Definitions of Box Model operations

Box Model

A **box model** is a directed graph whose vertices are **compartments** and edges are **transitions**. Each compartment has a **name**, which is a mathematical variable such as X. A transition is an ordered triple (s, t, r), where s and t are the **source** and **target** compartments of the transition, and r is its **rate**, which is a function of the compartments' names. We will use the notation $s \xrightarrow{r} t$ as a synonym for the above triple. Any variable involved in a transition rate that is not the name of a compartment is a **parameter** of the model. $V(M) = \{c_1, \ldots, c_n\}$, the vertex set of model M, is the set of its compartments, and $E(M)$ is the set of its edges. Let $X(M)$ be the set of the names of the compartments of model M, and let $P(M) = \{p_1, \ldots, p_m\}$ be the set of all its transitions' parameters; then each transition rate is a function $r(c_1, \ldots, c_n, p_1, \ldots, p_m)$ taking values in $\mathbb{R}$.

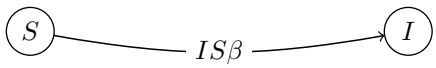
A box model is associated with an **ODE**, whose state variables are the compartments' names, and whose flow vector field is constructed from the transition rates:

$\frac{dX}{dt} = \sum_{\{e \in E(M) | \text{source}(e) = X\}} \text{rate}(e) - \sum_{\{e \in E(M) | \text{target}(e) = X\}} \text{rate}(e)$

for each compartment X.

There are also an SDE, a diffusion equation, individual-based models, and possibly other models that can be automatically generated to describe the behavior of this system.

Example: SI model.



This box model has two compartments, S and I. There is one transition from S to I, with rate βSI. Its ODE is

$\frac{dS}{dt} = -\beta SI$

$\frac{dI}{dt} = \beta SI.$

Products of box models

A **product** of box models, written $M_1 \times \cdots \times M_n$, where each M_i is a box model, is a box model whose set of compartments is the cross product, or Cartesian product, of the component box models' sets of compartments (see Appendix for definitions of graph product operations). The transitions include the edges of the Cartesian product of the components' graphs, but the product may include more transitions as well.

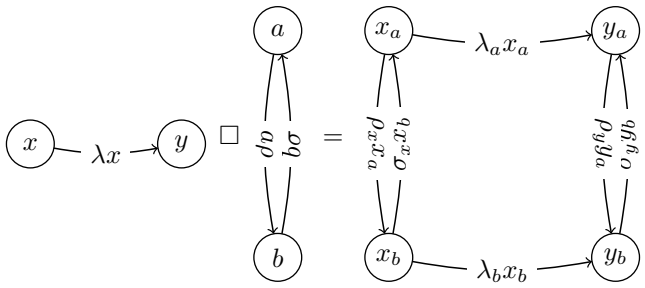
[TODO: it may include added compartments as well?]

- The compartments of the cross product are tuples $(c_1, \ldots, c_n)$ where each c_i is a compartment of M_i. The name of compartment $(c, d, e, \ldots, w)$ may be $c_{de\ldots w}$, or it may be named $X_{cde\ldots w}$, or some other naming may be used.
- For each transition T of component model M_i, with source s, target t, and rate r, there is a transition from each compartment $(c_1, \ldots, c_{i-1}, s, c_{i+1}, \ldots, c_n)$ of the product model to $(c_1, \ldots, c_{i-1}, t, c_{i+1}, \ldots, c_n)$. Its transition rate is derived from r.

I believe there are a few different products that are appropriate depending on the biology of the model, differing in what transitions are included and how their rates are constructed.

Simple Cross Product

Sometime it's sufficient to construct a product model with one transition for each edge of the graph Cartesian product. For example, imagine a simple infection model M_i, in which all compartments are stratified together by some demographic variable. Assume each component transition rate involves no compartments other than its source compartment. Then the stratified model is a simple product of the infection model with the stratification. The compartments of the product are labeled using subscripts, and the infection transitions are replicated in each stratum, with stratified compartment names substituted and subscript added to all parameters. For example, given a model with transition from x to y at rate λx, stratified by crossing with a simple model providing two demographic states a and b, we would construct a product model



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Thus by crossing with the a-b model, the single row of the x-y model gets replicated once for each compartment of the a-b model. Symmetrically, the full a-b model is replicated once for each compartment of the x-y model.

This simple Cartesian product of models is defined by the following formula.

Definition. The **simple cross product** of models $M_1, \ldots, M_n$ is defined as follows:

- $V(M_1 \,\square\, \cdots \,\square\, M_n) = V(M_1) \times \cdots \times V(M_n)$ (see Appendix for set product operations).
- $E(M_1 \,\square\, \cdots \,\square\, M_n) = \cup_{\{\,(v_1,\ldots,v_n) \in V(M_1)\times\cdots\times V(M_n)\,\}} \cup_{i\in\{1,\ldots,n\}} \cup_{\{\,w,r \mid v_i \xrightarrow{r} w \in E(M_i)\,\}}$ stratify$((v_1, \ldots, v_n), w, r, (M_1, \ldots, M_n), i)$

where

- stratify$((v_1, \ldots, v_n), w, r, (M_1, \ldots, M_n), i) = (v_1, \ldots, v_n) \xrightarrow{r_s} (v_1, \ldots, v_{i-1}, w, v_{1+i}, \ldots, v_n)$,

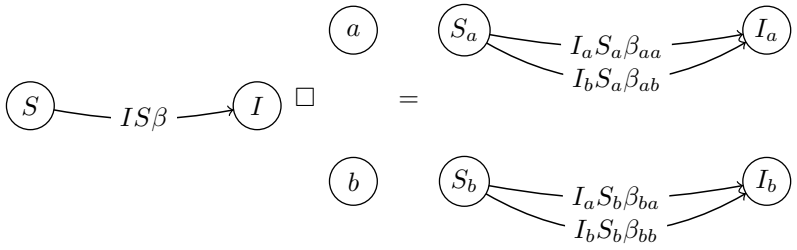
where r_s is the rate r with the name of v_i replaced by the name of the stratified vertex $(v_1, \ldots, v_n)$ and all parameters subscripted by $v_1, \ldots, v_{i-1}, v_{i+1}, \ldots, v_n$.

The name of a product compartment $(v_1, \ldots, v_n)$ can be constructed in various ways. It might be the name of v_1 subscripted by the names of the other compartments $v_2, \ldots, v_n$, or it might be X subscripted by all the compartments' names, or some other rule might be used.

Cross product with interactions

Unfortunately, the above definition of the cross product is not suitable for even a simple SI example with transition rate βSI, because this model violates the assumption that the rate involves no compartments other than S. In this model it's reasonable to believe that either stratified S class can be infected by individuals of both stratified I classes. This requires the S and I variables in that transition rate to be stratified separately, and a transition to be constructed

for every combination of stratified compartments. The correct product model is this one, with the one edge replicated four times, not only twice (with a trivial stratification model, for simplicity):



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If we used the simple cross product, we would not generate the correct sum over β and I variables.

To implement this, we need an extended product operation that provides stratification for the "catalyst" I in the βSI transition as well as the source S. The simple cross product operation can be extended in this way to become a full cross product operation.

Along with that extension, at this point I will introduce a complete definition of the cross product operation, including some details that will only become relevant in later examples.

Definition. A **cross product** $M_1 \,\square\, \cdots \,\square\, M_n$ of models $M_1, \ldots, M_n$ is a box model M such that

- $E(M) = \cup_{i \in \{1,\ldots,n\}} \cup_{s \xrightarrow{r} t \in E(M_i)} \Xi(s \xrightarrow{r} t, i)$

where

- $\Xi(s \xrightarrow{r} t, i) = \Xi_{\square}(s \xrightarrow{r} t, i) =$
$$\begin{cases} \{\, S \xrightarrow{\Phi_r(r,S,i_s,T)} T \mid S \in V_M, i_s \in \Sigma(s,S), \\ \quad T \in \Omega_1(S, i_s, s, t, r, i)\,\} \\ \quad \text{if } r \text{ is linear in } s \\ \{\, S \xrightarrow{\Phi_{2r}(r,S,i_s,C,i_c,T)} T \mid S \in V_M, i_s \in \Sigma(s,S), \\ \quad C \in V_M, i_c \in \Sigma(c,C), T \in \Omega_2(S, i_s, C, i_c, s, c, t, r, i)\,\} \\ \cup \{\, S \xrightarrow{\Phi_{1r}(S,i_s,i_c,s,t,r,i)} T \mid S \in V_M, i_s \in \Sigma(s,S), \\ \quad i_c \in \Sigma(c,S), T \in \Omega_{2i}(S, i_s, i_c, s, c, t, r, i)\,\} \\ \quad \text{if } r \text{ is bilinear in } s \text{ and } c \end{cases}$$
  generates the set of all product edges derived from the edge $s \xrightarrow{r} t$.
- $V_M = V(M_1) \times \cdots \times V(M_n)$.

- $\Sigma(v, V)$ is the set of **inclusions** of compartment v in the tuple V, which is a set of indices i for which the ith entry in the tuple is v. In this stratification example, we only require simple inclusion in the ith model, $\Sigma_1(v, (v_1, \ldots, v_n); i) = \{i\}$ if $v_i = v$, else $\{\}$, when stratifying a transition of that model. In some cases, as we will see, we will require a full inclusion function allowing "cross interactions", as we need to allow compartments from different component models to interact with each other: $\Sigma_c(v, (v_1, \ldots, v_n)) = \{\, j \mid v_j = v \,\}$.
- $\Omega_1(S, i_s, s, t, r, i) = \{\, (S_1, \ldots, S_{i_s-1}, t, S_{i_s+1}, \ldots, S_n) \,\}$ is a **unary operation** defining the set of output (target) compartments produced by a given transition acting on source compartment S. Here we provide a simple definition where S just goes to the corresponding compartment T in the same stratification of the model, but we allow for variant products defined by a different unary operation.
- $\Omega_2(S, i_s, C, i_c, s, c, t, r, i) = \{\, (S_1, \ldots, S_{i_s-1}, t, S_{i_s+1}, \ldots, S_n) \,\}$ is a **binary operation** defining the set of output (target) compartments produced by a given transition acting on source compartment V when compartment C is the catalyst. Here as well, we simply transform S into its stratified counterpart T, but we allow for variant operations in which the same S transitions to different targets depending on C.
- $\Omega_{2i}(S, i_s, i_c, s, c, t, r, i)$ is a variant binary operation providing additional transitions in the case that s and c are both components of the same compartment S. This allows for a within-compartment interaction that is distinct from an interaction between two individuals of the same compartment.
- Φ_r, Φ_{2r}, and Φ_{1r} are **rewritings** of transition rates. We construct a rewritten rate for each edge of the product model based on its original rate r, by replacing the source s by V, the catalyst c by C (if present), and adding subscripts to all parameters. Parameters are subscripted by the compartment names indicating the stratification of the source compartment, in the simple case. When a single transition is replicated to multiple output compartments, it's necessary to add subscripts indicating the output compartments; when it's replicated using multiple catalyst compartments, we need subscripts naming the catalyst, and when it's replicated multiple times using different inclusions of compartments we need subscripts distinguishing the inclusions as well. The software tries to be smart about applying as few subscripts as are necessary to provide unique parameters for each transition.
- The vertex set $V(M)$ is the set of compartments occurring as source or target vertices in the above set of edges, which may or may not be equal to the product set V_M.

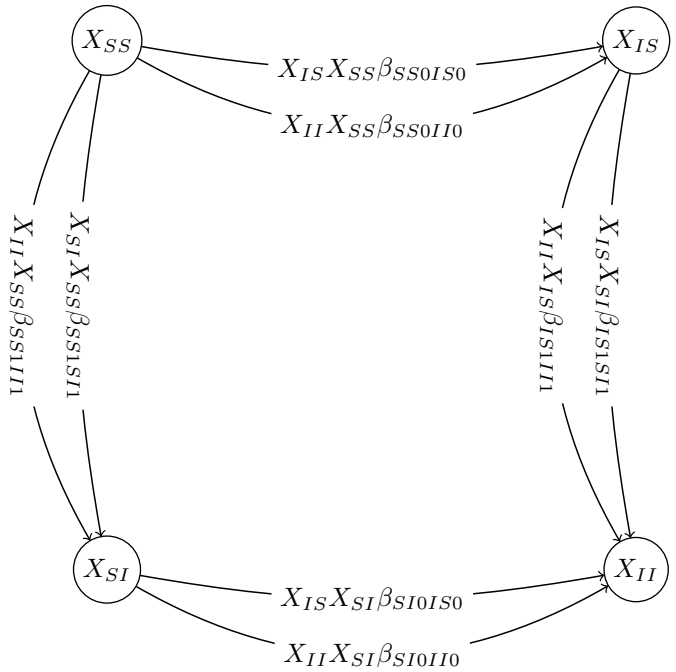
This is a fairly general framework for defining products, at least in a world of linear and bilinear reactions among compartments. If transitions arise whose rates are arbitrary functions of compartment sizes, we'll need to allow users to supply additional Ξ and Ω functions to generate product transitions and rewrite

their rates.

This product operation generates the correctly stratified SI model shown above. In this case it's not necessary to distinguish which inclusion function Σ it uses, because both produce the same result. In the next model it does make a difference.

Example: Infectious dynamics of couples (ordered pairs)

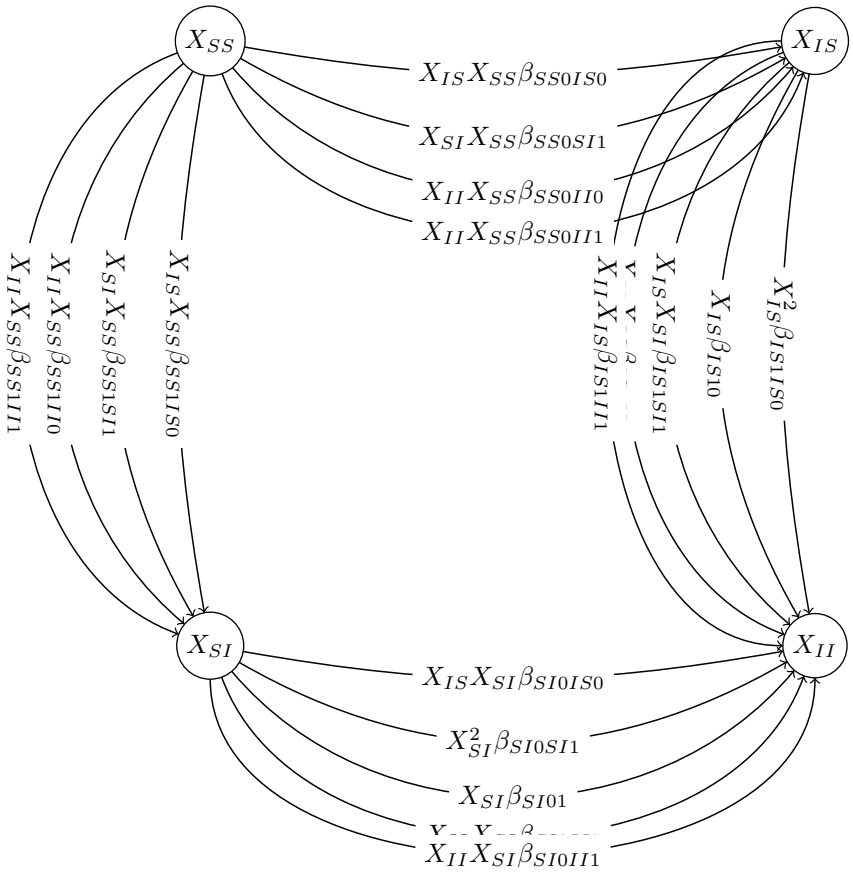
Consider a system of pairs of individuals, where either can be susceptible or infected at any time. The above definition with the simple inclusion function Σ_1 produces this model:



This models pairs of individuals taken from two completely separate, non-interacting populations. The second individual of a pair can't infect the first individual of any pair. We want a model that allows interactions across that division, where each S individual in either position of any paired compartment can be infected by any I individual in either position of any compartment: there are four such S types and four such I types, so there will be 16 of these infection transitions.

In all we will have 18 transitions, including within-compartment infection events in compartments SI and IS. Using the full inclusion function Σ_c, which generates

the full set of 18 interactions, we construct this model:



.

$$\begin{aligned}
\frac{dX_{SS}}{dt} &= -X_{II}X_{SS}\beta_{SS0II0} - X_{II}X_{SS}\beta_{SS0II1} - X_{IS}X_{SS}\beta_{SS0IS0} \\
&\quad - X_{SI}X_{SS}\beta_{SS0SI1} - X_{II}X_{SS}\beta_{SS1II0} - X_{II}X_{SS}\beta_{SS1II1} \\
&\quad - X_{IS}X_{SS}\beta_{SS1IS0} - X_{SI}X_{SS}\beta_{SS1SI1} \\
\frac{dX_{SI}}{dt} &= -X_{II}X_{SI}\beta_{SI0II0} - X_{II}X_{SI}\beta_{SI0II1} - X_{IS}X_{SI}\beta_{SI0IS0} \\
&\quad - X_{SI}^2\beta_{SI0SI1} + X_{II}X_{SS}\beta_{SS1II0} + X_{II}X_{SS}\beta_{SS1II1} \\
&\quad + X_{IS}X_{SS}\beta_{SS1IS0} + X_{SI}X_{SS}\beta_{SS1SI1} - X_{SI}\beta_{SI01}
\end{aligned}$$

$$\begin{aligned}\frac{dX_{IS}}{dt} &= -X_{II}X_{IS}\beta_{IS1II0} - X_{II}X_{IS}\beta_{IS1II1} - X_{IS}^2\beta_{IS1IS0} \\ &\quad - X_{IS}X_{SI}\beta_{IS1SI1} + X_{II}X_{SS}\beta_{SS0II0} + X_{II}X_{SS}\beta_{SS0II1} \\ &\quad + X_{IS}X_{SS}\beta_{SS0IS0} + X_{SI}X_{SS}\beta_{SS0SI1} - X_{IS}\beta_{IS10} \\ \frac{dX_{II}}{dt} &= X_{II}X_{IS}\beta_{IS1II0} + X_{II}X_{IS}\beta_{IS1II1} + X_{IS}^2\beta_{IS1IS0} \\ &\quad + X_{IS}X_{SI}\beta_{IS1SI1} + X_{II}X_{SI}\beta_{SI0II0} + X_{II}X_{SI}\beta_{SI0II1} \\ &\quad + X_{IS}X_{SI}\beta_{SI0IS0} + X_{SI}^2\beta_{SI0SI1} + X_{IS}\beta_{IS10} + X_{SI}\beta_{SI01}\end{aligned}$$

[Note: It's more common to consider pair models together with pair-formation and breakup events, with compartments for unpaired individuals. We can add this if needed.]

Example: Infectious dynamics of couples (unordered pairs)

In some cases we don't want to track the order of the individuals in a pair – we don't care about the difference between (S, I) and (I, S), and we just want to distinguish the number of people infected in each pair.

This unordered pair dynamics must be consistent with the above, ordered-pair model, because they are different descriptions of the same events. So we should be able to generate the unordered pair model from the ordered one, by combining compartments. We will define the unordered dynamics in that way, even though we may end up generating them in a more direct way for efficiency.

The formal construction of the unordered model, then, is

- construct the ordered pair model
- define unordered compartments by counting the number infected in each of the ordered compartments, that is, construct an **aggregation function** $A : V(M) \to V_{\text{new}}$ assigning the contents of each compartment to a new, aggregate compartment.
- write equations defining the size of each aggregate compartment as the sum of its preimages. In our example, these equations are $Z_0 = X_{SS}$; $Z_1 = X_{SI} + X_{IS}$; $Z_2 = X_{II}$.
- for each pair V, W of aggregate compartments, sum together all the transition rates from V to W in the ordered model, and use the sum equations to transform the sum into terms of the unordered compartment names.
- For graphical display, we separate the resulting sum into separate arrows, as it was before we summed them together.
- This step requires us to change the names of the parameters as well as the compartments, as some of them need to be assumed equal for this to work. Thus we have the following definition:

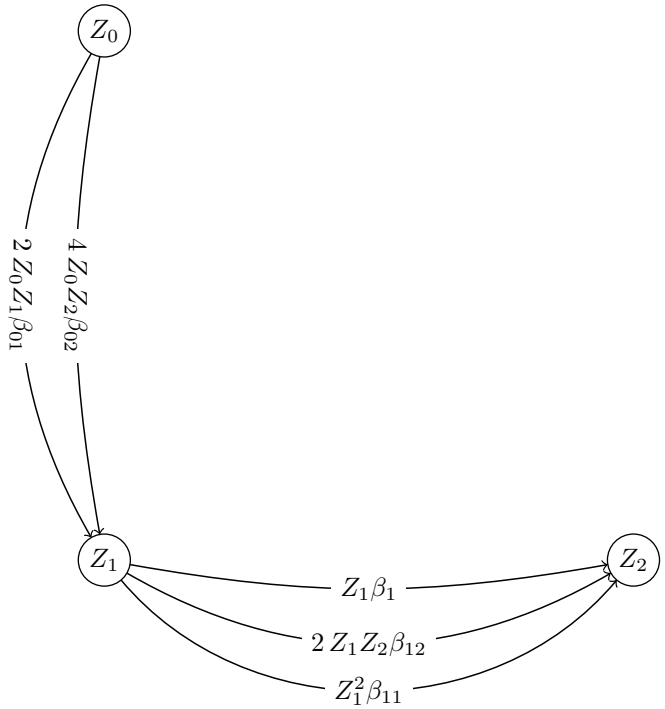
Definition. An **aggregation of compartments** of a compartment model is a model $A(M)$, given by a transformation of compartments $A(V)$ for V in $V(M)$ and a transformation of parameters $A(P)$ for the parameters P of M, in which

- The vertex set of $A(M)$ is the set $\{A(C) \mid C \in V(M)\}$ of aggregate compartments
- For each aggregate compartment C, there is an equality $C = \sum_{\{V|A(V)=C\}} A$, equating the aggregate compartment with the sum of its preimage compartments.
- The set of transitions of $A(M)$ is the set of edges $S \xrightarrow{\sum_{\{V \xrightarrow{r} W \in E(M) | A(V)=S, A(W)=T\}} A(r)} T$, where $A(r)$ is the transition rate expression r with all parameter names P replaced by $A(P)$, and with sums of unaggregated compartment names replaced by their equivalent aggregated compartment names.

This aggregation process doesn't work for general box models – the sum of transition rates doesn't necessarily reduce to terms of the aggregate quantities – so this can only be done in particular cases, and the parameters have to be relabeled just right so that the sums will come out right.

To construct our unordered-pair model, now, we define an aggregation function for compartments: $A(X_{pq}) = Z_c$, where c is the number of occurrences of I in the labels p and q. Along with this we use a congruent aggregation function for parameters, $A(\beta_{pqirsj}) = \beta_{cd}$, where c is the number of I in (p, q) and d is the number of I in (r, s). For the within-pair rate β_{pqi} we put β_c, using the count in (p, q).

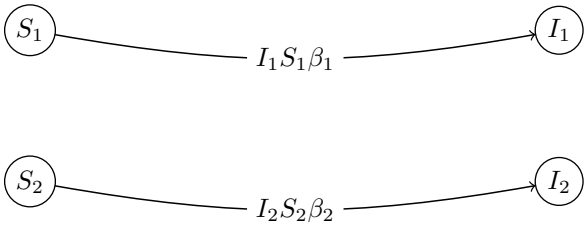
This aggregation produces the following model, with three states instead of four:



We can verify that this is equivalent to the original 18 transitions by noticing that Z_1 stands for two compartments of the unaggregated model. Thus each term involving a single Z_1 is two of the original transitions, and the Z_1^2 term is four of them. With that multiplication, the transitions can be seen to sum up to the original 18.

Combining infection models into a multi-infection model

Suppose there are two infectious agents, numbered 1 and 2. Each is involved in an SI process (and maybe other compartments downstream from I). Let us call these models M_1 and M_2:



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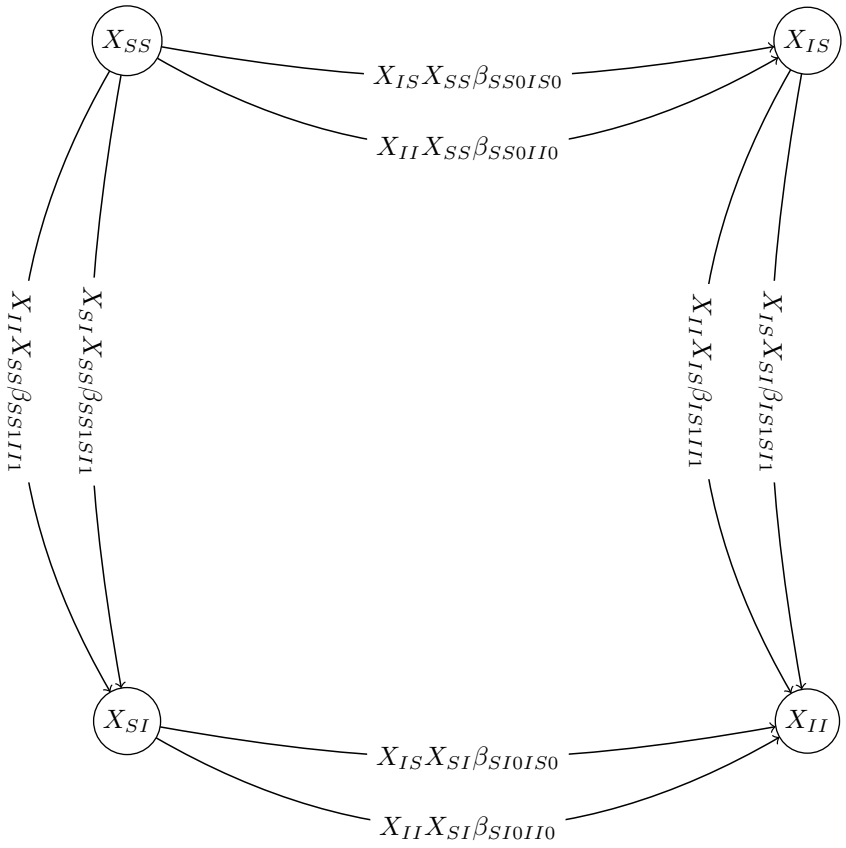
We wish to combine these infection processes into a single model M_{12}, in which a single susceptible population is infected by both agents, producing not only the I_1 and I_2 classes, but also one or more superinfected classes. Order of infection events might matter, in diseases in which an individual acquiring a second strain develops a weaker infection.

In this case, we need to use the simple inclusion function Σ_1, because there is no interaction between an individual infected with one strain and one susceptible to a different strain. With that, the cross product as defined gives us this product model:



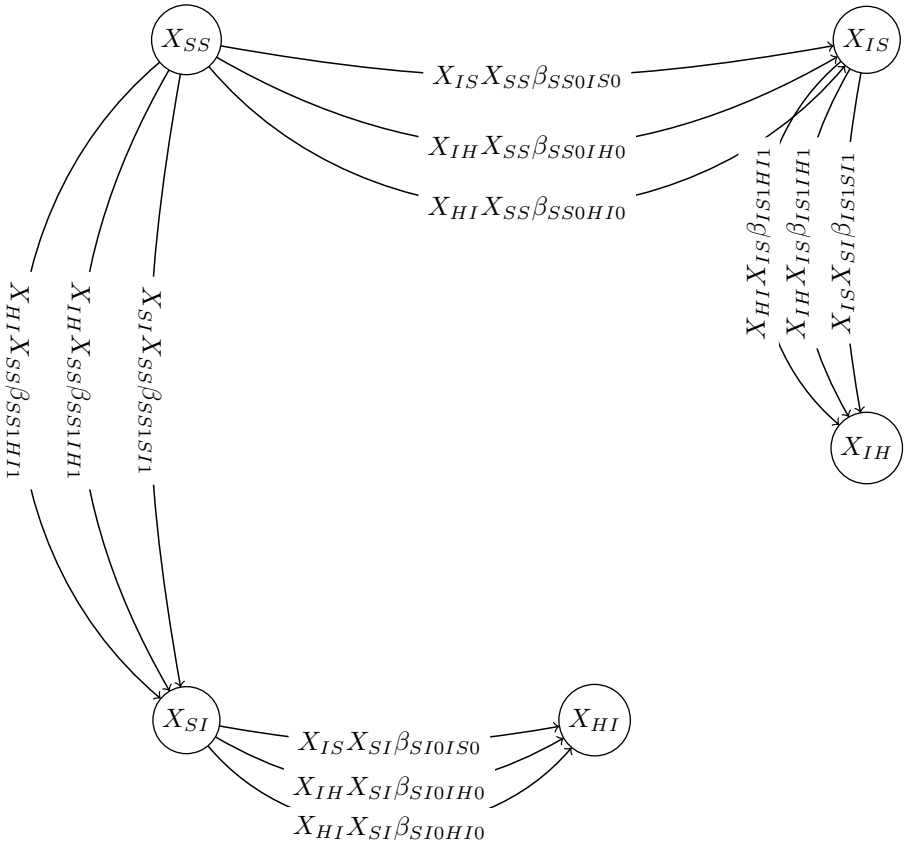
We need to modify this to account for order of infection, and to allow for the possibility that both strains can be transmitted in a single contact event.

[Note: we might want to explain why we didn't worry about double transmission events in the pair model]

To model partial superinfection, we need to introduce a "half-infected" class H, and provide a modified binary operation:

$$\Omega_H(S,i,C,i,S,I,I,r,i) = \begin{cases} \{\,(S_1,\ldots,S_{i_s-1},H,S_{i_s+1},\ldots,S_n)\,\} & \text{if } S \text{ includes } I \\ \{\,(S_1,\ldots,S_{i_s-1},I,S_{i_s+1},\ldots,S_n)\,\} & \text{if not} \end{cases}$$
$\Omega_H(S,i_s,C,i_c,s,c,t,r,i) = \{\}$ otherwise.

[TODO: the vertex set is generated by the Σ operation, not by the Cartesian product of vertex sets as claimed in the definition]



To account for simultaneous transmission of both strains, we need to construct a strong product rather than the cross product we have been studying. As described in the appendix, a strong product contains all the edges of the cross product, plus edges constructed from edges of multiple component graphs at once. In this model, the edges of the cross product are transitions where S changes to I in one or the other of the component models, i.e. where an individual acquires one of the disease strains. Transitions in which an individual acquires both strains in a single event are edges of the strong product.

The strong product of box models can be defined using most of the formal apparatus of the cross product, but with an edge generation function that

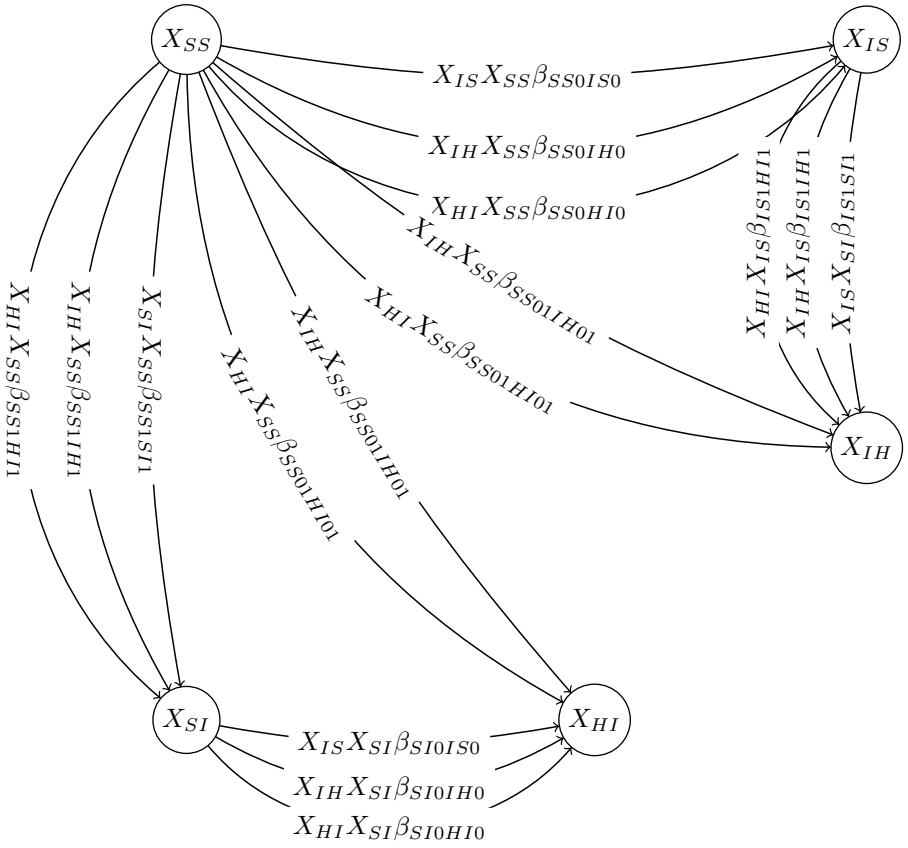
generates derived edges from each combination of models' edges, rather than from each edge individually.

Definition. A **strong product** $M_1 \boxtimes \cdots \boxtimes M_n$ of box models $M_1, \ldots, M_n$ is a box model M such that

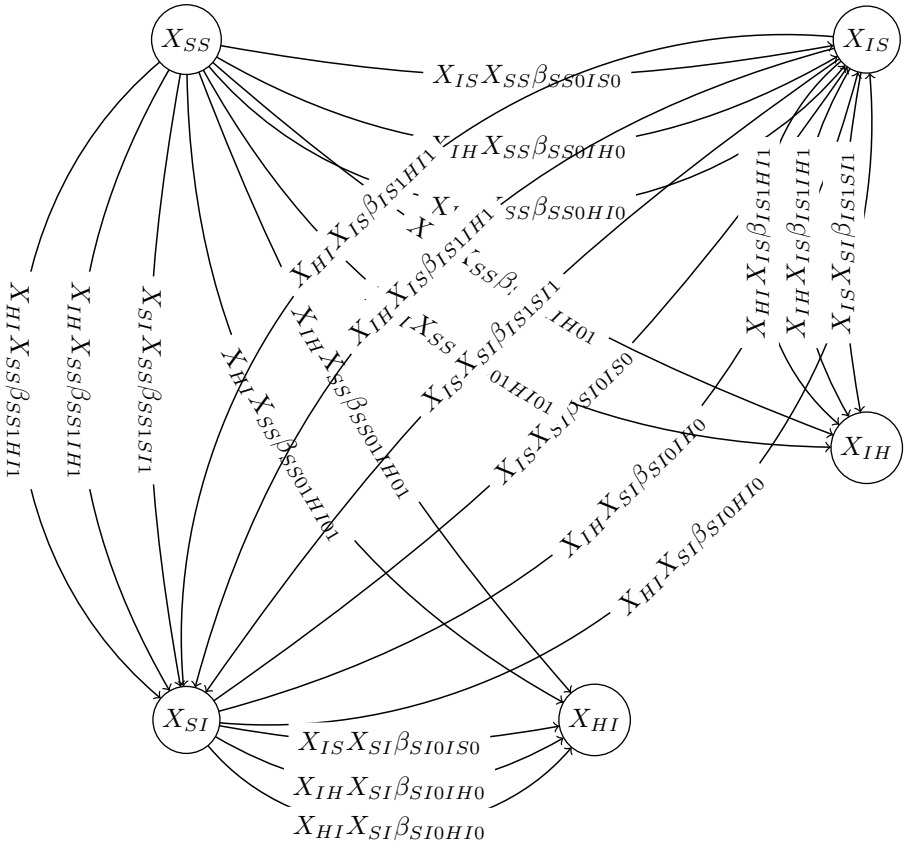
- $E(M) = \cup_{\sigma \subseteq \{1,\ldots,n\}} \cup_{\varepsilon \in \prod_{i \in \sigma} E(M_i)} \Xi_{\boxtimes}(\sigma, \varepsilon)$
- $\Xi_{\boxtimes}(\sigma, \varepsilon) = \begin{cases} \{\, S \xrightarrow{\tilde{\Phi}_r(r,S,\sigma,T)} T \mid S \in V_M, S \times \sigma \subseteq \Sigma_1(s, \{S\}), \\ \quad T \in \tilde{\Omega}_1(S, \sigma, \varepsilon) \,\} \\ \quad \text{if } e = s \xrightarrow{r} t \; \forall e \in \varepsilon \text{ and } r \text{ is linear in } s \\ \{\, S \xrightarrow{\tilde{\Phi}_{2r}(r,S,C,\sigma,C)} T \mid S \in V_M, \{S\} \times \sigma \subseteq \Sigma_1(s, \{S\}) \\ \quad C \in V_M, \{C\} \times \sigma \subseteq \Sigma_1(c, \{C\}), \\ \quad T \in \tilde{\Omega}_2(S, C, \sigma, \varepsilon) \,\} \\ \quad \text{if } e = s \xrightarrow{r} t \; \forall e \in \varepsilon \text{ and } r \text{ is bilinear in } s \text{ and } c. \end{cases}$
- $V_M = V(M_1) \times \cdots \times V(M_n)$.
- $\tilde{\Omega}_1$ and $\tilde{\Omega}_2$ generate the destination compartment for each transition given the transitions it's constructed from, and the source and catalyst compartments, and $\tilde{\Phi}_r$ and $\tilde{\Phi}_{2r}$ provide rewritten rate expressions.
- The vertex set $V(M)$ is the set of compartments occurring as source or target vertices in the above set of edges, which may or may not be equal to the product set V_M.

This definition is surely opaque but the upshot is that, in our example, for every way of locating one or more S labels in a compartment, and for every way of locating one or more I labels in a compartment, it uses the $\tilde{\Omega}_2$ function to generate a set of transitions resulting from the interactions of those pairs. [This is the strong product *without* cross interactions: there is also a strong product with cross interactions, but it's more complex and we don't need it for these applications.] In this model, we want the S and I labels to match up in the same positions (no cross interactions), so we provide an $\tilde{\Omega}_2$ function that yields outputs only in those cases.

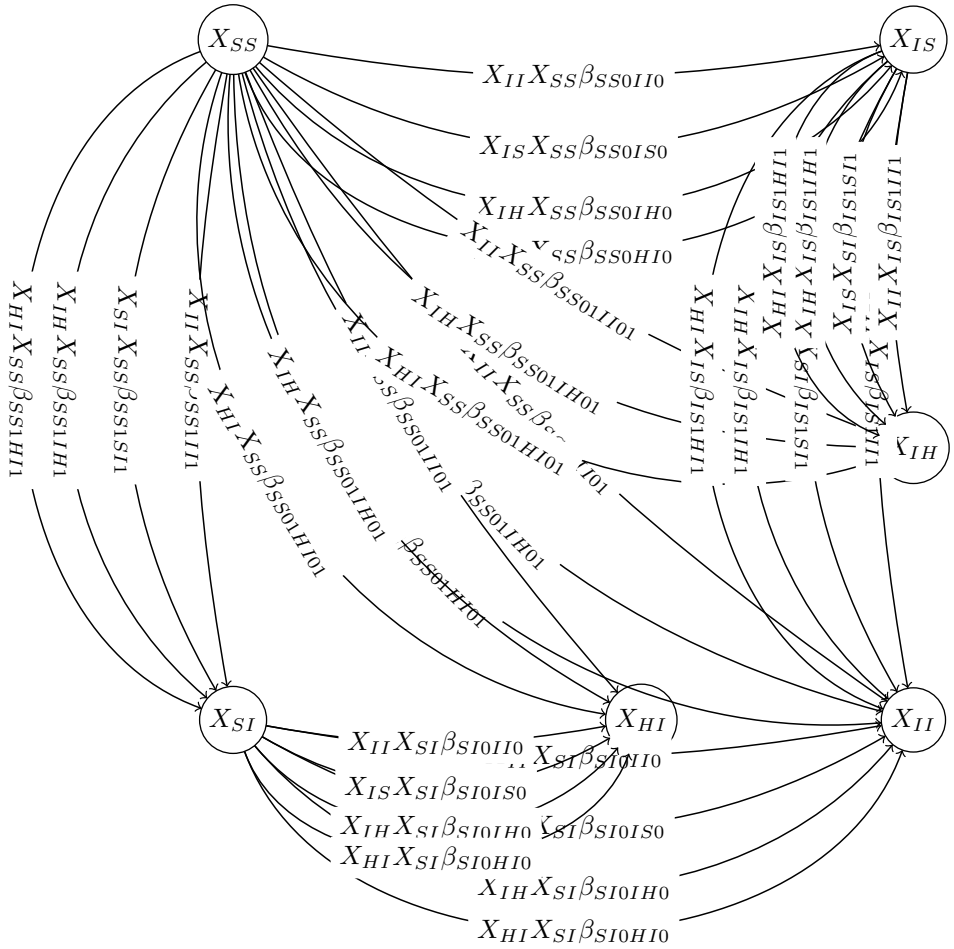
Using a strong product allows us to produce this model:



We can construct products based on different assumptions by writing slightly different $\tilde{\Omega}_2$ functions. Here is a variant in which an encounter with an infected individual can knock out one or more strains, as well as infecting the contact with new ones:



Here's a variant in which it's also possible to get infected with both strains equally, in addition to having one infection weaker than the other:



Forward equations for a box model

Given a box model, rather than ODE as defined above, we can generate Kolmogorov forward and backward equations for the model. Both are ODEs, but the forward equations are the ODE of a box model, so we define that system as a box model.

Given an integer number N of total individuals, the compartments, that is the state variables, for the forward equations are $p_{(i_1/N,\ldots,i_n/N)}$ for each $(i_1,\ldots,i_n) \in \{0,1,\ldots,N\}^n$, where n is the number of compartments. If total mass is conserved, as it often is in box models, we reduce the dimension by eliminating the last of the model's compartments, and assume that the sum of all compartments is 1.

For each compartment X let $\mathbf{e}_X$ be the vector $(0, \ldots, 0, 1, 0, \ldots, 0)$ with 1 in the place corresponding to compartment X.

The transitions are $p_S \xrightarrow{r(S)p_S} p_{S-\mathbf{e}_s/N+\mathbf{e}_t/N}$ for each transition with source, target, and rate s, t, r of the original box model, and for every state S, where $r(S)$ is the rate r evaluated at the state S.

The forward equations themselves are the ODE of this box model, as defined above.

For example, for a simple SI model with transition βSI, the forward equations for $N = 3$ are

$$\begin{aligned}
\frac{dp_{01}}{dt} &= \frac{2}{9}\,\beta p_{\frac{1}{3}\frac{2}{3}} \\
\frac{dp_{\frac{1}{3}\frac{2}{3}}}{dt} &= -\frac{2}{9}\,\beta p_{\frac{1}{3}\frac{2}{3}} + \frac{2}{9}\,\beta p_{\frac{2}{3}\frac{1}{3}} \\
\frac{dp_{\frac{2}{3}\frac{1}{3}}}{dt} &= -\frac{2}{9}\,\beta p_{\frac{2}{3}\frac{1}{3}} \\
\frac{dp_{10}}{dt} &= 0
\end{aligned}$$

To do: forward equations of large power of infection model

In this section, we will document the Sage code (yet to be written) that implements large powers of a single model efficiently (as in the $SI \times SI$ pair model presented above), binds its transition rate parameters to something sane, and constructs its forward equations in a way that collapses to something usable.

With an ordered-$n$tuple model, where there are N_i instances of I appearing in all the compartments, there are N_i infection transitions from each S entry in every composite compartment of the model to its infected counterpart compartment.

In the nth power of a k-state model, N_i is $1/k$ of the total number of entries in compartments, which is k^n/k or k^{n-1}. There are the same number of S entries. So in all, $k^{2(n-1)}$ infection transitions!!

Plus within-group events - in a compartment with c Ss and d Is, there are cd of these transitions, to the c different post-infection compartments.

Maybe I can generate these directly? I'm sure, if we let $\pi_i(C)$ be the ith entry of the tuple C (the ith projection function).

- $E(M^n) = \cup_{i=1,\ldots,k} \cup_{j=1,\ldots,k} \Big[\{ V \xrightarrow{\beta V^2} I_i(V) \mid V \in V(M)^n, \pi_i(V) = S, \pi_j(V) = S \}$
  $\cup \{ V \xrightarrow{\beta V W} I_i(V) \mid V \in V(M)^n, \pi_i(V) = S, W \in V(M)^n, \pi_j(W) = I \} \Big]$

where $I_i(V)$ is the compartment equal to V with the ith entry changed to I.

So in SI^n, the compartments are $\{S, I\}^n$. The transitions from a compartment V that has c Ss (and $n - c$ Is) are:

- $c(n - c)$ within-compartment transmissions
- $c2^{n-1}$ between-compartment transmissions

Let $i(V)$ be the number of I entries in V.

Every compartment is subject to the same force of infection, which is one piece for every I entry in every compartment:

$F_I = \sum_W i(W)W$.

We can aggregate transmission due to interaction between V and W: the rate is $(n - i(V))i(W)\beta VW$. Let's aggregate all β parameters into a single value β for this, without subscripts.

The combined transitions are

- $V \xrightarrow{\beta V F_I + i(V)\beta V} I_j(V)$ for each V, j, $\pi_j(V) = S$.

When we aggregate compartments into $Z_i = \cup_{i(V)=i} V$, the transitions become

- $Z_i \xrightarrow{r} Z_{i-1}$
- $r = \sum_{i(V)=i}(n - i)(\beta V F_I + i\beta V)$
- $F_I = \sum_j jZ_j$
- $r = (n - i)\beta Z_i F_I + i(n - i)\beta Z_i$
- $Z_i \xrightarrow{(n-i)\beta Z_i(i+\sum_j jZ_j)} Z_{i-1}$.

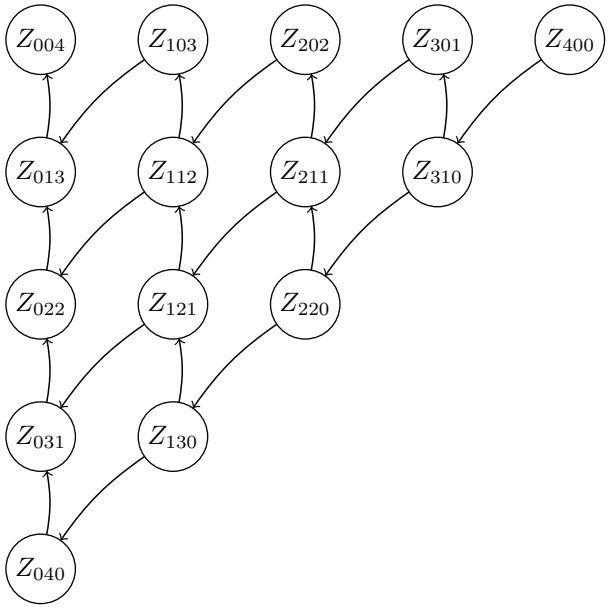
So I think there isn't much percentage in generating the ordered-$n$tuple powers for high n (too many compartments), but we can definitely produce these aggregated models efficiently. We don't have to back our parameter set all the way off to just β, we can use β_i and β_{ij} for the terms of that transition rate.

The above is the rule for any binary transition $V + C \mapsto W$, I guess. For a unary transition $V \xrightarrow{\alpha V} W$, I suppose it's just

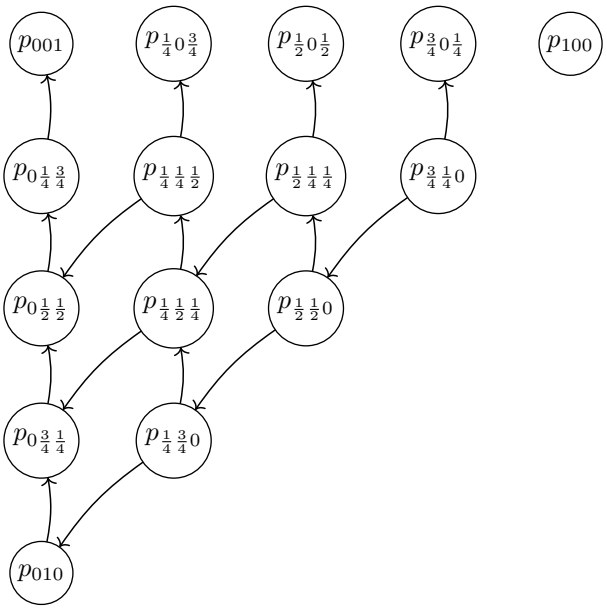
- $Z_i \xrightarrow{\alpha i Z_i} Z_{i-1}$ for a certain value of i.

In a general k-state model, rather than just one counting subscript we have $Z_{\mathbf{c}}$ where $\mathbf{c} = (c_1, \ldots, c_k)$ is the count of each of the k compartments in a tuple of compartments. Since $\sum c_i = n$, one could be omitted, but it's probably simpler to keep them all, at least for formal definitions.

So for an nth power of an SIR model:



That's interesting - this is very similar to the box model representation of the SIR model's master (forward) equations:



The transition rates are different though. In the forward equations, one box doesn't contribute force of infection to the other boxes (this is why the power model has transitions that the forward equations don't have). The forward equations are similar but not isomorphic to the power model's equations restricted to only within-group interactions.

Here are the forward equations:

$$\frac{dp_{001}}{dt} = \frac{1}{4}\,\gamma p_{0\frac{1}{4}\frac{3}{4}}$$

$$\frac{dp_{0\frac{1}{4}\frac{3}{4}}}{dt} = \frac{1}{2}\,\gamma p_{0\frac{1}{2}\frac{1}{2}} - \frac{1}{4}\,\gamma p_{0\frac{1}{4}\frac{3}{4}}$$

$$\frac{dp_{0\frac{1}{2}\frac{1}{2}}}{dt} = -\frac{1}{2}\,\gamma p_{0\frac{1}{2}\frac{1}{2}} + \frac{3}{4}\,\gamma p_{0\frac{3}{4}\frac{1}{4}} + \frac{1}{16}\,\beta p_{\frac{1}{4}\frac{1}{4}\frac{1}{2}}$$

$$\frac{dp_{0\frac{3}{4}\frac{1}{4}}}{dt} = \gamma p_{010} - \frac{3}{4}\,\gamma p_{0\frac{3}{4}\frac{1}{4}} + \frac{1}{8}\,\beta p_{\frac{1}{4}\frac{1}{2}\frac{1}{4}}$$

$$\frac{dp_{010}}{dt} = -\gamma p_{010} + \frac{3}{16}\,\beta p_{\frac{1}{4}\frac{3}{4}0}$$

$$\frac{dp_{\frac{1}{4}0\frac{3}{4}}}{dt} = \frac{1}{4}\,\gamma p_{\frac{1}{4}\frac{1}{4}\frac{1}{2}}$$

$$\frac{dp_{\frac{1}{4}\frac{1}{4}\frac{1}{2}}}{dt} = \frac{1}{2}\,\gamma p_{\frac{1}{4}\frac{1}{2}\frac{1}{4}} - \frac{1}{16}\,\beta p_{\frac{1}{4}\frac{1}{4}\frac{1}{2}} - \frac{1}{4}\,\gamma p_{\frac{1}{4}\frac{1}{4}\frac{1}{2}}$$

$$\frac{dp_{\frac{1}{4}\frac{1}{2}\frac{1}{4}}}{dt} = \frac{1}{8}\,\beta p_{\frac{1}{2}\frac{1}{4}\frac{1}{4}} - \frac{1}{8}\,\beta p_{\frac{1}{4}\frac{1}{2}\frac{1}{4}} - \frac{1}{2}\,\gamma p_{\frac{1}{4}\frac{1}{2}\frac{1}{4}} + \frac{3}{4}\,\gamma p_{\frac{1}{4}\frac{3}{4}0}$$

$$\frac{dp_{\frac{1}{4}\frac{3}{4}0}}{dt} = \frac{1}{4}\,\beta p_{\frac{1}{2}\frac{1}{2}0} - \frac{3}{16}\,\beta p_{\frac{1}{4}\frac{3}{4}0} - \frac{3}{4}\,\gamma p_{\frac{1}{4}\frac{3}{4}0}$$

$$\frac{dp_{\frac{1}{2}0\frac{1}{2}}}{dt} = \frac{1}{4}\,\gamma p_{\frac{1}{2}\frac{1}{4}\frac{1}{4}}$$

$$\frac{dp_{\frac{1}{2}\frac{1}{4}\frac{1}{4}}}{dt} = \frac{1}{2}\,\gamma p_{\frac{1}{2}\frac{1}{2}0} - \frac{1}{8}\,\beta p_{\frac{1}{2}\frac{1}{4}\frac{1}{4}} - \frac{1}{4}\,\gamma p_{\frac{1}{2}\frac{1}{4}\frac{1}{4}}$$

$$\frac{dp_{\frac{1}{2}\frac{1}{2}0}}{dt} = -\frac{1}{4}\,\beta p_{\frac{1}{2}\frac{1}{2}0} - \frac{1}{2}\,\gamma p_{\frac{1}{2}\frac{1}{2}0} + \frac{3}{16}\,\beta p_{\frac{3}{4}\frac{1}{4}0}$$

$$\frac{dp_{\frac{3}{4}0\frac{1}{4}}}{dt} = \frac{1}{4}\,\gamma p_{\frac{3}{4}\frac{1}{4}0}$$

$$\frac{dp_{\frac{3}{4}\frac{1}{4}0}}{dt} = -\frac{3}{16}\,\beta p_{\frac{3}{4}\frac{1}{4}0} - \frac{1}{4}\,\gamma p_{\frac{3}{4}\frac{1}{4}0}$$

$$\frac{dp_{100}}{dt} = 0$$

And here are the within-group interactions of the power model:

$$\frac{dZ_{004}}{dt} = Z_{013}\gamma_{013}$$

$$\frac{dZ_{013}}{dt} = -Z_{013}\gamma_{013} + 2\,Z_{022}\gamma_{022}$$

$$\frac{dZ_{022}}{dt} = Z_{112}^2\beta_{112} - 2\,Z_{022}\gamma_{022} + 3\,Z_{031}\gamma_{031}$$

$$\frac{dZ_{031}}{dt} = 2\,Z_{121}^2\beta_{121} - 3\,Z_{031}\gamma_{031} + 4\,Z_{040}\gamma_{040}$$

$$\frac{dZ_{040}}{dt} = 3\,Z_{130}^2\beta_{130} - 4\,Z_{040}\gamma_{040}$$

$$\frac{dZ_{103}}{dt} = Z_{112}\gamma_{112}$$

$$\frac{dZ_{112}}{dt} = -Z_{112}^2\beta_{112} - Z_{112}\gamma_{112} + 2\,Z_{121}\gamma_{121}$$

$$\frac{dZ_{121}}{dt} = -2\,Z_{121}^2\beta_{121} + 2\,Z_{211}^2\beta_{211} - 2\,Z_{121}\gamma_{121} + 3\,Z_{130}\gamma_{130}$$

$$\frac{dZ_{130}}{dt} = -3\,Z_{130}^2\beta_{130} + 4\,Z_{220}^2\beta_{220} - 3\,Z_{130}\gamma_{130}$$

$$\frac{dZ_{202}}{dt} = Z_{211}\gamma_{211}$$

$$\frac{dZ_{211}}{dt} = -2\,Z_{211}^2\beta_{211} - Z_{211}\gamma_{211} + 2\,Z_{220}\gamma_{220}$$

$$\frac{dZ_{220}}{dt} = -4\,Z_{220}^2\beta_{220} + 3\,Z_{310}^2\beta_{310} - 2\,Z_{220}\gamma_{220}$$

$$\frac{dZ_{301}}{dt} = Z_{310}\gamma_{310}$$

$$\frac{dZ_{310}}{dt} = -3\,Z_{310}^2\beta_{310} - Z_{310}\gamma_{310}$$

$$\frac{dZ_{400}}{dt} = 0$$

Appendix: graph products

There are several standard product operations on directed graphs. All are ways of assigning arrows to the same set of vertices, which is the Cartesian product (cross product) of the component graphs' vertex sets. We use several of them in our definitions of products of box models.

The **Cartesian product of sets** S_1, S_2, ..., S_n is the set $S_1 \times S_2 \times \ldots \times S_n = \{\, (s_1, s_2, \ldots, s_n) \mid s_1 \in S_1, s_2 \in S_2, \ldots, s_n \in S_n \,\}$. The elements of $S_1 \times S_2 \times \ldots \times S_n$ are referred to as **tuples** of elements of the component sets S_1, S_2, ..., S_n.

We define a **directed graph** (and we are not concerned with undirected graphs) as a set $\{\, (v, w, e) \,\} \subseteq V \times V \times E$, where V is the **vertex set** of the graph and E is its set of edge labels. Each of these tuples is visualized as an arrow from v to w with label e. For easy reading, we sometimes represent these arrows as $\{\, v \xrightarrow{e} w \,\}$. [In our definition of box models, the edge labels e are transition rates.] Note that this definition allows multiple edges between the same vertices v, w, so we are properly discussing directed multigraphs.

The cross product of graphs

The **cross product** $G_1 \Box G_2 \Box \cdots \Box G_n$ **of directed graphs** G_1, G_2, ..., G_n is a graph whose vertex set is the Cartesian product $V_1 \times V_2 \times \ldots \times V_n$ of the vertex sets V_i of each graph G_i, and whose edges are of the form $(v_1, v_2, \ldots, v_i, \ldots, v_n) \xrightarrow{e} (v_1, v_2, \ldots, w_i, \ldots, v_n)$, where the two tuples are identical in all but the i'th position, and where there is an edge connecting v_i to w_i in G_i.

Most definitions of this product do not provide labels for the edges of the product graph. In the body of this paper we construct these labels (transition rates) in a variety of ways.

The square symbol is chosen to suggest the shape of the cross product graph.

The tensor product

The **tensor product** of directed graphs G_1, ..., G_n is a graph $G_1 \times \cdots \times G_n$ whose vertex set is the Cartesian product of the graphs' vertex sets, and which has an edge from $(v_1, v_2, \ldots, v_n)$ to $(w_1, w_1, \ldots, w_n)$ if and only if there is an edge from v_i to w_i in *every* graph G_i.

The tensor product is the natural product in the category of graphs (with graph homomorphisms as the category's morphisms), because the tensor product of graphs is the graph that has a homomorphism to each of the component graphs, and such that any other graph that has a homomorphism to each component also has a homomorphism to the tensor product graph that commutes.

In some sense, it might make sense to think of this product as embodying an "and" or "all" operation, where the Cartesian product embodies an "exactly one of" operation.

The strong product

The **strong product** $G_1 \boxtimes G_2$ of two graphs G_1, G_2 is the union of the Cartesian product and tensor product of the graphs. That is, it contains all the edges of those two product graphs.

If we extend that definition verbatim to n graphs, we get an "all or exactly one" product. In modeling infectious dynamics we are probably more interested in a "one or more" product. Therefore I prefer the following definition:

The **strong product** of graphs G_1, ..., G_n, written $G_1 \boxtimes G_2 \boxtimes \cdots \boxtimes G_n$, is the graph whose vertex set is the Cartesian product of the graphs' vertex sets, and which has an edge from $(v_1, \ldots, v_n)$ to $(w_1, \ldots, w_n)$ if and only if, for every i, either there is an edge from v_i to w_i, or $v_i = w_i$.

This graph is a subgraph of the transitive closure of the Cartesian product graph, but it is not the transitive closure, because it's limited to transitive combinations of at most one edge from each component graph.