Exploring Transmission of Infectious Diseases on Networks with NETLOGO

Winfried Just Department of Mathematics, Ohio University

in collaboration with

Hannah Callender, University of Portland M. Drew LaMar, College of William and Mary Natalia Toporikova, Washington and Lee University

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The purpose of this talk

- Quoting the abstract: In this talk we will present a set of teaching materials ...
- In plain English: The presenter is going to give a sales talk, shamelessly bragging about his materials, and will tell us to adopt them.
- **Putting it more diplomatically:** I will tell you what teaching objectives the authors had in mind for these materials, how we structured them to achieve these objectives, and what makes them different from more traditional sources.
- **Moreover:** I hope for feedback from the audience that may help us in further developing these materials.

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We have two book chapters in

Raina Robeva (ed.), *Algebraic and Discrete Mathematical Methods* for Modern Biology, Academic Press, 2015:

[1] Winfried Just, Hannah Callender, M. Drew LaMar, and Natalia Toporikova; *Transmission of infectious diseases: Data, models, and simulations.* 193-215.

[2] Winfried Just, Hannah Callender, and M. Drew LaMar; *Disease transmission dynamics on networks: Network structure vs. disease dynamics.* 217-235.

A third book chapter is in preparation:

[3] Winfried Just and Hannah Callender; *Vaccination strategies for small worlds.*

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M. Drew LaMar, in consultation with the other authors, developed a customized simulation tool called **IONTW**, which stands for **I**nfections **O**n **N**e**TW**orks.

It is written in the NETLOGO programming language.

IONTW is freely available and can be used (to some extent) independently of the book chapters.

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The materials: Modules published on the web

A number of modules for more in-depth student explorations are published at

```
http://www.ohio.edu/people/just/IONTW/
https://qubeshub.org/iontw
```

They form a natural continuation of the book chapters, but can also be used independently, based on the condensed introduction to network-based models of disease transmission posted at these websites.

We strongly encourage submissions of additional modules or expansion of existing ones by our colleagues and students. Three of the current modules have been co-authored by my Ph.D. student Ying Xin.

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For whom did we write?

- Our first book chapter is intended for undergraduate students of the life sciences and mathematics.
- The second book chapter targets advanced undergraduate and beginning graduate students of mathematics or with a strong mathematical background.
- The modules on the web vary in level from elementary to advanced. The target audience and prerequisites for each are specified at the websites.
- The forthcoming third book chapter will lead into open research problems.

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Our goals

- Create a set of materials suitable for adoption as modules or supplementary reading in a math modeling in biology course or as a basis for REU projects.
- Use discovery-based learning throughout.
- Provide extensive coverage, with active student involvement, of the process of building, understanding, and critically evaluating mathematical models in biology.
- Illustrate the kinds of insights that can be gained from simulations on the one hand and from mathematical derivations on the other hand.

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Models of disease transmission the usual way

A standard introduction to mathematical models of disease transmission might begin like this:

(Definition of compartments and variables).

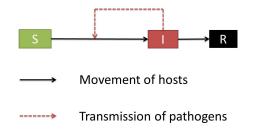


Figure: Schematic representation of SIR-models.

(Some DEs or difference equations.)

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Our treatment in the first book chapter [1]

We introduce students to the process of mathematical modeling by

- starting from the kind of data that can be collected,
- posing the questions we want to answer with the help of the model,
- spelling out the simplifying assumptions that are being made when biological processes are distilled into mathematical terminology,
- specifying agent-based models (ABMs),
- illustrating in detail how to explore ABMs with simulations,
- explaining what the computer does when it runs simulations.

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Infectious diseases are caused by pathogens (such as viruses, bacteria, fungi, or protozoans) that spread in populations of hosts (humans, animals, or plants). We focus on pathogens that are transmitted during direct contacts between hosts.

We may want to predict the final size of an outbreak.

The final size is the fraction F of hosts who experience infection during the outbreak.

How does the expected value of *F* behave if we increase population size *N*?

If $\lim_{N\to\infty} F = 0$, we predict only minor outbreaks, when $\lim_{N\to\infty} F > 0$, there is a risk of major outbreaks.

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The previous slide definened minor *vs.* major outbreaks in a condensed and mathematically abstract way.

In the materials themselves we use discovery-based learning for introducing most concepts.

Numerous student exercises of varying levels of difficulty form an integral part of our text.

A typical exercise or sequence of exercises uses the **IONTW** simulation tool and guides students towards discovering a particular mathematical insight.

Let us see how this works for the concept of minor *vs.* major outbreaks.

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Example continued: Instructions for the exercises

In general, we give very specific and detailed instructions for exercises that use software.

Open IONTW, press Defaults. Set infection-prob := 0.015 end-infection-prob := 1 num-nodes := 100

Click New, Set and then Go.

Use the **Disease Prevalence** plot to estimate and record the observed final size.

Repeat ten times using Reset, Set, and then Go.

Repeat 10 times each with

infection-prob := 0.015 num-nodes := 200

infection-prob := 0.0075 num-nodes := 200

Summarize your observations in a short paragraph.

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The results are in, now what?

Observed outcomes will vary from simulation run to simulation run. In some of our exercises, we teach students some rudiments of statistical inference, in particular, on how to choose appropriate batch sizes.

For other exercises, we make the connection with theoretical results.

The ones in our example naturally leads towards the definition of the basic reproductive ratio R_0 as a predictor of the possibility of major outbreaks and their final sizes.

- Theorems give us insight into the driving mechanisms.
- Theorems usually provide a clearer picture than simulations.
- One needs to very carefully parse a theorem to properly understand what it actually predicts.
- A theorem is applicable to a real-world situation only if its assumptions are roughly satisfied.

We put great emphasis on clearly spelling out the simplifying assumptions that lead to a given model and discussing how they might distort the predictions.

Our particular focus is on the uniform mixing assumption that underlies all compartment-level models. More precisely, explore how the uniform mixing assumption might distort predictions of certain more realistic models that contain representations of individual hosts.

In network-based models of disease transmission we assume that two hosts can make contact only if they are connected by an edge of a given graph G that represents the contact network.

The uniform mixing assumption becomes the special case when G is the complete graph.

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- Contains some theoretical results on the role of *R*₀ under uniform mixing.
- Introduces notions from graph theory in context.
- Explores the relation between the structure of the underlying contact network and the predicted dynamics.

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Example: An example with the same R_0

```
Open IONTW, press Defaults. Set
infection-prob := 0.375
end-infection-prob := 1
network-type := Nearest-neighbor 1
num-nodes := 100
d := 2
```

Look up R_0 in the **Command Center** and compare with the previous exercises.

Click **Set** and then **Go**.

Use the **Disease Prevalence** plot to estimate and record the observed final size.

Repeat ten times using Reset, Set, and then Go.

Summarize your observations in a short paragraph.

This exercise introduces the effect of clustering.

For any real population of realistic size we simply don't.

But we can estimate some structural parameters, like the mean degree of the nodes, based on statistical sampling, and treat the contact network as a random graph that shares these empirically verified properties with high probability.

Quite a few types of random graphs are implemented in **IONTW** and introduced in our materials.

They include Erdős-Rényi, small world (1 and 2 dimensions), preferential attachment, generic scale-free, spatially clustered, random regular graphs, as well as random graphs with a user-specified degree distribution.

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How to use the materials for REU projects?

- Most of the exercises of our web-based modules can be directly incorporated into REU projects. Sample solutions are accessible to instructors via a sign-up page.
- Many of our exercises also can be easily modified into similar ones that would provide a research experience.
- The intended outcome of an REU project may well be design of an additional module to be posted at our websites, or expansion of an existing one.
- The forthcoming book chapter [3] will combine material from several of the existing modules so that it builds up towards five open research problems. These problems are related to optimal vaccination strategies in models with a small-world contact network. They should be within reach of undergraduate students of mathematics.

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The software and online modules can be accessed at:

http://www.ohio.edu/people/just/IONTW/
(For download and local installation of IONTW.)

https://qubeshub.org/iontw
(A version of IONTW that runs on a web server; also
sample-solutions via instructor sign-up.)

The online parts of our book chapters can be found at:

http://booksite.elsevier.com/9780128012130/chapters.php

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