Online Supplement - Dose-optimal vaccine allocation over multiple populations

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Appendix S1   The herd effect function

In this paper we study the herd effect of vaccination, denoted by the function $G_j(f_j)$. In Section 3.2 we have defined $G_j(f_j)$ as the final fraction of people susceptible in population j after vaccinating a fraction f_j of the susceptible people at time τ. More precisely, for $f_j \in [0, s_j(\tau)]$

$$G_j(f_j) = \lim_{t \to \infty} s_j(t), \tag{1}$$

with $s_j(t)$ evolving according to the differential equations of the SIR model (1) for $t > \tau$. In this appendix we present and analyze an alternative formulation of the herd effect $G_j(f_j)$, which forms the basis of the structural analysis of the herd effect.

S1.1   Implicit formulation of the herd effect

Based on the differential equations of the SIR model we derive an implicit expression for the herd effect. From (1) the following equation follows, which presents the relation between $i_j(t)$ and $s_j(t)$ at any time t (Hethcote 1976):

$$i_j(t) = -s_j(t) + \frac{\log(s_j(t))}{\sigma_j} + s_{0,j} + i_{0,j} - \frac{\log(s_{0,j})}{\sigma_j} \tag{2}$$

Above relation characterizes the state of the system at any point in time, but prior to vaccination. Upon vaccination at time τ the state of the system changes from state $(s_j(\tau), i_j(\tau))$ to state $(s_j(\tau) - f_j, i_j(\tau))$. Hence, the state $(s_j(\tau) - f_j, i_j(\tau))$ directly after vaccination can be seen as a new initial state, where $i_j(\tau)$ can be obtained from (2). $G_j(f_j)$ is then obtained from (2) by setting $i_j(t) = 0$ and thus is the unique solution to:

$$0 = -G_j(f_j) + \frac{\log(G_j(f_j))}{\sigma_j} + s_j(\tau) - f_j + i_j(\tau) - \frac{\log(s(\tau) - f_j)}{\sigma_j}$$
$$\Leftrightarrow 0 = -G_j(f_j) + \frac{\log(G_j(f_j))}{\sigma_j} + s_{0,j} + i_{0,j} - \frac{1}{\sigma_j} \log\left(s_{0,j}\left(1 - \frac{f_j}{s_j(\tau)}\right)\right) - f_j \tag{3}$$

Above equation holds for all $i_{0,j} > 0$. The value of $G_j(f_j)$ in the limit $i_{0,j} \downarrow 0$ can be determined by substituting $i_{0,j} = 0$. (3) extends the *final size equation* to any initial state. The original final size equation can be recovered for $f_j = 0$, $s_{0,j} \to 1$ and $i_{0,j} \to 0$ (see e.g., Kermack and McKendrick (1927), Ma and Earn (2006), Diekmann et al. (2012) and Keeling and Shattock (2012)). We refer

to Appendix S5 for an alternative expression of $G_j(f_j)$ using the Lambert W function denoted by $W(x)$ (cf. Corless et al. 1996, Ma and Earn 2006).

S1.2   Derivatives of the herd effect

We present implicit equations for the first and second order derivative of the function $G(f)$ with respect to f (we drop the subscript j for convenience). These derivatives will appear in the next sections to prove the structural characteristics of the herd effect $G(f)$. Denote by $G'(f)$ and $G''(f)$ respectively the first and second order derivative of the function $G(f)$ with respect to f which can be derived from (3):

$$G'(f)\left[1 - \frac{1}{\sigma G(f)}\right] = \frac{1}{\sigma(s(\tau) - f)} - 1 \tag{4}$$

$$G''(f)\left[1 - \frac{1}{\sigma G(f)}\right] = \frac{1}{\sigma(s(\tau) - f)^2} - \frac{1}{\sigma}\left[\frac{G'(f)}{G(f)}\right]^2$$

$$\Leftrightarrow G''(f) = \frac{G(f)^2 - [G'(f)(s(\tau) - f)]^2}{(\sigma G(f) - 1)G(f)(s(\tau) - f)^2} \tag{5}$$

Appendix S2   Analysis of the herd effect - Lemmas and theorems

This appendix consists of theorems that describe the characteristics of the function $G(f)$. The proofs for Theorem 1, Theorem 2 and Theorem 3 are presented as well as other results required for these proofs. This appendix is structured as follows. We start with deriving bounds on the herd effect in Section S2.1. Section S2.2 focuses on the structure of the function $G(f)$. In Section S2.3 we formally derive and study the dose-optimal vaccination fraction.

We need that the differential equations (1) have a solution $s(t), i(t)$ and $r(t)$ for all t which conforms to intuition: all fractions are between 0 and 1, $s(t)$ is non-increasing over time and $r(t)$ non-decreasing over time. We omit this technical result for brevity.

S2.1   Bounds on the herd effect

In the following three theorems we formally proof which values are feasible for $G(f)$.

Theorem S2.1. *It holds that $G(f) > 0$ for all $f \in [0, s(\tau))$ and $\lim_{f \uparrow s(\tau)} G(f) = 0$.*

Proof. Consider the characterization of $G(f)$ in (22). Note that $W[0] = 0$ and $W[x] < 0$ for $\frac{-1}{e} \leq x < 0$ (Appendix S5). In our case $x = -\sigma \exp\{-\sigma B(f, \sigma)\}$, with $\lim_{f \uparrow s(\tau)} B(f, \sigma) = +\infty$. Thus, $x < 0$ for $f \in [0, s(\tau))$ and approaches 0 for $f \uparrow s(\tau)$. Therefore, $W[x] < 0$ and $G(f) > 0$ for $f \in [0, s(\tau))$ and $\lim_{f \uparrow s(\tau)} G(f) = 0$. $\qquad \square$

Theorem S2.2. *It holds that $G(f) < \frac{1}{\sigma}$ for all $f \in [0, s(\tau)]$ under the assumption that $i_0 > 0$.*

Proof. The differential equations in (1) show that $i(t)$ is maximized when $s(t) = 1/\sigma$. Note that $G(f)$ describes the fraction of people susceptible, when the pandemic has died out. Therefore, if $G(f) = 1/\sigma$, the function $i(t)$ is maximal when the pandemic has died out, so $i(t)$ is at most equal to 0. This contradicts our assumption that $i_0 > 0$. Using the same argument, it can be noted that it is not possible for $G(f)$ to be greater than $1/\sigma$. As long as $s(t) > 1/\sigma$, the number of infectives is increasing, thereby reducing $s(t)$. In a final state, when $i(+\infty) = 0$, it must always hold that the fraction of susceptible people is below $1/\sigma$, which completes the proof. $\qquad \square$

Theorem S2.3. *It holds that $G(f) < s(\tau) - f$ for all $f \in [0, s(\tau))$ for vaccination in an infected population.*

Proof. Upon vaccination the system changes from state $(s(\tau), i(\tau))$ to state $(s(\tau) - f, i(\tau))$. By assumption we have that $s(\tau) > 0$ and $i(\tau) > 0$ for vaccination in an infected population. By the differential equations in (1) this implies that the derivative of $s(t)$ directly after vaccination is negative. As $G(f) = \lim_{t \to +\infty} s(t)$ (2) and $s(t)$ is non-increasing over time, we have that $G(f) < s(\tau + \epsilon) \leq s(\tau) - f$. $\qquad\square$

S2.2 Analysis of the structure of the herd effect

This section is dedicated to deriving structural results on the herd effect $G(f)$. This is done by analyzing the derivatives of this function as presented in Section S1.2.

Lemma S2.1. *The function $G(f)$ is twice differentiable for all $f \in [0, s(\tau))$ in case of vaccination in an infected population ($i_0 > 0$) and twice differentiable for all $f \in [0, s(\tau))$ with $f \neq s(\tau) - \frac{1}{\sigma}$ in case of vaccination in a completely susceptible population (the limit $i_0 \downarrow 0$).*

Proof. We prove the following four statements consecutively:

(i). The function $G(f)$ is differentiable for all $f \in [0, s(\tau))$ for vaccination in an infected population.

(ii). In case of vaccination in a completely susceptible population (i.e., $s_0 > 0$, $i_0 = 0$ and $s(\tau) = s_0$) the function $G(f)$ is indifferentiable if and only if $f^* = s(\tau) - \frac{1}{\sigma}$ or $f = s(\tau)$.

(iii). The function $G(f)$ is twice differentiable for all $f \in [0, s(\tau))$ in case of vaccination in an infected population.

(iv). The function $G(f)$ is twice differentiable for all $f \in [0, s(\tau))$ except for $f = f^* = s(\tau) - \frac{1}{\sigma}$ in case of vaccination in a completely susceptible population.

We start the proof:

(i). Note that vaccination in an infected population means $i(\tau) > 0$ and $i_0 > 0$ which implies $G(f) < \frac{1}{\sigma}$ by Theorem S2.2. For $G(f) = \frac{1}{\sigma}$ the function $G'(f)$ is not defined as can be seen in (4). However, this does not occur for vaccination in an infected population (Theorem S2.2). The function $G(f) : [0, s(\tau)] \to \mathbb{R}$. We therefore also analyze the existence of the derivative at the boundaries $f = 0$ and $f = s(\tau)$. Because $G(0) < \frac{1}{\sigma}$ by Theorem S2.2:

$$\lim_{f \downarrow 0} G'(f) = \frac{1}{\left[1 - \frac{1}{\sigma G(0)}\right]} \left(\frac{1}{\sigma s(\tau)} - 1\right) \tag{6}$$

By Theorem S2.1 we have $\lim_{f \uparrow s(\tau)} G(f) = 0 < \frac{1}{\sigma}$ and thus $\lim_{f \uparrow s(\tau)} G'(f) < 0$.

(ii). First we will prove that the given vaccination fractions indeed render $G(f)$ to be indifferentiable. Consider the explicit expression for $G(f)$ in (22) and insert the parameter settings for vaccination in a completely susceptible population and the value for f^*:

$$G(f) = \frac{-1}{\sigma} W\left[-\sigma \exp\{-\log(\sigma) - 1\}\right] = \frac{-1}{\sigma} W[-\exp\{-1\}] = \frac{1}{\sigma}$$

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By (i) the function $G(f)$ is indifferentiable at f^*, because $G(f^*) = \frac{1}{\sigma}$. Part (i) also states that $G(f)$ is indifferentiable at $f = s(\tau)$. Now we will also prove that for vaccination in a completely susceptible population $G(f)$ is differentiable for all $f \in [0,1)$ for which $f \neq f^*$. By definition of the Lambert W function, $W(y(f))$, this function is differentiable for all $y(f) \notin \{0, -1/e\}$ (Corless et al. 1996). Let $G(f) = \frac{-1}{\sigma}W[y(f)]$, with $y(f) = -\sigma(s(\tau) - f)\exp\{-\sigma(s(\tau) - f)\}$ for vaccination in a completely susceptible population (22). Clearly $y(f) < 0$, since $f < s(\tau)$. Thus, we only need to investigate for which f the function $y(f) = -\exp\{-1\}$. Note that this only holds for: $\sigma(s(\tau) - f) = 1 \Leftrightarrow f = s(\tau) - \frac{1}{\sigma} = f^*$

(iii). By (4) and (5) $G(f)$ is twice differentiable unless one of the following conditions holds: $G(f) = \frac{1}{\sigma}, f = s(\tau), G(f) = 0$. In Theorem S2.1 we showed that $G(f) > 0$ for all $f \in [0,1)$. By Theorem S2.2 we know that $G(f) < \frac{1}{\sigma}$ for vaccination in an infected population and since $\lim_{f \uparrow s(\tau)} G(f) = 0$, part (iii) follows directly.

(iv). For vaccination in a completely susceptible population we showed that $G(f) = \frac{1}{\sigma} \Leftrightarrow f = f^*$ in part (ii), which proves part (iv).

$\square$

Theorem 1. *There is a unique vaccination fraction $f^* = \max\left(s(\tau) - \frac{1}{\sigma}, 0\right)$ that maximizes the herd effect: the herd effect $G(f)$ is increasing in f for all $f < f^*$, maximized for $f = f^*$ and decreasing for $f > f^*$.*

Proof. By Theorem S2.1 the function $G'(f)$ is not defined for $f = s(\tau)$, but we know that $\lim_{f \uparrow s(\tau)} G(f) = 0$. We analyze the derivative $G'(f)$ (4). Because $G(f) < \frac{1}{\sigma}$ for all $f \in [0, s(\tau)]$ (Theorem S2.2), the function $G(f)$ is maximized for $f = f^* = s(\tau) - \frac{1}{\sigma}$. It is increasing for $f < f^*$ and decreasing for $f > f^*$. Note that for $s(\tau) \leq \frac{1}{\sigma}$ we get $f^* \leq 0$ and thus the function $G(f)$ is only decreasing in that case. $\square$

Lemma S2.2. *Let $G''(f)$ be the second derivative of the function $G(f)$ with respect to f. Then for $i_0 > 0$ the following holds:*

(i). *$G''(f) = 0$ if and only if $G(f) = \frac{2}{\sigma} - (s(\tau) - f)$.*

(ii). *$G''(f) > 0$ if and only if $G(f) > \frac{2}{\sigma} - (s(\tau) - f)$.*

(iii). *$G''(f) < 0$ for $f \geq s(\tau) - \frac{1}{\sigma}$ and $G''(f) < 0$ if and only if $G(f) < \frac{2}{\sigma} - (s(\tau) - f)$ for $f < s(\tau) - \frac{1}{\sigma}$.*

Proof. We analyze $G''(f)$ which is presented in (5). Because $\lim_{f \uparrow s(\tau)} G(f) = 0$ (Theorem S2.1), the function $G''(f)$ is not defined for $f = s(\tau)$. We prove the three statements of the lemma:

(i). We analyze $G''(f) = 0$ and consider that $G(f) < \frac{1}{\sigma}$ (Theorem S2.2):

$$
\begin{aligned}
G''(f) = 0 &\Leftrightarrow \frac{G(f)^2 - [G'(f)(s(\tau) - f)]^2}{(\sigma G(f) - 1)G(f)(s(\tau) - f)^2} = 0 \\
&\Leftrightarrow G(f)^2 - \left[G'(f)(s(\tau) - f)\right]^2 = 0 \\
&\Leftrightarrow G(f)^2 = \left[\frac{[1 - \sigma(s(\tau) - f)]G(f)}{[\sigma G(f) - 1]}\right]^2 \\
&\Leftrightarrow [1 - \sigma(s(\tau) - f)]^2 = [\sigma G(f) - 1]^2
\end{aligned}
$$

(7)

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In the second step we use that $(\sigma G(f) - 1)G(f)(s(\tau) - f)^2 \neq 0$, which holds for all $f < s(\tau)$ by Theorems S2.1 and S2.2. In the third step we substitute (4). Thus $G''(f) = 0$ if and only if one of the following two relations holds:

$$1 - \sigma(s(\tau) - f) = \sigma G(f) - 1 \Leftrightarrow G(f) = \frac{2}{\sigma} - (s(\tau) - f) \qquad \text{if } f < s(\tau) - \frac{1}{\sigma}$$

$$1 - \sigma(s(\tau) - f) = 1 - \sigma G(f) \Leftrightarrow G(f) = (s(\tau) - f) \qquad \text{if } f > s(\tau) - \frac{1}{\sigma}$$

By Theorem S2.3 $G(f) < (s(\tau) - f)$ which implies that the second relation cannot hold. Thus, $G''(f) = 0$ if and only if the first relation holds. The function $G''(f) = 0$ on the interval $[0, s(\tau) - \frac{1}{\sigma})$ for the value of f which satisfies $G(f) = \frac{2}{\sigma} - (s(\tau) - f)$.

(ii). Consider the second expression in (5), by Theorems S2.1 and S2.2 we have: $(\sigma G(f) - 1)G(f)(s(\tau) - f)^2 < 0$ for $f < 1$ From (7) we derive:

$$G''(f) > 0 \Leftrightarrow G(f)^2 - \left[G'(f)(s(\tau) - f)\right]^2 < 0$$

$$\Leftrightarrow G(f)^2 < \left[\frac{[1 - \sigma(s(\tau) - f)]G(f)}{[\sigma G(f) - 1]}\right]^2$$

$$\Leftrightarrow [1 - \sigma(s(\tau) - f)]^2 > [\sigma G(f) - 1]^2$$

Thus $G''(f) > 0$ if and only if one of the following two relations hold:

$$1 - \sigma(s(\tau) - f) < \sigma G(f) - 1 \Leftrightarrow G(f) > \frac{2}{\sigma} - (s(\tau) - f) \qquad \text{if } f < s(\tau) - \frac{1}{\sigma}$$

$$1 - \sigma(s(\tau) - f) > 1 - \sigma G(f) \Leftrightarrow G(f) > (s(\tau) - f) \qquad \text{if } f \geq s(\tau) - \frac{1}{\sigma}$$

By Theorem S2.3 the second relation cannot hold and thus $G''(f) > 0$ if and only if $G(f) > \frac{2}{\sigma} - (s(\tau) - f)$, which can only hold for $f < s(\tau) - \frac{1}{\sigma}$.

(iii). Analogous to the previous proof we have: $G''(f) < 0 \Leftrightarrow [1 - \sigma(s(\tau) - f)]^2 < [\sigma G(f) - 1]^2$ Thus, $G''(f) < 0$ if and only if one of the following two relations hold:

$$1 - \sigma(s(\tau) - f) > \sigma G(f) - 1 \Leftrightarrow G(f) < \frac{2}{\sigma} - (s(\tau) - f) \qquad \text{if } f < s(\tau) - \frac{1}{\sigma}$$

$$1 - \sigma(s(\tau) - f) < 1 - \sigma G(f) \Leftrightarrow G(f) < (s(\tau) - f) \qquad \text{if } f \geq s(\tau) - \frac{1}{\sigma}$$

By Theorem S2.3 the second relation is satisfied and thus $G''(f) < 0$ for all $f \geq s(\tau) - \frac{1}{\sigma}$. For $f < s(\tau) - \frac{1}{\sigma}$ we have that $G''(f) < 0$ if and only if $G(f) < \frac{2}{\sigma} - (s(\tau) - f)$.

$\square$

Theorem S2.4. *The derivative of $G(f)$ with respect to f, denoted by $G'(f)$, is bounded from above by 1, i.e., $G'(f) < 1 \quad \forall f \in [0, s(\tau)]$*

Proof. From (4) we have:

$$G'(f)\left[1 - \frac{1}{\sigma G(f)}\right] = \frac{1}{\sigma(s(\tau) - f)} - 1 \Leftrightarrow G'(f) = \frac{\sigma G(f)}{\sigma G(f) - 1} \cdot \frac{1 - \sigma(s(\tau) - f)}{\sigma(s(\tau) - f)} \qquad (8)$$

From Lemma S2.2 we note that $G'(f)$ has an extreme under the following condition:

$$G(f) = \frac{2}{\sigma} - (s(\tau) - f) \tag{9}$$

By contradiction we assume that there exists a vaccination fraction $\bar{f}$ for which $G'(\bar{f}) \geq 1$ and assume that $\bar{f}$ meets condition (9), then:

$$G'(\bar{f}) = \frac{2 - \sigma(s(\tau) - \bar{f})}{\sigma(s(\tau) - \bar{f})} \geq 1 \Leftrightarrow \bar{f} > s(\tau) - \frac{1}{\sigma}$$

We arrive at a contradiction, because by Theorem 1 we have that $G'(f) < 0$ for all $f > s(\tau) - \frac{1}{\sigma}$. Thus, $G'(f) < 1$ for all f that are an extreme for $G'(f)$. This completes the proof that $G'(f) < 1$ for all $f \in (0, s(\tau))$. We consider the two boundary cases: $f = 0$ and $f = s(\tau)$. From Lemma S2.1 we know that $\lim_{f \uparrow s(\tau)} G'(f) < 0$ and thus the lemma is satisfied for $f = s(\tau)$. For $\lim_{f \downarrow 0} G'(f)$, we distinguish between three cases:

(i). if $G''(0) = 0$: then $f = 0$ is an extreme of the function $G'(f)$ for which the derivative is strictly smaller than 1.

(ii). if $G''(0) > 0$: then for a very small $\epsilon > 0$ we have $G'(\epsilon) > \lim_{f \downarrow 0} G'(f)$ and $G'(f) < 1$ for all $f \in (0, s(\tau)]$. Thus also $\lim_{f \downarrow 0} G'(f) < 1$.

(iii). if $G''(0) < 0$: then from Lemma S2.2 we have that $G(0) < \frac{2}{\sigma} - s(\tau)$. By (6) we have:

$$\lim_{f \downarrow 0} G'(f) = \frac{1}{\left[1 - \frac{1}{\sigma G(0)}\right]} \left(\frac{1}{\sigma s(\tau)} - 1)\right)$$

Since $G(f) < \frac{1}{\sigma}$ by Theorem S2.2, we have $\lim_{f \downarrow 0} G'(f) < 0$ in case $s(\tau) < \frac{1}{\sigma}$. In that case the theorem is satisfied. For $s(\tau) > \frac{1}{\sigma}$ we substitute $G(0) < \frac{2}{\sigma} - s(\tau)$ in (6):

$$\lim_{f \downarrow 0} G'(f) < \left[\frac{2 - \sigma s(\tau)}{1 - \sigma s(\tau)}\right] \left(\frac{1 - \sigma s(\tau)}{\sigma s(\tau)}\right) = \frac{2}{\sigma s(\tau)} - 1 < 1$$

This completes the proof that $G'(f) < 1$ for all $f \in [0, s(\tau)]$.

$\square$

Theorem 2. *There exists a unique vaccination fraction $\bar{f}$ with $0 \leq \bar{f} \leq f^*$ such that $G(f)$ is strictly convex ($G''(f) > 0$) for all $f < \bar{f}$ and strictly concave ($G''(f) < 0$) for all $f > \bar{f}$.*

Proof. By (5) note that $G''(f)$ is a continuous function for $f < s(\tau)$, because both $G(f)$ and $G'(f)$ are continuous by Lemma S2.1. Consider the function $M(f) = G(f) - \frac{2}{\sigma} + (s(\tau) - f)$. From Lemma S2.2 we have that $\bar{f}$ must satisfy $G(\bar{f}) = \frac{2}{\sigma} - (s(\tau) - \bar{f})$, i.e. $M(\bar{f}) = 0$. Denote by $M'(f)$ the derivative of $M(f)$ with respect to f: By Theorem S2.4 we have $M'(f) < 0$. This implies that $M(f) = 0$ has only one solution and thus there is only one $\bar{f}$ for which $G''(\bar{f}) = 0$. As $G''(f)$ is a continuous function this implies that on either side of $\bar{f}$ the function $G(f)$ is either convex or concave.

By Lemma S2.2 we have $G''(f) < 0$ for $f \geq s(\tau) - \frac{1}{\sigma}$ and thus $G(f)$ is concave for $f > \bar{f}$. Since $M'(f) < 0$ and $M(\bar{f}) = 0$ it holds that $M(f) > 0$ for $f < \bar{f}$. By Lemma S2.2 this implies that $G(f)$ is convex for all $f < \bar{f}$, which proves the convex-concave shape of the function $G(f)$. Note

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that this prove only holds for $i_0 > 0$. In case $i_0 = 0$ we refer to Lemma S2.3. By Lemma S2.2 $G(f)$ is concave for $f \geq f^*$, such that $\bar{f} \leq f^*$. This completes the proof of this theorem. $\square$

Lemma S2.3. *In case of vaccination in a completely susceptible population, the function $G(f)$ is convex for all $f < f^*$ and concave for all $f > f^*$, where $f^* = s(\tau) - \frac{1}{\sigma}$.*

Proof. By Lemma S2.1(ii) we have that $G(f^*) = \frac{1}{\sigma}$ for vaccination in a completely susceptible population. Since the vaccination fraction f^* also maximizes the function $G(f)$ (Theorem 1), it holds that $G(f) < \frac{1}{\sigma}$ for all $f \neq f^*$. In Lemma S2.2 we derived conditions for $G(f)$ to be convex or concave where we needed that $G(f) < \frac{1}{\sigma}$. These conditions can still be used if we apply them only to $f \neq f^*$.

$$G''(f) > 0 \Leftrightarrow G(f) > \frac{2}{\sigma} - (s(\tau) - f) \quad \text{and} \quad G''(f) < 0 \Leftrightarrow G(f) < \frac{2}{\sigma} - (s(\tau) - f)$$

Note that for f^* we have $G(f^*) = \frac{1}{\sigma} = \frac{2}{\sigma} - (s(\tau) - f^*)$. By Theorem 1 the function $G(f)$ is decreasing for $f > f^*$, whereas the expression $\frac{2}{\sigma} - (s(\tau) - f)$ is increasing in f. This implies that $G(f)$ is concave for all $f > f^*$. The function $G(f)$ is increasing for $f < f^*$, just as the expression on the right hand side in the conditions for convexity and concavity. By Theorem S2.4 the expression $\frac{2}{\sigma} - (s(\tau) - f)$ increases with a faster rate than $G(f)$. This implies that $G(f)$ is convex for all $f < f^*$. $\square$

Theorem 3. *For the structure of $G(f)$ we can distinguish three cases based on $s(\tau)$, the proportion of susceptibles at the moment of vaccination τ:*

(i) $C < s(\tau) < 1$: *We have $f^* > \bar{f} > 0$. Thus $G(f)$ is increasing and convex between 0 and $\bar{f}$, increasing and concave between $\bar{f}$ and f^*, and decreasing and concave above f^*.*

(ii) $1/\sigma < s(\tau) \leq C$: *We have $f^* > 0$ and $\bar{f} = 0$. Thus $G(f)$ is increasing and concave between 0 and f^*, and decreasing and concave above f^*.*

(iii) $0 \leq s(\tau) < 1/\sigma$: *We have $\bar{f} = f^* = 0$. Thus $G(f)$ is decreasing and concave everywhere.*

Proof. From Theorem 2 it follows that $\bar{f} \leq f^*$. It therefore suffices to proof the following two steps:

(a) $f^* > 0$ if $s(\tau) > 1/\sigma$ and $f^* = 0$ otherwise.

(b) $\bar{f} > 0$ if $s(\tau) > C$ and $\bar{f} = 0$ otherwise.

The proof is given below:

(a) This follows directly from Theorem 1: $f^* = \max\left(s(\tau) - \frac{1}{\sigma}, 0\right)$.

(b) We start from deriving the value C. By Theorem 2 the function $G(f)$ has a convex and a concave part for certain parameter settings. By Lemma S2.2 the following condition must hold for $G(f)$ to be convex: $G(f) > \frac{2}{\sigma} - (s(\tau) - f)$. Since $G(f)$ is convex for all values f below a certain threshold, the following condition requires that the function $G(f)$ has a convex part:

$$G(0) > \frac{2}{\sigma} - s(\tau) \tag{10}$$

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We solve above inequality with equality to obtain the value C. By substituting in (3) this results in the following, where $H(x) = -x + \frac{1}{\sigma} \log(x)$:

$$0 = -\frac{2}{\sigma} + s(\tau) + \frac{1}{\sigma} \log \left(\frac{2}{\sigma} - s(\tau) \right) + s_0 + i_0 - \frac{1}{\sigma} \log(s_0)$$

$$H \left[\frac{2}{\sigma} - s(\tau) \right] = H[s_0] - i_0$$

$$s(\tau) = \frac{W \left[-\sigma \exp\{k\sigma\} \right] + 2}{\sigma} = C \text{ with } k = H[s_0] - i_0$$

We know that $-1 < W \left[-\sigma \exp\{k\sigma\} \right] < 0$ (cf. Appendix S5) and thus $\frac{1}{\sigma} < C < \frac{2}{\sigma}$. Note that for $s(\tau) \leq \frac{1}{\sigma}$ condition (10) is never met by Theorem S2.2. By Theorem S2.1 the condition is always met for $s(\tau) \geq \frac{2}{\sigma}$. Thus only for $s(\tau) > C$ the function $G(f)$ has a convex part and for $s(\tau) = C$ we have $\tilde{f} = 0$.

This completes the proof of this theorem. □

S2.3 The dose-optimal vaccination fraction

We present the dose-optimal vaccination fraction $\tilde{f}$ and relate it to the vaccination fractions f^* and $\bar{f}$ as defined in Theorem 1 and Theorem 2 respectively.

Corollary 1. *The function $D(f)$ as defined by (4) is maximized by the unique vaccination fraction $\tilde{f}$ for which $G'(\tilde{f}) = D(\tilde{f})$. The function $D(f)$ is increasing for $f < \tilde{f}$ and decreasing for $f > \tilde{f}$.*

Proof. The function $D(f)$ is defined as follows: $D(f) = \frac{1}{f} [G(f) - G(0)]$.

$$\frac{d}{df} D(f) = \frac{1}{f} \left[G'(f) - D(f) \right]$$

$$\frac{d^2}{df^2} D(f) = \frac{1}{f} G''(f) - \frac{2}{f^2} [G'(f) - D(f)]$$

By the first derivative of $D(f)$, $\tilde{f}$ is clearly an extreme of the function $D(f)$. Observe that in the limit $f \downarrow 0$ is always a solution of the condition $G'(\tilde{f}) = D(f)$, by limit definition of the one-sided derivative. For parameter settings for which the function $G(f)$ does not have a convex part, the function $D(f)$ is maximized for $f = 0$. Namely, in that case $G(f)$ is concave, meaning that the slope of $G(f)$ is decreasing in f. The average slope on the interval $[0, f]$, measured by $D(f)$, is then also decreasing. Analogously, $D(f)$ is increasing as long as $G(f)$ is convex. This implies that $f = 0$ cannot maximize the function $D(f)$ if $G(f)$ has a convex domain and that $\tilde{f}$ is in the concave domain of $G(f)$.

Assume that $\tilde{f}$ is the first value in the concave domain for which $G'(\tilde{f}) = D(f)$. Because of concavity it holds that $G(f)$ for all $f > \tilde{f}$ is below the line through $G(0)$ and $G(\tilde{f})$. For all $f > \tilde{f}$ this implies:

$$\frac{1}{f} [G(f) - G(0)] < \frac{1}{\tilde{f}} \left[G(\tilde{f}) - G(0) \right]$$

Let f_1 be an arbitrarily selected value greater than $\tilde{f}$. Because of concavity the function $G(f)$ for all $f > f_1$ is below the line through $G(0)$ and $G(f_1)$. This implies that $D(f)$ is decreasing for $f > \tilde{f}$. Thus, there is only one strictly positive solution for the condition $G'(f) = D(f)$, which is in the concave and increasing domain of $G(f)$. By the second derivative of $D(f)$, $\tilde{f}$ gives a maximum. □

Lemma 1. *Consider the following three vaccination fractions: f^* as defined in Theorem 1, $\bar{f}$ as defined in Theorem 2 and $\tilde{f}$ as defined in Corollary 1. The following relation holds: $\bar{f} \leq \tilde{f} \leq f^*$*

Proof. By Lemma S2.2 we know that $G''(f) \leq 0 \Leftrightarrow G(f) \leq \frac{2}{\sigma} - (s(\tau) - f)$. Filling in the expression for $f^* = s(\tau) - \frac{1}{\sigma}$ results in $G(f^*) \leq \frac{1}{\sigma}$. This clearly holds by Theorem S2.2 and thus $\bar{f} \leq f^*$, due to Theorem 2. The optimal vaccination fraction $\tilde{f}$ is defined as the fraction that maximizes the function $D(f)$ and meets the condition $G'(\tilde{f}) = D(\tilde{f})$. Observe that $D(\tilde{f}) \geq 0$, because $\lim_{f \downarrow 0} D(f) = 0$ and $\tilde{f}$ maximizes $D(f)$. This implies that $G'(\tilde{f}) \geq 0$ and thus $\tilde{f} \leq f^*$ by Theorem 1. By argument we showed in Corollary 1 that $\tilde{f}$ cannot be in the convex domain of the function $G(f)$, such that $\bar{f} \leq \tilde{f}$. This completes the proof of this lemma. □

Lemma S2.4. *For increasing σ the dose-optimal vaccine fraction $\tilde{f}$ converges to f^*.*

Proof. The basic reproduction ratio is denoted by σ. By Lemma 1 it suffices to show that $\lim_{\sigma \uparrow +\infty} f^* - \bar{f} = 0$. By definition we have $\lim_{\sigma \uparrow +\infty} f^* = \lim_{\sigma \uparrow +\infty} s(\tau) - \frac{1}{\sigma} = s(\tau)$. Clearly, for $\sigma \uparrow +\infty$ and $\bar{f} = s(\tau)$ the condition $G(\bar{f}) = \frac{2}{\sigma} - (s(\tau) - \bar{f})$ is satisfied, as $\lim_{f \uparrow s(\tau)} G(f) = 0$ by Theorem S2.1. This completes the proof. □

Lemma S2.5. *In case of vaccination in a completely susceptible population $\bar{f} = \tilde{f} = f^*$.*

Proof. This result follows directly from Lemma 1 and Lemma S2.3. □

S2.4 The best vaccination moment

In Section 4.5 we state that it is optimal to vaccinate as early as possible in an ideal world. We prove this in the following lemma.

Lemma S2.6. *The herd effect $G(f)$ is increasing in $s(\tau)$.*

Proof. Let $G'_{s(\tau)}(f, s(\tau))$ be the derivative of $G(f, s(\tau))$ with respect to $s(\tau)$:

$$G'_{s(\tau)}(f, s(\tau)) \left[1 - \frac{1}{\sigma G(f, s(\tau))} \right] = \frac{-f}{\sigma s(\tau)[s(\tau) - f]}$$

Observe that the objective function is increasing in $s(\tau)$, because $G(f, s(\tau)) < \frac{1}{\sigma}$ by Theorem S2.2. Therefore, to maximize the herd effect one should vaccinate as soon as possible, i.e., when $s(\tau)$ is as high as possible. □

Appendix S3 Generality of the function $G(f)$

One of the extensions to the standard SIR compartmental model, is the SI^nR model with n different consecutive infectious stages. Let $s(t)$ and $r(t)$ denote the fraction of people respectively susceptible and removed at time t. The fractions of people susceptible in every state are given by $i_k(t)$ for $k = 1, ..., n$. Interpretation dictates that $s(t) + \sum_{k=1}^{n} i_k(t) + r(t) = 1$ for all t. Let β_k and γ_k denote respectively the transmission rate and recovery rate in infectious stage k. The differential

equations for the SI^nR model are:

$$\frac{ds}{dt} = -s \sum_{k=1}^{n} \beta_k i_k$$

$$\frac{di_1}{dt} = s \sum_{k=1}^{n} \beta_k i_k - \gamma_1 i_1$$

(11)

$$\frac{di_k}{dt} = \gamma_{k-1} i_{k-1} - \gamma_k i_k \quad k = 2, ..., n$$

$$\frac{dr}{dt} = \gamma_n i_n$$

Hyman et al. (1999) prove that $R_0 = \sum_{k=1}^{n} \frac{\beta_k}{\gamma_k}$ for this model, with R_0 denoting the basic reproduction ratio.

Theorem S3.1. *Up to a constant, the expression for $G(f)$ given in (3) also applies to the SI^nR model with $\sigma = \sum_{k=1}^{n} \frac{\beta_k}{\gamma_k}$.*

Proof. The following relation can be derived from (11), using $\sigma = \sum_{k=1}^{n} \frac{\beta_k}{\gamma_k}$. Analogous to Ma and Earn (2006) we define $G_k(t) = \sum_{j=k+1}^{n} i_j(t) + r(t)$, $G_n(t) = r(t)$. From (11) this implies that $\frac{d}{dt} G_k(t) = \gamma_k i_k$.

$$\int_0^\infty \frac{1}{s(t)} ds = -\sum_{k=1}^{n} \beta_k \int_0^\infty i_k(t) dt \Leftrightarrow$$

$$\log(s(t)) - \log(s(0)) = -\sum_{k=1}^{n} \frac{\beta_k}{\gamma_k} [G_k(t) - G_k(0)]$$

(12)

$$= \sigma \left[s(t) + \sum_{k=1}^{n} i_k(t) \right] - \sigma \left[s(0) + \sum_{k=1}^{n} i_k(0) \right]$$

$$- \sum_{k=1}^{n} \frac{\beta_k}{\gamma_k} \left[\sum_{m=k+1}^{n} i_m(t) - i_m(0) \right]$$

We let $t \to \infty$ and use that $i_k(\infty) = 0$ for $k = 1, ..., n$. This results in the following expression, which is equal to the expression for the SIR (3) model up to a constant:

$$0 = -s(\infty) + \frac{1}{\sigma} \log(s(\infty)) - \frac{1}{\sigma} \log(s(0)) + s(0) + \sum_{k=1}^{n} i_k(0) - \frac{1}{\sigma} \sum_{k=1}^{n} \frac{\beta_k}{\gamma_k} \sum_{m=k+1}^{n} i_m(0) \quad (13)$$

We vaccinate a fraction f of the population at time τ. Analogous to the analysis of the SIR model, we let $(s(\tau) - f, i_1(\tau), ..., i_n(\tau))$ be a new initial state and define the value $s(\infty)$ according to (13). The values for $i_k(\tau)$ for $k = 1, ..., n$ can be calculated according to (12). We define $G(f) = \lim_{t \to \infty} s(t)$, where $s(t)$ follows (11) for $t > \tau$. This results in the following:

$$0 = -G(f) + \frac{1}{\sigma} \log(G(f)) - \frac{1}{\sigma} \log \left(s(0) \left(1 - \frac{f}{s(\tau)} \right) \right) + s(0) + \sum_{k=1}^{n} i_k(0)$$

$$- f - \frac{1}{\sigma} \sum_{k=1}^{n} \frac{\beta_k}{\gamma_k} \sum_{m=k+1}^{n} i_m(0)$$

(14)

Above expression equals the expression for the SIR model (3) up to the final term, which is a constant. $\square$

Lemma 2. *The results of Theorem 1, Theorem 2, Theorem 3 and Corollary 1 also apply to the SI^nR model with $\sigma = \sum_{k=1}^{n} \frac{\beta_k}{\gamma_k}$. In particular, for each SI^nR model with given initial conditions there exist vaccination fractions $\bar{f}, \tilde{f}$ and f^* that together characterize the convex-concave and increasing-decreasing shape of the herd effect.*

Proof. By Theorem S3.1 the expression for $G(f)$ in the SI^nR model is equal to the expression in the SIR model up to a constant. This constant disappears after taking the derivative, implying that the first and second order derivative do not change. The structural properties of the function $G(f)$ thus carry over. $\square$

Appendix S4 Optimal vaccine allocation - Theorems and proofs

In this appendix we characterize the optimal solution to the vaccine allocation problem of Section 3.3. We first derive a basic result in Section S4.1: that it is suboptimal to leave vaccines unused. The main derivation of the optimality conditions is presented in Section S4.2.

S4.1 The total effect of vaccination

We formally show that it is optimal to use the entire available vaccine stockpile. Thereto we define the function $F_j(f_j)$ as the total effect of vaccinating with a fraction f_j in population j:

$$F_j(f_j) = G_j(f_j) + f_j \tag{15}$$

Observe that the dose-optimal vaccination fraction $\tilde{f}$ as defined by Corollary 1 does not only result in the highest additional herd effect per dose of vaccine, but also in the highest additional *total effect* per dose of vaccine. Formally, $\tilde{f}$ also maximizes the average slope of the total effect $F(f)$ on the interval $[0, f]$, calculated as $[F(f) - F(0)]/f$. As vaccinating with the fraction $\tilde{f}$ is very efficient per dose of vaccine, the optimal allocation tries to allocate as close as possible to $\tilde{f}$ in a subset of all the populations as can be seen in Theorem 5.

Theorem S4.1. *The fraction of people not infected during the epidemic, $F_j(f_j) = G_j(f_j) + f_j$, is increasing in f_j for all $f_j \in [0, s_j(\tau))$.*

Proof. We prove this theorem for a single population and therefore drop the subscript j in the proof. Let $F'(f)$ denote the derivative of $F(f)$ with respect to f: $F'(f) = \frac{d}{df}F(f) = G'(f) + 1$. By Theorem 1 $G'(f) > 0$ for all $f < s(\tau) - \frac{1}{\sigma}$ and $G'(f) < 0$ for all $f > s(\tau) - \frac{1}{\sigma}$. Hence, the function $F(f)$ is increasing for all $f < s(\tau) - \frac{1}{\sigma}$. $F(f)$ is increasing under the following condition:

$$F'(f) = G'(f) + 1 = \frac{\sigma G(f)}{\sigma G(f) - 1} \left[\frac{1}{\sigma(s(\tau) - f)} - 1 \right] + 1$$

$$= \frac{1}{\sigma G(f) - 1} \left[\frac{G(f)}{(s(\tau) - f)} - 1 \right] > 0$$

By Theorem S2.2 $F'(f) > 0$ if and only if $G(f) < (s(\tau) - f)$, which holds by Theorem S2.3 for all $f \in [0, s(\tau))$. Thus the function $F(f)$ is increasing for all $f \in [0, s(\tau))$. $\square$

Because the functions $F_j(f_j)$ are all non-decreasing there always exists an optimal solution for which all available vaccines are used:

Lemma S4.1. *The vaccine allocation problem always has an optimal solution for which $\sum_{j \in J} f_j N_j = V$.*

Proof. Let x_j for all $j \in J$ be a solution of the vaccine allocation problem and assume that $\sum_{j \in J} x_j N_j < V$. Let y_j for all $j \in J$ be the solution for which $y_j \geq x_j$ for all $j \in J$, such that $\sum_{j \in J} y_j N_j = V$. By Lemma S4.1 the functions $F_j(f)$ are non-decreasing and thus $F_i(y_i) \geq F_j(x_j)$ for all $j \in J$. This implies that: $\sum_{j \in J} N_j F_j(y_j) \geq \sum_{j \in J} N_j F_j(x_j)$. Hence, the proposed solution y_j for all $j \in J$ for which $\sum_{j \in J} y_j N_j = V$ is also an optimal solution. $\square$

S4.2 Optimality conditions

Theorem 2 establishes that resource allocation Problem (3) is a knapsack problem with S-shaped return functions: non-decreasing and convex for all x smaller than some value $\hat{x}$ and concave for all $x > \hat{x}$ (cf. Ginsberg (1974) and Ağralı and Geunes (2009)). As the vaccine allocation problem is a maximization problem with inequality constraints, necessary conditions for the optimum are given by the Karush-Kuhn-Tucker (KKT) conditions. Let δ be the KKT multiplier for the capacity constraint, λ_j for the non-negativity constraint $f_j \geq 0$ for all $j \in J$ and μ_j for the constraint $f_j \leq s_j(\tau)$ for all $j \in J$. Denote by $\mathbf{f}, \boldsymbol{\lambda}, \boldsymbol{\mu}$ the vectors with the variables f_j, λ_j and μ_j respectively. Let $\mathcal{L}(\mathbf{f}, \boldsymbol{\lambda}, \boldsymbol{\mu}, \delta)$ denote the Lagrange function of the maximization problem. The KKT conditions for this problem are given in (16). Observe that the *marginal efficiency* ω as introduced in Section 5.1 follows from the KKT condition that the partial derivative of $\mathcal{L}(\mathbf{f}, \boldsymbol{\lambda}, \boldsymbol{\mu}, \delta)$ with respect to f_j equals 0 for all $j \in J$.

$$\mathcal{L}(\mathbf{f}, \boldsymbol{\lambda}, \boldsymbol{\mu}, \delta) = \sum_{j \in J} N_j F_j(f_j) - \delta \left(\sum_{j \in J} f_j N_j - V \right) - \sum_{j \in J} (\mu_j(f_j - s_j(\tau)) - \lambda_j f_j)$$

$$\frac{\partial}{\partial f_j} \mathcal{L}(\mathbf{f}, \boldsymbol{\lambda}, \boldsymbol{\mu}, \delta) = 0 \quad \forall j \in J$$

$$\delta \left(\sum_{j \in J} f_j N_j - V \right) = 0 \qquad \qquad \delta \geq 0 \tag{16}$$

$$\lambda_j f_j = 0 \quad \forall j \in J \qquad \lambda_j \geq 0 \quad \forall j \in J$$

$$\mu_j(f_j - s_j(\tau)) = 0 \quad \forall j \in J \qquad \mu_j \geq 0 \quad \forall j \in J$$

We analyze the solution to (3) using the KKT conditions. We first present the solution to the general problem in Theorem S4.2. In Lemma S4.2 and Lemma S4.3 we discuss two simplifications. These enable us to proof the Central Insight in Theorem 4.

Theorem S4.2. *For every optimal solution to (3) there exist $J' \subseteq J$, $k \in J'$ and $\omega \geq 0$ such that:*

(i). *For all $j \in J' \setminus \{k\}$, f_j is the unique solution to $G'_j(f_j) = \omega$ for which $f_j \geq \bar{f}_j$.*

(ii). *$G'_k(f_k) = \omega$, and either f_k is the unique solution to this equation for which $f_k \geq \bar{f}_k$ or f_k is the unique solution for which $f_k < \bar{f}_k$.*

(iii). *Either $f_j = 0$ or $f_j = s_j(\tau)$ for every $j \in J \setminus J'$.*

Proof. The proof of this theorem consists of the following steps:

(a). Let $J' \subseteq J$ such that $0 < f_j < s_j(\tau)$ for all $j \in J'$. We prove that $G'_j(f_j) = \omega$ for all $j \in J'$.

(b). We prove that for at most one population there is a strictly positive vaccination fraction in the strictly convex domain, i.e. $0 < f_k < \bar{f}_k$ for at most one $k \in J'$.

We proof the two steps consecutively:

(a). This result follows from the KKT conditions. Note that for any population j for which $0 < f_j < s_j(\tau)$ the KKT conditions require that $\mu_j = 0$ and $\lambda_j = 0$. This gives the following:

$$\frac{\partial}{\partial f_j} \mathcal{L}(\mathbf{f}, \boldsymbol{\lambda}, \boldsymbol{\mu}, \delta) = N_j F'_j(f_j) - \delta N_j - \mu_j + \lambda_j$$
$$= N_j \left[F'_j(f_j) - \delta \right] = 0 \Leftrightarrow F'_j(f_j) = G'_j(f_j) + 1 = \delta$$

Hence, $G'_j(f_j) = \omega$, with $\omega = \delta - 1$.

(b). By contradiction assume there is an optimal solution with at least two strictly positive variables in the convex domain. W.l.o.g. let $0 < f_j < \bar{f}_j$ for $j = 1, 2$, i.e. the functions $F_1(f)$ and $F_2(f)$ are convex at respectively f_1 and f_2. Choose an $0 < \epsilon < \min \left\{ f_1, f_2 \frac{N_2}{N_1}, \bar{f}_1 - f_1, (\bar{f}_2 - f_2) \frac{N_2}{N_1} \right\}$ and let $\delta = \epsilon \frac{N_1}{N_2}$ such that:

$$f_1 N_1 + f_2 N_2 = (f_1 + \epsilon) N_1 + (f_2 - \delta) N_2$$

By the KKT conditions $F'_1(f_1) = F'_2(f_2)$ and by convexity of $F_1(f_1)$ and $F_2(f_2)$ the following can be derived:

$$N_1 F_1(f_1 + \epsilon) + N_2 F_2(f_2 - \delta) > N_1 F_1(f_1) + N_2 F_2(f_2) + \epsilon N_1 [F'_1(f_1) - F'_2(f_2)]$$
$$= N_1 F_1(f_1) + N_2 F_2(f_2)$$

Above relation shows that the objective function can be improved by a small change in the allocation. Thus, a solution with more than one strictly positive variable in the convex domain can never be optimal.

$\square$

Lemma S4.2. *If $s_j(\tau) > \frac{1}{\sigma_j}$ for all $j \in J$, then there is no optimal solution to (3) for which $f_j = 0$ and $f_k = s_k(\tau)$ for two populations $j, k \in J$. This implies that (iii) of Theorem S4.2 changes into: Either $f_j = 0$ for all $j \in J \setminus \{J' \cup \{k\}\}$ or $f_j = s_j(\tau)$ for all $j \in J \setminus \{J' \cup \{k\}\}$.*

Proof. By contradiction assume that $f_1 = 0$ and $f_2 = s_2(\tau)$ w.l.o.g. Let $\epsilon > 0$ and $\delta = \epsilon \frac{N_1}{N_2} < 1$ such that:
$$f_1 N_1 + f_2 N_2 = (f_1 + \epsilon) N_1 + (f_2 - \delta) N_2$$

The following holds:

$$N_1 F_1(\epsilon) + N_2 F_2(s_2(\tau) - \delta) - N_1 F_1(0) - N_2 F_2(s_2(\tau))$$
$$= N_1 [G_1(\epsilon) - G_1(0)] + N_2 [G_2(s_2(\tau) - \delta) - G_2(s_2(\tau))] > 0$$

For $s_j(\tau) > \frac{1}{\sigma_j}$ the function $G_j(f)$ is initially increasing by Theorem 1, implying that $G_1(\epsilon) > G_1(0)$. Furthermore, by Theorem S2.1 $G_j(f_j) > 0$ for all $0 \leq f_j < s_j(\tau)$ and $\lim_{f_j \uparrow s_j(\tau)} G_j(f_j) = 0$. This

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implies that $G_2(s_2(\tau) - \delta) > G_2(s_2(\tau))$. Thus, a small change in allocation can improve the solution. We arrive at a contradiction which completes the proof of this lemma. $\square$

Lemma S4.3. *If $s_j(\tau) > \frac{1}{\sigma_j}$ for all $j \in J$ and $V \le \sum_{j \in J} N_j f_j^*$ then there is no optimal solution to (3) with $f_j = s_j(\tau)$ for some $j \in J$. This implies that (iii) of Theorem S4.2 changes into: $f_j = 0$ for all $j \in J \setminus \{J' \cup \{k\}\}$.*

Proof. By contradiction assume that there is a population $k \in J$ for which $f_k = s_k(\tau)$ in the optimal solution. Since $s_k(\tau) > \frac{1}{\sigma_k}$ this implies that $f_k > f_k^* = s_k(\tau) - \frac{1}{\sigma_k}$. Because $V \le \sum_{j \in J} N_j f_j^*$ there must also be a population l for which $f_l < f_l^*$ in the optimal allocation. Let $\epsilon > 0$ be sufficiently small such that $f_l + \epsilon < f_l^*$ and $f_k - \epsilon \frac{N_l}{N_k} > f_k^*$. Then the following holds, where the inequality follows from Theorem 1:

$$N_l F_l(f_l + \epsilon) + N_k F_k \left(s_k(\tau) - \epsilon \frac{N_l}{N_k} \right) - N_l F_l(f_l) - N_k F_k(s_k(\tau))$$

$$N_l \left[G_l(f_l + \epsilon) - G_l(f_l) \right] + N_k \left[G_k(s_k(\tau)) - G_k \left(s_k(\tau) - \epsilon \frac{N_l}{N_k} \right) \right] > 0$$

A small change in allocation can improve the solution. Hence, there cannot be an optimal solution with $f_j = s_j(\tau)$ for some $j \in J$. We arrive at a contradiction which proves the first part of this lemma. The implication then directly follows from Lemma S4.2. $\square$

Theorem 4. *Every optimal solution to (3) can be characterized as follows:*

(i). *A subset of populations $J' \subseteq J$ is vaccinated with the regular fraction that corresponds to marginal efficiency ω.*

(ii). *Possibly another population k is also vaccinated with marginal efficiency ω, but with the exceptional fraction for which $f_k < \bar{f}_k$.*

(iii). *The remaining populations are not vaccinated at all.*

Proof. This theorem can be reformulated more analytically as follows: For every optimal solution to (3) there exist $J' \subseteq J$, $k \in J'$ and $\omega \ge 0$ such that:

(i). For all $j \in J' \setminus \{k\}$, f_j is the unique solution to $G_j'(f_j) = \omega$ for which $f_j \ge \bar{f}_j$.

(ii). $G_k'(f_k) = \omega$, and either f_k is the unique solution to this equation for which $f_k \ge \bar{f}_k$ or f_k is the unique solution for which $f_k < \bar{f}_k$.

(iii). $f_j = 0$ for all $j \in J \setminus J'$.

The proof then follows directly from Theorem S4.2, Lemma S4.2 and Lemma S4.3. $\square$

Theorem 5. *Consider a set of populations J with $\forall j\colon G_j(f) = G(f)$ and a total available amount of resources equal to V. Let $|J| = n$ and order the populations such that $N_1 \le \dots \le N_n$. The optimal allocation for particular cases is as follows:*

(a). *if $V < \tilde{f} N_1$, then allocate only to the smallest population. Set $f_1 = V/N_1$ and $f_j = 0$ for $j = 2, \dots, n$.*

(b). if $V = \sum_{j \in K} \tilde{f} N_j$ for a subset $K \subseteq J$, then set $f_j = \tilde{f}$ for $j \in K$ and $f_j = 0$ for $j \notin K$.

(c). if $V > \sum_{j \in J} \tilde{f} N_j$, then allocate pro rata over all the populations: $f_j = \frac{V}{\sum_{j \in J} N_j}$ for all $j \in J$.

Proof. This proof uses ideas that are also used in the proof of Proposition 1 of Ginsberg (1974).

(a). Step (b) in the proof of Theorem S4.2 shows that an optimal allocation results in at most one strictly positive vaccination fraction in the convex domain. By this result, the proposed allocation follows directly from convexity of the function $G(\cdot)$ for all $f < \bar{f} < \tilde{f}$.

(b). The proposed allocation results in the maximum attainable value for the objective function for V available vaccines and is thus optimal.

(c). We prove the optimality of the proposed allocation using the items of Theorem S4.2. More precisely, regarding item (iii) we show that $f_j = s(\tau)$ cannot occur for any $j \in J'$ and we analyze the two types of strategies that remain. Consider item (iii): for the special case of identical parameters it holds that $s_j(\tau) := s(\tau)$ for all $j \in J$. We can show that an allocation with $f_j = s(\tau)$ and $f_k < s(\tau)$ for arbitrary populations $j, k \in J$ cannot be optimal:

$$N_j F(f_j - \epsilon) + N_k F\left(f_k + \epsilon \frac{N_j}{N_k}\right) - N_j F(f_j) - N_k F(f_k) = \epsilon N_j (F'(f_k) - F'(f_j)) > 0$$

The inequality follows because of the structure of the function $F(\cdot)$. Thus, it is not optimal to set $f_j = s(\tau)$ for some $j \in J$. Using this result, there are two possible allocations remaining by Theorem S4.2:

(i) Either the amount V is allocated pro rata over the populations in $K \subseteq J$. i.e., $f_j = \frac{V}{\sum_{j \in K} N_j} = \hat{x}$ and $f_j = 0$ for all $j \notin K$.

(ii) Or an amount ξ is allocated to one population k and the remaining $(V - \xi)$ is allocated pro rata over all populations in $I \subseteq J \backslash \{k\}$. i.e., $f_k = \xi/N_k$, $f_j = \frac{V - \xi}{\sum_{j \in I} N_j} = \hat{y}$ for $j \in I$ and $f_j = 0$ for all $j \notin I \cup \{k\}$.

First we consider scheme (i) and prove that it is optimal to allocate pro rata over all populations, i.e., we show that it is optimal to let K equal J. Let z_j and x_j respectively denote the pro rata allocation over $K \subset J$ and over J, such that $z_j = \hat{z} = \frac{V}{\sum_{j \in K} N_j}$ for all $j \in K$ and $x_j = \hat{x} = \frac{V}{\sum_{j \in J} N_j}$ for all $j \in J$. Note that $\hat{z} > \hat{x} > \tilde{f}$, because $V > \sum_{j \in J} N_j \tilde{f}$ by assumption. This implies the following inequality by Corollary 1:

$$[F(\hat{z}) - F(0)]/\hat{z} < [F(\hat{x}) - F(0)]/\hat{x}$$
$$\Leftrightarrow \quad \sum_{j \in K} N_j F(\hat{z}) - \sum_{j \in K} N_j F(0) < \sum_{j \in J} N_j F(\hat{x}) - \sum_{j \in J} N_j F(0)$$
$$\Leftrightarrow \quad \sum_{j \in K} N_j F(\hat{z}) + \sum_{j \notin K} N_j F(0) < \sum_{j \in J} N_j F(\hat{x})$$

The first equivalence follows by substituting the definitions of $\hat{x}$ and $\hat{z}$ and the second equivalence follows by rearranging terms. The last inequality shows precisely that allocating pro rata over all populations gives a higher objective value than allocating pro rata over $K \subset J$.

Second, we now consider allocation scheme (ii), in which an amount of ξ is allocated to population k and the remaining $V - \xi$ is allocated pro rata over $I \subseteq J \backslash \{k\}$ to reach a

vaccination fraction $\hat{y}$. We will show that allocation scheme (ii) will never be superior to allocation scheme (i), in which the latter allocates pro rata over all populations to reach a vaccination fraction $\hat{x}$. By contradiction we assume that allocation (ii) is optimal and thus better than allocation (i).

We first show that the vaccination fraction $\hat{x}$ in allocation (i) is smaller than the vaccination fraction $\hat{y}$ in allocation (ii). By Theorem S4.2 ξ/N_k lies in the convex domain of $F(\cdot)$, which implies $\xi/N_k < \bar{f} < \tilde{f}$. We also know that $\tilde{f} < \hat{x} \leq \frac{1}{N_k}(\sum_{j \in J} N_j - \sum_{j \in I} N_j)\hat{x}$, where the first inequality follows because $\hat{x} > \tilde{f}$ by $V > \sum_{j \in J} N_j \tilde{f}$ and the second inequality because $I \subseteq J\backslash\{k\}$. By combining the inequalities, we have that:

$$\xi/N_k < \frac{1}{N_k}(\sum_{j \in J} N_j - \sum_{j \in I} N_j)\hat{x}$$

$$\Leftrightarrow \qquad \xi \sum_{j \in J} N_j < V \sum_{j \in J} N_j - V \sum_{j \in I} N_j$$

$$\Leftrightarrow \qquad \frac{V}{\sum_{j \in J} N_j} < \frac{V - \xi}{\sum_{j \in I} N_j}$$

The first equivalence follows from $\hat{x} = \frac{V}{\sum_{j \in J} N_j}$ and in the second equivalence we rewrite terms. Note that the last inequality is precisely $\hat{x} < \hat{y}$.

We now compare allocation (i) and (ii). Under the assumption that (ii) is better than (i), the following must hold:

$$N_k F(\xi/N_k) + \sum_{j \in I} N_j F(\hat{y}) + \sum_{j \notin I \cup \{k\}} N_j F(0) > \sum_{j \in J} N_j F(\hat{x})$$

$$\Leftrightarrow N_k G(\xi/N_k) + \sum_{j \in I} N_j G(\hat{y}) + \sum_{j \notin I \cup \{k\}} N_j G(0) > \sum_{j \in J} N_j G(\hat{x}) \tag{17}$$

The equivalence above follows from the fact that both allocations allocate the same amount of vaccines, i.e., the direct effect is the same. Hence, it suffices to consider the herd effect instead of the total effect. (17) implies the following:

$$N_k G\left(\frac{\xi}{N_k}\right) + \sum_{j \in I} N_j \left[\int_0^{\hat{y}} G'(f)df + G(0)\right] + \sum_{j \notin I \cup \{k\}} N_j G(0) > \sum_{j \in J} N_j \left[\int_0^{\hat{x}} G'(f)df + G(0)\right]$$

$$\Leftrightarrow \quad N_k G\left(\frac{\xi}{N_k}\right) + \sum_{j \in I} N_j \int_0^{\hat{y}} G'(f)df > \sum_{j \in J} \left[N_j \int_0^{\hat{x}} G'(f)df\right] + N_k G(0)$$

$$\Leftrightarrow \quad \sum_{j \in I} N_j \left[\int_0^{\hat{y}} G'(f)df - \int_0^{\hat{x}} G'(f)df\right] > \sum_{j \notin I} \left[N_j \int_0^{\hat{x}} G'(f)df\right] - N_k \left[G\left(\frac{\xi}{N_k}\right) - G(0)\right]$$

$$\Leftrightarrow \quad \sum_{j \in I} N_j \int_{\hat{x}}^{\hat{y}} G'(f)df > \sum_{j \notin I} N_j[G(\hat{x}) - G(0)] - N_k \left[G\left(\frac{\xi}{N_k}\right) - G(0)\right]$$

$$\tag{18}$$

The equivalences above follow from rearranging, cancelling and recombining terms. By Lemma 1 $\tilde{f}$ is in the concave domain, which also holds for all $f > \tilde{f}$. Since $\hat{y} > \hat{x} > \tilde{f}$ it holds that $G''(\hat{y}) < 0$ and $G''(\hat{x}) < 0$. This implies that $(\hat{y} - \hat{x})G'(\hat{x}) > \int_{\hat{x}}^{\hat{y}} G'(f)df$. We

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thus have the following:

$$\sum_{j \in I} N_j[(\hat{y} - \hat{x})G'(\hat{x})] > \sum_{j \in I} N_j \int_{\hat{x}}^{\hat{y}} G'(f)df$$

$$> \sum_{j \notin I} N_j[G(\hat{x}) - G(0)] - N_k[G(\xi/N_k) - G(0)] \qquad (19)$$

$$> \sum_{j \notin I} N_j G'(\hat{x})\hat{x} - N_k[G(\xi/N_k) - G(0)]$$

The second inequality follows from (18) and in the last inequality we use that $[G(f) - G(0)]/f > G'(f)$ for all $f > \tilde{f}$ by Corollary 1. The three inequalities in (19) together establish that:

$$\sum_{j \in I} N_j(\hat{y} - \hat{x})G'(\hat{x}) > \sum_{j \notin I} N_j G'(\hat{x})\hat{x} - N_k[G(\xi/N_k) - G(0)]$$

$$. \Leftrightarrow \quad G'(\hat{x}) \left[\sum_{j \in I} N_j(\hat{y} - \hat{x}) - \sum_{j \notin I} N_j \hat{x} \right] > -N_k[G(\xi/N_k) - G(0)] \qquad (20)$$

$$\Leftrightarrow \qquad -\xi G'(\hat{x}) > -N_k[G(\xi/N_k) - G(0)]$$

$$\Leftrightarrow \qquad G'(\hat{x}) < [G(\xi/N_k) - G(0)]/(\xi/N_k)$$

The first equivalence follows from rearranging terms and the second by definition of $\hat{x}$ and $\hat{y}$. The third equivalence follows from multiplying both sides of the inequality with $-1/\xi$.

We will now show that the last inequality in (20) will lead to a contradiction. Because the function $G(\cdot)$ is convex at ξ/N_k we have that $[G(\xi/N_k) - G(0)]/(\xi/N_k) < G'(\xi/N_k)$. Thus, under the assumption that (ii) is optimal it must hold that $G'(\hat{x}) < G'(\xi/N_k)$ by the last inequality of (20). If allocation (ii) is optimal we also have that $G'(\xi/N_k) = G'(\hat{y})$ by Theorem S4.2, and thus that $G'(\hat{x}) < G'(\hat{y})$. However, because $\hat{x} < \hat{y}$ and both fractions are in the concave domain of the function $G(\cdot)$ it holds that $G'(\hat{x}) > G'(\hat{y})$. We thus arrive at a contradiction, which implies that allocation scheme (ii) can never be better than allocation scheme (i) for $V > \sum_{j \in J} N_j \tilde{f}$. Thus, the optimal allocation for $V > \sum_{j \in J} N_j \tilde{f}$ is allocation (i): i.e., the pro rata allocation over all populations in J. This completes the proof of part (c) of this theorem.

$\square$

Appendix S5   The Lambert W function

This appendix considers the Lambert W function, or product log function (cf. Corless et al. (1996)). This function is denoted by $W(x)$ and solves:

$$x = W(x)e^{W(x)}. \qquad (21)$$

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The herd effect $G(f)$ can be expressed using the Lambert W function:

$$G(f) = \frac{-1}{\sigma} W\left(-\sigma \exp\{-\sigma B(f)\}\right)$$

$$\text{with } B(f) = s_0 + i_0 - \frac{1}{\sigma} \log\left(s_0\left(1 - \frac{f}{s(\tau)}\right)\right) - f \tag{22}$$

which can be verified by substituting (22) into (21), which leads to (3). In this study we consider only real valued x and the function $W(x)$ is then defined only for $x \geq -\frac{1}{e}$. For $x \in [-\frac{1}{e}, 0]$ the function $W(x)$ has two values, but two branches of $W(x)$ can be defined that are both single valued. The constraint $W(x) \leq -1$ can be added to construct the branch $W_{-1}(x)$ defined only for $x \in [-\frac{1}{e}, 0]$. The other branch $W_0(x)$ holds for all $x \geq -\frac{1}{e}$ and meets the constraint $W(x) \geq -1$. This branch is also referred to as the principal branch, denoted by $W_p(x)$.

Let $G(f) = \frac{-1}{\sigma} W[y(f)]$, with $y(f) = -\sigma s_0 \left(1 - \frac{f}{s(\tau)}\right) \exp\left\{-\sigma(s_0 + i_0 - f)\right\}$ (22). We will study $y(f)$ in more detail to determine which branch of the Lambert W function is needed for the calculation of $G(f)$.

Theorem S5.1. $-\frac{1}{e} \leq y(f) \leq 0$

Proof. We can easily see that $y(f) \leq 0$, because $\sigma > 0$, $s_0 > 0$ and $f \leq s(\tau)$. Analyze the extreme values of $y(f)$:

$$\frac{d}{df} y(f) = \sigma s_0 \exp\left\{-\sigma(s_0 + i_0 - f)\right\} \left[\frac{1}{s(\tau)} - \sigma\left(1 - \frac{f}{s(\tau)}\right)\right] = 0 \Leftrightarrow f = s(\tau) - \frac{1}{\sigma}$$

It suffices to show that $y(f) \geq -\frac{1}{e}$ for $f = s(\tau) - \frac{1}{\sigma}$:

$$-\frac{s_0}{s(\tau)} \exp\{-\sigma(s_0 + i_0 - s(\tau)) - 1\} \geq -\frac{1}{e}$$

$$\log(s_0) - \sigma\left(s_0 + i_0 - s(\tau)\right) \leq \log(s(\tau))$$

$$0 \leq -s(\tau) + \frac{1}{\sigma} \log(s(\tau)) + s_0 + i_0 - \frac{1}{\sigma} \log(s_0)$$

By (2) above relation holds, because $i(\tau) \geq 0$.

$\square$

By Theorem S2.2 we know that $G(f) < \frac{1}{\sigma}$ and thus $-1 < W(-\sigma \exp\{-\sigma B(f, \sigma)\}) < 0$. By Theorem S5.1 only the principal branch $W_0(x)$ is needed when using the Lambert W function for $G(f)$ in (22).

Appendix S6 Interacting populations

In Section 5.4 the optimal allocation is analyzed for geographically distant populations that interact with each other. We use the same initial states and population sizes as in Section 5.3.

In this appendix we study the relative performance of ignoring interaction by either using the optimal allocation for non-interacting populations or by using the equitable allocation, which allocates pro rata over all populations. In Figure 1 we illustrate the performance of these two solutions relative to the optimal allocation for the interacting case. We evaluate the additional herd effect and observe that the non-interacting solution performs close to optimal and outperforms

the equitable allocation. Note that the additional herd effect becomes negative for large vaccine stockpiles, because vaccinating many people leaves very few people susceptible. This implies that herd effect can be lower for large vaccine stockpiles than for no vaccination, resulting in a negative additional herd effect.
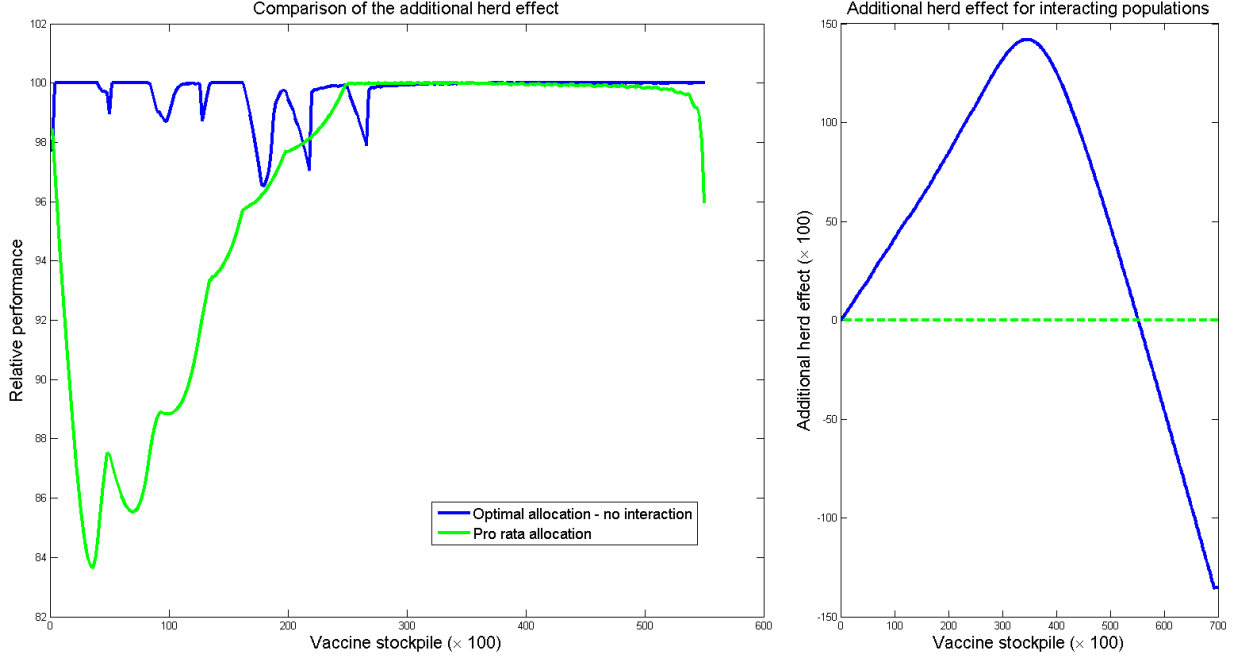

Figure 1: The left figure illustrates the relative performance of the optimal allocation for the non-interacting case (Figure 7) and the equitable pro rata allocation evaluated in the model as described in Section 5.4 with interactionfactor $c = 0.01$. We evaluate the additional herd effect for vaccine stockpiles up to size 550, because the right figure shows that for larger vaccine stockpiles the additional herd effect becomes negative.

We also study the optimal allocation for increasing levels of interaction. Figures 2, 3, 4 and 5 display the optimal allocation in case interaction between populations is respectively 0.01, 0.02, 0.05 and 0.1 times the interaction within a population. This corresponds to interaction between populations being a factor 100, 50, 20 or 10 times weaker than interaction within a population. The figures are discussed in Section 5.4.

Each of the graphs present the optimal vaccine allocation (the solid lines) over three interacting populations for different sizes of vaccine stockpile. The dashed and dotted lines indicate the important vaccination fractions: the dashed line in the middle equals $\tilde{V}_j = \tilde{f}_j N_j$, the upper dotted line equals $V_j^* = f_j^* N_j$ and the lower dotted line equals $\bar{V}_j = \bar{f}_j N_j$.
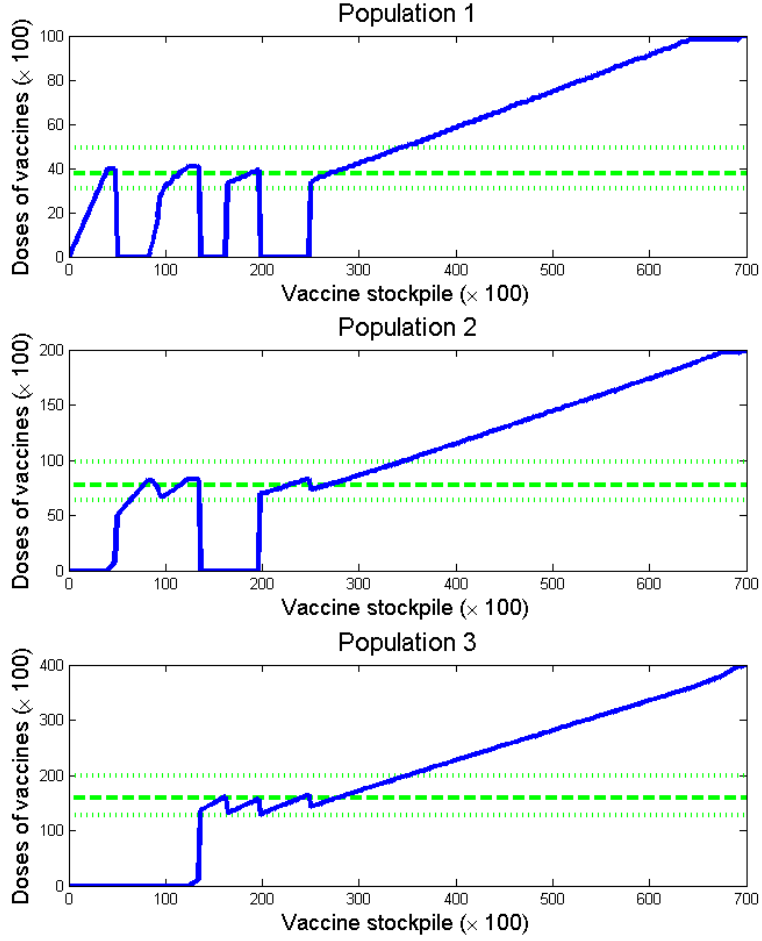
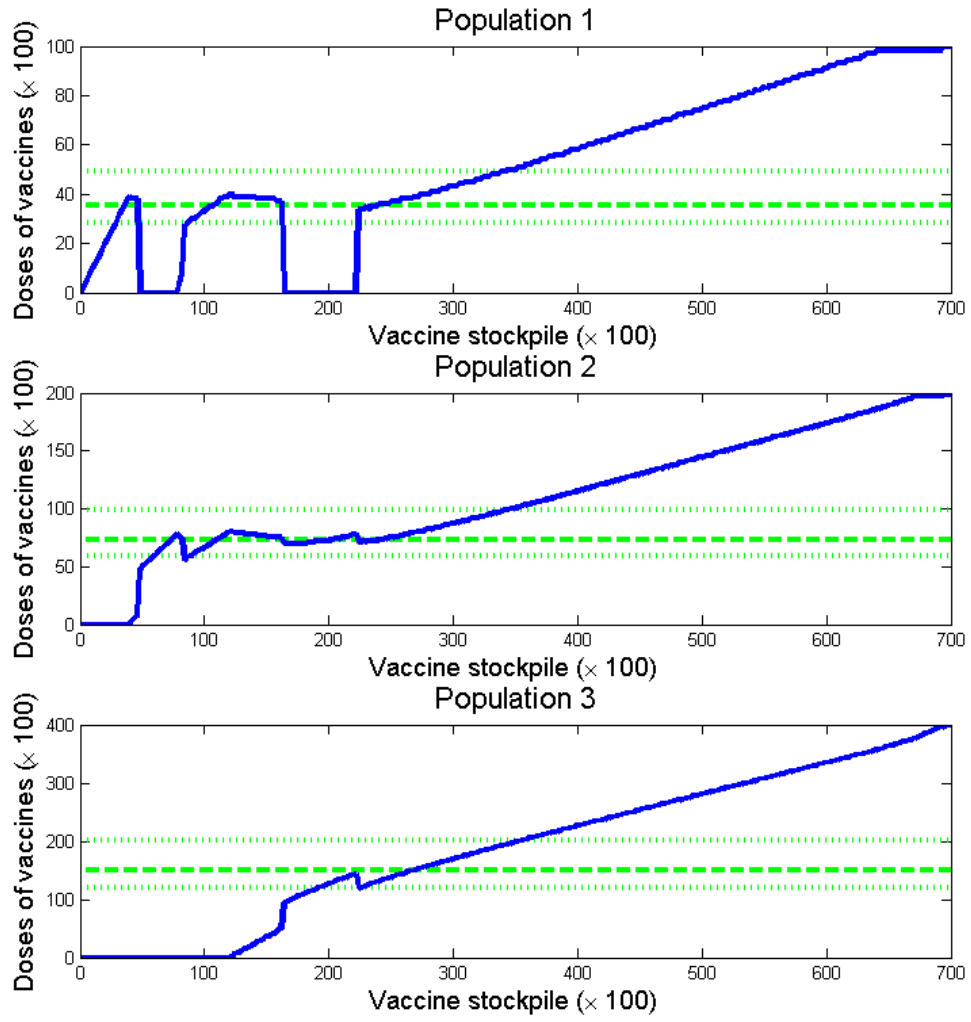Figure 2: The graphs present the optimal vaccine allocation (the solid lines) over three interacting populations for different sizes of vaccine stockpile. The dashed and dotted lines indicate the important vaccination fractions: the dashed line in the middle equals $\tilde{V}_j = \tilde{f}_j N_j$, the upper dotted line equals $V_j^* = f_j^* N_j$ and the lower dotted line equals $\bar{V}_j = \bar{f}_j N_j$.

Figure 3: The optimal allocation in case interaction between populations is 0.02 times the interaction within a population.
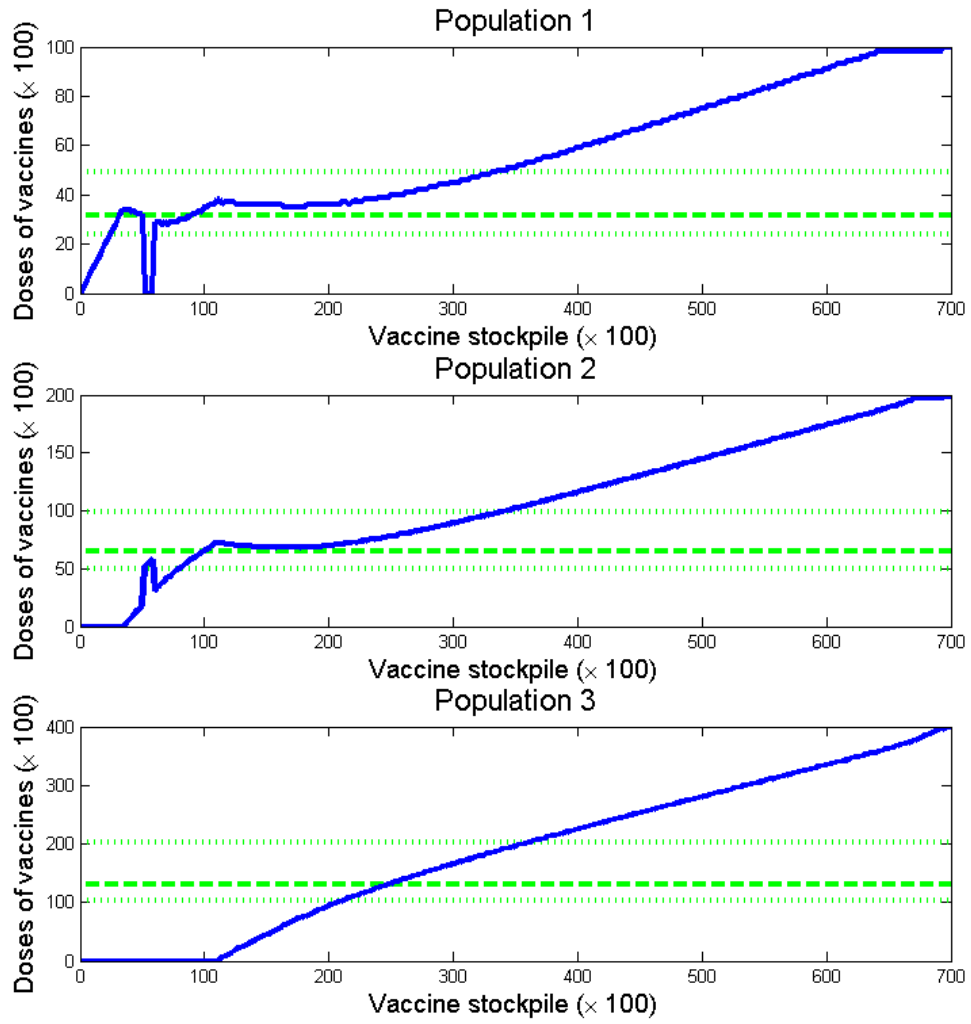
Figure 4: The optimal allocation in case interaction between populations is 0.05 times the interaction within a population.
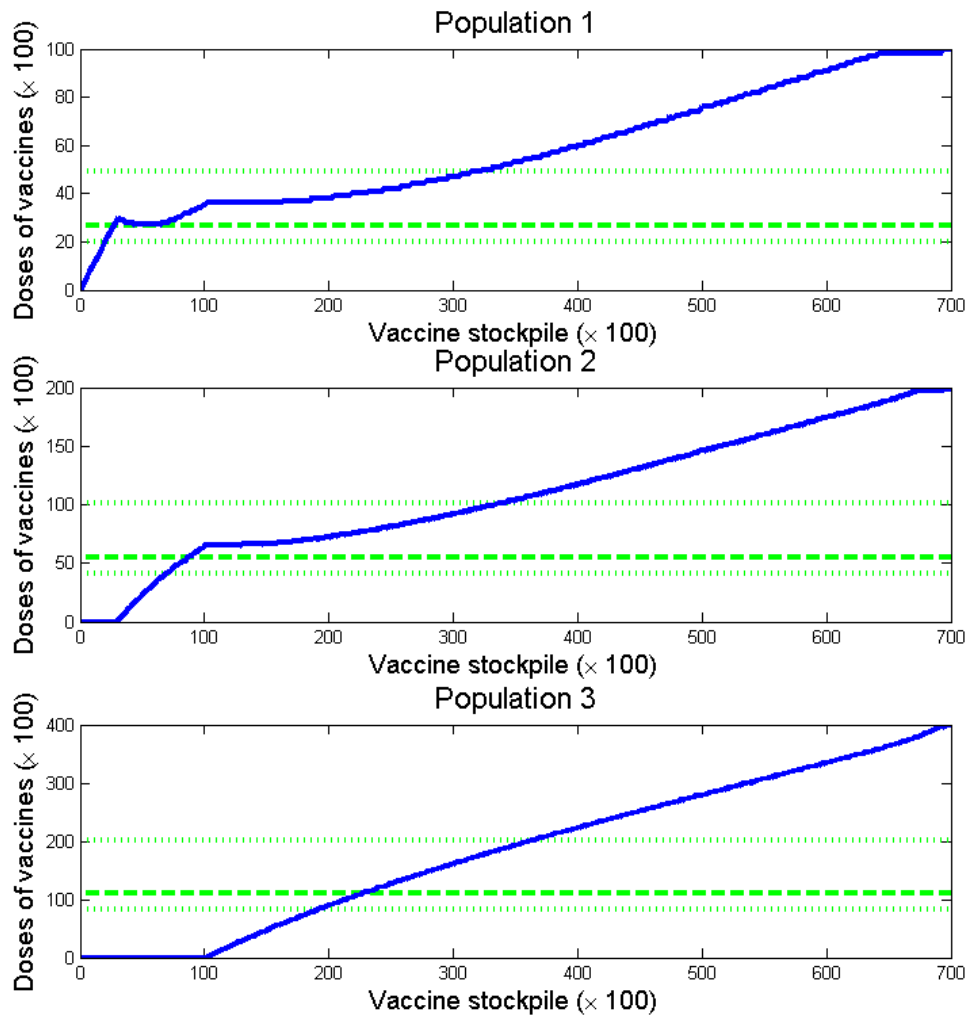
Figure 5: The optimal allocation in case interaction between populations is 0.1 times the interaction within a population.

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