# Definitions of Box Model objects

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. Any variable involved in a transition rate that is not the name of a compartment is a **parameter** of the model. Let $C_M = \{c_1, \ldots, c_n\}$ be the set of 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 $r(c_1, \ldots, c_n, p_1, \ldots, p_m) \in \mathbb{R}$.

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:

$\frac{dX}{dt} = \sum_{\text{edges } e \text{ entering } X} \text{rate}(e) - \sum_{\text{edges } e \text{ leaving } X} \text{rate}(e)$ 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.
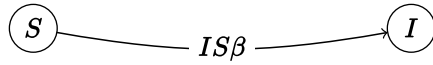
This box model has two compartments, S and I. There is one transition from S to I, with rate βSI. Its ODE is

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

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

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. The transitions include the edges of the Cartesian product of the components' graphs, but the product may include more transitions 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. The product may include other transitions derived from T as well.

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.

Before providing examples, here are some useful definitions:

- A **stratification** $S(X)$ of a variable X in a product of models $M_1 \times \cdots \times M_n$, where X is a compartment of model M_i, is a compartment $(c_1, \ldots, c_{i-1}, X, c_{i+1}, \ldots, c_n)$, where each c_j is a compartment of M_j.

- A stratification $S(P)$ of a parameter P of model M_i, where S is defined as above, is the ordered pair $(P, (c_1, \ldots, c_{i-1}, c_{i+1}, \ldots, c_n))$. The name given to that stratified parameter may be $P_{c_1 \ldots c_{i-1} c_{i+1} \ldots c_n}$, or some other naming may be used. As we will see, parameters may be stratified multiple times, which corresponds to adding more subscripts.

Example: Simple Cartesian Product

In many cases each model provides strata for the other(s), in some sense. Sometime it's sufficient to construct a product model with one transition for each edge of the graph Cartesian product. Assume each component transition rate involves no compartments other than its source compartment. The compartments are labeled using subscripts, and transitions are copied to each stratum, by substituting the subscripted name of the source compartment and subscripting all parameters. For example, given a model with transition from X to Y at rate λX, stratified by crossing with a model of two states a and b, we would construct a model
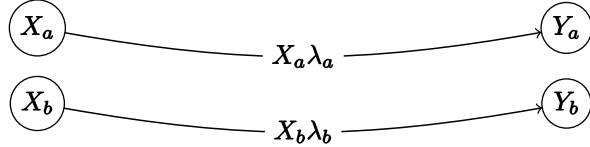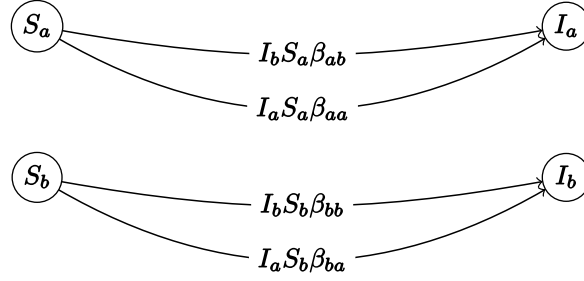

In the simple Cartesian product of models, we construct transitions by the following rule:

- for each component model B_i
    - for each transition of B_i, from s to t with rate r
        * for each stratification $S(s)$ of s
            · include a transition from $S(s)$ to $S(t)$, whose transition rate is constructed from r by replacing s by $S(s)$ and replacing all parameters P by $S(P)$.

Example: Stratifying multiple interacting compartments

The above stratification 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:

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

To get this right, we may need to construct transitions as follows:

- for each component model B_i
    - for each transition of B_i, from s to t with rate r
        * for every tuple of stratifications $(S(s), S_1(X_1), \dots, S_k(X_k))$, where $X_1, \dots, X_k$ are all the compartments other than s whose names appear in r
            · include a transition from $S(s)$ to $S(t)$ whose rate is constructed from r by replacing s by $S(s)$, each X_j by $S_j(X_j)$, and each parameter P by $S_n(\cdots S_1(S(P)) \cdots)$.

That would suffice for the above example. Still, transitions whose rates are arbitrary functions of compartment sizes will probably not be handled adequately by this rule, and we'll need to allow users to supply their own rules for creation of transitions in the product model.

Can I redefine this and the previous case using a binary relation of the form source + catalyst → (destination, rate)?

I think so: it will require a concept of **inclusion** of a compartment in another. The compartments of a compartment model are a partition of the population, and a product model's compartments are set-theoretical intersections of the component model's compartments. For example, compartment S_b in the above example is the intersection of the sets S and b. Thus S_b is a subset of S and of b. For precision, we'll say there is an **inclusion** of V in v when V is a subset of v. But note there may be multiple such inclusions, for example when V is (v, v). The "for every" clauses in the definition below must be applied once to each such inclusion, not once to each supercompartment v. We make the possible different inclusions ι explicit by writing $V \xrightarrow{\iota} v$.

Given that, here is a definition of the cross product:

The vertex set of the cross product of box models is the Cartesian product of their vertex sets. Its edges are defined by the following relation:

- For every edge (v, w, r) of each component model
    - if the rate is a constant multiple of the source v
        * for every inclusion of every compartment V in v
            · produce a transition from V to the corresponding W with stratified rate
    - if the rate r is a product of the source v and a second compartment c, which we will call a **catalyst**
        * for every inclusion of every compartment V in v, for every inclusion of every compartment C in c
            · produce a transition from V to corresponding W with appropriately stratified rate

or $M = M_1 \times \cdots \times M_n$ if

$$E(M) = \cup_{M_i} \cup_{(v,w,r) \in E(M_i)} \text{strat}(v, w, r)$$

where

$$\text{strat}(v, w, r) = \begin{cases} \{(V, \text{dest}(w, V), \text{rel}(r, \iota)) \mid v \xrightarrow{\iota} V\} & \text{comp}(r) = \{v\} \\ \{(V, \text{dest}(w, V), \text{rel}(r, \iota, \iota')) \mid v \xrightarrow{\iota} V, c \xrightarrow{\iota'} C\} & \text{comp}(r) = \{v, c\} \end{cases}$$

Example: Infectious dynamics of couples (ordered pairs)

Also, that multiple stratification isn't right for a model of pairs (or larger groupings) of people. Here is what we get if we use that definition as is:

$$X_{SS} \qquad X_{II}X_{SS}\beta_{SI} \qquad X_{IS}X_{SS}\beta_{SS} \qquad X_{IS}$$
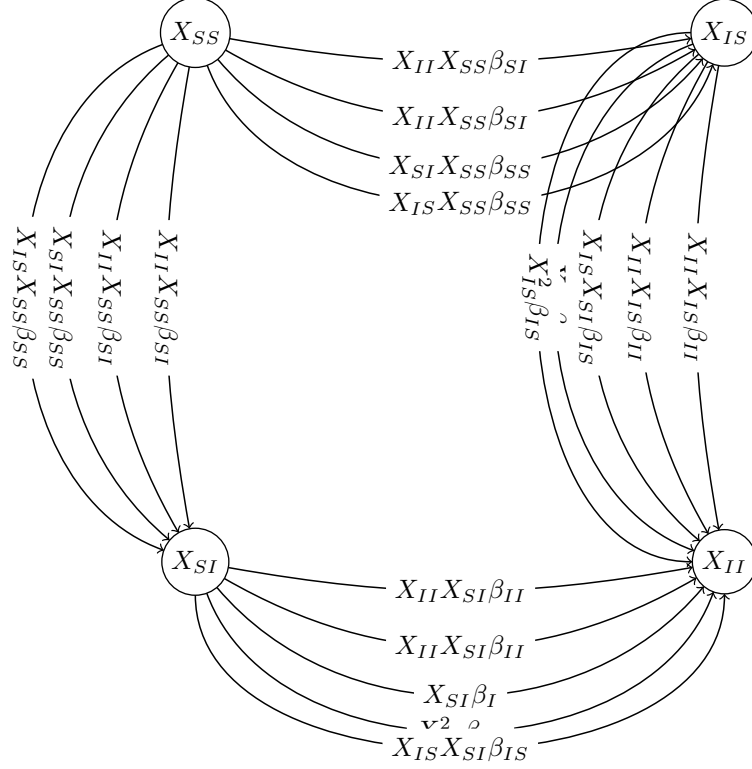
$$X_{SI}X_{SS}\beta_{SS} \qquad X_{II}X_{SS}\beta_{SI} \qquad X_{IS}X_{SI}\beta_{IS} \qquad X_{II}X_{IS}\beta_{II}$$

$$X_{SI} \qquad X_{II}X_{SI}\beta_{II} \qquad X_{IS}X_{SI}\beta_{IS} \qquad X_{II}$$
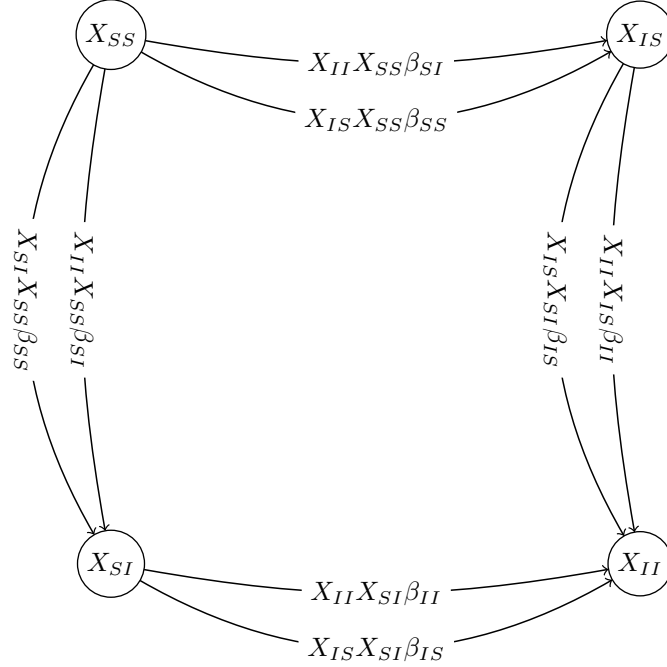
This models pairs of individuals taken from two completely separate, non-interacting populations. The second individual of a pair can't infect the first individual of any pair. We want a model that allows interactions across that division, where each S individual in either position of any paired compartment 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 we need to generate 16 infection transitions.

Actually we need to generate two more in addition to those, for within-pair infection events in compartments SI and IS. In total, we'll generate this model:

The nodes are X_{SS}, X_{IS}, X_{SI}, X_{II}.

Edges from X_{SS} to X_{IS} (top):
- $X_{II}X_{SS}\beta_{SI}$
- $X_{II}X_{SS}\beta_{SI}$
- $X_{SI}X_{SS}\beta_{SS}$
- $X_{IS}X_{SS}\beta_{SS}$

Edges from X_{SS} to X_{SI} (left):
- $X_{IS}X_{SS}\beta_{SS}$
- $X_{SI}X_{SS}\beta_{SS}$
- $X_{II}X_{SS}\beta_{SI}$
- $X_{II}X_{SS}\beta_{SI}$

Edges to X_{II} from X_{IS} (right):
- $X_{IS}^2\beta_{IS}$
- $X_{IS}X_{SI}\beta_{IS}$
- $X_{II}X_{IS}\beta_{II}$
- $X_{II}X_{IS}\beta_{II}$

Edges from X_{SI} to X_{II} (bottom):
- $X_{II}X_{SI}\beta_{II}$
- $X_{II}X_{SI}\beta_{II}$
- $X_{SI}\beta_{I}$
- $X_{IS}X_{SI}\beta_{IS}$

.

$$\frac{dX_{SS}}{dt} = -4\,X_{II}X_{SS}\beta_{SI} - 2\,X_{IS}X_{SS}\beta_{SS} - 2\,X_{SI}X_{SS}\beta_{SS}$$

$$\frac{dX_{SI}}{dt} = -2\,X_{II}X_{SI}\beta_{II} - X_{IS}X_{SI}\beta_{IS} - X_{SI}^2\beta_{IS}$$
$$+ 2\,X_{II}X_{SS}\beta_{SI} + X_{IS}X_{SS}\beta_{SS} + X_{SI}X_{SS}\beta_{SS} - X_{SI}\beta_{I}$$

$$\frac{dX_{IS}}{dt} = -2\,X_{II}X_{IS}\beta_{II} - X_{IS}^2\beta_{IS} - X_{IS}X_{SI}\beta_{IS}$$
$$+ 2\,X_{II}X_{SS}\beta_{SI} + X_{IS}X_{SS}\beta_{SS} + X_{SI}X_{SS}\beta_{SS} - X_{IS}\beta_{I}$$

$$\frac{dX_{II}}{dt} = 2\,X_{II}X_{IS}\beta_{II} + 2\,X_{II}X_{SI}\beta_{II} + X_{IS}^2\beta_{IS}$$
$$+ 2\,X_{IS}X_{SI}\beta_{IS} + X_{SI}^2\beta_{IS} + X_{IS}\beta_{I} + X_{SI}\beta_{I}$$

[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.]

We can do the above product in three steps:

- Stratify the SI model doubly, by position in the pair (first or second), and by partner's infectious class. This gives us stratified compartments of the form $(S, 1, I)$ (susceptible first partner, with an infectious counterpart), $(I, 2, S)$ (infectious second partner, with a susceptible counterpart), etc. There are 8 of these compartments – four S compartments and four I compartments – and 16 transitions, one for each possible contact from an I compartment to an S compartment.

- Merge equivalent classes, relabeling $(S, 1, I)$ and $(I, 2, S)$ as (S, I), etc. This reduces the 8 compartments to 4, giving us the square we want, with 16 transitions.

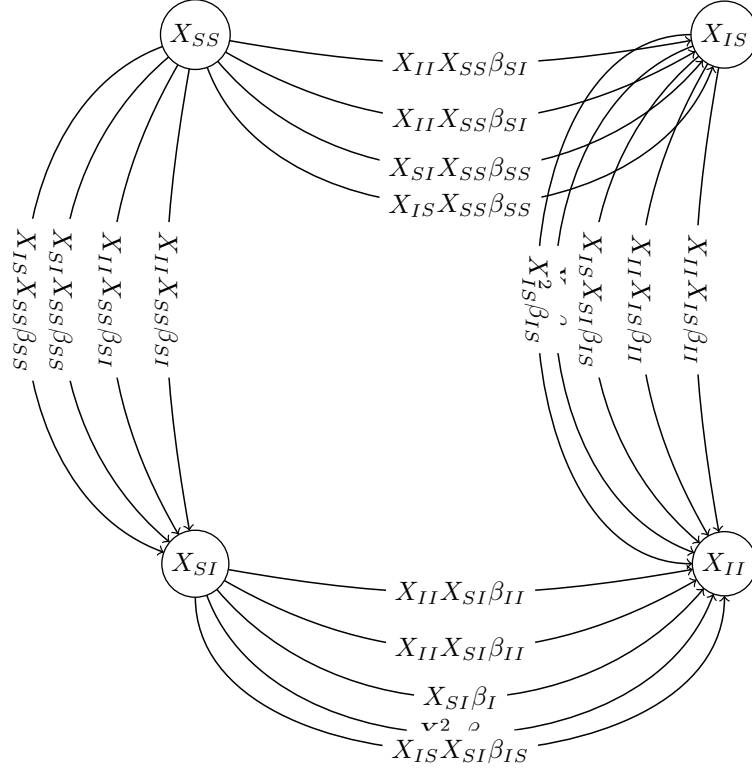- Add the two within-pair infection events, from (S, I) and (I, S) to (I, I).

The first of these is the Cartesian product operation with multiple stratification that we defined above. The others are other operations that are probably also worth defining formally:

Relabeling compartments

A **relabeling** of compartment model M by a state-relabeling function $R : C_M \to C_R$ which maps compartments into a set of relabeled compartments C_R, and a similarly defined parameter-relabeling function $R : P_M \to P_R$, is a compartment model $R(M)$ in which

- the compartments of $R(M)$ are the set $\{R(C) | C \in C_M\}$
- the transitions of $R(M)$ are $(R(s), R(t), R(r))$ for every transition (s, t, r) of M, where $R(r)(c'_1, \ldots, c'_{n'}, p'_1, \ldots, p'_{m'}) = r(R(c_1), \ldots, R(c_n), R(p_1), \ldots, R(p_m))$, given $C_R = \{c'_1, \ldots, c'_{n'}\}$, and $P_R = \{p'_1, \ldots, p'_{m'}\}$.

Here is the above square, relabeled so that order within each pair isn't distinguished. [TO DO: no it isn't]

Nodes and transition rates:

X_{SS} X_{IS} X_{SI} X_{II}

From X_{SS} to X_{IS}:
- $X_{II}X_{SS}\beta_{SI}$
- $X_{II}X_{SS}\beta_{SI}$
- $X_{SI}X_{SS}\beta_{SS}$
- $X_{IS}X_{SS}\beta_{SS}$

From X_{SS} to X_{SI} (left):
- $X_{IS}X_{SS}\beta_{SS}$
- $X_{SI}X_{SS}\beta_{SS}$
- $X_{II}X_{SS}\beta_{SI}$
- $X_{II}X_{SS}\beta_{SI}$

From X_{IS} to X_{II} (right):
- $X_{IS}^2\beta_{IS}$
- $X_{IS}X_{SI}\beta_{IS}$
- $X_{II}X_{IS}\beta_{II}$
- $X_{II}X_{IS}\beta_{II}$

From X_{SI} to X_{II} (bottom):
- $X_{II}X_{SI}\beta_{II}$
- $X_{II}X_{SI}\beta_{II}$
- $X_{SI}\beta_{I}$
- $X_{IS}^2\beta$
- $X_{IS}X_{SI}\beta_{IS}$

Constructing within-pair events and adding to a box model

These two operations also need to be formalized. Once that's done we'll be able to say

$$M^2 = R(M \times M_{12} \times M_{SI}) + \text{within-pair transitions}(R(M \times M_{12} \times M_{SI}))$$

with suitably defined objects M_{12}, M_{SI}, R.

Example: Infectious dynamics of couples (unordered pairs)

If we want to consider pairs without distinguishing the two individuals by gender or otherwise differentiating the first from second individual, we reduce the model to fewer compartments – for instance, in our example, we will have one (S, I) class standing for both (S, I) and (I, S).

The unordered pair dynamics must be consistent with the 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're likely to 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
- collect the compartments of that model into equivalence classes: in the SI case, $\{\{(S,S)\}, \{(S,I),(I,S)\}, \{(I,I)\}\}$. Sum over those classes to generate the reduced compartments: in this case $Z_{SI} = X_{SI} + X_{IS}$ where we use the letter Z for reduced (unordered) compartment variables and X for the compartments of the ordered-pair model M^2.
- Construct reduced transition rates by transforming all X variables to Z variables, and assign their source and target vertices to the appropriate Z variables.

Note that this is a different way of combining compartments than the combining we did when constructing the ordered pair model. There we simply defined one compartment to be a synonym of the other and merged them by moving the arrows from one to the other; here we define a new compartment to be the sum of the old compartments and transform the transition rate expressions as well as relocating their arrows. Here is a definition for this operation:

An **aggregation of compartments** of a compartment model is a transformation $A(M)$ of that model by a pair of mappings $A : C_M \to C_A$ and $A : P_M \to P_A$, defined as for a relabeling, such that

- The compartments of $A(M)$ are the set $\{A(C)|C \in C_M\}$
- There is an equation $C_i' = \sum C_j$ for each compartment C_i' of $A(M)$, where the sum is over all the compartments C_j such that $A(C_j) = C_i'$.
- The set of transitions of $A(M)$ is the set of triples $(A(s), A(t), (C_1', \ldots, C_{n'}', P_1', \ldots, P_{m'}') \mapsto \sum_{\{(s',t',r')|A(s')=A(s),A(t')=A(t)\}} r'(C_1, \ldots, C_n, P_1, \ldots, P_m))$ generated by all transitions (s, t, r) of M. The sum is simplified to a function of the C_i' variables using the above sum equations.

That is, the transitions of the model M are summed together where their sources and targets are mapped to the same places by the aggregation, and sums of compartments of M are simplified in terms of the compartments of $A(M)$. This reduction doesn't work for general box models, so this can only be done in particular cases. Also, it's probably necessary to relabel the parameters just so using $A(P_i)$, so that the sums will come out right.

Given that definition, we define a **sorting operation** Z such that $Z((S,I)) = Z((I,S)) = (S,I)$ (we sort the compartments in the order S, I, R). Using that as an aggregation function, the definition above gives us $Z_{SI} = X_{SI} + X_{IS}$, and we define the unordered pair model as

$M_U = Z(M^2)$

where M^2 is the ordered-pair model defined above. (Note: To make the transitions reduce to Z expressions we'll have to construct the right renaming for the indexed β parameters.)

## 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:

$$S_1 \xrightarrow{\quad I_1 S_1 \beta_1 \quad} I_1$$

$$S_2 \xrightarrow{\quad I_2 S_2 \beta_2 \quad} I_2$$
.
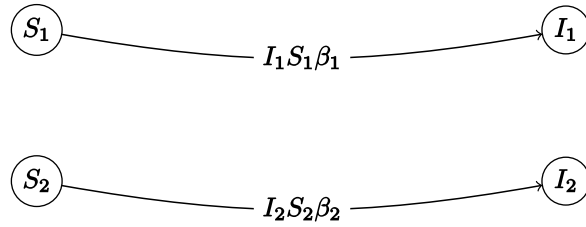
We wish to combine these infection processes into a single model $M_1 \boxtimes M_2$, in which a single susceptible class is infected by both agents, producing not only the I_1 and I_2 classes, but also an I_{12} class which is infected by both, and potentially an I_{21} class as well, if the order of infection events is important. This has some characteristics of the strong product of the models' graphs, because it includes at least one diagonal arrow, representing multiple infection from a single contact, as well as the horizontal and vertical arrows representing simple infection events:

.
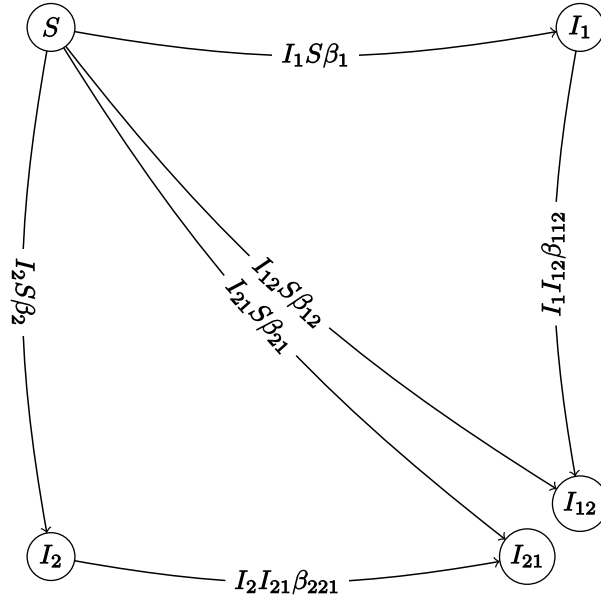
There may also be cases in which one infection excludes the other:
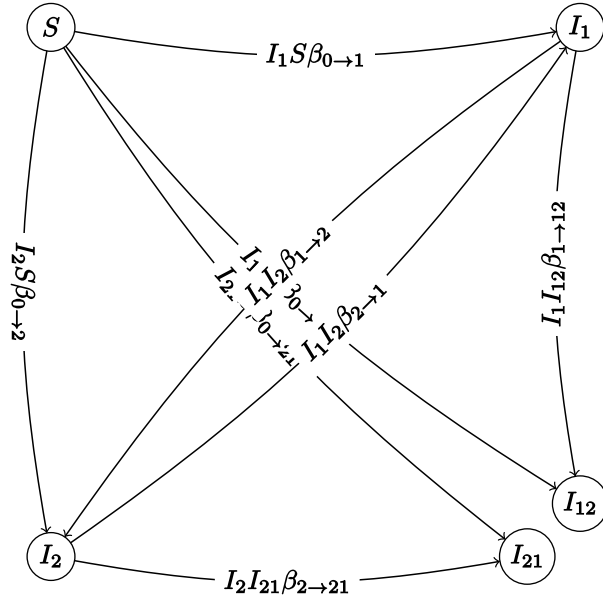
How are we to define this product of simple SI models? Each of the two original infection arrows becomes four: the simple infection event from S, the superinfection event from the other model's I class, an replacement event in which it replaces the other model's infection, and one of the two double-infection events.

We can probably use that list to define the "multiple-infection product". But how does this product generalize to n generic compartment models with some quadratic transition rates and some other rates?

This product is distinguished from the ones above in three ways:

- The order of events makes a difference: infection by agent 1 and then agent 2 is different from infection by agent 2 and then agent 1.
- It's possible to "jump forward" over two transitions at once, from S to I_{12} for example.
- There are "lateral" transitions, for instance from I_1 to I_2 by contact with an I_2 individual, rather than the more standard transition to I_{12} that would be triggered by that contact.

Let's take those in order.

Distinguishing the order of events

In a simple, standard cross product of models, compartments I_{12} and I_{21} would both be the same compartment (I_1, I_2). The difference is whether an individual

arrives from compartment I_1 or from I_2 (we'll consider the double-infection transition from a contact between S and I_{12} separately, below).

We can formalize this by identifying the compartments of the product model with, not the vertices of the Cartesian product of graphs, but directed paths in the graph. Instead of ordered pairs such as (S_1, I_2), each compartment of the product model would be a sequence of ordered pairs, such as $((S_1, S_2), (S_1, I_2), (I_1, I_2))$. Instead of producing a square graph, this construction produces a branching tree:
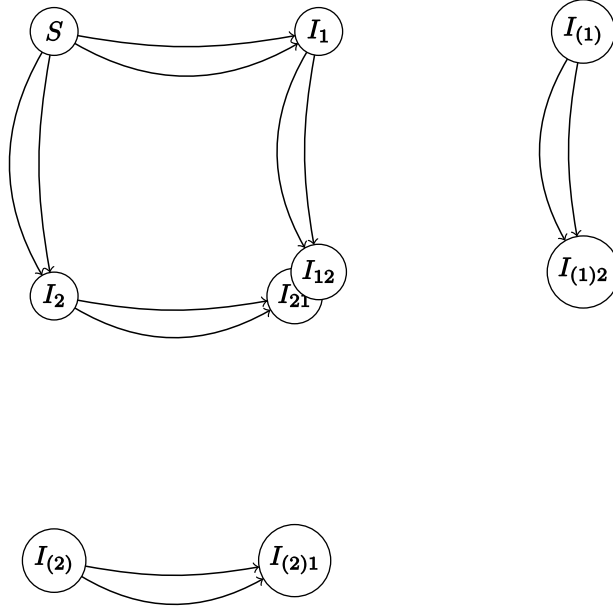
It generates some extra edges, starting at places other than (S_1, S_2). We should think about whether those might ever be meaningful.

We can generate just the component we want by specifying a starting compartment. In this case the starting compartment is the pair (S_1, S_2), which is labelled S in the diagram.
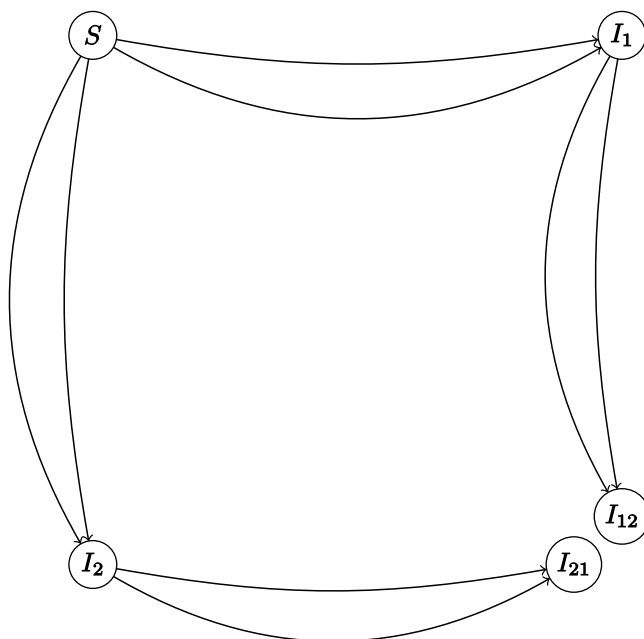
This diagram also makes clear that the sketch above doesn't have enough arrows. There are multiple kinds of interactions driving transitions across each pair of compartments. There must be more than that as well: nearly every possible encounter between two types needs at least one transition, sometimes more.

I have an implementation of this product using a recursive binary relation. I want to understand a little better what it has to do with the other formulations in this paper, then I'll write it up.

Here is a hierarchical coinfection model generated by software:

X_{SS} X_{IS}

$X_{IH}X_{SS}\beta_{SS0IH0}$

$X_{HI}X_{SS}\beta_{SS0HI0}$

$X_{IS}X_{SS}\beta_{SS0IS0}$

$X_{IH}X_{SS}\beta_{SS01IH01}$

$X_{HI}X_{SS}\beta_{SS01HI01}$

$X_{IH}X_{SS}\beta_{SS01IH01}$

$X_{HI}X_{SS}\beta_{SS01HI01}$

$X_{SI}X_{SS}\beta_{SS1SI1}$

$X_{HI}X_{SS}\beta_{SS1HI1}$

$X_{IH}X_{SS}\beta_{SS1IH1}$

$X_{IS}X_{SI}\beta_{IS1SI1}$

$X_{HI}X_{IS}\beta_{IS1HI1}$

$X_{IH}X_{IS}\beta_{IS1IH1}$

X_{IH}

X_{SI} X_{HI}

$X_{IH}X_{SI}\beta_{SI0IH0}$

$X_{HI}X_{SI}\beta_{SI0HI0}$

$X_{IS}X_{SI}\beta_{SI0IS0}$
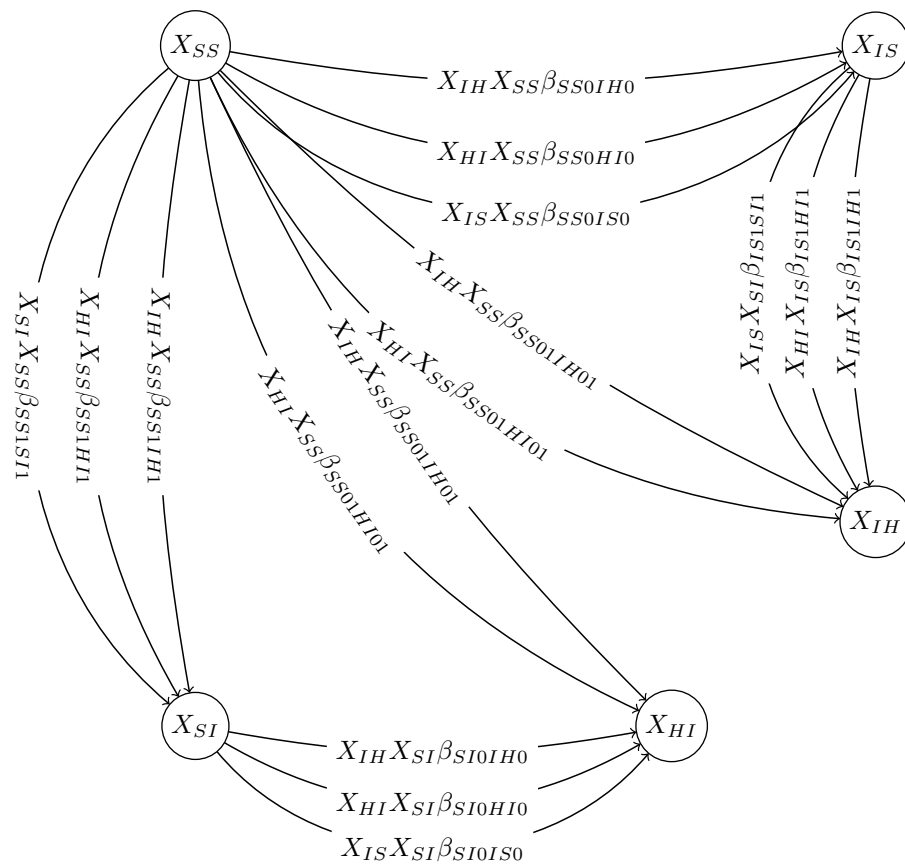
Here is a variant in which an encounter with an infected individual can knock out one or more of your strains, as well as giving you new ones:

X_{SS}

X_{IS}

$X_{IH} X_{SS} \beta_{SS0IH0}$

$X_{HI} X_{SS} \beta_{SS0HI0}$

$X_{IS} X_{SI} \beta_{IS1SI1}$

$X_{SS} \beta_{SS0IS0}$

$X_{IS} X_{SI} \beta_{IS1HI1}$

$X_{HI} X_{IS} \beta_{IS1HI1}$

$X_{IS} \beta_{IS1HI1}$

$X_{SI} X_{SS} \beta_{SS1SI1}$

$X_{HI} X_{SS} \beta_{SS1HI1}$

$X_{IH} X_{SS} \beta_{SS1IH1}$

$X_{IS} X_{SI} \beta_{IS1SI1}$

$X_{HI} X_{IS} \beta_{IS1HI1}$

$X_{IH} X_{IS} \beta_{IS1IH1}$

$X_{HI} X_{SS} \beta_{SS0HI01}$

$X_{IH} X_{SS} \beta_{SS0IH01}$

$X_{IH} X_{IS} \beta_{IS0IH0}$

$X_{HI} X_{IS} \beta_{IS0HI0}$

$X_{IS} X_{SI} \beta_{IS0IS0}$

X_{IH}

X_{SI}

X_{HI}

$X_{IH} X_{SI} \beta_{SI0IH0}$

$X_{HI} X_{SI} \beta_{SI0HI0}$

$X_{IS} X_{SI} \beta_{SI0IS0}$
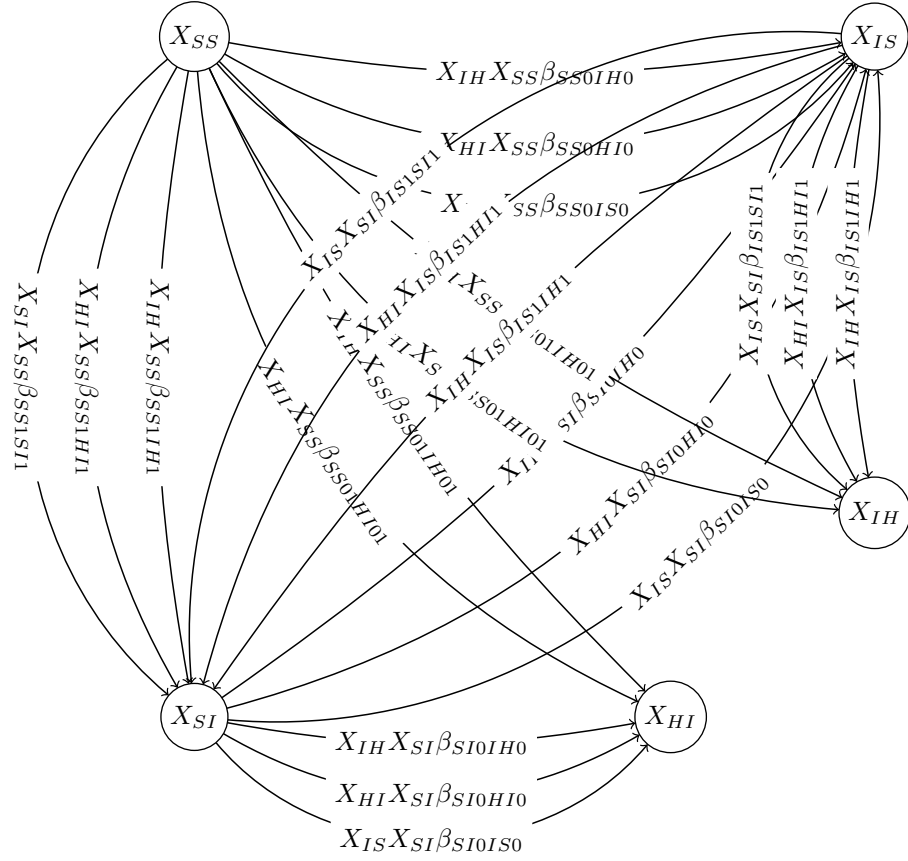
Here's a variant in which it's possible to get infected with both strains equally:

X_{SS} X_{IS} X_{IH} X_{II} X_{SI} X_{HI}

$X_{HI}X_{SS}\beta_{SS0HI0}$

$X_{IH}X_{SS}\beta_{SS0IH0}$

$X_{II}X_{SS}\beta_{SS0II0}$

$X_{IS}X_{SS}\beta_{SS0IS}$

$X_{HI}X_{SS}\beta_{SS01HI01}$

$X_{HI}X_{SS}\beta$

$X_{IH}X_{SS}\beta_{SS01IH01}$

$X_{II}X_{SS}\beta_{SS01II01}$

$X_{II}X_{SS}\beta_{SS01II01}$

$X_{II}X_{SS}\beta_{SS01IH01}$

$X_{SI}X_{SS}\beta_{SS1SI51}$

$X_{II}X_{SS}\beta_{SS1II1}$

$X_{IH}X_{SS}\beta_{SS1IH1}$

$X_{HI}X_{SS}\beta_{SS1HI1}$

$X_{IS}X_{SI}\beta_{IS1SI1}$

$X_{II}X_{IS}\beta_{IS1II1}$

$X_{IS}X_{SI}\beta_{IS1SI1}$

$X_{II}X_{IS}\beta_{IS1II1}$

$X_{IH}X_{IS}\beta_{IS1IH1}$

$X_{HI}X_{IS}\beta_{IS1HI1}$

$X_{HI}X_{SI}\beta_{SI0HI0}$

$X_{IH}X_{SI}\beta_{SI0IH0}$

$X_{II}X_{SI}\beta_{SI0II0}$

$X_{IS}X_{SI}\beta_{SI0IS0}$

$X_{IS}X_{SI}\beta_{SI0IS0}$

Here's a hand-drawn box model with hierarchical coinfection where one strain can knock out the other. If this is the model we want I can look for a general rule that generates it.

16

Transitive transitions ("jump-overs")

The above implementation doesn't generate the diagonal arrows. First let's consider the "forward" arrows from S to the co-infection compartments I_{12} and I_{21}. These are the events that make this a "strong product", the ones that combine two events of the cross product into one. Semantically, these denote events in which two transitions of the cross product happen in a single encounter: one individual gives the subject two infections at the same time.

First of all, here is an unadorned strong product of M_1 and M_2:
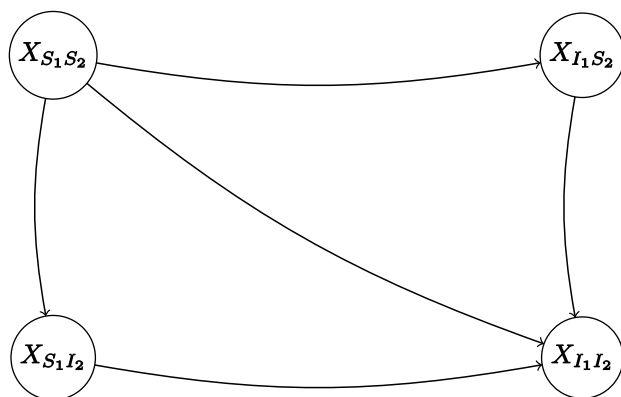
Clearly we need more structure than that. Try this:
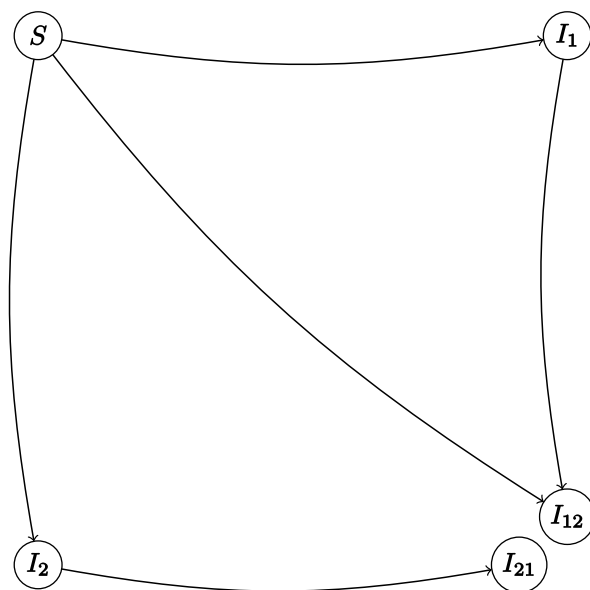
Lateral transitions

(to come)

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 it as a box model.

Given an integer number N of total individuals, the compartments, that is the state variables, for the forward equations are $p_{(\frac{i_1}{N}, \ldots, \frac{i_n}{N})}$ 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, under the assumption 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

$$(p_S, p_{S - \frac{\mathbf{e}_s}{N} + \frac{\mathbf{e}_t}{N}}, r(S)p_S)$$

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

$$\frac{dp_{01}}{dt} = \frac{2}{9} \beta p_{\frac{1}{3} \frac{2}{3}}$$

$$\frac{dp_{\frac{1}{3} \frac{2}{3}}}{dt} = -\frac{2}{9} \beta p_{\frac{1}{3} \frac{2}{3}} + \frac{2}{9} \beta p_{\frac{2}{3} \frac{1}{3}}$$

$$\frac{dp_{\frac{2}{3} \frac{1}{3}}}{dt} = -\frac{2}{9} \beta p_{\frac{2}{3} \frac{1}{3}}$$

$$\frac{dp_{10}}{dt} = 0$$

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, $\ldots$, 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, $\ldots$, 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. [In our definition of box models, the elements of 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 Cartesian product of graphs

The **Cartesian product** (or cross product) $G_1 \times G_2 \times \ldots \times G_n$ **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 $((v_1, v_2, \ldots, v_i, \ldots, v_n), (v_1, v_2, \ldots, w_i, \ldots, v_n), e)$, 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 Cartesian product of graphs is sometimes written $G_1 \,\square\, G_2 \,\square\, \cdots \,\square\, G_n$, which is visually resonant with the shape of the product graph.

The tensor product

The **tensor product** of directed graphs G_1, ..., G_n is a graph $G_1 \cdot G_2 \cdot \ldots \cdot G_n$ 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.

This is often written $G_1 \times \cdots \times G_n$ when the $\square$ operator is used for Cartesian products, since this product produces X-shaped diagrams.

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

the edges of the two product graphs.

If we extend that definition 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 propose 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 contains edges belonging to the transitive closure of the Cartesian product graph, but it is not the transitive closure, because it's limited to transitive combinations of exactly zero or one edge from each component graph.