# Structured compartment models of infection in Python

We consider a population aggregated by age into M groups labelled by  $i=1,2,\ldots M$ . In what follows, we provide several mathematical models of infection which have been implemented in PyRoss. We consider a structured metapopulation

$$\boldsymbol{n} = (n_1, \dots n_{M \times L}) \tag{1}$$

consisting of M age-compartments and L classes of epidemiological states. The  $\xi$ -th reaction can be written down in its most general form as

$$\sum_{i=1}^{M\times L} f_i^{\xi} Y_i \to \sum_{i=1}^{M\times L} g_i^{\xi} Y_i$$

where  $Y_i$  stands for an age-compartment of a epidemiological state (of dimension  $M \times L$ ), and  $f^{\xi}$ ,  $g^{\xi}$  keeps track of the number of each participating in the  $\xi$ -th reaction. The change in the metapopulation as a result of the  $\xi$ -th reaction reaction is,

$$\xi$$
-th transition step:  $n \xrightarrow{w_{\xi}} n + r_{\xi}$  (2)

where  $r^{\xi}$  is the vector of change for reaction  $\xi$ :  $r^{x} = g^{\xi} - f^{x}$ , and the combinatorial forward rate constant is

$$w_{\xi}(t, \boldsymbol{\theta}, \boldsymbol{n}) = k_{\xi}(t) \prod_{i} \frac{x_{i}!}{(x_{i} - f_{i}^{\xi})!}, \tag{3}$$

which gives the chemical master equation (CME) of interest:

$$\partial_t P(\boldsymbol{n}, t) = \sum_{\xi} \left[ w_{\xi}(t, \boldsymbol{\theta}, \boldsymbol{n} - \boldsymbol{r}_{\xi}) P(\boldsymbol{n} - \boldsymbol{r}_{\xi}, t) - w_{\xi}(t, \boldsymbol{\theta}, \boldsymbol{n}) P(\boldsymbol{n}, t) \right]. \tag{4}$$

## I. SIR

The population within age group i is partitioned into susceptibles  $S_i$ , infectives  $I_i$ , and removed individuals  $R_i$ . The sum of these is the size of the population in age group i,  $N_i = S_i + I_i + R_i$  ([1–5]). For this model, vital dynamics and the change in age structure on the time scale of the epidemic in this model is ignored. Therefore each  $N_i$  and, consequently, the total population size

$$N = \sum_{i=1}^{M} N_i \tag{5}$$

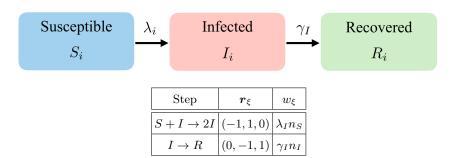


Table I. Schematics of the SIR model and elementary reaction steps and their rates. The parameters for this model are:  $\theta(\beta, \gamma_I)$ . The reaction takes the state  $n = (n_S, n_I, n_R)$  to the state  $n + r_{\xi}$ . For simplicity we consider M = 1, and thus, the sum in  $\lambda_i$ , (12), becomes trivial. we define  $\lambda_I = \beta C n_I / N$ .

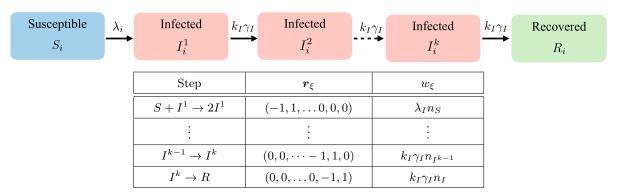


Table II. Schematics of the SIkR model and elementary reaction steps and their rates. The parameters for this model are:  $\theta(k_I, \beta, \gamma_I)$ . The reaction takes the state  $\boldsymbol{n} = (n_S, n_{I^1}, \dots, n_{I^{k_I}}, n_R)$  to the state  $\boldsymbol{n} + \boldsymbol{r}_{\xi}$ . For simplicity we consider M = 1, and thus, the sum in  $\lambda_i$ , (12), becomes trivial. we define  $\lambda_I = \beta C n_I / N$ .

remain constant in time. We assume that the rate of infection of a susceptible individual in age group i is

$$\lambda_i(t) = \beta \sum_{j=1}^M \left( C_{ij}(t) \frac{I_j}{N_j} \right), \quad i, j = 1, \dots M$$
 (6)

where  $\beta$  is the probability of infection on contact (assumed intrinsic to the pathogen) and  $C^a_{ij}$  and  $C^s_{ij}$  are, respectively, the number of contacts between asymptomatic and symptomatic infectives in age-group j with susceptibles in age-group i (reflecting the structure of social contacts). We take the age-independent recovery rate  $\gamma$  to be identical for both asymptomatic and symptomatic individuals whose fractions are, respectively,  $\alpha_i$  and  $\bar{\alpha}_i = 1 - \alpha_i$ . The social contact matrix  $C_{ij}$  denotes the average number of contacts made per day by an individual in class i with an individual in class j. Clearly, the total number of contacts between group i to group j must equal the total number of contacts from group j to group i, and thus,  $N_iC_{ij} = N_jC_{ji}$ .

The above class SIR can be instantiated in PyRoss using breakatwhitespacepyross.deterministic.SIR. A detailed notebook is present in the examples folder of PyRoss [6].

## II. SIKR

We now use method of stages to write an age-structured k-staged SIkR model  $\dot{I}_k(t) = \gamma_I N_I (I_{k-1} - I_k)$ 

$$\dot{S}_{i} = -\lambda_{i}(t)S_{i}, 
\dot{I}_{i}^{1} = \lambda_{i}(t)S_{i} - k_{I}\gamma_{I}I_{i}^{1}, 
\dot{I}_{i}^{2} = k\gamma_{I}I_{i}^{1} - k_{I}\gamma_{I}I_{i}^{2}, 
\vdots 
\dot{I}_{i}^{k} = k_{I}\gamma_{I}I_{i}^{k-1} - k_{I}\gamma_{I}I_{i}^{k}, 
\dot{R}_{i} = k_{I}\gamma_{I}I_{i}^{k}.$$
(7)

The rate of infection of a susceptible individual in age group i is

$$\lambda_i(t) = \beta \sum_{j=1}^M \sum_{n=1}^k C_{ij} \frac{I_j^n}{N_j},\tag{8}$$

The above class SIkR can be instantiated in PyRoss using breakatwhitespacepyross.deterministic.SIkR. A detailed notebook is present in the examples folder of PyRoss [6].

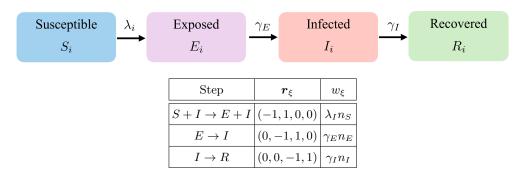


Table III. Schematics of the SEIR model and elementary reaction steps and their rates. The parameters for this model are:  $\theta(\beta, \gamma_I, \gamma_E)$ . The reaction takes the state  $n = (n_S, n_E, n_I, n_R)$  to the state  $n + r_{\xi}$ . For simplicity we consider M = 1, and thus, the sum in  $\lambda_i$ , (12), becomes trivial. we define  $\lambda_I = \beta C n_I / N$ .

#### III. SEIR

We can add an exposed class, that has caught the infection but is not infectious, to the SIR model to obtain an SEIR model.

$$\dot{S}_{i} = -\lambda_{i}(t)S_{i}, 
\dot{E}_{i} = \lambda_{i}(t)S_{i} - \gamma_{E}E_{i} 
\dot{I}_{i} = \gamma_{E}E_{i} - \gamma_{I}I_{i}, 
\dot{R}_{i} = \gamma_{I}I_{i}.$$
(9)

The rate of infection remains unchanged as before, but the equations now change. The rate of infection of a susceptible individual in age group i is

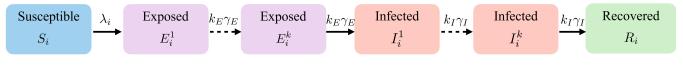
$$\lambda_i(t) = \beta \sum_{j=1}^M \left( C_{ij} \frac{I_j}{N_j} \right), \tag{10}$$

The above class SEIR can be instantiated in PyRoss using breakatwhitespacepyross.deterministic.SEIR. A detailed notebook is present in the examples folder of PyRoss [6].

#### IV. SEKIKR

The above method of stages for SIR can be extended to SEIR model to obtain an age-structured k-staged SEkIkR model to obtain

$$\dot{S}_{i} = -\lambda_{i}(t)S_{i}, 
\dot{E}_{i}^{1} = \lambda_{i}(t)S_{i} - k_{E}\gamma_{E}E_{i}^{1} 
\dot{E}_{i}^{2} = k_{E}\gamma_{E}E_{i}^{1} - k_{E}\gamma_{E}E_{i}^{2} 
\vdots 
\dot{E}_{i}^{k} = k_{E}\gamma_{E}E_{i}^{k-1} - k_{E}\gamma_{E}E_{i}^{k} 
\dot{I}_{i}^{1} = k_{E}\gamma_{E}E_{i}^{k} - k_{I}\gamma_{I}I_{i}^{1}, 
\dot{I}_{i}^{2} = k_{I}\gamma_{I}I_{i}^{1} - k_{I}\gamma_{I}I_{i}^{2}, 
\vdots 
\dot{I}_{i}^{k} = k_{I}\gamma_{I}I_{i}^{(k-1)} - k_{I}\gamma_{I}I_{i}^{k}, 
\dot{R}_{i} = k_{I}\gamma_{I}I_{i}^{k}.$$
(11)



Step	$oldsymbol{r}_{\xi}$	$w_{\xi}$
$S + I^1 \to E^1 + I^1$	$(-1,1,0\ldots,0,0,0,\ldots,0,0)$	$\lambda_I n_S$
$E^1 \to E^2$	$(0,-1,1,\ldots,0,0,0,\ldots,0,0)$	$k_E \gamma_E n_E$
<u>:</u>	i:	:
$E^{k-1} \to E^k$	$(0,0,0\ldots,-1,1,0,\ldots,0,0)$	$k_E \gamma_E n_E$
$E^k \to I^1$	$(0,0,0\ldots,0,-1,1,\ldots,0,0)$	$k_E \gamma_E n_E$
:	:	:
$I^k \to R$	$(0,0,0\ldots,0,0,0,\ldots,-1,1)$	$k_I \gamma_I n_I$

Table IV. Schematics of the SEkIkR model and elementary reaction steps and their rates. The parameters for this model are:  $\theta(k_I, k_E, \beta, \gamma_I, \gamma_E)$ . The reaction takes the state  $\mathbf{n} = (n_S, n_{E^1}, \dots, n_{E^{k_E}}, n_{I^1}, \dots, n_{I^{k_I}}, n_R)$  to the state  $\mathbf{n} + \mathbf{r}_{\xi}$ . For simplicity we consider M = 1, and thus, the sum in  $\lambda_i$ , (12), becomes trivial. we define  $\lambda_I = \beta C n_I / N$ .

The rate of infection of a susceptible individual in age group i is as in SIkR. The above class SEkIkR can be instantiated in PyRoss using breakatwhitespacepyross.deterministic.SEkIkR. A detailed notebook is present in the examples folder of PyRoss [6].

#### V. SIIR

The population within age group i is partitioned into susceptibles  $S_i$ , asymptomatic infectives  $I_i^a$ , symptomatic infectives  $I_i^s$  and removed individuals  $R_i$ . The sum of these is the size of the population in age group i,  $N_i = S_i + I_i^a + I_i^s + R_i$  [1–4]. We ignore vital dynamics and the change in age structure on the time scale of the epidemic in this model. We assume that the rate of infection of a susceptible individual in age group i is

$$\lambda_i(t) = \beta \sum_{j=1}^{M} \left( C_{ij}^a(t) \frac{I_j^a}{N_j} + C_{ij}^s(t) \frac{I_j^s}{N_j} \right), \quad i, j = 1, \dots M$$
 (12)

where  $\beta$  is the probability of infection on contact (assumed intrinsic to the pathogen) and  $C_{ij}^a$  and  $C_{ij}^s$  are, respectively, the number of contacts between asymptomatic and symptomatic infectives in age-group j with susceptibles in age-group i (reflecting the structure of social contacts).

With these assumptions the progress of the epidemic is governed by the age-structured SIR model

$$\dot{S}_{i} = -\lambda_{i}(t)S_{i}, 
\dot{I}_{i}^{a} = \alpha_{i}\lambda_{i}(t)S_{i} - \gamma_{I^{a}}I_{i}^{a}, 
\dot{I}_{i}^{s} = \bar{\alpha}_{i}\lambda_{i}(t)S_{i} - \gamma_{I^{s}}I_{i}^{s}, 
\dot{R}_{i} = \gamma_{I^{a}}I_{i}^{a} + \gamma_{I^{s}}I_{i}^{s}.$$
(13)

The age structure of the population is specified the proportions  $N_i/N$  and the contact structure by the matrices  $C^a_{ij}$  and  $C^s_{ij}$ . We assume that symptomatic infectives reduce their contacts compared to asymptomatic infectives and set  $C^s_{ij} = f^s C^a_{ij} \equiv f^s C_{ij}$ , where  $0 \le f^s \le 1$  is the proportion by which this self-isolation takes place. Here

The rate of infection of a susceptible individual in age group i is

$$\lambda_i(t) = \beta \sum_{j=1}^{M} \left( C_{ij}^a(t) \frac{I_j^a}{N_j} + C_{ij}^s(t) \frac{I_j^s}{N_j} \right), \quad i, j = 1, \dots M$$
 (14)

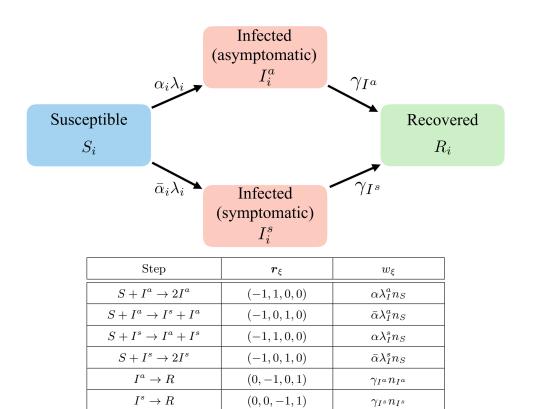


Table V. Schematics of the SIIR model and elementary reaction steps and their rates. The parameters for this model are:  $\theta(\alpha_i, \beta, \gamma_{I^a}, \gamma_{I^s})$ . The reaction takes the state  $n = (n_S, n_{I^a}, n_{I^s}, n_R)$  to the state  $n + r_{\xi}$ . For simplicity we consider M = 1, and thus, the sum in  $\lambda_i$ , (12), becomes trivial. we define  $\lambda_I^a = \beta C^a n_{I^a}/N$  and  $\lambda_I^s = \beta C^s n_{I^s}/N$  such that  $\lambda = \lambda_I^a + \lambda_I^s$ . This can be easily generalized to the age-structured model.

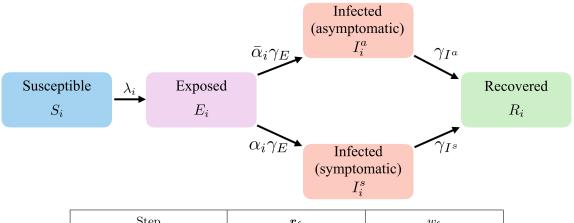
where  $\beta$  is the probability of infection on contact (assumed intrinsic to the pathogen) and  $C_{ij}^a$  and  $C_{ij}^s$  are, respectively, the number of contacts between asymptomatic and symptomatic infectives in age-group j with susceptibles in age-group i (reflecting the structure of social contacts). We take the age-independent recovery rate  $\gamma$  to be identical for both asymptomatic and symptomatic individuals whose fractions are, respectively,  $\alpha_i$  and  $\bar{\alpha}_i = 1 - \alpha_i$ . The social contact matrix  $C_{ij}$  denotes the average number of contacts made per day by an individual in class i with an individual in class i. Clearly, the total number of contacts between group i to group i must equal the total number of contacts from group i to group i, and thus,  $N_iC_{ij} = N_jC_{ji}$ .

- $\gamma_{I^a}$  is the recovery rate for asymptomatic infectives
- $\gamma_{I^s}$  is the recovery rate for symptomatic infectives
- $\beta$  is the probability of infection on contact
- $\alpha_i$  is the fraction of asymptomatic infectives
- $f^s$  is the fraction for reduction in contacts of the symptomatic infectives

In what follows, we add more features to SIR model and derive more detailed models. The above class SIIR can be instantiated in PyRoss using breakatwhitespacepyross.deterministic.SIR. A detailed notebook is present in the examples folder of PyRoss [6].

## VI. SEIIR

We can add an exposed class, that has caught the infection but is not infectious, to the SIR model to obtain an SEIR model. The rate of infection remains unchanged as before, but the equations now change to



Step	$oldsymbol{r}_{\xi}$	$w_{\xi}$
$S + I^a, I^s \rightarrow E + I^a, I^s$	(-1, 1, 0, 0, 0)	$\lambda_I^a n_S, \lambda_I^s n_S$
$E \to I^a$	(0,-1,1,0,0)	$lpha\gamma_E n_E$
$E \to I^s$	(0,-1,0,1,0)	$ar{lpha}\gamma_E n_E$
$I^a \to R$	(0,0,-1,0,1)	$\gamma_{I^a}n_{I^a}$
$I^s \to R$	(0,0,0,-1,1)	$\gamma_{I^s}n_{I^s}$

Table VI. Schematics of the SEIIR model, elementary reaction steps and their rates. The parameters for this model are:  $\theta(\alpha_i, \beta, \gamma_E, \gamma_{I^a}, \gamma_{I^s})$ . The reaction takes the state  $n = (n_S, n_E, n_{I^a}, n_{I^s}, n_R)$  to the state  $n + r_{\xi}$ . The infection rates  $\lambda_I^a$  and  $\lambda_I^s$  are defined in V.

$$\dot{S}_{i} = -\lambda_{i}(t)S_{i}, 
\dot{E}_{i} = \lambda_{i}(t)S_{i} - \gamma_{E}E_{i} 
\dot{I}_{i}^{a} = \alpha_{i}\gamma_{E}E_{i} - \gamma_{I^{a}}I_{i}^{a}, 
\dot{I}_{i}^{s} = \bar{\alpha}_{i}\gamma_{E}E_{i} - \gamma_{I^{a}}I_{i}^{s}, 
\dot{R}_{i} = \gamma_{I^{a}}I_{i}^{a} + \gamma_{I^{s}}I_{i}^{s}.$$
(15)

$$\lambda_i(t) = \beta \sum_{j=1}^M \left( C_{ij}^a \frac{I_j^a}{N_j} + C_{ij}^s \frac{I_j^s}{N_j} \right), \tag{16}$$

Assuming an exponentially distributed incubation time distribution,  $1/\gamma_E$  can be interpreted as the average incubation period. Here the population remains constant. The above class SEIIR can be instantiated in PyRoss using breakatwhitespacepyross.deterministic.SEIR. A detailed notebook is present in the examples folder of PyRoss [6].

## VII. SEKIKIKR

We can add an exposed class, that has caught the infection but is not infectious, to the SIR model to obtain an SEIR model. The rate of infection remains unchanged as before, but the equations now change to

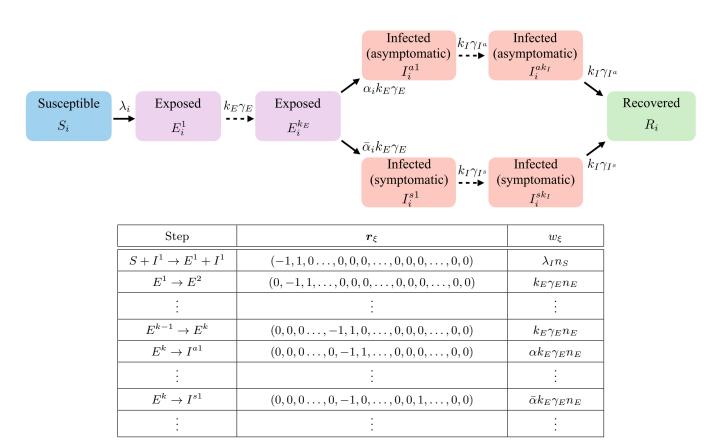


Table VII. Schematics of the SEkIkR model and elementary reaction steps and their rates. The parameters for this model are:  $\theta(k_I, k_E, \alpha_i, \beta, \gamma_{I^a}, \gamma_{I^s}, \gamma_E)$ . The reaction takes the state  $n = (n_S, n_{E^1}, \dots, n_{E^kE}, n_{I^{a_1}}, \dots, n_{I^{ak_I}}, n_{I^{s_1}}, \dots, n_{I^{sk_I}}, n_R)$  to the state  $n + r_{\xi}$ . For simplicity we consider M = 1, and thus, the sum in  $\lambda_i$ , (12), becomes trivial. we define  $\lambda_I = \beta C n_I / N$ .

$$\dot{S}_{i} = -\lambda_{i}(t)S_{i}, 
\dot{E}_{i}^{1} = \lambda_{i}(t)S_{i} - k_{E}\gamma_{E}E_{i}^{1} 
\dot{E}_{i}^{2} = k_{E}\gamma_{E}E_{i}^{1} - k_{E}\gamma_{E}E_{i}^{2} 
\vdots 
\dot{E}_{i}^{k_{E}} = k_{E}\gamma_{E}E_{i}^{k_{E}-1} - k_{E}\gamma_{E}E_{i}^{k_{E}} 
\dot{I}_{i}^{a1} = \alpha_{i}k_{E}\gamma_{E}E_{i}^{k} - k_{I}\gamma_{Ia}I_{i}^{a1}, 
\dot{I}_{i}^{a2} = k_{I}\gamma_{Ia}I_{i}^{a1} - k_{I}\gamma_{Ia}I_{i}^{a2}, 
\vdots 
\dot{I}_{i}^{ak_{I}} = k_{Ia}\gamma_{Ia}I_{i}^{a(k_{I}-1)} - k_{I}\gamma_{Ia}I_{i}^{ak_{I}}, 
\dot{I}_{i}^{i2} = \alpha_{i}k_{E}\gamma_{E}E_{i}^{k_{E}} - k_{I}\gamma_{Is}I_{i}^{a1}, 
\dot{I}_{i}^{i2} = k_{I}\gamma_{Is}I_{i}^{s1} - k_{I}\gamma_{Is}I_{i}^{s2}, 
\vdots 
\dot{I}_{i}^{sk_{I}} = k_{I}\gamma_{Is}I_{i}^{s1} - k_{I}\gamma_{Is}I_{i}^{s2}, 
\vdots 
\dot{I}_{i}^{sk_{I}} = k_{I}\gamma_{Is}I_{i}^{s(k_{I}-1)} - k_{I}\gamma_{Is}I_{i}^{sk_{I}}, 
\dot{R}_{i} = k_{I}\gamma_{Ia}I_{i}^{ak_{I}} + k_{I}\gamma_{Is}I_{i}^{sk_{I}}.$$

$$\lambda_i(t) = \beta \sum_{j=1}^{M} \sum_{n=1}^{k_I} \left( C_{ij}^a \frac{I_j^{an}}{N_j} + C_{ij}^s \frac{I_j^{sn}}{N_j} \right), \tag{18}$$

The above class SEkIkIkR can be instantiated in PyRoss using breakatwhitespacepyross.deterministic.SEkIkIkR. A detailed notebook is present in the examples folder of PyRoss [6].

#### VIII. SEI5R

We now extend SEIR model to have fives types of infectives ( $I_i^h$ : infectives who are hospitalized,  $I_i^c$ : infectives who are in ICU, and  $I_i^m$ : mortality) to obtain:

$$\dot{S}_{i} = -\lambda_{i}(t)S_{i} + \sigma_{i}, 
\dot{E}_{i} = \lambda_{i}(t)S_{i} - \gamma_{E}E_{i} 
\dot{I}_{i}^{a} = \alpha_{i}\gamma_{E}E_{i} - \gamma_{I^{a}}I_{i}^{a}, 
\dot{I}_{i}^{s} = \bar{\alpha}_{i}\gamma_{E}E_{i} - \gamma_{I^{s}}I_{i}^{s}, 
\dot{I}_{i}^{h} = h_{i}\gamma_{I^{s}}I_{i}^{s} - \gamma_{I^{h}}I_{i}^{h}, 
\dot{I}_{i}^{c} = c_{i}\gamma_{I^{h}}I_{i}^{h} - \gamma_{I^{c}}I_{i}^{c}, 
\dot{I}_{i}^{m} = m_{i}\gamma_{I^{c}}I_{i}^{c}, 
\dot{R}_{i} = \gamma_{I^{a}}I_{i}^{a} + \bar{h}_{i}\gamma_{I^{s}}I_{i}^{s} + \bar{c}_{i}\gamma_{I^{h}}I_{i}^{h} + \bar{m}_{i}\gamma_{I^{c}}I_{i}^{c}. 
\dot{N}_{i} = \sigma_{i} - m_{i}\gamma_{I^{c}}I_{i}^{c}$$
(19)

The rate of infection of a susceptible individual in age group i is

$$\lambda_i(t) = \beta \sum_{j=1}^{M} \left( C_{ij}^a \frac{I_j^a}{N_j} + C_{ij}^s \frac{I_j^s}{N_j} + C_{ij}^h \frac{I_j^h}{N_j} \right), \tag{20}$$

Here  $\bar{h}_i = 1 - h_i$ ,  $\bar{m}_i = 1 - m_i$ ,  $C^s_{ij} = f^s C^a_{ij} \equiv f^s C_{ij}$  and  $C^s_{ij} = f^h C^a_{ij} \equiv f^h C_{ij}$ .  $I^c$  is ICU cases and  $I^m$  is the mortality due to the infection. The above class SEI5R can be instantiated in PyRoss using breakatwhitespacepyross. deterministic.SEI5R. A detailed notebook is present in the examples folder of PyRoss [6].

### IX. SEI8R

We now extend SEIR model to have eight types of infectives ( $I_i^h$ : infectives who are hospitalized,  $I_i^c$ : infectives who are in ICU, and  $I_i^m$ : mortality) to obtain:

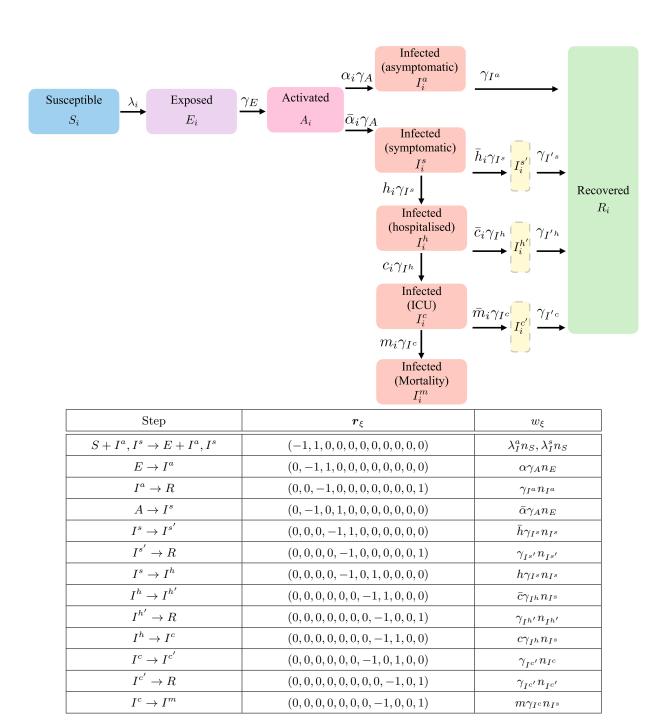


Table VIII. Schematics of the SEI8R model, elementary reaction steps and their rates. The parameters for this model are:  $\theta(\alpha_i, \beta, \gamma_E, \gamma_{I^a}, \gamma_{I^s}, \gamma_{I^h}, \gamma_{I^c}, \gamma_{I^{h'}}, \gamma_{I^{c'}}, h_i, c_i, m_i)$ . Elementary reaction steps and their rates for the SEAI8R model for M=1. The reaction takes the state  $\boldsymbol{n}=(n_S, n_E, n_{I^a}, n_{I^s}, n_{I^s'}, n_{I^h}, n_{I^{c'}}, n_{I^c}, n_{I^c'}, n_{I^m}, n_R)$  to the state  $\boldsymbol{n}+\boldsymbol{r}_{\xi}$ . The infection rates  $\lambda_I^a$  and  $\lambda_I^s$  are defined in .

$$\dot{S}_{i} = -\lambda_{i}(t)S_{i} + \sigma_{i}, 
\dot{E}_{i} = \lambda_{i}(t)S_{i} - \gamma_{E}E_{i} 
\dot{I}_{i}^{a} = \alpha_{i}\gamma_{E}E_{i} - \gamma_{I^{a}}I_{i}^{a}, 
\dot{I}_{i}^{s} = \bar{\alpha}_{i}\gamma_{E}E_{i} - \gamma_{I^{s}}I_{i}^{s}, 
\dot{I}_{i}^{s'} = \bar{h}_{i}\gamma_{I^{s}}I_{i}^{s} - \gamma_{I^{s'}}I_{i}^{s'} 
\dot{I}_{i}^{h} = h_{i}\gamma_{I^{s}}I_{i}^{s} - \gamma_{I^{h}}I_{i}^{h}, 
\dot{I}_{i}^{h'} = \bar{c}_{i}\gamma_{I^{h}}I_{i}^{h} - \gamma_{I^{h'}}I_{i}^{h'} 
\dot{I}_{i}^{c} = c_{i}\gamma_{I^{h}}I_{i}^{h} - \gamma_{I^{c}}I_{i}^{c}, 
\dot{I}_{i}^{c'} = \bar{m}_{i}\gamma_{I^{c}}I_{i}^{c} - \gamma_{I^{c'}}I_{i}^{c'} 
\dot{I}_{i}^{m} = m_{i}\gamma_{I^{c}}I_{i}^{c}, 
\dot{R}_{i} = \gamma_{I^{a}}I_{i}^{a} + \gamma_{I^{s'}}I_{i}^{s'} + \gamma_{I^{h'}}I_{i}^{h'} + \gamma_{I^{c'}}I_{i}^{c'}. 
\dot{N}_{i} = \sigma_{i} - m_{i}\gamma_{I^{c}}I_{i}^{c}$$
(21)

$$\lambda_i(t) = \beta \sum_{j=1}^{M} \left( C_{ij}^a \frac{I_j^a}{N_j} + C_{ij}^s \frac{I_j^s}{N_j} + C_{ij}^h \frac{I_j^h}{N_j} \right), \tag{22}$$

Here  $\bar{h}_i = 1 - h_i$ ,  $\bar{m}_i = 1 - m_i$ ,  $C^s_{ij} = f^s C^a_{ij} \equiv f^s C_{ij}$  and  $C^s_{ij} = f^h C^a_{ij} \equiv f^h C_{ij}$ .  $I^c$  is ICU cases and  $I^m$  is the mortality due to the infection. The above class SEI8R can be instantiated in PyRoss using breakatwhitespacepyross. deterministic. SEI8R. A detailed notebook is present in the examples folder of PyRoss [6].

## X. SEAIIR

This model is an extension of the SEIR model, introducing the additional class A, which is both asymptomatic and infectious. In other words, this models shows what ensues if *everyone* who gets infected, undergoes a latency period where they are both asymptomatic and infectious. This class is potentially quite important, as there is some evidence that people are infectious before they start showing symptoms

$$\dot{S}_{i} = -\lambda_{i}(t)S_{i}$$

$$\dot{E}_{i} = \lambda_{i}(t)S_{i} - \gamma_{E}E_{i}$$

$$\dot{A}_{i} = \gamma_{E}E_{i} - \gamma_{A}A_{i}$$

$$\dot{I}_{i}^{a} = \alpha_{i}\gamma_{A}A_{i} - \gamma_{I^{a}}I_{i}^{a}$$

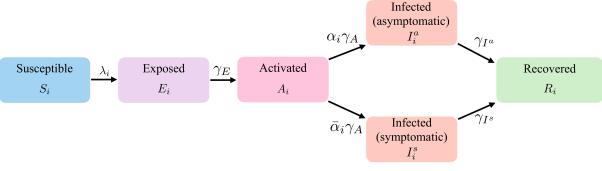
$$\dot{I}_{i}^{s} = \bar{\alpha}_{i}\gamma_{A}A_{i} - \gamma_{I^{s}}I_{i}^{s}$$

$$\dot{R}_{i} = \gamma_{I^{a}}I_{i}^{a} + \gamma_{I^{s}}I_{i}^{s}$$
(23)

The rate of infection of a susceptible individual in age group i is

$$\lambda_i(t) = \beta \sum_{j=1}^{M} \left( C_{ij}^a \frac{I_j^a}{N_j} + C_{ij}^a \frac{A_j}{N_j} + C_{ij}^s \frac{I_j^s}{N_j} \right), \tag{24}$$

The A and  $I^a$  classes should behave virtually the same (so their contact matrices should be equal). The two are kept distinct to keep track of the fact that some people remain asymptomatic even in the I stage. Since it's difficult to find data on the ratio of  $I^s$  to  $I^a$ , it is possible to disregard the distinction and simply use I instead. The above class SEI5R can be instantiated in PyRoss using breakatwhitespacepyross.deterministic.SEAIR. A detailed notebook is present in the examples folder of PyRoss [6].



Step	$r_{\xi}$	$w_{\xi}$
$S+A, I^a, I^s \to E+A, I^a, I^s$	(-1, 1, 0, 0, 0)	$\lambda_A^a n_S, \lambda_I^a n_S, \lambda_I^s n_S$
$E \to A$	(0,-1,1,0,0)	$\gamma_E n_E$
$A  o I^a$	(0,0,-1,1,0)	$lpha\gamma_A n_A$
$A \to I^s$	(0,0,-1,0,1)	$ar{lpha}\gamma_A n_A$
$I^a  o R$	(0,0,0,-1,0)	$\gamma_{I^a}n_{I^a}$
$I^s \to R$	(0,0,0,0,-1)	$\gamma_{I^s}n_{I^s}$

Table IX. Schematics of the SEAIIR model, elementary reaction steps and their rates. The parameters for this model are:  $\theta(\alpha_i, \beta, \gamma_E, \gamma_A, \gamma_{I^a}, \gamma_{I^s})$ . Elementary reaction steps and their rates for the SEAIR model. The reaction takes the state  $\boldsymbol{n} = (n_S, n_E, n_A, n_{I^a}, n_{I^s})$  to the state  $\boldsymbol{n} + \boldsymbol{r}_{\alpha}$  for M = 1. In addition to the infection rates  $\lambda_I^a$  and  $\lambda_I^s$ , we define  $\lambda_A^a = \beta C^a n_A/N$ . Thus, for this simplified model we can write for the total rate of infection, (??),  $\lambda = \lambda_A^a + \lambda_I^a + \lambda_I^s$ .

#### XI. SEAI5R

We now extend SEIR model to have fives types of infectives ( $I_i^h$ : infectives who are hospitalized,  $I_i^c$ : infectives who are in ICU, and  $I_i^m$ : mortality) to obtain:

$$\dot{S}_{i} = -\lambda_{i}(t)S_{i} + \sigma_{i},$$

$$\dot{E}_{i} = \lambda_{i}(t)S_{i} - \gamma_{E}E_{i}$$

$$\dot{A}_{i} = \gamma_{E}E_{i} - \gamma_{A}A_{i}$$

$$\dot{I}_{i}^{a} = \alpha_{i}\gamma_{A}A_{i} - \gamma_{I^{a}}I_{i}^{a},$$

$$\dot{I}_{i}^{s} = \bar{\alpha}_{i}\gamma_{A}A_{i} - \gamma_{I^{s}}I_{i}^{s},$$

$$\dot{I}_{i}^{h} = h_{i}\gamma_{I^{s}}I_{i}^{s} - \gamma_{I^{h}}I_{i}^{h},$$

$$\dot{I}_{i}^{c} = c_{i}\gamma_{I^{h}}I_{i}^{h} - \gamma_{I^{c}}I_{i}^{c},$$

$$\dot{I}_{i}^{m} = m_{i}\gamma_{I^{c}}I_{i}^{c},$$

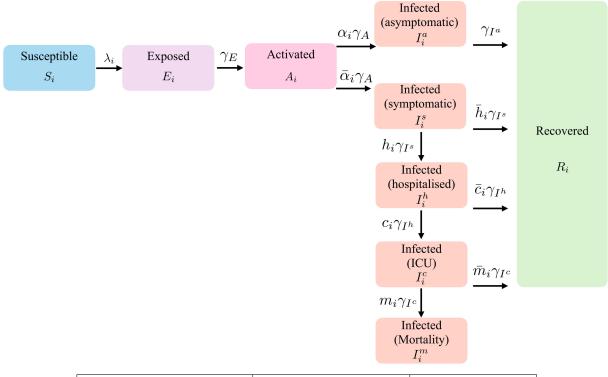
$$\dot{R}_{i} = \gamma_{I^{a}}I_{i}^{a} + \bar{h}_{i}\gamma_{I^{s}}I_{i}^{s} + \bar{c}_{i}\gamma_{I^{h}}I_{i}^{h} + \bar{m}_{i}\gamma_{I^{c}}I_{i}^{c}.$$

$$\dot{N}_{i} = \sigma_{i} - m_{i}\gamma_{I^{c}}I_{i}^{m}$$
(25)

The rate of infection of a susceptible individual in age group i is

$$\lambda_i(t) = \beta \sum_{j=1}^{M} \left( C_{ij}^a \frac{I_j^a}{N_j} + C_{ij}^a \frac{A_j}{N_j} + C_{ij}^s \frac{I_j^s}{N_j} + C_{ij}^h \frac{I_j^h}{N_j} \right), \tag{26}$$

Here  $\bar{h}_i = 1 - h_i$ ,  $\bar{m}_i = 1 - m_i$ ,  $C^s_{ij} = f^s C^a_{ij} \equiv f^s C_{ij}$  and  $C^s_{ij} = f^h C^a_{ij} \equiv f^h C_{ij}$ .  $I^c$  is ICU cases and  $I^m$  is the mortality. The above class SEAI5R can be instantiated in PyRoss using breakatwhitespacepyross.deterministic.SEAI5R. A detailed notebook is present in the examples folder of PyRoss [6].



Step	$oldsymbol{r}_{\xi}$	$w_{\xi}$
$S + I^a, I^s \to E + I^a, I^s$	(-1, 1, 0, 0, 0, 0, 0, 0, 0)	$\lambda_I^a n_S, \lambda_I^s n_S$
$E \to A$	(0,-1,1,0,0,0,0,0)	$\gamma_E n_E$
$A \rightarrow I^a$	(0,0,-1,1,0,0,0,0,0)	$lpha\gamma_A n_E$
$I^a \to R$	(0,0,0,-1,0,0,0,0,1)	$\gamma_{I^a}n_{I^a}$
$A \rightarrow I^s$	(0,0,-1,0,1,0,0,0,0)	$ar{lpha}\gamma_A n_E$
$I^s \to R$	(0,0,0,0,-1,0,0,0,1)	$ar{h}\gamma_{I^s}n_{I^s}$
$I^s  o I^h$	(0,0,0,0,-1,1,0,0,0)	$h\gamma_{I^s}n_{I^s}$
$I^h \to R$	(0,0,0,0,0,-1,0,0,1)	$ar{c}\gamma_{I^h}n_{I^s}$
$I^h  o I^c$	(0,0,0,0,0,-1,1,0,0)	$c\gamma_{I^h}n_{I^s}$
$I^c \to R$	(0,0,0,0,0,0,-1,0,1)	$m\gamma_{I^c}n_{I^s}$
$I^c  o I^m$	(0,0,0,0,0,0,-1,1,1)	$m\gamma_{I^c}n_{I^s}$

Table X. Schematics of the SEAI5R model, elementary reaction steps and their rates. The parameters for this model are:  $\theta(\alpha_i, \beta, \gamma_E, \gamma_A, \gamma_{I^a}, \gamma_{I^s}, \gamma_{I^b}, \gamma_{I^c}, h_i, c_i, m_i)$ . Elementary reaction steps and their rates for the SEAI5R model for M = 1. The reaction takes the state  $\mathbf{n} = (n_S, n_E, n_A, n_{I^a}, n_{I^s}, n_{I^h}, n_{I^c}, n_{I^m}, n_R)$  to the state  $\mathbf{n} + \mathbf{r}_{\xi}$ . The infection rates  $\lambda_I^a$  and  $\lambda_I^s$  are defined in .

#### XII. SEAI8R

We now extend SEIR model to have eight types of infectives ( $I_i^h$ : infectives who are hospitalized,  $I_i^c$ : infectives who are in ICU, and  $I_i^m$ : mortality) to obtain:

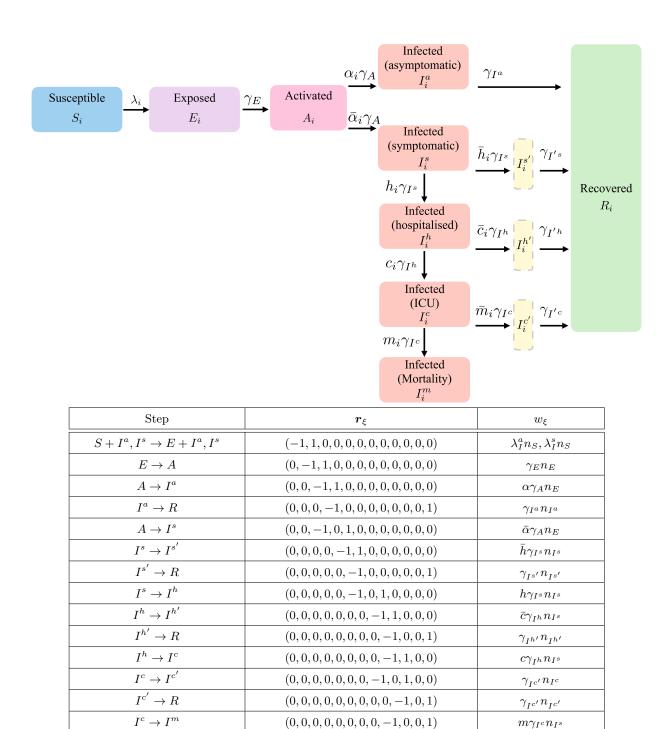


Table XI. Schematics of the SEAI8R model, elementary reaction steps and their rates. The parameters for this model are:  $\theta(\alpha_i, \beta, \gamma_E, \gamma_A, \gamma_{I^a}, \gamma_{I^s}, \gamma_{I^h}, \gamma_{I^c}, \gamma_{I^{h'}}, \gamma_{I^{c'}}, h_i, c_i, m_i)$ . Elementary reaction steps and their rates for the SEAI8R model for M=1. The reaction takes the state  $\mathbf{n}=(n_S, n_E, n_A, n_{I^a}, n_{I^s}, n_{I^s'}, n_{I^h}, n_{I^{h'}}, n_{I^c}, n_{I^{c'}}, n_{I^m}, n_R)$  to the state  $\mathbf{n}+\mathbf{r}_{\xi}$ . The infection rates  $\lambda_I^a$  and  $\lambda_I^s$  are defined in .

$$\dot{S}_{i} = -\lambda_{i}(t)S_{i} + \sigma_{i}, 
\dot{E}_{i} = \lambda_{i}(t)S_{i} - \gamma_{E}E_{i} 
\dot{A}_{i} = \gamma_{E}E_{i} - \gamma_{A}A_{i} 
\dot{I}_{i}^{a} = \alpha_{i}\gamma_{A}A_{i} - \gamma_{I^{a}}I_{i}^{a}, 
\dot{I}_{i}^{s} = \bar{\alpha}_{i}\gamma_{A}A_{i} - \gamma_{I^{s}}I_{i}^{s}, 
\dot{I}_{i}^{s'} = \bar{h}_{i}\gamma_{I^{s}}I_{i}^{s} - \gamma_{I^{s'}}I_{i}^{s'} 
\dot{I}_{i}^{b'} = h_{i}\gamma_{I^{s}}I_{i}^{s} - \gamma_{I^{h}}I_{i}^{h}, 
\dot{I}_{i}^{h'} = \bar{c}_{i}\gamma_{I^{h}}I_{i}^{h} - \gamma_{I^{h'}}I_{i}^{h'} 
\dot{I}_{i}^{c} = c_{i}\gamma_{I^{h}}I_{i}^{h} - \gamma_{I^{c}}I_{i}^{c}, 
\dot{I}_{i}^{c'} = \bar{m}_{i}\gamma_{I^{c}}I_{i}^{c} - \gamma_{I^{c'}}I_{i}^{c'} 
\dot{I}_{i}^{m} = m_{i}\gamma_{I^{c}}I_{i}^{c}, 
\dot{R}_{i} = \gamma_{I^{a}}I_{i}^{a} + \gamma_{I^{s'}}I_{i}^{s'} + \gamma_{I^{h'}}I_{i}^{h'} + \gamma_{I^{c'}}I_{i}^{c'}. 
\dot{N}_{i} = \sigma_{i} - m_{i}\gamma_{I^{c}}I_{i}^{c}$$
(27)

$$\lambda_{i}(t) = \beta \sum_{j=1}^{M} \left( C_{ij}^{a} \frac{I_{j}^{a}}{N_{j}} + C_{ij}^{s} \frac{I_{j}^{s}}{N_{j}} + C_{ij}^{h} \frac{I_{j}^{h}}{N_{j}} \right), \tag{28}$$

Here  $\bar{h}_i = 1 - h_i$ ,  $\bar{m}_i = 1 - m_i$ ,  $C^s_{ij} = f^s C^a_{ij} \equiv f^s C_{ij}$  and  $C^s_{ij} = f^h C^a_{ij} \equiv f^h C_{ij}$ .  $I^c$  is ICU cases and  $I^m$  is the mortality due to the infection. The above class SEAI8R can be instantiated in PyRoss using breakatwhitespacepyross. deterministic. SEAI8R. A detailed notebook is present in the examples folder of PyRoss [6].

#### XIII. SEAIIRQ

We now introduce the Q-class, which represents people who have been tested and put into quarantine (and can therefore not infect anyone else). This point of Q-class is to model proper contact tracing. The dynamics of the SEAIRQ model is given as:

$$\dot{S}_{i} = -\lambda_{i}(t)S_{i}$$

$$\dot{E}_{i} = \lambda_{i}(t)S_{i} - (\gamma_{E} + \tau_{E})E_{i}$$

$$\dot{A}_{i} = \gamma_{E}E_{i} - (\gamma_{A} + \tau_{A})A_{i}$$

$$\dot{I}_{i}^{a} = \alpha_{i}\gamma_{A}A_{i} - (\gamma_{I^{a}} + \tau_{I^{a}})I_{i}^{a}$$

$$\dot{I}_{i}^{s} = \bar{\alpha}_{i}\gamma_{A}A_{i} - (\gamma_{I^{s}} + \tau_{I^{s}})I_{i}^{s}$$

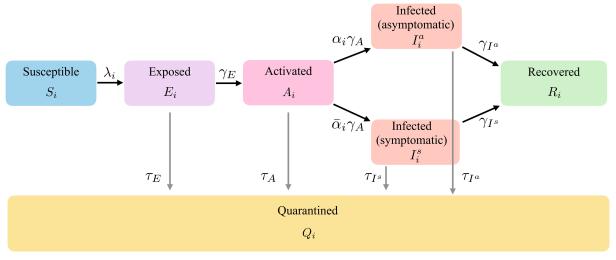
$$\dot{R}_{i} = \gamma_{I^{a}}I_{i}^{a} + \gamma_{I^{s}}I_{i}^{s}$$

$$\dot{Q}_{i} = \tau_{S}S_{i} + \tau_{E}E_{i} + \tau_{A}A_{i} + \tau_{I^{s}}I_{i}^{s} + \tau_{I^{a}}I_{i}^{a}$$
(29)

The rate of infection of a susceptible individual in age group i is

$$\lambda_i(t) = \beta \sum_{j=1}^{M} \left( C_{ij}^a \frac{I_j^a}{N_j} + C_{ij}^a \frac{A_j}{N_j} + C_{ij}^s \frac{I_j^s}{N_j} \right), \tag{30}$$

Here  $\tau_{E,A,I^s,I^a}$  is the testing rate in the population, these are in general different for different classes. We have presumed that people in the incubation stage E can also be tested. The  $\tau_S$  terms model the effects of false-positives, resulting in susceptibles being put into quarantine. Note that this model does not keep track of what happens to

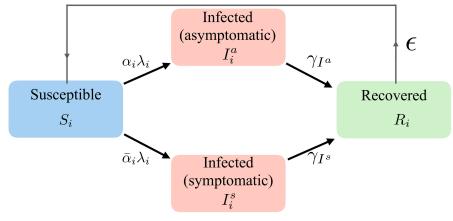


Step	$r_{\xi}$	$w_{\xi}$
$S+A, I^a, I^s \to E+A, I^a, I^s$	(-1, 1, 0, 0, 0, 0, 0)	$\lambda_A^a n_S, \lambda_I^a n_S, \lambda_I^s n_S$
$S \rightarrow Q$	(-1,0,0,0,0,1,0)	$ au_S n_S$
$E \to A$	(0,-1,1,0,0,0,0)	$\gamma_E n_E$
$E \to Q$	(0,-1,0,0,0,1,0)	$ au_E n_E$
$A  o I^a$	(0,0,-1,1,0,0,0)	$lpha\gamma_A n_A$
$A  o I^s$	(0,0,-1,0,1,0,0)	$ar{lpha}\gamma_A n_A$
$A \rightarrow Q$	(0,0,-1,0,0,1,0)	$ au_A n_A$
$I^a \to Q$	(0,0,0,-1,0,1,0)	$ au_{I^a}n_{I^a}$
$I^a \to R$	(0,0,0,-1,0,0,1)	$\gamma_{I^a} n_{I^a}$
$I^s  o Q$	(0,0,0,0,-1,1,0)	$ au_{I^s}n_{I^s}$
$I^s  o R$	(0,0,0,0,-1,0,1)	$\gamma_{I^s} n_{I^s}$

Table XII. Schematics of the SEAIIRQ model, elementary reaction steps and their rates. The parameters for this model are:  $\theta(\alpha_i, \beta, \gamma_E, \gamma_A, \gamma_{I^a}, \gamma_{I^s}, \tau_E, \tau_A, \tau_{I^a}, \tau_{I^s})$ . Elementary reaction steps and their rates for the SEAIRQ model. The reaction takes the state  $\mathbf{n} = (n_S, n_E, n_A, n_{I^a}, n_{I^s}, n_Q, n_R)$  to the state  $\mathbf{n} + \mathbf{r}_{\xi}$  for M = 1. In addition to the infection rates  $\lambda_I^a$  and  $\lambda_I^s$ , see Table V on page 5, we define  $\lambda_A^a = \beta C^a n_A/N$ . Thus, for this simplified model we can write for the total rate of infection, (??),  $\lambda = \lambda_A^a + \lambda_I^a + \lambda_I^s$ .

people once they're put into Q (which is especially important to do if  $\tau_S > 0$ ). Since Q is a closed system, this can all be done after the initial SEAIR simulation has been completed.

Here  $\tau_{E,A,I^s,I^a}$  is the testing rate in the population, these are in general different for different classes. We have presumed that people in the incubation stage E can also be tested. The  $\tau_S$  terms model the effects of false-positives, resulting in susceptibles being put into quarantine. Note that this model does not keep track of what happens to people once they're put into Q (which is especially important to do if  $\tau_S > 0$ ). Since Q is a closed system, this can all be done after the initial SEAIR simulation has been completed. The above class SEAIRQ can be instantiated in PyRoss using breakatwhitespacepyross.deterministic.SEAIRQ. A detailed notebook is present in the examples folder of PyRoss [6].



Step	$r_{\xi}$	$w_{\xi}$
$S + I^a \rightarrow 2I^a$	(-1, 1, 0, 0)	$\alpha \lambda_I^a n_S$
$S + I^a \rightarrow I^s + I^a$	(-1,0,1,0)	$\bar{\alpha}\lambda_I^a n_S$
$S + I^s \rightarrow I^a + I^s$	(-1,1,0,0)	$\alpha \lambda_I^s n_S$
$S + I^s \rightarrow 2I^s$	(-1,0,1,0)	$\bar{\alpha}\lambda_I^s n_S$
$I^a \to R$	(0,-1,0,1)	$\gamma_{I^a}n_{I^a}$
$I^s \to R$	(0,0,-1,1)	$\gamma_{I^s}n_{I^s}$
$R \to S$	(1,0,0,-1)	$\epsilon n_R$

Table XIII. Schematics of the SIRS model, elementary reaction steps and their rates. The parameters for this model are:  $\theta(\alpha_i, \beta, \gamma_{I^a}, \gamma_{I^s}, \epsilon)$ . Elementary reaction steps and their rates for the non-age-structred SIRS model. The reaction takes the state  $\mathbf{n} = (n_S, n_{I^a}, n_{I^s}n_R)$  to the state  $\mathbf{n} + \mathbf{r}_{\xi}$ . For this simplified model the sum in  $\lambda_i$ , (6), becomes trivial. Thus, let's define  $\lambda_I^a = \beta C^a n_{I^a}/N$  and  $\lambda_I^s = \beta C^s n_{I^s}/N$  such that  $\lambda = \lambda_I^a + \lambda_I^s$ . This can be easily generalized to the age-structured model.

#### XIV. SIIRS

We now extend the age-structured SIR model to allow for recovered persons to be susceptible and change in population of each age group. The dynamics of the resulting SIRS model is:

$$\dot{S}_{i} = -\lambda_{i}(t)S_{i} + \sigma_{i} + \epsilon(\gamma_{I^{a}}I_{i}^{a} + \gamma_{I^{s}}I_{i}^{s})$$

$$\dot{I}_{i}^{a} = \alpha_{i}\lambda_{i}(t)S_{i} - \gamma_{I^{a}}I_{i}^{a} + l_{i}$$

$$\dot{I}_{i}^{s} = \bar{\alpha}_{i}\lambda_{i}(t)S_{i} - \gamma_{I^{a}}I_{i}^{s}$$

$$\dot{R}_{i} = \gamma_{I^{a}}I_{i}^{a} + \gamma_{I^{s}}I_{i}^{s}.$$

$$\dot{N}_{i} = \sigma_{i} + l_{i}$$
(31)

Here  $\epsilon$  is fraction of recovered who is susceptible.  $\sigma_i$  denotes of the arrival of new susceptibles, while  $l_i$  are new asymptomatic infectives. This means that  $N_i$  is now dynamical. The rate of infection of a susceptible individual in age group i is

$$\lambda_i(t) = \beta \sum_{j=1}^M \left( C_{ij}^a \frac{I_j^a}{N_j} + C_{ij}^s \frac{I_j^s}{N_j} \right), \tag{32}$$

The above class SIRS can be instantiated in PyRoss using breakatwhitespacepyross.deterministic.SIRS. A detailed notebook is present in the examples folder of PyRoss [6].

#### XV. WHAT ELSE?

In PyRoss we can also implement any other model which you can come-up with using breakatwhitespacepyross. deterministic.Spp. The class Spp (pronounced "S plus plus") can simulate any generic compartmental model, which can be specified using a Python dictionary. For example a SIR model (I) is:

- [1] R. M. Anderson, B. Anderson, and R. M. May, *Infectious diseases of humans: dynamics and control* (Oxford university press, 1992).
- [2] M. J. Keeling and P. Rohani, Modeling infectious diseases in humans and animals (Princeton University Press, 2011).
- [3] S. Towers and Z. Feng, "Social contact patterns and control strategies for influenza in the elderly," Math. Biosci. 240, 241–249 (2012).
- [4] N. M. Ferguson et al., "Strategies for mitigating an influenza pandemic," Nature 442, 448-452 (2006).
- [5] Rajesh Singh and R Adhikari, "Age-structured impact of social distancing on the covid-19 epidemic in india," arXiv preprint arXiv:2003.12055 (2020).
- [6] "https://github.com/rajeshrinet/pyross," .