Lecture 10: Sampling, sweeps, & uncertainty

Complex Systems 530

3/10/20

Welcome back!

- Networks lab check in
- Final project details
- Plan for the next few weeks

Final Project: Presentation

- **Dates**
- **Length**: tentatively, we will plan for (potentially to be changed depending on scheduling needs):
  - 1 person: 10 minutes + 2 for questions
  - 2 people: 12 minutes + 2 for questions
- Everyone in the group must present
- Ask at least one question of another group (or more!)

Final Project: Paper

- **Due date: Final exam day, 4/30/2020**, via Canvas (grades are due 72 h later, so this is a hard deadline!)
- **Write-up:** roughly 8-12 pages, but shorter or longer is fine so long as you fully cover the motivation, problem, methods/model, results, etc.
- **Model code:** I should be able to both review the code and run it myself if in NetLogo or Python.
  - Your code must be **documented, clear, and readable**.
  - Be sure to also document the version of python and any packages you used.

Paper components

- **Introduction.** problem overview and literature review—what gap or question are you addressing? What has been done before?

- **Methods: model description.** Describe how your model works in terms of its: agents, interactions, environment, model schedule/timing

  - You can use the PARTE and/or ODD frameworks as a guide

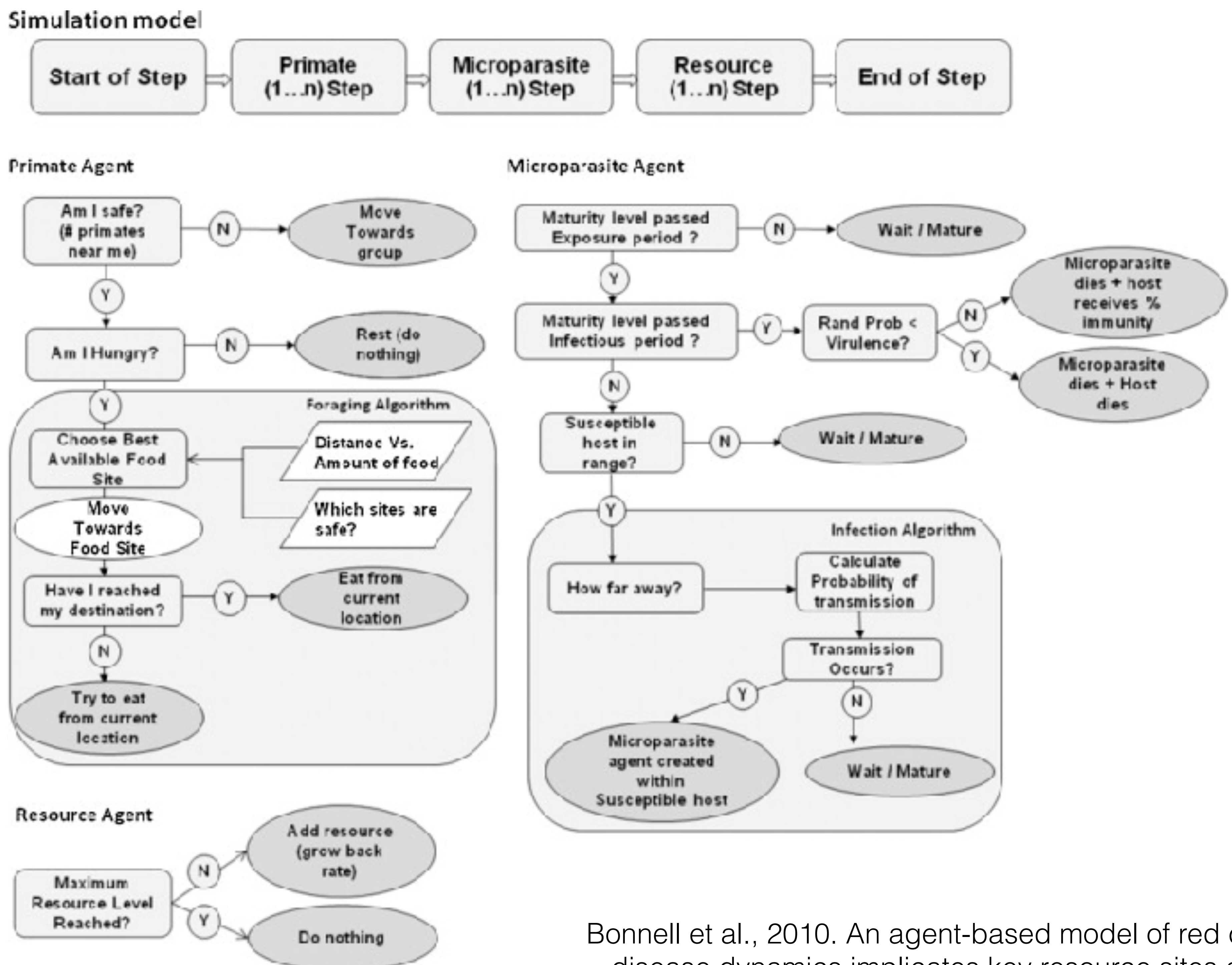
  - Flow charts & visuals are good!

How to write up an ABM

- PARTE - Properties, Actions, Rules, Time, Environment
    - Agents are defined by their properties, actions, and rules
- ODD Protocol - Overview, Design concepts, and Details
    - Describes the model purpose, structure, and design concepts around which the model was built (e.g. emergence, adaptation, etc.)
- You will get more practice on the next lab!

PARTE: https://www.ncbi.nlm.nih.gov/books/NBK305917/ ODD: https://www.sciencedirect.com/science/article/pii/S030438001000414X

Flow Chart Example



Bonnell et al., 2010. An agent-based model of red colobus resources and disease dynamics implicates key resource sites as hot spots of disease transmission. https://www.vetmed.wisc.edu/goldberglab/pdf/P071.pdf

Paper components

- **Methods: model analysis.** Describe the parameter settings you swept through, the analyses you ran. If your model is stochastic, you may need to run multiple trials at the same parameter settings.

- **Results.** Provide qualitative and quantitative summaries of how your model behaves. Provide graphs and plots of model outcomes at different settings as needed.

Paper components

- **Discussion.** Return to the question or problem in your intro—what do your results say about this problem? Put this in a broader context. Describe the strengths, limitations, and potential future directions of your work.

  - If you think there are still some bugs driving your model's behavior, this is the place to discuss this

  - Also a good place to talk about how you might verify, validate, or extend the model in the future

A note about verification as you build your model

- Your model will have bugs, be wrong, do things you didn’t intend/think through, etc.
- Unit testing and thinking and building with small examples and modules is key
  - Figure out small test cases where almost the entire model is either absent or set to a constant and you know what the one piece you're working with should do. Then move on to the next piece/ submodel, etc.

Plan for the next few weeks

- Sensitivity analysis and exploring the parameter space
- Visualizing and interpreting results
- Different levels of agent cognition - game theory & decision theory
- Model calibration & estimating parameters from data
- Model comparison & inference robustness
- More complex environments (e.g. GIS)

ABM complexity & dimensionality

ABM complexity & issues of dimensionality

- So far, our ABMs have obeyed fairly simple rules—reasonably easy to describe with a bulleted list (even if this can leave a lot of ambiguity still)

- This already leads to a high dimensional input/parameter space

- But many ABMs used in practice include more detailed mechanisms, more complicated processes to capture realistic details or more intricate questions

Parameter/input space

- Voting model
  - Grid size (width, height)
  - Initial fraction/probability of yes/no votes
  - Neighborhood size

SIR model on a network

- Network generation parameters (e.g. total number of nodes and probability of an edge for an Erdös-Renyi graph)

- Probability of transmission

- Probability of recovery

- Initial conditions (numbers of S, I, and R individuals)

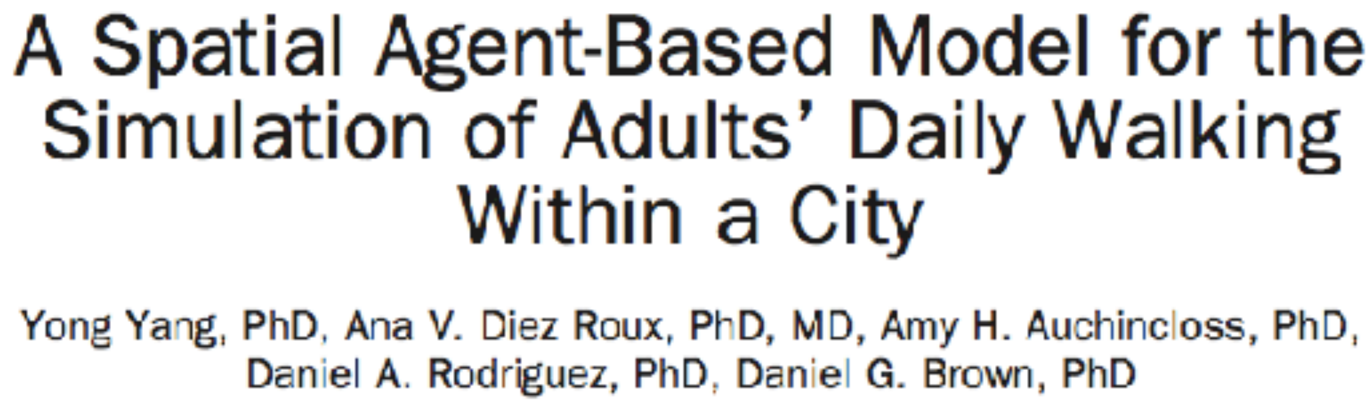
Power grid network model

- Network parameters: number of nodes, number of connections for each new node (scale free graph)
- Node capacity distribution parameters (in this case the mean and SD for a normal distribution)
- Initial electrical load parameters (in this case the bounds for a uniform distribution)
- Initial node states (e.g. fraction of failed nodes at start time)

Ants Model

- Food sources: number of sources, sizes, locations
- Nest location, nest scent gradient parameters
- Population size
- Chemical (pheromone) parameters: how much, diffusion rate, evaporation rate
- Ant movement parameters (angles to wiggle), chemical detection upper & lower bounds, chemical and nest scent angle bounds, how much chemical to drop, etc.

Example: Walking & Health


A Spatial Agent-Based Model for the Simulation of Adults' Daily Walking Within a City

Yong Yang, PhD, Ana V. Diez Roux, PhD, MD, Amy H. Auchincloss, PhD, Daniel A. Rodriguez, PhD, Daniel G. Brown, PhD

- Models walking behaviors in an Ann Arbor-sized city as a function of health, SES, neighborhood safety, commutin patterns, and other features
- Time is discrete steps, with 1 step = 1 day

Yang et al / Am J Prev Med 2011;40(3):353–361

Environment

- Environment: 800 x 800 grid
  - Each cell = 10 m x 10 m
    (64 km city ~ Ann Arbor)
  - Neighborhoods - 40 x 40 cells
    - Neighborhood properties: safety, asthetics, other environmental elements

Environment properties

- Elements in the environment (based on Ann Arbor census)
  - 200 groceries
  - 800 non-food shops
  - 1500 social places
  - 12000 workplaces
  - 60000 households

Agents

- 108,000 individuals
  - 48,000 couples, and 12,000 single people
  - Range of properties related to walking, SES, health, etc.
  - E.g. walking ability is determined by:

$$A_b = U^4(0,1) \times \left(\frac{\mathrm{Min}(|137 - \mathrm{Age}|, 100)}{100} \right)$$

Table 1. Properties of individuals and selected model parameters

Individual-level properties	Values and meaning
Gender	Assigned as male or female with equal probability
Age	Random integer from the uniform distribution ranging between 18 and 87 years; the difference between a couple is no more than 3 years
SES	Integer value ranging between 1 and 5, with higher values indicating higher SES. Members of a family are assumed to have the same SES. In select scenarios, SES is assumed to be positively correlated with increasing distance from the city's center
Family size	Family size can be 1 (with probability of 20%) or 2 (with probability of 80%)
Friends	Each individual has 3 to 5 friends who can influence her/his walking attitude, randomly selected from the people with the same or similar SES value (difference no more than 2)
Dog ownership	Each individual has a 20% probability of having a dog (dog owners have a higher probably of walking within the neighborhood)
Household	Each person is randomly assigned to a household (except in scenarios involving residential segregation by SES)
Work and workplace	If aged ≤69 years, the probability of working is 95%; people aged >69 years are assumed to not work. Working people are randomly assigned a workplace in the city. This can be a grocery store, a non-food shop, a social place, or another workplace in the city
Walking ability (A_b)	Value ranges from 0 to 1, the higher the value, the longer distance an individual can walk
Attitude toward walking (A_t)	Value ranges from 0 to 1, the higher the value, the higher probability an individual will walk

CALIBRATED MODEL PARAMETERS

Activity	Daily probability of performing the activity	Maximum walking distance for the activity (miles)
Work[a]	1 for individuals with a job; 0 for others	1.125
Food shopping	0.4	2
Other shopping	0.25	1.5
Visiting a social place	0.2	2.5
Leisure within neighborhood	0.33	5.5

[a]Only among employed

Actions & Rules

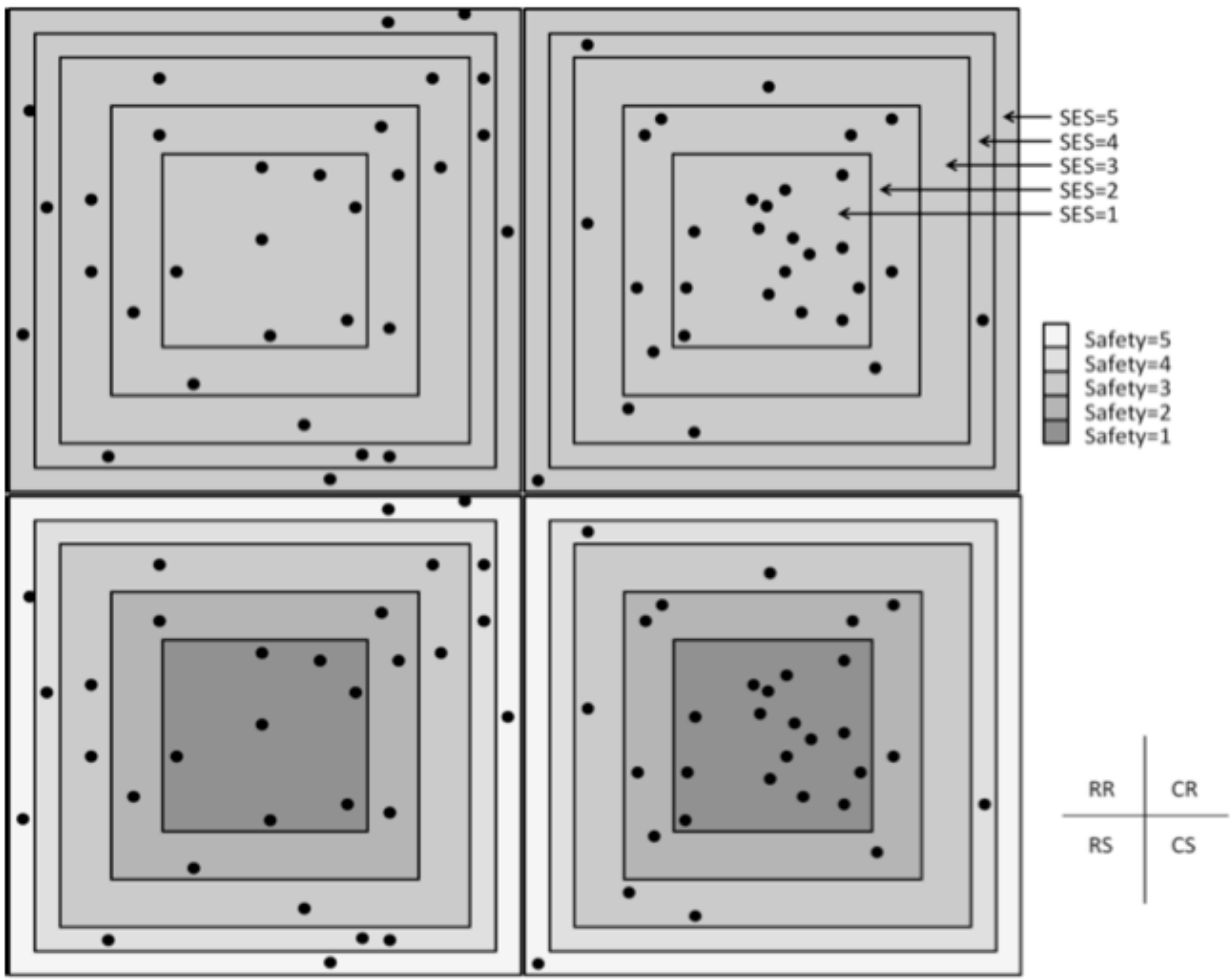
- Individuals can walk for three purposes: (1) to work; (2) forbasic needs (such as food shopping, other shopping, andvisits to social places); and (3) for leisure.
- Walk with a certain probability each day (e.g., non-food shopping takes place every 4 days on average, resulting in a daily probability of 0.25).
- Maximum walking distance for each type of activity. Person-specific maximum distances are calculated as the product of maximum distances and the person-specific ability (Ab).

Actions & Rules

- Example: Work. If the distance between the person’s household and workplace is less than the person-specific maximum walking distance for work, then the decision to walk is a random draw with probability equal to attitude At.

- Attitudes update each time step with feedback from household members, safety, aesthetics of the route, etc.

Example: Walking & Health



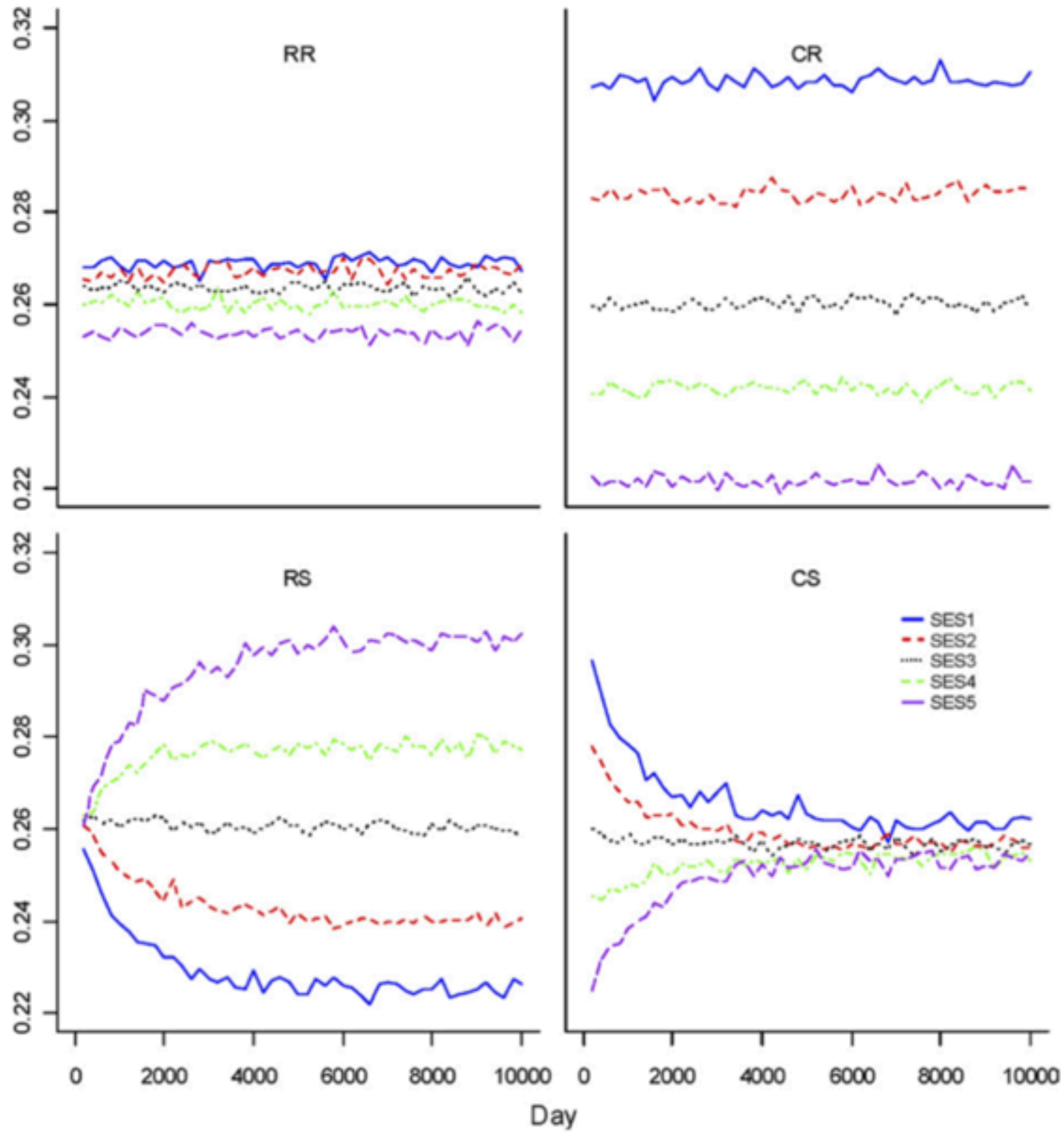


Figure 1. Average walking trips per day per person for different SES groups over time for four scenarios

CR, more non-household locations in the core and random safety level; CS, more non-household locations and lower safety level in the core; RR, randomly distributed non-household locations and random safety level; RS, randomly distributed non-household location and lower safety level in the core

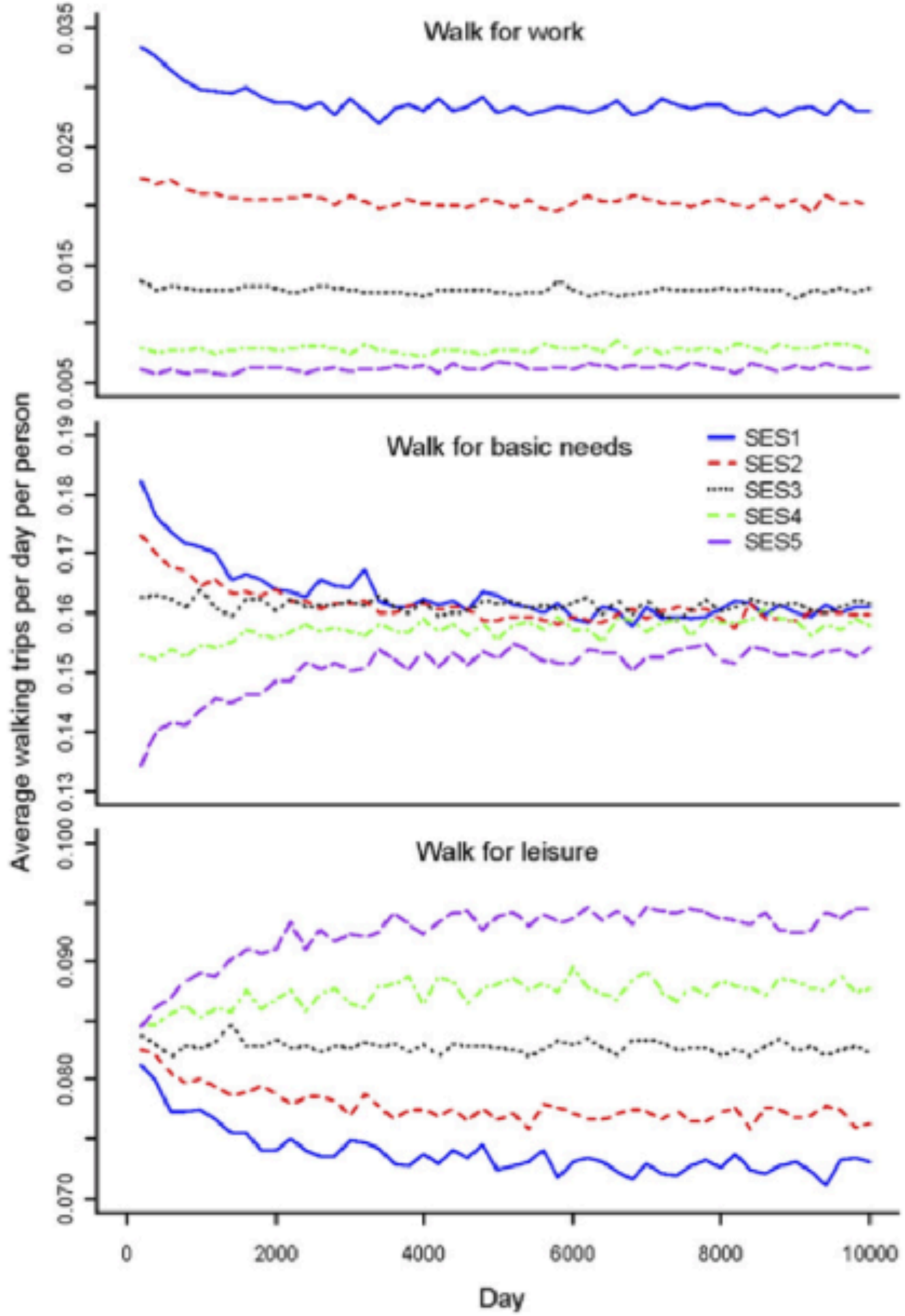


Figure 2. Average walking trips per day per person for different purposes and for different SES groups over time in the CS scenario

CS, more non-household locations and lower safety level in the core

Complexity & high-dimensionality with ABMs

- Many different inputs and possible outputs
- Too complicated to explore by hand
- Need ways to:
  - Visualize and interpret the variation in behaviors
  - Explore which parameters/inputs have the most effect on model outputs of interest

Complexity & high-dimensionality with ABMs

- Also underscores the importance of being targeted and thoughtful in your question!
- Freedom of design means you can easily end up with way too many variables to analyze effectively
- Decide what scenarios to run (e.g. four city setups), what questions to answer, and then keep it as simple as possible

High dimensionality of ABM

- Benefit: ability to explore relationships between large spaces of system inputs & system outputs
- Also allows for exploration of stochastic processes and evolution of systems across time and space
- However, very high dimensionality of data to deal with in analysis

High dimensionality of ABM

Level	Inputs/Parameters	Outputs
Agent	Initial distributions of agent types, attributes, preference structure, direction, number, density	Final distribution of resources, density, proportion in a given state, position
Interaction	Type of strategy, connection topology, adaptation	Strategy prevalence, network structure
Environment	Resources, type, layout	Resources, percent of environment in a given state

Sensitivity, uncertainty, & sampling

Goals

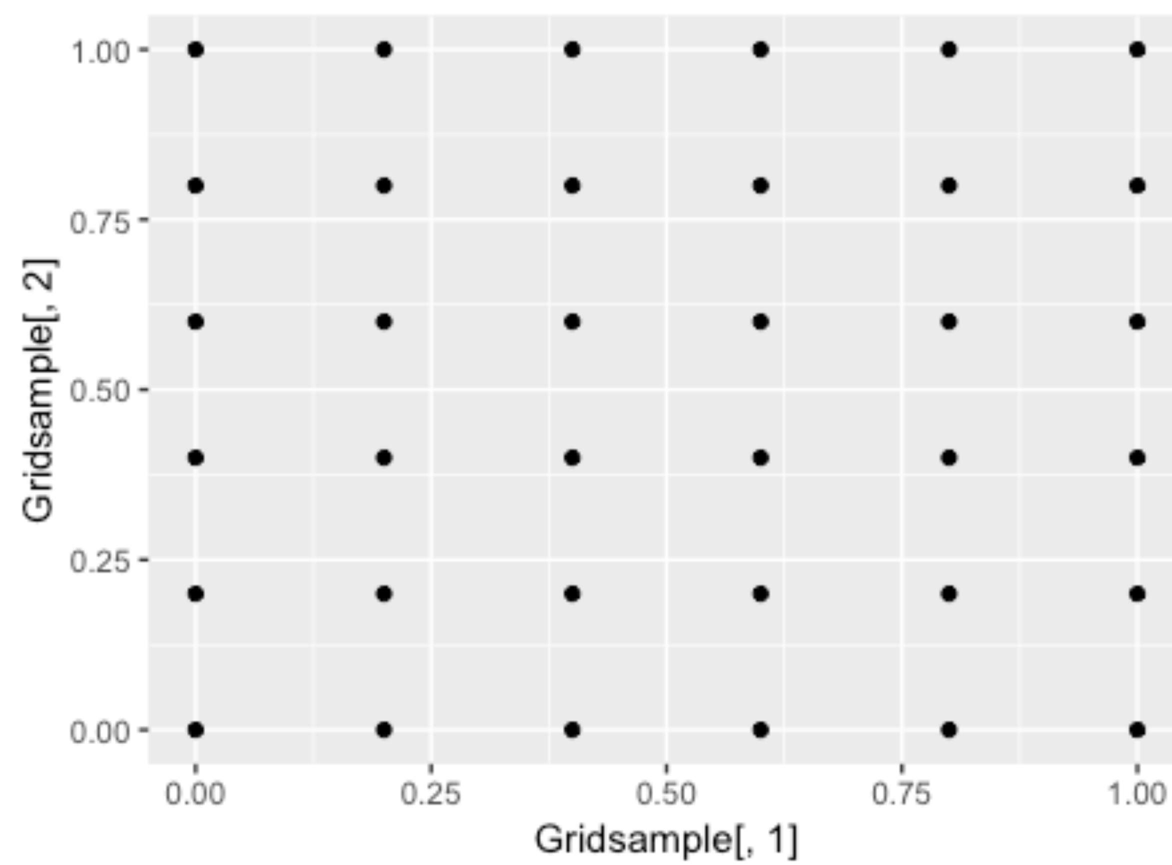
- Understand the variation in model outputs & behaviors (often termed **uncertainty quantification**)
- Understand which inputs/parameters drive that variation (**sensitivity analysis**)

Exploring the space of model behaviors

- How to explore model behaviors?
- So far, we have focused on adjusting specific variables and parameters, and seeing how the model behavior changed by running the model a few times and visually assessing
- We need a more comprehensive, systematic approach

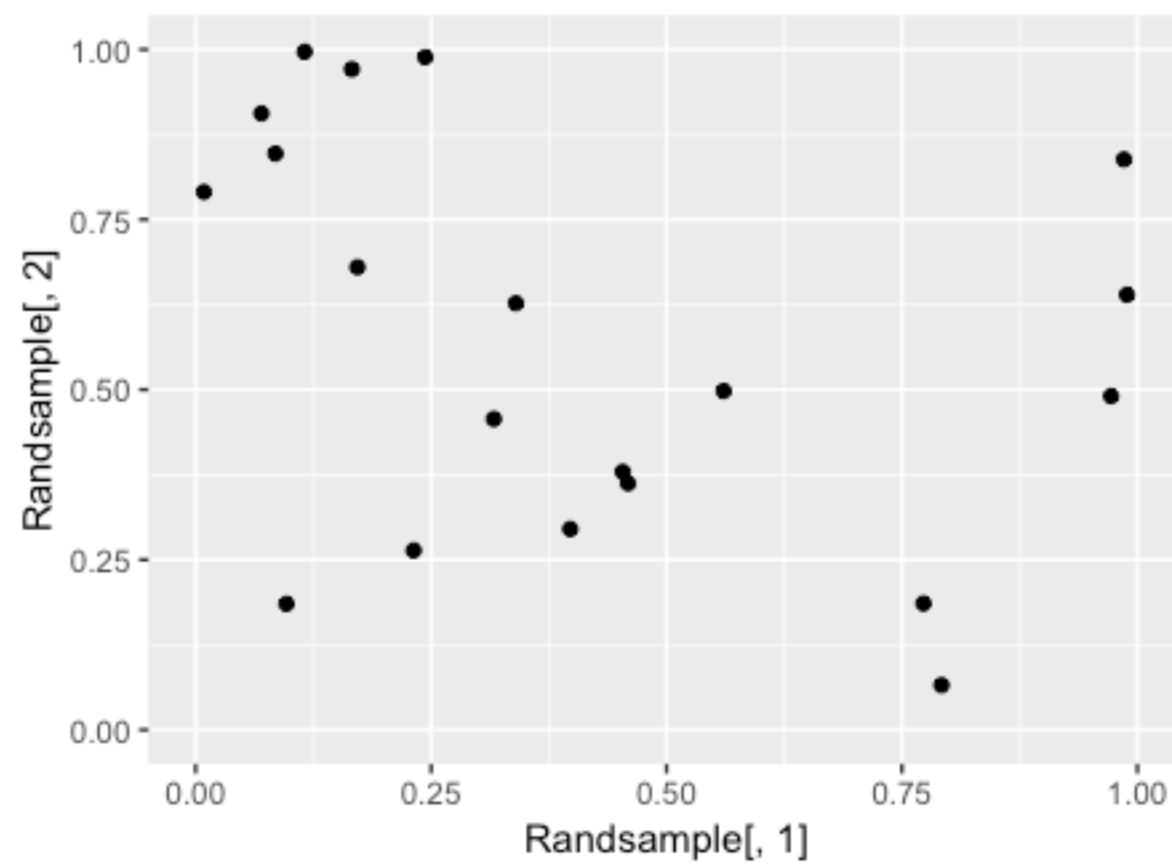
Sampling parameter space

- **Grid sampling**
- Typically choose uniform distribution of points
- Good coverage of space
- Computationally expensive! Becomes infeasible as dimension increases



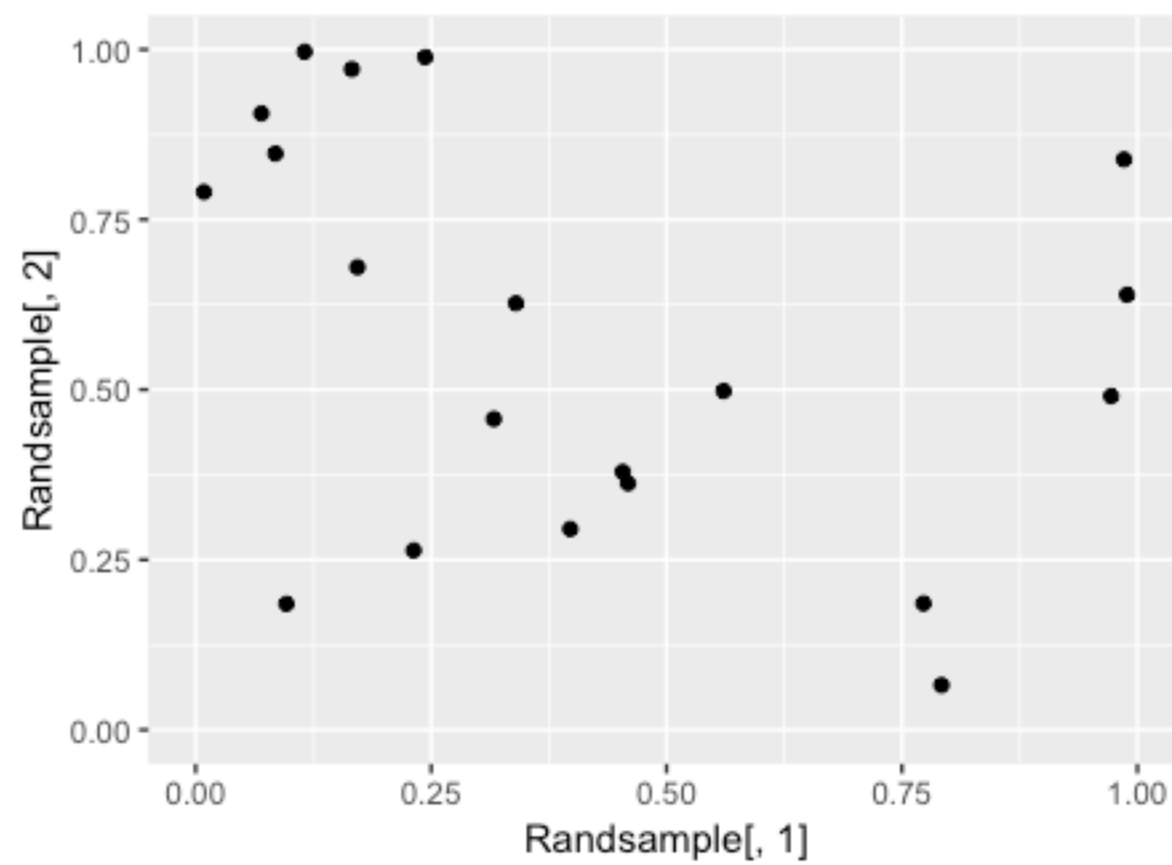
Sampling parameter space

- **Random sampling** (Monte Carlo)
- Often done with uniform distribution, but can choose any distribution
- However, may leave big blank spots, require many samples to fully explore the space



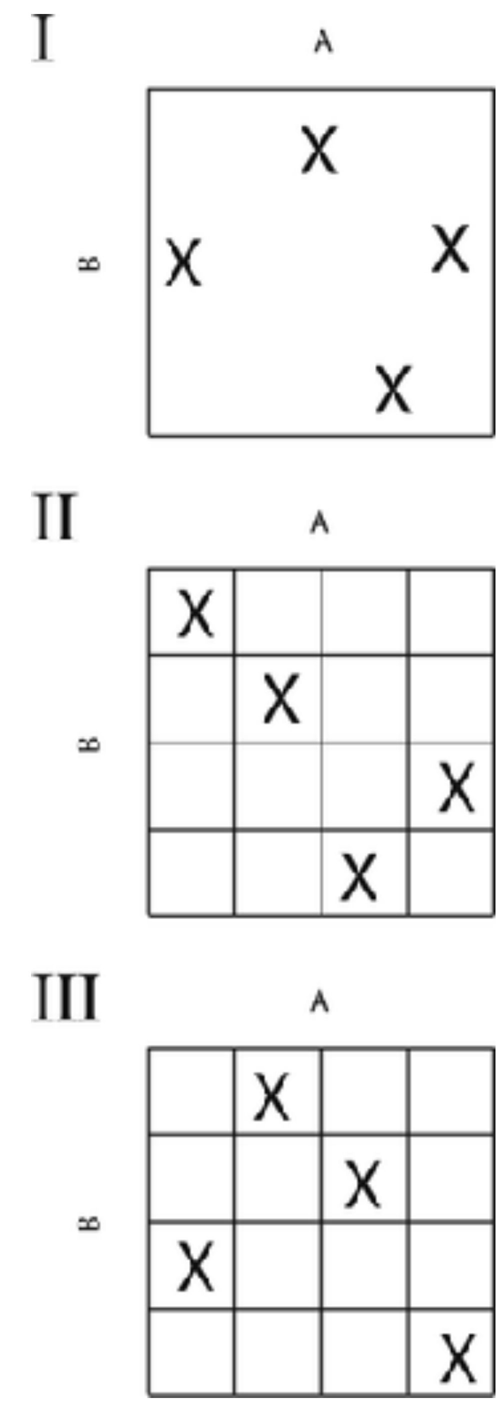
Sampling parameter space

- More efficient ways to explore the space?
  - Latin hypercube sampling (& variants, orthogonal, etc.)
  - Sobol sampling (& other low-discrepancy sequences)



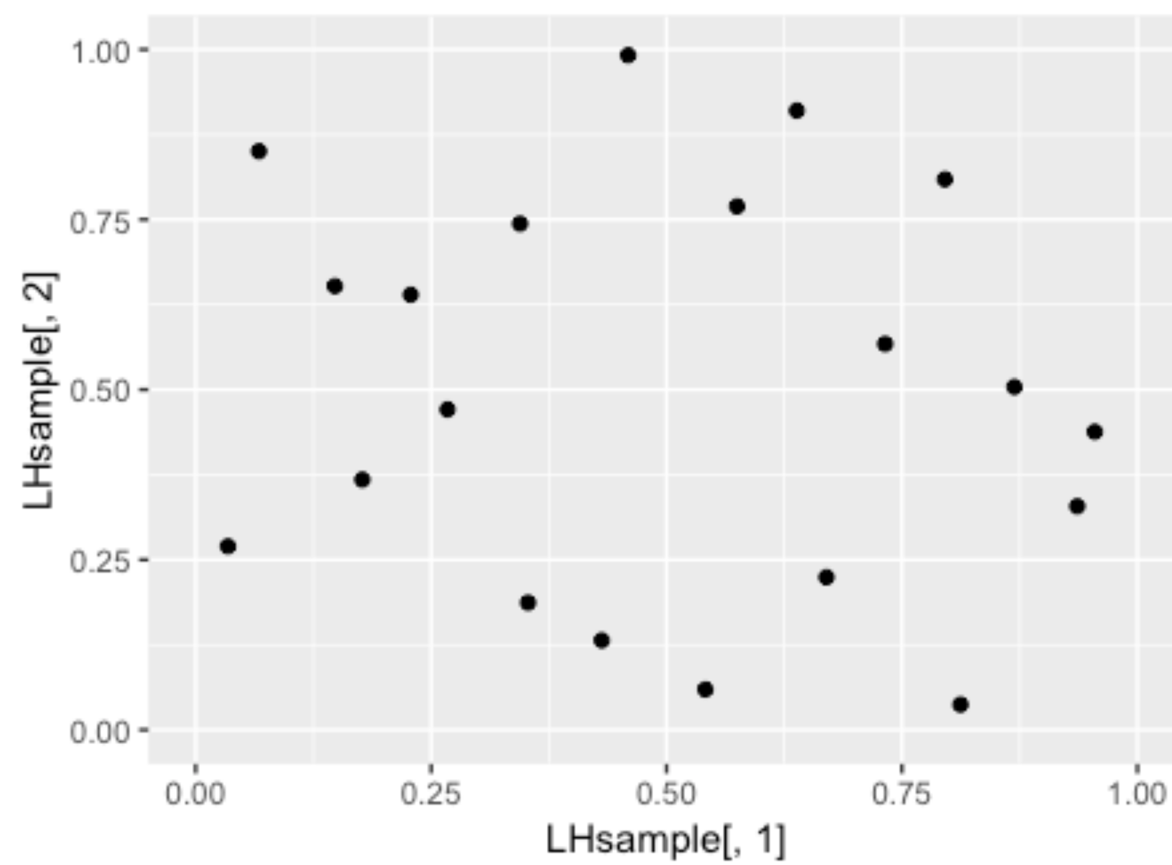
Latin hypercube sampling

- Kind of like sudoku
- Divide space into a grid of rows & columns
- Choose one square in each row and each column
- Choose a random point within that square



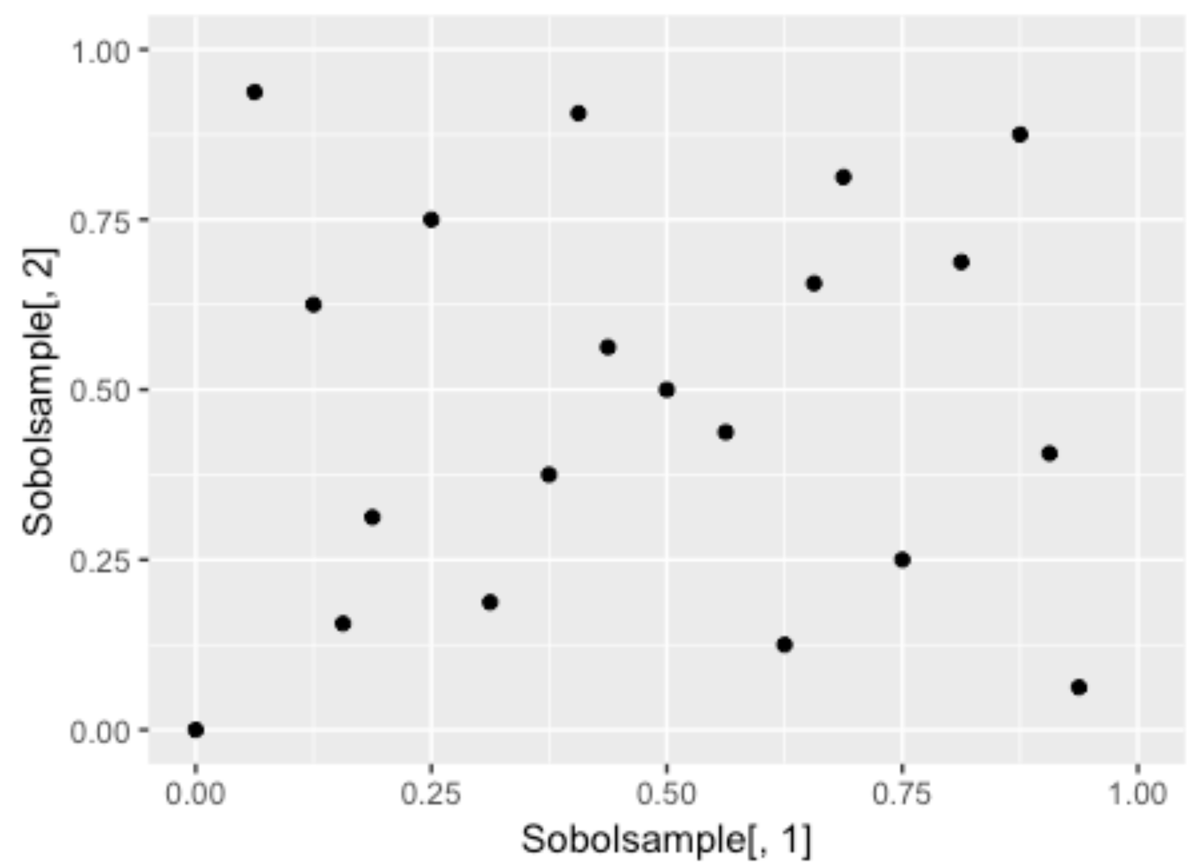
Latin hypercube sampling

- Still an element of randomness
- Ensures better coverage of the space/faster convergence to the sampled distribution



Sobol sampling

- Low-discrepancy sequence (see also Halton, Faure)
- Generates a sequence that samples the space evenly but requires few points
- Convergence can be better than LHS



Kucherenko et al., Exploring multi-dimensional spaces: a Comparison of Latin Hypercube and Quasi Monte Carlo Sampling Techniques. https://arxiv.org/abs/1505.02350

How many samples to take?

- Tough to say! Balance computational intensiveness with good coverage (often >>100, e.g. in the 1K to 10K range depending on number of parameters)
- May need to run more than one sample for a given point due to stochasticity (since different runs may give different behaviors)
- Some methods have rules of thumb, e.g. for LHS, $N_S > (4/3) \times N_P$ has been proposed, but you will often want much more than this bound

Blower and Dowlatabadi (1994), McKay et al. (1979)

Choosing outputs

- Given that we’ll be running large numbers of samples, evaluating the model behavior visually will be difficult!
- Choose your model outputs based on your question of interest—be thoughtful about this!
- Can often be hard to pick metrics that accurately capture the behaviors you're interested in examining

Visualizing & interpreting results

- Histograms and scatterplots—simple but useful!
- Boxplots, violin plots, ridgeline plots, heatmaps
- Basic descriptive stats (means, medians, SD, quantiles)
- We will explore other/fancier options as we go

Example

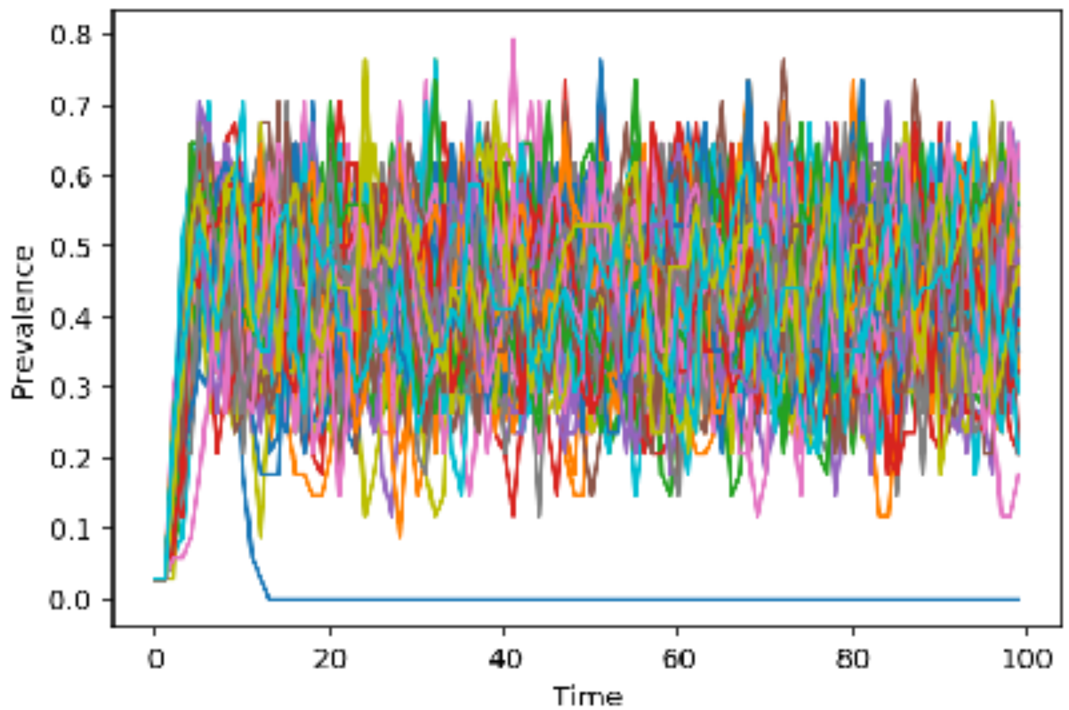
- SIR on the karate club network, with edge regrowth

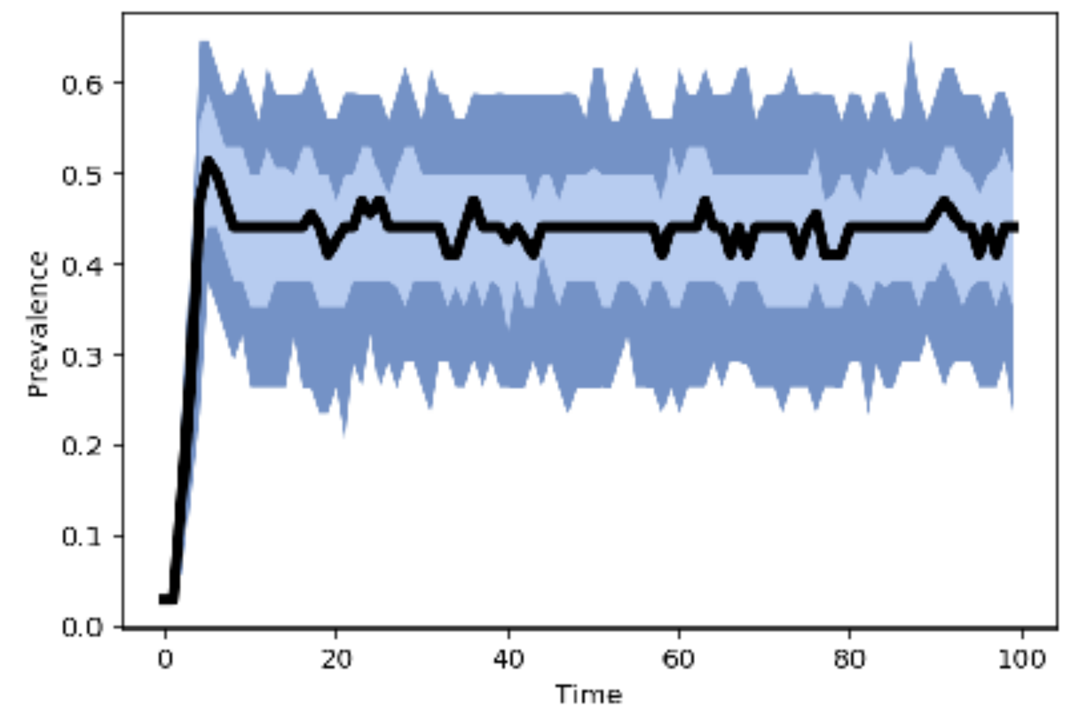
- **Parameters to sample**: infection probability, recovery probability, tie-breaking probability, tie-regrowth probability

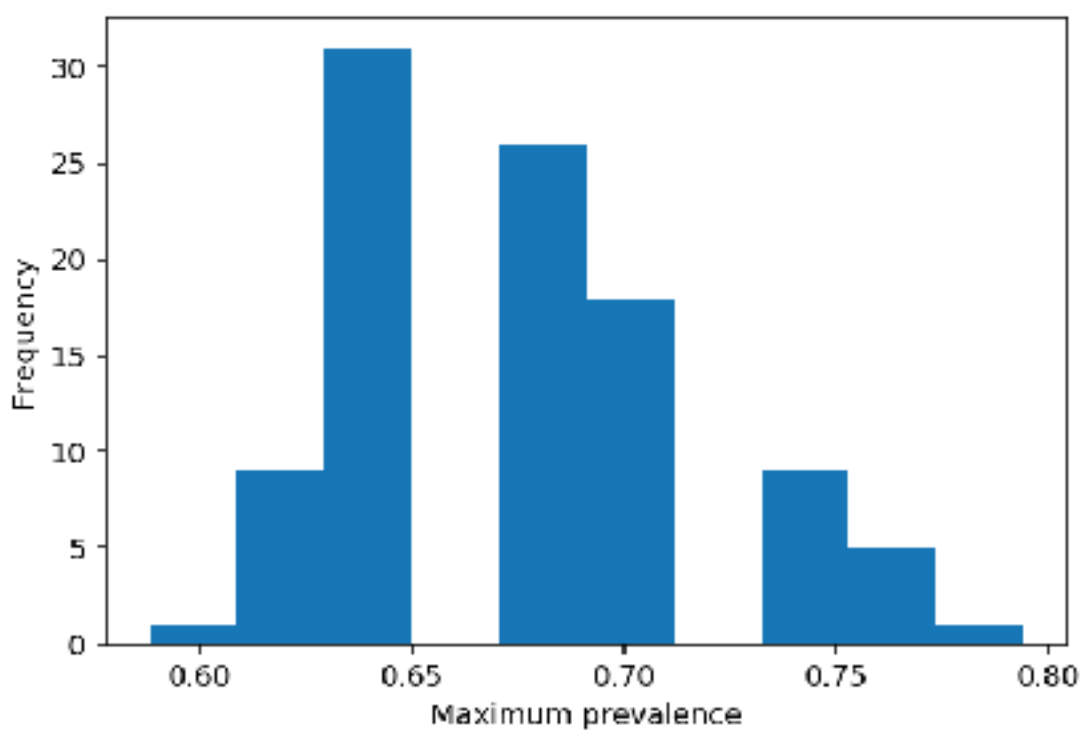
- **Outputs**: maximum prevalence (fraction infected), duration of the epidemic (within the 100 timesteps simulated)

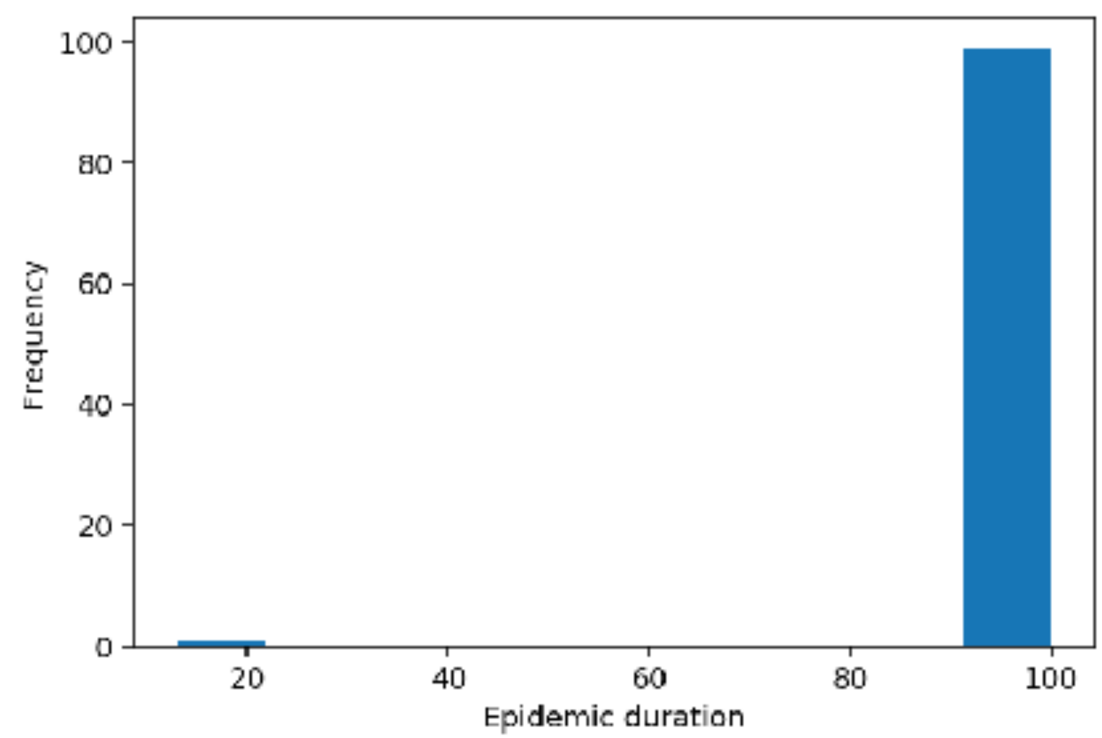
- Pause to work with code

Stochastic variation

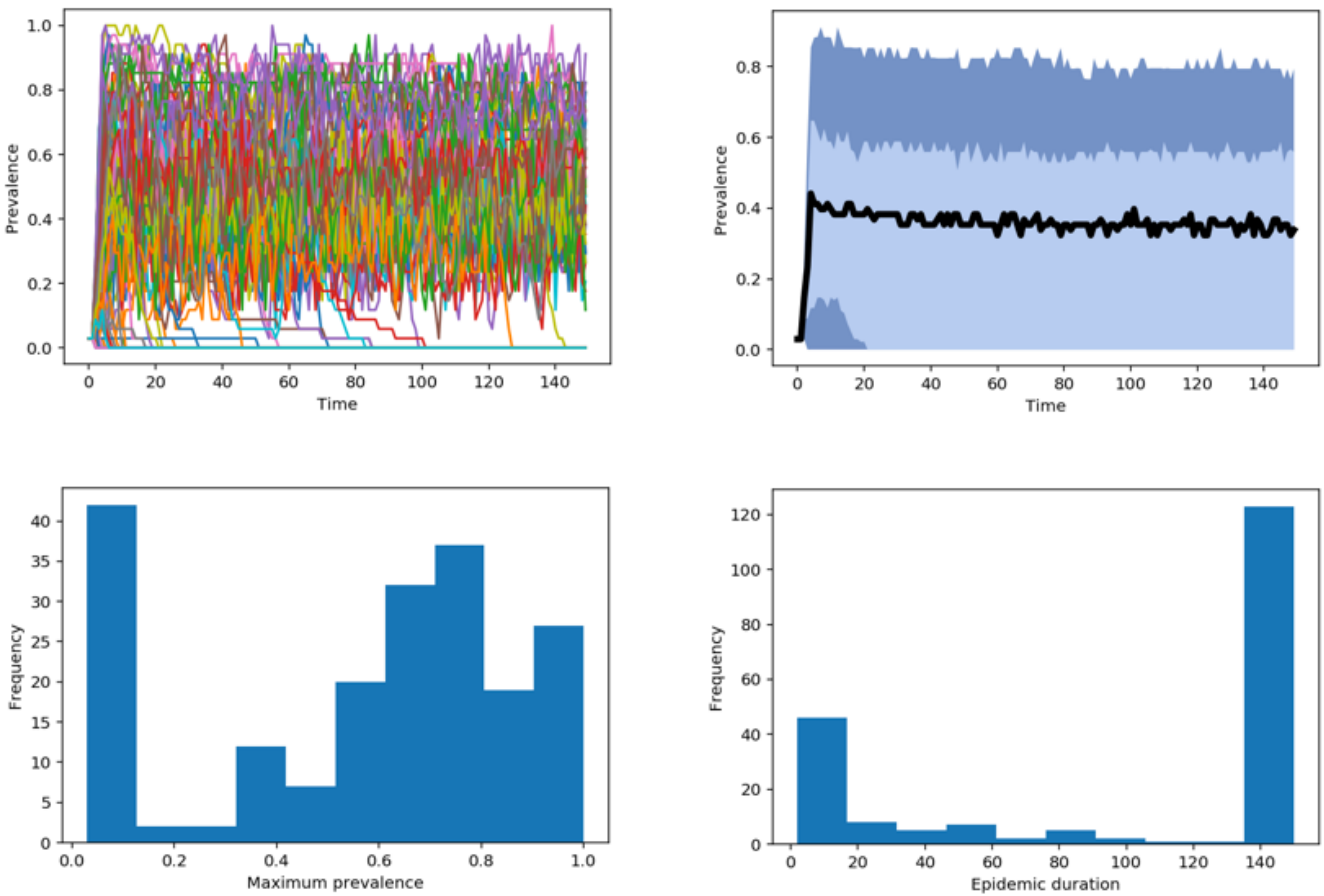




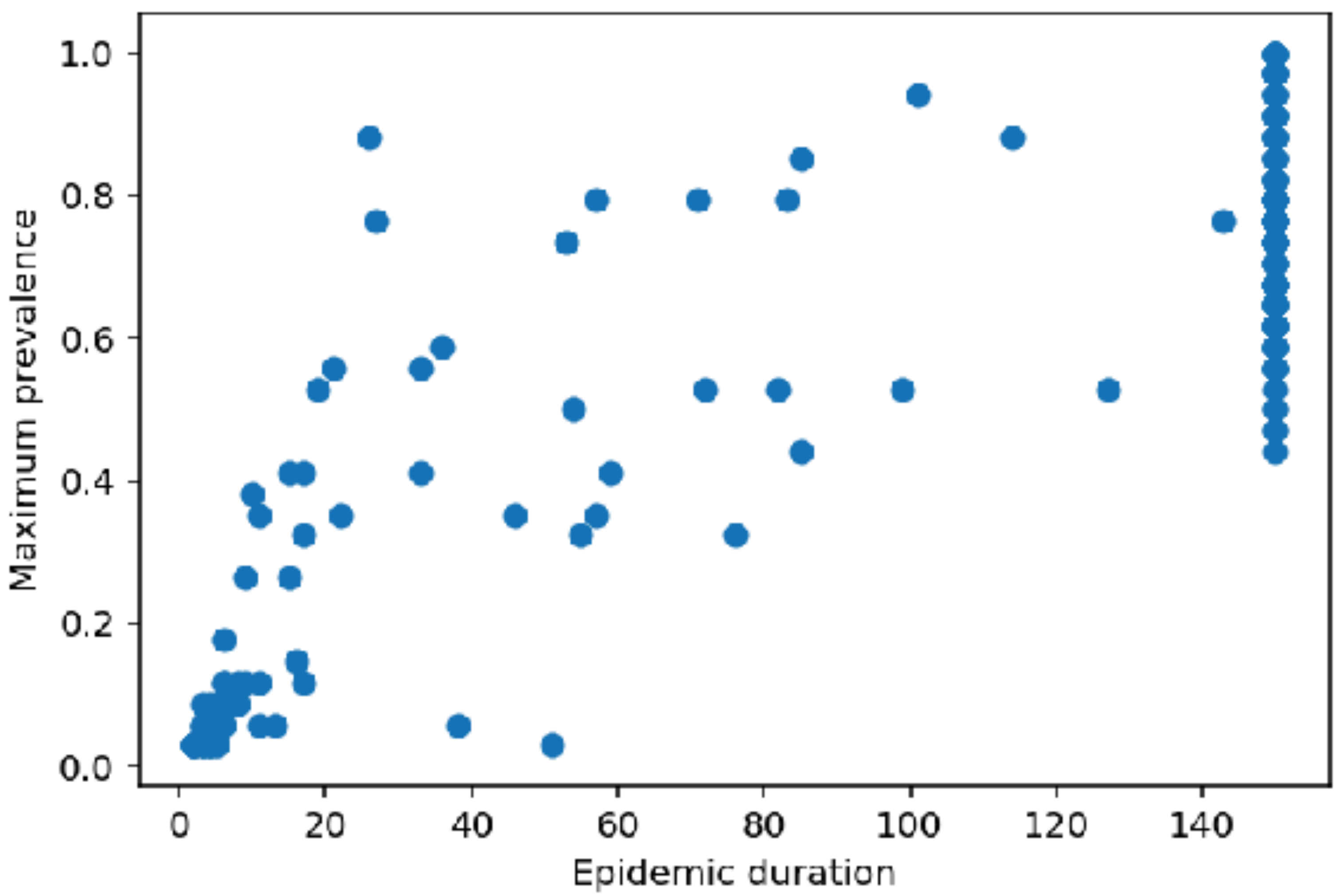


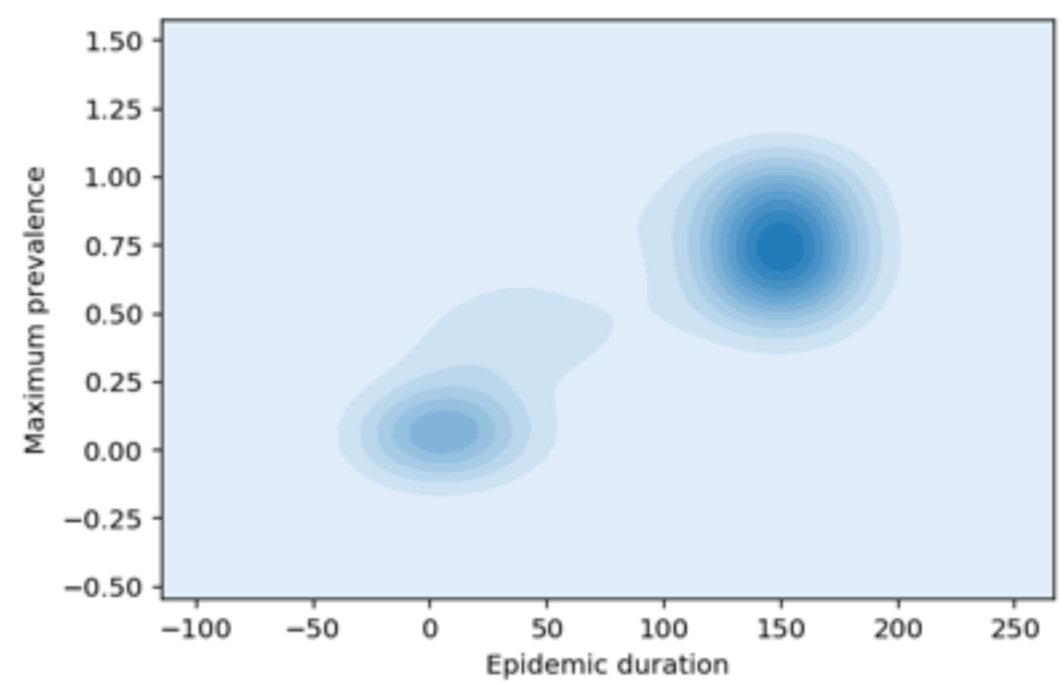


Sampling parameter space



Sampling parameter space





For next time…

- Readings
  - PARTE framework
  - ODD protocol
  - Example ABMs also posted on the website