

Exact solution of the Kermack and McKendrick SIR differential equations

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1 September 2020

5 March 2021

Abstract

Several exact expansions as well as lower and upperbounds of the Kermack and McKendrick SIR equations are presented.

1 SIR governing equations

In their seminal paper [1], Kermack and McKendrick derive the differential equations for SIR epidemics in a homogeneous population (i.e. complete graph) with constant infection rate β and curing rate δ

$$\frac{dx}{dt} = -\beta xy \quad \frac{dy}{dt} = \beta xy - \delta y \quad \frac{dz}{dt} = \delta y \quad (1)$$

where x, y, z denotes the number of susceptible, infected and removed items in a fixed population of size $N = x + y + z$. We follow here the original notation of Kermack and McKendrick [1], whereas today, one usually writes $x = S$, $y = I$ and $z = R$. The set (1) is a special case of the general Kermack-McKendrick theory for constant rates. The Kermack-McKendrick differential equations with constant rates β and δ in (1) describe the basic SIR model for a disease without re-infections and appear in nearly each book and course on epidemics (see e.g. [2, 3, 4, 5]). Even today in Corona times, predictions and first order estimates of infected individuals are based on the SIR equations (1).

Here, we present exact solutions, which, at the best of our knowledge, have not yet appeared inspite of the fundamental role of the SIR differential equation (1) in the theory of epidemics. Numerous approximate solutions of (1) exist (see e.g. [6, 7]) and the first approximation is presented by Kermack and McKendrick [1], which is here revisited and generalized. Tedious mathematical derivations are placed in Appendices.

As usual in SIS epidemics, we denote the effective infection rate $\tau = \frac{\beta}{\delta}$, which is equal to the basic reproduction number R_0 . A key observation of Kermack and McKendrick [1] is that

$$\frac{dx}{dz} = -\tau x$$

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whose solution is $\log \frac{x(t)}{x_0} = -\tau z(t)$, because initially there are no removed, $z(0) = 0$, while $x_0 = x(0)$ is the initial number of susceptible items. Writing $y = N - x - z$ in the last SIR differential equation in (1) and introducing $x = x_0 e^{-\tau z}$ yields

$$\frac{dz}{dt} = \delta (N - x_0 e^{-\tau z} - z) \quad (2)$$

Hence, the set of differential equations in (1) is equivalent to

$$x = x_0 e^{-\tau z} \quad y = N - x - z \quad \frac{dz}{dt} = \delta (N - x_0 e^{-\tau z} - z)$$

where only one differential equation (2) remains.

Kermack and McKendrick [1] integrate (2) with the scaled time $t^* = \delta t$, taken into account that $z(0) = 0$, and present the exact result

$$t^* = \int_0^z \frac{du}{N - x_0 e^{-\tau u} - u} \quad (3)$$

If the effective infection rate τ is a function of time t , then the differential equation (2) cannot be directly integrated anymore. In other words, the confinement to constant rates greatly simplifies the analysis of the SIR differential equations. This paper mainly concentrates on the differential (2) and the integral (3).

The parameter N is eliminated if we define the fraction of susceptible items by $\xi = \frac{x}{N}$, of infected by $\eta = \frac{y}{N}$ and of removed by $\zeta = \frac{z}{N}$ so that

$$\xi + \eta + \zeta = 1$$

but the initial conditions with a zero recovered fraction, $\zeta_0 = 0$, obey

$$\xi_0 = 1 - \eta_0$$

The differential equation (2) is transformed into

$$\frac{d\zeta}{dt^*} = 1 - \xi_0 e^{-\tau \zeta} - \frac{1}{N} \zeta \quad (4)$$

The integral (3) for the scaled time becomes

$$t^* = \frac{1}{N} \int_0^{N\zeta} \frac{du}{1 - \xi_0 e^{-\tau u} - \frac{1}{N} u}$$

We define the *normalized effective infection rate* by $\theta = N\tau$ and, expect from SIS epidemics [8] on the complete graph, that the epidemic threshold $\tau_c \approx \frac{1}{N}$ and $\theta_c \approx 1$. In other words, the generalization to networks would be $\theta_G = \frac{\tau}{\tau_c}$, where τ_c is the epidemic threshold for SIR spread in a graph G . Let $w = \frac{u}{N}$, then we arrive at the (scaled) time $t^* = \delta t$, measured in units of the average curing time $\frac{1}{\delta}$, as a function of the fraction ζ of removed items in a homogeneous population or complete graph,

$$t^* = t_\theta^*(\zeta) = \int_0^\zeta \frac{dw}{1 - \xi_0 e^{-\theta w} - w} \quad (5)$$

The last differential equation in (1) in terms of fractions, $\frac{d\zeta}{dt^*} = \eta$, indicates that the fraction ζ of removed strictly increases with time t^* until the fraction of infected η equals zero, where ζ attains a

maximum ζ_{\max} . Since the fraction of infected $\eta = 1 - \xi_0 e^{-\theta\zeta} - \zeta \geq 0$, it follows that $1 - \zeta \geq \xi_0 e^{-\theta\zeta}$ and equality when $\eta = 0$ corresponds to the maximal fraction ζ_{\max} of removed items. At $w = \zeta_{\max}$, the denominator of the integral in (5) is zero and the corresponding time $t_{\theta}^*(\zeta_{\max})$ is obtained after infinitely long time. We require physically that the fraction of removed $\zeta \in [0, \zeta_{\max})$. The maximal fraction ζ_{\max} is expressed in terms of the Lambert function [9] in (31) in Appendix A. Fig. 1 plots the maximum removed fraction ζ_{\max} computed by (31) as a function of the initial fraction ξ_0 of susceptible for various normalized effective infection rates θ , starting from $\theta = 0.2$ up to $\theta = 2.0$ in steps of 0.2.

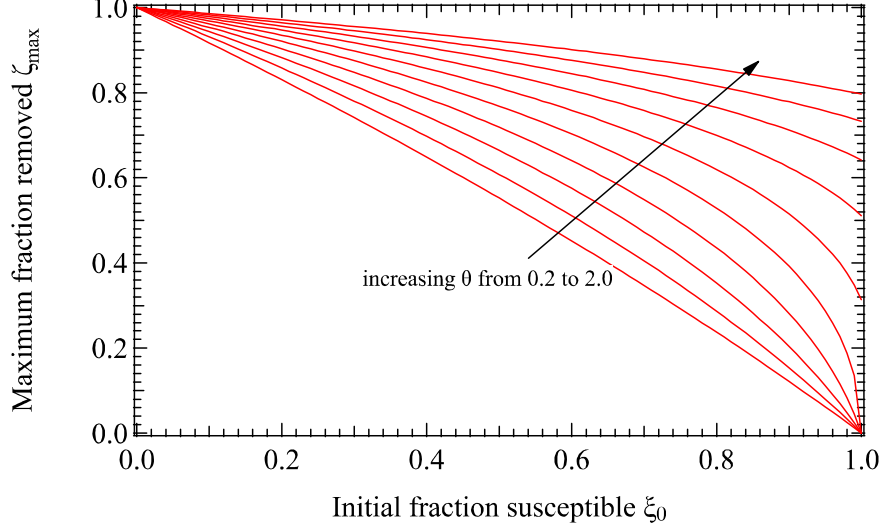


Figure 1: The maximum fraction ζ_{\max} of removed items in an SIR epidemics versus the initial fraction ξ_0 of susceptible, for various normalized effective infection rates θ .

Another approach of the scaled Kermack-McKendrick SIR equations (1) and closer aligned to the SIS epidemics focuses on the fraction η of infected, rather than on the fraction ξ of removed items,

$$\frac{d\eta}{dt^*} = (N\tau\xi - 1)\eta$$

and eliminates the fraction ξ of susceptible items via the conservation law $\xi + \eta + \zeta = 1$,

$$\frac{d\eta}{dt^*} = -\eta + N\tau(1 - \eta - \zeta)\eta$$

The differential equation $\frac{d\zeta}{dt^*} = \eta$ with $\zeta(0) = \zeta_0 = 0$, equivalent to $\zeta = \int_0^{t^*} \eta(u) du$, then yields

$$\frac{d\eta}{dt^*} = -\eta + N\tau\eta \left(1 - \eta - \int_0^{t^*} \eta(u) du \right) \quad (6)$$

After dividing both sides by η and integrating with respect to the normalized time $t^* = \delta t$, we have

$$\log \frac{\eta(t^*)}{\eta_0} = (N\tau - 1)t^* - N\tau \int_0^{t^*} \eta(u) du - N\tau \int_0^{t^*} du \int_0^v \eta(v) dv$$

Finally with $\int_0^{t^*} du \int_0^v \eta(v) dv = \int_0^{t^*} (t^* - u) \eta(u) du$, we arrive at the integral equation

$$\log \frac{\eta(t^*)}{\eta_0} = (N\tau - 1)t^* - N\tau \int_0^{t^*} (1 + t^* - u) \eta(u) du \quad (7)$$

which is also written in terms of the normalized effective infection rate $\theta = N\tau$, commonly referred to as the reproduction number $R_0 = \theta$, as

$$\eta(t^*) = \eta_0 e^{(\theta-1)t^*} e^{-\theta \int_0^{t^*} (1+t^*-u)\eta(u)du} \quad (8)$$

Since the integral in (8) is non-negative, it holds that $\eta(t^*) \leq \eta_0 e^{(\theta-1)t^*}$, which illustrates the role of the critical threshold $\theta_c = 1$ (or reproduction number $R_0 = 1$). Indeed, for a normalized effective infection strength $\theta > \theta_c = 1$, the fraction η of infected items *never* grows faster (in time) than an exponential with rate $\theta - 1 > 0$. On the other hand, below the critical threshold $\theta < \theta_c$, the fraction η of infected items *always* decays faster than an exponential with rate $\theta - 1 < 0$.

2 Solution of the SIR governing equation (4)

Formally, the exact solution (3) of the Kermack and McKendrick SIR differential equation (2) expresses the scaled time $t^* = H(\zeta)$ in terms of the fraction ζ of removed items, where the integral is

$$H(w) = \int_0^w \frac{du}{h(u)}$$

with $h(u) = 1 - \xi_0 e^{-\theta u} - u$. Since $h(u) \geq 0$, the integral $H(w)$ is increasing in $w \geq 0$. Moreover, fractions are contained in $[0, 1]$ and $h(u) \leq 1$, which implies that $H(w) \geq w$. Clearly¹, there exists an inverse function H^{-1} so that $\zeta = H^{-1}(t^*)$ and $t^* = H(\zeta)$, similarly as $t = \arcsin y$, where $\arcsin y = \int_0^y \frac{du}{\sqrt{1-u^2}}$ and $y = \sin t$. From the key property of inverse functions

$$H(H^{-1}(t^*)) = t^*$$

differentiation yields

$$\frac{dH^{-1}(t^*)}{dt^*} = \frac{1}{\left. \frac{dH(x)}{dx} \right|_{x=H^{-1}(t^*)}} = h(H^{-1}(t^*))$$

which is nothing else than the differential equation (2).

Since the integral (3) is not analytically known, Kermack and McKendrick approximate $e^{-\theta\zeta} = 1 - \theta\zeta + \frac{1}{2}\theta^2\zeta^2 + O(\zeta^3)$ up to third order in (4) to obtain

$$\frac{d\zeta}{dt^*} = 1 - \xi_0 + (\xi_0\theta - 1)\zeta - \frac{\xi_0\theta^2}{2}\zeta^2$$

which is a Riccati differential equation

$$\frac{dw}{dt} = aw - bw^2 - c \quad (9)$$

whose solution is

$$w(t) = \frac{a}{2b} + \frac{\Upsilon}{2b} \tanh\left(\frac{t}{2}\Upsilon + \operatorname{arctanh}\left(\frac{2by_0 - a}{\Upsilon}\right)\right) \quad (10)$$

¹If $t^* = H(z)$ is continuous and strictly increasing from t_1^* to t_2^* as z increases from z_1 to z_2 , then there is a unique inverse function $z = H^{-1}(t^*)$, which is also continuous and strictly increasing from z_1 to z_2 as t^* increases from t_1^* to t_2^* . This theorem is proved in [10, p. 206].

where $\Upsilon = \sqrt{a^2 - 4bc}$. The solution (10) appeared already in [1] and is reviewed in [5, Sec. 2.3]. The Riccati differential equation (9) is directly integrated as

$$t_3 = \int_{w_0}^w \frac{du}{au - bu^2 - c}$$

which equals (after rewriting $au - bu^2 - c = \frac{\Upsilon^2}{4b} \left\{ 1 - \left(\frac{2b}{\Upsilon} \left(u - \frac{a}{2b} \right) \right)^2 \right\}$)

$$t_3 = \int_{w_0}^w \frac{du}{\frac{\Upsilon^2}{4b} \left\{ 1 - \left(\frac{2b}{\Upsilon} \left(u - \frac{a}{2b} \right) \right)^2 \right\}} = \frac{2}{\Upsilon} \operatorname{arctanh} \frac{2b}{\Upsilon} \left(u - \frac{a}{2b} \right) \Big|_{w_0}^w$$

Inversion (i.e. solving for w) leads to (10). Inserting $a = (\xi_0\theta - 1)$, $b = \frac{\xi_0\theta^2}{2}$ and $c = -(1 - \xi_0)$ provides us with the approximation t_3 for the time t^* as function of the fraction ζ of removed items in the population,

$$t_3 = \frac{2}{\Upsilon} \left\{ \operatorname{arctanh} \left(\frac{\xi_0\theta^2\zeta - (\xi_0\theta - 1)}{\Upsilon} \right) + \operatorname{arctanh} \frac{(\xi_0\theta - 1)}{\Upsilon} \right\} \quad (11)$$

with

$$\Upsilon = \sqrt{(\xi_0\theta - 1)^2 + 2\theta^2\xi_0(1 - \xi_0)}$$

Since [11, p. 103]

$$e^{-\theta\zeta} < 1 - \theta\zeta + \frac{1}{2}\theta^2\zeta^2$$

we conclude that (11) derived from the third order approximation in $e^{-\theta\zeta}$ upper bounds the correct time,

$$t_\theta^*(\zeta) < t_3$$

Consequently, the inverse relation deduced from (11) indicates that

$$\frac{2}{\Upsilon} \left\{ \operatorname{arctanh} \left(\frac{\xi_0\theta^2\zeta - (\xi_0\theta - 1)}{\Upsilon} \right) + \operatorname{arctanh} \frac{(\xi_0\theta - 1)}{\Upsilon} \right\} > t_\theta^*(\zeta)$$

and

$$\zeta(t^*) > \frac{1}{\xi_0\theta^2} \left\{ (\xi_0\theta - 1) + \Upsilon \tanh \left(\frac{\Upsilon}{2} t^* - \operatorname{arctanh} \frac{(\xi_0\theta - 1)}{\Upsilon} \right) \right\} \quad (12)$$

In other words, the “tanh”-approximation underestimates the fraction of removed items. Equivalently, the conservation law $\xi + \eta + \zeta = 1$ implies that the “tanh”-approximation overestimates the fraction η of infection items, as demonstrated earlier for SIS epidemics [12],[13].

2.1 The “tanh”-approximation for the average path length in small-world graphs

The “tanh”-approximation also appears in an approximate, but ingenious computation in [14] of the average path length in small-world graphs [15]. The Watts-Strogatz small-world graph $G_{WS}(p_r, k, N)$ has N nodes regularly placed and consecutively numbered on a ring. Each node i has $2k$ links connected to its direct neighbors $i - k, i - k + 1, \dots, i - 1, i + 1, \dots, i + k$ and the basic law of the degree $\sum_{j=1}^N d_j = 2L$ then tells us that the number of links $L = kN$. Each end point of a link has probability p_r to be rewired to a random node; in total, there are $s = p_r kN$ rewired links, called shortcuts. Newman *et al.* [14] consider a continuous version of the Watts-Strogatz small-world graph

$G_{WS}(p_r, k, N)$, where the one-dimensional ring lattice is treated as a continuum and shortcuts are assumed to have zero length. The neighborhood $b(r)$ of segment length r around a random point (node) on the circle consists of the set of points that can be reached by following paths of length r or less on the graph $G_{WS}(p_r, k, N)$. The fraction $q(r)$ of points that belongs to a neighborhood $b(r)$ follows from [14] as

$$r = -\frac{1}{4k^2 p_r} \int_0^q \frac{dv}{v^2 - v - \frac{1}{2Nkp_r}} \quad (13)$$

The average path length or hopcount (i.e. number of links in the shortest path) is deduced in [14] as $E[H] = -\int_0^1 r dq$. After introducing (13) and performing a partial integration, we find the basic result of Newman *et al.*

$$E[H] = \frac{1}{4k^2 p_r} \int_0^1 \frac{(1-v) dv}{v^2 - v - \frac{1}{2Nkp_r}} = \frac{1}{2k^2 p_r} \frac{1}{\sqrt{1 + \frac{2}{Nkp_r}}} \arctan \frac{1}{\sqrt{1 + \frac{2}{Nkp_r}}}$$

The scaled approximate time t_3 satisfies

$$t_3 = -\frac{1}{\frac{\xi_0 \theta^2}{2}} \int_0^\zeta \frac{du}{u^2 - \frac{2}{\xi_0 \theta^2} (\xi_0 \theta - 1) u - \frac{2(1-\xi_0)}{\xi_0 \theta^2}}$$

and suggests the analogy between a segment length r versus scaled time t_3 and between the fraction q of points that belongs to a (random) neighborhood $b(r)$ versus the fraction ζ of removed items in an SIR epidemics.

2.2 Partial fraction expansion

Here, we present a formal generalization to any order m in $O(\zeta^m)$. First up to $O(\zeta^4)$, the bound for any real θ [11, p. 103]

$$e^{-\theta\zeta} > 1 - \theta\zeta + \frac{1}{2}\theta^2\zeta^2 - \frac{1}{6}\theta^3\zeta^3$$

illustrates that increasing m alternatively provides lower and upper bounds. Introduced into Kermack and McKendrick differential equation (5) shows² that

$$\frac{d\zeta}{dt^*} < (1 - \xi_0) + (\xi_0 \theta - 1) \zeta - \frac{\xi_0 \theta^2}{2} \zeta^2 + \frac{1}{6} \xi_0 \theta^3 \zeta^3$$

The third order polynomial $p_3(\zeta)$ at the right-hand side can be factored as

$$p_3(\zeta) = A(\zeta - \zeta_1)(\zeta - \zeta_2)(\zeta - \zeta_3)$$

where $A = \frac{1}{6}\xi_0\theta^3$. The zeros ζ_1, ζ_2 and ζ_3 can be analytically expressed by Cardano's formulas for the cubic. Thus, we have

$$\frac{d\zeta}{dt^*} < A(\zeta - \zeta_1)(\zeta - \zeta_2)(\zeta - \zeta_3)$$

²This differential equation with a third order polynomial resembles that of Weierstrass's elliptic $\mathcal{P}(z)$ function [16, p. 247],

$$\left(\frac{d\mathcal{P}(z)}{dz}\right)^2 = 4\mathcal{P}^3(z) - g_2\mathcal{P}(z) + g_3$$

from which

$$\frac{d\zeta}{(\zeta - \zeta_1)(\zeta - \zeta_2)(\zeta - \zeta_3)} < Adt^*$$

After integration and partial fraction expansion (provided all zeros ζ_1 , ζ_2 and ζ_3 are different)

$$\frac{1}{(\zeta - \zeta_1)(\zeta - \zeta_2)(\zeta - \zeta_3)} = \frac{a_1}{(\zeta - \zeta_1)} + \frac{a_2}{(\zeta - \zeta_2)} + \frac{a_3}{(\zeta - \zeta_3)}$$

we find, with $a_1 = \frac{1}{(\zeta_1 - \zeta_2)(\zeta_1 - \zeta_3)}$, $a_2 = \frac{1}{(\zeta_2 - \zeta_1)(\zeta_2 - \zeta_3)}$ and $a_3 = \frac{1}{(\zeta_3 - \zeta_1)(\zeta_3 - \zeta_2)}$,

$$\int_0^\zeta \frac{a_1 dw}{(w - \zeta_1)} + \int_0^\zeta \frac{a_2 dw}{(w - \zeta_2)} + \int_0^\zeta \frac{a_3 dw}{(w - \zeta_3)} < At^*$$

Hence, we arrive at

$$\log \left(\frac{\zeta - \zeta_1}{\zeta_1} \right)^{a_1} \left(\frac{\zeta - \zeta_2}{\zeta_2} \right)^{a_2} \left(\frac{\zeta - \zeta_3}{\zeta_3} \right)^{a_3} < At^*$$

from which the lower bound follows

$$\left(\frac{\zeta - \zeta_1}{\zeta_1} \right)^{a_1} \left(\frac{\zeta - \zeta_2}{\zeta_2} \right)^{a_2} \left(\frac{\zeta - \zeta_3}{\zeta_3} \right)^{a_3} < e^{At^*}$$

In general, we cannot solve ζ from this inequality. After increasing the order to $O(\zeta^5)$, the quartic with zeros $\omega_1, \omega_2, \omega_3$ and ω_4 leads to the upper bound

$$\left(\frac{\zeta - \omega_1}{\omega_1} \right)^{\alpha_1} \left(\frac{\zeta - \omega_2}{\omega_2} \right)^{\alpha_2} \left(\frac{\zeta - \omega_3}{\omega_3} \right)^{\alpha_3} \left(\frac{\zeta - \omega_4}{\omega_4} \right)^{\alpha_4} > e^{At^*}$$

Formally, the partial fraction method can be extended to any polynomial and to the exact case itself, as shown below.

Cauchy's integral theorem [17] states that

$$\frac{1}{1 - \xi_0 e^{-\theta w} - w} = \frac{1}{2\pi i} \int_{C(w)} \frac{1}{1 - \xi_0 e^{-\theta z} - z} \frac{dz}{(z - w)}$$

where the contour $C(w)$ encloses in counter-clockwise sense a region around the point $z = w$, where the integrand is analytic. Since

$$\lim_{r \rightarrow \infty} \frac{1}{1 - \xi_0 e^{-\theta r e^{i\omega}} - r e^{i\omega}} = 0$$

for any angle ω , the integrand vanishes for $|z| \rightarrow \infty$ and we can deform the contour to enclose the entire complex plane without the point $z = w$, in clockwise sense,

$$\frac{1}{2\pi i} \int_{C(w)} \frac{1}{1 - \xi_0 e^{-\theta z} - z} \frac{dz}{(z - w)} = -\frac{1}{2\pi i} \int_{C \setminus \{w\}} \frac{1}{1 - \xi_0 e^{-\theta z} - z} \frac{dz}{(z - w)}$$

The function $\frac{1}{1 - \xi_0 e^{-\theta z} - z}$ has poles at the zeros of $1 - \xi_0 e^{-\theta z} - z$, where only $0 \leq \arg z < 2\pi$ is enclosed by the contour. The simple zero \tilde{z} obeys $1 - \tilde{z} = \xi_0 e^{-\theta \tilde{z}}$, which, as shown in Section A, can be transformed to $qe^{-q} = a$ with $a = \theta \xi_0 e^{-\theta} \in [0, \xi_0]$. Section A.1 illustrates that there are infinitely many complex zeros $\{\tilde{z}_k\}_{k \geq 0}$, whose precise form can only be computed numerically. Cauchy's residue theorem tells us that

$$\begin{aligned} \frac{1}{1 - \xi_0 e^{-\theta w} - w} &= \sum_{\tilde{z}_k} \frac{1}{w - \tilde{z}_k} \lim_{z \rightarrow \tilde{z}_k} \frac{z - \tilde{z}_k}{1 - \xi_0 e^{-\theta z} - z} = \sum_{\tilde{z}_k} \frac{1}{w - \tilde{z}_k} \frac{1}{\xi_0 \theta e^{-\theta \tilde{z}_k} - 1} \\ &= \sum_{\tilde{z}_k} \frac{1}{w - \tilde{z}_k} \frac{1}{\theta - 1 - \theta \tilde{z}_k} \end{aligned}$$

This result is the partial fraction expansion of $\frac{1}{1-\xi_0 e^{-\theta w} - w}$ in terms of its complex zeros. The scaled time in (5) becomes

$$\begin{aligned} t^* &= \int_0^\zeta \frac{dw}{1 - \xi_0 e^{-\theta w} - w} \\ &= \sum_{\tilde{z}_k} \int_0^\zeta \frac{dw}{w - \tilde{z}_k} \frac{1}{\theta - 1 - \theta \tilde{z}_k} = \sum_{\tilde{z}_k} \log \left(\frac{\tilde{z}_k - \zeta}{\tilde{z}_k} \right) \frac{1}{\theta - 1 - \theta \tilde{z}_k} \end{aligned}$$

and

$$e^{t^*} = \prod_{\tilde{z}_k} \left(1 - \frac{\zeta}{\tilde{z}_k} \right)^{\frac{1}{\theta - 1 - \theta \tilde{z}_k}}$$

Section A.1 shows that there is only one real zero ζ_{\max} specified in (31), while all other zeros,

$$\tilde{z}_k = 1 - \frac{x_k + iy_k}{\theta} = \frac{\theta - x_k - iy_k}{\theta}$$

are complex conjugate (with $x_k > 0$), where $q = x_k + iy_k$ satisfies $qe^{-q} = a > 0$. Thus, for real w , we obtain

$$\begin{aligned} \frac{1}{1 - \xi_0 e^{-\theta w} - w} &= \frac{1}{w - \zeta_{\max}} \frac{1}{\theta - 1 - \theta \zeta_{\max}} + 2\theta \sum_{y_k > 0} \operatorname{Re} \left(\frac{1}{\theta w + x_k - \theta + iy_k} \frac{1}{x_k - 1 + iy_k} \right) \\ &= \frac{1}{w - \zeta_{\max}} \frac{1}{\theta - 1 - \theta \zeta_{\max}} + 2\theta \sum_{y_k > 0} \frac{(\theta w + x_k - \theta)(x_k - 1) - y_k^2}{((\theta w + x_k - \theta)^2 + y_k^2)(x_k - 1)^2 + y_k^2} \end{aligned}$$

and analogously, after some tedious calculations,

$$t^* = \frac{\log \left(1 - \frac{\zeta}{\zeta_{\max}} \right)}{\theta - 1 - \theta \zeta_{\max}} + 2 \sum_{y_k > 0} \frac{\log \left| 1 + \frac{2x_k - \theta(2 - \zeta)}{(\theta - x_k)^2 + y_k^2} \theta \zeta \right| (x_k - 1) + y_k \arctan \frac{\theta \zeta y_k}{(\theta - x_k)^2 + y_k^2 + \theta \zeta (x_k - \theta)}}{(x_k - 1)^2 + y_k^2} \quad (14)$$

where $x_k^2 + y_k^2 = a^2 e^{2x_k}$ grows exponentially fast. Because the complex zeros $\tilde{z}_k = 1 - \frac{x_k + iy_k}{\theta}$ can only be numerically computed, we do not further investigate this novel approach (14), but concentrate on series expansions in Section 4.

3 Bounds on the scaled time t^*

Before turning to an exact series expansion of the scaled time t^* in Section 4, we present a set of different bounds.

The integral (5) is analytically computable in two extreme limits of the normalized effective infection rate θ . First, if $\theta \rightarrow \infty$, then

$$t_{\theta \rightarrow \infty}^*(\zeta) = \lim_{\theta \rightarrow \infty} \int_0^\zeta \frac{dw}{1 - \xi_0 e^{-\theta w} - w} = \int_0^\zeta \frac{dw}{1 - w}$$

and

$$t_{\theta \rightarrow \infty}^*(\zeta) = -\log(1 - \zeta)$$

Thus, if the infectiousness is unlimitedly strong $\theta \rightarrow \infty$, then the removed fraction is $\zeta_{\{\theta \rightarrow \infty\}}(t^*) = (1 - e^{-t^*})$. The other extremal case for $\theta \rightarrow 0$ is

$$t_{\theta \rightarrow 0}^*(\zeta) = \lim_{\theta \rightarrow 0} \int_0^\zeta \frac{dw}{1 - \xi_0 e^{-\theta w} - w} = \int_0^\zeta \frac{dw}{1 - \xi_0 - w}$$

and

$$t_{\theta \rightarrow 0}^*(\zeta) = -\log \left(1 - \frac{\zeta}{1 - \xi_0} \right)$$

Thus, if the infectious power is absent $\theta \rightarrow 0$, then the removed fraction is $\zeta_{\{\theta \rightarrow 0\}}(t^*) = (1 - \xi_0)(1 - e^{-t^*})$. In summary, the fraction $\zeta_\tau(t^*)$ of removed items as a function of the scaled time t^* is bounded by

$$(1 - \xi_0)(1 - e^{-t^*}) \leq \zeta_\tau(t^*) \leq (1 - e^{-t^*})$$

Alternatively, the scaled time $t^* = t_\theta^*(\zeta) = \int_0^\zeta \frac{dw}{(1 - \xi_0 e^{-\theta w}) - w}$ is bounded by

$$-\log \left(1 - \frac{\zeta}{1 - \xi_0} \right) \leq t_\theta^*(\zeta) \leq -\log(1 - \zeta) \quad (15)$$

Since $1 - \frac{\zeta}{1 - \xi_0} = \frac{1 - \xi_0 - \zeta}{1 - \xi_0}$, while the fraction of infected $\eta = 1 - \xi_0 e^{-\theta \zeta} - \zeta$ at any time, the above inequality suggests a reasonable estimate,

$$t_\theta^*(\zeta) > -\log \left(1 - \frac{\zeta}{1 - \xi_0 e^{-\theta \zeta}} \right) \quad (16)$$

Numerical computations indicate that the right-hand side is a (strict) lower bound for $t_\theta^*(\zeta)$.

Since the fraction of removed $\zeta \in [0, 1]$, it holds that $1 - \xi_0 e^{-\theta w} - w \leq 1 - \xi_0 e^{-\theta \zeta}$ and the integral (5) is bounded as

$$t_\theta^*(\zeta) \geq \int_0^\zeta \frac{dw}{1 - \xi_0 e^{-\theta w}} = \frac{1}{\theta} \log \left(\frac{e^{\theta \zeta} - \xi_0}{1 - \xi_0} \right)$$

We rewrite $\frac{1}{\theta} \log \left(\frac{e^{\theta \zeta} - \xi_0}{1 - \xi_0} \right) = \zeta - \frac{1}{\theta} \log \left(1 - \frac{\xi_0 - \xi_0 e^{-\theta \zeta}}{1 - \xi_0 e^{-\theta \zeta}} \right)$, where $\frac{\xi_0 - \xi_0 e^{-\theta \zeta}}{1 - \xi_0 e^{-\theta \zeta}} \leq 1$, and find

$$t_\theta^*(\zeta) \geq \zeta - \frac{1}{\theta} \log \left(1 - \frac{\xi_0 - \xi_0 e^{-\theta \zeta}}{1 - \xi_0 e^{-\theta \zeta}} \right) \geq \zeta$$

where the last inequality follows directly from (5), because $1 - \xi_0 e^{-\theta w} - w \leq 1$ for $w \in [0, \zeta]$. The scaled time $t_\theta^*(\zeta)$ is always larger than the fraction of removed at that time. The above suggests us to rewrite (5) with

$$\frac{1}{1 - \xi_0 e^{-\theta w} - w} = \frac{1}{(1 - \xi_0 e^{-\theta w}) \left(1 - \frac{w}{1 - \xi_0 e^{-\theta w}} \right)}$$

Since the fraction of infected $\eta = 1 - \xi_0 e^{-\theta \zeta} - \zeta \geq 0$ and $1 - \xi_0 e^{-\theta w} - w \geq 0$ for any $w \in [0, \zeta]$ – the integration parameter w physically represents the fraction of removed at a time $t' \in [0, t]$ –, the last inequality is equivalent to $1 \geq \frac{w}{1 - \xi_0 e^{-\theta w}}$. Geometric series expansion then yields

$$\frac{1}{1 - \xi_0 e^{-\theta w} - w} = \sum_{k=0}^{\infty} \frac{w^k}{(1 - \xi_0 e^{-\theta w})^{k+1}} = \frac{1}{1 - \xi_0 e^{-\theta w}} + \sum_{k=1}^{\infty} \frac{w^k}{(1 - \xi_0 e^{-\theta w})^{k+1}}$$

Hence³, the integral (5) equals

$$\begin{aligned} t_\theta^*(\zeta) &= \int_0^\zeta \frac{dw}{1 - \xi_0 e^{-\theta w} - w} = \int_0^\zeta \frac{dw}{1 - \xi_0 e^{-\theta w}} + \sum_{k=1}^{\infty} \int_0^\zeta \frac{w^k dw}{(1 - \xi_0 e^{-\theta w})^{k+1}} \\ &= \frac{1}{\theta} \log \left(\frac{e^{\theta \zeta} - \xi_0}{1 - \xi_0} \right) + \sum_{k=1}^{\infty} \int_0^\zeta \frac{w^k dw}{(1 - \xi_0 e^{-\theta w})^{k+1}} \end{aligned}$$

but none of the positive terms in the k -sum is analytically integrable. However, the rather trivial bounds

$$\frac{1}{(1 - \xi_0 e^{-\theta \zeta})^{k+1}} \int_0^\zeta w^k dw \leq \int_0^\zeta \frac{w^k dw}{(1 - \xi_0 e^{-\theta w})^{k+1}} \leq \frac{1}{(1 - \xi_0)^{k+1}} \int_0^\zeta w^k dw$$

lead to

$$\sum_{k=1}^{\infty} \frac{1}{k+1} \left(\frac{\zeta}{1 - \xi_0 e^{-\theta \zeta}} \right)^{k+1} \leq \sum_{k=1}^{\infty} \int_0^\zeta \frac{w^k dw}{(1 - \xi_0 e^{-\theta w})^{k+1}} \leq \sum_{k=1}^{\infty} \frac{1}{k+1} \left(\frac{\zeta}{1 - \xi_0} \right)^{k+1}$$

With $\sum_{k=1}^{\infty} \frac{x^{k+1}}{k+1} = -\log(1-x) - x$, we thus obtain the bounds for $T_\theta^*(\zeta) = t_\theta^*(\zeta) - \frac{1}{\theta} \log \left(\frac{e^{\theta \zeta} - \xi_0}{1 - \xi_0} \right)$,

$$-\log \left(1 - \frac{\zeta}{1 - \xi_0 e^{-\theta \zeta}} \right) - \frac{\zeta}{1 - \xi_0 e^{-\theta \zeta}} \leq T_\theta^*(\zeta) \leq -\log \left(1 - \frac{\zeta}{1 - \xi_0} \right) - \frac{\zeta}{1 - \xi_0} \quad (17)$$

The bounds in (17) are clearly sharper than the bounds in (15), which are limiting cases in the normalized effective infection rate θ . Instead of bounding the integral as here, an exact series approach is presented in Theorem 1.

Numerical evaluations indicate that the scaled time $t^* = t_\theta^*(\zeta)$ is accurately bounded as

$$\frac{1}{\theta} \log \left(\frac{e^{\theta \zeta} - \xi_0}{1 - \xi_0} \right) - \frac{\zeta}{1 - \xi_0 e^{-\theta \zeta}} - \log \left(1 - \frac{\zeta}{1 - \xi_0 e^{-\theta \zeta}} \right) < t_\theta^*(\zeta) < t_3 \quad (18)$$

In other words, the best lower bound deduced here appears in (17) and the best upper bound is t_3 specified in (11). Finally, we observe that the last sum in the complex zeros expansion (14) only contains positive terms. Hence, in terms of the maximum fraction ζ_{\max} of removed items specified in (31) in Appendix A, we find another lower bound

$$t_\theta^*(\zeta) > \frac{\log \left(1 - \frac{\zeta}{\zeta_{\max}} \right)}{\theta (1 - \zeta_{\max}) - 1}$$

which is reasonably accurate.

4 Series for the scaled time t^* in (3)

Our major exact result is

³Any Taylor series can be integrated within its region of convergence, because it represents then an analytic function in the complex plane.

Theorem 1 In the complete graph K_N on N nodes, the SIR time $t^* = \delta t$, measured in units of the average curing time $\frac{1}{\delta}$, can be expanded in a converging series for $\zeta < \zeta_{\max}$ specified in (31),

$$t^* = \frac{\zeta}{1 - \frac{\zeta}{2} - \xi_0 e^{-\frac{\theta\zeta}{2}}} \left\{ 1 + 2 \sum_{m=1}^{\infty} \left[\sum_{k=1}^{2m} \frac{k! \sum_{j=0}^k \binom{2m}{j} \left(\xi_0 e^{-\frac{\theta\zeta}{2}} \right)^{k-j} (-\theta)^{2m-j} \mathcal{S}_{2m-j}^{(k-j)}}{\left(1 - \frac{\zeta}{2} - \xi_0 e^{-\frac{\theta\zeta}{2}} \right)^k} \right] \frac{\left(\frac{\zeta}{2} \right)^{2m}}{(2m+1)!} \right\} \quad (19)$$

where $\mathcal{S}_m^{(k)}$ is the Stirling Number of the second kind.

The proof is given in Appendix C. The Taylor series in (41) can be inverted using Lagrange series. Our characteristic coefficients [18, Sec. 2] can produce that Lagrange series formally to any desired order term. Unfortunately, that exact Lagrange series of ζ in terms of t^* is quite involved and omitted. Instead, we derive the Taylor series of $\zeta(t^*)$ around an arbitrary point t_0^* in Section 5.

All terms in the m -series in (19) are positive. Hence, summing terms up to $m \leq K$ provides a lower bound, that is increasingly sharp for increasing K . However, the k -series in (19) is alternating and causes numerical instabilities for large m . In Appendix D, we present an alternative Taylor series which is numerically stable. Moreover, we demonstrate that the entire Taylor series can, in principle be analytically evaluated term by term. The first split-off of terms yields

$$t^* = \frac{1}{1 - \theta \xi_0 e^{-\theta z_0}} \ln \left(\frac{1 - \xi_0 e^{-\theta z_0} (1 + z_0 \theta)}{1 - \zeta - \xi_0 e^{-\theta z_0} (1 + (z_0 - \zeta) \theta)} \right) + \sum_{m=1}^{\infty} \left[\sum_{k=1}^{m-1} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{\theta (1 - z_0 - \xi_0 e^{-\theta z_0})} \right)^k \sum_{j=1}^{m-k} \binom{k}{j} \left(\frac{\xi_0 \theta e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \right)^j j! T(j, m-k) \right] \frac{\theta^m z_0^{m+1} - \theta^m (z_0 - \zeta)^{m+1}}{(1 - z_0 - \xi_0 e^{-\theta z_0}) (m+1)} \quad (20)$$

The second split-off, specified by the upper-index $k = m - 2$ in the k -sum, is

$$t^* = \frac{1}{1 - \theta \xi_0 e^{-\theta z_0}} \log \left(\frac{1 - \xi_0 e^{-\theta z_0} (1 + z_0 \theta)}{1 - \zeta - \xi_0 e^{-\theta z_0} (1 + (z_0 - \zeta) \theta)} \right) \left\{ 1 - \frac{\xi_0 \theta^2 e^{-\theta z_0} (1 - z_0 - \xi_0 e^{-\theta z_0})}{(1 - \theta \xi_0 e^{-\theta z_0})^2} \right\} + \frac{1}{2} \left(\frac{\xi_0 \theta^2 e^{-\theta z_0}}{1 - \theta \xi_0 e^{-\theta z_0}} \right) \left\{ \frac{(z_0 - \zeta)^2}{1 - \zeta - \xi_0 e^{-\theta z_0} (1 + (z_0 - \zeta) \theta)} - \frac{z_0^2}{1 - \xi_0 e^{-\theta z_0} (1 + z_0 \theta)} \right\} + \frac{\zeta \xi_0 \theta^2 e^{-\theta z_0}}{(1 - \theta \xi_0 e^{-\theta z_0})^2} + \sum_{m=1}^{\infty} \left[\sum_{k=1}^{m-2} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{\theta (1 - z_0 - \xi_0 e^{-\theta z_0})} \right)^k \sum_{j=1}^{m-k} \binom{k}{j} \left(\frac{\xi_0 \theta e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \right)^j j! T(j, m-k) \right] \frac{\theta^m z_0^{m+1} - \theta^m (z_0 - \zeta)^{m+1}}{(1 - z_0 - \xi_0 e^{-\theta z_0}) (m+1)} \quad (21)$$

The third split-off with upper-index $k = m - 3$ is

$$\begin{aligned}
t^* = & \frac{1}{1 - \theta \xi_0 e^{-\theta z_0}} \log \left(\frac{1 - \xi_0 e^{-\theta z_0} (1 + z_0 \theta)}{1 - \zeta - \xi_0 e^{-\theta z_0} (1 + (z_0 - \zeta) \theta)} \right) \\
& \times \left\{ 1 - \frac{\xi_0 \theta^2 e^{-\theta z_0} (1 - z_0 - \xi_0 e^{-\theta z_0})}{(1 - \theta \xi_0 e^{-\theta z_0})^2} + \frac{\xi_0 \theta^3 e^{-\theta z_0} (1 - z_0 - \xi_0 e^{-\theta z_0})^2}{2 (1 - \theta \xi_0 e^{-\theta z_0})^3} + \frac{3 \xi_0^2 \theta^4 e^{-2\theta z_0} (1 - z_0 - \xi_0 e^{-\theta z_0})^2}{2 (1 - \theta \xi_0 e^{-\theta z_0})^4} \right\} \\
& + \frac{1}{2} \left(\frac{\xi_0 \theta^2 e^{-\theta z_0}}{1 - \theta \xi_0 e^{-\theta z_0}} \right) \left\{ \frac{(z_0 - \zeta)^2}{1 - \zeta - \xi_0 e^{-\theta z_0} (1 + (z_0 - \zeta) \theta)} - \frac{z_0^2}{1 - \xi_0 e^{-\theta z_0} (1 + z_0 \theta)} \right\} \\
& \times \left\{ 1 - \frac{\theta (1 - z_0 - \xi_0 e^{-\theta z_0})}{3 (1 - \theta \xi_0 e^{-\theta z_0})} - \frac{3 \xi_0 \theta^2 e^{-\theta z_0} (1 - z_0 - \xi_0 e^{-\theta z_0})}{2 (1 - \theta \xi_0 e^{-\theta z_0})^2} \right\} \\
& + \frac{\xi_0^2 \theta^4 e^{-2\theta z_0} (1 - z_0 - \xi_0 e^{-\theta z_0})^2}{8 (1 - \theta \xi_0 e^{-\theta z_0})^3} \left\{ \frac{(z_0 - \zeta)^2}{(1 - \zeta - \xi_0 e^{-\theta z_0} (1 + (z_0 - \zeta) \theta))^2} - \frac{z_0^2}{(1 - \xi_0 e^{-\theta z_0} (1 + z_0 \theta))^2} \right\} \\
& + \frac{\zeta \xi_0 \theta^2 e^{-\theta z_0}}{(1 - \theta \xi_0 e^{-\theta z_0})^2} \left\{ 1 - \frac{\theta (1 - z_0 - \xi_0 e^{-\theta z_0})}{2 (1 - \theta \xi_0 e^{-\theta z_0})} - \frac{3 \xi_0 \theta^2 e^{-\theta z_0} (1 - z_0 - \xi_0 e^{-\theta z_0})}{2 (1 - \theta \xi_0 e^{-\theta z_0})^2} \right\} \\
& + \sum_{m=1}^{\infty} \left[\sum_{k=1}^{m-3} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{\theta (1 - z_0 - \xi_0 e^{-\theta z_0})} \right)^k \sum_{j=1}^{m-k} \binom{k}{j} \left(\frac{\xi_0 \theta e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \right)^j j! T(j, m-k) \right] \frac{\theta^m z_0^{m+1} - \theta^m (z_0 - \zeta)^{m+1}}{(1 - z_0 - \xi_0 e^{-\theta z_0}) (m+1)}
\end{aligned} \tag{22}$$

When neglecting the m -sum in (20), (21) and (22) increasingly sharper lower bounds for t^* are established. Although we can continue the computations as shown in Appendix D, the analytic terms (without m -sum) are already involved. Only when compared close to divergence point where $\zeta \rightarrow \zeta_{\max}$, differences are apparent, but for a less extreme parameter range, the best candidate (22) with expansion point $z_0 = \frac{\zeta}{2}$ is sufficiently accurate.

4.1 Another type of expansion

Another application of (42) is based upon

$$\frac{1}{1 - u - \xi_0 e^{-\theta u}} = \frac{1}{\theta \xi_0 e^{-\theta u} - 1} \frac{d}{du} \log (1 - u - \xi_0 e^{-\theta u})$$

For $f(u) = \frac{d}{du} \log (1 - u - \xi_0 e^{-\theta u})$ and $g(u) = \frac{1}{\theta \xi_0 e^{-\theta u} - 1}$, we obtain from (42)

$$\begin{aligned}
\int_0^\zeta \frac{du}{1 - u - \xi_0 e^{-\theta u}} &= \int_0^\zeta \left(\sum_{k=0}^{m-1} \frac{g^{(k)}(\zeta)}{k!} (u - \zeta)^k \right) \frac{d}{du} \log (1 - u - \xi_0 e^{-\theta u}) du \\
&+ \frac{(-1)^m}{(m-1)!} \int_0^\zeta dx g^{(m)}(x) \int_0^x (x - u)^{m-1} \frac{d}{du} \log (1 - u - \xi_0 e^{-\theta u}) du
\end{aligned} \tag{23}$$

Partial integration of (23) leads after tedious manipulations to

$$\begin{aligned}
\int_0^\zeta \frac{du}{1 - \xi_0 e^{-\theta u} - u} &= \left\{ \log \left(\frac{1 - \xi_0 e^{-\theta \zeta} - \zeta}{1 - \xi_0} \right) \right\} g(\zeta) - \int_0^\zeta dx g^{(1)}(x) \log \left(\frac{1 - \xi_0 e^{-\theta x} - x}{1 - \xi_0} \right) \\
&+ \log(1 - \xi_0) \left\{ 1_{\{m>1\}} \int_0^\zeta dx \frac{(-1)^m g^{(m)}(x)}{(m-1)!} x^{m-1} - \sum_{k=1}^{m-1} \frac{g^{(k)}(\zeta)}{k!} (-\zeta)^k \right\} \\
&- \sum_{k=0}^{m-2} \frac{g^{(k+1)}(\zeta)}{k!} \int_0^\zeta (u - \zeta)^k \log(1 - \xi_0 e^{-\theta u} - u) du \\
&+ \int_0^\zeta dx \frac{(-1)^m g^{(m)}(x)}{(m-2)!} \int_0^x (x - u)^{m-2} \log(1 - \xi_0 e^{-\theta u} - u) du
\end{aligned} \tag{24}$$

The first term in (24)

$$t_\theta^*(\zeta) \approx \frac{\log \left(\frac{1 - \xi_0 e^{-\theta \zeta} - \zeta}{1 - \xi_0} \right)}{e^{-\theta \zeta} + \log \theta \xi_0 - 1}$$

turns out to be a reasonably accurate estimate of t^* for not too large θ . In fact, for $\theta \leq 1$, numerical computations seem to indicate that the above first term is a tighter lower bound than (16).

4.2 Time of the peak infection

The maximum number of infected obeys $\frac{dy}{dt} = \beta xy - \delta y = 0$, from which the peak number $y_p = 1 - x_p - z_p$ of infected occurs when $x_p = \frac{1}{\tau}$. Using $\log \frac{x(t)}{x_0} = -\tau z(t)$, it holds that $\frac{\log x_0 \tau}{\tau} = z_p$ and the peak number of infected $y_p = 1 - \frac{1 + \log x_0 \tau}{\tau}$. Turning to the fraction of removed $\zeta_p = \frac{\log \xi_0 \theta}{\theta}$ at a maximum fraction of infected η_p and using (5) expresses the time $t_{\text{peak}}^* = \delta t_{\text{peak}}$, expressed in units of the average curing time $\frac{1}{\delta}$, at which the peak infection occurs with $\theta = N\tau$ as

$$t_{\text{peak}}^* = \int_0^{\frac{\log \xi_0 \theta}{\theta}} \frac{dw}{1 - \xi_0 e^{-\theta w} - w}$$

It just remains to substitute $\zeta_p = \frac{\log \xi_0 \theta}{\theta}$, $e^{-\theta \frac{\zeta_p}{2}} = \frac{1}{\sqrt{\xi_0 \theta}}$ and $\xi_0 e^{-\theta \frac{\zeta_p}{2}} = \sqrt{\frac{\xi_0}{\theta}}$ into one of the series (20), (21) and (22) to find a good lower bound for t_{peak}^* .

5 Differential equation (2)

So far, we have concentrated on the function $t^* = H(\zeta)$ and now we focus on $\zeta = H^{-1}(t^*)$. We start a Taylor series approach and introduce $\zeta(t^*) = \sum_{k=0}^\infty \zeta_k(t_0^*) (t^* - t_0^*)^k$ into the Kermack and McKendrick differential equation (2), written in fractions,

$$\frac{d\zeta(t^*)}{dt^*} = 1 - \xi_0 e^{-\theta \zeta(t^*)} - \zeta(t^*)$$

Invoking our general Taylor expansion (see Appendix B)

$$e^{-\theta \zeta(t^*)} = e^{-\theta \zeta_0(t_0^*)} \left(1 + \sum_{m=1}^\infty \left[\sum_{k=1}^m \frac{(-\theta)^k}{k!} s[k, m]_{|\zeta(t)}(t_0^*) \right] (t^* - t_0^*)^m \right) \tag{25}$$

where $s[k, m]|_{\zeta(t)}(t_0^*)$ is the characteristic coefficient of $\zeta(t)$ around t_0^* , yields

$$\sum_{m=0}^{\infty} (m+1) \zeta_{m+1}(t_0^*) (t^* - t_0^*)^m = 1 - \xi_0 e^{-\theta \zeta_0(t_0^*)} - \zeta_0(t_0^*) \\ - \sum_{m=1}^{\infty} \left[\xi_0 e^{-\theta \zeta_0(t_0^*)} \sum_{k=1}^m \frac{(-\theta)^k}{k!} s[k, m]|_{\zeta(t)}(t_0^*) + \zeta_m(t_0^*) \right] (t^* - t_0^*)^m$$

Equating corresponding powers in $t^* - t_0^*$ results in $\zeta_1(t_0^*) = 1 - \xi_0 e^{-\tau \zeta_0(t_0^*)} - \zeta_0(t_0^*)$, which is the differential equation at the scaled time t_0^* , and in the recursion

$$\zeta_m(t_0^*) = -\frac{1}{m} \left(\xi_0 e^{-\theta \zeta_0(t_0^*)} \sum_{k=1}^{m-1} \frac{(-\theta)^k}{k!} s[k, m-1]|_{\zeta(t)}(t_0^*) + \zeta_{m-1}(t_0^*) \right) \quad (26)$$

that essentially extends the first order differential equation to all higher orders. For example, for $m = 2$ in (26), we obtain

$$\zeta_2(t_0^*) = -\frac{1}{2} \left(1 - \theta \xi_0 e^{-\tau \zeta_0(t_0^*)} \right) \zeta_1(t_0^*) \\ = -\frac{1}{2} \left(1 - \theta \xi_0 e^{-\tau \zeta_0(t_0^*)} \right) \left(1 - \xi_0 e^{-\tau \zeta_0(t_0^*)} - \zeta_0(t_0^*) \right)$$

We can iterate the recursion (26) up to any m . However, the unknown $\zeta_0(t_0^*) = \zeta(t_0^*)$ will appear in each Taylor coefficient $\zeta_m(t_0^*)$.

5.1 Structure of the Taylor coefficient $\zeta_m(t_0^*)$

With $A = \xi_0 e^{-\theta \zeta_0(t_0^*)}$, $Z = 1 - \zeta_0(t_0^*)$ and $x = \theta Z$, we list a few iterations of the recursion (26),

$$\begin{aligned}
\zeta_1(t_0^*) &= -A + Z \\
\zeta_2(t_0^*) &= -\frac{A^2\theta}{2} + \frac{A}{2!}(x+1) - \frac{Z}{2!} \\
\zeta_3(t_0^*) &= -\frac{A^3\theta^2}{3} + \frac{A^2\theta}{3!}(3x+2) - \frac{A}{3!}(x+1)^2 + \frac{Z}{3!} \\
\zeta_4(t_0^*) &= -\frac{A^4\theta^3}{4} + \frac{A^3\theta^2}{4!}(12x+7) - \frac{A^2\theta}{4!}(7x^2+11x+3) + \frac{A}{4!}(x^3+4x^2+3x+1) - \frac{Z}{4!} \\
\zeta_5(t_0^*) &= -\frac{A^5\theta^4}{5} + \frac{A^4\theta^3}{5!}(60x+33) - \frac{A^3\theta^2}{5!}(50x^2+69x+17) \\
&\quad + \frac{A^2\theta}{5!}(15x^3+43x^2+28x+4) - \frac{A}{5!}(x^4+7x^3+11x^2+4x+1) + \frac{Z}{5!} \\
\zeta_6(t_0^*) &= -\frac{A^6\theta^5}{6} + \frac{A^5\theta^4}{6!}24(15x+8) - \frac{A^4\theta^3}{6!}(390x^2+499x+120) \\
&\quad + \frac{A^3\theta^2}{6!}2(90x^3+219x^2+131x+18) - \frac{A^2\theta}{6!}(31x^4+142x^3+174x^2+62x+5) \\
&\quad + \frac{A}{6!}(x^5+11x^4+32x^3+26x^2+5x+1) - \frac{Z}{6!} \\
\zeta_7(t_0^*) &= -\frac{A^7\theta^6}{7} + \frac{A^6\theta^5}{7!}120(21x+11) - \frac{A^5\theta^4}{7!}(3360x^2+4096x+979) \\
&\quad + \frac{A^4\theta^3}{7!}(2100x^3+4630x^2+2641x+370) - \frac{A^3\theta^2}{7!}2(301x^4+1131x^3+1218x^2+421x+36) \\
&\quad + \frac{A^2\theta}{7!}(63x^5+424x^4+850x^3+594x^2+129x+6) \\
&\quad - \frac{A}{7!}(x^6+16x^5+76x^4+122x^3+57x^2+6x+1) + \frac{Z}{7!}
\end{aligned}$$

which suggest that

$$\zeta_m(t_0^*) = \frac{(-1)^{m-1}Z}{m!} - \frac{(A\theta)^m}{\theta m} + \frac{(-1)^{m-1}}{\theta m!} \sum_{j=1}^{m-1} (-A\theta)^j p(x; m, j) \quad (27)$$

where

$$p(x; m, j) = \sum_{k=0}^{m-j} a_k(m, j) x^k \quad (28)$$

is a polynomial of degree $m-j$ in x with integer coefficients $a_k(m, j)$, where $1 \leq j \leq m-1$. Around any time point t_0^* , the Taylor coefficient $\zeta_m(t_0^*)$ possesses a general form, where only A, Z and x change with $\zeta_0(t_0^*) = \zeta(t_0^*)$. An explicit solution requires the general form of the coefficients $a_k(m, j)$ in the polynomial $p(x; m, j)$, that are independent of t_0^* . The coefficients $a_k(m, j)$ are generated by a complicated recursion via (26) and it is unlikely that an explicit form can be obtained. For some particular cases, we give their explicit form in Appendix E.

5.2 Taylor series

Introducing (27) in the Taylor series $\zeta(t^*) = \zeta_0(t_0^*) + \sum_{m=1}^{\infty} \zeta_m(t_0^*)(t^* - t_0^*)^m$ gives us

$$\begin{aligned} \zeta(t^*) &= \zeta_0(t_0^*) - \frac{1}{\theta} \sum_{m=1}^{\infty} \frac{(A\theta(t^* - t_0^*))^m}{m} - Z \sum_{m=1}^{\infty} \frac{(t_0^* - t)^m}{m!} \\ &\quad + \frac{1}{\theta} \sum_{m=1}^{\infty} \left(\sum_{j=1}^m (-1)^{m-1-j} (A\theta)^j p(x; m, j) \right) \frac{(t^* - t_0^*)^m}{m!} \end{aligned}$$

Provided that $|A\theta(t^* - t_0^*)| < 1$, we obtain, with $A = \xi_0 e^{-\theta \zeta_0(t_0^*)}$, $Z = 1 - \zeta_0(t_0^*)$ and $x = \theta Z$, Taylor series of the removed fraction $\zeta(t^*)$ around the scaled time t_0^* ,

$$\begin{aligned} \zeta(t^*) &= \zeta_0(t_0^*) + Z \left(1 - e^{t_0^* - t^*} \right) - \frac{1}{\theta} \log(1 - \theta A(t^* - t_0^*)) \\ &\quad - \frac{1}{\theta} \sum_{m=1}^{\infty} \left(\sum_{j=1}^m (-A\theta)^j \sum_{k=0}^{m-j} a_k(m, j) x^k \right) \frac{(t_0^* - t^*)^m}{m!} \end{aligned} \quad (29)$$

Assuming that $p(x; m, j) = O(m^a m!)$ for finite a , then the radius R of convergence of the Taylor series $\zeta(t^*) = \sum_{k=0}^{\infty} \zeta_k(t_0^*)(t^* - t_0^*)^k$ is $|t^* - t_0^*| < R = \frac{e^{\theta \zeta_0(t_0^*)}}{\xi_0 \theta}$. The minimum radius of convergence as function of the normalized effective infection rate θ occurs at $\theta_{\min} = \frac{1}{\zeta_0(t_0^*)}$. Within the radius of convergence, the Taylor series (29) converges as quickly as a geometric series. The numerical solution of the differential equation (2) with Mathematica is very accurate. The Taylor series in (29) attains 6 digits with about 15 terms when $|t^* - t_0^*| = 1$ for $\xi_0 = 0.6$ and $\theta = 2$ at any $\zeta(t_0^*)$.

If $\zeta(t_0^*)$ is known at one time point t_0^* , all values of $\zeta(t^*)$ can be obtained, by analytical continuation [19, 17], even if the Taylor series (29) has a finite radius of convergence. Indeed, starting from $(t_0^*, \zeta(t_0^*))$, the couple $(t_1^*, \zeta(t_1^*))$ is found via the Taylor series sufficiently accurately, which is fed into the new Taylor series around t_1^* to produce $(t_2^*, \zeta(t_2^*))$ and so on. The usual starting expansion point $t_0^* = 0$, for which $\zeta_0(t_0^*) = 0$ and thus $A = \xi_0$ and $Z = 1$. If we choose the step small enough⁴, say $t_k^* - t_{k-1}^* = \frac{1}{10}$ for $k > 1$, then the above explicitly listed coefficients $\zeta_m(t_0^*)$ up to $O((t^* - t_0^*)^8)$ may provide a sufficient accuracy for each $\zeta(t_k^*)$. The Taylor series (19) of the inverse function couples a chosen value of ζ to the corresponding time t_0^* , whereas the Taylor series $\zeta(t^*) = \sum_{k=0}^{\infty} \zeta_k(t_0^*)(t^* - t_0^*)^k$ returns ζ for a chosen value t^* .

6 Conclusion

After an overview of the McKendrick differential equations with constant rates β and δ in (1), we have presented a formal exact solution (at the end of Section 2) and bounds for the scaled time t^* (Section

⁴The famous Euler transform, which is a special case of an univalent and conformal Möbius transform [16, Vol. 2], $w = \frac{az+b}{cz+d}$, and whose summability is treated by Hardy in [20, chap. VIII],

$$f(z) = f_0 + \sum_{m=1}^{\infty} \left[\sum_{k=1}^m \binom{m-1}{k-1} f_k q^{m-k} \right] \left(\frac{z}{1+qz} \right)^m \quad (30)$$

usually extends the convergence range of z compared to the corresponding Taylor series $f(z) = f_0 + \sum_{m=1}^{\infty} f_m z^m$. Here, we set the Euler transform aside, because numerical computation is not our main aim.

3). A Taylor series-based approach to subsequentially approximate the integral (5) for the scaled time t^* in the SIR epidemic process is presented. The method allows analytic evaluation up to any desired accuracy, at the expense of many terms. Similarly, the Taylor series $\zeta(t^*) = \sum_{k=0}^{\infty} \zeta_k(t_0^*) (t^* - t_0^*)^k$ is derived around t_0^* . The corresponding Taylor coefficients $\zeta_k(t_0^*)$ can be recursively computed up to any order, but the explicit form of $\zeta_k(t_0^*)$ for any k has not been found.

Acknowledgements I am very grateful to M. Achterberg and B. Prasse for pointing me to errors.

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A The Lambert function

The function $1 - \xi_0 e^{-\theta\zeta} - \zeta$ is negative if $\zeta > \tilde{\zeta}$, where $\tilde{\zeta}$ is the zero that obeys $1 - \xi_0 e^{-\theta\tilde{\zeta}} = \tilde{\zeta}$. With $u = 1 - \tilde{\zeta}$, we rewrite that equation as

$$u = 1 - \tilde{\zeta} = \xi_0 e^{-\theta} e^{\theta(1-\tilde{\zeta})} = \xi_0 e^{-\theta} e^{\theta v}$$

or

$$\theta v e^{-\theta v} = \theta \xi_0 e^{-\theta} = a$$

where $a = \theta \xi_0 e^{-\theta} \leq \xi_0$ is positive real number in $[0, 1]$. Finally, let $q = \theta u = \theta(1 - \tilde{\zeta})$, then we arrive at simplest possible form

$$q e^{-q} = a$$

In terms of the Lambert function $v = W(z)$, whose inverse function is $z = W^{-1}(v) = v e^v$, the above equation for the zero is $W^{-1}(-q) = -a$, which is equivalent to $q = -W(-a)$. Hence, the zero $\tilde{\zeta} = 1 - \frac{q}{\theta}$ equals

$$\tilde{\zeta} = \zeta_{\max} = 1 + \frac{1}{\theta} W(-\theta \xi_0 e^{-\theta}) \quad (31)$$

The Lambert function $v = W(z)$, its applications and history is discussed by Corless *et al.* [9]. Physically, the zero $\tilde{\zeta}$ equals the maximum possible removed fraction ζ_{\max} that is reached after infinitely long time when $\frac{dz}{dt^*} = 0$ and the integrand $\frac{1}{1 - \xi_0 e^{-\theta w} - w}$ reaches the real pole at $w = \tilde{\zeta}$. If θ is small, then the zero $\tilde{\zeta} = 1 - \xi_0 e^{-\theta\tilde{\zeta}} \simeq 1 - \xi_0$, while if θ is large, then $\tilde{\zeta} \simeq 1$. If $\xi_0 = 1$, then $\tilde{\zeta} = 1 - e^{-\theta\tilde{\zeta}}$, which has the zero solution $\tilde{\zeta} = 0$, only if $\theta \leq 1$. Indeed, the inequality [11, p. 103], $e^{-\theta\tilde{\zeta}} < 1 - \theta\tilde{\zeta} + \frac{1}{2}\theta^2\tilde{\zeta}^2$, leads to the bound

$$\theta\tilde{\zeta} - \frac{1}{2}\theta^2\tilde{\zeta}^2 < 1 - e^{-\theta\tilde{\zeta}} = \tilde{\zeta}$$

which reduces, provided that $\tilde{\zeta} \neq 0$, to the inequality

$$\tilde{\zeta} > \frac{2(\theta - 1)}{\theta^2}$$

that is feasible only if $\theta > 1$. If $\theta > 1$ and small, then the above bound is an accurate estimate for $\tilde{\zeta}$ in (31).

A.1 Complex zeros of $q e^{-q} = a$ for $a \in [0, 1]$

We will determine all complex numbers $q = x + iy$ that satisfy $q e^{-q} = a$ subject to $0 \leq \arg q \leq 2\pi$. After separating real and imaginary part in $(x + iy) = a e^{x+iy}$, we obtain

$$\begin{cases} x = a e^x \cos y \\ y = a e^x \sin y \end{cases}$$

Their ratio is

$$x = y \cot y$$

and $y = ae^x \sin y$ shows that $y = 0$ is a solution corresponding to $x = ae^x$. From the last equation, we can eliminate $x = \log \frac{y}{a \sin y}$ and substitute in their ratio,

$$\log \frac{y}{a \sin y} = y \cot y$$

which is even in y , but only numerically solvable for y .

Further, using $\cos^2 y + \sin^2 y = 1$ results in a circle around the origin with radius ae^x or $y^2 = a^2 e^{2x} - x^2 = (ae^x - x)(ae^x + x)$. Since y is real, we either have (a) $ae^x - x \geq 0$ and $ae^x + x \geq 0$ or (b) $ae^x - x \leq 0$ and $ae^x + x \leq 0$. The set (a) is equivalent to $a \geq xe^{-x}$ and $-a \leq xe^{-x}$, implying that $x > 0$ (because $a > 0$). The set (b), $0 < ae^x \leq x$ and $0 > -ae^x \geq x$ is not possible. Introducing $y = \pm \sqrt{a^2 e^{2x} - x^2}$ into $x = y \cot y$ yields

$$x = \sqrt{a^2 e^{2x} - x^2} \cot \sqrt{a^2 e^{2x} - x^2}$$

The plot of the last equation shows that all solutions for x are positive and the number of solutions grows exponentially fast with x ! Hence, there are infinitely many complex zeros. For each positive solution x , there are two values for y , symmetric around the real-axis. In other words, the zeros appear in complex conjugate pairs.

The equations can be expressed in terms of the Lambert function. We rewrite the first equation as

$$-a \cos y = -xe^{-x} = W^{-1}(-x)$$

from which

$$x = -W(a \cos y)$$

If $0 \leq a \cos y \leq a \leq 1$, then $x \in (-W(1), 0] = (-0.567, 0]$. If $-\frac{1}{e} \leq a \cos y \leq 0$, then there are two solutions for x , either $x \in [0, 1]$ or $x > 1$. Substituted into $x = y \cot y$, then yields

$$y = -W(a \cos y) \tan y$$

Unfortunately, there is no elegant closed form for a complex zero.

A.2 The integral (5) in terms of the Lambert function

Using the derivative of $W(W^{-1}(v)) = v$, we obtain

$$\left. \frac{dW(x)}{dx} \right|_{x=W^{-1}(v)=ve^v} = \frac{1}{\frac{dW^{-1}(v)}{dv}} = \frac{1}{e^v + ve^v} = \frac{1}{e^v + x} = \frac{1}{\frac{x}{v} + x}$$

Thus, with $W(x) = v$ that obeys $x = W(x)e^{W(x)}$, we arrive at

$$\frac{dW(x)}{dx} = \frac{1}{e^{W(x)} + x} = \frac{1}{x} \frac{W(x)}{1 + W(x)}$$

Reconsidering the integral (5)

$$\begin{aligned} t^* &= \int_0^\zeta \frac{dw}{1 - \xi_0 e^{-\theta w} - w} = \int_0^\zeta \frac{dw}{(1-w) - \xi_0 e^{-\theta} e^{\theta(1-w)}} = \int_{1-\zeta}^1 \frac{dv}{v - \xi_0 e^{-\theta} e^{\theta v}} \\ &= \int_{\theta(1-\zeta)}^\theta \frac{du}{u - a e^u} = - \int_{\theta(1-\zeta)}^\theta \frac{e^{-u} du}{a - u e^{-u}} = - \int_{\theta(1-\zeta)}^\theta \frac{e^{-u} du}{a + W^{-1}(-u)} \end{aligned}$$

where $a = \xi_0 \theta e^{-\theta} = -\xi_0 W^{-1}(-\theta)$. Let $x = W^{-1}(-u)$, then $u = -W(x)$ and

$$t^* = \int_{W^{-1}(-\theta(1-\zeta))}^{W^{-1}(-\theta)} \frac{e^{W(x)} \frac{dW(x)}{dx} dx}{a + x} = \int_{W^{-1}(-\theta(1-\zeta))}^{W^{-1}(-\theta)} \frac{dx}{(1 + x e^{-W(x)}) (a + x)}$$

Finally, with $x = W(x) e^{W(x)}$ and $W^{-1}(x) = x e^x$, we arrive at

$$t^* = \int_{\theta e^{-\theta}}^{\theta(1-\zeta)e^{-\theta(1-\zeta)}} \frac{dx}{(1 + W(-x)) (\xi_0 \theta e^{-\theta} - x)}$$

We mention another possible route. Since $\frac{d}{du} (u e^{-u} - a) = -u e^{-u} + e^{-u} = (1-u) e^{-u}$, we have

$$t^* = \int_{\theta(1-\zeta)}^\theta \frac{e^{-u} du}{u e^{-u} - a} = \int_{\theta(1-\zeta)}^\theta \frac{d(u e^{-u} - a)}{(1-u)(u e^{-u} - a)}$$

Partial integration yields

$$t^* = \frac{\log(\theta e^{-\theta} (1 - \xi_0))}{1 - \theta} - \frac{\log(\theta e^{-\theta} ((1 - \zeta) e^{\theta \zeta} - \xi_0))}{1 - \theta (1 - \zeta)} - \int_{\theta(1-\zeta)}^\theta \frac{\log(u e^{-u} - a)}{(1-u)^2} du$$

which can be problematic if $\theta(1-\zeta) < 1$ and $\theta > 1$, due to the pole at $u = 1$. Invoking contour integration – Cauchy's principal value – can be considered.

B Characteristic coefficients of a complex function

If $f(z)$ has a Taylor series around z_0 ,

$$f(z) = \sum_{k=0}^{\infty} f_k(z_0) (z - z_0)^k \quad \text{with } f_k(z_0) = \frac{1}{k!} \left. \frac{d^k f(z)}{dz^k} \right|_{z=z_0}$$

then the general relation where $G(z)$ is analytic around $f(z_0)$ is

$$G(f(z)) = G(f(z_0)) + \sum_{m=1}^{\infty} \left(\sum_{k=1}^m \frac{1}{k!} \left. \frac{d^k G(p)}{dp^k} \right|_{p=f(z_0)} s[k, m]_{f(z)}(z_0) \right) (z - z_0)^m \quad (32)$$

where the characteristic coefficient [18] of a complex function $f(z)$ has the combinatorial form

$$s[k, m]_{f(z)}(z_0) = \sum_{\sum_{i=1}^k j_i = m, j_i > 0} \prod_{i=1}^k f_{j_i}(z_0)$$

which obeys the recursion relation

$$\begin{aligned} s[1, m]_{f(z)}(z_0) &= f_m(z_0) \\ s[k, m]_{f(z)}(z_0) &= \sum_{j=1}^{m-k+1} f_j(z_0) s[k-1, m-j]_{f(z)}(z_0) \quad (k > 1) \end{aligned} \quad (33)$$

For $k \leq m$ and $m > 0$, the characteristic coefficient of a function $f(z)$ around z_0 also equals

$$s[k, m]_{f(z)}(z_0) = \frac{1}{m!} \left. \frac{d^m}{dz^m} [f(z) - f(z_0)]^k \right|_{z=z_0} \quad (34)$$

illustrating that $s[k, m]_{f(z)}(z_0) = 0$ for a constant function. The characteristic coefficient $s[k, m]_{f(z)}(z_0)$ is a fundamental building block in the theory of generalized Taylor series. Clearly, (32) reduces to Taylor series of $G(z)$ for $f(z) = z$ and, thus, $s[k, m]_z(z_0) = \delta_{k,m}$.

C Proof of Theorem 1

We present three proofs, a direct computation involving our characteristic coefficients (Section B), a verification proof, that avoids characteristic coefficients and a proof based on repeated partial integrations.

A) If the Taylor series of a complex function $f(z) = \sum_{k=0}^{\infty} f_k(z_0) (z - z_0)^k$, then

$$\frac{1}{f(z)} = \frac{1}{f_0(z_0)} + \sum_{m=1}^{\infty} \left[\sum_{k=1}^m \frac{(-1)^k}{(f_0(z_0))^{k+1}} s[k, m](z_0) \right] (z - z_0)^m \quad (35)$$

where $s[k, m](z_0)$ is the characteristic coefficient of the function $f(z)$ around z_0 .

The Taylor series of the entire function $h(z) = 1 - \xi_0 e^{-\theta z} - z$ of the complex variable z around z_0 is

$$\begin{aligned} h(z) &= 1 - \xi_0 e^{-\theta z} - z = 1 - z_0 - (z - z_0) - \xi_0 e^{-\theta z_0} e^{-\theta(z-z_0)} \\ &= 1 - \xi_0 e^{-\theta z_0} - z_0 + \left(\theta \xi_0 e^{-\theta z_0} - 1 \right) (z - z_0) - \xi_0 e^{-\theta z_0} \sum_{k=2}^{\infty} \frac{(-\theta)^k}{k!} (z - z_0)^k \end{aligned}$$

Since the characteristic coefficient of e^z around $z_0 = 0$ is known as

$$\mathcal{S}_m^{(k)} = \frac{m!}{k!} s[k, m]|_{e^z}(0) \quad (36)$$

where $\mathcal{S}_m^{(k)}$ is the Stirling numbers of the second kind [21], we apply the property

$$s[k, m]|_{f(\alpha z)} = \alpha^m s[k, m]|_{f(z)} \quad (37)$$

to obtain

$$s[k, m]|_{e^{-\tau z}} = (-\tau)^m \frac{k!}{m!} \mathcal{S}_m^{(k)}$$

From (34), it follows that $s[k, m]|_{e^{-\tau z}}(z_0) = e^{-k\tau z_0} s[k, m]|_{e^{-\tau z}}(0)$ and

$$s[k, m]|_{e^{-\tau z}}(z_0) = e^{-k\tau z_0} (-\tau)^m \frac{k!}{m!} \mathcal{S}_m^{(k)}$$

Next, the characteristic coefficient of $N - z$ follows directly from (34)

$$s[k, m]|_{N-z}(z_0) = (-1)^k 1_{\{k=m\}}$$

With a little more effort, we find that

$$s[k, m]|_{\alpha f(z) + \beta g(z)}(z_0) = \sum_{j=0}^k \binom{k}{j} \alpha^{k-j} \beta^j \sum_{n=0}^m s[k-j, m-n]|_{f(z)}(z_0) s[j, n]|_{g(z)}(z_0) \quad (38)$$

Applying (38) to $g(z) = 1 - z$ and $f(z) = e^{-\theta z}$ with $\alpha = (-\xi_0)$ yields

$$\begin{aligned} s[k, m]|_{1-\zeta-\xi_0 e^{-\theta \zeta}}(z_0) &= \sum_{j=0}^k \binom{k}{j} (-\xi_0)^{k-j} \sum_{n=0}^m s[k-j, m-n]|_{e^{-\theta z}} s[j, n]|_{1-z} \\ &= (-\xi_0)^k \sum_{j=0}^k \binom{k}{j} (-\xi_0)^{-j} \sum_{n=0}^m e^{-(k-j)\theta z_0} (-\theta)^{m-n} \frac{(k-j)!}{(m-n)!} \mathcal{S}_{m-n}^{(k-j)} (-1)^j 1_{\{j=n\}} \end{aligned}$$

and

$$s[k, m]|_{1-\zeta-\xi_0 e^{-\theta \zeta}}(z_0) = \frac{k!}{m!} (-1)^k \sum_{j=0}^k \binom{m}{j} (\xi_0 e^{-\theta z_0})^{k-j} (-\theta)^{m-j} \mathcal{S}_{m-j}^{(k-j)} \quad (39)$$

We are now ready to apply (35)

$$\frac{1}{1-\zeta-\xi_0 e^{-\theta \zeta}} = \frac{1}{1-z_0-\xi_0 e^{-\theta z_0}} + \sum_{m=1}^{\infty} \left[\sum_{k=1}^m \frac{k! \sum_{j=0}^k \binom{m}{j} (\xi_0 e^{-\theta z_0})^{k-j} (-\theta)^{m-j} \mathcal{S}_{m-j}^{(k-j)}}{(1-z_0-\xi_0 e^{-\theta z_0})^{k+1}} \right] \frac{(\zeta-z_0)^m}{m!} \quad (40)$$

Finally, $t^* = H(\zeta) = \int_0^z \frac{du}{1-u-\xi_0 e^{-\theta u}}$ follows after integration of the Taylor series (40) as

$$t^* = H(\zeta) = \frac{\zeta}{1-z_0-\xi_0 e^{-\theta z_0}} + \sum_{m=1}^{\infty} \left[\sum_{k=1}^m \frac{k! \sum_{j=0}^k \binom{m}{j} (\xi_0 e^{-\theta z_0})^{k-j} (-\theta)^{m-j} \mathcal{S}_{m-j}^{(k-j)}}{(1-z_0-\xi_0 e^{-\theta z_0})^{k+1}} \right] \frac{(\zeta-z_0)^{m+1} - (-z_0)^{m+1}}{(m+1)!} \quad (41)$$

The Taylor series (41) converges reasonably fast if we choose $z_0 = \frac{\zeta}{2}$, which minimizes both $(\zeta - z_0)^{m+1}$ and $(-z_0)^{m+1}$. In that case,

$$(\zeta - z_0)^{m+1} - (-z_0)^{m+1} = \left(\frac{\zeta}{2}\right)^{m+1} - \left(-\frac{\zeta}{2}\right)^{m+1} = \left(\frac{\zeta}{2}\right)^{m+1} (1 + (-1)^m)$$

and only even terms in m remain. With the choice $z_0 = \frac{\zeta}{2}$, the Taylor series (41) becomes (19).

B) Reversing the m - and k -sum in (40) gives us

$$\begin{aligned} \frac{1}{1-\zeta-\xi_0 e^{-\theta \zeta}} &= \frac{1}{1-z_0-\xi_0 e^{-\theta z_0}} + \sum_{k=1}^{\infty} \frac{k! \sum_{j=0}^k (\xi_0 e^{-\theta z_0})^{k-j}}{(1-z_0-\xi_0 e^{-\theta z_0})^{k+1}} \sum_{m=k}^{\infty} \binom{m}{j} (-\theta)^{m-j} \mathcal{S}_{m-j}^{(k-j)} \frac{(\zeta-z_0)^m}{m!} \\ &= \frac{1}{1-z_0-\xi_0 e^{-\theta z_0}} + \sum_{k=1}^{\infty} \frac{k! \sum_{j=0}^k \frac{(\xi_0 e^{-\theta z_0})^{k-j}}{j!} (-\theta)^{-j}}{(1-z_0-\xi_0 e^{-\theta z_0})^{k+1}} \sum_{m=k}^{\infty} \mathcal{S}_{m-j}^{(k-j)} \frac{(\theta(z_0-\zeta))^m}{(m-j)!} \end{aligned}$$

Further,

$$\sum_{m=k}^{\infty} \mathcal{S}_{m-j}^{(k-j)} \frac{(\theta(z_0-\zeta))^m}{(m-j)!} = (\theta(z_0-\zeta))^j \sum_{m=k-j}^{\infty} \mathcal{S}_m^{(k-j)} \frac{(\theta(z_0-\zeta))^m}{m!}$$

and invoking the generating function of the Stirling Numbers of the Second Kind [21, Sec. 24.1.4]

$$(e^x - 1)^k = k! \sum_{m=k}^{\infty} \mathcal{S}_m^{(k)} \frac{x^m}{m!}$$

yields

$$\sum_{m=k}^{\infty} \mathcal{S}_{m-j}^{(k-j)} \frac{(\theta(z_0-\zeta))^m}{(m-j)!} = (\theta(z_0-\zeta))^j \frac{(e^{\theta(z_0-\zeta)} - 1)^{k-j}}{(k-j)!}$$

Hence,

$$\begin{aligned}
\frac{1}{1 - \zeta - \xi_0 e^{-\theta \zeta}} &= \frac{1}{1 - z_0 - \xi_0 e^{-\theta z_0}} + \sum_{k=1}^{\infty} \frac{\sum_{j=0}^k \binom{k}{j} (\xi_0 e^{-\theta z_0} (e^{\theta(z_0 - \zeta)} - 1))^{k-j} (\zeta - z_0)^j}{(1 - z_0 - \xi_0 e^{-\theta z_0})^{k+1}} \\
&= \frac{1}{1 - z_0 - \xi_0 e^{-\theta z_0}} + \sum_{k=1}^{\infty} \frac{(\zeta - z_0 + \xi_0 (e^{-\theta \zeta} - e^{-\theta z_0}))^k}{(1 - z_0 - \xi_0 e^{-\theta z_0})^{k+1}} \\
&= \frac{1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \left(1 + \sum_{k=1}^{\infty} \left(\frac{\zeta - z_0 + \xi_0 (e^{-\theta \zeta} - e^{-\theta z_0})}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^k \right)
\end{aligned}$$

and

$$\begin{aligned}
\frac{1}{1 - \zeta - \xi_0 e^{-\theta \zeta}} &= \frac{1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \sum_{k=0}^{\infty} \left(\frac{(1 - z_0 - \xi_0 e^{-\theta z_0}) - (1 - \zeta - \xi_0 e^{-\theta \zeta})}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^k \\
&= \frac{1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \sum_{k=0}^{\infty} \left(1 - \frac{1 - \zeta - \xi_0 e^{-\theta \zeta}}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^k \\
&= \frac{1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \frac{1}{1 - 1 + \frac{1 - \zeta - \xi_0 e^{-\theta \zeta}}{1 - z_0 - \xi_0 e^{-\theta z_0}}} = \frac{1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \frac{1}{\frac{1 - \zeta - \xi_0 e^{-\theta \zeta}}{1 - z_0 - \xi_0 e^{-\theta z_0}}}
\end{aligned}$$

resulting in an identity and demonstrating that the Taylor series (40) is correct. Moreover, convergence requires that $\left| 1 - \frac{1 - \zeta - \xi_0 e^{-\theta \zeta}}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right| < 1$, which is equivalent in terms of fractions to

$$\frac{\zeta - z_0 + \xi_0 (e^{-\theta \zeta} - e^{-\theta z_0})}{1 - z_0 - \xi_0 e^{-\theta z_0}} \leq 1$$

or

$$\zeta \leq 1 - \xi_0 e^{-\theta \zeta}$$

which is always satisfied for any (physical) fraction of removed items $\zeta \leq \zeta_{\max}$, because, as shown in Section A, the maximum possible fraction of removed items ζ_{\max} satisfies

$$\zeta_{\max} = 1 - \xi_0 e^{-\theta \zeta_{\max}}$$

Consequently, all terms in $\sum_{k=0}^{\infty} \left(1 - \frac{1 - \zeta - \xi_0 e^{-\theta \zeta}}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^k$ are positive, as well as in the integrated power series.

C) From the general relation [22]

$$\int_a^b f(x) g(x) dx = \int_a^b \left(\sum_{k=0}^{m-1} \frac{g^{(k)}(b)}{k!} (u-b)^k \right) f(u) du + \frac{(-1)^m}{(m-1)!} \int_a^b dx g^{(m)}(x) \int_a^x (x-u)^{m-1} f(u) du \quad (42)$$

we find, for $f(u) = 1$ and $g(u) = \frac{1}{1 - u - \xi_0 e^{-\theta u}}$,

$$\begin{aligned}
\int_0^{\zeta} \frac{du}{1 - u - \xi_0 e^{-\theta u}} &= \int_0^{\zeta} \left(\sum_{k=0}^{m-1} \frac{g^{(k)}(\zeta)}{k!} (u - \zeta)^k \right) du + \frac{(-1)^m}{(m-1)!} \int_0^{\zeta} dx g^{(m)}(x) \int_0^x (x-u)^{m-1} du \\
&= \sum_{k=0}^{m-1} \frac{g^{(k)}(\zeta)}{k!} \int_0^{\zeta} (u - \zeta)^k du + \frac{(-1)^m}{(m-1)!} \int_0^{\zeta} dx g^{(m)}(x) \int_0^x (x-u)^{m-1} du
\end{aligned}$$

and, with $\int_0^z (u-z)^k du = \frac{(u-z)^{k+1}}{k+1} \Big|_0^z = \frac{(-1)^k z^{k+1}}{k+1}$,

$$\int_0^\zeta \frac{du}{1-u-\xi_0 e^{-\theta u}} = \sum_{k=0}^{m-1} \frac{(-1)^k g^{(k)}(\zeta)}{(k+1)!} \zeta^{k+1} - \frac{(-1)^m}{m!} \int_0^\zeta x^m g^{(m)}(x) dx$$

Hence,

$$\begin{aligned} \int_0^\zeta \frac{du}{1-u-\xi_0 e^{-\theta u}} &= \sum_{k=0}^{m-1} \frac{d^k}{du^k} \left(\frac{1}{1-u-\xi_0 e^{-\theta u}} \right) \Big|_{u=\zeta} \frac{(-1)^k \zeta^{k+1}}{(k+1)!} \\ &\quad - \frac{(-1)^m}{m!} \int_0^\zeta t^m \frac{d^m}{du^m} \left(\frac{1}{1-u-\xi_0 e^{-\theta u}} \right) \Big|_{u=t} dt \end{aligned}$$

which leads for $m \rightarrow \infty$ to the Taylor series (41) for $z_0 = \zeta$. Consequently,

$$\frac{d^m}{du^m} \left(\frac{1}{1-u-\xi_0 e^{-\theta u}} \right) \Big|_{u=\zeta} = \sum_{k=1}^m \frac{k! \sum_{j=0}^k \binom{m}{j} (\xi_0 e^{-\theta \zeta})^{k-j} (-\theta)^{m-j} \mathcal{S}_{m-j}^{(k-j)}}{(1-\zeta-\xi_0 e^{-\theta \zeta})^{k+1}} \quad (43)$$

and, also with the characteristic coefficient (39),

$$\frac{d^m}{du^m} \left(\frac{1}{1-u-\xi_0 e^{-\theta u}} \right) \Big|_{u=\zeta} = m! \sum_{k=1}^m \frac{(-1)^k s[k, m]|_{1-\zeta-\xi_0 e^{-\theta \zeta}}(\zeta)}{(1-\zeta-\xi_0 e^{-\theta \zeta})^{k+1}}$$

D Further developments of the Taylor series

D.1 Other expression for the characteristic coefficient $s[k, m]|_{1-\zeta-\xi_0 e^{-\theta \zeta}}(z_0)$

Denoting $s^*[k, m] = s[k, m]|_{\forall j: f_j \rightarrow f_{j+1}}$, which means that we shift each Taylor coefficients one upwards, then we can show [22], for $m > k$, that

$$s[k, m](z_0) = \sum_{j=1}^{m-k} \binom{k}{j} f_1^{k-j} s^*[j, m-k](z_0)$$

and, in general, $s[m, m](z_0) = f_1^m(z_0)$. For the function $h(z) = 1 - \xi_0 e^{-\theta z} - z$, with Taylor coefficients $h_0(z_0) = 1 - z_0 - \xi_0 e^{-\theta z_0}$, $h_1(z_0) = \xi_0 \theta e^{-\theta z_0} - 1$ and $h_j(z_0) = -\xi_0 e^{-\theta z_0} \frac{(-\theta)^j}{j!}$ for $j > 1$, we have

$$s[k, m]|_{1-\zeta-\xi_0 e^{-\theta \zeta}}(z_0) = \sum_{j=1}^{m-k} \binom{k}{j} \left(\theta \xi_0 e^{-\theta z_0} - 1 \right)^{k-j} s^*[j, m-k](z_0)|_{1-\zeta-\xi_0 e^{-\theta \zeta}}$$

where $s^*[k, m](z_0)|_{1-\zeta-\xi_0 e^{-\theta \zeta}} = s^*[k, m](z_0)|_{-\xi_0 e^{-\theta \zeta}}$ and $s[k, m]|_{(-\xi_0) e^{\theta z}}(z_0) = (-1)^{k+m} \xi_0^k \theta^m e^{k\theta z_0} \frac{k!}{m!} \mathcal{S}_m^{(k)}$.

With

$$\begin{aligned} s^*[k, m]|_{(-\xi_0) e^{\theta z}}(z_0) &= \sum_{j=0}^k \binom{k}{j} (-1)^{k-j} (\xi_0 \theta)^{k-j} e^{-(k-j)\theta z_0} s[j, m+j]|_{(-\xi_0) e^{\theta z}}(z_0) \\ &= (-1)^m \sum_{j=0}^k \binom{k}{j} (-1)^{k-j} (\xi_0 \theta)^{k-j} e^{(k-j)\theta z_0} \xi_0^j \theta^{m+j} e^{j\theta z_0} \frac{j!}{(m+j)!} \mathcal{S}_{m+j}^{(j)} \\ &= (-1)^m \xi_0^k \theta^{m+k} e^{-k\theta z_0} k! \sum_{j=0}^k \frac{(-1)^{k-j}}{(k-j)!(m+j)!} \mathcal{S}_{m+j}^{(j)} \end{aligned}$$

leads, for $k < m$, to

$$s[k, m]|_{1-\zeta-\xi_0 e^{-\theta\zeta}}(z_0) = (-1)^{m-k} \theta^{m-k} \sum_{j=1}^{m-k} \binom{k}{j} \left(\theta \xi_0 e^{-\theta z_0} - 1 \right)^{k-j} (\xi_0 \theta)^j e^{-j\theta z_0} j! T(j, m-k)$$

where the sum

$$T(j, m) = \sum_{q=0}^j \frac{(-1)^{j-q}}{(j-q)!(m+q)!} \mathcal{S}_{m+q}^{(q)} = \frac{(-1)^j}{j!} \delta_{m0} + \sum_{q=1}^j \frac{(-1)^{j-q}}{(j-q)!(m+q)!} \mathcal{S}_{m+q}^{(q)} \quad (44)$$

is always positive and equals the $s[k, m]|_{ze^{-\tau z}}(0)$. From (39), we find

$$s[m, m]|_{1-\zeta-\xi_0 e^{-\theta\zeta}}(z_0) = (-1)^m \sum_{j=0}^m \binom{m}{j} \left(-\theta \xi_0 e^{-\theta z_0} \right)^{m-j} = \left(\theta \xi_0 e^{-\theta z_0} - 1 \right)^m$$

We are now ready to apply (35)

$$\begin{aligned} \frac{1}{1-\zeta-\xi_0 e^{-\theta\zeta}} &= \frac{1}{1-z_0-\xi_0 e^{-\theta z_0}} \\ &+ \sum_{m=1}^{\infty} \left[\sum_{k=1}^m \frac{\theta^{m-k} \sum_{j=1}^{m-k} \binom{k}{j} \left(\theta \xi_0 e^{-\theta z_0} - 1 \right)^{k-j} (\xi_0 \theta)^j e^{-j\theta z_0} j! T(j, m-k)}{(1-z_0-\xi_0 e^{-\theta z_0})^{k+1}} \right] (z_0 - \zeta)^m \end{aligned} \quad (45)$$

D.2 Splitting off the $k = m$ term in (41)

We split-off the $k = m$ term in the Taylor series (41) around the point z_0 ,

$$\begin{aligned} t^* &= \frac{\zeta}{1-z_0-\xi_0 e^{-\theta\zeta_0}} + \sum_{m=1}^{\infty} \frac{(1-\theta\xi_0 e^{-\theta z_0})^m}{(1-z_0-\xi_0 e^{-\theta z_0})^{m+1}} \frac{(\zeta-z_0)^{m+1}}{(m+1)} \\ &- \sum_{m=1}^{\infty} \frac{(1-\theta\xi_0 e^{-\theta z_0})^m}{(1-z_0-\xi_0 e^{-\theta z_0})^{m+1}} \frac{(-z_0)^{m+1}}{(m+1)} \\ &+ \sum_{m=1}^{\infty} \left[\sum_{k=1}^{m-1} \frac{k! \sum_{j=0}^k \binom{m}{j} (\xi_0 e^{-\theta z_0})^{k-j} (-\theta)^{m-j} \mathcal{S}_{m-j}^{(k-j)}}{(1-z_0-\xi_0 e^{-\theta z_0})^{k+1}} \right] \frac{(\zeta-z_0)^{m+1} - (-z_0)^{m+1}}{(m+1)!} \end{aligned}$$

It holds that

$$\begin{aligned} Y(y) &= \sum_{m=1}^{\infty} \frac{(1-\theta\xi_0 e^{-\theta z_0})^m}{(1-z_0-\xi_0 e^{-\theta z_0})^{m+1}} \frac{y^{m+1}}{(m+1)} = \sum_{m=2}^{\infty} \frac{(1-\theta\xi_0 e^{-\theta z_0})^{m-1}}{(1-z_0-\xi_0 e^{-\theta z_0})^m} \frac{y^m}{m} \\ &= \frac{1}{1-\theta\xi_0 e^{-\theta z_0}} \sum_{m=2}^{\infty} \frac{1}{m} \left(\frac{y(1-\theta\xi_0 e^{-\theta z_0})}{1-z_0-\xi_0 e^{-\theta z_0}} \right)^m \\ &= \frac{1}{1-\theta\xi_0 e^{-\theta z_0}} \left\{ -\ln \left(1 - \frac{y(1-\theta\xi_0 e^{-\theta z_0})}{1-z_0-\xi_0 e^{-\theta z_0}} \right) - \frac{y(1-\theta\xi_0 e^{-\theta z_0})}{1-z_0-\xi_0 e^{-\theta z_0}} \right\} \end{aligned}$$

and

$$\begin{aligned}
R_m &= \sum_{m=1}^{\infty} \frac{(1 - \theta \xi_0 e^{-\theta z_0})^m}{(1 - z_0 - \xi_0 e^{-\theta z_0})^{m+1}} \frac{(\zeta - z_0)^{m+1}}{(m+1)} - \sum_{m=1}^{\infty} \frac{(1 - \theta \xi_0 e^{-\theta z_0})^m}{(1 - z_0 - \xi_0 e^{-\theta z_0})^{m+1}} \frac{(-z_0)^{m+1}}{(m+1)} \\
&= \frac{1}{1 - \theta \xi_0 e^{-\theta z_0}} \left\{ -\ln \left(\frac{1 - z_0 - \xi_0 e^{-\theta z_0} - (\zeta - z_0)(1 - \theta \xi_0 e^{-\theta z_0})}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right) - \frac{\zeta(1 - \theta \xi_0 e^{-\theta z_0})}{(1 - z_0 - \xi_0 e^{-\theta z_0})} \right\} \\
&\quad + \frac{1}{1 - \theta \xi_0 e^{-\theta z_0}} \ln \left(\frac{1 - z_0 - \xi_0 e^{-\theta z_0} + z_0(1 - \theta \xi_0 e^{-\theta z_0})}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right) \\
&= \frac{1}{1 - \theta \xi_0 e^{-\theta z_0}} \ln \left(\frac{1 - \xi_0 e^{-\theta z_0}(1 + z_0 \theta)}{1 - \zeta - \xi_0 e^{-\theta z_0}(1 + (z_0 - \zeta)\theta)} \right) - \frac{\zeta}{(1 - z_0 - \xi_0 e^{-\theta z_0})}
\end{aligned}$$

Hence,

$$\begin{aligned}
t^* &= \frac{1}{1 - \theta \xi_0 e^{-\theta z_0}} \ln \left(\frac{1 - \xi_0 e^{-\theta z_0}(1 + z_0 \theta)}{1 - \zeta - \xi_0 e^{-\theta z_0}(1 + (z_0 - \zeta)\theta)} \right) + \\
&\quad \sum_{m=1}^{\infty} \left[\sum_{k=1}^{m-1} \frac{k! \sum_{j=0}^k \binom{m}{j} (\xi_0 e^{-\theta z_0})^{k-j} (-\theta)^{m-j} \mathcal{S}_{m-j}^{(k-j)}}{(1 - z_0 - \xi_0 e^{-\theta z_0})^{k+1}} \right] \frac{(\zeta - z_0)^{m+1} - (-z_0)^{m+1}}{(m+1)!} \quad (46)
\end{aligned}$$

Integration of the Taylor series in (45), $t^* = \int_0^{\zeta} \frac{dw}{1 - w - \xi_0 e^{-\theta w}}$ yields, similarly as in (46),

$$\begin{aligned}
t^* &= \frac{1}{1 - \theta \xi_0 e^{-\theta z_0}} \ln \left(\frac{1 - \xi_0 e^{-\theta z_0}(1 + z_0 \theta)}{1 - \zeta - \xi_0 e^{-\theta z_0}(1 + (z_0 - \zeta)\theta)} \right) \\
&\quad + \sum_{m=1}^{\infty} \left[\sum_{k=1}^{m-1} \frac{(\xi_0 e^{-\theta z_0} - \frac{1}{\theta})^k \sum_{j=1}^{m-k} \binom{m-k}{j} \left(\frac{\xi_0 \theta e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \right)^j j! T(j, m-k)}{(1 - z_0 - \xi_0 e^{-\theta z_0})^{k+1}} \right] \frac{(-\theta)^m (w - z_0)^{m+1}}{(m+1)} \Big|_0^{\zeta}
\end{aligned}$$

and (20). The series (20) is numerically stabler than (46), because all terms in the sums are positive.

The last sum can be rewritten as

$$\begin{aligned}
M &= \sum_{m=1}^{\infty} \left[\sum_{k=1}^{m-1} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{\theta(1 - z_0 - \xi_0 e^{-\theta z_0})} \right)^k \sum_{j=1}^{m-k} \binom{m-k}{j} \left(\frac{\xi_0 \theta e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \right)^j j! T(j, m-k) \right] \frac{\theta^m z_0^{m+1} - \theta^m (z_0 - \zeta)^{m+1}}{(1 - z_0 - \xi_0 e^{-\theta z_0})(m+1)} \\
&= \sum_{m=1}^{\infty} \left[\sum_{l=1}^{m-1} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{\theta(1 - z_0 - \xi_0 e^{-\theta z_0})} \right)^{m-l} \sum_{j=1}^l \binom{m-l}{j} \left(\frac{\xi_0 \theta e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \right)^j j! T(j, l) \right] \frac{\theta^m z_0^{m+1} - \theta^m (z_0 - \zeta)^{m+1}}{(1 - z_0 - \xi_0 e^{-\theta z_0})(m+1)}
\end{aligned}$$

Reversing the m - and l -sum yields

$$\begin{aligned}
M &= \sum_{l=1}^{\infty} \sum_{m=l+1}^{\infty} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{\theta(1 - z_0 - \xi_0 e^{-\theta z_0})} \right)^{m-l} \sum_{j=1}^l \binom{m-l}{j} \left(\frac{\xi_0 \theta e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \right)^j j! T(j, l) \frac{\theta^m z_0^{m+1} - \theta^m (z_0 - \zeta)^{m+1}}{(1 - z_0 - \xi_0 e^{-\theta z_0})(m+1)} \\
&= \sum_{l=1}^{\infty} \sum_{j=1}^l \left(\frac{\xi_0 \theta e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \right)^j j! T(j, l) \sum_{m=1}^{\infty} \binom{m}{j} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^m \frac{\theta^l (z_0^{m+l+1} - (z_0 - \zeta)^{m+l+1})}{(1 - z_0 - \xi_0 e^{-\theta z_0})(m+l+1)}
\end{aligned}$$

and

$$\begin{aligned}
M &= \sum_{l=1}^{\infty} \sum_{j=1}^l \left(\frac{\xi_0 \theta e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \right)^j T(j, l) \sum_{m=1}^{\infty} \frac{m!}{(m-l)!} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^m \frac{\theta^l \left(z_0^{m+l+1} - (z_0 - \zeta)^{m+l+1} \right)}{(1 - z_0 - \xi_0 e^{-\theta z_0}) (m + l + 1)} \\
&= \frac{1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \sum_{l=1}^{\infty} \sum_{j=1}^l \left(\frac{\xi_0 \theta e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \right)^j T(j, l) \left\{ \sum_{m=1}^{\infty} \frac{\frac{m!}{(m-l)!} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} z_0 \right)^m}{m + l + 1} \right\} \theta^l z_0^{l+1} \\
&\quad - \frac{1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \sum_{l=1}^{\infty} \sum_{j=1}^l \left(\frac{\xi_0 \theta e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \right)^j T(j, l) \left\{ \sum_{m=1}^{\infty} \frac{\frac{m!}{(m-l)!} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} (z_0 - \zeta) \right)^m}{m + l + 1} \right\} \theta^l (z_0 - \zeta)^{l+1}
\end{aligned}$$

The m -sum, which is of the type $\sum_{m=1}^{\infty} \frac{\frac{m!}{(m-l)!} x^m}{m+l+1}$, can be evaluated, because $\frac{m!}{(m-l)!(m+l+1)}$ is polynomial in m plus $\frac{\alpha}{m+l+1}$. The polynomials corresponds to derivatives of $(1-x)^{-q}$ and the $\frac{\alpha}{m+l+1}$ will generate a logarithm. Below we compute the case terms up to $l = 2$, but concentrated on (20).

D.3 Splitting off the $k = m - 1$ term in (41)

We split-off the $k = m - 1$ term in (20),

$$\begin{aligned}
t^* &= \frac{1}{1 - \theta \xi_0 e^{-\theta z_0}} \ln \left(\frac{1 - \xi_0 e^{-\theta z_0} (1 + z_0 \theta)}{1 - \zeta - \xi_0 e^{-\theta z_0} (1 + (z_0 - \zeta) \theta)} \right) \\
&\quad + \frac{1}{2} \left(\frac{\xi_0 \theta^2 e^{-\theta z_0}}{(1 - \theta \xi_0 e^{-\theta z_0})^2} \right) \sum_{m=1}^{\infty} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^m \frac{(m-1) \left\{ z_0^{m+1} - (z_0 - \zeta)^{m+1} \right\}}{(m+1)} \\
&\quad + \sum_{m=1}^{\infty} \left[\sum_{k=1}^{m-2} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{\theta (1 - z_0 - \xi_0 e^{-\theta z_0})} \right)^k \sum_{j=1}^{m-k} \binom{k}{j} \left(\frac{\xi_0 \theta e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \right)^j j! T(j, m-k) \right] \frac{\theta^m z_0^{m+1} - \theta^m (z_0 - \zeta)^{m+1}}{(1 - z_0 - \xi_0 e^{-\theta z_0}) (m+1)}
\end{aligned}$$

Now,

$$R_{m-1} = \frac{1}{2} \left(\frac{\xi_0 \theta^2 e^{-\theta z_0}}{(1 - \theta \xi_0 e^{-\theta z_0})^2} \right) \sum_{m=1}^{\infty} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^m \frac{m-1}{m+1} \left\{ z_0^{m+1} - (z_0 - \zeta)^{m+1} \right\}$$

and with $\frac{m-1}{m+1} = 1 - \frac{2}{m+1}$, the sum becomes

$$\begin{aligned}
Q &= \sum_{m=1}^{\infty} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^m \frac{m-1}{m+1} \left\{ z_0^{m+1} - (z_0 - \zeta)^{m+1} \right\} \\
&= \sum_{m=1}^{\infty} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^m \left\{ z_0^{m+1} - (z_0 - \zeta)^{m+1} \right\} - 2 \sum_{m=1}^{\infty} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^m \left\{ \frac{z_0^{m+1} - (z_0 - \zeta)^{m+1}}{m+1} \right\} \\
&= \frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \left\{ \zeta_0^2 \sum_{m=0}^{\infty} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} z_0 \right)^m - (z_0 - \zeta)^2 \sum_{m=0}^{\infty} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} (z_0 - \zeta) \right)^m \right\} \\
&\quad - 2 \frac{1 - z_0 - \xi_0 e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \left\{ \sum_{m=1}^{\infty} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^m \frac{\{z_0^m - (z_0 - \zeta)^m\}}{m} - \frac{\theta \xi_0 e^{-\theta z_0} - 1}{(1 - z_0 - \xi_0 e^{-\theta z_0})} \zeta \right\} \\
&= \frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \left\{ \frac{z_0^2}{1 - \frac{\theta \xi_0 e^{-\theta z_0} - 1}{(1 - z_0 - \xi_0 e^{-\theta z_0})} z_0} - \frac{(z_0 - \zeta)^2}{1 - \frac{\theta \xi_0 e^{-\theta z_0} - 1}{(1 - z_0 - \xi_0 e^{-\theta z_0})} (z_0 - \zeta)} \right\} \\
&\quad - 2 \frac{1 - z_0 - \xi_0 e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \left\{ -\log \left(\frac{1 - \frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} z_0}{1 - \frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} (z_0 - \zeta)} \right) - \frac{\theta \xi_0 e^{-\theta z_0} - 1}{(1 - z_0 - \xi_0 e^{-\theta z_0})} \zeta \right\}
\end{aligned}$$

and

$$\begin{aligned}
Q &= \left(\theta \xi_0 e^{-\theta z_0} - 1 \right) \left\{ \frac{z_0^2}{1 - \xi_0 e^{-\theta z_0} (1 + z_0 \theta)} - \frac{(z_0 - \zeta)^2}{1 - \zeta - \xi_0 e^{-\theta z_0} (1 + (z_0 - \zeta) \theta)} \right\} \\
&\quad + 2 \frac{1 - z_0 - \xi_0 e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \log \left(\frac{1 - \xi_0 e^{-\theta z_0} (1 + z_0 \theta)}{1 - \zeta - \xi_0 e^{-\theta z_0} (1 + (z_0 - \zeta) \theta)} \right) + 2\zeta
\end{aligned}$$

Substituting Q yields (21).

The form (21) is again better, but after summing the last m -sum, we converge to the same results as in the Taylor series (20) and (41).

D.4 Splitting off the $k = m - 2$ term in (41)

We may continue in summing in this way. A next split-off in the k -sum for $k = m - 2$ is

$$R_{m-2} = \sum_{m=1}^{\infty} \left[\left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{\theta (1 - z_0 - \xi_0 e^{-\theta z_0})} \right)^{m-2} \sum_{j=1}^2 \binom{m-2}{j} \left(\frac{\xi_0 \theta e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \right)^j j! T(j, 2) \right] \frac{\theta^m z_0^{m+1} - \theta^m (z_0 - \zeta)^{m+1}}{(1 - z_0 - \xi_0 e^{-\theta z_0}) (m+1)}$$

With $T(1, 2) = \frac{1}{6}$ and $T(2, 2) = \frac{1}{8}$, we find

$$\begin{aligned}
R_{m-2} &= \sum_{m=1}^{\infty} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{\theta (1 - z_0 - \xi_0 e^{-\theta z_0})} \right)^{m-2} \frac{(m-2)}{6} \left(\frac{\xi_0 \theta e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \right) \frac{\theta^m z_0^{m+1} - \theta^m (z_0 - \zeta)^{m+1}}{(1 - z_0 - \xi_0 e^{-\theta z_0}) (m+1)} \\
&\quad + \sum_{m=1}^{\infty} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{\theta (1 - z_0 - \xi_0 e^{-\theta z_0})} \right)^{m-2} \frac{(m-2)(m-3)}{8} \left(\frac{\xi_0 \theta e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \right)^2 \frac{\theta^m z_0^{m+1} - \theta^m (z_0 - \zeta)^{m+1}}{(1 - z_0 - \xi_0 e^{-\theta z_0}) (m+1)} \\
&= \frac{\xi_0 \theta^3 e^{-\theta z_0} (1 - z_0 - \xi_0 e^{-\theta z_0})}{6 (\theta \xi_0 e^{-\theta z_0} - 1)^3} \sum_{m=1}^{\infty} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^m \frac{(m-2) (z_0^{m+1} - (z_0 - \zeta)^{m+1})}{(m+1)} \\
&\quad + \frac{\xi_0^2 \theta^4 e^{-2\theta z_0} (1 - z_0 - \xi_0 e^{-\theta z_0})}{8 (\theta \xi_0 e^{-\theta z_0} - 1)^4} \sum_{m=1}^{\infty} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^m \frac{(m-2)(m-3) (z_0^{m+1} - (z_0 - \zeta)^{m+1})}{(m+1)}
\end{aligned}$$

We recognize that the first series is similar to Q , because $\frac{m-2}{m+1} = 1 - \frac{3}{m+1}$ and thus equal to

$$Q_* = \left(\theta \xi_0 e^{-\theta z_0} - 1 \right) \left\{ \frac{z_0^2}{1 - \xi_0 e^{-\theta z_0} (1 + z_0 \theta)} - \frac{(z_0 - \zeta)^2}{1 - \zeta - \xi_0 e^{-\theta z_0} (1 + (z_0 - \zeta) \theta)} \right\} \\ + 3 \frac{1 - z_0 - \xi_0 e^{-\theta z_0}}{\theta \xi_0 e^{-\theta z_0} - 1} \log \left(\frac{1 - \xi_0 e^{-\theta z_0} (1 + z_0 \theta)}{1 - \zeta - \xi_0 e^{-\theta z_0} (1 + (z_0 - \zeta) \theta)} \right) + 3\zeta$$

while, with $\frac{(m-2)(m-3)}{m+1} = (m-6) + \frac{12}{m+1} = m-6 \left(1 - \frac{2}{m+1} \right)$, the last sum contains precisely Q and a new series

$$R_{m-2} = \frac{\xi_0 \theta^3 e^{-\theta z_0} (1 - z_0 - \xi_0 e^{-\theta z_0})}{6 (\theta \xi_0 e^{-\theta z_0} - 1)^2} \left\{ \frac{z_0^2}{1 - \xi_0 e^{-\theta z_0} (1 + z_0 \theta)} - \frac{(z_0 - \zeta)^2}{1 - \zeta - \xi_0 e^{-\theta z_0} (1 + (z_0 - \zeta) \theta)} \right\} \\ + \frac{\xi_0 \theta^3 e^{-\theta z_0} (1 - z_0 - \xi_0 e^{-\theta z_0})^2}{2 (\theta \xi_0 e^{-\theta z_0} - 1)^3} \frac{1}{\theta \xi_0 e^{-\theta z_0} - 1} \log \left(\frac{1 - \xi_0 e^{-\theta z_0} (1 + z_0 \theta)}{1 - \zeta - \xi_0 e^{-\theta z_0} (1 + (z_0 - \zeta) \theta)} \right) \\ + \frac{\xi_0 \theta^3 e^{-\theta z_0} (1 - z_0 - \xi_0 e^{-\theta z_0})}{2 (\theta \xi_0 e^{-\theta z_0} - 1)^3} \zeta \\ + \frac{\xi_0^2 \theta^4 e^{-2\theta z_0} (1 - z_0 - \xi_0 e^{-\theta z_0})}{8 (\theta \xi_0 e^{-\theta z_0} - 1)^4} \sum_{m=1}^{\infty} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^m m \left(z_0^{m+1} - (z_0 - \zeta)^{m+1} \right) \\ - 6 \frac{\xi_0^2 \theta^4 e^{-2\theta z_0} (1 - z_0 - \xi_0 e^{-\theta z_0})}{8 (\theta \xi_0 e^{-\theta z_0} - 1)^4} Q$$

The new series

$$W = \sum_{m=1}^{\infty} \left(\frac{\theta \xi_0 e^{-\theta z_0} - 1}{1 - z_0 - \xi_0 e^{-\theta z_0}} \right)^m m \left(z_0^{m+1} - (z_0 - \zeta)^{m+1} \right)$$

follows from $\frac{1}{(1-x)^2} = \frac{d}{dx} \left(\frac{1}{1-x} \right) = \sum_{m=1}^{\infty} m x^{m-1}$ as

$$W = \left(\theta \xi_0 e^{-\theta z_0} - 1 \right) \left(1 - z_0 - \xi_0 e^{-\theta z_0} \right) \left\{ \frac{z_0^2}{(1 - \xi_0 e^{-\theta z_0} (1 + z_0 \theta))^2} - \frac{(z_0 - \zeta)^2}{(1 - \zeta - \xi_0 e^{-\theta z_0} (1 + (z_0 - \zeta) \theta))^2} \right\}$$

Hence,

$$R_{m-2} = \frac{\xi_0 \theta^3 e^{-\theta \zeta_0} (1 - \zeta_0 - \xi_0 e^{-\theta \zeta_0})}{6 (1 - \theta \xi_0 e^{-\theta \zeta_0})^2} \left\{ \frac{\zeta_0^2}{1 - \xi_0 e^{-\theta \zeta_0} (1 + \zeta_0 \theta)} - \frac{(\zeta_0 - \zeta)^2}{1 - \zeta - \xi_0 e^{-\theta \zeta_0} (1 + (\zeta_0 - \zeta) \theta)} \right\} \\ + \frac{\xi_0 \theta^3 e^{-\theta \zeta_0} (1 - \zeta_0 - \xi_0 e^{-\theta \zeta_0})^2}{2 (1 - \theta \xi_0 e^{-\theta \zeta_0})^3} \frac{1}{1 - \theta \xi_0 e^{-\theta \zeta_0}} \log \left(\frac{1 - \xi_0 e^{-\theta \zeta_0} (1 + \zeta_0 \theta)}{1 - \zeta - \xi_0 e^{-\theta \zeta_0} (1 + (\zeta_0 - \zeta) \theta)} \right) \\ - \frac{\xi_0 \theta^3 e^{-\theta \zeta_0} (1 - \zeta_0 - \xi_0 e^{-\theta \zeta_0})}{2 (1 - \theta \xi_0 e^{-\theta \zeta_0})^3} \zeta \\ - \frac{\xi_0^2 \theta^4 e^{-2\theta \zeta_0} (1 - \zeta_0 - \xi_0 e^{-\theta \zeta_0})^2}{8 (1 - \theta \xi_0 e^{-\theta \zeta_0})^3} \left\{ \frac{\zeta_0^2}{(1 - \xi_0 e^{-\theta \zeta_0} (1 + \theta \zeta_0))^2} - \frac{(\zeta_0 - \zeta)^2}{(1 - \zeta - \xi_0 e^{-\theta \zeta_0} (1 + \theta (\zeta_0 - \zeta)))^2} \right\} \\ + 3 \frac{\xi_0^2 \theta^4 e^{-2\theta \zeta_0} (1 - \zeta_0 - \xi_0 e^{-\theta \zeta_0})}{4 (1 - \theta \xi_0 e^{-\theta \zeta_0})^3} \left\{ \frac{\zeta_0^2}{1 - \xi_0 e^{-\theta \zeta_0} (1 + \zeta_0 \theta)} - \frac{(\zeta_0 - \zeta)^2}{1 - \zeta - \xi_0 e^{-\theta \zeta_0} (1 + (\zeta_0 - \zeta) \theta)} \right\} \\ + 3 \frac{\xi_0^2 \theta^4 e^{-2\theta \zeta_0} (1 - \zeta_0 - \xi_0 e^{-\theta \zeta_0})^2}{2 (1 - \theta \xi_0 e^{-\theta \zeta_0})^4} \left\{ \frac{1}{1 - \theta \xi_0 e^{-\theta \zeta_0}} \log \left(\frac{1 - \xi_0 e^{-\theta \zeta_0} (1 + \zeta_0 \theta)}{1 - \zeta - \xi_0 e^{-\theta \zeta_0} (1 + (\zeta_0 - \zeta) \theta)} \right) \right\} \\ - 3 \frac{\zeta \xi_0^2 \theta^4 e^{-2\theta \zeta_0} (1 - \zeta_0 - \xi_0 e^{-\theta \zeta_0})}{2 (1 - \theta \xi_0 e^{-\theta \zeta_0})^4}$$

Collecting all results in (22). The last sum in (22) is small and $O\left(\zeta_0^5 - (\zeta_0 - \zeta)^5\right)$ and only plays a role when $\zeta \rightarrow \zeta_{\max}$. Also, smaller θ result in faster convergence (only checked for $\zeta_0 = \frac{\zeta}{2}$). In summary, we have shown that, to any desired accuracy, the integral (5) can be analytically approximated. Moreover, ignoring the remaining m -sum, all analytic terms lower bound the integral (5).

E Coefficients $a_k(m, j)$ of the polynomial $p(x; m, j)$ in (28)

We revisit and rewrite the form (27) as

$$\zeta_m(t_0^*) = \frac{(-1)^{m-1} Z}{m!} - \frac{(-1)^m}{m! \theta} \sum_{j=1}^m (-A\theta)^j \sum_{k=0}^{m-j} a_k(m, j) x^k$$

where $p(x; m, j) = \sum_{k=0}^{m-j} a_k(m, j) x^k$ reduces for $p(x; m, m) = a_0(m, m) = (m-1)!$. The first order polynomial $p(x; m, m-1) = a_0(m, m-1) + a_1(m, m-1)x$ for $m \geq 2$ and we list the coefficients for a few m ,

m	$a_0(m, m-1)$	$a_1(m, m-1)$
2	1	1
3	2	3
4	7	12
5	33	60
6	192	360
7	1320	2520
8	10440	20160
9	93240	181440
10	927360	1814400

By inspection, we deduce that $a_1(m, m-1) = \frac{m!}{2}$ and $a_0(m, m-1) = \frac{m!}{4} + \frac{(m-2)!}{2}$.

The second order polynomial $p(x; m, m-2) = a_0(m, m-2) + a_1(m, m-2)x + a_2(m, m-2)x^2$ has coefficients

m	$a_0(m, m-2)$	$a_1(m, m-2)$	$a_2(m, m-2)$
3	1	2	1
4	3	11	7
5	17	69	50
6	120	499	390
7	979	4096	3360
8	8991	37640	31920
9	91586	382920	332640
10	1024022	4273080	3780000

By inspection, we obtain $a_2(m, m-2) = \frac{m!(3m-5)}{24}$ and

$$a_1(m, m-2) = \frac{(m-3)!}{72} (24 - 68m + 57m^2 - 34m^3 + 9m^4)$$

The latter is found as solution of a difference equation

$$\frac{3!a_1(m, m-2)}{(m-3)!} - \frac{3!a_1(m, m-3)}{(m-4)!} = 3(m-1)^2 - (m-2)(m-4)$$

leading to a summation of the right-hand side⁵. However, $a_0(m, m-2)$ possesses a more complicated law, which has defeated us so far.

The highest order polynomial $p(x; m, 1) = \sum_{k=0}^{m-1} a_k(m, 1) x^k$ has $a_0(m, 1) = a_{m-1}(m, 1) = 1$ and $a_1(m, 1) = m-1$. The coefficient $a_{m-2}(m, 1) = \frac{(m-1)(m-2)}{2} + 1$.

⁵Summations of powers of integers can be expressed as Bernoulli polynomials [23].