Lecture 10: Sensitivity analysis

Complex Systems 530

Sensitivity analysis

- Uncertainty quantification: examines the variation in model outputs & behaviors
- **Sensitivity analysis**: examines which inputs/ parameters drive that variation
    - If you change parameter p1, how much change in our output y (or other quantity of interest) do you see?

Goals

- Capture the frequency/distribution of different outputs/behaviors observed across parameter space as a function of the parameters

- Search for extremes/oddities, i.e. potentially uncommon behaviors that match a criteria (e.g. costly, interesting), illustrate the extreme range of behaviors

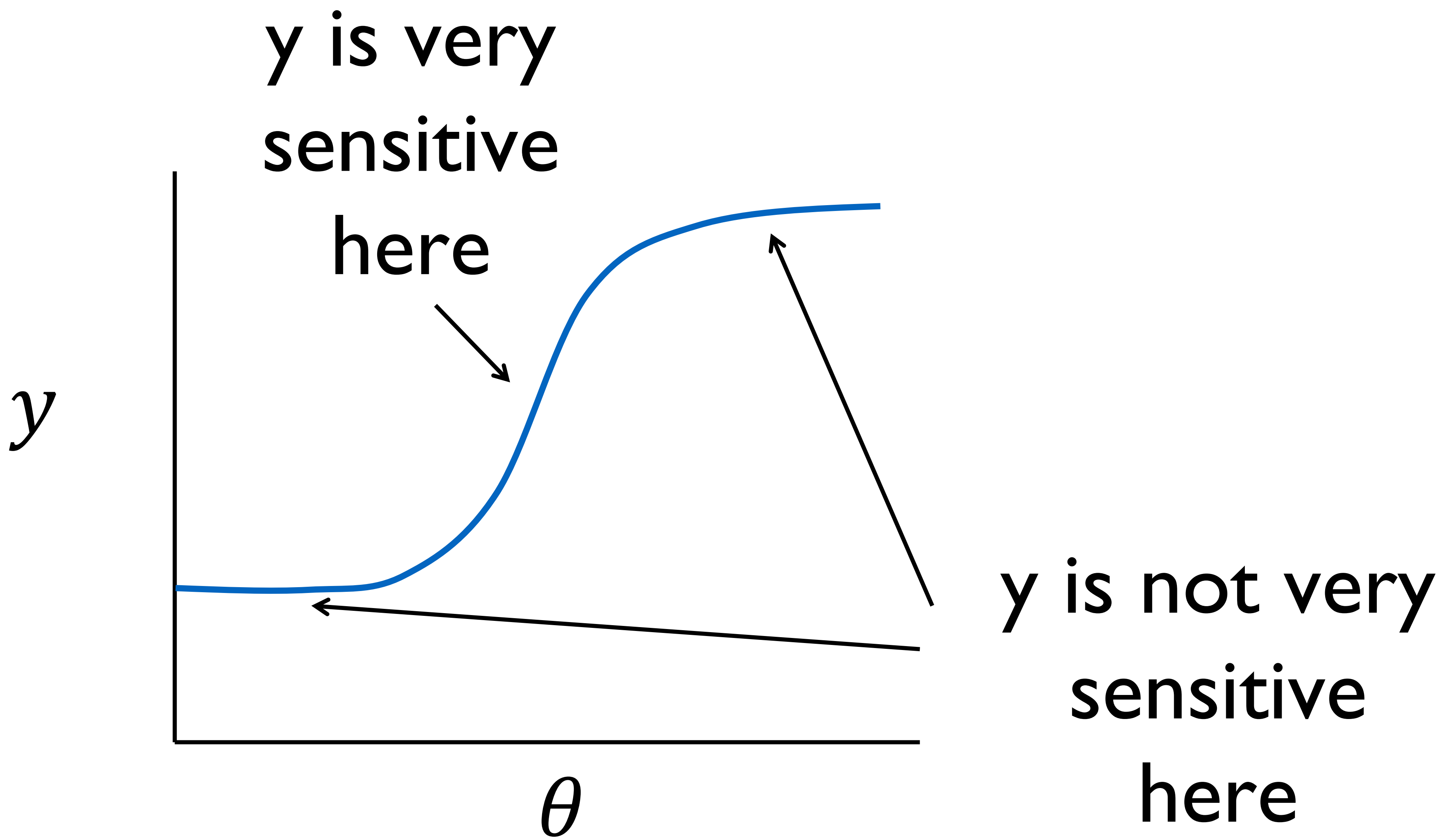
Goals

- Find sensitive/insensitive parameters or parameter combinations
  - Use these to decide what parameters to adjust/tune/intervene on
  - Reduce model complexity by fixing insensitive parameters

Basic setup

- Adjust a parameter or multiple parameters of interest
- Evaluate the model behavior/output
- Look for trends in how output changes as a function of parameters

Sensitivity is inherently a local attribute



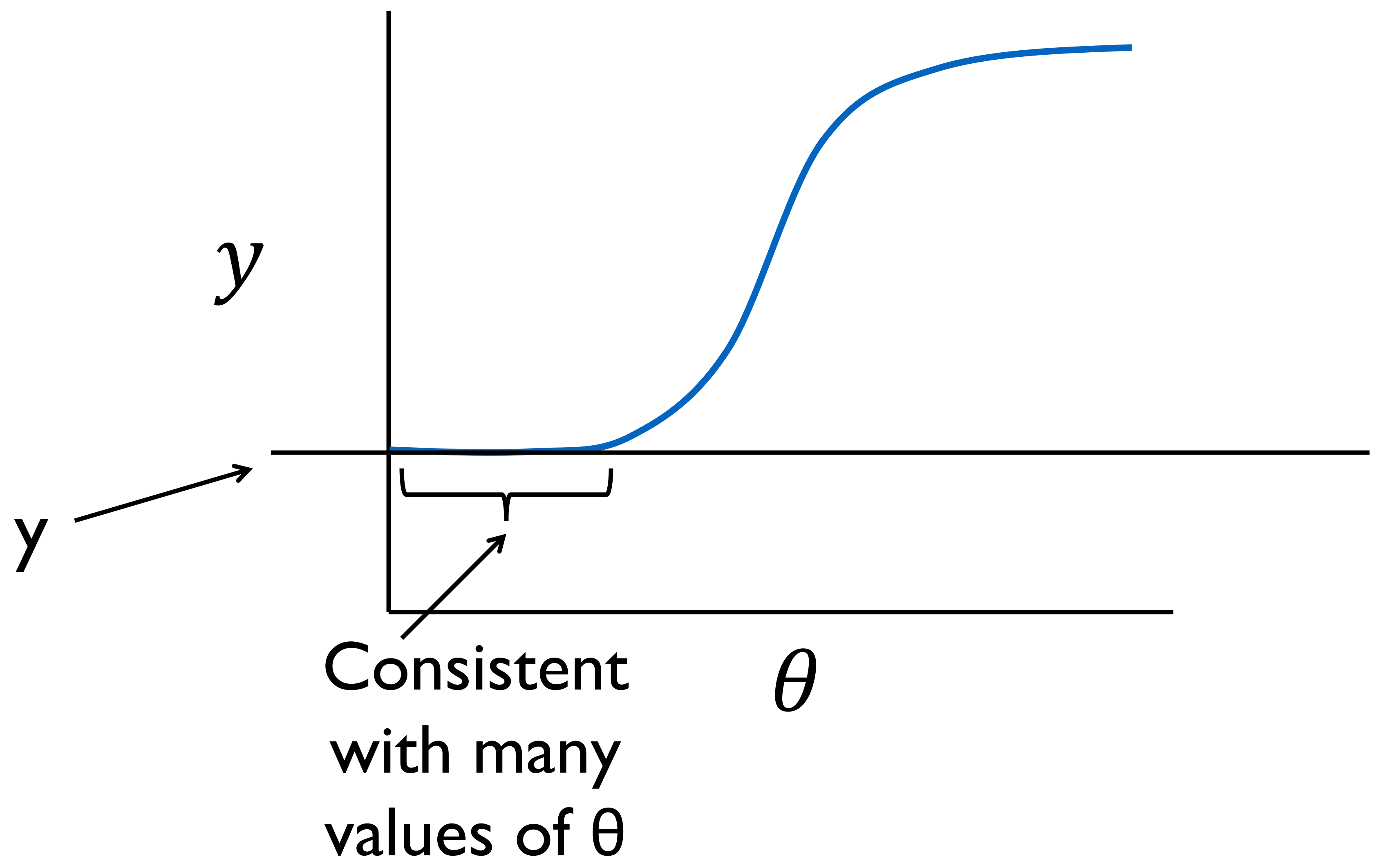
Sensitivity/robustness tradeoff

- How dependent is the model behavior on specific parameter values, initial conditions, inputs?
- Sensitivity - how much does the model output change as a function of the parameter(s)?
- Robustness - is the model able to reproduce similar behavior across a range of parameter space?

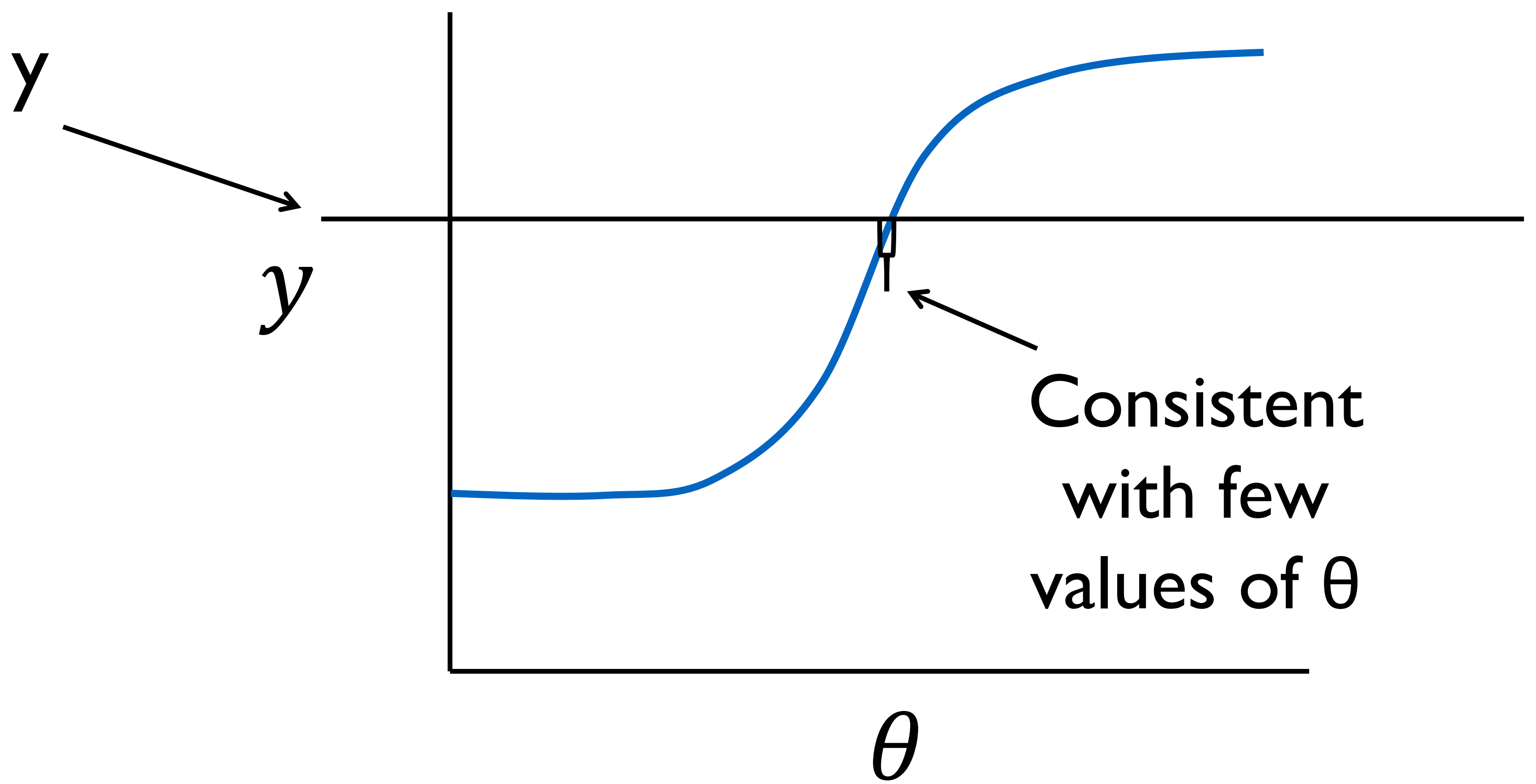
Sensitivity/robustness/ identifiability tradeoff

- When a behavior is robust, we may have more confidence in the behavior—but, this means we cannot be sure of what parameters generated the behavior
  - Unidentifiability
- Similarly, when the output is highly sensitive, we may be better able to infer what parameter conditions must be

Sensitivity/robustness/ identifiability tradeoff



Sensitivity/robustness/ identifiability tradeoff



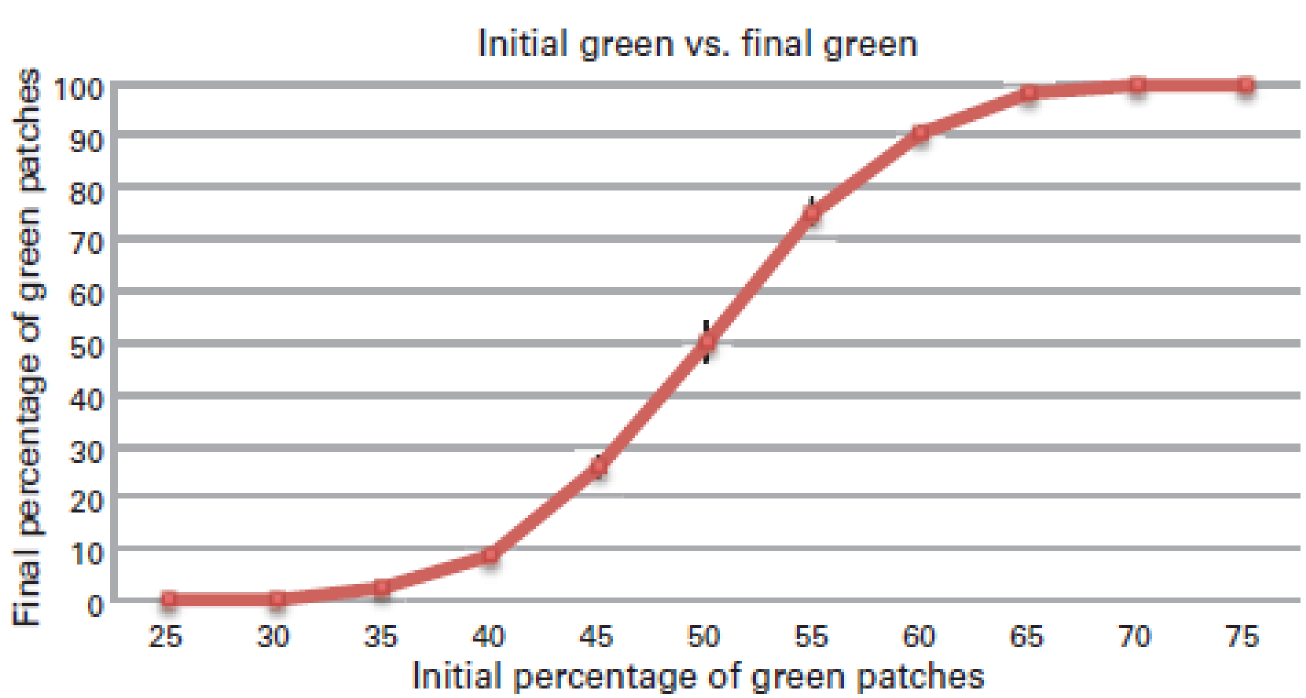
Local Methods

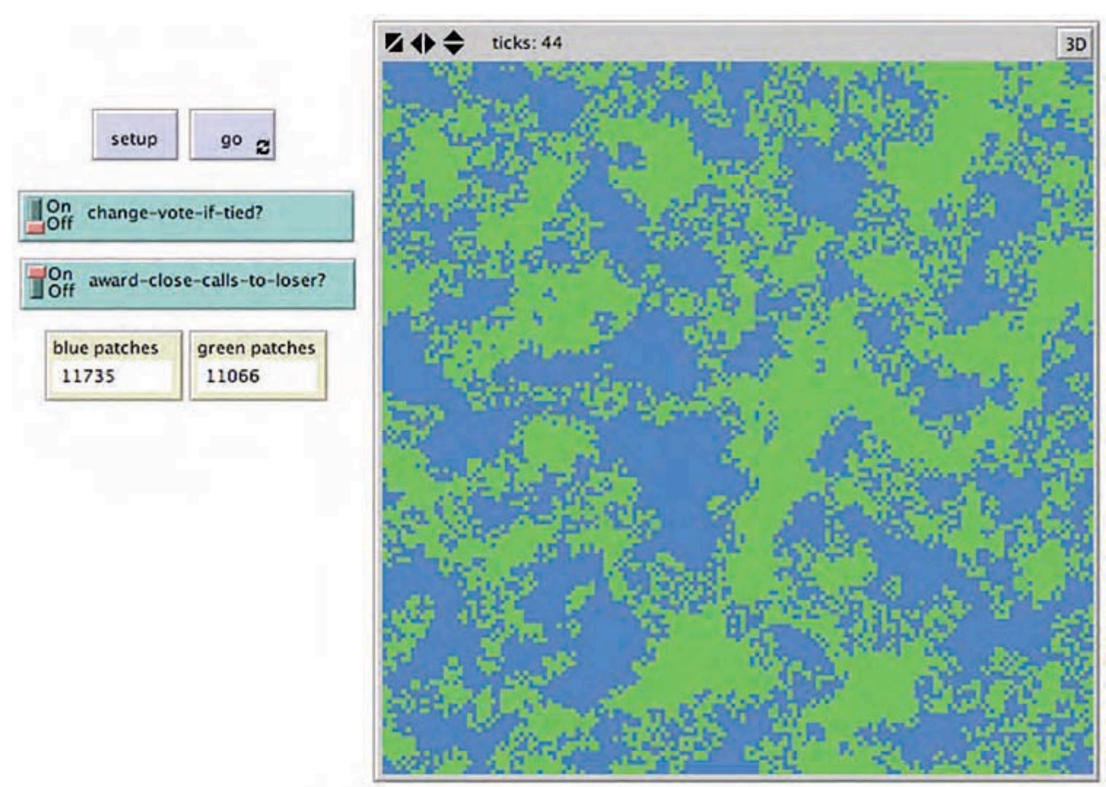
- One-at-a-time approaches
- Derivative methods for local sensitivity

One-at-a-time approach

- Adjust one parameter at a time, fixing the rest to pre-specified values

- Example: voting model initial fraction yes/no





Derivative-based local sensitivity

- Model $\dot{x} = f\left(x, t, p\right)$
- Output $y = g(x, t, p)$

- Output **sensitivity** to parameter variations

$$dy / dp$$

- Meaning depends on magnitude of y and p—often more useful to look at **relative sensitivity**

$$\frac{dy / y}{dp / p} = \frac{dy}{dp}\frac{p}{y}$$

How to calculate local sensitivity?

- Many methods—practically speaking, often done simply by testing small perturbations (e.g. 5% change) of the parameters and seeing how the output changes

$$\frac{dy\,/\,y}{dp\,/\,p} \approx \frac{\Delta y\,/\,y}{\Delta p\,/\,p} = \frac{\%\text{ change in } y}{\%\text{ change in } p}$$

Forward sensitivity equations for ODEs

- Extended ODE system that allows simulation of the model and the sensitivity functions at the same time

$$
\begin{aligned}
\frac{dx}{dt} &= g(t, x(t,\theta), \theta) \\
\frac{d}{dt}\frac{\partial x}{\partial \theta} &= \frac{\partial g}{\partial x}\frac{\partial x}{\partial \theta} + \frac{\partial g}{\partial \theta},
\end{aligned}
$$

- Take your ODE system and apply ∂/∂θ (with chain rule and assuming you can switch derivative order)

SIR model

$$\frac{dS}{dt} = -\beta S \frac{I}{N}$$
$$\frac{dI}{dt} = \beta S \frac{I}{N} - \gamma I$$
$$\frac{dR}{dt} = \gamma I$$

y = I(t)

- We assume the initial conditions $(S(0), I(0), R(0))$ and the population size N are known.
- The vector of model parameters is $\theta = (\beta, \gamma)$.
- The basic reproductive number is $\mathcal{R}_0 = \beta/\gamma$. Whenever $\beta/\gamma > 1$ then an outbreak occurs.

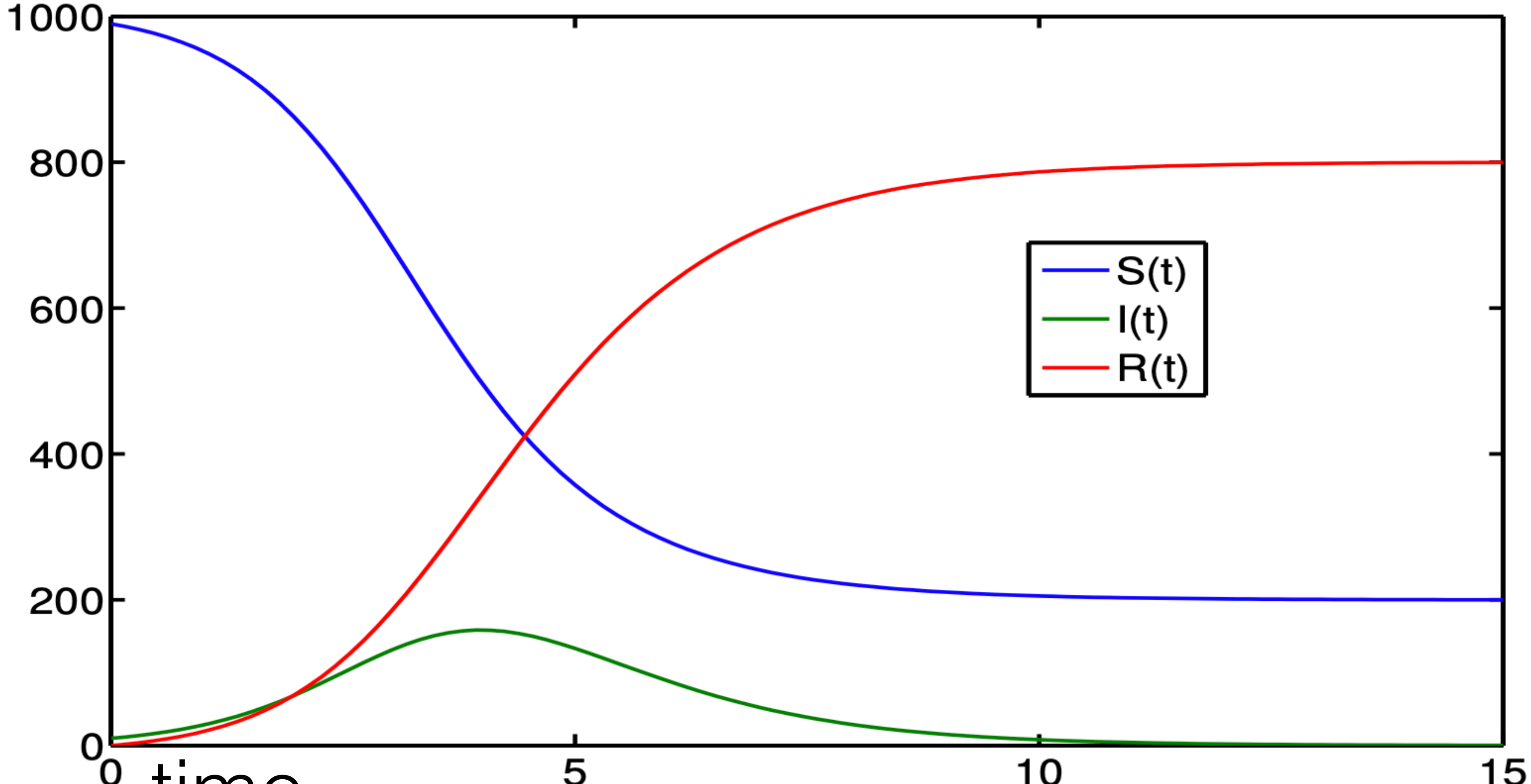
Borrowed from Ariel Cintron-Arias NIMBioS 2014 Parameter Estimation Tutorial

$$\frac{dS}{dt} = -\beta S \frac{I}{N}$$

$$\frac{dI}{dt} = \beta S \frac{I}{N} - \gamma I$$

$$\frac{dR}{dt} = \gamma I$$

y = I(t)



time

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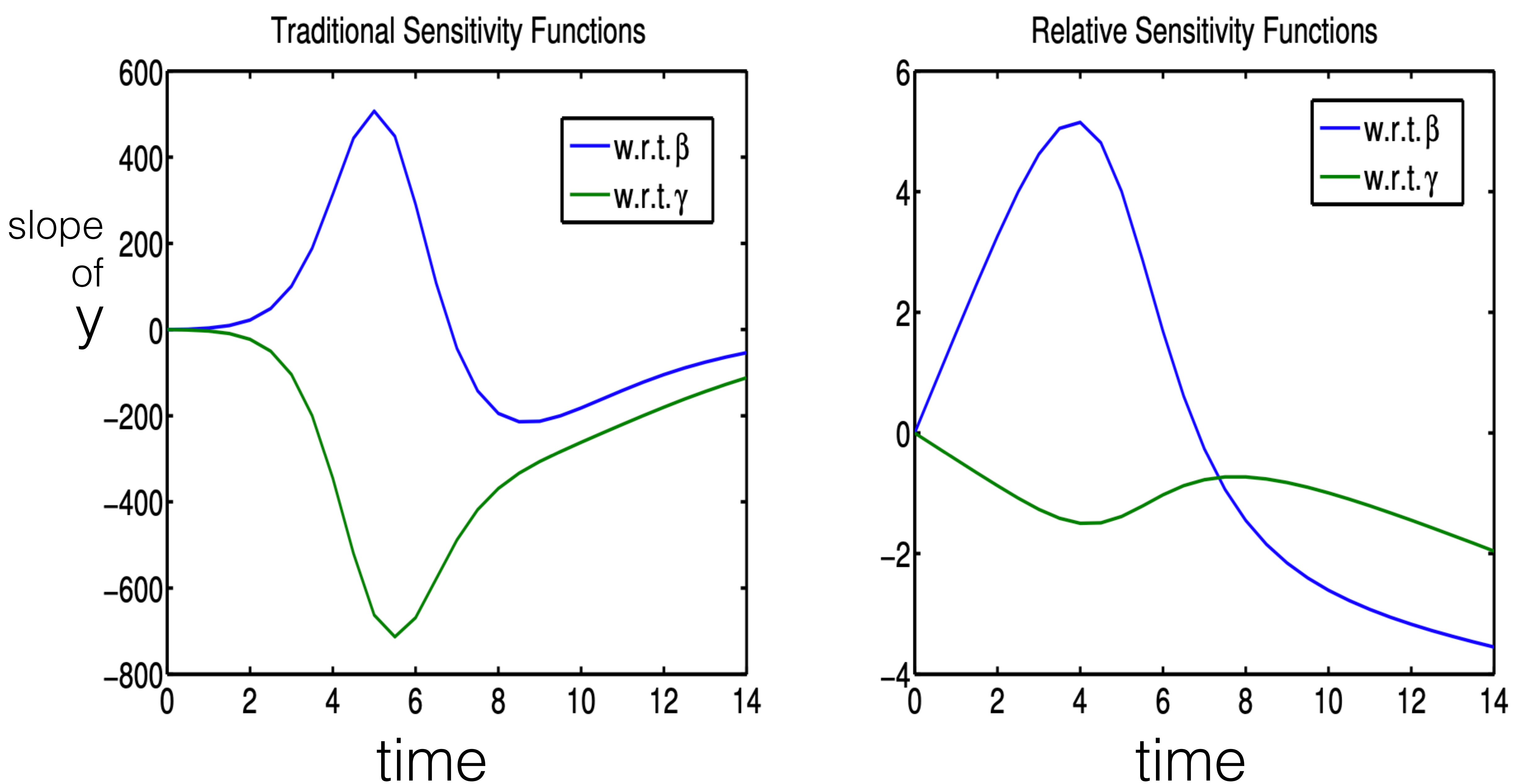
$$\begin{aligned} \frac{d}{dt}x(t) &= g(x(t,\hat{\theta}),\hat{\theta}), \\ \frac{d}{dt}\phi(t) &= \frac{\partial g}{\partial x}\phi(t) + \frac{\partial g}{\partial \theta}, \end{aligned}$$

where $\phi(t) = \frac{\partial x}{\partial \theta}(t,\theta)$, $\frac{\partial g}{\partial x} = \begin{bmatrix} -\hat{\beta}\frac{I}{N} & -\hat{\beta}\frac{S}{N} & 0 \\ \hat{\beta}\frac{I}{N} & \hat{\beta}\frac{S}{N} - \hat{\gamma} & 0 \\ 0 & \hat{\gamma} & 0 \end{bmatrix}$ and

$$\frac{\partial g}{\partial \theta} = \begin{bmatrix} -S\frac{I}{N} & 0 \\ S\frac{I}{N} & -I \\ 0 & I \end{bmatrix}.$$

Borrowed from Ariel Cintron-Arias NIMBioS 2014 Parameter Estimation Tutorial

Sensitivity functions



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Sensitivity Analysis

- Sensitivity is inherently a local attribute
- But often we want to know about **global sensitivity** over a wide range of values of θ
- Especially when we have a lot of parameters and want to drop some insensitive ones
- Helps to know where to allocate resources in general for a variety of scenarios

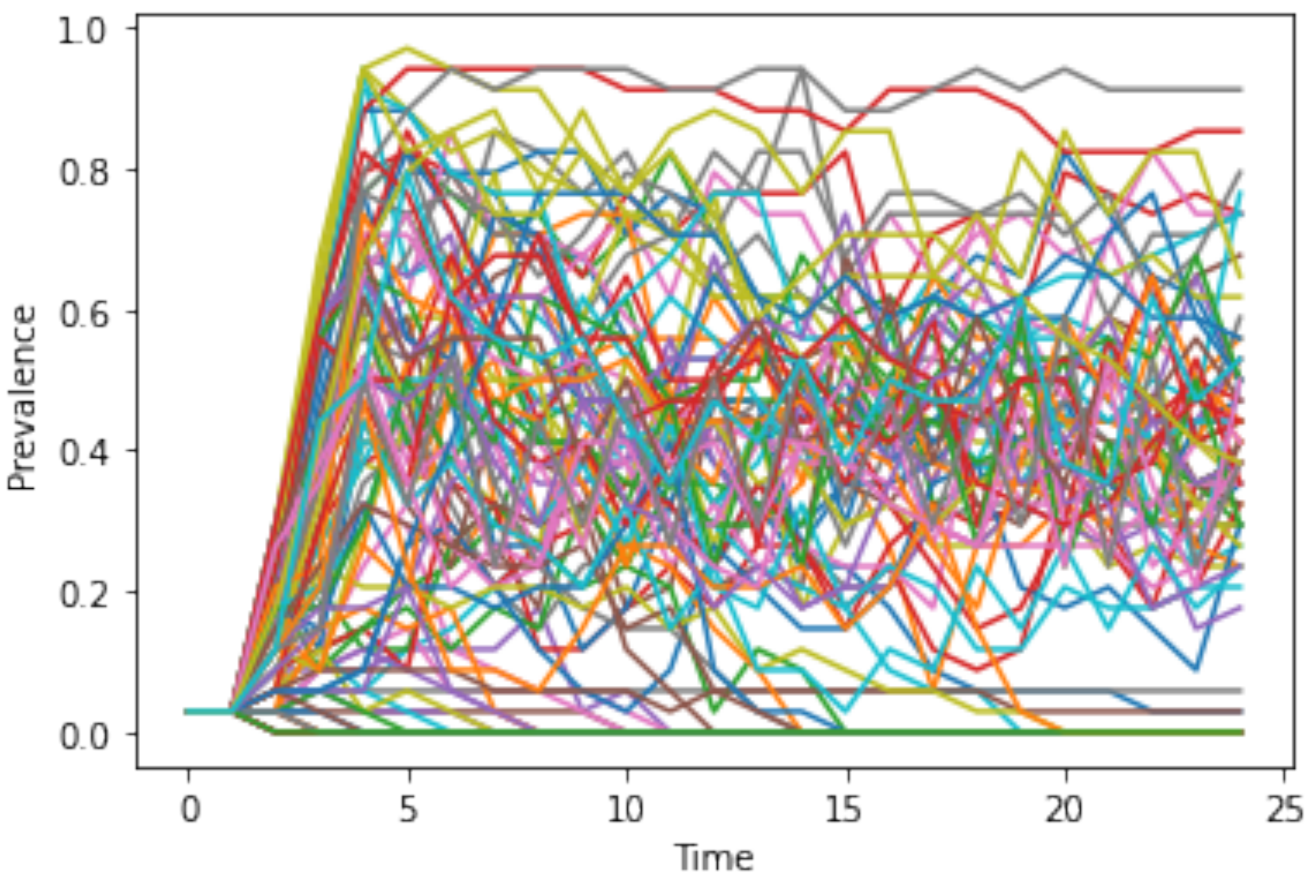
Global Methods

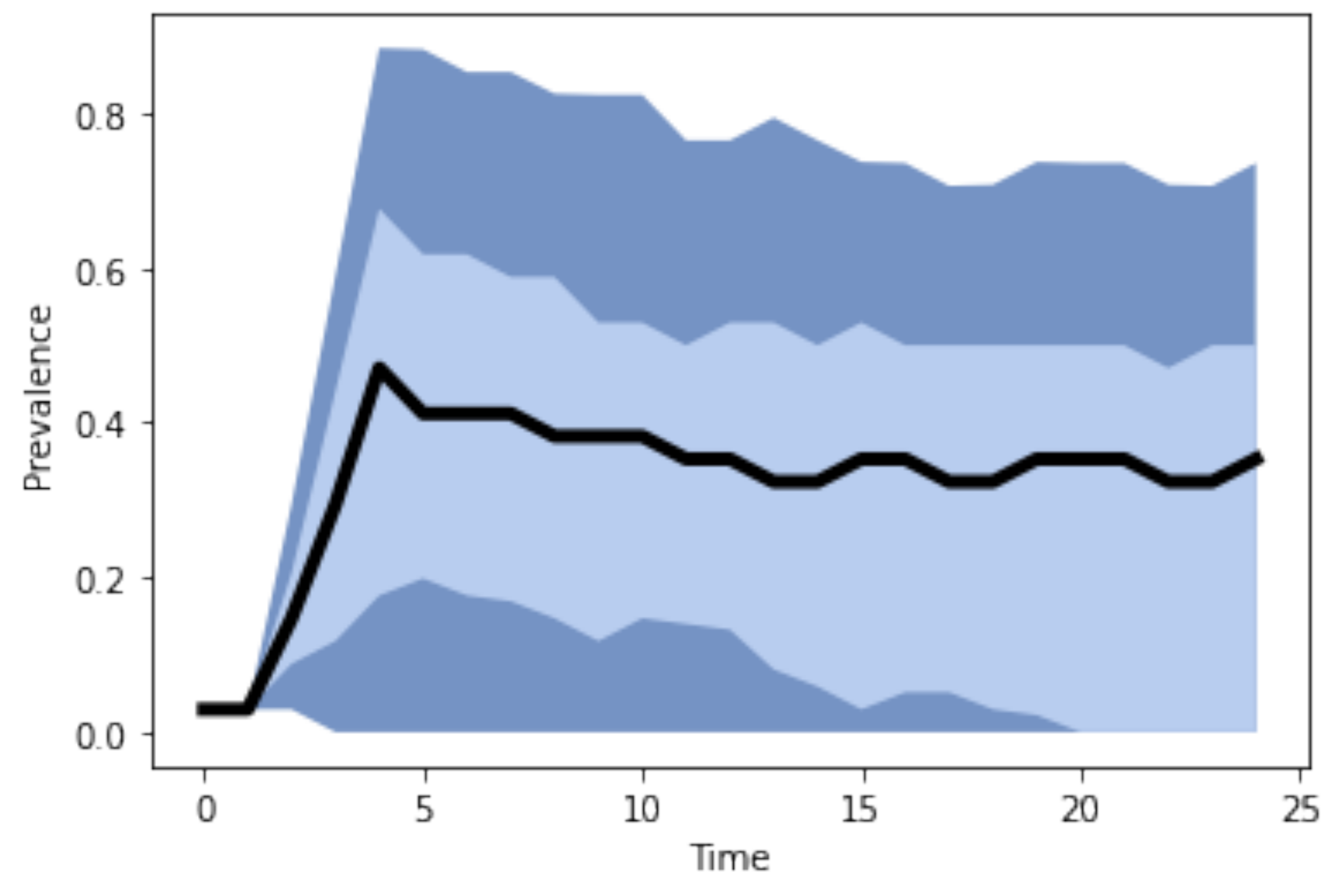
- Sampling-based methods
  - Visual approaches! (sample and look at scatterplots, etc.)
  - Regression-based methods
  - Variance-based methods

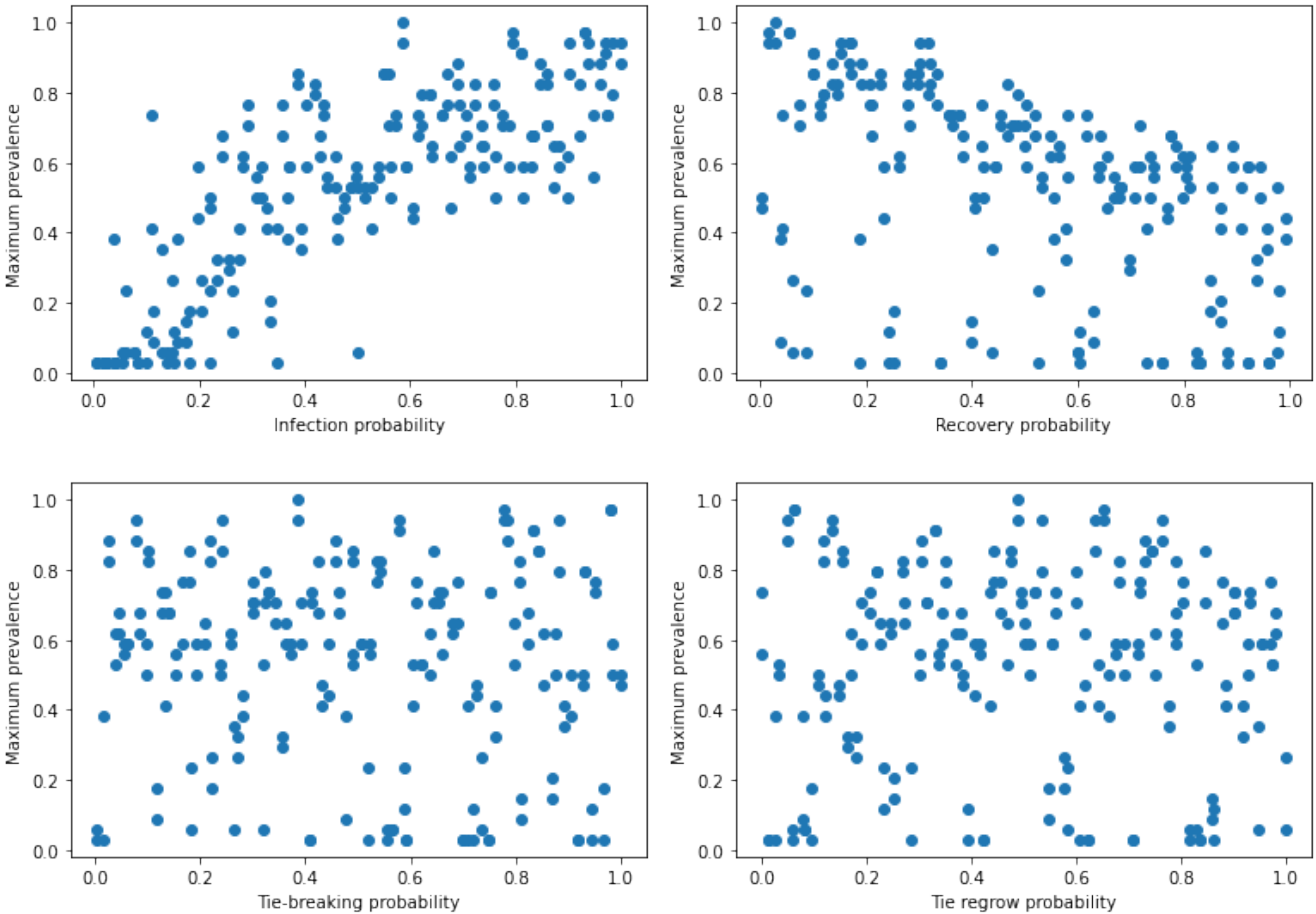
Sampling & visualization

- Sample parameter space, then plot relationships between parameters and model output(s)
- Example: SIS model on the karate club network with tie breaking and regrowth

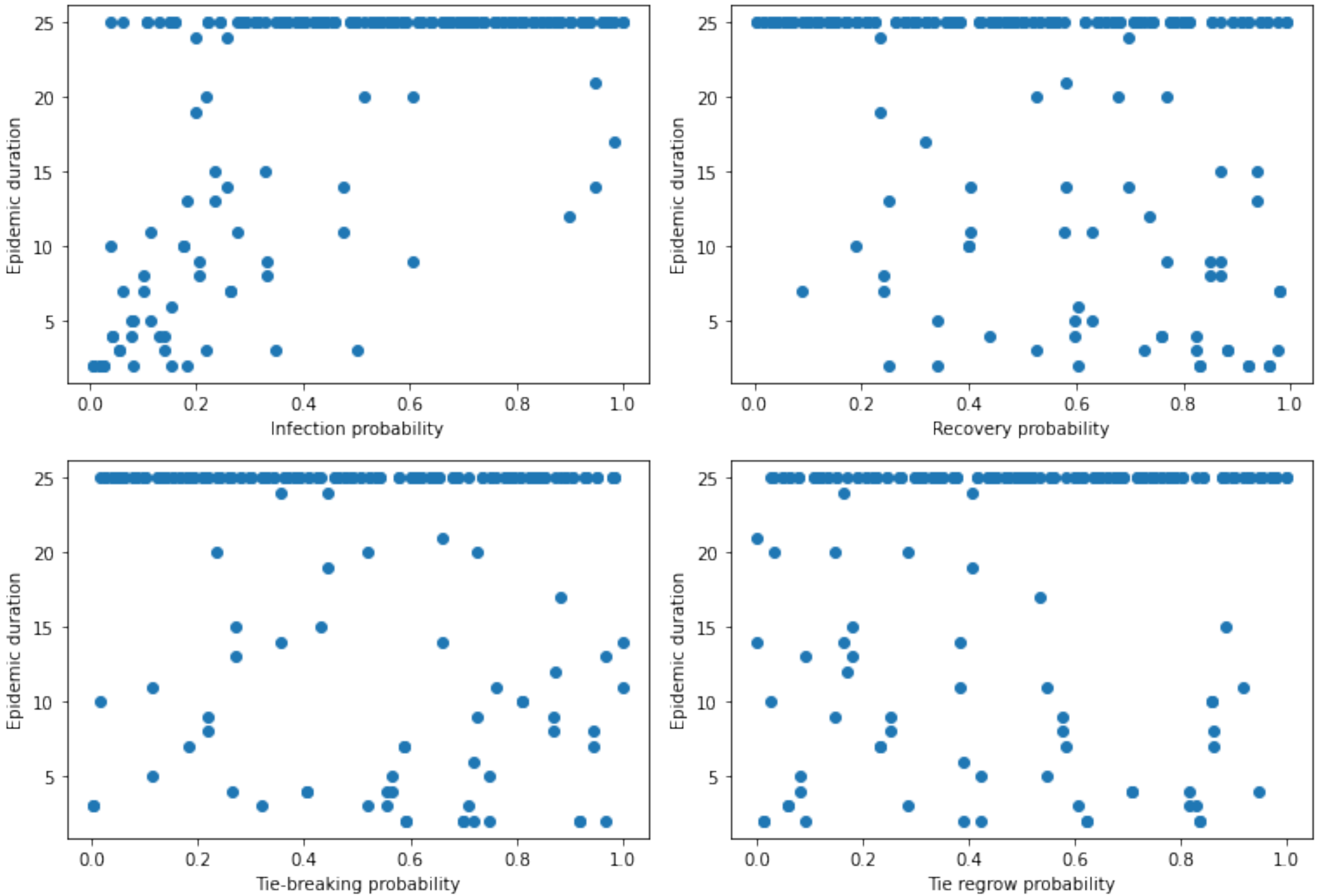
Model dynamics



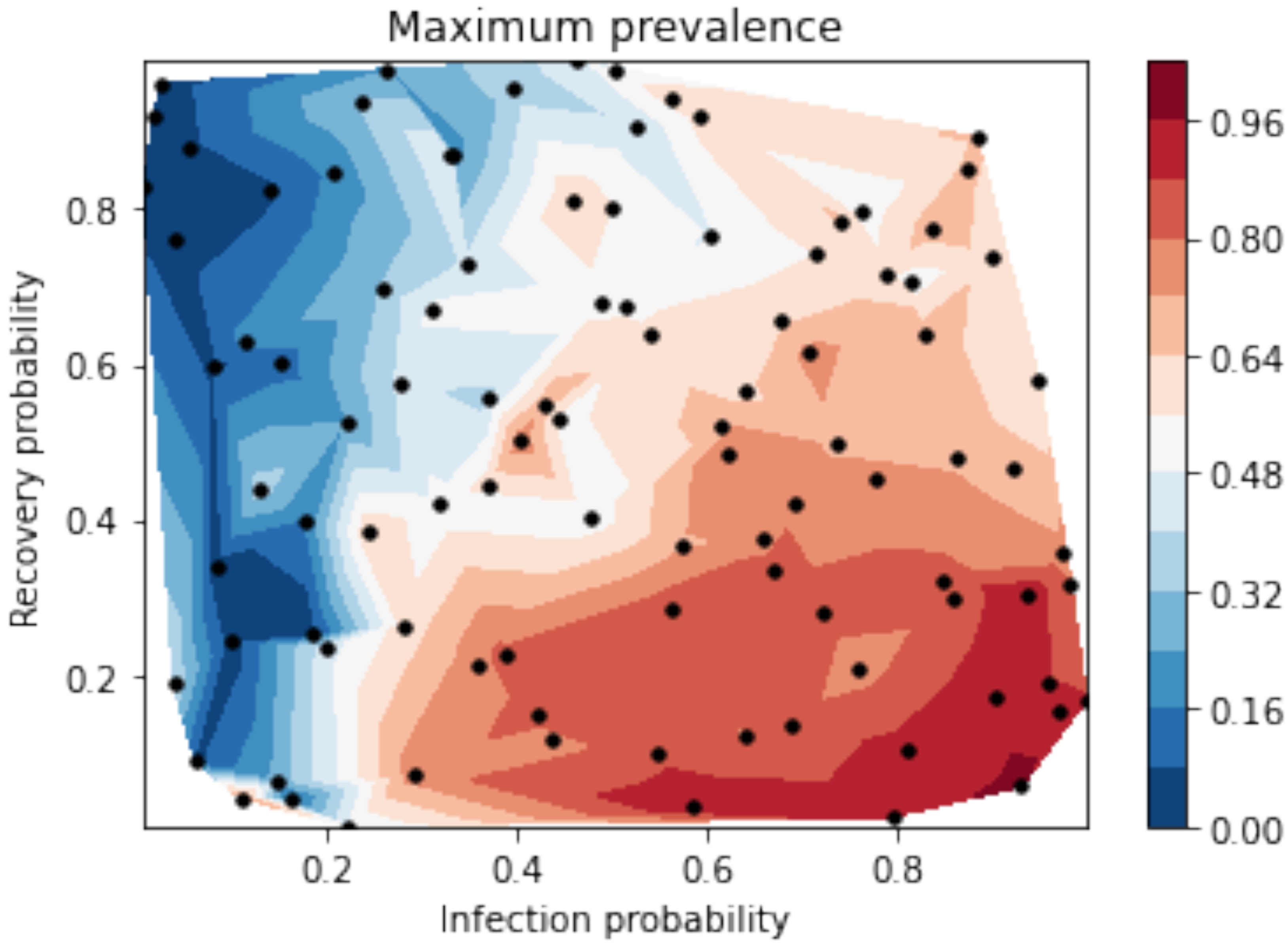


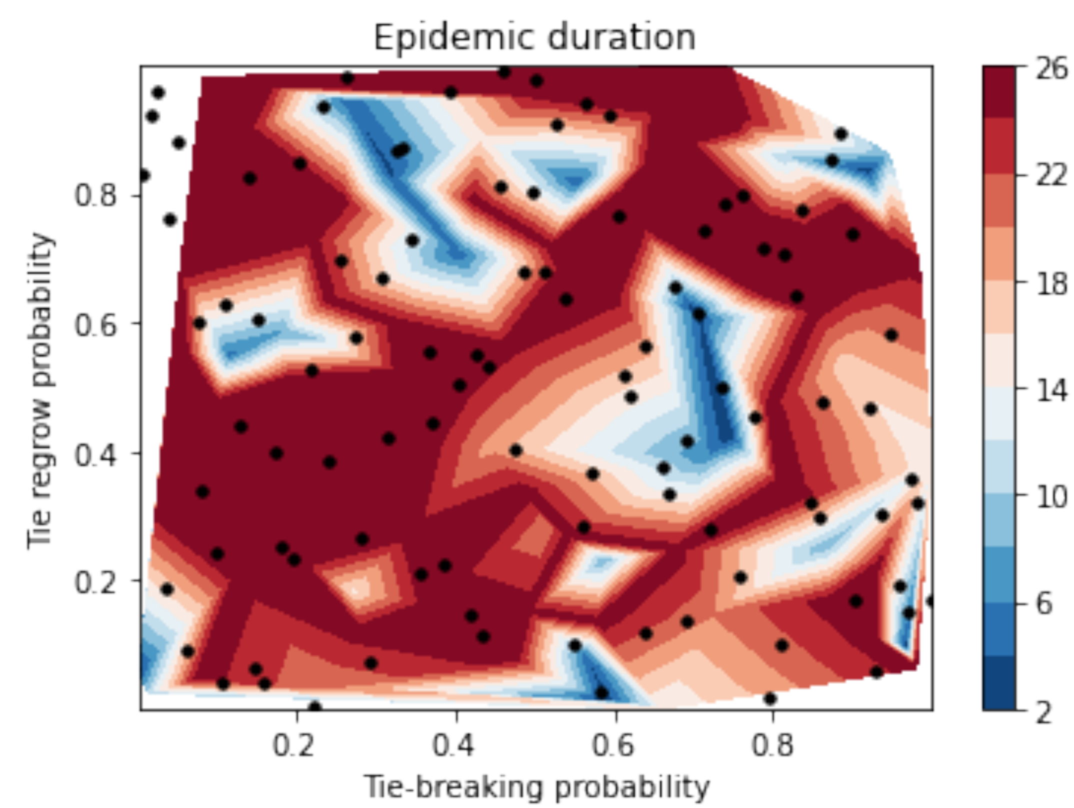


Maximum prevalence
Infection probability
Recovery probability
Tie-breaking probability
Tie regrow probability
0.0
0.2
0.4
0.6
0.8
1.0

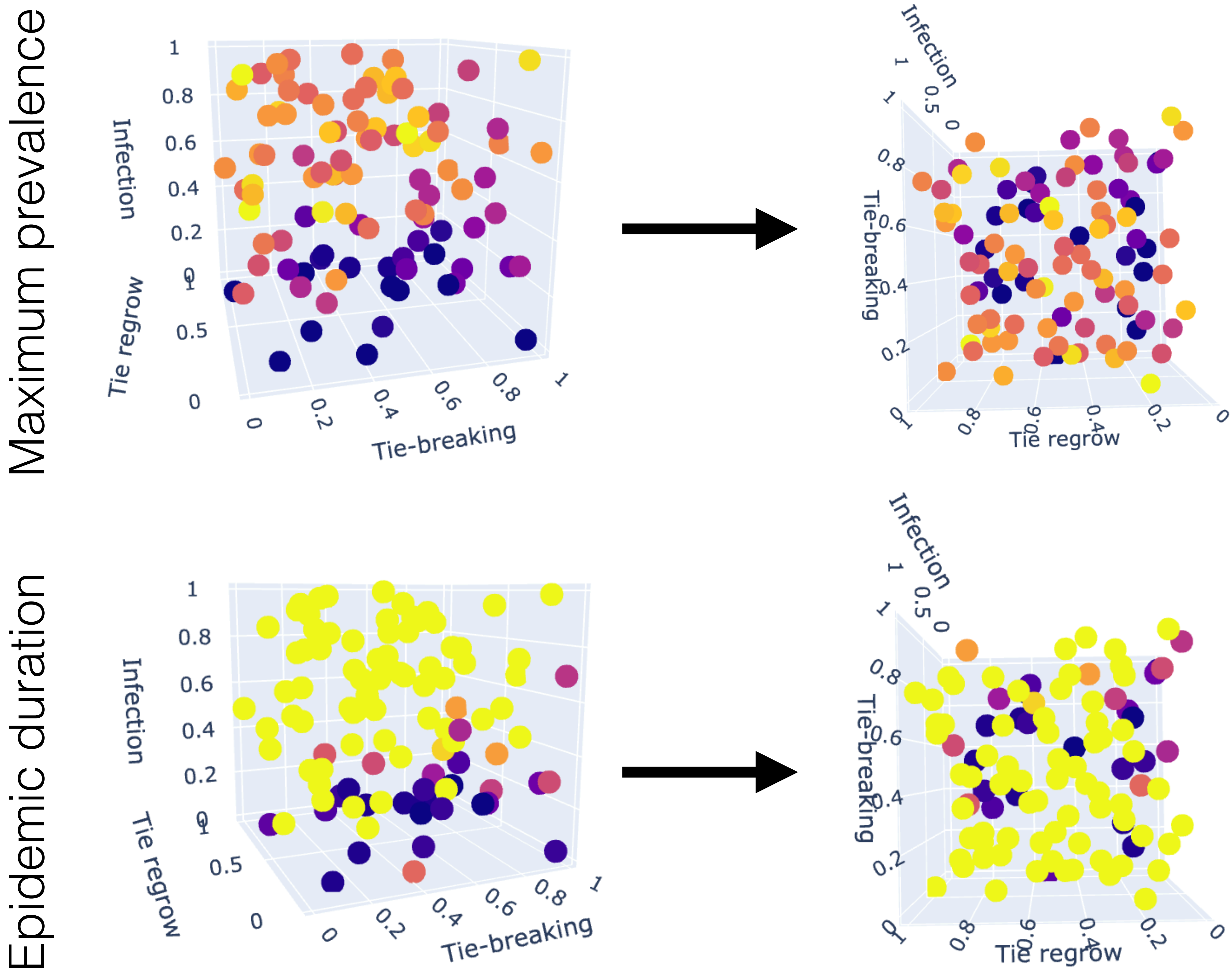


Epidemic duration
Infection probability
Recovery probability
Tie-breaking probability
Tie regrow probability
0.0
0.2
0.4
0.6
0.8
1.0
5
10
15
20
25





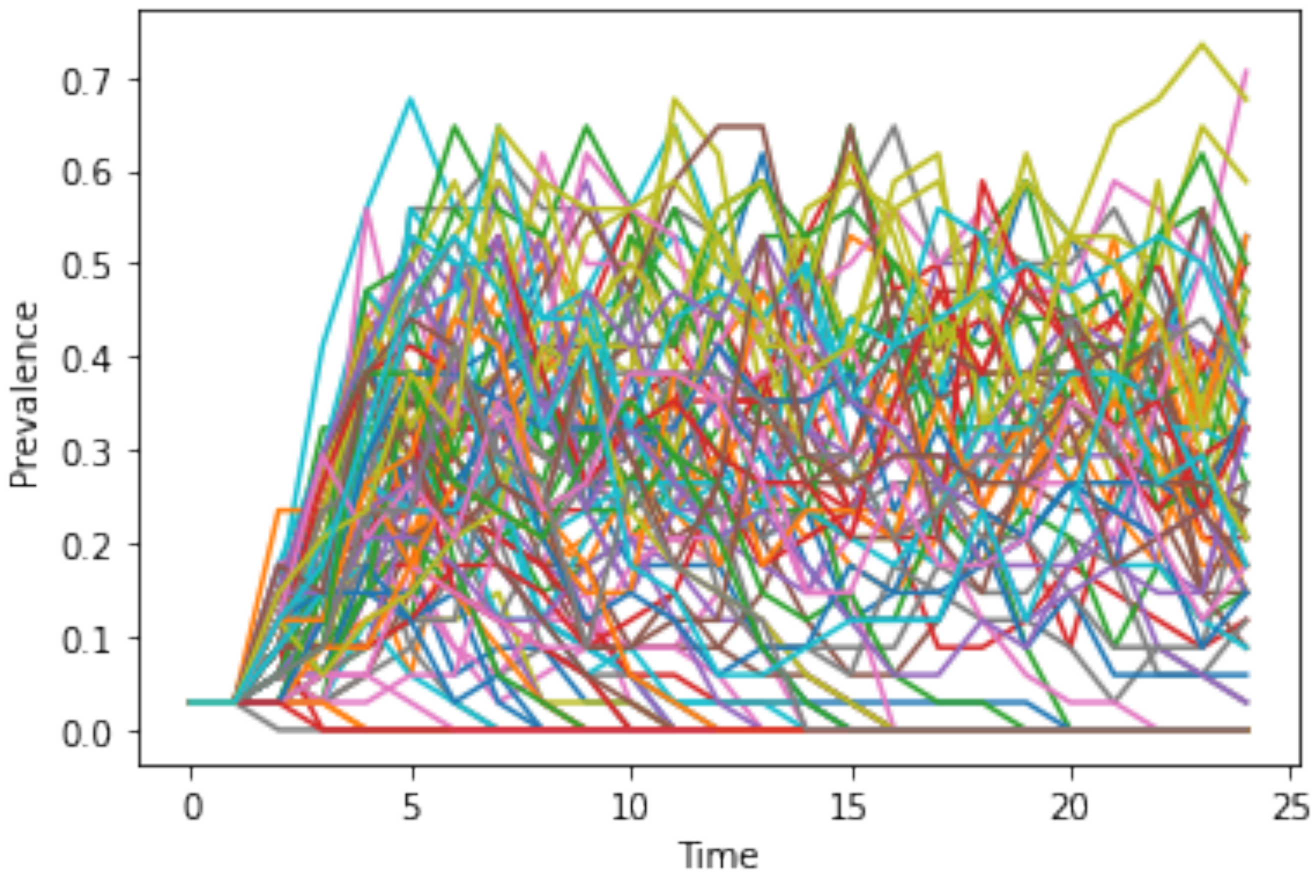
Tie breaking/regrowth—hard to see the effects because the other parameter values matter strongly

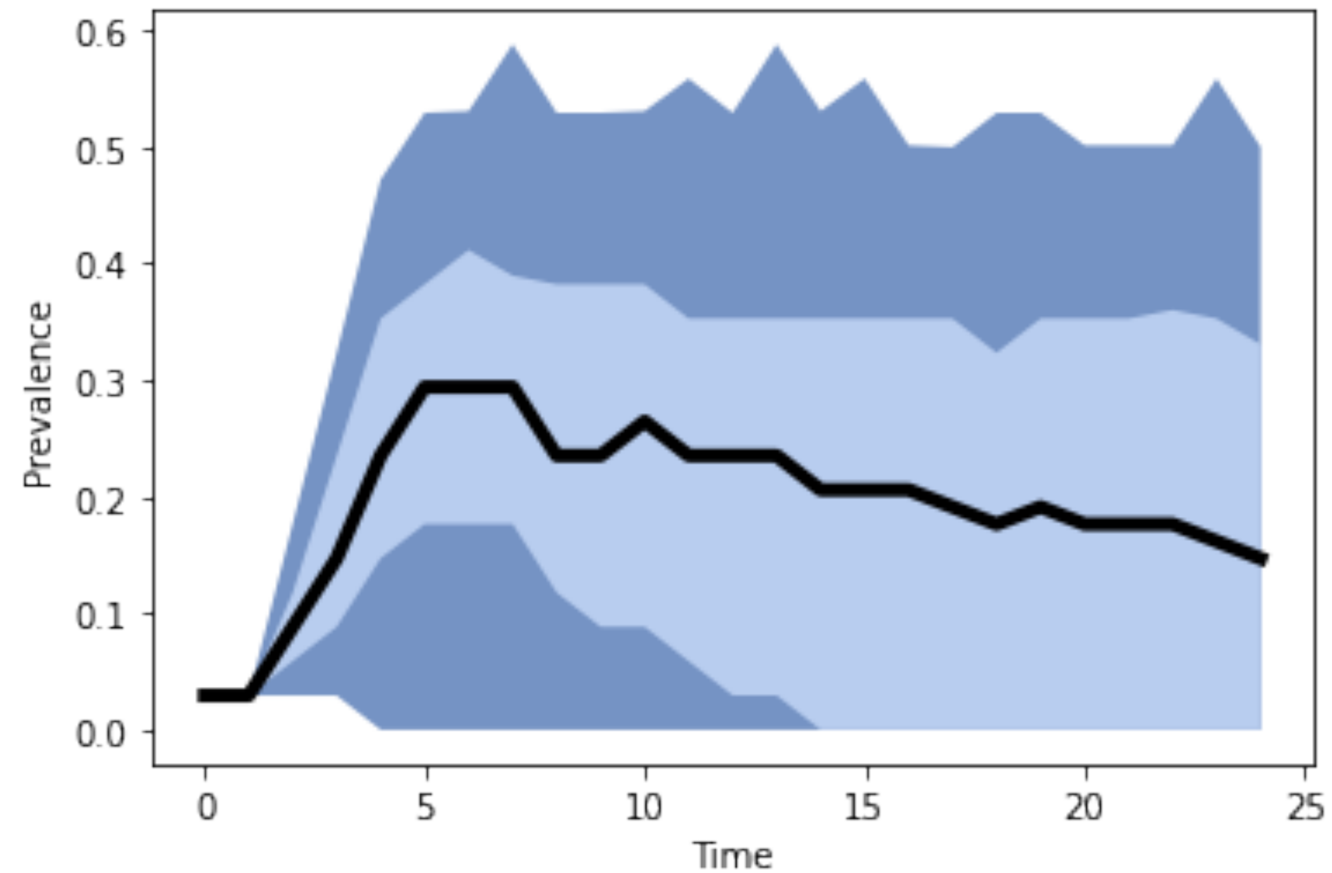


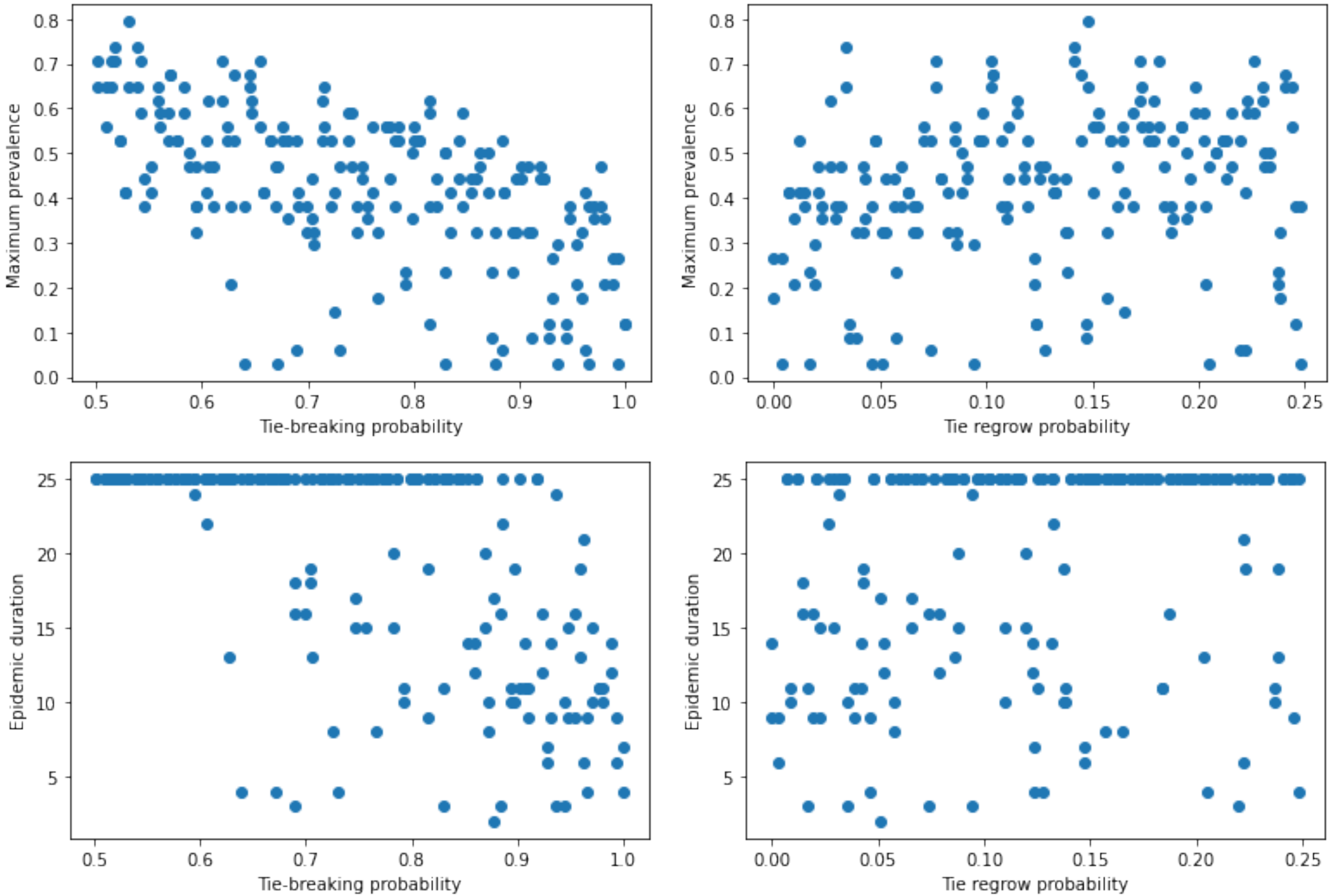
Maximum prevalence
Epidemic duration
Infection
Tie regrow
Tie-breaking

Try with a more restricted parameter range

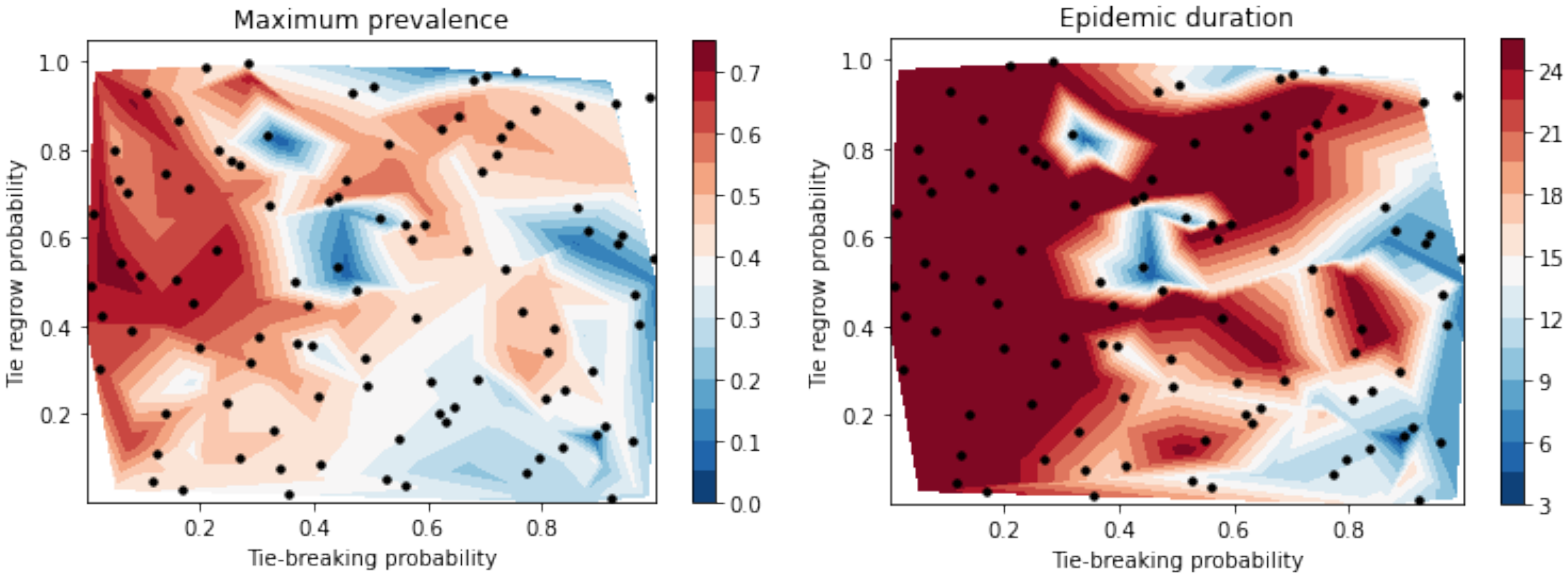
```
p_i = params[i,0]*0.2 + 0.2 # infection probability per contact - restrict to the range [0.2,0.4]
p_r = params[i,1]*0.2 + 0.4 # recovery probability - restrict to the range [0.4,0.6]
p_0 = params[i,2] # probability of breaking tie if infected neighbor
p_1 = params[i,3] # probability of regrowing tie if non-infected
```





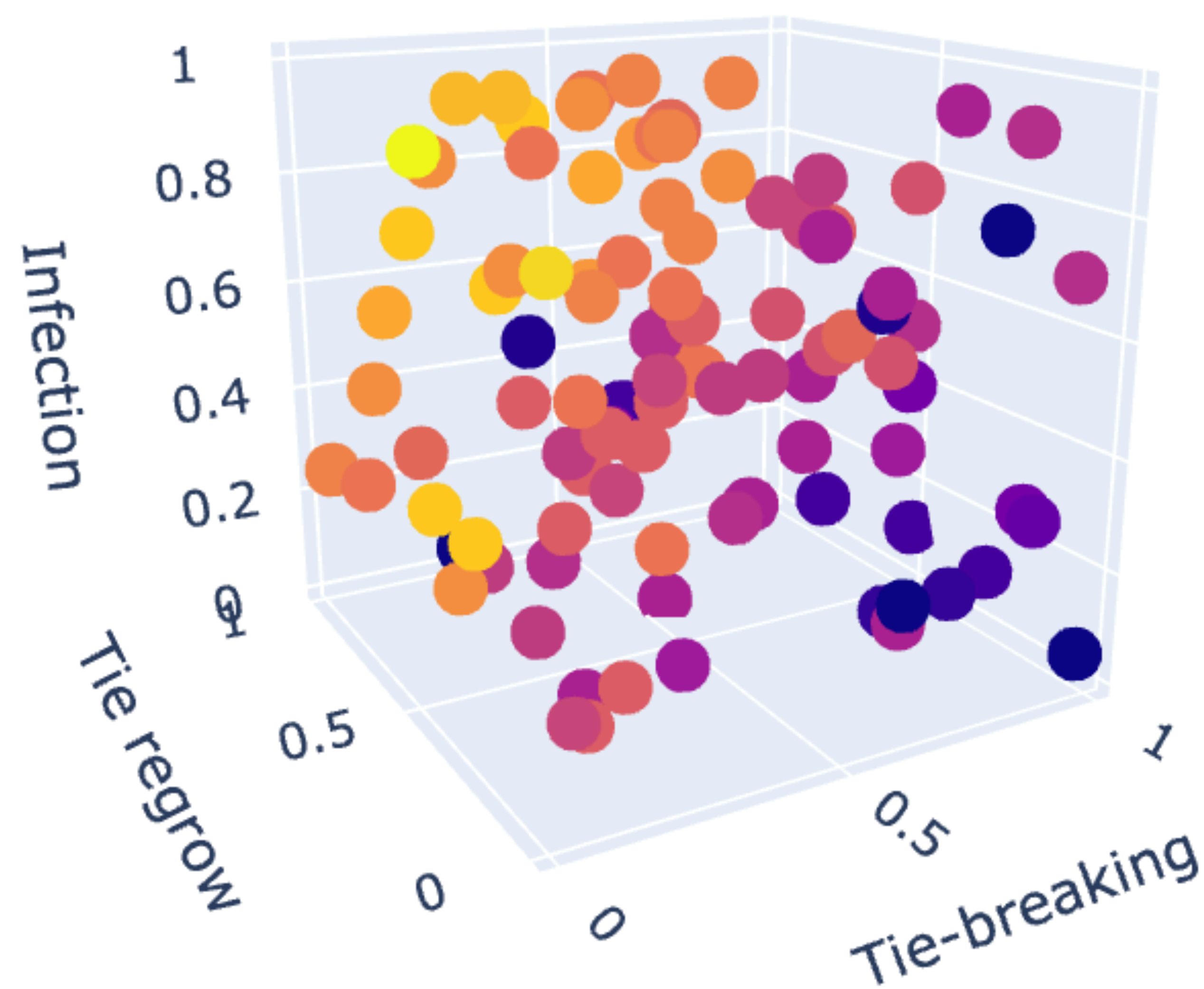


Maximum prevalence
Tie-breaking probability
Maximum prevalence
Tie regrow probability
Epidemic duration
Tie-breaking probability
Epidemic duration
Tie regrow probability



Maximum prevalence
Tie regrow probability
Tie-breaking probability
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
Epidemic duration
Tie regrow probability
Tie-breaking probability
3
6
9
12
15
18
21
24

Maximum prevalence



Regression based methods

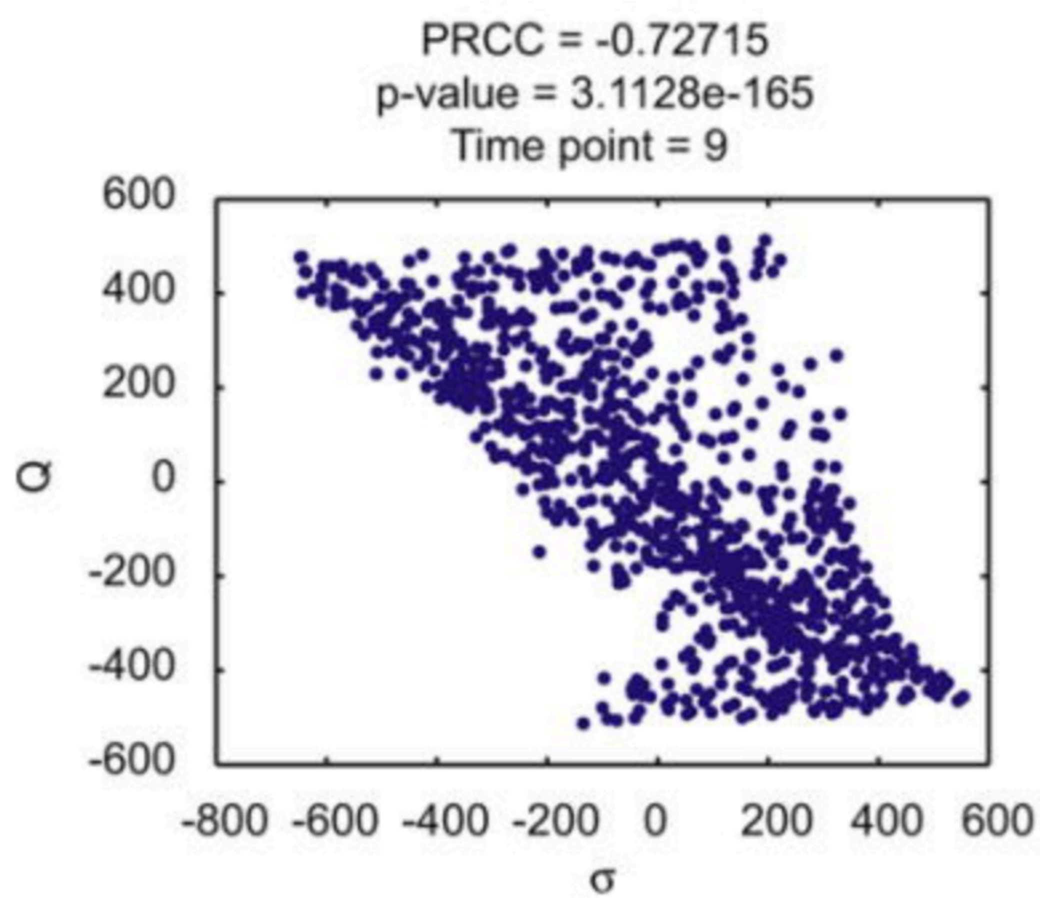
- Fit linear trend to the data
- Pearson correlation coefficient - correlate parameter and output
    - However, only works for linear relationships
- For nonlinear but monotonic relationships, rank-based correlation coefficients are often useful (draw example)

Partial rank correlation coefficient

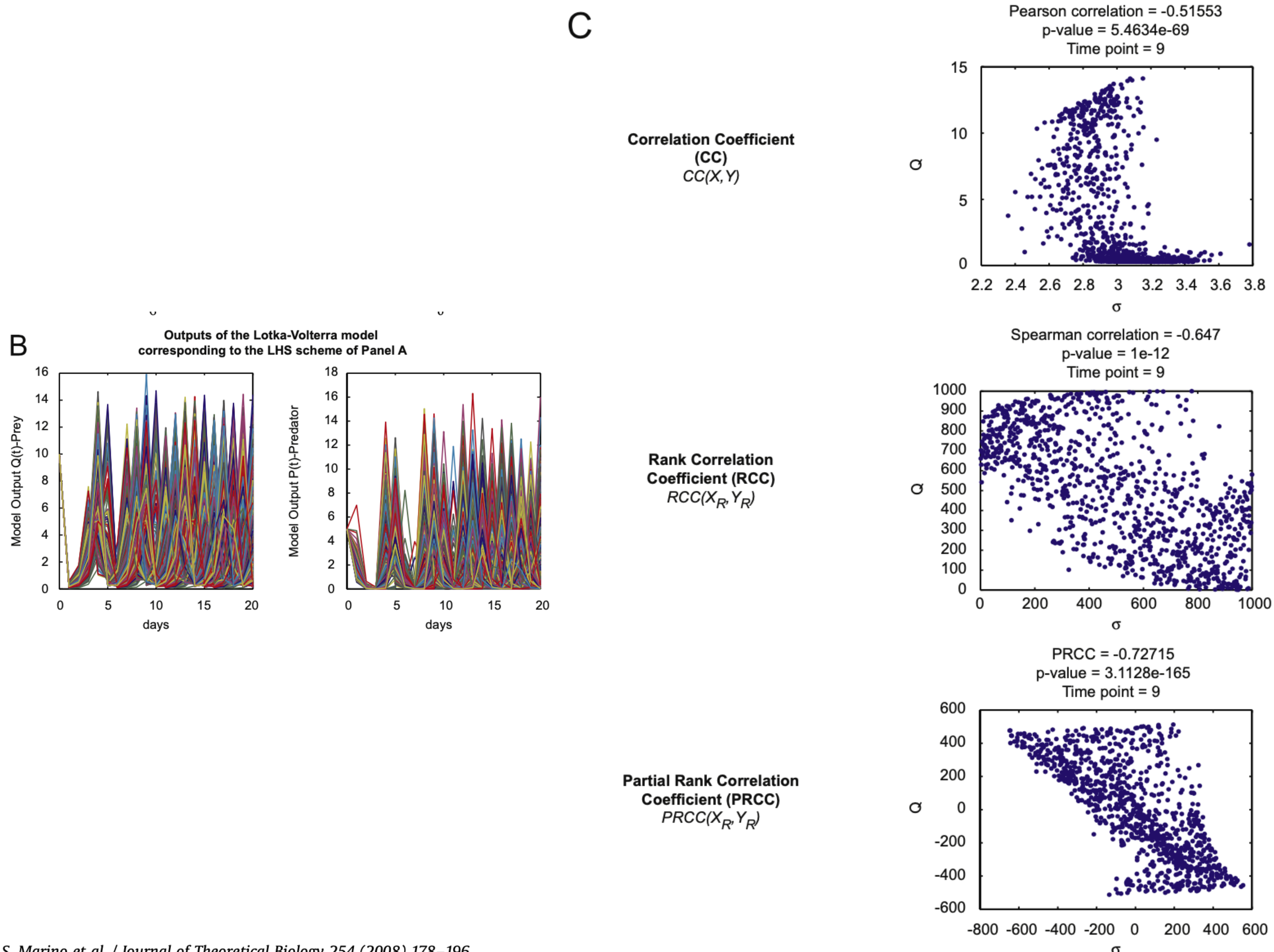
- A rank correlation coefficient that accounts for the effects of the other parameters

- Requires a generally monotonic relationship (allowing for noise) with the output

Partial Rank Correlation Coefficient (PRCC)
$PRCC(X_R, Y_R)$



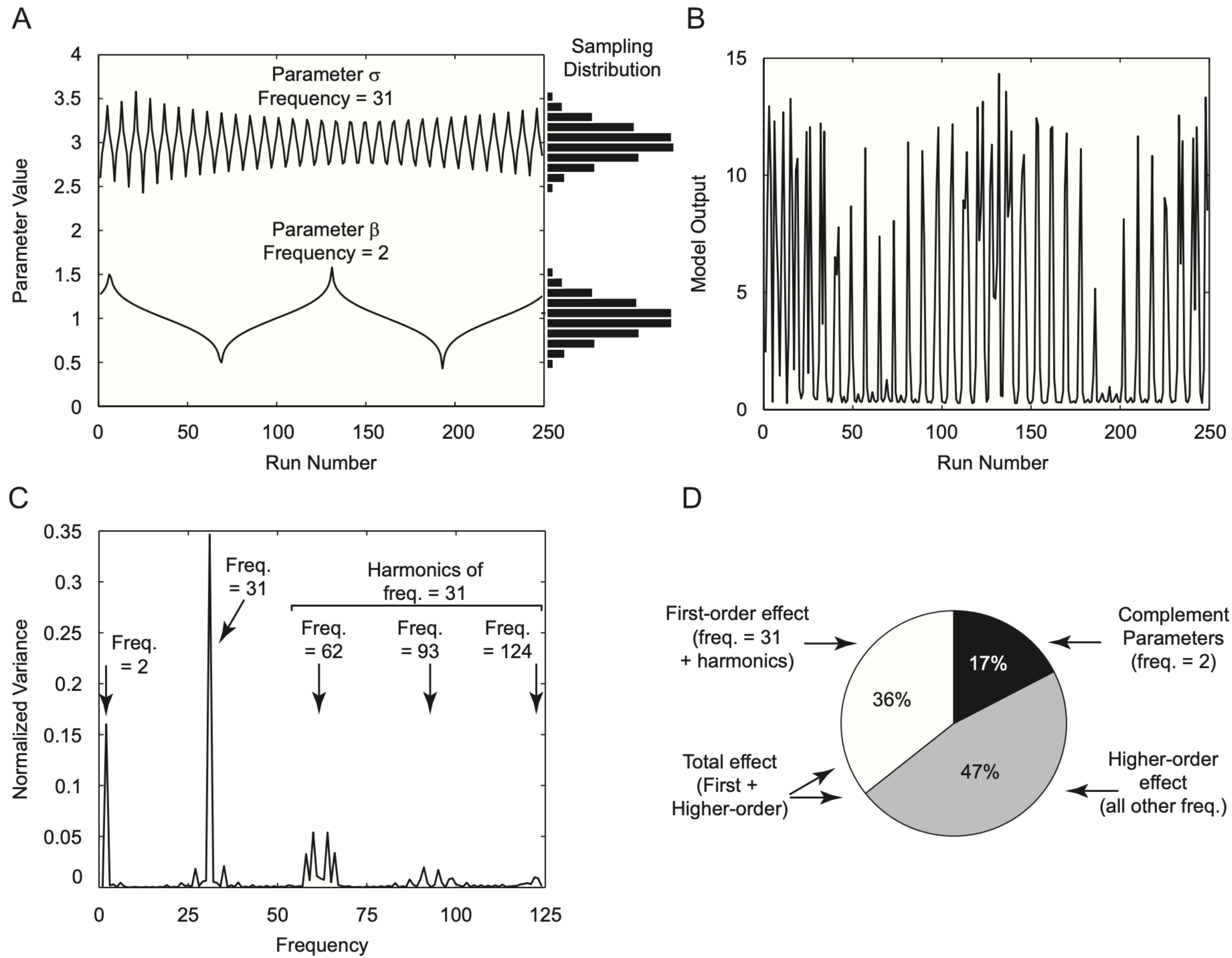
https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2570191/



S. Marino et al. / Journal of Theoretical Biology 254 (2008) 178–196

Variance-based methods

- Decomposition of variance (also called the Sobol method—unrelated to Sobol sampling though)
- Determines how much of the variance in output is due to each parameter
- Analogous to an ANOVA
- Direct calculation
- Faster options, e.g. eFAST

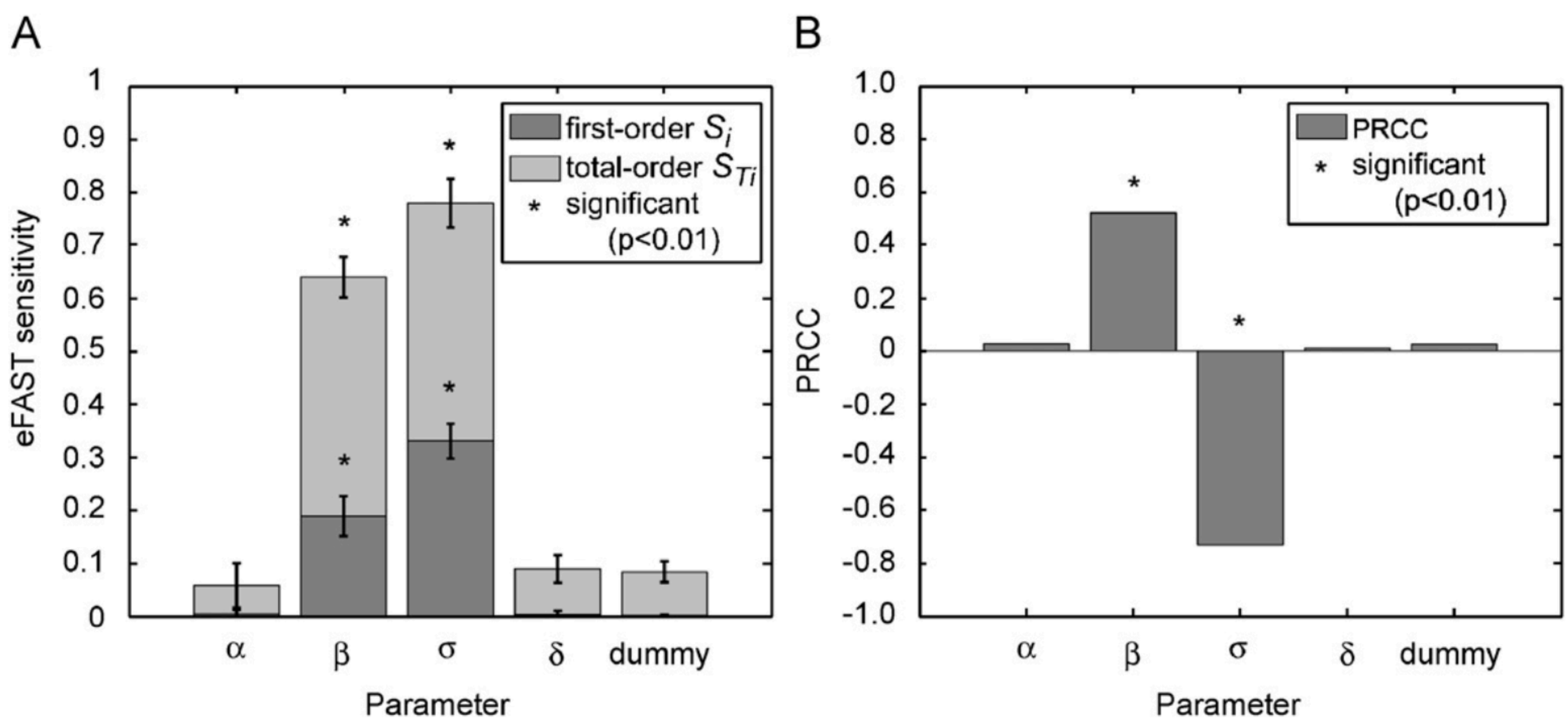


A
Parameter σ
Frequency = 31
Parameter β
Frequency = 2
Sampling Distribution
Parameter Value
Run Number
B
Model Output
Run Number
C
Freq. = 2
Freq. = 31
Harmonics of freq. = 31
Freq. = 62
Freq. = 93
Freq. = 124
Normalized Variance
Frequency
D
First-order effect (freq. = 31 + harmonics)
Complement Parameters (freq. = 2)
Total effect (First + Higher-order)
Higher-order effect (all other freq.)
17%
36%
47%

Word of caution: interpreting statistical results on model outputs

- What does the p-value on one of these regression or variance-based statistics mean?
- What is the source of the uncertainty in these estimates?
- We will discuss this more later

Use of dummy parameters to evaluate sensitivity



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Other Global Methods

- Many other approaches—using PCA & similar ideas (e.g. active subspaces), clustering methods, etc.

- Active nonlinear testing—different goal, instead of trying to capture variation, search for extremes, ‘break points’

Active nonlinear tests (ANTs)

- Different goal—instead of trying to capture variation in output/behavior, ANTs try to find extremes or ‘break points’ where behavior change
  - Search for ‘break points’ where behavior changes
- Similar in some ways to a bifurcation analysis
- Doesn't give a sense of what things are more likely, but more a sense of what things are possible

Miller 1998 - https://sfi-edu.s3.amazonaws.com/sfi-edu/production/uploads/sfi-com/dev/uploads/filer/08/15/0815718f-06ca-47d7-bbc6-61ed00511c91/96-03-011.pdf

Active nonlinear tests (ANTs)

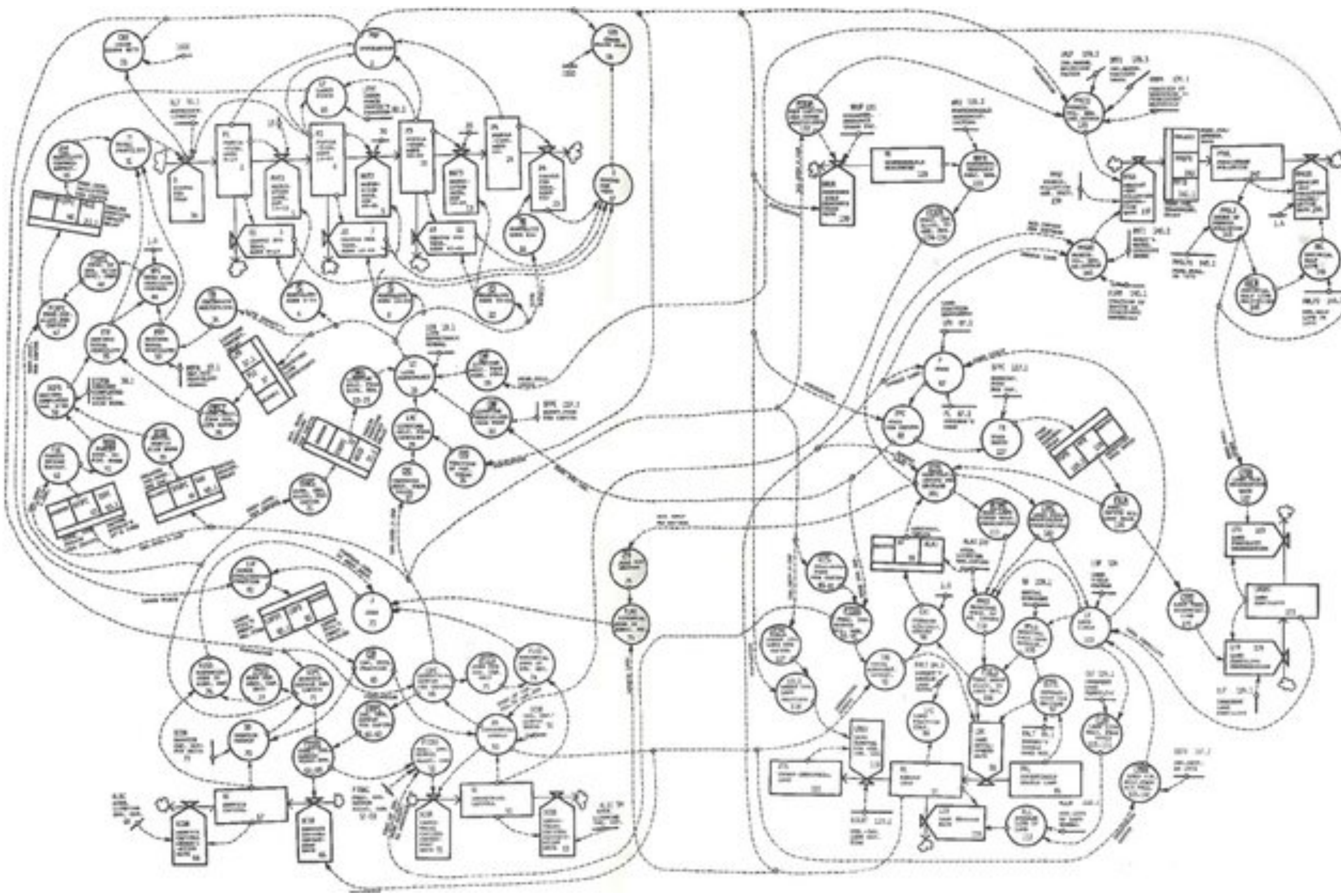
- Main idea: use an optimization method to maximize the deviation from the original output
- Find maximally ‘different’ behavior from the original
- Depending on your definition of ‘deviation’ and output, can search for alternate versions of ‘different’
- Wide range of different optimization approaches

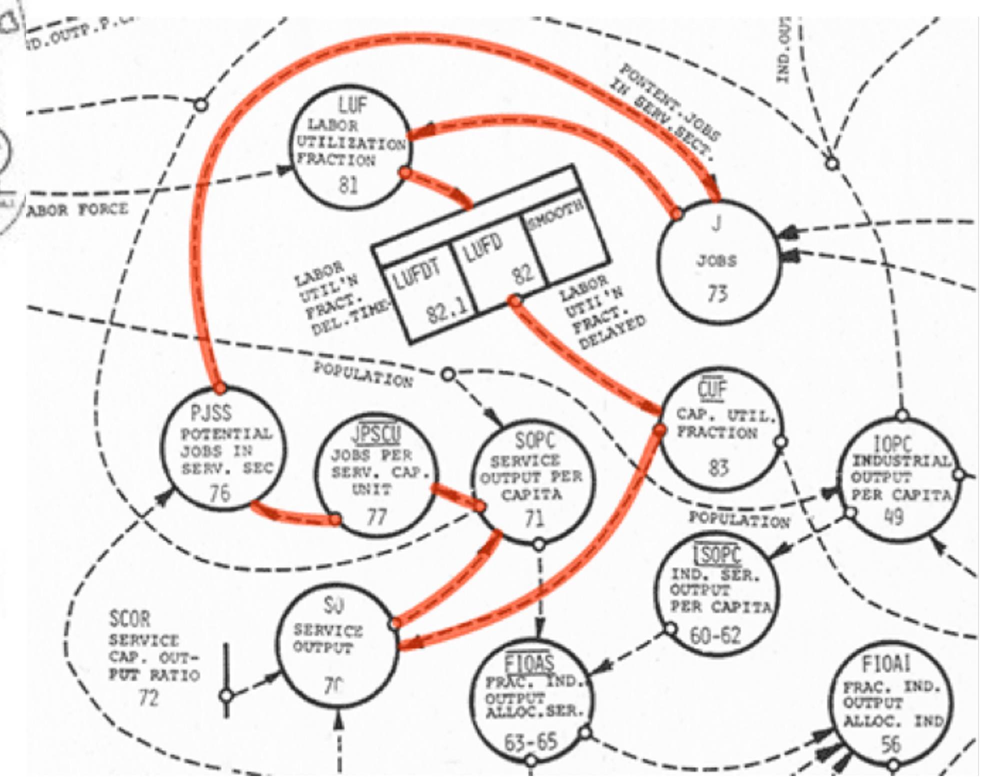
Miller 1998 - https://sfi-edu.s3.amazonaws.com/sfi-edu/production/uploads/sfi-com/dev/uploads/filer/08/15/0815718f-06ca-47d7-bbc6-61ed00511c91/96-03-011.pdf

Example: World3

- Ambitious, complex global system model developed in 1974 (Note - not an ABM!)
- Designed to simulate system dynamics relevant to human sustainability
- Model schematics:
  - 272 model variables with 96 that need to be initialized
  - 150 equations
  - 508 parameters needed to specify functional forms

Example: World3





Example: World3

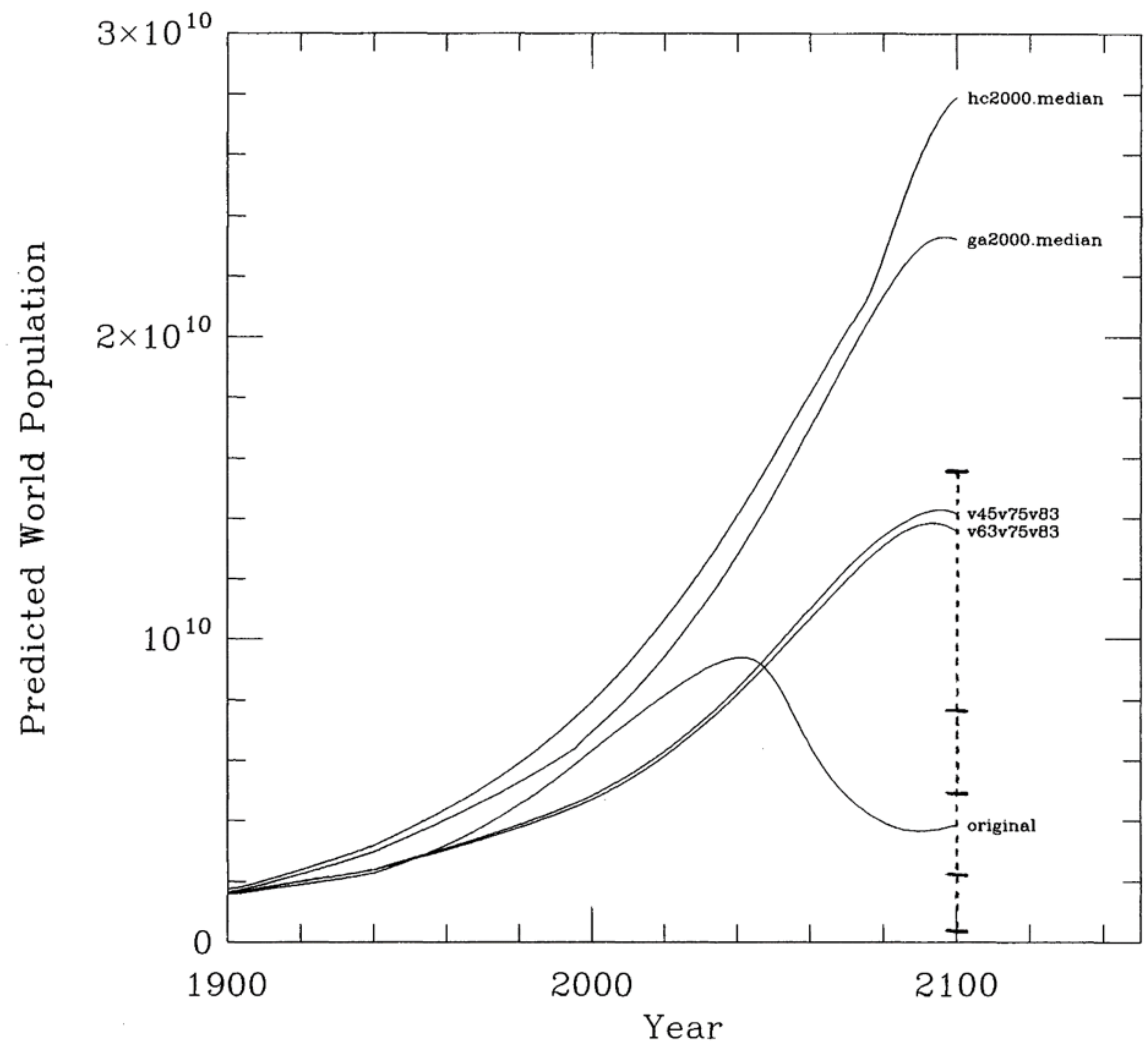
- ANT 1: Maximize estimated pop. in 2100
- ANT 2: minimize pop. peak while conforming to original pre-2000 estimates (i.e. cost function includes a penalty for deviating from pre-2000 estimates)

Example: World3

- Optimization algorithms:
- For each ANT, 2 different optimization algorithms were independently applied in 30 trials for the sake of comparison
  - Hill-climbing algorithm
  - Genetic algorithm
- A random-search of the parameter space was also done to provide a baseline of comparison

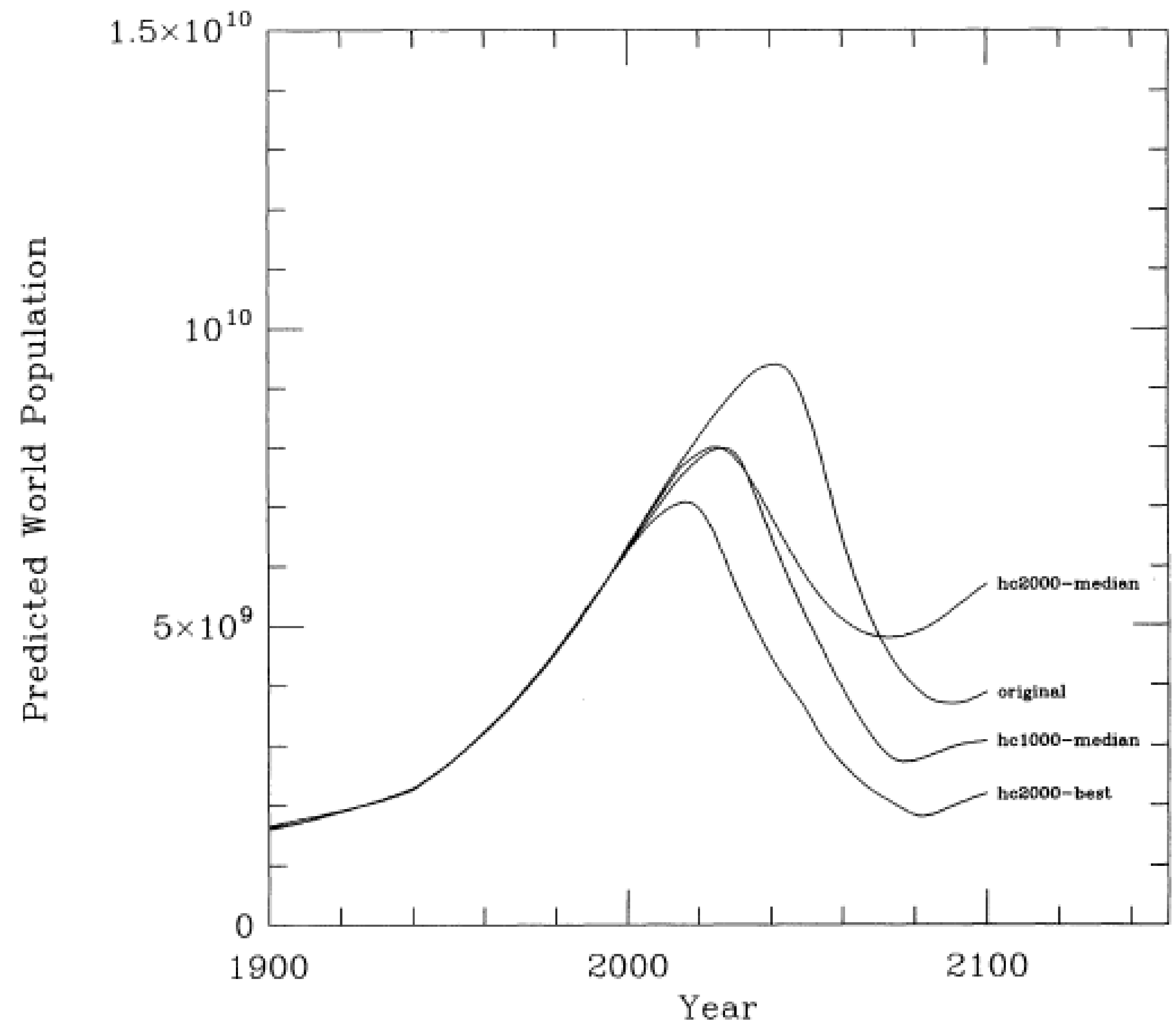
Example: World3

- Results: ANT 1
- Can substantially increase population estimate in 2100 (can "break" the model)



Example: World3

- Results: ANT 3
- Possible to notably reduce population prediction, even with pre-2000 constraint



Active nonlinear tests (ANTs)

- Note that most ANTs do not mean the resulting parameter values are the only ones that will generate a similar deviation from the original

- Nor that other parameter sets with similar deviation values will look anything like the one or ones the optimization algorithm finds!

- In most cases, consider these examples showing that the model can do the behaviors found in the ANT

Dimension reduction & parameter selection

- Fixing insensitive parameters
- Parameter subset selection methods
  - Find subsets of parameters or potentially new parameter combinations that explain most of the behavior (by fixing parameters or parameter combinations that are insensitive
  - Active subspaces, PCA

Surrogate models

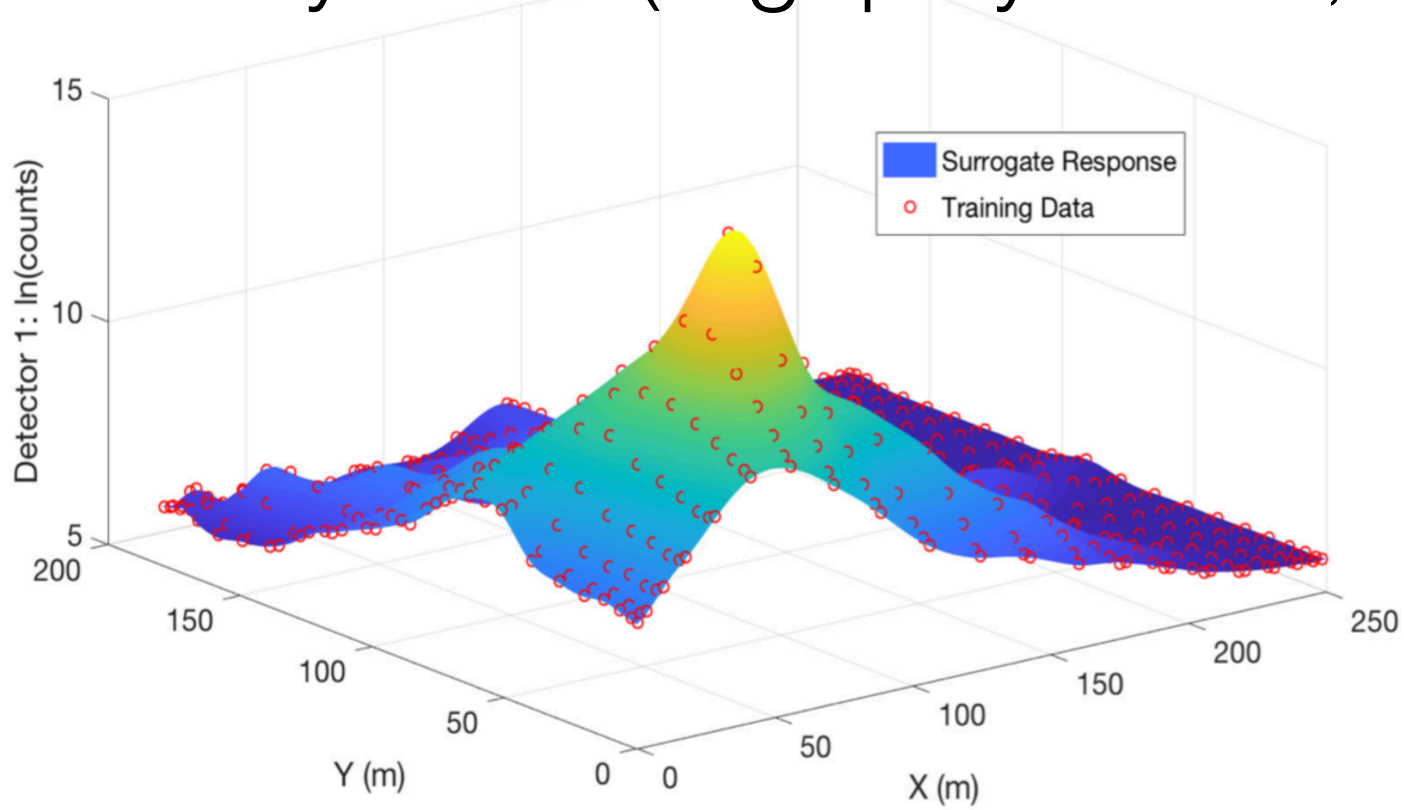
- Global sensitivity methods can be highly computationally expensive—many ABMs take too long to run to be feasible with the number of samples needed to explore space

- ANTs can sort of help, but still require many evaluations and don't give a sense of frequency/distribution of outputs/behavior

- Surrogate models (also called emulators, response surfaces) provide another option

Surrogate models

- Idea is to fit a surface or function to the model output(s) as a function of the parameters
  - Choose a functional form that is cheap to evaluate many times (e.g. polynomial, linear)



Cook JA, Smith RC, Hite JM, Stefanescu R, Mattingly J. Application and Evaluation of Surrogate Models for Radiation Source Search. Algorithms. 2019 Dec;12(12):269.

Surrogate models

- Use a smaller number of points to fit the surface, then sample a large number of points to run sensitivity analysis

- Re-run using the true model on regions of interest

For next time…

- Readings
    - Marino, Simeone, et al. "A methodology for performing global uncertainty and sensitivity analysis in systems biology." Journal of theoretical biology 254.1 (2008): 178-196.
    - Additional papers on the website