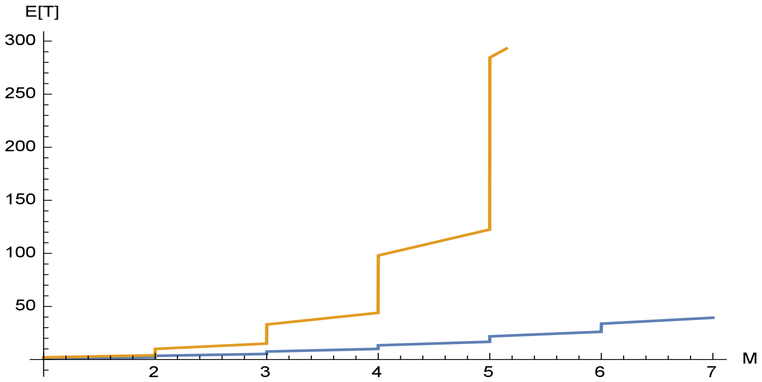
Starting with a full urn, the time to fill any of the other urns is

$$\mathbb{E}_{full_1}\left[T_{full_{any}}\right] = M \sum_{k=0}^{M-1} \frac{d^k}{k+1}.$$

Hitting time graphical representation



blue: time to empty a specific urn
orange: time to fill a specific urn

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(4) Solved for general formulae for hitting times for various scenarios of the Ehrenfest urn model.

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