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Separation of Concerns in an Edge-Based Compartmental Modeling Framework

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Abstract: A well-known framework with strong potential for epidemic prediction and the ability to incorporate realistic contact structures is edge-based compartmental modeling (EBCM). However, models built from this framework lead to a multiplication of ordinary differential equations and many parameters to be estimated, which make the models complex and difficult to extend or to reuse. The Kendrick approach has shown promising results in generalizing compartmental models to take into account aspects of contact networks while preserving the separation of concerns, thus allowing to define modular, extensible and reusable models. But this generalization of compartmental models to contact network aspects is still limited to a few contact networks. In this paper, we present an attempt to extend Kendrick’s approach from an approximation of EBCM models to further support aspects of contact networks, thereby improving the predictive quality of models with significant heterogeneity in contact structure, while maintaining the simplicity of compartmental models. This extension consists of an integration of the basic reproductive number $R_0$ into the compartmental SIR framework. This attempted is validated using Miller’s mass action and the approximation of EBCM configuration model.

1 Introduction

Mathematical modeling and computer simulation have been widely used in epidemiology to find appropriate control strategies and means of control (Levin and Durrett, 1996). One of the most common models in mathematical modeling using the compartmental framework is the mass action model (see Figure 1). The basic assumption in this model is that susceptible and infectious individuals meet at random and can spread the disease (Cuddington and Beisner, 2005; Keeling and Rohani, 2011). Susceptible individuals ($S$) can become infected from the force of infection $λ(S, I, N) = βI$ where $β$ is the contact transmission rate and $N$ is the population size. Infectious individuals ($I$) can be recovered at the recovery rate $γ$.

\begin{equation}
\begin{cases}
S' = -βIS \\
I' = βIS - γI \\
R' = γI
\end{cases}
\end{equation}

Figure 1: Flow diagram of the mass action mathematical model

Compartmental models are typically first defined as ordinary differential equations (ODEs) such as Equation 1. These models can be studied analytically and/or simulated using algorithms such as RungeKutta. However, it is considered more realistic to adopt a stochastic viewpoint on these models considering them as Continuous-Time Markov Chains (CTMCs). The latter can be derived from the ODEs modulo some widely accepted, albeit simplifying, probabilistic assumptions.

Although the mass action model is known largely
for its conceptual and mathematical simplicity (Kermack and McKendrick, 1927), it has been found to have some shortcomings, including the fact that it incorrectly assumes that all individuals have the same contact rate and implicitly assumes that all partnerships are infinitely short (Miller et al., 2012; Wang et al., 2018).

(Miller et al., 2012; Kiss et al., 2017; Wang et al., 2018) built on these limitations of the mass action model to introduce the edge-based compartmental modelling (EBCM) framework. It is a compartment-based model extension approach where the contacts between individuals are materialized by the edges (Miller et al., 2012; Wang et al., 2018). The main idea is to integrate the heterogeneous mixture by considering the population as a network of individuals where the contacts follow a given probability distribution. Thus, it consists in incorporating into the ordinary differential equations of the mass action model, a kind of social heterogeneity (heterogeneous contact rate), while taking into account the impact of the partnership duration.

The results obtained from this incorporation have enabled realistic and more predictable contact structures to be considered. However, the modification of the compartmental framework of mass action results in more and more multiple and complex differential equations, especially when new concerns (age, sex, control strategy, etc.) and parameters are taken into account (Balde et al., 2019). Moreover, another difficulty of the EBCM framework is that the models it contains are not easily scalable, extensible and therefore not reusable.

Kendrick’s approach (Bui et al., 2016, Bui et al., 2019) has shown its ability to define concerns (age, sex, spatial heterogeneity, etc.) as independent (possibly incomplete) models that are then combined into stochastic automata networks (SANs) (Plateau and Stewart, 2000) using a tensorial sum operator. Stochastic dependencies between concerns are then introduced in a second phase so that independent concerns can be reused and combined in other models much more easily. In Fodjo et al., 2022, the authors showed that this approach, based on compartmental models, could be extended to take into account certain aspects of contact networks while enabling the building of reusable models. But this generalization of compartmental models to contact network aspects is still limited to a few contact networks (Poisson, Exponential and Scale free).

While it is well known that taking into account aspects of contact networks in compartmental models leads to more realistic and predictive models, there is also a large body of work that recognizes the crucial importance of the basic reproductive number \( R_0 \) in predicting epidemics (Meyers et al., 2005; Danon et al., 2011; Molina and Stone, 2012; Heesterbeek et al., 2015; Zhang et al., 2015; Trapman et al., 2016; Yang and Xu, 2019). This parameter refers to the number of new cases caused by a single randomly infected individual in a completely susceptible population. When \( R_0 < 1 \), epidemics are impossible, while when \( R_0 > 1 \), they are possible. (Aparicio and Pascual, 2007) suggest modifying the SIR compartmental framework to incorporate the parameter \( R_0 \) into the ordinary differential equations. In this study, in order to take the aspects of contact networks, \( R_0 \) is approximated to Poisson, Exponential and Scale free contact networks.

In this work, we propose an attempt to extend Kendrick’s approach from an approximation of the EBCM approach while maintaining the separation of concerns and preserving the simplicity of compartmental models. This approximation consists in constructing a concern in the sense of Kendrick’s approach (i.e. as a stochastic automaton that can then be combined) from the \( R_0 \) of each EBCM model. The extension of the Kendrick approach is done by incorporating the base reproduction rate \( R_0 \) into the compartmental SIR framework. The simulation results obtained are similar to those of the EBCM configuration model presented in (Miller et al., 2012).

2 Miller et al.’s mass action model and edge-based compartmental configuration models

In this section, and for the purposes of this work, we will restrict ourselves to the standard mass action model of (Miller et al., 2012) and the edge-based compartmental configuration model.

2.1 Miller et al.’s mass action model

This model is constructed like the system of Equations (1) with some modifications. Such as the fact that the authors of (Miller et al., 2012) assume that an infected individual causes new infections at the rate \( \hat{\beta}S(t) \), where \( \hat{\beta} \) is the transmission rate per infected individual. Recovery occurs at the rate of \( \gamma \).

\[
\begin{align*}
S' &= \frac{-\hat{\beta}IS}{S + I + R} \\
I' &= \frac{\hat{\beta}IS - \gamma I}{S + I + R} \\
R' &= \gamma I
\end{align*}
\]

(2)
Moreover, when building the mass action model (see system of Equations 1), many works [Cuddington and Beisser, 2005; Keeling and Rohani, 2011; Marcheva, 2015] interpret the transmission rate $\beta$ as the product of the contact rates and the transmission probability. But in the specific case of the mass action model of Miller et al.’s, the authors assume that the transmission rate per infected person $\hat{\beta} = \beta(k)$ where $(k)$ is the average degree of the contact network considered.

### 2.2 EBCM configuration model

The flow diagram of the EBCM configuration model is shown in Figure 2. The compartments $S$, $I$, and $R$ represent the proportions of susceptible, infected, and recovered, respectively, as in the case of the mass action model in section 2.1. To calculate $S(t)$, $I(t)$, and $R(t)$, the authors note that these are the probabilities that a random test node $u$ is in each compartment. We calculate $S(t)$ noting that this is also the probability that none of $u$’s partners has yet transmitted to $u$. The probability that a randomly selected partner $v$ has not yet transmitted the infection to $u$.

For large networks, (Miller et al., 2012; Wang et al., 2018) assumed that the neighbors of the node test $u$ are independent. Given a degree $k$, $u$ is susceptible at time $t$ with probability $s(k,\theta(t)) = \theta(t)^k$. Thus, $S(t) = \sum_k P(k)s(k,\theta(t)) = \psi(\theta(t))$. The ODEs of the EBCM configuration model are obtained in (3).

$$\begin{align*}
S &= \psi(\theta) \\
I &= 1 - S - R
\end{align*}$$

The $\phi_S$, $\phi_I$ and $\phi_R$ compartments of Figure 2 represent respectively the probabilities that a partner $v$ is susceptible, infected and recovered but has not yet transmitted the infection to $u$. The compartment $1 - \theta$, represents the probability that there is infection (it is done with the rate $\beta\phi_I$ between the compartment $\phi_I$ and $1 - \theta$).

In order to determine $\theta$, consider that $(\theta = \phi_S + \phi_I + \phi_R)$. At time $t = 0$, $\theta = \phi_S \approx 1$. Because we consider that there has not yet been an infection, so $\phi_I = \phi_R \approx 0$.

The central parameter of this calculation is the determination of $\phi_I$. Thus,

$$\phi_I = \theta - \phi_S - \phi_R$$

(4)

It remains to calculate $\phi_S$ and $\phi_R$ explicitly to obtain $\phi_I$. If we finally consider that the $v$ is infected and that there was an infection, then

$$\theta' = -\beta\phi_I$$

(5)

To determine $\phi_R$, the authors use the fact that in Figure 2 the fluxes from $\phi_I$ to $\phi_R$ and from $\phi_I$ to $(1 - \theta)$ are proportional to one another. Both $\phi_R$ and $(1 - \theta)$ are equal to zero at time zero since we assume that no infection or recovery events can occur prior to time zero. By integrating the relation

$$\frac{d\phi_R}{dt} = \gamma d(1 - \theta)$$

(6)

and using the initial condition

$$\phi_R(0) = (1 - \theta(0)) = 0$$

(7)

Thus,

$$\phi_R = \frac{\gamma(1 - \theta)}{\beta}$$

(8)

To determine $\phi_I$, the authors rely on the fact that a partner $v$ has a degree $k$ with probability $P_v(k) = kP(k)/k$. Given a degree $k$, $v$ is susceptible with probability $\psi(k^{-1})$. This allows us to obtain

$$\phi_S = \sum_k P_v(k)\theta(k^{-1}) = \sum_k kP(k)/(k)\theta(k^{-1}) = \psi(\theta)$$

(9)

Therefore, from the relation $\psi$ they obtain

$$\phi_I = \theta - \phi_S - \phi_R = \theta - \frac{\psi'(\theta)}{\psi(1)} - \frac{\gamma(1 - \theta)}{\beta}$$

(10)

While it is easy to recognize that the EBCM configuration model captures much more population structure than the mass action model, it is also important to note that the complexity and number of differential equations increases significantly. As we have seen, to obtain Equation (10), the authors of (Miller et al., 2012) had to develop new Equations $3, 5, 6, 7, 8, 9$ in addition to the one of the system of (3).

### 3 Generalizing Kendrick’s approach

The challenge of this work is to show that Kendrick’s approach can be extended to support aspects of contact networks using an approximation of the EBCM approach. This would improve the predictive quality of models with significant heterogeneity in the structure of contacts while preserving the separation of concerns. This would result in modular models.
extension points

From the relations 11 and 12 the identification of the relation 12, given by (2) described in section 2.1 is given by the Kendric code. In the final generic definitions of the models and in 2022). Thus we use names with the subscript “gen” to indicate that they are generic points, i.e. variable points.

Thus from the relation 11 the identification of the extension points \( \alpha_{gen}, \mu_{gen} \) and \( \tau_{gen} \) is intended to signify that they are applied to a model based on a network of contacts and to indicate that they are generic points, i.e. variable points.

\[
\lambda = \alpha_{gen} \mu_{gen} \tau_{gen} \tag{11}
\]

For our modeling and simulation purposes, we use the same convention as the authors of Fodjo et al., 2022. Thus we use names with the subscript “gen” in the final generic definitions of the models and in the Kendric code.

The force of infection of the mass action model given by (2) described in section 2.1 is given by the relation 12.

\[
\lambda = \beta I = \beta \langle k \rangle I \tag{12}
\]

From the relations 11 and 12, the identification of the extension points \( \alpha_{gen}, \mu_{gen} \) and \( \tau_{gen} \) gives:

\[
\begin{cases}
\alpha_{gen} = \langle k \rangle \\
\mu_{gen} = I \\
\tau_{gen} = \beta
\end{cases}
\tag{13}
\]

In section 2.2, we have presented the EBCM configuration model and the array of ODEs and parameters to be estimated from the model. This constitutes more effort of understanding, programming for the model designers/modelers/developers. Our goal is to cope with the complexity of ordinary differential equations in the EBCM framework while defining extensible and reusable models.

In order to cope with the complexity of the ordinary differential equations of the EBCM framework while defining extensible and reusable models, we propose to use an approximation of each EBCM model from the mathematical formulation of \( R_0 \).

Indeed, (Aparicio and Pascual, 2007) showed that it was possible to modify the simple compartmental framework in order to integrate the parameter \( R_0 \) into the model equations.

We propose to this effect to approximate the EBCM models, by incorporating each \( R_0 \) of EBCM model in the compartmental framework SIR (Susceptible, Infected, Recovered) as shown in (Aparicio and Pascual, 2007), so as to define these EBCM model approximations as concerns in the sense of the Kendrick approach (i.e. a stochastic automaton that can be composed) as illustrated in (Fodjo et al., 2022) and then to be able to determine the force of infection \( \lambda \) which it would then be possible to decompose into different points of extensions \( \alpha_{gen}, \mu_{gen} \) and \( \tau_{gen} \).

Thus, the results of this incorporation of \( R_0 \) into the SIR compartmental framework would give 14:

\[
\begin{align*}
S' &= -R_0SI \\
I' &= R_0SI - \gamma I \\
R' &= \gamma I
\end{align*}
\tag{14}
\]

Miller et al., 2012 gave the following formulation in the case of the EBCM configuration model:

\[
R_0 = \frac{\beta}{(\beta + \gamma)} \langle k^2 - k \rangle \tag{15}
\]

From 14, the force of infection of the EBCM approximation is given by the relation

\[
\lambda = R_0 I = \frac{\beta}{(\beta + \gamma)} \langle k^2 - k \rangle I \tag{16}
\]

Thus from the relation 11, the identification of the extension points allows us to obtain:

\[
\begin{cases}
\alpha_{gen} = \frac{\langle k^2 - k \rangle}{\langle k \rangle} \\
\mu_{gen} = I \\
\tau_{gen} = \frac{\beta}{(\beta + \gamma)}
\end{cases}
\tag{17}
\]

In the relationship 17, the term \( \alpha_{gen} = \frac{\langle k^2 - k \rangle}{\langle k \rangle} \) is obtained from the python code of the EoN module for each degree distribution (Homogeneous, Poisson, Bimodal and PowerLaw) specified for the graph generation. For example, the code to obtain \( \alpha_{gen} \) from the configuration model generated from a Bimodal

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3It is the average number of individuals with whom a susceptible individual is in contact or the average degree of nodes in a contact network.

4This is the proportion of contacts that are infectious.

5The rate per contact at which disease is transmitted between an infectious individual and a susceptible individual.

6This parameter was an approximation of the different contact networks considered.

degree distribution\textsuperscript{8}. We proceed in a similar way for distributions of degree Homogeneous\textsuperscript{9} and Power-Law degree distribution\textsuperscript{10}, but for the particular case of the Poisson degree distribution, \( \langle k^2 \rangle - \langle k \rangle = \langle k \rangle^2 \) (Miller et al., 2012) thus, \( a_{gen} = \frac{\langle k^2 \rangle - \langle k \rangle}{\langle k \rangle} = \frac{\langle k \rangle^2}{\langle k \rangle} = \langle k \rangle \).

4 Validation and discussion

To validate our approach, we replicated the EBCM configuration model experiments of Miller et al. (2012) using the approximation of the EBCM configuration model on the distribution\textsuperscript{11} (Homogeneous, Poisson, Bimodal, and PowerLaw) in Kendrick (Bui et al., 2019; Fodjo et al., 2022). In our implementations, the variable points of the \( \lambda \) parameter of \textsuperscript{11} are named “alphagen”, “itgen” and “taugen”. The models are built in different entities that are easy to define in modules, extensible and reusable. Indeed, each model generally includes an entity of definition of the concerns then of composition of model (see Figure 6), an entity of initialization of parameters (see Figure 7) and finally an entity of simulation (lines 36 to 41) and visualization (lines 43 to 49) (see Figure 8).

The challenge was to check if Kendrick’s approach to separation of concerns could capture approaches such as Miller et al.’s mass action model or the approximation of the EBCM configuration model while maintaining the familiar compartmental framework. The implementation of the mass action model (see Figure 9) allowed us to obtain the black curve of Figure 9b. For this implementation, the code is subdivided into two major parts. The first one is the definition of the basic concern SIR (Susceptible, Infected and Recovered) where \( \lambda \) is defined (see Figure 3). In this implementation, \( \lambda \) is defined in a general way (see lines 9 to 10). The second part of the code, is the implementation of the mass action concern named here “maConcern” as shown in Figure 4. In this definition, lines 16 to 22 allow to redefine the extension points “alphagen”, “itgen” and “taugen”. Then in line 24 we compose the basic concern and the mass action concern in line 24.

As for the implementation of the approximation of the EBCM configuration model in Kendrick, we proceed in a similar way to the mass action model. But in the case of this model (see Figure 6), the extension point “alphagen” is obtained according to the specified degree distribution. In the case of the Bi-

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\textsuperscript{8}https://github.com/YvanGuifo/EBCM-ConfigurationModel/blob/main/generate_heterogeneity_CMHomogeneous.py

\textsuperscript{9}https://github.com/YvanGuifo/EBCM-ConfigurationModel/blob/main/generate_heterogeneity_CMPowerLaw.py

\textsuperscript{10}https://github.com/YvanGuifo/EBCM-ConfigurationModel/blob/main/generate_heterogeneity_CMPowerLaw.py

\textsuperscript{11}The Python and Kendrick code of our experiments is available under https://github.com/YvanGuifo/EBCM-ConfigurationModel
modal degree distribution for example, the value of "alphagen" is given in line (17 to 18) of Figure 6. Note that in our implementations, for approximation of the EBCM configuration model what varies from one degree distribution to another is the value of "alphagen". After having defined the concerns of the basic SIR model (see Figure 3) and the approximation of the EBCM configuration model (see Figure 6), we compose the different concerns as illustrated in Figure 5. The results obtained enable us to have in Figure 9b the curves of the various distributions of degrees of the model of configuration EBCM implemented in Kendrick.

It can be seen that, whether it is the mass action model of Miller et al.’s. or the approximation of the EBCM configuration model, Kendrick’s approach allows us to easily define the concerns ("maConcern" and "cmBimodal" in the case of the approximation of the EBCM configuration model on a Bimodal degree distribution) in a way that is separate from the basic SIR concern “sirConcern”. Therefore, the basic concern “sirConcern” can be reused without “maConcern” or “cmBimodal”. Kendrick’s approach enabled us to define “myConcern” and “cmBimodal” as independent models that can then be composed.

Regarding the results obtained while implementing the EBCM configuration model on the Power-law degree distributions (see orange curves of Figures 9a and 9b), the same dynamics are observed but with a difference regarding the infectious. This can be explained by the fact that some individuals (super-spreaders) have an abnormally high number of contacts at the beginning of the epidemic. We often note a strong propensity of individuals to attach themselves preferentially to the individual with more contacts in this type of network. We also note that the moment of the epidemic peak is reached at the same time.

EBCM configuration model simulations on homogeneous, Poisson, and bimodal degree distributions using our EBCM model approximation approach (see Figure 9a) yield improved curve heights (lower curves) compared to a typical configuration model approach on homogeneous, Poisson, and bimodal degree distributions simulated with EoN (see Figure 9a). Furthermore, we note that the curves of Figure 9b have the same dynamics as those seen in Figure 9a and significantly improve the predictive quality that one would expect from a mass action model (black curve). We also note that the timing of the epidemic peak of the homogeneous, Poisson and bimodal curves in Figure 9b is slightly slower compared to the respective homogeneous, Poisson, and bimodal curves in Figure 9a.

Our approach to approximating EBCM models can be applied to mean field social heterogeneity (MFSH) algorithms and a fixed-degree dynamic model (DFD) (Miller et al., 2012; Istvan et al., 2019).

5 Conclusion

In this paper, we proposed to generalize Kendrick’s approach to the consideration of realistic contact structures from the edge-based compartmental modeling (EBCM) framework while preserving the separation of concerns in compartmental epidemic models (Bui et al., 2016). To do this, we applied the solution of (Fodjo et al., 2022) which involved defining the usual λ parameter of epidemic models as a kind of model method with three extension points, which allowed us to easily capture aspects of contact network models.

In order to validate this integration, we applied the approach of (Fodjo et al., 2022) to the mass action and the approximation of the EBCM configuration model of (Miller et al., 2012) and we were able to obtain similar results close to those of (Miller et al., 2012).

12It’s model where contact rates in the population are assigned using a $P(k)$ or $\rho(k)$ distribution, while considering that the contact duration is negligible.

13It’s model in which each node in the dynamic network has a constant-valued degree, assigned using the $P(k)$ distribution.
Both models (mass action model and the approximation of the EBCM configuration model) were defined as a very simple and distinct concern of the basic SIR model in Kendrick.

If it is obvious that we were able to obtain similar results from the EBCM configuration model from the approximation of the EBCM configuration model in Kendrick, it is still a bit limiting. This is because it requires to have beforehand a mathematical formulation of $R_0$ of each EBCM model that we wish to implement as a concern in the Kendrick sense and to be able to find the appropriate decomposition of the extension points of the relation. However, the approach we propose avoids having to build an explicit contact network, and moreover we do not have to define a multitude of differential equations. Another encouraging aspect is the fact that most of the EBCM models proposed in the literature have a mathematical formulation of $R_0$, which gives us a wide range of models to explore for future work. In the same way, we also think that in the future, it would be interesting to be able to implement typical EBCM models (without model approximation approach) as concerns that could be composed when adding new concerns.

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