Decay towards the overall-healthy state in SIS epidemics on networks

Piet Van Mieghem*

Delft University of Technology

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Abstract

The decay rate of SIS epidemics on the complete graph K_N is computed analytically, based on a new, algebraic method to compute the second largest eigenvalue of a stochastic three-diagonal matrix up to arbitrary precision. The latter problem has been addressed around 1950, mainly via the theory of orthogonal polynomials and probability theory. The accurate determination of the second largest eigenvalue, also called the *decay parameter*, has been an outstanding problem appearing in general birth-death processes and random walks. Application of our general framework to SIS epidemics shows that the maximum average lifetime of an SIS epidemics in any network with N nodes is not larger (but tight for K_N) than

$$E[T] \sim \frac{1}{\delta} \frac{\frac{\tau}{\tau_c}\sqrt{2\pi}}{\left(\frac{\tau}{\tau_c}-1\right)^2} \frac{\exp\left(N\left\{\log\frac{\tau}{\tau_c}+\frac{\tau_c}{\tau}-1\right\}\right)}{\sqrt{N}} = O\left(e^{N\ln\frac{\tau}{\tau_c}}\right)$$

for large N and for an effective infection rate $\tau = \frac{\beta}{\delta}$ above the epidemic threshold τ_c. Our order estimate of $E[T]$ sharpens the order estimate $E[T] = O\left(e^{bN^a}\right)$ of Draief and Massoulié [6]. Combining the lower bound results of Mountford *et al.* [14] and our upper bound, we conclude that for almost all graphs, the average time to absorption for $\tau > \tau_c$ is $E[T] = O\left(e^{c_G N}\right)$, where $c_G > 0$ depends on the topological structure of the graph G and τ.

1 Introduction

We consider a simple dynamic process, a Susceptible-Infected-Susceptible (SIS) epidemic, on an undirected and unweighted graph G with N nodes and L links, that can be represented by a $N \times N$ symmetric adjacency matrix A. In a SIS epidemic process, the viral state of a node i at time t is specified by a Bernoulli random variable $X_i(t) \in \{0,1\}$: $X_i(t) = 0$ for a healthy, but susceptible node and $X_i(t) = 1$ for an infected node. A node i at time t can be in one of the two states: *infected*, with probability $v_i(t) = \Pr[X_i(t) = 1]$ or *healthy*, with probability $1 - v_i(t)$, but susceptible to the infection. We assume that the curing process per node i is a Poisson process with rate δ and that the

*Faculty of Electrical Engineering, Mathematics and Computer Science, P.O Box 5031, 2600 GA Delft, The Netherlands; *email*: P.F.A.VanMieghem@tudelft.nl

infection rate per link is a Poisson process with rate β. Obviously, only when a node is infected, it can infect its direct neighbors, that are still healthy. Both the curing and infection Poisson process are independent. The effective infection rate is defined by $\tau = \frac{\beta}{\delta}$. This is the general continuous-time description of the simplest type of a SIS epidemic process on a network. This SIS process with curing rate $\delta = 1$ is sometimes also called the contact process.

Kermack and McKendrick [11], whose work is nicely reviewed in [4], have already demonstrated in 1927 that epidemics generally, thus also the SIS process in particular, possess "threshold behavior". For effective infection rates below the epidemic threshold, $\tau < \tau_c$, the SIS-infection on networks dies out exponentially fast [23], while for $\tau > \tau_c$, the infection becomes endemic, which means that a non-zero fraction of the nodes remains infected for a very long time. The precise definition (for finite N) and the computation of the SIS epidemic threshold is still an active field of research [15], though a sharp lower bound exists for any graph, $\tau_c \geq \frac{1}{\lambda_1}$, where λ_1 is the largest eigenvalue of the adjacency matrix of the network [23].

Besides the epidemic threshold, the Markovian SIS process also possesses an important second property: an absorbing state equal to the overall-healthy state in which the virus has been eradicated from the network. Draief and Massoullié [6] prove that the time T for the SIS Markov process to hit the absorbing state when the effective infection rate $\tau < \tau_c$ is, on average, not larger than $E[T] \leq \frac{\log N+1}{\delta-\beta\lambda_1}$. On the other hand, when $\tau > \tau_c$, they show that the average time to absorption grows for large N as

$$E[T] = O\left(e^{bN^a}\right) \tag{1}$$

for some constants $a, b > 0$. Hence, the average "lifetime" of the epidemic below and above the epidemic phase transition are hugely different, which is a general characteristic of a phase transition. Mountford *et al.* [14] proved that, above the epidemic threshold in trees with bounded degree, i.e. the maximum degree $d_{\max} < a$, where a is finite, but $d_{\max} \geq 2$ (thus excluding e.g. the star), $E[T] = O(e^{cN})$ for large N and a real number $c > 0$. Moreover, improving a result of Chatterjee and Durrett [5], they show that for any $\tau > 0$ and large N, the time to absorption or extinction on a power law graph grows exponentially in N.

Fill [8] gave a nice stochastic interpretation of the time T to absorption in a continuous-time birth and death process with an absorbing state zero and N other states, described by the infinitestimal generator Q. Given that the process starts in state N, then the absorption time T is equal to a sum of independent exponential random variables, whose rates are the nonzero eigenvalues of $-Q$. Miclo [13] has extended Fill's result to a finite Markov chain, which is irreducible and reversible outside the absorbing point. Very recently, Economou *et al.* [7] have analysed the SIS model with heterogeneous infection rates via a block matrix formalism. In their analysis, they gave the general expression for distribution of the absorption time T as $\Pr[T \leq t] = 1 - \left(x_0^T e^{Q^* t}\right)_{2^N-1}$, where x_0 is the column vector with the initial states and Q^* is the infinitesimal generator (see [7] for the labelling of states) in which the row and column corresponding to the absorbing state are removed. Artalejo [3] has shown that the time T_q to extinction from the quasi-stationary (or metastable) state obeys $\Pr[T_q \leq t] = 1 - e^{\zeta t}$, where $\zeta \leq 0$ is the second largest eigenvalue[1] of the infinitesimal generator Q.

[1] More precisely, the largest eigenvalue of the submatrix Q_S of Q associated to the transient and finte set S of states, that is assumed to be irreducible. When the latter condition of irreducibility is omitted, $\Pr[T_q \leq t]$ is still exponentially distributed [3, Theorem 1], but with a more complicated mean $E[T_q]$ than $\frac{1}{\zeta}$.

Here, we derive a sharper estimate than $E[T] = O\left(e^{bN^a}\right)$ for the longest possible mean absorption time in any graph, by computing the spectral decomposition of a tri-diagonal, stochastic matrix P in (9), which is presented in Appendix A. Invoking the Lagrange series on the characteristic polynomial of P, the second largest eigenvalue $1+\zeta$ (with $\zeta \leq 0$) of P is deduced in Appendix B. Generally, for the state vector $x[k]$ of a discrete-time Markov process at discrete-time k with a real second largest eigenvalue, it holds that any vector norm $||x[k]-\pi|| \sim (1+\zeta)^k + O\left(|1+z_3|^k\right)$, where π is the corresponding steady-state vector and z_3 is the third largest (in absolute value) eigenvalue of P. The number of infected nodes in a SIS epidemic process on the complete graph can be determined [21] via a birth and death process, the continuous-time variant of a general random walk, whose infinitesimal generator Q is a tri-diagonal matrix. As shown in Section 2, the second largest eigenvalue ζ of the infinitesimal generator Q can thus be interpreted as the decay rate of the SIS epidemics on the complete graph towards the overall-healthy state and, approximately, the average lifetime of an SIS epidemics is about $E[T] \simeq \frac{1}{|\zeta|}$. Now, given a fixed infection rate β and curing rate δ, among all networks with N nodes, the SIS infection spreads fastest in the complete graph K_N with N nodes, because each node can be infected by a maximum possible number of neighbors. Hence, the longest time T to hit the overall-healthy state and, equivalently, the minimum decay rate ζ among all graphs are attained in the complete graph K_N.

Our main result for SIS epidemics is the accurate expression of the decay rate ζ in K_N for effective infection rates $\tau > \tau_c$ and large N

$$-\zeta = \frac{1}{F(\tau)} + O\left(\frac{N^2 \log N}{x^{2N-1}}\right) \tag{2}$$

where $x = \tau N \simeq \frac{\tau}{\tau_c} > 1$ and where

$$F(\tau) = \frac{1}{\delta} \sum_{j=1}^{N} \sum_{r=0}^{j-1} \frac{(N-j+r)!}{j\,(N-j)!} \tau^r \tag{3}$$

The double sum in (3) is hard to compute for large N and, after surprisingly much effort as illustrated in Appendix C, we established in Theorem 6 the correct behavior[2] of

$$F\left(\frac{x}{N}\right) \sim \frac{1}{\delta} \frac{x\sqrt{2\pi}}{(x-1)^2} \frac{\exp\left(N\left\{\log x + \frac{1}{x} - 1\right\}\right)}{\sqrt{N}} \tag{4}$$

for large N and fixed $x = \tau N > 1$. Roughly, for x slightly above than 1, we deduce from the asymptotic expression (4) of $F(\tau)$ that $E[T] = O\left(e^{N \ln \frac{\tau}{\tau_c}}\right)$. The exponentially accurate order estimate (2) thus specifies the parameters $a = 1$ and $b = \ln \frac{\tau}{\tau_c}$ (or more correctly $b = \ln \frac{\tau}{\tau_c} + \frac{\tau_c}{\tau} - 1$) in the general estimate (1). Earlier in [22], we have derived the exact $2^N \times 2^N$ infinitesimal generator Q for an SIS process on any graph and have numerically computed the second smallest eigenvalue of Q for the complete graph. For small networks up to $N = 13$, fitting results suggested that $E[T] = O\left(e^{b(\tau)N^2}\right)$. Hence, the current analytic result $E[T] = O\left(e^{N \ln \frac{\tau}{\tau_c}}\right)$ shows that $a \leq 1$, in contrast to our earlier extrapolated order estimates that hinted at $a \leq 2$.

[2] In October 2017, we discovered accidently that the asymptotic expression (4) was established before by Andersson and Djehiche [2] in 1998. In particular, their Theorem 1A states that, for large N, the scaled random variable $\frac{T}{E[T]}$ tends to an exponential random variable with mean 1 and $E[T]$ is given by the right-hand side of (4). The exact form (3) of $E[T] = F(\tau)$ was not derived in [2].

The probabilistic interpretation of the absorption time T by Fill [8] leads us to conclude that $E[T] = F(\tau)$, for any value of the effective infection rate τ (and not, as above in (2), only for $\tau > \tau_c$). Thus, starting from the all-infected state, the *exact*[3] average absorption time T in the SIS process on the complete graph is given by $F(\tau)$ in (3). Moreover, as shown in Appendix B, the first term in the Lagrange series for the second largest eigenvalue ζ of an infinitesimal generator Q equals the inverse of the sum of the inverse (non-zero) eigenvalues of Q, which may suggest that, in general Markov chains with an absorbing state, $-\zeta = \frac{1}{E[T]} + r$, where r are higher order terms in the Lagrange series.

Finally, combining the lower bound results in [14] and the upper bound in (2), we conclude that for almost all graphs, the average time to absorption for $\tau > \tau_c$ is $E[T] = O\left(e^{c_G N}\right)$, where $c_G > 0$ depends on the topological structure of the graph G. The interesting open next question lies in the accurate determination of c_G for a given graph G, different from K_N.

2 Markovian $\varepsilon-$SIS epidemics

We first define the Markovian $\varepsilon-$SIS epidemics on networks. Besides an infection process with rate β per infected neighbor and a nodal curing process with rate δ as in the SIS model, each node contains a Poissonean self-infection process with rate ε. All three Poisson processes are independent. This ε-SIS epidemic process on the complete graph K_N is a birth and death process with birth rate $\lambda_j = (\beta j + \varepsilon)(N - j)$ and death rate $\mu_j = j\delta$, as shown in [21]. When the process $X(t)$ at time t is at state j, precisely j nodes in K_N are infected. For $\varepsilon > 0$, all rates are positive and the birth and death process is irreducible, i.e. without absorbing state. Thus, the theory developed in Appendix A is applicable when we substitute

$$p_j \to (\beta j + \varepsilon)(N - j)$$
$$q_j \to j\delta$$

In an irreducible, n states, continuous-time Markov process, the $1 \times n$ state vector $s(t)$, with component i equal to $s_i(t) = \Pr[X(t) = i]$, satisfies

$$s(t) = s(0)\, e^{Qt}$$

where the spectral decomposition of the $n \times n$ matrix (see e.g. [19]) is

$$e^{Qt} = u\pi + \sum_{j=2}^{n} e^{\mu_j t} x_j y_j^T$$

and x_j and y_j are the $n \times 1$ right- and left-eigenvector belonging to the i-th largest eigenvalue μ_j of Q. The right-eigenvector belonging to the largest eigenvalue $\mu_1 = 0$ of Q is $x_0 = u$, the all-one vector. We denote $\mu_2 = \zeta$. For large t, the tendency of $s(t)$ towards the steady-state vector π equals

$$s(t) - \pi \approx w e^{\zeta t}$$

where $s(0)\, u = 1$ and $w = s(0)\, x_2 y_2^T$ is not a function of the time t.

[3] The exact relation $E[T] = F(\tau)$ has been verified by using a hitting time analysis in [16].

In Appendix B, we demonstrate the general bound $\zeta < -\frac{f_0}{f_1}$, where f_k are the coefficients (24) of the characteristic polynomial of a tri-band matrix. Hence, the continuous-time Markov process specified by a tri-diagonal infinitesimal generator Q converges always faster to the steady-state than $O\left(\exp\left(-\frac{f_0}{f_1}t\right)\right)$. This means [21] for an $\varepsilon-$SIS-epidemic process on the complete graph that the epidemics tends to the SIS *metastable* state with a time constant faster than $T(\varepsilon) = \frac{f_1}{f_0}$ time units. In the limit $\varepsilon \to 0$, where the $\varepsilon-$SIS-epidemic process behaves as the classical SIS epidemics in which the steady-state is the overall healthy state (which is the absorbing state for the SIS Markov process), the decay rate of the epidemics towards this absorbing state is never slower than $\frac{1}{T(0)}$.

The remainder of this section consists of (a) the determination of the coefficients f_k for the ε-SIS epidemic process on the complete graph K_N (Section 2.1), (b) the limit form of the these coefficients for large N and (c) the three regimes, depending on whether $\tau \geq \tau_c$,$\tau \simeq \tau_c$ and $\tau < \tau_c$, of the resulting decay rate ζ in SIS epidemics ($\varepsilon \to 0$) for large N, in which our main result (2) is derived.

2.1 Coefficients f_0, f_1 and f_2 in $\varepsilon-$SIS epidemics

The inverse of the probability that no node in K_N is infected is [21]

$$f_0 = \frac{1}{\pi_0} = \sum_{k=0}^{N} \binom{N}{k} \tau^k \frac{\Gamma\left(\frac{\varepsilon^*}{\tau} + k\right)}{\Gamma\left(\frac{\varepsilon^*}{\tau}\right)} = 1 + \sum_{k=1}^{N} \binom{N}{k} \tau^k \frac{\Gamma\left(\frac{\varepsilon^*}{\tau} + k\right)}{\Gamma\left(\frac{\varepsilon^*}{\tau}\right)}$$

where $\varepsilon^* = \frac{\varepsilon}{\delta}$ and $\tau = \frac{\beta}{\delta}$. Since $\lim_{\varepsilon \to 0} \frac{1}{\Gamma\left(\frac{\varepsilon^*}{\tau}\right)} = 0$,

$$\lim_{\varepsilon \to 0} f_0 = 1$$

agreeing with the fact that the steady-state in Markovian SIS epidemics is equal to the overall-healthy state, which is the absorbing state zero. Using

$$\prod_{m=0}^{j-1} q_{m+1} = \prod_{m=0}^{j-1} (m+1)\,\delta = j!\delta^j$$

and

$$\prod_{m=0}^{j-1} p_m = \prod_{m=0}^{j-1} (\beta m + \varepsilon)(N - m) = \frac{N!\beta^j}{(N-j)!} \prod_{m=0}^{j-1} \left(m + \frac{\varepsilon}{\beta}\right) = \frac{N!\beta^j \Gamma\left(\frac{\varepsilon}{\beta} + j\right)}{(N-j)!\Gamma\left(\frac{\varepsilon}{\beta}\right)}$$

into the general expression (37) for f_1 yields

$$f_1 = \frac{1}{\delta} \sum_{j=1}^{N} \frac{\tau^{j-1}}{j} \sum_{r=0}^{j-1} \sum_{k=0}^{j-1-r} \frac{\binom{N-j+r}{r}\binom{N}{j-1-r-k}}{\binom{j-1}{r}} \frac{\Gamma\left(\frac{\varepsilon^*}{\tau} + j\right)\Gamma\left(\frac{\varepsilon^*}{\tau} + j - 1 - r - k\right)}{\Gamma\left(\frac{\varepsilon^*}{\tau} + j - r\right)\Gamma\left(\frac{\varepsilon^*}{\tau}\right)} \frac{1}{\tau^k}$$

and $\lim_{\varepsilon \to 0} f_1 = F(\tau)$, specified in (3).

From the definition (24),

$$f_2 = \frac{1}{q_1 q_2} + \sum_{j=3}^{N} \frac{c_2(j)}{\prod_{m=0}^{j-1} q_{m+1}}$$

where $c_2(j)$ follows from (33), we arrive at

$$
\begin{aligned}
f_2 = & \frac{1}{2\delta^2} + \frac{1}{\delta^2}\sum_{j=3}^{N}\frac{(N-2)!\tau^{j-2}\Gamma\left(\frac{\varepsilon^*}{\tau}+j\right)}{j!\,(N-j)!\Gamma\left(\frac{\varepsilon^*}{\tau}+2\right)} \\
& + \left(\frac{\tau(N-1)+\varepsilon^*(2N-1)+3}{2\delta^2}\right)\sum_{j=3}^{N}\sum_{k=3}^{j}\frac{(k-1)!\,(N-k)!\tau^{j-k}\Gamma\left(\frac{\varepsilon^*}{\tau}+j\right)}{j!\,(N-j)!\Gamma\left(\frac{\varepsilon^*}{\tau}+k\right)} \\
& + \frac{1}{\delta^2}\sum_{j=3}^{N}\sum_{k=3}^{j}\sum_{s=1}^{k-3}\sum_{l_1=0}^{k-s-1}\sum_{l_2=0}^{k-s-l_1-1}\frac{\Gamma\left(\frac{\varepsilon^*}{\tau}+k-s-1-l_1-l_2\right)\Gamma\left(\frac{\varepsilon^*}{\tau}+k-s\right)\Gamma\left(\frac{\varepsilon^*}{\tau}+j\right)}{\Gamma\left(\frac{\varepsilon^*}{\tau}+k-s-l_1\right)\Gamma\left(\frac{\varepsilon^*}{\tau}\right)\Gamma\left(\frac{\varepsilon^*}{\tau}+k\right)} \\
& \times \frac{N!\,(N-(k-s-l_1))!\,(N-k)!\,(k-s-1-l_1)!\,(k-1)!\tau^{j-1-s-l_2}}{j!\,(N-(k-s-1-l_1-l_2))!\,(N-(k-s))!\,(N-j)!\,(k-s-l_1-l_2-1)!\,(k-s)!}
\end{aligned}
$$

After some tedious calculations, we find that

$$
\begin{aligned}
\lim_{\varepsilon\to 0} f_2 = & \frac{1}{2\delta^2} + \frac{1}{\delta^2}\sum_{j=3}^{N}\frac{(N-2)!\tau^{j-2}}{j\,(N-j)!} + \left(\frac{\tau(N-1)+3}{2\delta^2}\right)\sum_{j=3}^{N}\sum_{k=3}^{j}\frac{(N-k)!\tau^{j-k}}{j\,(N-j)!} \\
& + \frac{1}{\delta^2}\sum_{j=3}^{N}\sum_{k=3}^{j}\sum_{s=1}^{k-3}\sum_{m=0}^{k-s-1}\frac{(N-(k-s-m))!\,(N-k)!\tau^{j-k+m}}{j\,(N-j)!\,(k-s)\,(N-(k-s))!}
\end{aligned} \tag{5}
$$

2.2 Asymptotics of f_0, f_1 and f_2 in $\varepsilon-$SIS epidemics for large N

For large N, $\lim_{\varepsilon\to 0} f_1$ in (3) behaves as

$$
\begin{aligned}
\lim_{\varepsilon\to 0} f_1 = F(\tau) &= \frac{1}{\delta}\sum_{j=1}^{N}\sum_{r=0}^{j-1}\frac{(N-j+r)!}{j\,(N-j)!}\tau^r \\
&\sim \frac{1}{\delta}\sum_{j=1}^{N}\frac{1}{j}\sum_{r=0}^{j-1}N^r\tau^r = \frac{1}{\delta}\sum_{j=1}^{N}\frac{1}{j}\frac{(N\tau)^j-1}{N\tau-1}
\end{aligned}
$$

where we have used [1, 6.1.47]

$$
\frac{\Gamma(N-a)}{\Gamma(N-b)} = N^{a-b}\left(1+\frac{(a-b)(a+b-1)}{2N}+O\left(N^{-2}\right)\right) \tag{6}
$$

to first order. The accurate asymptotic behavior of $F(\tau)$ is deduced in Appendix C.3. Hence, using $x = N\tau$, we find

$$
\delta\lim_{\varepsilon\to 0} f_1 = \frac{1+O\left(\frac{1}{N}\right)}{(x-1)}\sum_{j=1}^{N}\frac{x^j-1}{j} \tag{7}
$$

From (7), the three regimes for x lead to the following growth. If $N\tau = x < 1$, then

$$
\begin{aligned}
\delta\lim_{\varepsilon\to 0} f_1 &= \frac{1+O\left(\frac{1}{N}\right)}{(1-x)}\left(\sum_{j=1}^{N}\frac{1}{j}-\sum_{j=1}^{N}\frac{x^j}{j}\right) \\
&= \frac{1+O\left(\frac{1}{N}\right)}{(1-x)}\left(H_N+\log(1-x)\right) = O(\log N)
\end{aligned}
$$

If $x > 1$, then

$$\delta \lim_{\varepsilon \to 0} f_1 = \frac{1 + O\left(\frac{1}{N}\right)}{(x-1)} \sum_{j=1}^{N} \frac{x^j - 1}{j} = O\left(\frac{x^{N-1}}{N}\right)$$

whereas for $x = 1$

$$\delta \lim_{\varepsilon \to 0} f_1 = \left(1 + O\left(\frac{1}{N}\right)\right) \sum_{j=1}^{N} 1 = N\left(1 + O\left(\frac{1}{N}\right)\right) = O(N)$$

Invoking (6), the asymptotic expression of $\lim_{\varepsilon \to 0} f_2$ in (3) for large N is

$$\lim_{\varepsilon \to 0} f_2 \sim \frac{1}{2\delta^2} + \frac{1}{\delta^2} \sum_{j=3}^{N} \frac{(N\tau)^{j-2}}{j} + \left(\frac{\tau N + 3}{2\delta^2}\right) \sum_{j=3}^{N} \sum_{k=3}^{j} \frac{(N\tau)^{j-k}}{j} + \frac{1}{\delta^2} \sum_{j=3}^{N} \sum_{k=3}^{j} \sum_{s=1}^{k-3} \sum_{m=0}^{k-s-1} \frac{(N\tau)^{j-k+m}}{j(k-s)}$$

Using $x = N\tau$, we have

$$\delta^2 \lim_{\varepsilon \to 0} f_2 \sim \frac{1}{2} + \left(\frac{3x+1}{2(x-1)}\right) \sum_{j=3}^{N} \frac{x^{j-2}}{j} - \frac{x+3}{2(x-1)} \sum_{j=3}^{N} \frac{1}{j} + R_4$$

where

$$R_4 = \sum_{j=3}^{N} \sum_{k=3}^{j} \sum_{s=1}^{k-3} \sum_{m=0}^{k-s-1} \frac{x^{j-k+m}}{j(k-s)}$$

which can be simplified to

$$R_4 = \frac{1}{(x-1)^2} \sum_{j=3}^{N} \frac{x^j}{j} \sum_{m=3}^{j-1} \frac{1}{m} \left(1 - x^{m-j} - x^{-m} + x^{-j}\right)$$

After further rearrangement of terms in R_4, we arrive at

$$\begin{aligned}
\delta^2 \lim_{\varepsilon \to 0} f_2 \sim{}& \frac{1}{2} + \left(\frac{3x+1}{2(x-1)}\right) \sum_{j=3}^{N} \frac{x^{j-2}}{j} - \frac{x+3}{2(x-1)} \sum_{j=3}^{N} \frac{1}{j} \\
&+ \frac{1}{(x-1)^2} \sum_{j=3}^{N} \frac{x^j}{j} \left(\sum_{m=3}^{j-1} \frac{1}{m} - \sum_{m=j+1}^{N} \frac{1}{m}\right) + \frac{1}{2(x-1)^2} \left(\sum_{j=3}^{N} \frac{1}{j}\right)^2 \\
&- \frac{1}{(x-1)^2} \sum_{j=1}^{N-3} \frac{x^j}{j} \left(\sum_{m=3}^{3+j} \frac{1}{m} - \sum_{m=N+1-j}^{N} \frac{1}{m}\right)
\end{aligned}$$

If $x < 1$, then

$$\begin{aligned}
\delta^2 \lim_{\varepsilon \to 0} f_2 &\sim \frac{1}{2(x-1)^2} \left(\sum_{j=3}^{N} \frac{1}{j}\right)^2 - \frac{x+3}{2(x-1)} \sum_{j=3}^{N} \frac{1}{j} + O(1) \\
&= O\left(\log^2 N\right)
\end{aligned}$$

whereas for $x > 1$, collecting the largest power in x yields

$$\delta^2 \lim_{\varepsilon \to 0} f_2 \sim \frac{x^{N-2}}{N} \left(\frac{3}{2} + \sum_{m=3}^{N-1} \frac{1}{m}\right) = O\left(\frac{\log N}{N} x^{N-2}\right)$$

For $x = 1$, we can show that

$$\delta^2 \lim_{\varepsilon \to 0} f_2 \sim \frac{N^2}{4} - \frac{9}{4}N + 4 \sum_{j=1}^{N} \frac{1}{j} - 2 = O\left(N^2\right)$$

2.3 Scaling of ζ with N in SIS epidemics (when $\varepsilon \downarrow 0$)

In the limit for $\varepsilon \to 0$, the upper bound (36) for ζ becomes, with (3),

$$\zeta < -\frac{f_0}{f_1} = \frac{\delta}{\sum_{j=1}^{N} \frac{1}{j(N-j)!} \sum_{r=0}^{j-1} (N-j+r)!\tau^r} \tag{8}$$

Using the asymptotic expressions for $\lim_{\varepsilon\to 0} f_1 = 1$, $\lim_{\varepsilon\to 0} f_1$ and $\lim_{\varepsilon\to 0} f_2$, the second order Lagrange series (38) for ζ is

$$\zeta \approx -\frac{1}{f_1} - \frac{f_2}{f_1^3}$$

Thus, for $x = N\tau > 1$,

$$-\zeta \approx O\left(\frac{N}{x^{N-1}} + \frac{N^2 \log N}{x^{2N-1}}\right) = O\left(\frac{N}{x^{N-1}}\right)$$

illustrating that the first term in the Lagrange series is sufficient, leading to our main result (2). Numerical computations support this result. For $x < 1$,

$$-\zeta \approx O\left(\frac{1}{\log N} + \frac{\log^2 N}{\log^3 N}\right) = O\left(\frac{1}{\log N}\right)$$

Since now the first and second term are of equal order, both need to be taken into account. A second order Lagrange expansion is not sufficient and higher order terms need to be evaluated in order to guarantee accuracy of ζ. In view of the dramatic increase in the computations, we refrain from pursuing this track and content ourselves with numerical calculations. Finally, when $x = 1$, we have

$$-\zeta \approx O\left(\frac{1}{N} + \frac{N^2}{N^3}\right) = O\left(\frac{1}{N}\right)$$

leading to a similar conclusion as the case for $x < 1$. In fact, we can compute this zero a little more precise as

$$-\zeta \approx \left(1 + O\left(\frac{1}{N}\right)\right)\left(\frac{\delta}{N}\left(1 + \frac{\frac{N^2}{4} - \frac{9}{4}N + 4\sum_{j=1}^{N}\frac{1}{j} - 2}{N^2}\right)\right) = \frac{5\delta}{4N}\left(1 + O\left(\frac{1}{N}\right)\right)$$

We also observe that $-\zeta$ is a rate, which is here naturally expressed in units of the curing rate δ.

Fig. 1 shows the accuracy (for $\varepsilon = 10^{-5}$) of the second order Lagrange series (38), the upper bound (39) derived from the Newton identities and the exact (numerical) computation of the second largest eigenvalue of the infinitesimal generator matrix Q of the continuous-time ε-SIS Markov process on the complete graph N, for which the epidemic threshold τ_c is slightly larger than $1/N$. These numerical results confirm the order estimates (even for $\varepsilon \to 0$) above, at and below the epidemic threshold. Both Lagrange's second order and Newton's upper bound are increasingly sharp for increasing values of τ above the epidemic threshold. Our exact asymptotics in (2) of the order of $-\zeta = O\left(\frac{N}{x^{N-1}}\right)$ for $x >> 1$ is difficult to verify for $N > 10$ since numerical root finders only provide an accuracy of about 10^{-10}. For $1 < x < 2.5$, (2) is verified up to $N = 100$. The relative accuracy for $\varepsilon < \frac{1}{N}$ is about the same as the results shown in Fig. 1.

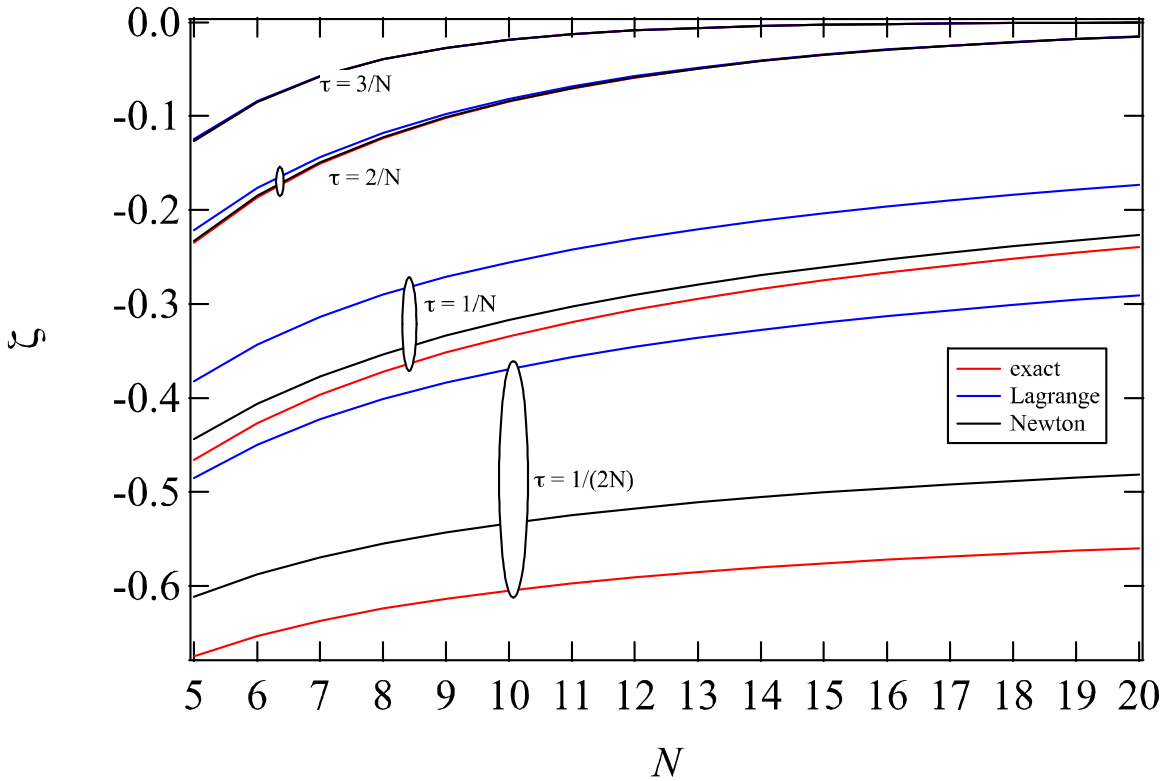

Figure 1: The second largest zero ζ, exactly computed in red, by a second order Lagrange series (38) in blue and by Newton's identity (39) in black as a function of N for $\varepsilon = 10^{-5}$ and four values for the effective infection rate $\tau = \{1/(2N), 1/N, 2/N, 3/N\}$.

3 Conclusion

Our asymptotic order results agree with the general estimates of the average lifetime of a SIS epidemics in Draief and Massoulié [6]. For large t, the probability of survival of the SIS epidemics or probability that the life-time T of an SIS epidemics exceeds t time units equals about

$$\Pr[T > t] \simeq e^{-|\zeta| t}$$

Hence, the life time of an epidemics (for large t) can be interpreted as being exponentially distributed with mean $\frac{1}{|\zeta|}$. In particular, above the epidemic threshold (equal to $x > 1$ to first order in N), the SIS epidemics in K_N dies out exponentially in time t with decay rate ζ, which tends to zero at least as fast as $e^{-N \ln \frac{\tau}{\tau_c}}$, where $x = \frac{\tau}{\tau_c} > 1$ is measured in units of the epidemic threshold $\tau_c \sim \frac{1}{N}$ for large N. This means that the probability that an SIS epidemic in any network survives longer than t time units is smaller than about $e^{-te^{-N \ln \frac{\tau}{\tau_c}}}$ or that the average life time is at most $E[T] \simeq \frac{1}{|\zeta|} \simeq O\left(e^{N \ln \frac{\tau}{\tau_c}}\right)$, which is unrealistically long. Hence, for sufficiently large N and an effective infection rate $\tau > \tau_c$, the SIS epidemics hardly ever dies in reality. When τ approaches τ_c, the decay rate ζ of the SIS epidemics decreases at least as fast as $O\left(\frac{1}{N}\right)$, equivalent to an average life time $E[T] \simeq O(N)$. Below the epidemic threshold $x = \frac{\tau}{\tau_c} < 1$, the decay rate ζ decreases at least as fast as $O\left(\frac{1}{\log N}\right)$ and the average life time is about $E[T] = O(\log N)$.

Finally, the lower bound results in [14] together with our upper bound in (2) leads us to conclude that for almost all graphs, the average time to absorption for $\tau > \tau_c$ is $E[T] = O\left(e^{c_G N}\right)$, where $c_G > 0$. The precise expression of c_G for a given graph G stays on the agenda of future work.

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A General tri-diagonal matrices

We study the eigen-structure of tri-diagonal matrices of the form

$$P = \begin{bmatrix} r_0 & p_0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ q_1 & r_1 & p_1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & q_2 & r_2 & p_2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & q_{N-1} & r_{N-1} & p_{N-1} \\ 0 & 0 & 0 & 0 & \cdots & 0 & q_N & r_N \end{bmatrix} \tag{9}$$

where p_j and q_j are probabilities and where P obeys the stochasticity requirement $Pu = u$, where u is the all-one vector. The matrix P frequently occurs in Markov theory, in particular, P is the transition probability matrix of the generalized random walk. The stochasticity requirement reflects the fact that a Markov process must be in any of the $N+1$ states. If $p_j = p$ and $q_j = q$, the matrix P reduces to a Toeplitz form for which the eigenvalues and eigenvectors can be explicitly written, as shown in

[19]. Here, we consider the general tri-diagonal matrix (9) and show how orthogonal polynomials enter the scene. The theory for the discrete-time generalized random walk is readily extended to that for the continuous-time general birth-death process. While our approach is more algebraic, Karlin and McGregor [10] have presented a different, more probabilistic and function-theoretic method, which is reviewed and complemented by Van Doorn and Schrijner [17].

When P is written as a block matrix

$$P = \begin{bmatrix} A_{k\times k} & B_{k\times(N+1-k)} \\ C_{(N+1-k)\times k} & D_{(N+1-k)\times(N+1-k)} \end{bmatrix}$$

then the matrix B and C only consist of one non-zero element, so that, using the basic vector e_j whose j-th component equals 1 while all others are zero, $B = p_{k-1}\,(e_k)_{k\times 1}\,.\,(e_1)^T_{1\times(N+1-k)}$ and $C = q_k\,(e_1)_{(N+1-k)\times 1}\,(e_k)^T_{1\times k}$. The determinant of P evaluated with Schur's formula

$$\det\begin{bmatrix} A & B \\ C & D \end{bmatrix} = \det A \det\left(D - CA^{-1}B\right)$$

shows that

$$\begin{aligned} CA^{-1}B &= p_{k-1}q_k\,(e_1)_{(N+1-k)\times 1}\,(e_k)^T_{1\times k}\,A^{-1}\,(e_k)_{k\times 1}\,.\,(e_1)^T_{1\times(N+1-k)} \\ &= p_{k-1}q_k\left(A^{-1}\right)_{kk}(e_1)_{(N+1-k)\times 1}\,.\,(e_1)^T_{1\times(N+1-k)} \end{aligned}$$

Thus, the matrix $CA^{-1}B$ only contains one non-zero element on position $(1,1)$. Only the first element in $\widetilde{D} = D - CA^{-1}B$ is changed from r_k in D to $r_k - p_{k-1}q_k\left(A^{-1}\right)_{kk}$ in $\widetilde{D}$ and $p_{k-1}q_k\left(A^{-1}\right)_{kk}$ can be considered as the coupling between the first $k-1$ states in the generalized random walk and the remaining other states. If $p_{k-1} = 0$ or/and $q_k = 0$, then $\det P = \det A \det D$, which is the product of two individual tri-diagonal determinants. In that case, the Markov chain is reducible. Hence, in the sequel, we assume that all elements of P are non-zero and time-independent so that the Markov chain is irreducible.

A.1 A similarity transform

We apply a similarity transform analogous to that of the Jacobi matrix for orthogonal polynomials as studied in [20, Section 10.6]. If there exists a similarity transform that makes the matrix P symmetric, then all eigenvalues of P are real, because a similarity transform preserves the eigenvalues. The simplest similarity transform is $H = \mathrm{diag}(h_1, h_2, \ldots, h_{N+1})$ such that

$$\widetilde{P} = HPH^{-1} = \begin{bmatrix} r_0 & \frac{h_1}{h_2}p_0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ \frac{h_2}{h_1}q_1 & r_1 & \frac{h_2}{h_3}p_1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & \frac{h_3}{h_2}q_2 & r_2 & \frac{h_3}{h_4}p_2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \frac{h_N}{h_{N-1}}q_{N-1} & r_{N-1} & \frac{h_N}{h_{N+1}}p_{N-1} \\ 0 & 0 & 0 & 0 & \cdots & 0 & \frac{h_{N+1}}{h_N}q_N & r_N \end{bmatrix}$$

Thus, in order to produce a symmetric matrix $\widetilde{P} = \widetilde{P}^T$, we need to require that $\left(\widetilde{P}\right)_{i,i-1} = \left(\widetilde{P}\right)_{i-1,i}$ for all $1 \le i \le N$, implying that,

$$\frac{h_{i+1}}{h_i}q_i = \frac{h_i}{h_{i+1}}p_{i-1}$$

whence

$$\left(\frac{h_{i+1}}{h_i}\right)^2 = \frac{p_{i-1}}{q_i}$$

Assuming that all p_i and q_i are positive[4], we find that $h_{i+1} = \sqrt{\frac{p_{i-1}}{q_i}} h_i$ for $1 \leq i \leq N$ and we can choose $h_1 = 1$ such that

$$h_i = \sqrt{\prod_{k=1}^{i-1} \frac{p_{k-1}}{q_k}} \tag{10}$$

and

$$\frac{h_{i+1}}{h_i} q_i = \frac{h_i}{h_{i+1}} p_{i-1} = \sqrt{p_{i-1} q_i}$$

After the similarity transform H, the symmetric matrix $\widetilde{P}$ becomes

$$\widetilde{P} = \begin{bmatrix} r_0 & \sqrt{p_0 q_1} & 0 & 0 & \cdots & 0 & 0 & 0 \\ \sqrt{p_0 q_1} & r_1 & \sqrt{p_1 q_2} & 0 & \cdots & 0 & 0 & 0 \\ 0 & \sqrt{p_1 q_2} & r_2 & \sqrt{p_2 q_3} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \sqrt{p_{N-2} q_{N-1}} & r_{N-1} & \sqrt{p_{N-1} q_N} \\ 0 & 0 & 0 & 0 & \cdots & 0 & \sqrt{p_{N-1} q_N} & r_N \end{bmatrix} \tag{11}$$

In conclusion, if all p_i and q_i are positive, then all eigenvalues of P are real. Rather than solving the eigenvector $\widetilde{x}$ from the eigenvalue equation $\widetilde{P}\widetilde{x} = \lambda \widetilde{x}$, we determine the eigenvector x as a function of λ from the original matrix P for reasons explained below and use the similarity transform $\widetilde{x} = Hx$, where H is independent of λ, later for the left-eigenvectors of P.

A.2 Eigenvectors of P

The right-eigenvector x of P belonging to eigenvalue λ satisfies $(P - \lambda I)x = 0$ so that

$$\begin{cases} (r_0 - \lambda)\, x_0 + p_0 x_1 = 0 \\ q_j x_{j-1} + (r_j - \lambda)\, x_j + p_j x_{j+1} = 0 \quad 1 \leq j < N \\ q_N x_{N-1} + (r_N - \lambda)\, x_N = 0 \end{cases}$$

We replace the last equation, that breaks the structure, by

$$q_N x_{N-1} + (r_N - \lambda)\, x_N + p_N x_{N+1} = 0$$

and the condition that $p_N x_{N+1} = 0$. Using $r_j = 1 - q_j - p_j$ for $0 \leq j \leq N$ with $q_0 = 0$ and $p_N = 0$ and making the dependence on $\xi = \lambda - 1$ explicit, the above set simplifies, subject to the condition $p_N x_{N+1}(\xi) = 0$, to

$$\begin{cases} x_1(\xi) = \frac{p_0 + \xi}{p_0} x_0(\xi) \\ x_{j+1}(\xi) = \frac{p_j + q_j + \xi}{p_j} x_j(\xi) - \frac{q_j}{p_j} x_{j-1}(\xi) \quad 1 \leq j < N \end{cases} \tag{12}$$

For the stochastic matrix P, that obeys $Pu = u$, there holds that $r_N = 1 - q_N$ so that $p_N = 0$ and that the condition $p_N x_{N+1} = 0$ seems to be obeyed. In the theory of orthogonal polynomials (see e.g.

[4] If $p_{i-1} = 0$ (or $q_i = 0$), then the states 0 up to $i - 1$ are uncoupled from the states i up to N.

[20, Chapter 10]), a similar trick is used where the orthogonal polynomial $x_{N+1}(\xi)$ needs to vanish, because p_N is not necessarily zero in absence of the stochasticity requirement $Pu = u$. The zeros of the orthogonal polynomial $x_{N+1}(\xi)$ are then equal to the eigenvalues of the corresponding Jabobi matrix. Moreover, the powerful interlacing property for the zeros of the set $\{x_j(\xi)\}_{0\leq j\leq N+1}$ applies. We will return to the condition $p_N x_{N+1} = 0$ below.

Solving (12) iteratively for $j < N$,

$$\begin{aligned} x_2(\xi) &= \frac{x_0(\xi)}{p_0 p_1}\left(\xi^2 + (q_1 + p_1 + p_0)\xi + p_1 p_0\right) \\ x_3(\xi) &= \frac{x_0(\xi)}{p_2 p_1 p_0}\left(\xi^3 + (q_1 + q_2 + p_2 + p_1 + p_0)\xi^2\right) \\ &\quad + (q_2 q_1 + q_2 p_0 + p_2 q_1 + p_2 p_1 + p_2 p_0 + p_1 p_0)\xi + p_2 p_1 p_0 \end{aligned}$$

reveals that $\frac{x_j(\xi)}{x_0(\xi)}$ is a polynomial of degree j in ξ with positive coefficients, whose zeros are all non-positive[5]. This simple form is the main reason to consider the eigenvector components of P instead of $\widetilde{P}$. By inspection, the general form of $x_j(\xi)$ for $1 \leq j \leq N$ is

$$x_j(\xi) = \frac{x_0(\xi)}{\prod_{m=0}^{j-1} p_m} \sum_{k=0}^{j} c_k(j)\xi^k \tag{13}$$

with[6]

$$c_j(j) = 1; \quad c_{j-1}(j) = \textstyle\sum_{m=0}^{j-1}(p_m + q_m); \quad c_0(j) = \prod_{m=0}^{j-1} p_m; \tag{14}$$

where $q_0 = p_N = 0$. By substituting (13) into (12),

$$\sum_{k=1}^{j-1} c_k(j+1)\xi^k = \sum_{k=1}^{j-1}\left[(q_j + p_j)c_k(j) - q_j p_{j-1} c_k(j-1) + c_{k-1}(j)\right]\xi^k$$

and equating the corresponding powers in ξ, a recursion relation for the coefficients $c_k(j)$ for $0 \leq k < j$ is obtained with $c_j(j) = 1$,

$$c_k(j+1) = (q_j + p_j)c_k(j) - q_j p_{j-1} c_k(j-1) + c_{k-1}(j) \tag{15}$$

from which all coefficients can be determined as shown in Section A.3. The stochasticity requirement $Pu = u$ implies that the right-eigenvector belonging to the largest eigenvalue $\lambda = 1$, equivalently to $\xi = \lambda - 1 = 0$, equals $x(0) = u$.

We now express the left-eigenvectors of P in terms of the right-eigenvector by using the similarity transform H. Since $\widetilde{P}$ is symmetric, the left- and right-eigenvectors are the same [20, p. 222-223]. The left-eigenvector x of P equals $x = H^{-1}\widetilde{x}$, while the right-eigenvector y of P equals $y = H\widetilde{x}$. Hence, we find that $y = H^2 x$ and explicitly with (13) and (10),

$$y_j(\xi) = \frac{y_0(\xi)}{\prod_{m=0}^{j-1} q_{m+1}} \sum_{k=0}^{j} c_k(j)\xi^k \tag{16}$$

[5] If P is a stochastic, irreducible matrix, then the Perron-Frobenius Theorem [20] states that the largest (in absolute value) eigenvalue is one, hence $-1 < \lambda = \xi + 1 \leq 1$.

[6] We use the convention that $\sum_{k=a}^{b} f(k) = 0$ and $\prod_{k=a}^{b} f(k) = 1$ if $a > b$.

For any matrix, the left- and right-eigenvectors obey the orthogonality equation

$$x^T(\xi)\, y(\xi') = x^T(\xi)\, y(\xi)\, \delta_{\xi\xi'} \tag{17}$$

that holds for any pair of eigenvalues $\lambda = \xi + 1$ and $\lambda' = \xi' + 1$ of that matrix. For symmetric matrices, usually, the normalization

$$\widetilde{x}^T(\xi)\, \widetilde{x}(\xi') = \delta_{\xi\xi'} \tag{18}$$

is chosen, which implies, after the similarity transform $H = \mathrm{diag}(h_i)$, that $x^T(\xi)\, y(\xi') = \widetilde{x}^T(\xi)\, \widetilde{x}(\xi') = \delta_{\xi\xi'}$ and that $x^T(\xi)\, H^2 x(\xi') = \delta_{\xi\xi'}$ and similarly that $y^T(\xi)\, H^{-2} y(\xi') = \delta_{\xi\xi'}$. These normalizations of the eigenvector components imply, using (13) and (16) and with the definition of the polynomial for $0 \le j \le N+1$

$$\rho_j(\xi) = \sum_{k=0}^{j} c_k(j)\xi^k \tag{19}$$

that

$$x_0(\xi)\, y_0(\xi) = x_0^2(\xi) = y_0^2(\xi) = \left(1 + \sum_{j=1}^{N} \frac{\rho_j^2(\xi)}{\prod_{m=0}^{j-1} q_{m+1} p_m}\right)^{-1} \tag{20}$$

The orthogonality equation (17) together with our choice of normalization, $\widetilde{x}^T(\xi)\, \widetilde{x}(\xi') = \delta_{\xi\xi'}$, lead to a couple of important consequences.

Using the general form (13), the initially made condition $p_N x_{N+1} = 0$ translates to

$$p_N x_{N+1}(\xi) = \frac{x_0(\xi)\, \rho_{N+1}(\xi)}{\prod_{m=0}^{N-1} p_m} = 0$$

Since $\rho_j(\xi)$ is a polynomial, (20) indicates that neither $x_0(\xi)$ nor $y_0(\xi)$ can vanish for finite ξ so that the initial condition is met provided

$$\rho_{N+1}(\xi) = 0 \tag{21}$$

which closely corresponds to results in the theory of orthogonal polynomials. Thus, $\rho_j(\xi)$ should be considered as orthogonal polynomial, rather than $x_j(\xi)$ due to the scaling of $x_0(\xi)$, defined in (20). For the set of orthogonal polynomials $\{\rho_j(\xi)\}_{0 \le j \le N+1}$ *interlacing* applies, which means that the zeros of $\rho_j(\xi)$ interlace with those of $\rho_l(\xi)$ for all $1 \le l \ne j \le N+1$. Moreover, the eigenvalues of P are equal to the zeros of $\rho_{N+1}(\xi)$ in (21).

For stochastic matrices, the left-eigenvector $y(0)$ belonging to $\xi = 0$ equals the steady-state vector π (see [19]). For $\xi = 0$, the orthogonality relation (17) becomes $u^T y(\xi') = 0$ and $u^T y(0) = u^T \pi = 1$, from which the j-th component in (16) of the left-eigenvector $y(0) = \pi$ follows, for $1 \le j \le N$, as

$$\pi_j = y_j(0) = \frac{y_0(0)\, c_0(j)}{\prod_{m=0}^{j-1} q_{m+1}} = \frac{\prod_{m=0}^{j-1} \frac{p_m}{q_{m+1}}}{1 + \sum_{k=1}^{N} \prod_{m=0}^{k-1} \frac{p_m}{q_{m+1}}} \tag{22}$$

which precisely equal the well-known steady-state probabilities of the generalized random walk [19, p. 207]. For $\xi \ne 0$, the orthogonality relation (17) and the fact that $y_0(\xi)$ is non-zero for finite ξ imply that

$$0 = 1 + \sum_{j=1}^{N} \frac{1}{\prod_{m=0}^{j-1} q_{m+1}} \sum_{k=0}^{j} c_k(j)\xi^k = 1 + \sum_{j=1}^{N} \prod_{m=0}^{j-1} \frac{p_m}{q_{m+1}} + \sum_{k=1}^{N} \left(\sum_{j=k}^{N} \frac{c_k(j)}{\prod_{m=0}^{j-1} q_{m+1}} \right) \xi^k$$

We write the right-hand side polynomial as

$$\sum_{k=0}^{N} f_k \xi^k = f_N \prod_{k=1}^{N} (\xi - z_k) \tag{23}$$

where $f_0 = \frac{1}{\pi_0}$ by (22) and where, for $k > 0$,

$$f_k = \sum_{j=k}^{N} \frac{c_k(j)}{\prod_{m=0}^{j-1} q_{m+1}} \tag{24}$$

and, explicitly,

$$f_N = \frac{1}{\prod_{m=0}^{N-1} q_{m+1}}$$
$$f_{N-1} = \frac{1}{\prod_{m=0}^{N-2} q_{m+1}} + \frac{\sum_{m=0}^{N-1} (p_m + q_m)}{\prod_{m=0}^{N-1} q_{m+1}}$$

Relation (24) illustrates that all coefficients f_k are non-negative. Moreover, the orthogonality relation (17) implies that the polynomial $\sum_{k=0}^{N} f_k \xi^k$ possesses the same zeros as $\frac{c_P(\xi)}{\xi}$, where

$$c_P(\xi) = \det(P - (\xi + 1) I) = \xi \prod_{k=1}^{N} (z_k - \xi)$$

is the $N+1$ degree characteristic polynomial of the matrix P, in particular,

$$\frac{c_P(\xi)}{(-1)^N \xi} = \frac{1}{f_N} \sum_{k=0}^{N} f_k \xi^k \tag{25}$$

Finally, since the eigenvalues of P also obey (21) so that

$$\frac{c_P(\xi)}{(-1)^N \xi} = \frac{1}{f_N} \sum_{k=0}^{N} f_k \xi^k = \sum_{k=1}^{N+1} c_k(N+1) \xi^{k-1}$$

after equating corresponding powers in ξ, we find that

$$c_{k+1}(N+1) = \frac{f_k}{f_N} = \sum_{j=k}^{N} c_k(j) \prod_{m=j}^{N-1} q_{m+1} \tag{26}$$

In summary, the stochasticity property of P provides us with an additional relation (26) on the coefficients of $c_P(\xi)$, that is not necessarily obeyed for general orthogonal polynomials.

A.3 Solving the recursion (15)

We now propose two different types of solutions of the recursion (15) for the coefficients $c_k(j)$ of $x_j(\xi)$ in (13).

Theorem 1 *A recursion relation for $c_{j-m}(j)$, valid for $2 \le m \le j$, is*

$$c_{j-m}(j) = \sum_{l=0}^{j-1} \left((q_l + p_l) c_{l-m+1}(l) - q_l p_{l-1} c_{l-m+1}(l-1) \right) \tag{27}$$

Proof: Letting $k = j - m$ in (15) yields

$$c_{j+1-(m+1)}(j+1) = (q_j + p_j)\, c_{j-m}(j) - q_j p_{j-1} c_{j-1-(m-1)}(j-1) + c_{j-(m+1)}(j)$$

With $t_m(j) = c_{j-m}(j)$, the above equation transforms into the difference equation

$$t_{m+1}(j+1) = t_{m+1}(j) + (q_j + p_j)\, t_m(j) - q_j p_{j-1} t_{m-1}(j-1)$$

whose solution is

$$t_{m+1}(j) = \sum_{l=0}^{j-1} \left((q_l + p_l)\, t_m(l) - q_l p_{l-1} t_{m-1}(l-1) \right)$$

With the initial values $t_0(j) = 1$ and $t_1(j) = \sum_{m=0}^{j-1} (p_m + q_m)$ from (14), all $t_m(j)$ can be iteratively found from (27). □

Thus, letting $m = 2$ in (27) yields

$$c_{j-2}(j) = \sum_{l=0}^{j-1} \left((q_l + p_l) \sum_{m=0}^{l-1} (p_m + q_m) - q_l p_{l-1} \right) \tag{28}$$

Next, for $m = 3$ in (27), we have

$$c_{j-3}(j) = \sum_{l=0}^{j-1} \left((q_l + p_l) \sum_{l_1=0}^{l-1} \left((q_{l_1} + p_{l_1}) \sum_{m=0}^{l_1-1} (p_m + q_m) - q_{l_1} p_{l_1-1} \right) - q_l p_{l-1} \sum_{m=0}^{l-2} (p_m + q_m) \right)$$

and so on.

For the polynomial in (23), the next general expression will prove more useful.

Theorem 2 *The explicit general expression for the coefficients $c_k(j)$ in terms of $c_{k-1}(l)$ for all $l \geq k-1$ is*

$$\begin{aligned} c_k(j) = & \prod_{m=k}^{j-1} p_m + \sum_{l=0}^{j-k-1} \prod_{m=k}^{j-l-1} q_m \prod_{m=j-l}^{j-1} p_m + \sum_{m=0}^{k-1} (p_m + q_m) \sum_{l=0}^{j-k-1} \prod_{m=k+1}^{j-l-1} q_m \prod_{m=j-l}^{j-1} p_m \\ & + \sum_{l=0}^{j-k-1} \sum_{s=1}^{j-l-k-1} c_{k-1}(j-l-s) \prod_{m=j-l+1-s}^{j-l-1} q_m \prod_{m=j-l}^{j-1} p_m \end{aligned} \tag{29}$$

Proof: Rewriting (15) as

$$c_k(j+1) - p_j c_k(j) = q_j \left\{ c_k(j) - p_{j-1} c_k(j-1) \right\} + c_{k-1}(j)$$

and defining $b_k(j) = c_k(j) - p_{j-1} c_k(j-1)$ shows that the second order recursion (15) in j can be decomposed into two first order recursions in j

$$\begin{cases} c_k(j) = p_{j-1} c_k(j-1) + b_k(j) \\ b_k(j) = q_{j-1} b_k(j-1) + c_{k-1}(j-1) \end{cases}$$

Since $k < j$, the choice for $j = k+1$ yields

$$\begin{aligned} b_k(k+1) &= c_k(k+1) - p_k c_k(k) \\ &= \sum_{m=0}^{k} (p_m + q_m) - p_k = q_k + \sum_{m=0}^{k-1} (p_m + q_m) \end{aligned}$$

Iterating the first recursion downwards yields

$$\begin{aligned}
c_k(j) &= p_{j-1}p_{j-2}c_k(j-2) + p_{j-1}b_k(j-1) + b_k(j) \\
&= p_{j-1}p_{j-2}p_{j-3}c_k(j-3) + p_{j-1}p_{j-2}b_k(j-2) + p_{j-1}b_k(j-1) + b_k(j) \\
&= p_{j-1}p_{j-2}p_{j-3}p_{j-4}c_k(j-4) + p_{j-1}p_{j-2}p_{j-3}b_k(j-3) + p_{j-1}p_{j-2}b_k(j-2) + p_{j-1}b_k(j-1) + b_k(j)
\end{aligned}$$

from which we deduce that

$$c_k(j) = c_k(j-p)\prod_{m=j-p}^{j-1} p_m + \sum_{l=0}^{p-1} b_k(j-l)\prod_{m=j-l}^{j-1} p_m$$

When $j-p=k$, then $c_k(k)=1$ and thus

$$c_k(j) = \prod_{m=k}^{j-1} p_m + \sum_{l=0}^{j-k-1} b_k(j-l)\prod_{m=j-l}^{j-1} p_m \tag{30}$$

Similarly, we iterate the second recursion downwards,

$$\begin{aligned}
b_k(j) &= q_{j-1}q_{j-2}b_k(j-2) + q_{j-1}c_{k-1}(j-2) + c_{k-1}(j-1) \\
&= q_{j-1}q_{j-2}q_{j-3}b_k(j-3) + q_{j-1}q_{j-2}c_{k-1}(j-3) + q_{j-1}c_{k-1}(j-2) + c_{k-1}(j-1)
\end{aligned}$$

which suggests that

$$b_k(j) = b_k(j-p)\prod_{m=j-p}^{j-1} q_m + \sum_{l=1}^{p} c_{k-1}(j-l)\prod_{m=j+1-l}^{j-1} q_m$$

For $j-p=k+1$ or $p=j-k-1$, we have

$$\begin{aligned}
b_k(j) &= b_k(k+1)\prod_{m=k+1}^{j-1} q_m + \sum_{l=1}^{j-k-1} c_{k-1}(j-l)\prod_{m=j+1-l}^{j-1} q_m \\
&= \prod_{m=k}^{j-1} q_m + \prod_{m=k+1}^{j-1} q_m \sum_{m=0}^{k-1}(p_m+q_m) + \sum_{l=1}^{j-k-1} c_{k-1}(j-l)\prod_{m=j+1-l}^{j-1} q_m
\end{aligned} \tag{31}$$

Combining (30) and (31) yields (29). □

For $k=1$ and using $c_0(j)=\prod_{m=0}^{j-1} p_m$, we find from (29) that

$$c_1(j) = \sum_{l=0}^{j-1}\sum_{s=0}^{j-1-l}\prod_{m=0}^{j-2-l-s} p_m \prod_{m=j-l-s}^{j-1-l} q_m \prod_{m=j-l}^{j-1} p_m \tag{32}$$

Introducing the expression (32) for $c_1(j)$ into (29) produces the explicit form for $c_2(j)$,

$$\begin{aligned}
c_2(j) &= \prod_{m=2}^{j-1} p_m + (p_0+p_1+q_1+q_2)\sum_{l=0}^{j-3}\prod_{m=3}^{j-l-1} q_m \prod_{m=j-l}^{j-1} p_m \\
&+ \sum_{l=0}^{j-3}\sum_{s=1}^{j-l-3}\sum_{l_1=0}^{j-l-s-1}\sum_{l_2=0}^{j-l-s-l_1-1}\prod_{m=0}^{j-l-s-2-l_1-l_2} p_m \prod_{m=j-l-s-l_1-l_2}^{j-l-s-1-l_1} q_m \prod_{m=j-l-s-l_1}^{j-l-s-1} p_m \prod_{m=j-l+1-s}^{j-l-1} q_m \prod_{m=j-l}^{j-1} p_m
\end{aligned} \tag{33}$$

and so on. In this way, all coefficients $c_k(j)$ in the polynomial (13) can be explicitly determined[7]. Since all p_j and q_j are probabilities and thus non-negative, the recursion (29) together with $c_0(j)=\prod_{m=0}^{j-1} p_m$ illustrates that all coefficients $c_k(j)$ are non-negative.

[7] For $j=k$ in (29), we find indeed that $c_k(k)=1$ (based on our convention).

A.4 The second set of orthogonality conditions

Since the matrix $\widetilde{X}$, with the eigenvectors $\widetilde{x}$ of the symmetric matrix $\widetilde{P}$ as columns, is orthogonal, it holds that

$$\widetilde{X}^T\widetilde{X} = \widetilde{X}\widetilde{X}^T = I$$

and the last equation means that

$$\sum_{\lambda\in\{\lambda_1,\lambda_2,\ldots,\lambda_N,\lambda_{N+1}\}} \widetilde{x}_j(\lambda)\,\widetilde{x}_m(\lambda) = \delta_{jm}$$

where $\lambda_1 = 1 \geq \lambda_2 \geq \cdots \geq \lambda_{N+1}$ are the eigenvalues of P corresponding to the zeros of $c_P(\xi)$ by $\xi = \lambda - 1$ and

$$\sum_{\lambda\in\{\lambda_1,\lambda_2,\ldots,\lambda_N,\lambda_{N+1}\}} h_{j+1}h_{m+1}x_j(\lambda)\,x_m(\lambda) = \delta_{jm}$$

Using (13) and (10) yields

$$\sum_{\lambda\in\{\lambda_1,\lambda_2,\ldots,\lambda_N,\lambda_{N+1}\}} x_0^2(\lambda-1)\sum_{k=0}^{j} c_k(j)\,(\lambda-1)^k \sum_{l=0}^{k} c_l(k)\,(\lambda-1)^l = \sqrt{\prod_{m=1}^{j} q_m \prod_{m=1}^{k} q_m}\,\delta_{jk}$$

which we rewrite, with the definition (19), as

$$\sum_{\lambda\in\{\lambda_1,\lambda_2,\ldots,\lambda_N,\lambda_{N+1}\}} x_0^2(\lambda-1)\,\rho_j(\lambda-1)\,\rho_k(\lambda-1) = \delta_{jk}\prod_{m=1}^{k} q_m$$

Finally, introducing the Dirac delta-function, the left-hand side is rewritten as an integral

$$\begin{aligned} I &= \sum_{\lambda\in\{\lambda_1,\lambda_2,\ldots,\lambda_N,\lambda_{N+1}\}} x_0^2(\lambda-1)\,\rho_j(\lambda-1)\,\rho_k(\lambda-1) \\ &= \sum_{j=1}^{N+1}\int_{-1}^{1} \delta(\lambda-\lambda_j)\,x_0^2(\lambda-1)\,\rho_j(\lambda-1)\,\rho_k(\lambda-1)\,d\lambda \end{aligned}$$

because the eigenvalues of P lie between $[-1,1]$. Further,

$$\begin{aligned} I &= \int_{-1}^{1} d\lambda x_0^2(\lambda-1)\,\rho_j(\lambda-1)\,\rho_k(\lambda-1)\,\delta(\det(P-\lambda I))\left|\frac{d\det(P-xI)}{dx}\bigg|_{x=\lambda}\right| \\ &= \int_{-2}^{0} d\xi x_0^2(\xi)\,\rho_j(\xi)\,\rho_k(\xi)\,\delta(\det(P-(\xi+1)I))\left|\frac{d\det(P-xI)}{dx}\bigg|_{x=\xi+1}\right| \end{aligned}$$

Defining the weight function as

$$\begin{aligned} w(\xi) &= x_0^2(\xi)\,\delta(\det(P-(\xi+1)I))\left|\frac{d\det(P-xI)}{dx}\bigg|_{x=\xi+1}\right| \\ &= x_0^2(\xi)\,\delta(c_P(\xi))\left|\frac{dc_P(\xi)}{d\xi}\right| = \sum_{j=1}^{N+1} x_0^2(\xi_j)\,\delta(\xi-\xi_j) \end{aligned}$$

we finally obtain the orthogonality condition for the orthogonal polynomials r_j and r_k as

$$\int_{-2}^{0} w(\xi)\,\rho_j(\xi)\,\rho_k(\xi)\,d\xi = \delta_{jk}\prod_{m=1}^{k} q_m$$

In summary, the derivation provides an explicit way to determine the weight function $w(\xi)$ in the orthogonality relation corresponding to a tri-diagonal stochastic matrix P.

A.5 The Christoffel-Darboux formula for eigenvectors of P

We derive the Christoffel-Darboux formula (see [20, p. 357]) for the matrix P. Indeed, multiply the equation for $x_{j+1}(\xi)$ in (12) by $x_j(\omega)$

$$p_j x_{j+1}(\xi) x_j(\omega) = \xi x_j(\xi) x_j(\omega) + (p_j + q_j) x_j(\xi) x_j(\omega) - q_j x_{j-1}(\xi) x_j(\omega)$$

Letting $\xi \to \omega$ in (12) and multiply both sides by $x_j(\xi)$,

$$p_j x_{j+1}(\omega) x_j(\xi) = \omega x_j(\xi) x_j(\omega) + (p_j + q_j) x_j(\xi) x_j(\omega) - q_j x_j(\xi) x_{j-1}(\omega)$$

Subtracting both equation yields,

$$p_j \{x_{j+1}(\xi) x_j(\omega) - x_{j+1}(\omega) x_j(\xi)\} + q_j \{x_{j-1}(\xi) x_j(\omega) - x_j(\xi) x_{j-1}(\omega)\} = (\xi - \omega) x_j(\xi) x_j(\omega)$$

Now, we transform to $x_j(\xi) = \frac{\widetilde{x}_j(\xi)}{h_{j+1}}$,

$$\frac{p_j}{h_{j+2}h_{j+1}} \{\widetilde{x}_{j+1}(\xi) \widetilde{x}_j(\omega) - \widetilde{x}_{j+1}(\omega) \widetilde{x}_j(\xi)\} + \frac{q_j}{h_j h_{j+1}} \{\widetilde{x}_{j-1}(\xi) \widetilde{x}_j(\omega) - \widetilde{x}_{j-1}(\omega) \widetilde{x}_j(\xi)\} = \frac{(\xi - \omega)}{h_{j+1}^2} \widetilde{x}_j(\xi) \widetilde{x}_j(\omega)$$

Using (10) shows that $\frac{p_j}{h_{j+2}h_{j+1}} = \frac{\sqrt{p_j q_{j+1}}}{h_{j+1}^2}$ and $\frac{q_j}{h_j h_{j+1}} = \frac{\sqrt{p_{j-1} q_j}}{h_{j+1}^2}$ so that

$$g_{j+1} - g_j = (\xi - \omega) \widetilde{x}_j(\xi) \widetilde{x}_j(\omega)$$

where

$$g_j = \sqrt{p_{j-1} q_j} \{\widetilde{x}_{j-1}(\omega) \widetilde{x}_j(\xi) - \widetilde{x}_{j-1}(\xi) \widetilde{x}_j(\omega)\}$$

Summing over $j \in [0, m]$,

$$(\xi - \omega) \sum_{j=0}^{m} \widetilde{x}_j(\xi) \widetilde{x}_j(\omega) = \sum_{j=0}^{m} g_{j+1} - \sum_{j=0}^{m} g_j = g_{m+1} - g_0$$

where $g_0 = 0$ because $\widetilde{x}_{-1} = 0$. Hence, we arrive at the Christoffel-Darboux sum for the eigenvectors of $\widetilde{P}$,

$$(\xi - \omega) \sum_{j=0}^{m} \widetilde{x}_j(\xi) \widetilde{x}_j(\omega) = \sqrt{p_m q_{m+1}} \{\widetilde{x}_m(\omega) \widetilde{x}_{m+1}(\xi) - \widetilde{x}_m(\xi) \widetilde{x}_{m+1}(\omega)\}$$

which extends the orthogonality relation (18). Transformed back to $x_j(\xi)$ using (10) yields

$$(\xi - \omega) \sum_{j=0}^{m} h_{j+1}^2 x_j(\xi) x_j(\omega) = p_m h_{m+1}^2 \{x_m(\omega) x_{m+1}(\xi) - x_m(\xi) x_{m+1}(\omega)\} \tag{34}$$

Since $\omega = 0$ is an eigenvalue with corresponding eigenvector $x(0) = \frac{1}{N+1} u$, each other real eigenvalue $\xi \neq 0$ must obey

$$\xi \sum_{j=0}^{m} h_{j+1}^2 x_j(\xi) = p_m h_{m+1}^2 \{x_{m+1}(\xi) - x_m(\xi)\}$$

Taking $p_N = 0$ into account, the Christoffel-Darboux formula (34) extends (18) to all $0 \leq m \leq N$.

B Second largest zero of $c_P(\xi)$

The zero of a complex function can be expressed as a Lagrange series [24, 12]. When all Taylor coefficients f_k of a function expanded around a point z_0 are known, our framework of characteristic coefficients, first published in [18], provides all coefficients in the corresponding Lagrange series in terms of f_k. In particular, the second largest zero ζ closest to $\xi = 0$, based on the Lagrange expansion (see e.g. [20, p. 305]) up to order 4 in $\frac{f_0}{f_1}$, is

$$\zeta \approx -\frac{f_0}{f_1} - \frac{f_2}{f_1}\left(\frac{f_0}{f_1}\right)^2 + \left[-2\left(\frac{f_2}{f_1}\right)^2 + \frac{f_3}{f_1}\right]\left(\frac{f_0}{f_1}\right)^3 + O\left(\left(\frac{f_0}{f_1}\right)^4\right) \tag{35}$$

Since all Taylor coefficients f_k of the characteristic polynomial $c_P(\xi)$ around $\xi = 0$ are known, we can formally compute the zero ζ to *any order or accuracy.* The fact that all coefficients f_k are non-zero and that $\xi = 0$ is the largest zero of $c_P(\xi)$ guarantees that the Lagrange series converges fast. In fact, the first term in (35) equals the first iteration in the Newton-Raphson method and the point $z_0 = 0$ is an ideal expansion point. This article demonstrates this computation up to second order, hence, using the explicit knowledge of f_0, f_1 and f_2. Proceeding further with f_3 is possible, however, at the expense of huge computations, from which we refrained, mainly because numerical computations in Section 2 demonstrate a good accuracy of ζ only based on the three coefficients f_0, f_1 and f_2.

The sum[8] of the inverse of the zeros of $\frac{c_P(\xi)}{\xi}$ follows from the Newton identities [20, p. 305] as

$$\sum_{k=1}^{N} \frac{1}{z_k} = -\frac{f_1}{f_0}$$

from which

$$-\zeta = \frac{1}{\frac{f_1}{f_0} + \sum_{k=2}^{N} \frac{1}{z_k}}$$

Since all zeros z_k of $\frac{c_P(\xi)}{\xi}$ are negative, we have

$$-\zeta = \frac{1}{\frac{f_1}{f_0} + \sum_{k=2}^{N} \frac{1}{z_k}} > \frac{f_0}{f_1}$$

[8] The sum of the zeros of $\frac{c_P(\xi)}{\xi}$ (taking into account that $p_N = 0$) equals

$$\sum_{k=1}^{N} z_k = -\frac{f_{N-1}}{f_N} = -\sum_{m=0}^{N} (p_m + q_m)$$

Since $0 \le p_m + q_m = 1 - r_m \le 1$ and $p_N = q_0 = 0$, the average of the zeros lies between zero and minus one. The product of the zeros follows from (23) as

$$\prod_{k=1}^{N} (-z_k) = \frac{f_0}{f_N} = \frac{\prod_{m=0}^{N-1} q_{m+1}}{\pi_0} = \prod_{m=0}^{N-1} q_{m+1} + \sum_{j=1}^{N-1} \prod_{m=j}^{N-1} q_{m+1} \prod_{m=0}^{j-1} p_m + \prod_{m=0}^{N-1} p_m$$

which is, by the Perron-Frobenius Theorem strictly smaller than 1. Finally, we also compute $\sum_{k=1}^{N} z_k^2 = \left(\frac{f_{N-1}}{f_N}\right)^2 - 2\frac{f_{N-2}}{f_N}$ from the Newton identities with (28) as

$$\sum_{k=1}^{N} z_k^2 = \sum_{m=0}^{N} \left\{(q_m + p_m)^2 + 2q_m p_{m-1}\right\}$$

so that

$$\zeta < -\frac{f_0}{f_1} \tag{36}$$

demonstrating that $-\frac{f_0}{f_1}$ is an upper bound for ζ. This observation also follows from the above Lagrange series (35).

From (24), we have that $f_0 = \frac{1}{\pi_0}$, where π_0 is the zero component of the state-state vector of P (eigenvector belonging to eigenvalue $\lambda = 1$), and

$$f_1 = \frac{1}{q_1} + \sum_{j=2}^{N} \frac{c_1(j)}{\prod_{m=0}^{j-1} q_{m+1}}$$

which becomes with (32),

$$f_1 = \frac{1}{q_1} + \sum_{j=2}^{N} \frac{1}{\prod_{m=0}^{j-1} q_{m+1}} \sum_{r=0}^{j-1} \prod_{s=j-r}^{j-1} p_s \sum_{k=0}^{j-1-r} \prod_{m=0}^{j-2-r-k} p_m \prod_{l=j-r-k}^{j-1-r} q_l \tag{37}$$

The number of terms in f_1 equals $1 + \sum_{j=1}^{N-1} \sum_{r=0}^{j} \sum_{k=0}^{j-r} 1 = \frac{N(N+1)(N+2)}{6} = \binom{N+2}{3}$. Hence, the *lower* bound for $-\zeta$ is

$$\frac{f_0}{f_1} = \frac{1 + \sum_{j=1}^{N} \prod_{m=0}^{j-1} \frac{p_m}{q_{m+1}}}{\frac{1}{q_1} + \sum_{j=2}^{N} \frac{1}{\prod_{m=0}^{j-1} q_{m+1}} \sum_{r=0}^{j-1} \prod_{s=j-r}^{j-1} p_s \sum_{k=0}^{j-1-r} \prod_{m=0}^{j-2-r-k} p_m \prod_{l=j-r-k}^{j-1-r} q_l}$$

Similarly, combining (24), (33) and (37) yields $\frac{f_2}{f_1}$, and so establishing the Lagrange series for ζ up to second order in $\frac{f_0}{f_1}$,

$$\zeta \approx -\frac{f_0}{f_1} - \frac{f_2}{f_1} \left(\frac{f_0}{f_1}\right)^2 \tag{38}$$

The inverse of the squares of the zeros of $\frac{c_P(\xi)}{\xi}$ equals [20, p. 305]

$$\sum_{k=1}^{N} \frac{1}{z_k^2} = \left(\frac{f_1}{f_0}\right)^2 - \frac{2f_2}{f_0} \geq 0$$

from which

$$\frac{1}{\zeta^2} = \left(\frac{f_1}{f_0}\right)^2 - \frac{2f_2}{f_0} - \sum_{k=2}^{N} \frac{1}{z_k^2}$$

and

$$\zeta^2 = \frac{1}{\left(\frac{f_1}{f_0}\right)^2 - \frac{2f_2}{f_0} - \sum_{k=2}^{N} \frac{1}{z_k^2}} \geq \left(\frac{f_0}{f_1}\right)^2 \frac{1}{1 - \frac{2f_2}{f_0}\left(\frac{f_0}{f_1}\right)^2}$$

where the inequality follows because all zeros are real. Thus, a sharper upper bound for ζ is found

$$\zeta \leq -\frac{f_0}{f_1} \frac{1}{\sqrt{1 - \frac{2f_2}{f_0}\left(\frac{f_0}{f_1}\right)^2}} \tag{39}$$

After expansion of the right-hand side in (39), we find

$$|\zeta| \geq \left(\frac{f_0}{f_1}\right) \left(1 + \frac{f_2}{f_0}\left(\frac{f_0}{f_1}\right)^2 + \frac{3}{2}\left\{\frac{f_2}{f_0}\left(\frac{f_0}{f_1}\right)^2\right\}^2 + O\left(\left\{\frac{f_2}{f_0}\left(\frac{f_0}{f_1}\right)^2\right\}^3\right)\right)$$

which should be compared with the Lagrange expansion up to third order,

$$-\zeta \approx \left(\frac{f_0}{f_1}\right)\left(1+\frac{f_2}{f_1}\left(\frac{f_0}{f_1}\right)+\left[2\left(\frac{f_2}{f_1}\right)^2-\frac{f_3}{f_1}\right]\left(\frac{f_0}{f_1}\right)^2\right)$$
$$=\left(\frac{f_0}{f_1}\right)\left(1+\frac{f_2}{f_0}\left(\frac{f_0}{f_1}\right)^2+2\left\{\frac{f_2}{f_0}\left(\frac{f_0}{f_1}\right)^2\right\}^2-\frac{f_3}{f_1}\left(\frac{f_0}{f_1}\right)^2\right)$$

In summary, based on the knowledge of the coefficients f_0, f_1 and f_2, the second largest zero ζ of $c_P(\xi)$ is approximated by a Lagrange series (38) up to second order, possesses an upper[9] bound (36) and a sharper bound (39).

Incidentally, we have also shown how subsequent terms in the Lagrange series can be computed from the Newton identities for the sum of inverse powers of the zeros. The combination of the knowledge of the Newton identities with the Lagrange series around a certain complex number can shed additional insight into the convergence of the Lagrange series.

C The function $F(\tau)$

We have shown that $\zeta \approx -\frac{1}{f_1}$ for $\tau > \frac{1}{N}$, which led to the result (2). We reconsider $F(\tau) = \lim_{\varepsilon\to 0} f_1$ in (3), which is also rewritten as

$$\beta F(\tau) = \sum_{j=1}^{N}\sum_{r=1}^{j}\frac{(N-1-j+r)!}{j(N-j)!}\tau^r \tag{40}$$

In this section, we explore properties of $F(\tau)$: in Section C.1, $F(\tau)$ is expressed as a Laplace transform, from which alternative exact forms for $F(\tau)$ are deduced in Section C.2. Finally, Section C.3 presents the asymptotic form (4) of $F(\tau)$ for $\tau = \frac{x}{N}$, with fixed x and large N.

C.1 $F(\tau)$ as a Laplace transform

Theorem 3 *For $\tau > \tau_c$, $F(\tau) = \lim_{\varepsilon\to 0} f_1$ can be expressed as a Laplace transform*

$$F(\tau) = \frac{1}{\beta}\int_0^\infty\left(\int_1^\infty \frac{dx}{x^{N+1}}\frac{(u+x)^N-1}{(u+x)-1}\right)e^{-\frac{1}{\tau}u}du \tag{41}$$

Proof: We rewrite (3) as

$$F(\tau) = \frac{1}{\delta}\sum_{j=1}^{N}\frac{x_j}{j}$$

with

$$x_j = \sum_{r=0}^{j-1}\frac{(N-j+r)!}{(N-j)!}\tau^r$$

[9] The interlacing property of the orthogonal polynomials provides us with lower bounds for ζ. The interlacing theorem for orthogonal polynomials states that between two zeros of $\rho_k(\xi)$, defined in (19), there is at least on zero of $\rho_l(\xi)$ with $l > k$. The best lower bound for ζ thus equals the second largest zero of $\rho_N(\xi)$, which is, unfortunately, more difficult to compute than ζ itself, because the largest zero is negative and unknown in contrast to $\rho_{N+1}(\xi)$ where it is zero.

which obeys the recursion

$$x_{j+1} = x_j(N-j)\tau + 1 \tag{42}$$

with $x_1 = 1$. Furthermore, $x_k = 0$ for $k < 1$. Indeed,

$$\begin{aligned} x_{j+1} &= \sum_{r=0}^{j} \frac{(N-j-1+r)!}{(N-j-1)!}\tau^r = \tau\,(N-j)\sum_{r=-1}^{j-1}\frac{(N-j+r)!}{(N-j)!}\tau^r \\ &= x_j(N-j)\tau + \tau\,(N-j)\,\frac{(N-j-1)!}{(N-j)!}\tau^{-1} = x_j(N-j)\tau + 1 \end{aligned}$$

Now, consider

$$g\,(z,N) = \sum_{j=0}^{N-1} x_{j+1}z^j = \frac{1}{z}\sum_{j=1}^{N} x_j z^j \tag{43}$$

with $g\,(0,N) = x_1 = 1$ so that

$$\int_0^1 g\,(z,N)\,dz = \sum_{j=0}^{N-1}\frac{x_{j+1}}{j+1} = \sum_{j=1}^{N}\frac{x_j}{j} = \delta F\,(\tau)$$

After multiplying both sides of the recursion (42) with z^j and summing over j, we obtain

$$\begin{aligned} g\,(z,N) &= \sum_{j=0}^{N-1} x_{j+1}z^j = \tau\sum_{j=0}^{N-1} x_j(N-j)z^j + \sum_{j=0}^{N-1} z^j \\ &= \tau N\sum_{j=1}^{N} x_j z^j - \tau\sum_{j=0}^{N} j x_j z^j + \frac{z^N-1}{z-1} \end{aligned}$$

since $x_0 = 0$. With the definition (43) and

$$\frac{d}{dz}\left(zg\,(z,N)\right) = \frac{1}{z}\sum_{j=0}^{N} j x_j z^j$$

we find

$$g\,(z,N) = \tau N z g\,(z,N) - \tau z\frac{d}{dz}\left(zg\,(z,N)\right) + \frac{z^N-1}{z-1}$$

Thus,

$$\frac{d}{dz}\left(zg\,(z,N)\right) = \left(N - \frac{1}{\tau z}\right)g\,(z,N) + \frac{z^N-1}{\tau z\,(z-1)}$$

The differential equation for g becomes

$$-\tau z^2\frac{d}{dz}\left(g\,(z,N)\right) + \left(\tau\,(N-1)\,z - 1\right)g\,(z,N) = -\frac{z^N-1}{z-1}$$

The homogeneous differential equation is rewritten as

$$\frac{d}{dz}\left(\log h\,(z,N)\right) = \frac{\tau\,(N-1)\,z - 1}{\tau z^2} = \frac{(N-1)}{z} - \frac{1}{\tau z^2}$$

Integration yields

$$\log h\,(z,N) = (N-1)\ln z + \frac{1}{\tau z} + \ln C$$

where C is a constant. Thus,

$$h(z,N) = Cz^{N-1}e^{\frac{1}{\tau z}}$$

Using the variation of a constant method yields

$$g(z,N) = C(z)\, z^{N-1}e^{\frac{1}{\tau z}}$$

where the function $C(z)$ must obey the differential equation. Hence, after substitution, we have

$$g'(z,N) = C'(z)\, z^{N-1}e^{\frac{1}{\tau z}} + C(z)\frac{d}{dz}\left(z^{N-1}e^{\frac{1}{\tau z}}\right)$$

and

$$-\tau z^2 C'(z)\, z^{N-1}e^{\frac{1}{\tau z}} - \tau z^2 C(z)\frac{d}{dz}\left(z^{N-1}e^{\frac{1}{\tau z}}\right) + (\tau(N-1)z-1)\, C(z)\, z^{N-1}e^{\frac{1}{\tau z}} = -\frac{z^N-1}{z-1}$$

Since

$$\begin{aligned}-\tau z^2 C(z)\frac{d}{dz}\left(z^{N-1}e^{\frac{1}{\tau z}}\right) &= -\tau z^2 C(z)(N-1)\, z^{N-2}e^{\frac{1}{\tau z}} + \tau z^2 C(z)\, z^{N-1}e^{\frac{1}{\tau z}}\left(\frac{1}{\tau z^2}\right)\\ &= \{-\tau z(N-1)+1\}\, z^{N-1}C(z)\, e^{\frac{1}{\tau z}}\end{aligned}$$

we see (as required by the method of the variation of a constant) that

$$C'(z) = \frac{1}{\tau}\frac{z^N-1}{(z-1)\, z^{N+1}}e^{-\frac{1}{\tau z}}$$

from which $C'(0)=0$ for any finite N. After integration, we arrive at

$$g(z,N) = \frac{1}{\tau}z^{N-1}e^{\frac{1}{\tau z}}\left(\int_0^z \frac{u^N-1}{(u-1)\, u^{N+1}}e^{-\frac{1}{\tau u}}du + C(0)\right)$$

where the constant $C(0)$ needs to be chosen so that $g(0,N)=1$. The only possible value is $C(0)=0$ in order to have a finite limit for $\lim_{z\to 0} g(z,N)$. Then,

$$g(z,N) = \frac{1}{\tau}z^{N-1}e^{\frac{1}{\tau z}}\int_0^z \frac{u^N-1}{(u-1)\, u^{N+1}}e^{-\frac{1}{\tau u}}du$$

Substituting $u=\frac{1}{y}$,

$$g(z,N) = \frac{1}{\tau}z^{N-1}e^{\frac{1}{\tau z}}\int_{\frac{1}{z}}^{\infty} \frac{\left(1-y^N\right)}{(1-y)}e^{-\frac{1}{\tau}y}dy \tag{44}$$

Finally,

$$\begin{aligned}\delta F(\tau) &= \frac{1}{\tau}\int_0^1 dz\; z^{N-1}e^{\frac{1}{\tau z}}\int_{\frac{1}{z}}^{\infty}\frac{\left(1-y^N\right)}{(1-y)}e^{-\frac{1}{\tau}y}dy\\ &= \frac{1}{\tau}\int_1^{\infty} dx\;\frac{1}{x^{N+1}}\int_x^{\infty}\frac{\left(1-y^N\right)}{(1-y)}e^{-\frac{1}{\tau}(y-x)}dy\end{aligned}$$

Let $u=y-x$ in the y-integral, then

$$\delta F(\tau) = \frac{1}{\tau}\int_1^{\infty} dx\;\frac{1}{x^{N+1}}\int_0^{\infty}\frac{\left(1-(u+x)^N\right)}{(1-u-x)}e^{-\frac{1}{\tau}u}du$$

so that $F(\tau)$ can be written as a Laplace transform (41). □

C.2 $F(\tau)$ in terms of exponential integrals

The integrand in (41) can be rewritten as

$$h_N(u) = \int_1^\infty \frac{dx}{x^{N+1}} \frac{(u+x)^N - 1}{(u+x)-1} = \int_0^1 \frac{(yu+1)^N - y^N}{(yu+1)-y} dy$$

so that we obtain an alternative integral

$$\beta F(\tau) = \int_0^\infty \left(\int_0^1 \frac{(yu+1)^N - y^N}{(yu+1)-y} dy \right) e^{-\frac{1}{\tau}u} du$$

or

$$\beta F(\tau) = \int_0^1 \left(\int_0^\infty \frac{(yu+1)^N e^{-\frac{1}{\tau}u}}{yu+1-y} du \right) dy - \int_0^1 y^N \left(\int_0^\infty \frac{e^{-\frac{1}{\tau}u}}{yu+1-y} du \right) dy \tag{45}$$

which will be exploited below.

In the next Theorem 4, we show that $F(\tau)$ can be expressed in terms of the exponential integrals $E_n(x)$ of integer order n, defined in [1, Chapter 5] as

$$E_n(x) = \int_1^\infty \frac{e^{-xt}}{t^n} dt$$

Theorem 4 *For $\tau > \frac{1}{N}$, $F(\tau) = \lim_{\varepsilon \to 0} f_1$ equals*

$$F(\tau) = \frac{N!}{\beta} \sum_{k=1}^{N+1} \frac{L_k(\tau)}{(N+1-k)!} - \frac{1}{\beta} \int_0^\infty \frac{e^w E_{N+1}(w)\, dw}{w + \frac{1}{\tau}} \tag{46}$$

where

$$L_k(\tau) = \int_0^\infty \frac{e^w E_k(w)}{\left(w + \frac{1}{\tau}\right)^k} dw \tag{47}$$

Proof: We start with the second u-integral in (45) for $\beta F(\tau)$,

$$\begin{aligned}
\int_0^\infty \frac{e^{-\frac{1}{\tau}u}}{yu+1-y} du &= \frac{e^{\frac{1}{\tau}\left(\frac{1}{y}-1\right)}}{y} \int_0^\infty \frac{e^{-\frac{1}{\tau}\left(u+\frac{1}{y}-1\right)}}{u+\frac{1}{y}-1} du \\
&= \frac{e^{\frac{1}{\tau}\left(\frac{1}{y}-1\right)}}{y} \int_0^\infty \int_{\frac{1}{\tau}}^\infty e^{-p\left(u+\frac{1}{y}-1\right)} dp du \\
&= \frac{e^{\frac{1}{\tau}\left(\frac{1}{y}-1\right)}}{y} \int_{\frac{1}{\tau}}^\infty e^{-p\left(\frac{1}{y}-1\right)} \int_0^\infty e^{-pu} du dp \\
&= \frac{1}{y} \int_{\frac{1}{\tau}}^\infty \frac{e^{-\left(p-\frac{1}{\tau}\right)\left(\frac{1}{y}-1\right)}}{p} dp \\
&= \frac{1}{y} \int_0^\infty \frac{e^{-w\left(\frac{1}{y}-1\right)}}{w+\frac{1}{\tau}} dw
\end{aligned}$$

where the reversal of integrations is allowed by absolute convergence (Fubinni's Theorem). The second u-integral in (45) for $\beta F(\tau)$ becomes

$$\int_0^1 y^N \left(\int_0^\infty \frac{e^{-\frac{1}{\tau}u}}{yu+1-y} du \right) dy = \int_0^\infty \frac{e^w dw}{w+\frac{1}{\tau}} \left(\int_0^1 e^{-w\frac{1}{y}} y^{N-1} dy \right)$$
$$= \int_0^\infty \frac{e^w dw}{w+\frac{1}{\tau}} \left(\int_1^\infty \frac{e^{-wx}}{x^{N+1}} dx \right)$$

or

$$\int_0^1 y^N \left(\int_0^\infty \frac{e^{-\frac{1}{\tau}u}}{yu+1-y} du \right) dy = \int_0^\infty \frac{e^w E_{N+1}(w)\, dw}{w+\frac{1}{\tau}} \tag{48}$$

We now focus on the first integral in (45) and start with

$$\int_0^\infty \frac{(yu+1)^N e^{-\frac{1}{\tau}u}}{yu+1-y} du = \frac{e^{\frac{1}{\tau}\left(\frac{1}{y}-1\right)}}{y} \int_0^\infty \frac{(yu+1)^N e^{-\frac{1}{\tau}\left(u+\frac{1}{y}-1\right)}}{u+\frac{1}{y}-1} du$$
$$= \frac{e^{\frac{1}{\tau}\left(\frac{1}{y}-1\right)}}{y} \int_0^\infty (yu+1)^N \int_{\frac{1}{\tau}}^\infty e^{-p\left(u+\frac{1}{y}-1\right)} dp du$$
$$= \frac{e^{\frac{1}{\tau}\left(\frac{1}{y}-1\right)} y^N}{y} \int_{\frac{1}{\tau}}^\infty e^{-p\left(\frac{1}{y}-1\right)} \left(\int_0^\infty \left(u+\frac{1}{y}\right)^N e^{-pu} du \right) dp$$

and

$$\int_0^\infty \left(u+\frac{1}{y}\right)^N e^{-pu} du = e^{\frac{p}{y}} \int_{\frac{1}{y}}^\infty w^N e^{-pw} dw = \frac{e^{\frac{p}{y}}}{p^{N+1}} \int_{\frac{p}{y}}^\infty t^N e^{-t} dt$$
$$= \frac{N!}{p^{N+1}} \sum_{j=0}^N \frac{\left(\frac{p}{y}\right)^j}{j!}$$

where the incomplete Gamma function for integer k

$$\int_x^\infty t^k e^{-t} dt = k! e^{-x} \sum_{j=0}^k \frac{x^j}{j!}$$

is used. Hence[10],

$$\int_0^\infty \frac{(yu+1)^N e^{-\frac{1}{\tau}u}}{yu+1-y} du = \frac{e^{\frac{1}{\tau}\left(\frac{1}{y}-1\right)} y^N}{y} \int_{\frac{1}{\tau}}^\infty e^{-p\left(\frac{1}{y}-1\right)} \left(\frac{N!}{p^{N+1}} \sum_{j=0}^N \frac{\left(\frac{p}{y}\right)^j}{j!} \right) dp$$
$$= N! e^{\frac{1}{\tau}\left(\frac{1}{y}-1\right)} y^{N-1} \sum_{j=0}^N \frac{\left(\frac{1}{y}\right)^j}{j!} \int_{\frac{1}{\tau}}^\infty \frac{e^{-p\left(\frac{1}{y}-1\right)}}{p^{N+1-j}} dp$$

[10] Notice that we cannot use the approximation for large N,

$$\sum_{j=0}^N \frac{\left(\frac{p}{y}\right)^j}{j!} \lesssim e^{\frac{p}{y}}$$

because then the p-integral diverges.

We consider now the first integral in the expression (45) for $\beta F(\tau)$,

$$\int_0^1 \left(\int_0^\infty \frac{(yu+1)^N e^{-\frac{1}{\tau}u}}{yu+1-y} du \right) dy = N! \int_0^1 e^{\frac{1}{\tau}\left(\frac{1}{y}-1\right)} y^{N-1} \sum_{j=0}^{N} \frac{\left(\frac{1}{y}\right)^j}{j!} \int_{\frac{1}{\tau}}^\infty \frac{e^{-p\left(\frac{1}{y}-1\right)}}{p^{N+1-j}} dp dy$$

$$= N! \sum_{j=0}^{N} \frac{1}{j!} \int_{\frac{1}{\tau}}^\infty \frac{e^{p-\frac{1}{\tau}}}{p^{N+1-j}} dp \int_0^1 e^{\left(\frac{1}{\tau}-p\right)\frac{1}{y}} y^{N-1-j} dy$$

$$= N! \sum_{j=0}^{N} \frac{1}{j!} \int_0^\infty \frac{e^w}{\left(w+\frac{1}{\tau}\right)^{N+1-j}} dw \int_0^1 e^{-w\frac{1}{y}} y^{N-1-j} dy$$

Since

$$\int_0^1 e^{-w\frac{1}{y}} y^{N-1-j} dy = \int_1^\infty \frac{e^{-wu}}{u^{N+1-j}} du = E_{N+1-j}(w)$$

we find that

$$\int_0^1 \left(\int_0^\infty \frac{(yu+1)^N e^{-\frac{1}{\tau}u}}{yu+1-y} du \right) dy = N! \sum_{j=0}^{N} \frac{1}{j!} \int_0^\infty \frac{e^w E_{N+1-j}(w)}{\left(w+\frac{1}{\tau}\right)^{N+1-j}} dw$$

$$= N! \sum_{k=1}^{N+1} \frac{L_k(\tau)}{(N+1-k)!} \tag{49}$$

which proves the theorem. □

An expression that avoids the summation is

$$\int_0^\infty \frac{(yu+1)^N e^{-\frac{1}{\tau}u}}{yu+1-y} du = \frac{e^{\frac{1}{\tau}\left(\frac{1}{y}-1\right)} y^N}{y} \int_{\frac{1}{\tau}}^\infty dp \frac{e^p}{p^{N+1}} \int_{\frac{p}{y}}^\infty t^N e^{-t} dt$$

Then,

$$\int_0^1 \left(\int_0^\infty \frac{(yu+1)^N e^{-\frac{1}{\tau}u}}{yu+1-y} du \right) dy = e^{-\frac{1}{\tau}} \int_0^1 dy e^{\frac{1}{\tau y}} y^{N-1} \int_{\frac{1}{\tau}}^\infty dp \frac{e^p}{p^{N+1}} \int_{\frac{p}{y}}^\infty t^N e^{-t} dt$$

$$= e^{-\frac{1}{\tau}} \int_{\frac{1}{\tau}}^\infty dp \frac{e^p}{p^{N+1}} \int_0^1 dy e^{\frac{1}{\tau y}} y^{N-1} \int_{\frac{p}{y}}^\infty t^N e^{-t} dt$$

$$= \frac{e^{-\frac{1}{\tau}}}{\tau^N} \int_{\frac{1}{\tau}}^\infty dp \frac{e^p}{p^{N+1}} \int_{\frac{1}{\tau}}^\infty du \frac{e^u}{u^{N+1}} \int_{\tau p u}^\infty t^N e^{-t} dt$$

We will not further use this triple integral, although it suggests a change of variables $s = p + u$ and $r = pu$, which, as we found, did not lead to useful results.

C.2.1 Other exact series for $\beta F(\tau)$

The expression (46) for $\beta F(\tau)$ in Theorem 4 will be further explored by using properties of the exponential integral.

After partial integration of $E_k(w) = \int_1^\infty \frac{e^{-wt}}{t^k} dt$, we obtain the recursion,

$$E_{k+1}(w) = \frac{1}{k} e^{-w} - \frac{w}{k} E_k(w) \tag{50}$$

After p iteration, we find

$$E_k(w) = e^{-w}\sum_{j=0}^{p-1}\frac{(-1)^j(k-j-2)!w^j}{(k-1)!} + \frac{(-1)^p(k-p-1)!w^p}{(k-1)!}E_{k-p}(w) \tag{51}$$

Introducing (51) into (47) gives

$$L_k(\tau) = \sum_{j=0}^{p-1}\frac{(-1)^j(k-j-2)!}{(k-1)!}\int_0^\infty \frac{w^j dw}{\left(w+\frac{1}{\tau}\right)^k} + \frac{(-1)^p(k-p-1)!}{(k-1)!}\int_0^\infty \frac{w^p e^w}{\left(w+\frac{1}{\tau}\right)^k}E_{k-p}(w)\,dw$$

Further, we use the Beta function integral,

$$\int_0^\infty \frac{w^j dw}{\left(w+\frac{1}{\tau}\right)^k} = \tau^k\int_0^\infty \frac{w^j dw}{(\tau w+1)^k} = \tau^{k-j-1}\int_0^\infty \frac{u^j du}{(u+1)^k} = \tau^{k-j-1}\frac{\Gamma(j+1)\Gamma(k-j-1)}{\Gamma(k)}$$

so that

$$L_k(\tau) = \sum_{j=0}^{p-1}\frac{(-1)^j((k-j-2)!)^2 j!}{((k-1)!)^2}\tau^{k-j-1} + \frac{(-1)^p(k-p-1)!}{(k-1)!}\int_0^\infty \frac{w^p e^w}{\left(w+\frac{1}{\tau}\right)^k}E_{k-p}(w)\,dw$$

Finally, if $p = k-1$, then

$$L_k(\tau) = \sum_{j=0}^{k-2}\frac{(-1)^j((k-j-2)!)^2 j!}{((k-1)!)^2}\tau^{k-j-1} + \frac{(-1)^{k-1}}{(k-1)!}\int_0^\infty \frac{w^{k-1}e^w}{\left(w+\frac{1}{\tau}\right)^k}E_1(w)\,dw$$

Introduced in (49) yields

$$\begin{aligned}\int_0^1\left(\int_0^\infty \frac{(yu+1)^N e^{-\frac{1}{\tau}u}}{yu+1-y}du\right)dy &= N!\sum_{k=0}^{N}\frac{1}{(N-k)!}\sum_{j=0}^{k-1}\frac{(-1)^j((k-j-1)!)^2 j!}{(k!)^2}\tau^{k-j}\\ &\quad+\sum_{k=0}^{N}\frac{N!}{(N-k)!}\frac{(-1)^k}{k!}\int_0^\infty \frac{w^k e^w}{\left(w+\frac{1}{\tau}\right)^{k+1}}E_1(w)\,dw\end{aligned}$$

The first sum can be rewritten as

$$\begin{aligned}T &= \sum_{k=1}^{N}\frac{1}{(N-k)!}\sum_{j=0}^{k-1}\frac{(-1)^j((k-j-1)!)^2 j!}{(k!)^2}\tau^{k-j}\\ &= \sum_{k=1}^{N}\frac{1}{(N-k)!}\sum_{m=1}^{k}\frac{(-1)^{k-m}((m-1)!)^2(k-m)!}{(k!)^2}\tau^m\\ &= \sum_{m=1}^{N}\left(\sum_{k=m}^{N}\frac{1}{(N-k)!}\frac{(-1)^{k-m}(k-m)!}{(k!)^2}\right)((m-1)!)^2\tau^m\\ &= \frac{1}{N!}\sum_{m=1}^{N}\left(\sum_{k=m}^{N}\binom{N}{k}\frac{(-1)^{k-m}(k-m)!}{k!}\right)((m-1)!)^2\tau^m\end{aligned}$$

while the last sum equals

$$\begin{aligned}\sum_{k=0}^{N}\frac{N!}{(N-k)!}\frac{(-1)^k}{k!}\int_0^\infty \frac{w^k e^w}{\left(w+\frac{1}{\tau}\right)^{k+1}}E_1(w)\,dw &= \int_0^\infty \frac{e^w E_1(w)}{w+\frac{1}{\tau}}\sum_{k=0}^{N}\binom{N}{k}\left(\frac{-w}{w+\frac{1}{\tau}}\right)^k dw\\ &= \frac{1}{\tau^N}\int_0^\infty \frac{e^w E_1(w)}{\left(w+\frac{1}{\tau}\right)^{N+1}}dw\end{aligned}$$

After combining the above, we arrive at

$$\int_0^1 \left(\int_0^\infty \frac{(yu+1)^N e^{-\frac{1}{\tau}u}}{yu+1-y} du \right) dy = \sum_{m=1}^N C_m \tau^m + \tau \int_0^\infty \frac{e^w E_1(w)}{(\tau w+1)^{N+1}} dw \tag{52}$$

with

$$C_m = ((m-1)!)^2 \sum_{k=m}^N \binom{N}{k} \frac{(-1)^{k-m}(k-m)!}{k!} \tag{53}$$

Theorem 5 *The Taylor series of $\beta F(\tau)$ is defined by*

$$\beta F(\tau) = \sum_{j=1}^N B_j \tau^j \tag{54}$$

with

$$B_j = \sum_{k=j}^N \frac{(N-k+j-1)!}{(N-k)!k} \tag{55}$$

Moreover, another form for B_j is

$$B_j = ((j-1)!)^2 \sum_{k=j}^N \binom{N}{k} \frac{(-1)^{k-j}(k-j)!}{k!} \tag{56}$$

Proof: Reversing the j- and r-sum in (40) yields

$$\beta F(\tau) = \sum_{j=1}^N \left(\sum_{r=j}^N \frac{(N-r+j-1)!}{(N-r)!r} \right) \tau^j$$

which proves (54) and (55). We will now prove that $B_j = C_j$, where C_j is defined in (53). First, we prove that

$$\int_0^\infty \frac{e^w E_n(w)}{(\tau w+1)} dw = \int_0^\infty \frac{e^w E_1(w)}{(\tau w+1)^n} dw$$

Introducing the definition of the exponential integral of order n yields

$$\begin{aligned}
\int_0^\infty \frac{e^w E_n(w)}{(\tau w+1)} dw &= \int_0^\infty \frac{e^w dw}{(\tau w+1)} \int_1^\infty \frac{e^{-wt}}{t^n} dt \\
&= \int_1^\infty \frac{dt}{t^n} \int_0^\infty \frac{e^{-w(t-1)} dw}{(\tau w+1)} \\
&= \int_0^\infty \frac{du}{(u+1)^n} \int_0^\infty \frac{e^{-wu} dw}{(\tau w+1)}
\end{aligned}$$

Let $y = \tau w + 1$, then

$$\begin{aligned}
\int_0^\infty \frac{e^w E_n(w)}{(\tau w+1)} dw &= \frac{1}{\tau} \int_0^\infty \frac{du}{(u+1)^n} \int_1^\infty \frac{e^{-(y-1)\frac{u}{\tau}} dy}{y} \\
&= \frac{1}{\tau} \int_0^\infty \frac{e^{\frac{u}{\tau}} du}{(u+1)^n} \int_1^\infty \frac{e^{-y\frac{u}{\tau}} dy}{y} \\
&= \frac{1}{\tau} \int_0^\infty \frac{e^{\frac{u}{\tau}} E_1\left(\frac{u}{\tau}\right)}{(u+1)^n} du = \int_0^\infty \frac{e^w E_1(w)}{(\tau w+1)^n} du
\end{aligned}$$

From (48), we find that

$$\beta F(\tau) = \int_0^1 \left(\int_0^\infty \frac{(yu+1)^N e^{-\frac{1}{\tau}u}}{yu+1-y} du \right) dy - \tau \int_0^\infty \frac{e^w E_1(w)}{(\tau w+1)^{N+1}} dw$$

The uniqueness of the Taylor series implies that (54) equals the Taylor series in (52). □

C.2.2 The coefficients B_j

We present other properties of the Taylor coefficients B_j, defined in (55). Starting from

$$\sum_{r=1}^{N} \frac{(N+j-1-r)!}{(N-r)!r} = \sum_{r=1}^{j-1} \frac{(N+j-1-r)!}{(N-r)!r} + \sum_{r=j}^{N} \frac{(N+j-1-r)!}{(N-r)!r}$$

and using (see [19, p. 410]),

$$\sum_{r=1}^{N} \frac{(N+j-1-r)!}{(N-r)!r} = \frac{(N+j-1)!}{N!} [\psi(N+j) - \psi(j)] = \frac{(N+j-1)!}{N!} \sum_{k=j}^{N+j-1} \frac{1}{k}$$

shows that

$$B_j = \frac{(N+j-1)!}{N!} \sum_{k=j}^{N+j-1} \frac{1}{k} - \sum_{r=1}^{j-1} \frac{(N+j-1-r)!}{(N-r)!r} \tag{57}$$

A recursion for the Taylor coefficient

$$B_j(N) = \sum_{r=j}^{N} \frac{(N+j-1-r)!}{(N-r)!r}$$

is

$$B_{j+1}(N) = B_{j+1}(N-1) + jB_j(N) - \frac{(N-1)!}{(N-j)!} \tag{58}$$

Indeed,

$$\begin{aligned} B_{j+1}(N) &= \sum_{r=j+1}^{N} \frac{(N+j-r)!}{(N-r)!r} = \sum_{r=j+1}^{N} \frac{(N+j-r)(N+j-1-r)!}{(N-r)!r} \\ &= \sum_{r=j+1}^{N} \frac{(N+j-1-r)!}{(N-r-1)!r} + j \sum_{r=j+1}^{N} \frac{(N+j-1-r)!}{(N-r)!r} \\ &= B_{j+1}(N-1) + j \left(B_j(N) - \frac{(N-1)!}{(N-j)!j} \right) \end{aligned}$$

C.3 Order estimate of $F(\tau)$ for large N

The exponential integral is bounded [1, 5.1.9] by

$$\frac{1}{x+n} < e^x E_n(x) \leq \frac{1}{x+n-1} \tag{59}$$

The bound (59) will play a crucial role in the proof of Theorem 6 below. In the determination of the order of $F(\tau)$ for large N (and fixed $x = N\tau$), the bound (59) can be used when the last term in the summation is treated separately

$$\int_0^1 \left(\int_0^\infty \frac{(yu+1)^N e^{-\frac{1}{\tau}u}}{yu+1-y} du \right) dy = N! \sum_{j=0}^{N} \frac{1}{j!} \int_0^\infty \frac{e^w E_{N+1-j}(w)}{\left(w+\frac{1}{\tau}\right)^{N+1-j}} dw$$
$$= N! \sum_{j=0}^{N-1} \frac{1}{j!} \int_0^\infty \frac{e^w E_{N+1-j}(w)}{\left(w+\frac{1}{\tau}\right)^{N+1-j}} dw + \int_0^\infty \frac{e^w E_1(w)}{w+\frac{1}{\tau}} dw$$

The definition (47) of $L_k(\tau)$ and the inequality $E_k(w) < E_{k-1}(w)$ shows that, for $k > 1$,

$$L_k(\tau) = \int_0^\infty \frac{e^w E_k(w)}{\left(w+\frac{1}{\tau}\right)^k} dw < \int_0^\infty \frac{e^w E_{k-1}(w)}{\left(w+\frac{1}{\tau}\right)^{k-1}} \frac{1}{\left(w+\frac{1}{\tau}\right)} dw < \tau L_{k-1}(\tau)$$

and

$$\frac{dL_k(\tau)}{d\tau} = \frac{k}{\tau^2} \int_0^\infty \frac{e^w E_k(w)}{\left(w+\frac{1}{\tau}\right)^{k+1}} dw > \frac{k}{\tau^2} L_{k+1}(\tau)$$

Using $\frac{dE_n(x)}{dx} = -E_{n-1}(x)$, after partial integration of $L_k(\tau)$, we obtain, for $k > 1$,

$$L_k(\tau) = \frac{\tau^{k-1}}{(k-1)^2} + \frac{1}{(k-1)} \int_0^\infty \frac{e^w \left(E_k(w) - E_{k-1}(w)\right)}{\left(w+\frac{1}{\tau}\right)^{k-1}} dw$$

Since $E_k(w) < E_{k-1}(w)$, we find, for $k > 1$, that

$$L_k(\tau) < \frac{\tau^{k-1}}{(k-1)^2} \tag{60}$$

The function $L_1(\tau)$ requires a different treatment,

$$L_1(\tau) = \int_0^\infty \frac{e^w E_1(w)}{w+\frac{1}{\tau}} dw = \int_0^\infty \frac{e^w dw}{\left(w+\frac{1}{\tau}\right)} \int_w^\infty \frac{e^{-t}}{t} dt$$
$$= \int_0^\infty dw \int_w^\infty dt \frac{e^{-(t-w)}}{\left(w+\frac{1}{\tau}\right) t} = \int_0^\infty dw \int_0^\infty dy \frac{e^{-y}}{\left(w+\frac{1}{\tau}\right)(y+w)}$$
$$= \int_0^\infty e^{-y} dy \int_0^\infty \frac{dw}{\left(w+\frac{1}{\tau}\right)(y+w)}$$

The integral, computed after partial fraction expansion,

$$\int_0^\infty \frac{dw}{\left(w+\frac{1}{\tau}\right)(y+w)} = \frac{1}{\left(\frac{1}{\tau}-y\right)} \left\{ \int_0^\infty \frac{dw}{(y+w)} - \int_0^\infty \frac{dw}{\left(w+\frac{1}{\tau}\right)} \right\}$$
$$= \frac{\ln(y\tau)}{y-\frac{1}{\tau}} = \frac{\ln(y) - \ln\left(\frac{1}{\tau}\right)}{y-\frac{1}{\tau}}$$

shows that $\frac{\ln(y\tau)}{y-\frac{1}{\tau}}$ is decreasing in y and $\frac{1}{\tau}$. Moreover, we find that

$$L_1(\tau) = \int_0^\infty \frac{\ln(y\tau) e^{-y}}{y-\frac{1}{\tau}} dy = \int_0^\infty \frac{\ln(u) e^{-\frac{u}{\tau}}}{u-1} du$$

Thus,

$$L_1(\tau) = \int_0^\infty \frac{e^w E_1(w)}{\left(w + \frac{1}{\tau}\right)} dw = \int_0^\infty \frac{\ln(u)\, e^{-\frac{u}{\tau}}}{u-1} du$$

Now, let $t = \frac{1}{\tau}$, then

$$\begin{aligned}\frac{dL_1(t)}{dt} &= -\int_0^\infty \frac{u \ln(u)\, e^{-tu}}{u-1} du = -\int_0^\infty \frac{(u-1+1)\ln(u)\, e^{-tu}}{u-1} du \\ &= -\int_0^\infty \ln(u)\, e^{-tu} du - \int_0^\infty \frac{\ln(u)\, e^{-tu}}{u-1} du\end{aligned}$$

With

$$\begin{aligned}\int_0^\infty \ln(u)\, e^{-tu} du &= \frac{1}{t}\int_0^\infty \ln\left(\frac{y}{t}\right) e^{-y} dy = \frac{1}{t}\int_0^\infty \ln(y)\, e^{-y} dy - \frac{\ln t}{t}\int_0^\infty e^{-y} dy \\ &= -\frac{\gamma}{t} - \frac{\ln t}{t}\end{aligned}$$

because $\int_0^\infty e^{-y} \ln y dy = \Gamma'(1) = -\gamma = -0.5227$, we obtain the first-order differential equation

$$\frac{dL_1(t)}{dt} = \frac{\gamma + \ln t}{t} - L_1(t)$$

Since $\frac{u\ln(u)}{u-1} \leq \sqrt{u}$ (with equality for $u = 1$ and tight for $0 \leq u \leq 1$),

$$0 \leq -\frac{dL_1(t)}{dt} < \int_0^\infty \sqrt{u} e^{-tu} du = \frac{1}{t\sqrt{t}}\Gamma\left(\frac{3}{2}\right)$$

the differential equation provides us with

$$\tau(\gamma - \ln\tau) < L_1(\tau) < \tau(\gamma - \ln\tau) + \tau^{\frac{3}{2}}\frac{\sqrt{\pi}}{2}$$

and the upper bound is tight for $\tau < 1$, but loose for $\tau > 1$. Since we are interested in small $\tau = \frac{x}{N}$, the upper bound suffices and illustrates that $L_1\left(\frac{x}{N}\right) = O\left(\frac{\ln N}{N}\right)$.

The main result here is the following theorem

Theorem 6 *For $\tau = \frac{x}{N}$, $F(\tau) = \lim_{\varepsilon\to 0} f_1$ behaves for large N and fixed $x > 1$ as*

$$F\left(\frac{x}{N}\right) \sim \frac{1}{\delta}\frac{x\sqrt{2\pi}}{(x-1)^2}\frac{\exp\left(N\left\{\log x + \frac{1}{x} - 1\right\}\right)}{\sqrt{N}}$$

Proof: Using the bounds (59) for the exponential integral, the negative term in (46)

$$\int_0^\infty \frac{dw}{\left(w + \frac{1}{\tau}\right)(w + N - 1)} < \int_0^\infty \frac{e^w E_{N+1}(w)\, dw}{w + \frac{1}{\tau}} \leq \int_0^\infty \frac{dw}{\left(w + \frac{1}{\tau}\right)(w + N)}$$

With

$$\begin{aligned}\int_0^\infty \frac{dw}{\left(w + \frac{1}{\tau}\right)(w + m)} &= -\left(m - \frac{1}{\tau}\right)\ln\frac{w+m}{w + \frac{1}{\tau}}\Bigg|_0^\infty \\ &= \left(m - \frac{1}{\tau}\right)\ln m\tau\end{aligned}$$

we arrive at

$$\left(N-1-\frac{1}{\tau}\right)\ln\left(N-1\right)\tau<\int_0^1 y^N\left(\int_0^\infty\frac{e^{-\frac{1}{\tau}u}}{yu+1-y}du\right)dy\leq\left(N-\frac{1}{\tau}\right)\ln N\tau$$

which demonstrates, since $x=N\tau>1$ and fixed, that the negative term in (46) grows as $N\left(1-\frac{1}{x}\right)\log x$ for large N.

Using the bounds (59) in the expression (47) of $L_k\left(\tau\right)$ yields, for $0\leq j<N$,

$$\int_0^\infty\frac{dw}{\left(w+\frac{1}{\tau}\right)^{N+1-j}\left(w+N+1-j\right)}<\int_0^\infty\frac{e^wE_{N+1-j}\left(w\right)dw}{\left(w+\frac{1}{\tau}\right)^{N+1-j}}\leq\int_0^\infty\frac{dw}{\left(w+\frac{1}{\tau}\right)^{N+1-j}\left(w+N-j\right)}$$

The upper bound is further

$$\begin{aligned}\int_0^\infty\frac{e^wE_{N+1-j}\left(w\right)dw}{\left(w+\frac{1}{\tau}\right)^{N+1-j}}&\leq\int_0^\infty\frac{dw}{\left(w+\frac{1}{\tau}\right)^{N+1-j}\left(w+N-j\right)}<\frac{1}{N-j}\int_0^\infty\frac{dw}{\left(w+\frac{1}{\tau}\right)^{N+1-j}}\\&=\frac{\tau^{N-j}}{\left(N-j\right)^2}\end{aligned}$$

which also follows from (60). Hence,

$$\int_0^1\left(\int_0^\infty\frac{\left(yu+1\right)^Ne^{-\frac{1}{\tau}u}}{yu+1-y}du\right)dy<L_1\left(\tau\right)+N!\tau^N\sum_{j=0}^{N-1}\frac{\tau^{-j}}{j!}\frac{1}{\left(N-j\right)^2}\tag{61}$$

When making the rather crude approximation

$$\sum_{j=0}^{N-1}\frac{\tau^{-j}}{j!}\frac{1}{\left(N-j\right)^2}<\sum_{j=0}^{N-1}\frac{\tau^{-j}}{j!}<e^{\frac{1}{\tau}}$$

we obtain the upper bound

$$\beta F\left(\tau\right)<L_1\left(\tau\right)+N!\tau^Ne^{\frac{1}{\tau}}\tag{62}$$

A much better approximation, that is asymptotically correct for large N and constant $x>1$, is

$$\sum_{j=0}^{N-1}\frac{\left(\frac{N}{x}\right)^j}{j!}\frac{1}{\left(N-j\right)^2}\approx\frac{e^{\frac{N}{x}}}{\left(1-\frac{1}{x}\right)^2N^2}$$

The arguments require order estimates for sums $\sum_{m=a}^b u_m$, where $u_m=e^{-y}\frac{y^m}{m!}$, derived in a theorem by Hardy [9, p. 200]. Since $\tau=\frac{x}{N}$, with $x=1+\delta>1$, we obtain

$$\sum_{j=0}^{N-1}\frac{\tau^{-j}}{j!}=\sum_{j=0}^{N-1}\frac{\left(\frac{N}{x}\right)^j}{j!}=\sum_{j=0}^{\frac{N}{x}(1+\delta)-1}\frac{\left(\frac{N}{x}\right)^j}{j!}$$

The largest term in the j-sum occurs at $j=\frac{N}{x}$. Hardy shows, that for large N and $0<\delta<1$, the sum is very close to $e^{\frac{N}{x}}$ with error at most $O\left(e^{-\frac{1}{3}\delta^2}\right)$. Moreover, for $|h|\leq y^\zeta$ (and $\frac{1}{2}<\zeta<\frac{2}{3}$), $u_m=e^{-y}\frac{y^m}{m!}$ with $m=[y]+h$ equals

$$u_m=\sqrt{\frac{1}{2\pi\left[y\right]}}e^{-\frac{h^2}{2[y]}}\left\{1+O\left(\frac{|h|+1}{y}\right)+O\left(\frac{h^3}{y^2}\right)\right\}$$

Since the terms $u_{[y]+h}$ are increasingly peaked around the maximum $y = \frac{N}{x}$, we can approximate

$$e^{-\frac{1}{\tau}} \sum_{j=0}^{N-1} \frac{\tau^{-j}}{j!} \frac{1}{(N-j)^2} \approx \frac{1}{\left(N - \left[\frac{N}{x}\right]\right)^2} \sum_{h=-\left[\frac{N}{x}\right]^{\zeta}}^{\left[\frac{N}{x}\right]^{\zeta}} \frac{e^{-\frac{xh^2}{2N}}}{\sqrt{2\pi \left[\frac{N}{x}\right]}} \approx \frac{1}{N^2 \left(1 - \frac{1}{x}\right)^2}$$

Hence, for large N and fixed $x = \tau N$ in the dominant term (61) for $\beta F(\tau)$, we arrive at

$$\begin{aligned} \beta F\left(\frac{N}{x}\right) &\approx L_1\left(\frac{x}{N}\right) + N!\left(\frac{x}{N}\right)^N \sum_{j=0}^{N-1} \frac{\left(\frac{N}{x}\right)^j}{j!} \frac{1}{(N-j)^2} \\ &\sim O\left(\frac{\ln N}{N}\right) + N!\left(\frac{x}{N}\right)^N \frac{e^{\frac{N}{x}}}{\left(1 - \frac{1}{x}\right)^2 N^2} \end{aligned}$$

Using Stirling's approximation $N! \approx \sqrt{2\pi N} N^N e^{-N}$ and $\beta = \tau\delta = \frac{x}{N}\delta$, we finally obtain

$$F\left(\frac{N}{x}\right) \sim \frac{1}{\delta} \frac{N}{x} \frac{\sqrt{2\pi N} N^N e^{-N}}{N^N \left(1 - \frac{1}{x}\right)^2 N^2} \left(x e^{\frac{1}{x}}\right)^N$$

which proves the theorem after some simplifications. □