CSI 709/CSS 739
Verification and Validation of Models

Computational Techniques to Support Simulation Model Validation

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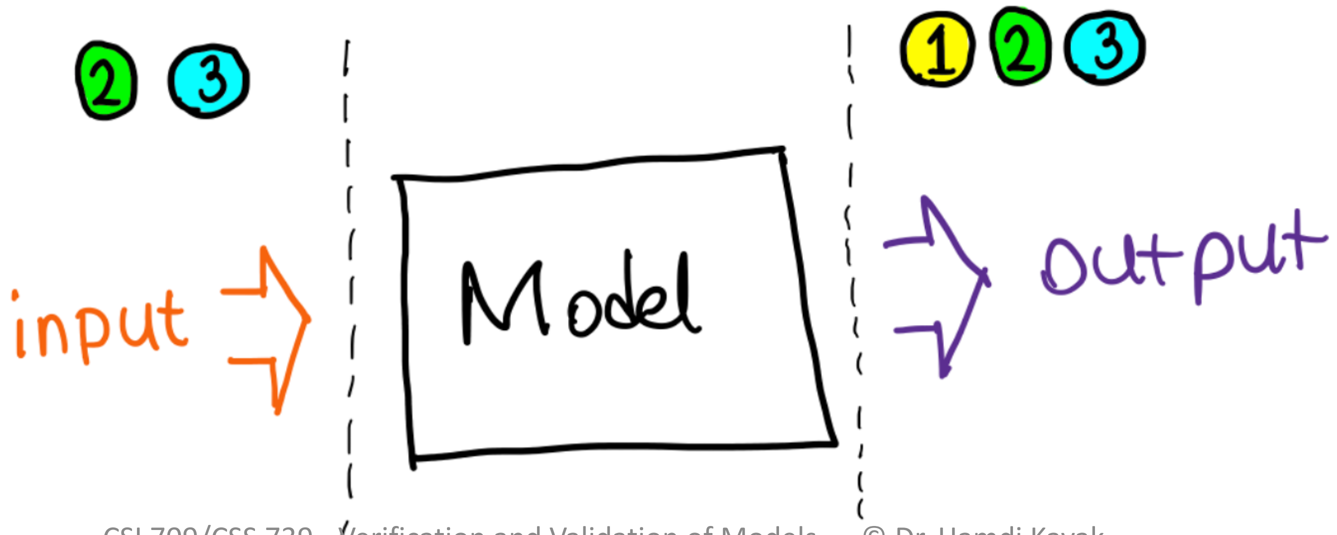
Objective of this lecture

- Exploring some computational techniques to conduct more thorough V&V for simulation models.

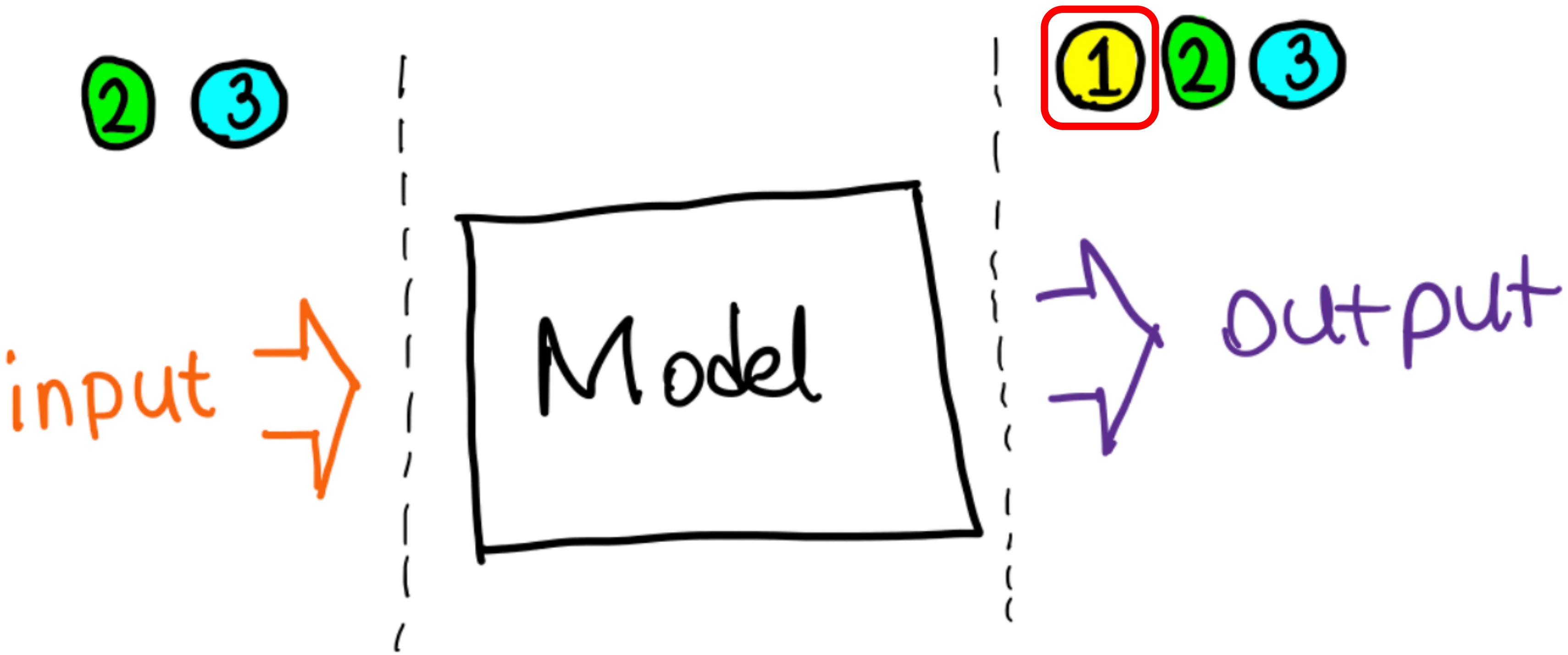
1 Non-terminating simulations

2 Model parameter value estimation

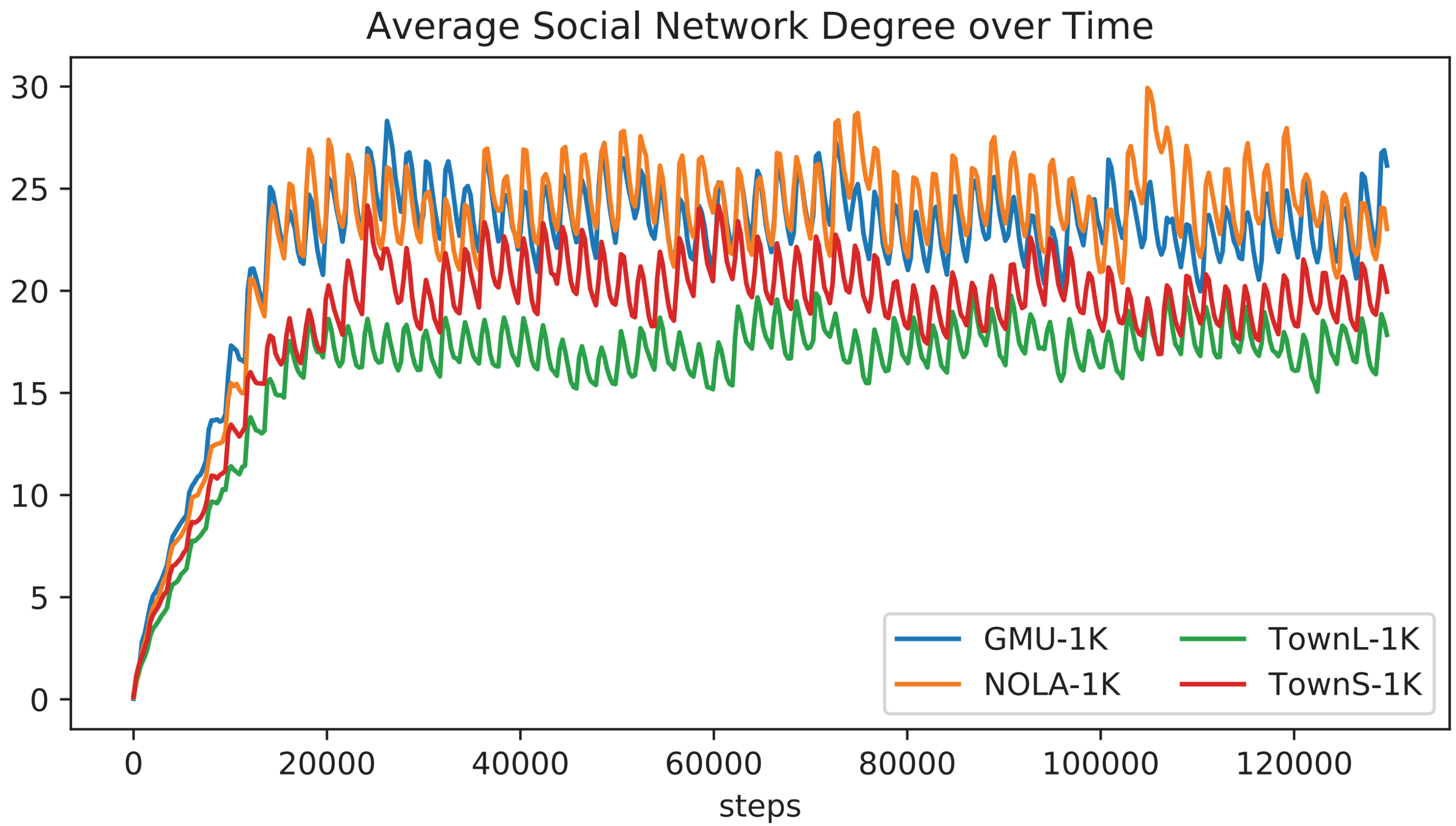
3 Model sensitivity



1. Non-terminating simulations
2. Model parameter value estimation
3. Model sensitivity



What are your observations about this plot?



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Simulation types

Terminating simulation

- The behavior of interest in the model has a specific initial state and a natural ending event (E).
- Runs for a specific duration until E occurs.
- Examples:
  - A grocery store model with an opening time of 6:00 am and closing time of 10:00 pm when no more customers are inside.
  - A WMD model aims to simulate people's behavior to a nuclear bomb until the initial lethal effects of the bomb are no longer present.

Non-terminating simulation

- The behavior of interest in the model does not have a natural ending event.
- Runs for a duration identified by the modeler.
- The interest is usually to study long-term behaviors.
- Examples:
  - An assembly line simulation that runs almost non-stop with infrequent disruptions.
  - A patterns of life model that simulates the fabric of everyday life and people's movement.

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To identify whether a simulation is terminating or not terminating, one needs to look at **"the objectives of the simulation"** and **"the nature of the system"** (Banks et al., 2013)

Terminating vs. not terminating categorization is usually considered for Discrete-Event Simulation (DES) models. However, it can be applied to other simulation model types (e.g., ABMs, hybrid models).

Non-terminating simulation types

STEADY-STATE

STEADY-STATE CYCLIC

OTHER

Non-terminating simulation types*

- **Steady-state**
  - Example manufacturing operation:
    - "Operation starts empty and idle at t = 0.
    - System operates **2 eight-hour shifts per day, 5 days per week**.
    - System state at day's end is the initial state for beginning the next day.
    - Interested in long-term average daily production."

*Source: Mielke

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- **Steady-state cyclic**
  - Example manufacturing operation:
    - "Operation starts empty and idle at t = 0.
    - System operates **2 eight-hour shifts per day, Monday through Friday**.
    - System operates **1 eight-hour shift on Saturday and Sunday**.
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    - Interested in long-term average daily production."
- **Other**
  - Example call center operation:
    - "Operation starts empty and idle at t = 0.
    - System operates **3 eight-hour shifts per day, 7 days per week**.
    - Call volume varies by the day of the week.
    - Weekly call volume depends on season of the year.
    - Yearly call volume varies with economy.
    - Interested in average delay experienced by a caller."
- **Steady-state cyclic**
  - Example manufacturing operation:
    - "Operation starts empty and idle at t = 0.
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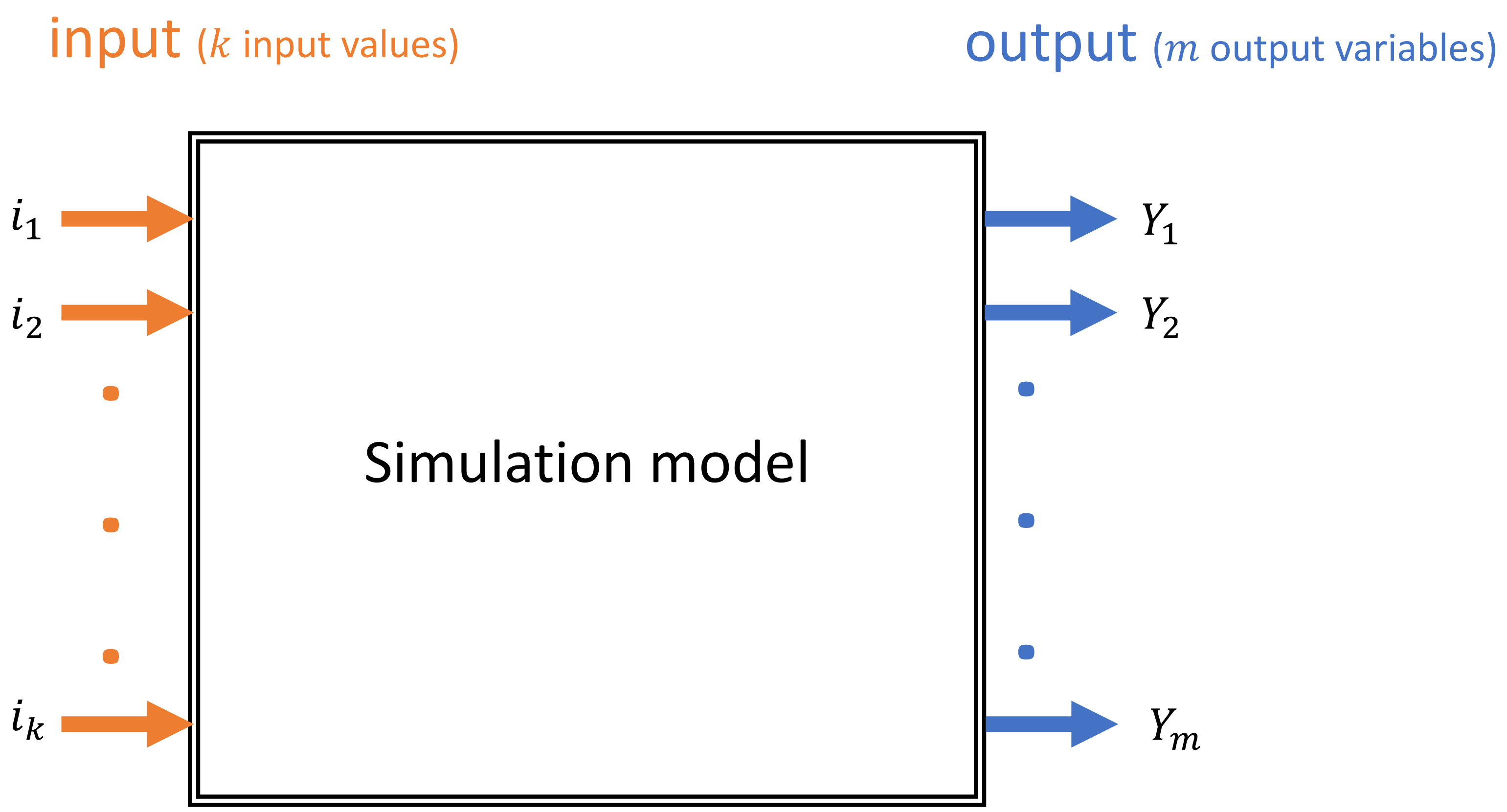
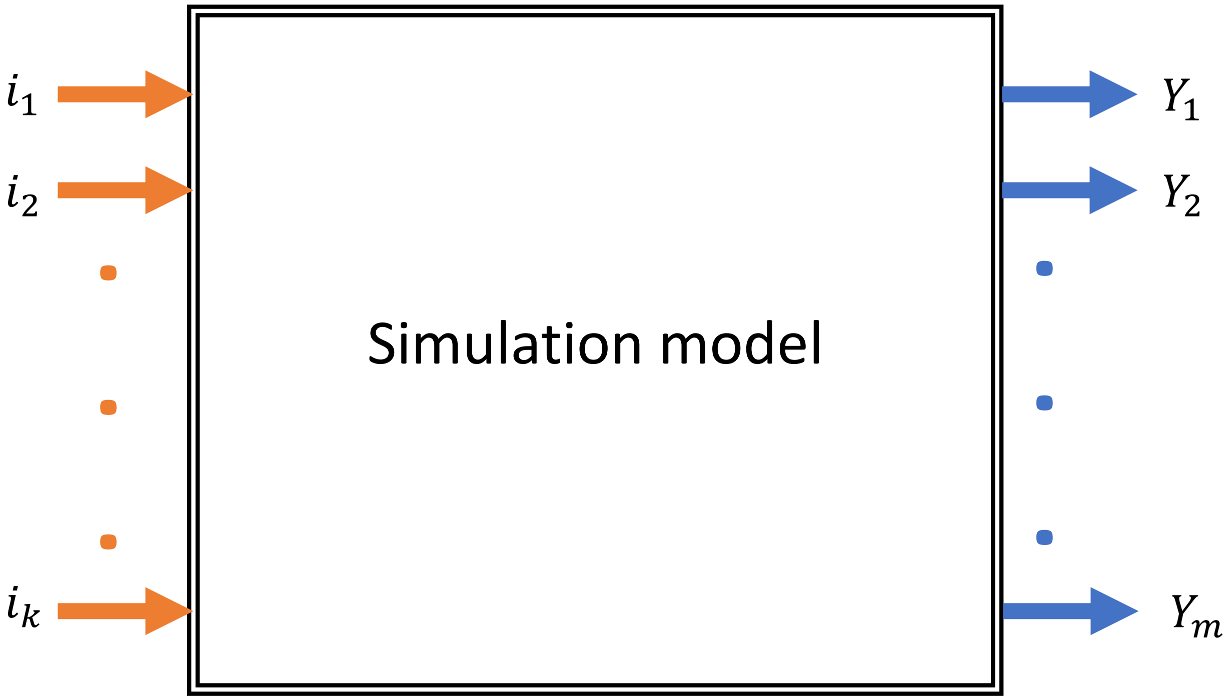
Simulation input/output formalization



Simulation input/output formalization

input (k input values) output (m output variables)

$$I = \{\mathrm{i}_1, \mathrm{i}_2, \ldots, \mathrm{i}_\mathrm{k}\}$$



$$Y = \{Y_1, Y_2, \ldots, Y_m\}$$

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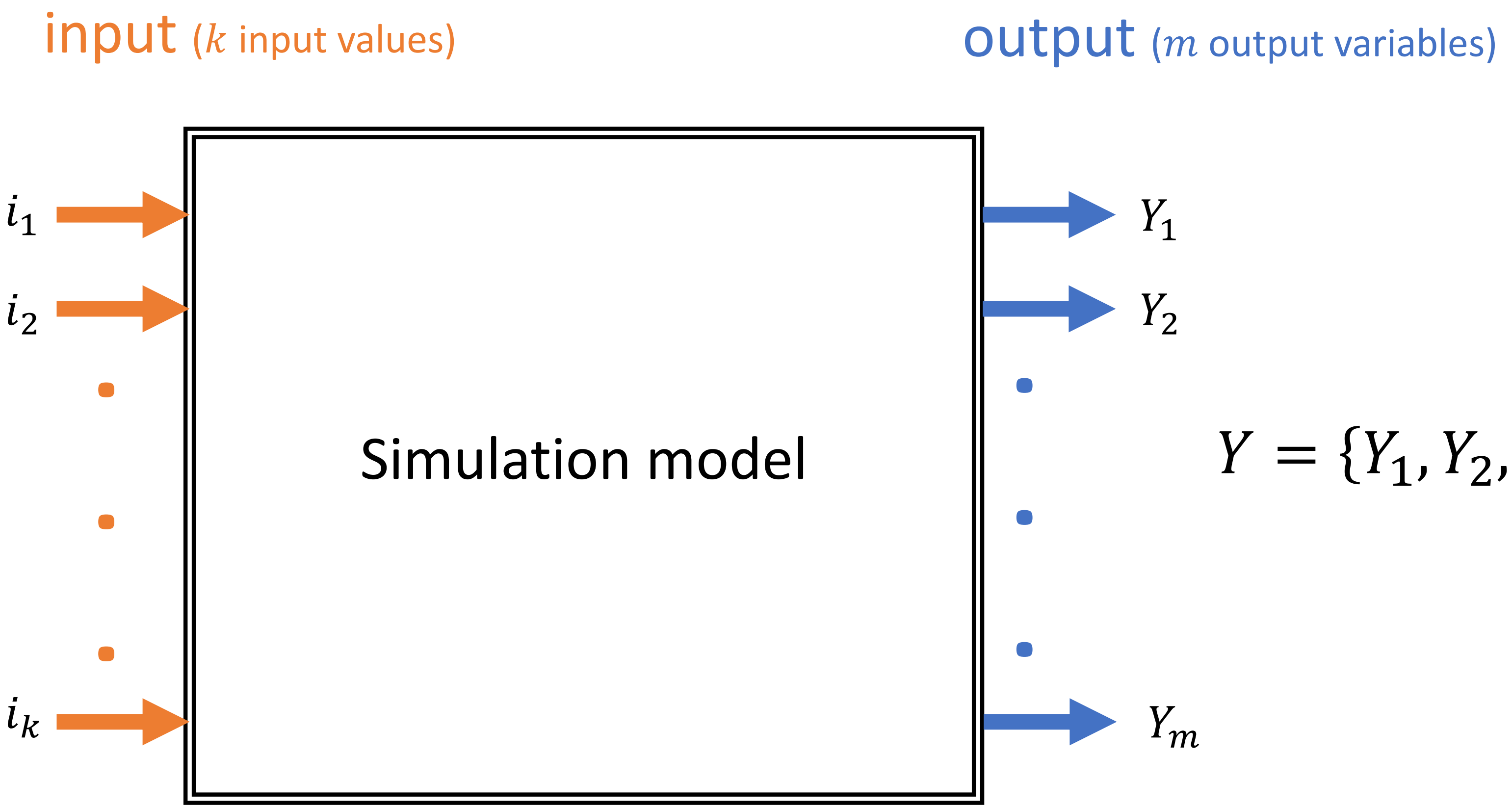

$Y = \{Y_1, Y_2, \dots, Y_m\}$

$$Y_i = \{y_{i1}, y_{i2}, \dots, y_{ij}\}$$

we observe j values for output variable i

Simulation output data

- Most simulation models are stochastic and non-terminating.
- Assume that we are interested in the output variable $Y_i = \{y_{i1}, y_{i2}, \dots, y_{ij}\}$.
- Run $\boldsymbol{n}$ times w/ the same input set (I) and observe j values in each run.

$$\begin{array}{cccccccccl}
\boldsymbol{y_{i1}^{(1)}} & \boldsymbol{y_{i2}^{(1)}} & \boldsymbol{y_{i3}^{(1)}} & \cdots & \boldsymbol{y_{ik}^{(1)}} & \boldsymbol{y_{i(k+1)}^{(1)}} & \cdots & \boldsymbol{y_{ij}^{(1)}} & \longleftarrow & \text{Run } \mathbf{1} \\
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\cdot & \cdot & \cdot & & \cdot & \cdot & & \cdot & & \\
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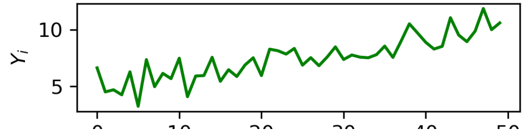
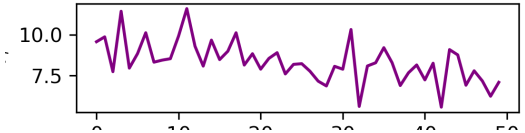
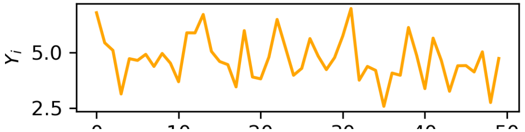
\end{array}$$







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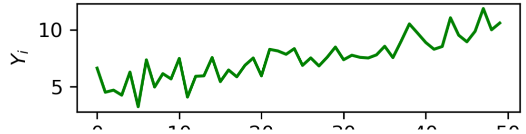
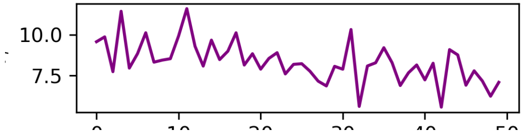
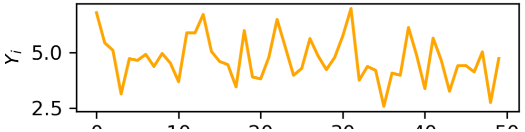
- Run n times w/ the same input set (I) and observe j values in each run.

$$
\begin{array}{cccccccccl}
\boxed{\begin{array}{c} \boldsymbol{y_{i1}^{(1)}} \\ \boldsymbol{y_{i1}^{(2)}} \\ \vdots \\ \boldsymbol{y_{i1}^{(n)}} \end{array}} &
\begin{array}{c} \boldsymbol{y_{i2}^{(1)}} \\ \boldsymbol{y_{i2}^{(2)}} \\ \vdots \\ \boldsymbol{y_{i2}^{(n)}} \end{array} &
\begin{array}{c} \boldsymbol{y_{i3}^{(1)}} \\ \boldsymbol{y_{i3}^{(2)}} \\ \vdots \\ \boldsymbol{y_{i3}^{(n)}} \end{array} &
\begin{array}{c} \cdots \\ \cdots \\ \\ \cdots \end{array} &
\begin{array}{c} \boldsymbol{y_{ik}^{(1)}} \\ \boldsymbol{y_{ik}^{(2)}} \\ \vdots \\ \boldsymbol{y_{ik}^{(n)}} \end{array} &
\begin{array}{c} \boldsymbol{y_{i(k+1)}^{(1)}} \\ \boldsymbol{y_{i(k+1)}^{(2)}} \\ \vdots \\ \boldsymbol{y_{i(k+1)}^{(n)}} \end{array} &
\begin{array}{c} \cdots \\ \cdots \\ \\ \cdots \end{array} &
\begin{array}{c} \boldsymbol{y_{ij}^{(1)}} \\ \boldsymbol{y_{ij}^{(2)}} \\ \vdots \\ \boldsymbol{y_{ij}^{(n)}} \end{array} &
\begin{array}{c} \longleftarrow \\ \longleftarrow \\ \\ \longleftarrow \end{array} &
\begin{array}{l} \text{Run } \mathbf{1} \\ \text{Run } \mathbf{2} \\ \\ \text{Run } \boldsymbol{n} \end{array}
\end{array}
$$







n samples from output variable Y_i at the first observation

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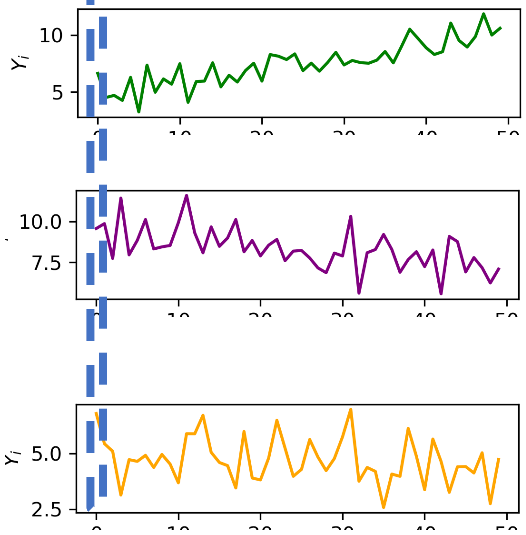
y_{i1}^{(2)} & y_{i2}^{(2)} & y_{i3}^{(2)} & \cdots & y_{ik}^{(2)} & y_{i(k+1)}^{(2)} & \cdots & y_{ij}^{(2)} & \longleftarrow \text{Run } 2 \\
. & . & . & & . & . & & . & \\
y_{i1}^{(n)} & y_{i2}^{(n)} & y_{i3}^{(n)} & \cdots & y_{ik}^{(n)} & y_{i(k+1)}^{(n)} & \cdots & y_{ij}^{(n)} & \longleftarrow \text{Run } n
\end{array}
$$



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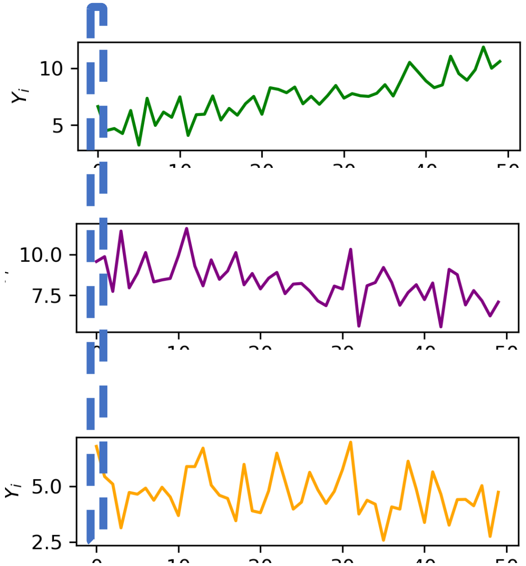

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. & . & . & & . & . & & . & & \\
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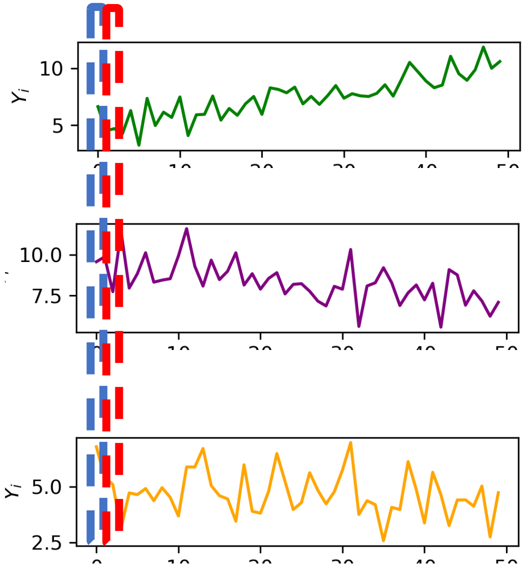

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How to know if simulation is in steady-state?

- There is often the first k observations such that distribution from $k+1$ and beyond are roughly the same, a.k.a., **steady-state**.
- Thus, the first k observations are usually called **transient**.
- We need to ignore transient state observations

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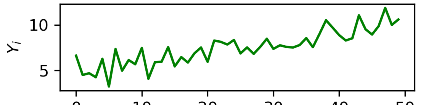

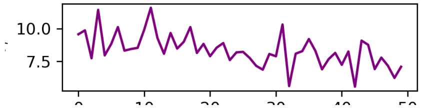

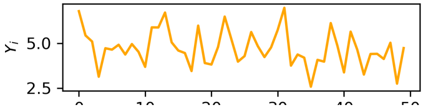

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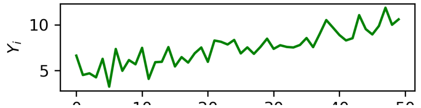

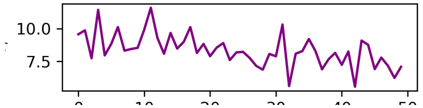

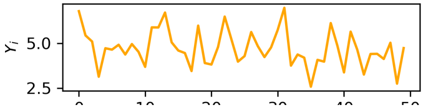

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\end{array}
$$

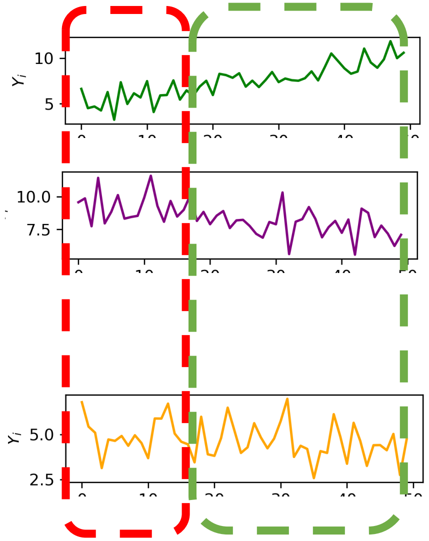
transient-state

steady-state

Run **1**

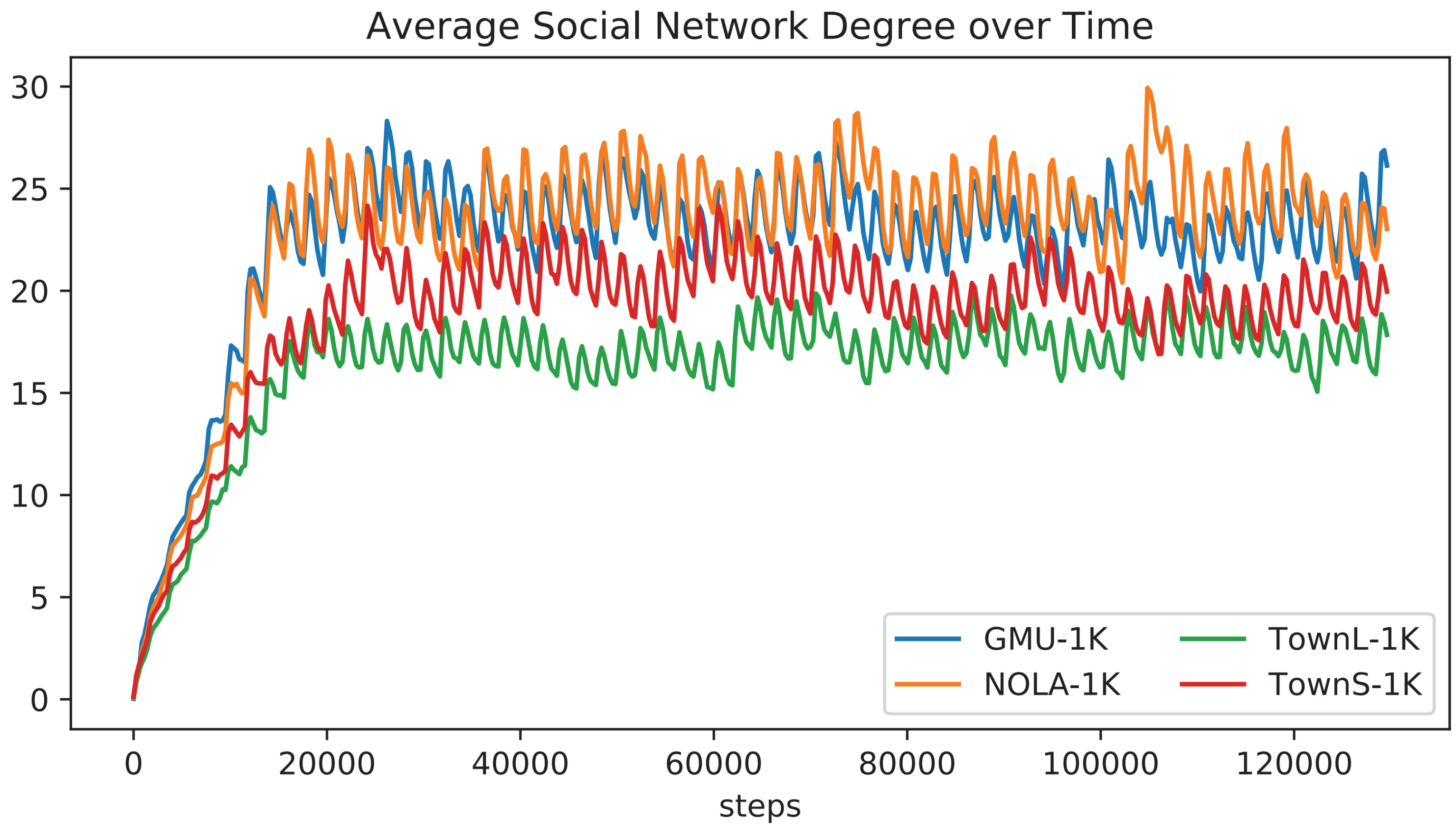
Run **2**

Run n



Recall the plot again

Can you show the **transient** and **steady-state** behavior?



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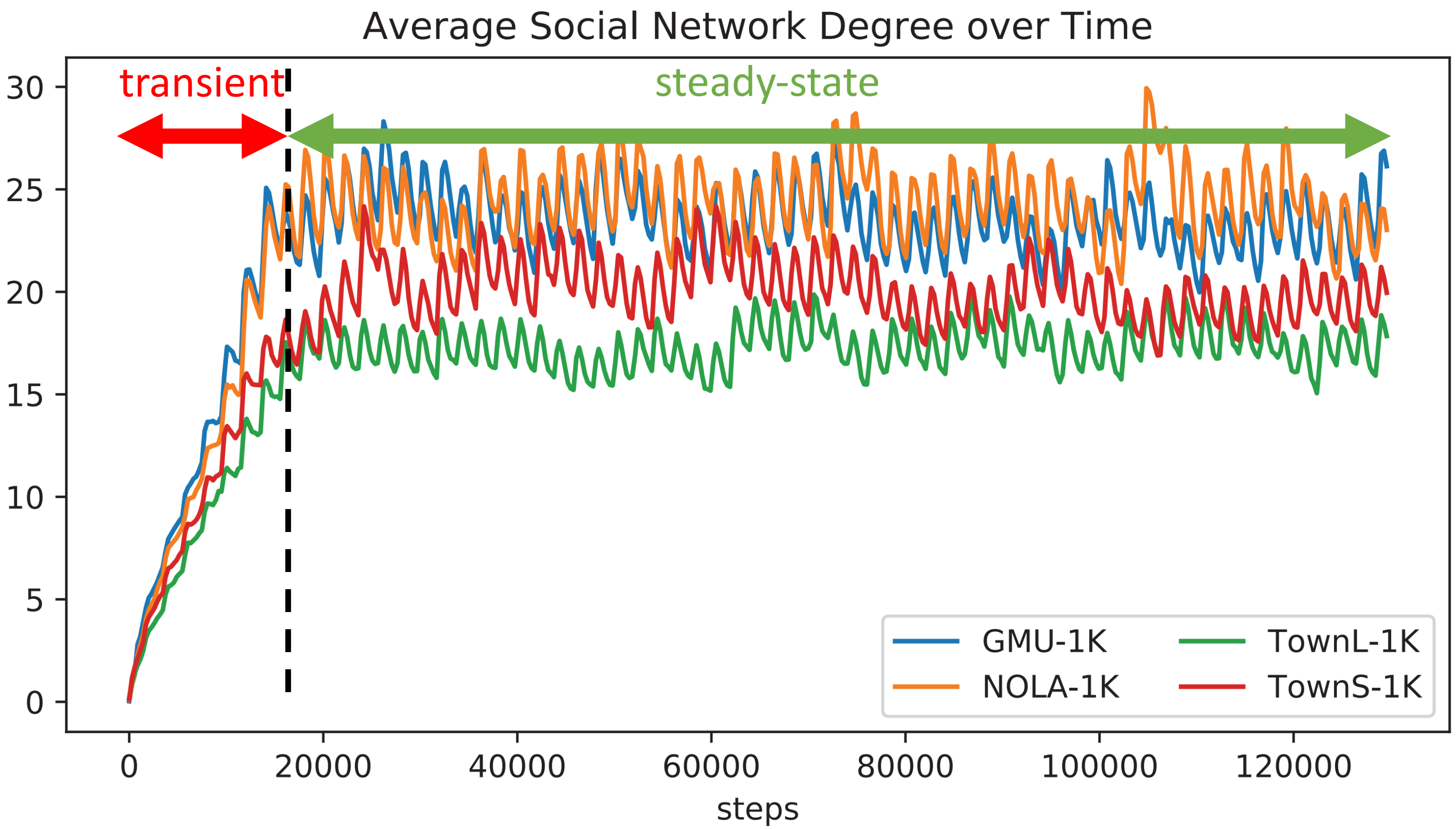

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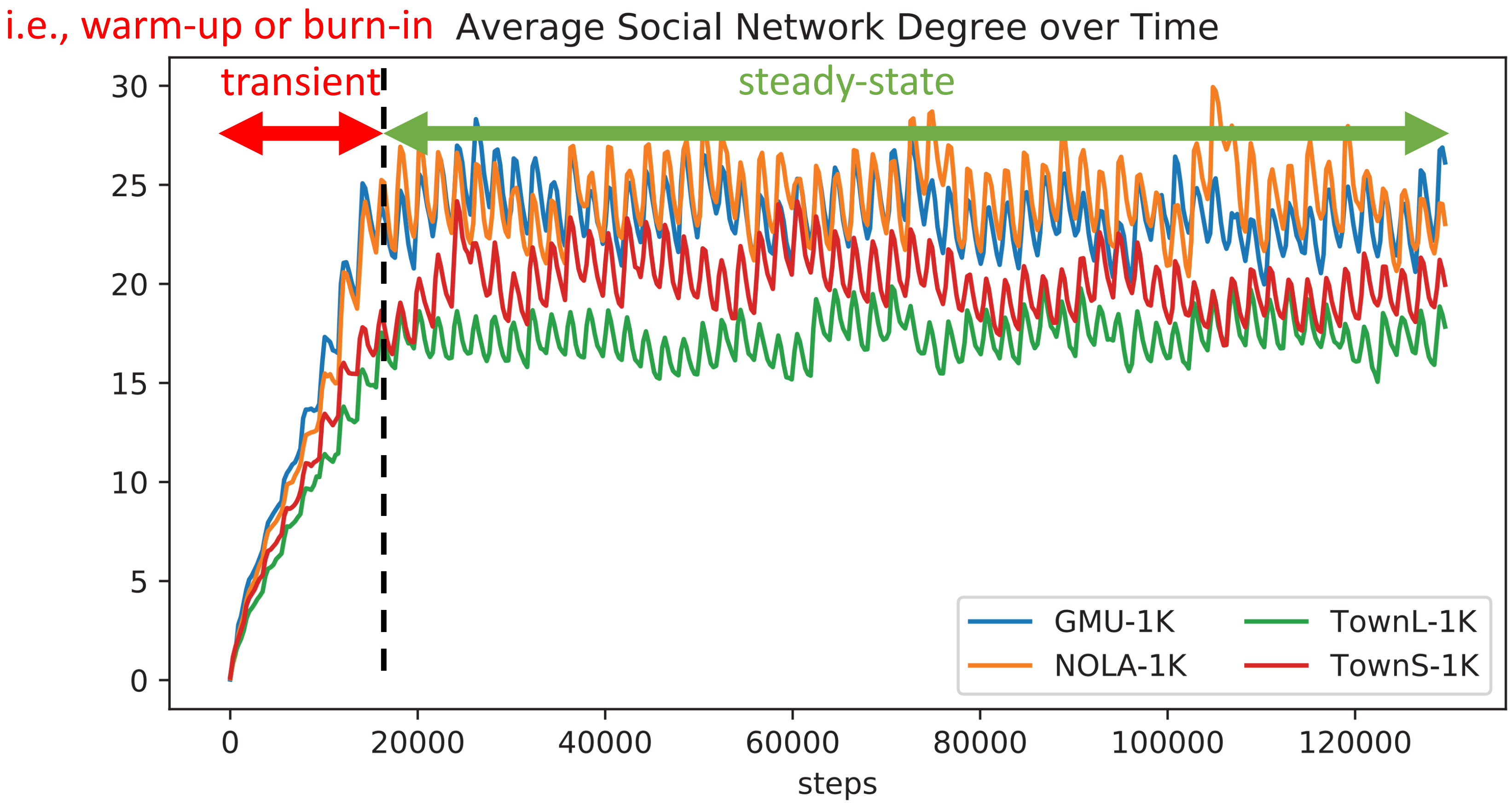

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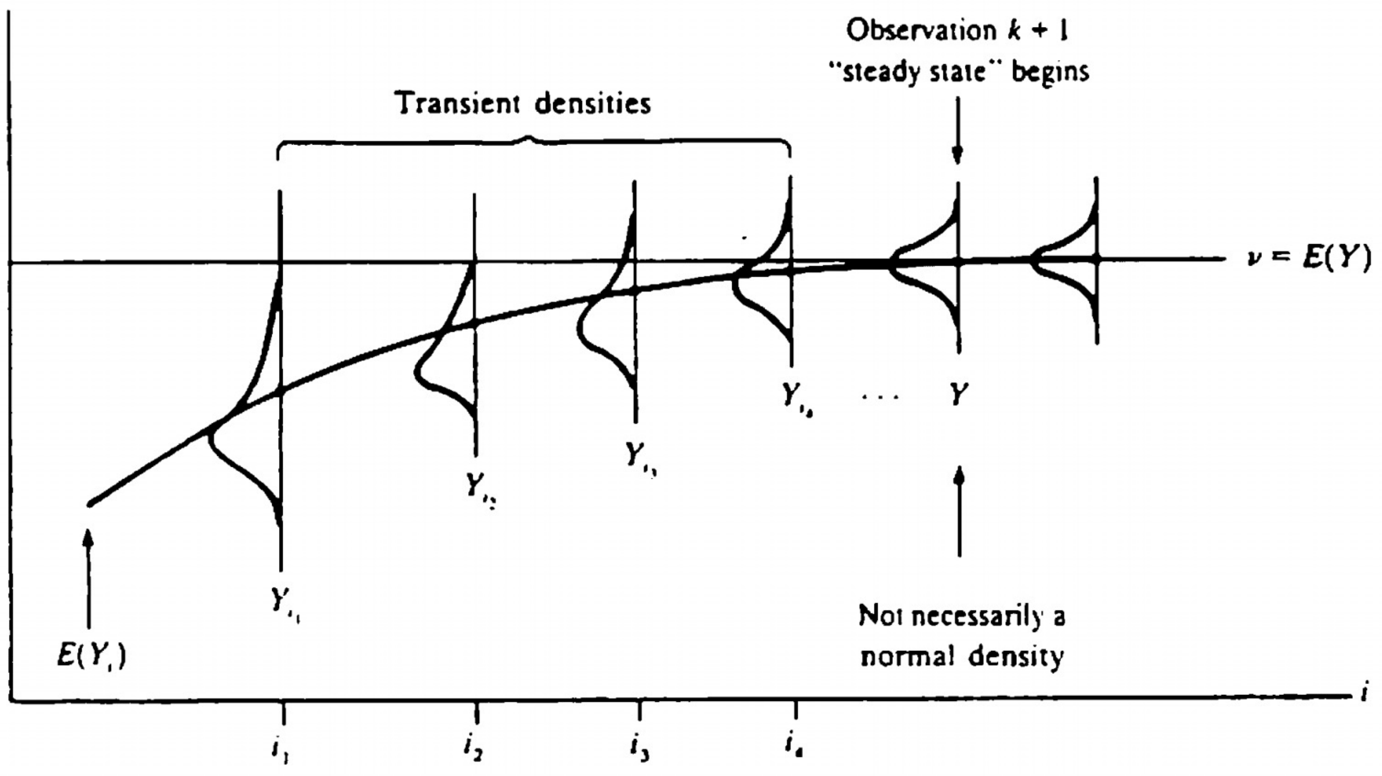
How to detect the transient state?

Mahajan & Ingalls (2004) summarizes several methods

- Graphical
- Statistical
- Heuristic
- Initialization Bias

Welch’s Graphical Method



Law (1990)

Conway Rule heuristic

- "Truncate a series of measurements until the first of the series is neither the maximum nor the minimum of the remaining set" (Conway, 1963).
- Gafarian et al. (1978)

1. Decide n and m the number of exploratory replications and the length of the exploratory replications.
2. Compute y^{+}_{jr} and y^{-}_{jr} using following formulae:

$$y^{+}_{jr} = \max(y_{jl} : l = r,\dots,m)\ j = 1,\dots n \qquad (6)$$

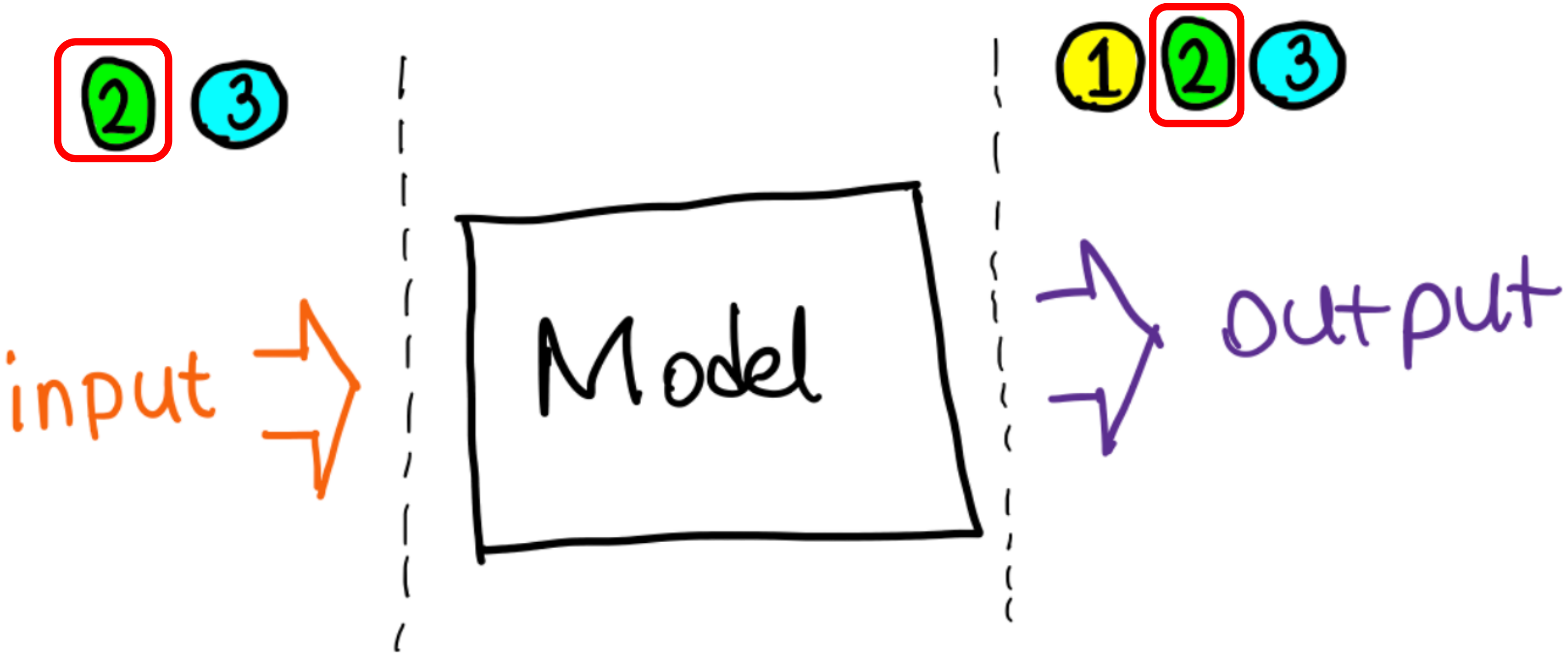
$$y^{-}_{jr} = \min(y_{jl} : l = r,\dots,m)\ j = 1,\dots n \qquad (7)$$

3. For $r = 1, 2, \dots, m$ determine t_j such that $t_{j=\min_r}\{Y^{-}_{jr} < Y_{jr} < Y^{+}_{jr}\}$ occurs for the first time.
4. Estimate of the truncation point t^* is given by $\max\{t_1, t_2, t_3, \dots, t_n\}$

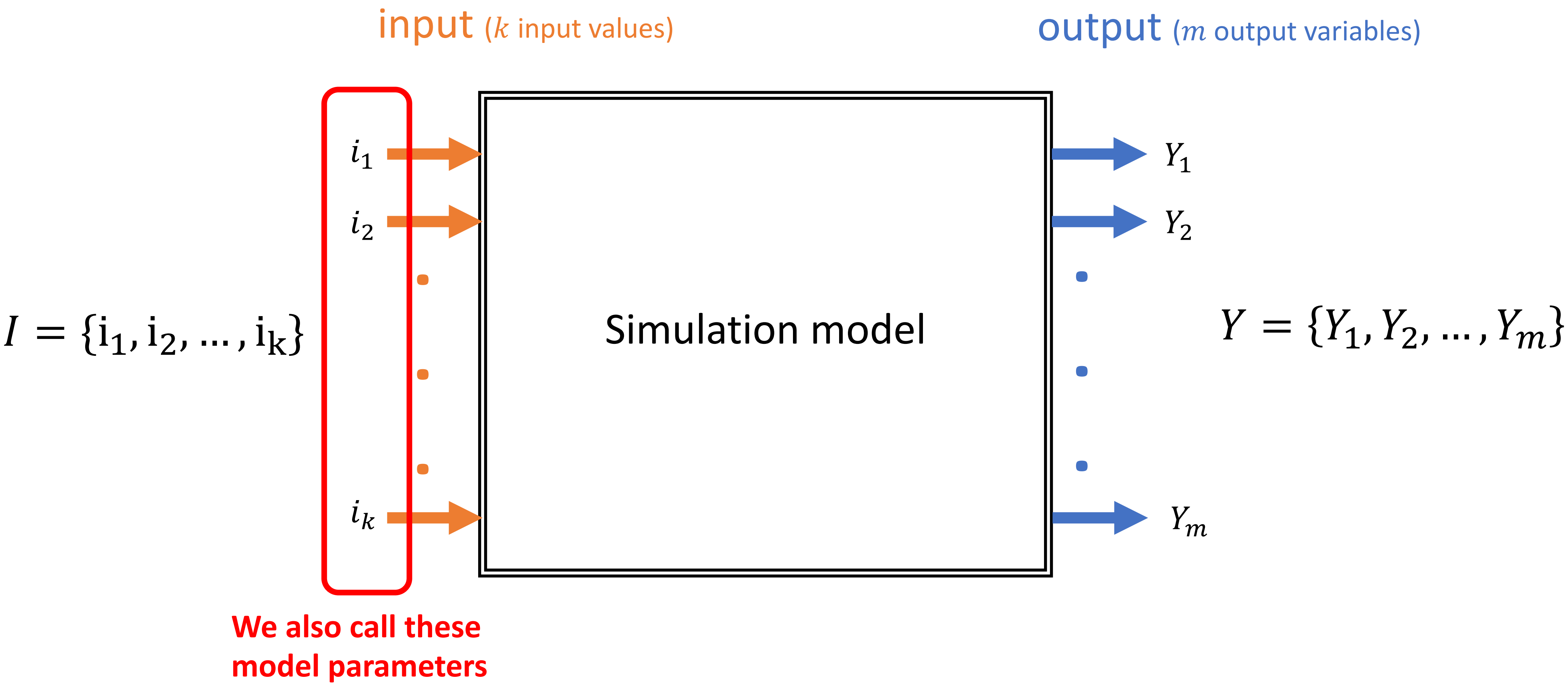
Why do we identify transient state, again?

- Transient state data should be removed from our analysis.
- Selecting inaccurate cut-off point (k) can lead to one of the two results
  - Including transient data in our analysis if $k \ll k_{actual}$
  - Removing meaningful simulation data in our analysis if $k \gg k_{actual}$
- Various techniques are introduced and compared in Mahajan and Ingalls (2004)

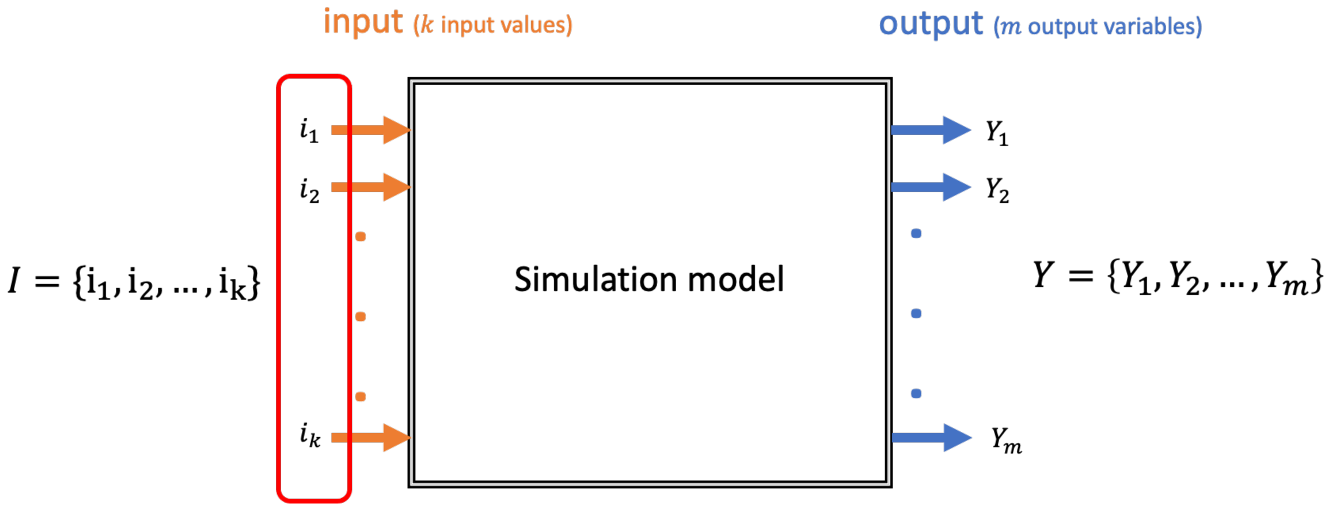
1. Non-terminating simulations
2. Model parameter value estimation
3. Model sensitivity



Simulation input/output formalization

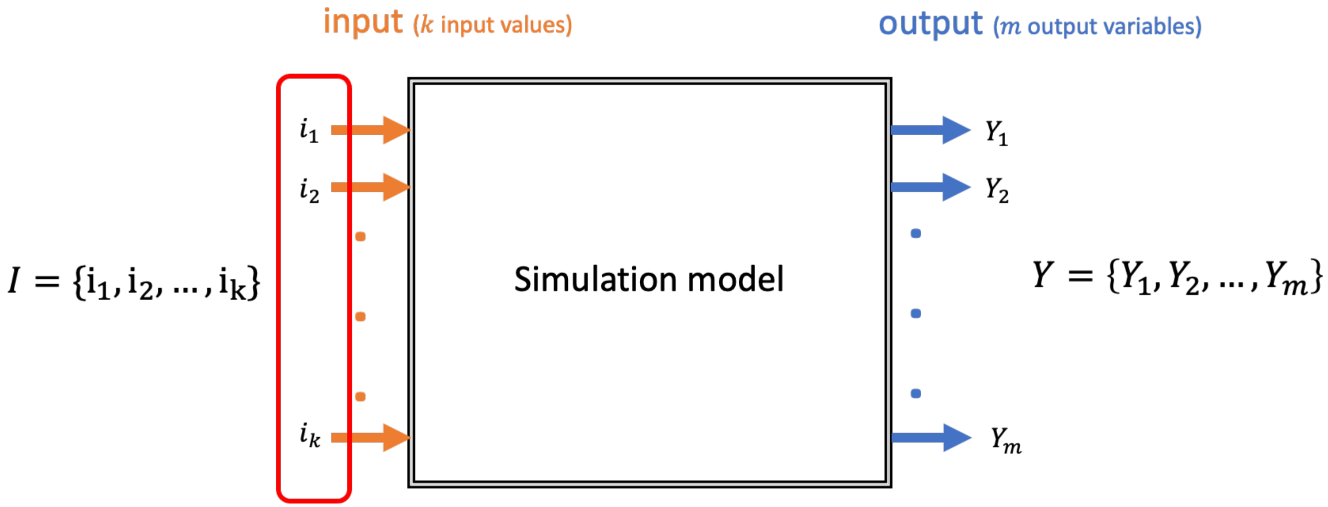


Model parameters



- These model parameter values (i.e., input values, I) are **critical**.
- If the values are not accurate, we cannot rely on simulation results.
  - Garbage in, garbage out

Model parameters



- In some cases, data for model parameter values are **directly available**. E.g.:
  - Population size in a social model
  - Number of cashiers in a specific grocery store model
  - Part assembling time in an assembly line model
  - Mass of a planet in a solar system model
  - …

Model parameters

- In some cases, data for model parameter values can be obtained using **secondary sources** if cannot be directly found.

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Active data sources

- Surveys from a similar population
  - E.g.: a behavioral measure for a topic can be obtained from another geographic area with similar population characteristics.
- Crowd sourcing
  - E.g.: participants respond to decision-based questions in a smartphone app.
  - E.g.: participants use platforms like Amazon Mechanical Turk.

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Passive data sources

- Social media:
  - E.g.: Twitter (Padilla et al. 2016)
- Cell phone:
  - E.g.: call detail records characterizing movement patterns
  - E.g.: trip data providing traffic status (Uber Movement, etc.).
- Wi-Fi connections:
  - E.g.: Safegraph foot traffic data

Padilla, J. J., Diallo, S. Y., Kavak, et al. (2016). Semi-automated initialization of simulations: an application to healthcare. The Journal of Defense Modeling and Simulation, 13(2), 171-182.

Model parameters

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Model parameters

- In other cases, data for model parameter values can be **unfeasible**, **unethical**, or **too costly to obtain** directly or via secondary sources.
- Examples
  - Constants that vary based on different environmental factors.
    - E.g.: *growth rates* in a predator-pray model
  - Behavior variables
    - E.g.: *driver's reaction time* and *speed acceptance* in a transportation model.
      - Ciuffo, B., Punzo, V., & Torrieri, V. (2008). Comparison of simulation-based and model-based calibrations of traffic-flow microsimulation models. *Transportation Research Record*, *2088*(1), 36-44.
  - Unobservable parameters
    - E.g.: *breast cancer natural history* parameters in a cancer epidemiology model.
      - Cevik, M., Ergun, M. A., Stout, N. K., Trentham-Dietz, A., Craven, M., & Alagoz, O. (2016). Using active learning for speeding up calibration in simulation models. *Medical Decision Making*, *36*(5), 581-593.

Simulation model calibration

- “Calibration is the activity of adjusting the unknown rate parameters until the outputs of the model fit the observed data” (Kennedy and O'Hagan, 2001).

Simulation model calibration

- "Calibration is the activity of adjusting the unknown rate parameters until the outputs of the model fit the observed data" (Kennedy and O'Hagan, 2001).
- Certain application domains use calibration more than others. What are the commonalities between these domains?
    - Traffic models
    - Economic models
    - Policy models

Simulation model calibration: preparation

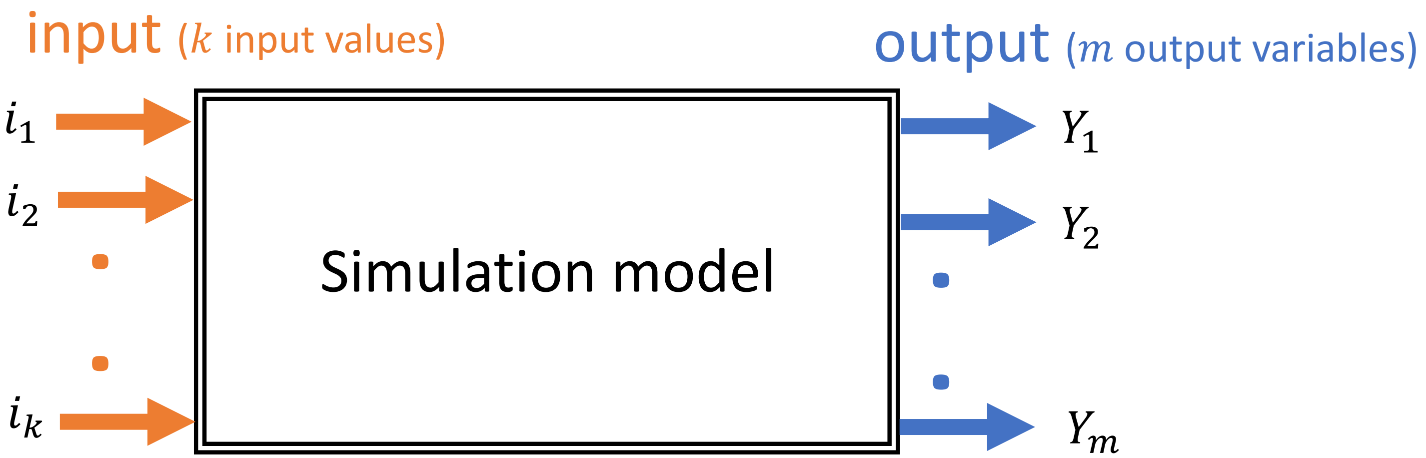
Preparation step

1) Identify a set of input parameters w/ unknown values (I_c).

2) Identify a set of output variables of interest (Y_c).

3) Get (real-world) data to measure the selected output variables ($Y_c^{(real)}$).

4) Set initial values for I_c.



Calibration in detail

Calibration step

1) Run the model and collect output data (Y_c).

2) Compare output data (Y_c) against real-world data ($Y_c^{(real)}$)

3) Is difference low enough?

No

Adjust parameter values (I_c)

Yes

Store (I_c)

End

Check the goodness of fit here

- Squared error
- Mean error
- Mean normalized error
- Mean absolute error
- Root mean square error
- …

Did we reach a reasonably low value?

Change the values in a way that it can improve the fit.

These three steps can be formulated as an optimization problem in which the objective function is to minimize the difference between Y_c and $Y_c^{(real)}$.

- Heuristics
- Dynamic programming
- …

Calibration example: projectile motion

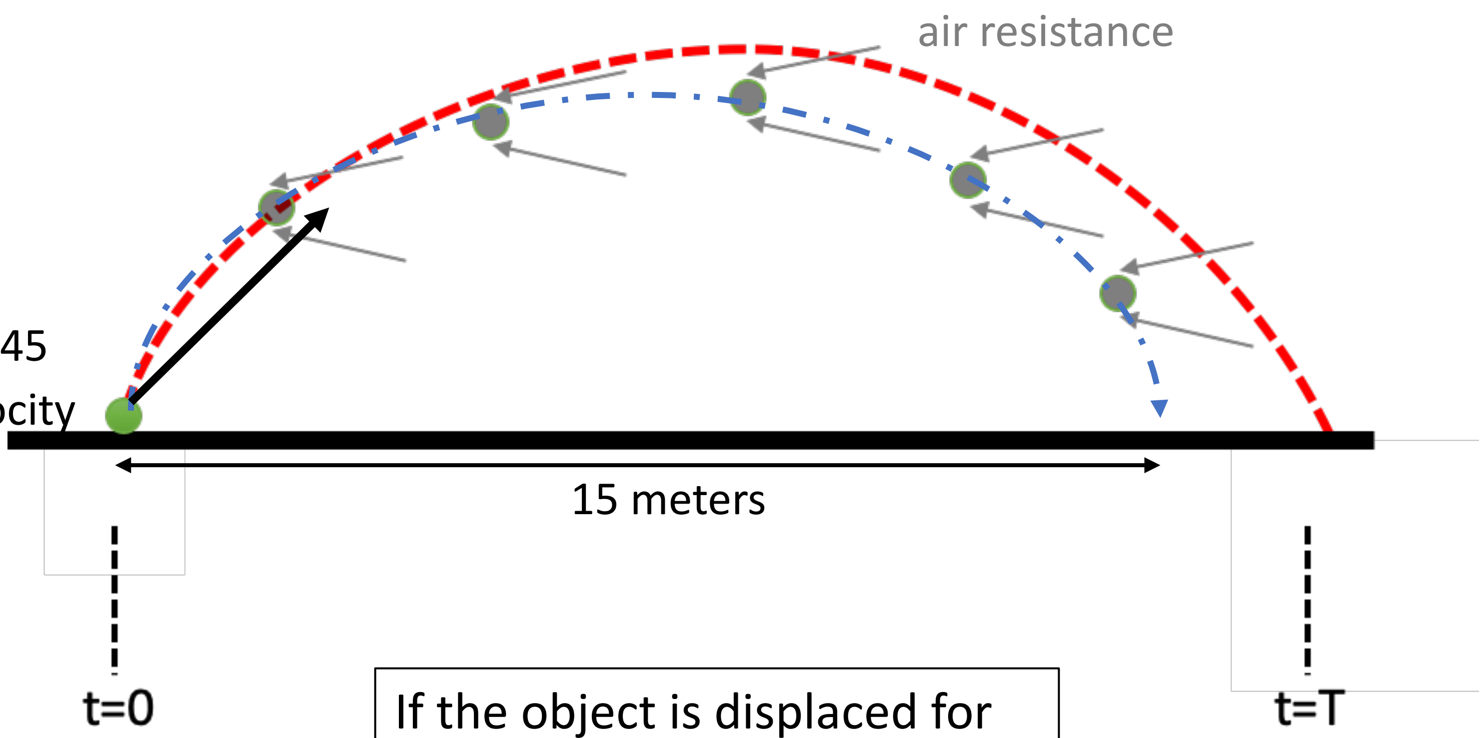
Parameters

$m = 1$

$g = 9.81$

$v_h = 10, v_v = 10$

The object is thrown at 45 degrees with $10\sqrt{2}$ velocity



If the object is displaced for 15 meters when touches the ground, calibrate the model to find air resistance (k).

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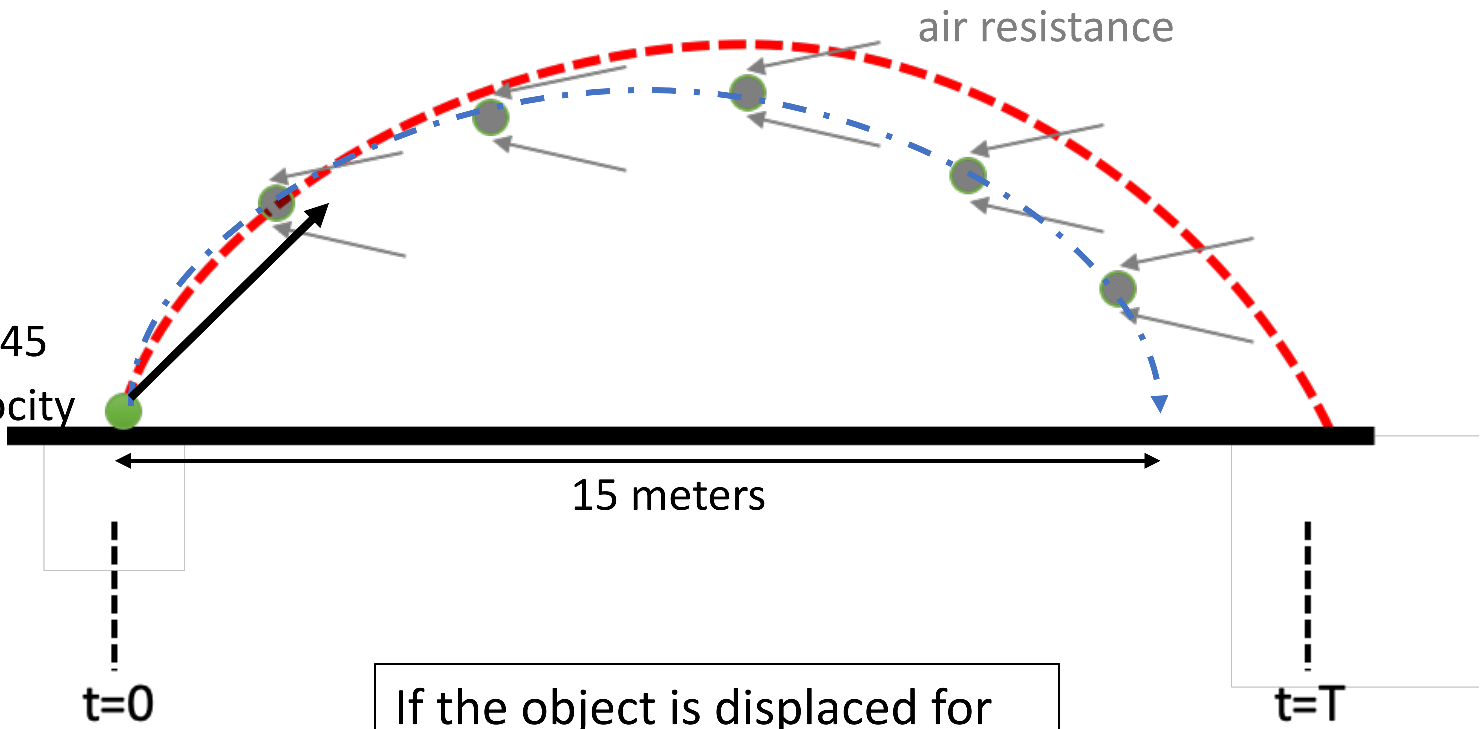

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Variables for projectile motion model

- System states
  - Position (x, y)
  - Speed (horizontal speed, vertical speed)
- Variables
  - Mass
  - Air resistance coefficient
  - Gravity

Dynamics for projectile motion

- $u = (x, y)$ - two dimensional position of our mass (m).
- Our mass is under the influence of two forces
  - Gravity mg or the vector of $(0, -9.81m)$.
  - Air resistance $F = -ku$'.
- Newton's Second Law of Motion (F=ma)
  - $F + mg = m \cdot u''$ can be rearranged by plugging $F = -ku'$ and leaving u'' alone.
    - $u'' = -\frac{k}{m}u' + g$ (second order ODE).
- Transform to a single-order ODE by plugging $\mathrm{v} = (u, u')$ thus $v' = (u', u'')$
  - $v' = (u', u'') = (u', -\frac{k}{m}u' + g)$ which can be represented as a function of v.

Parameters

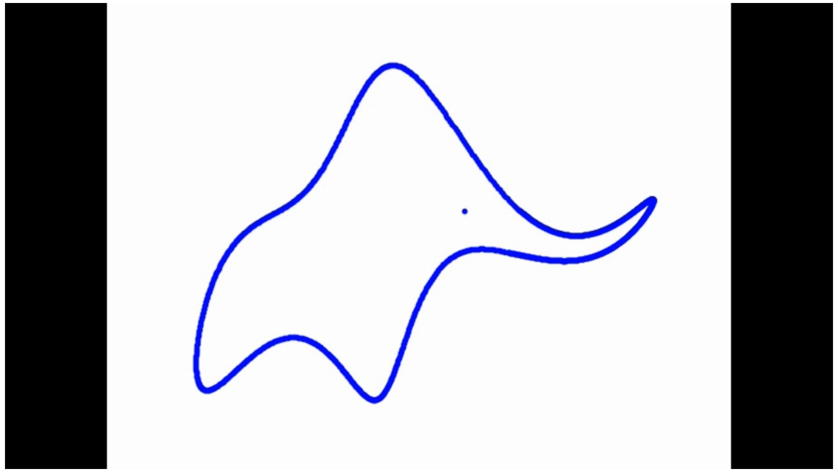
- Initial position (x, y): $(0, 0)$
- Final position: (15,0) – assume we collected this from the real-world
- Velocity $(horizontal, vertical)$: $(10, 10)$
- Parameter to be calibrated k which is set 0.1 initially.

- Goal find k which can predict the 15-meter disposition properly.

Calibration challenges

- Too many input parameters -> large search space
- Too many variables in the objective function
- Overfit (calibrating unrelated parameters)

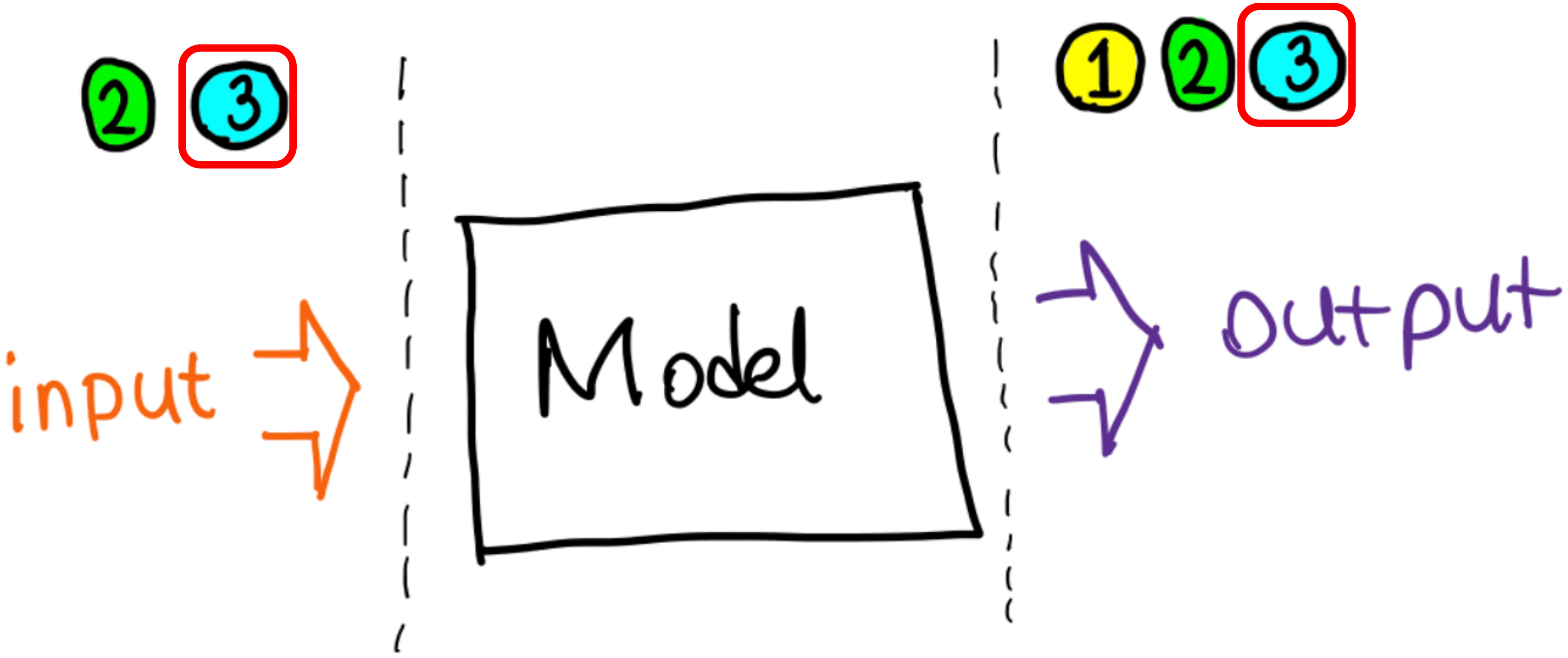
recall
"With four parameters I can fit an elephant, and with five I can make him wiggle his trunk."
– John von Neumann
check https://youtu.be/CVDYh5liQkA



1 Non-terminating simulations

2 Model parameter value estimation

3 Model sensitivity



Model sensitivity

- Ideally, models are tolerant to small changes in input parameter values.
- Tolerance to parameter value changes shows how robust the simulation model is.
- We study such tolerance cases using **sensitivity analysis**.

Hypothetical equation model

- Write a Python code for the following equation
  - $x_{n+1} = r\, x_n\, (1 - x_n)$
- Start with r=2, and $x_0 = 0.1$
- Compute for 100 iterations.
- Plot the results.
- What value does it settle on?

Hypothetical equation model

$$x_{n+1} = r\, x_n\, (1 - x_n)$$

- If the value of r is 2.5 what is the final value of the graph?
- If the value of r is 2.8 what is the final value of the graph?
- Before trying it, predict the value for r = 3.
- r=3.3?
- r=3.5?
- r=4.0?

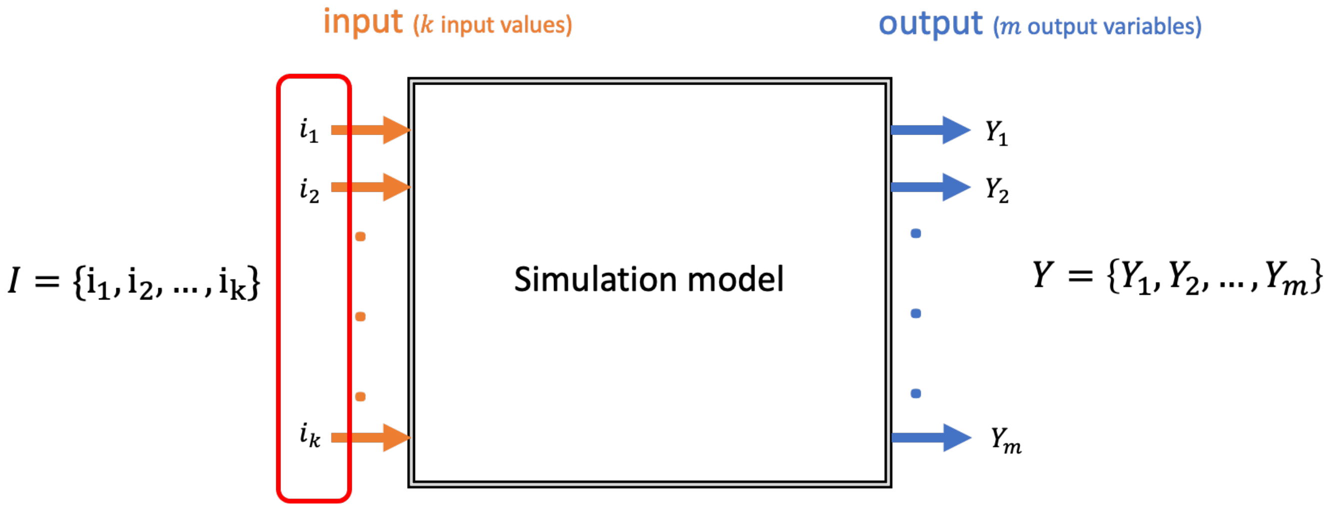
Sensitivity analysis

- "Sensitivity analysis is a validation method that compares magnitude and variability in simuland behavior to magnitude and variability in the model results" (Sokolowski & Banks, 2010).
- Thus, the challenge is to **systematically** vary input parameter values to observe output values.
  - Input-output relationship can be tested using "partial correlation" etc.
- If the simulation model is stochastic, we need to run multiple times to observe changes in the aggregated behavior (e.g., average).

How to vary input values?

- If you have one input to vary, it is a relatively simple problem.
  - Keep everything constant, sample from the min-max range of values
- If you have multiple inputs to vary
  1. Systematically
     - Design of experiments
       - Full factorial design
       - Selecting certain combinations. E.g., Latin Hypercube Sampling
  2. Randomized

Full Factorial Design



- Captures all possible combinations.
- If all k model parameters are binary, we will have 2^k combinations to run.
- If all model parameters are continuous, we will first need to identify discrete points within each range and then run all possible combinations.

Latin Hypercube Sampling (LHS)

- "is a way to sample the space of all combinations of the input variables" (Collins).
- Reduces the number of runs to a reasonable number.
- Your results should approximate to the case should you sampled the whole space.

LHS

- Step 1: Identify number of runs (n).
- Step 2: For each of k input variables
  - Identify range of possible values
  - Divide the range into n equally-probable bins.
  - Choose a value randomly from each bin.
- Step 3: Randomly combine these values from each bin w/out replacement. Meaning, make n combinations.
- Step 4: Run the model with all n combinations.
  - If the model is stochastic, you may want to run each combination multiple times.

LHS bin combinations

- $n = 2$

- $n = 3$

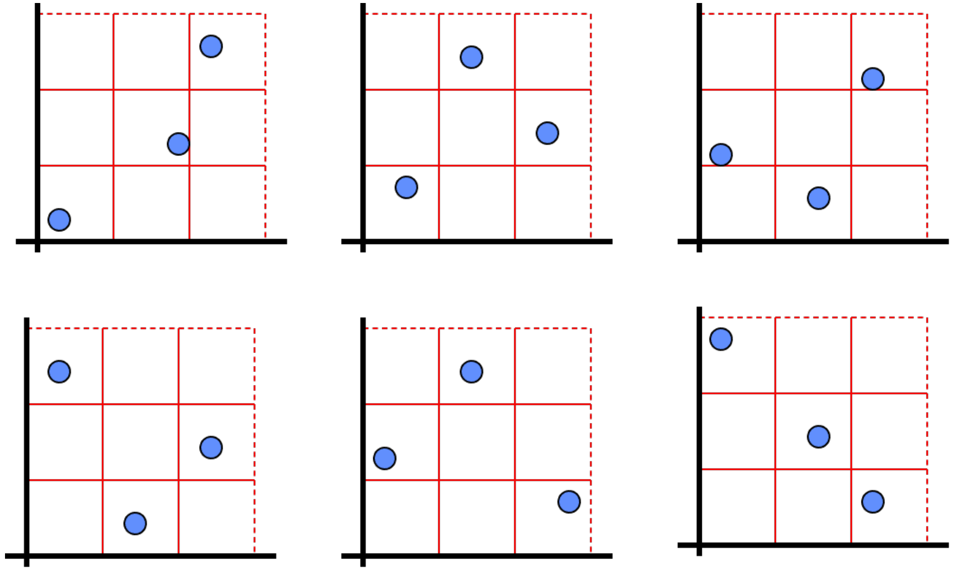
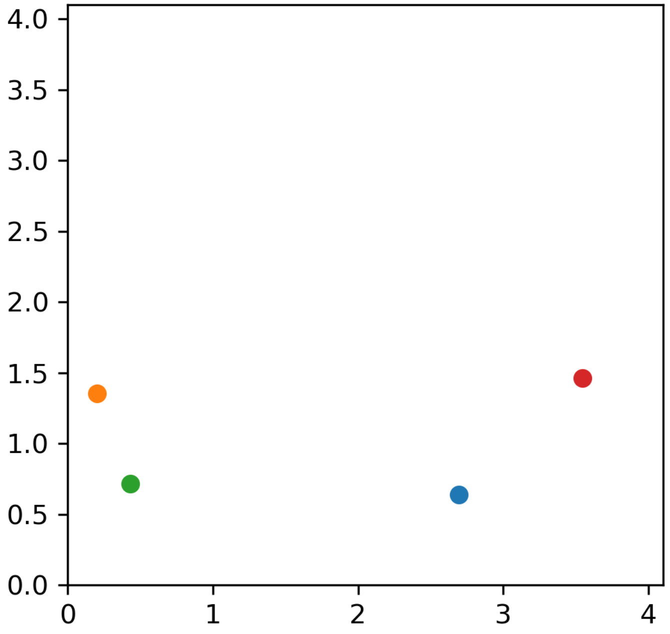
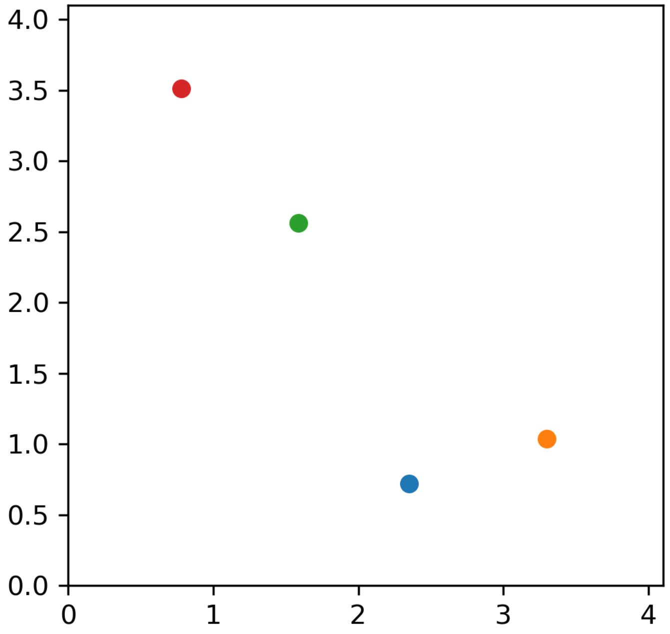


Figure source: Collins

LHS vs. random sampling

Value ranges: [0,4]
n = 4





Can you guess which one is which?

How many runs are needed for stochastic models per parameter configuration?

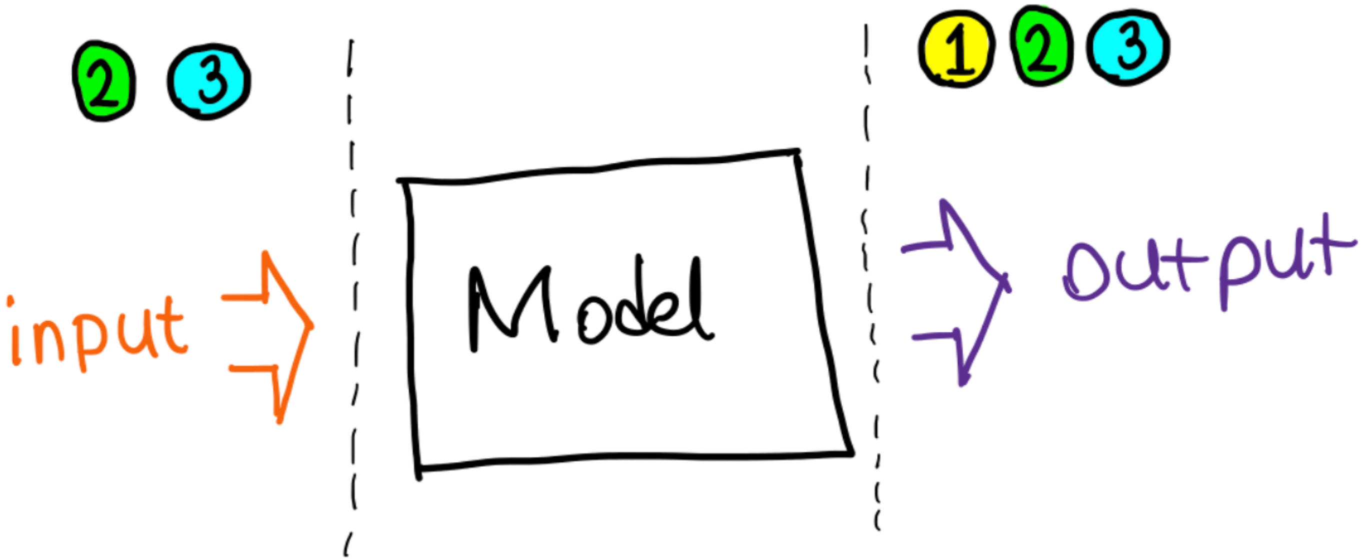
- There is no magical formula.
- Identify output variables of interest.
- Vary number of runs from lower to higher numbers
  - (e.g., [10, 100, 1000, 10k])
- Capture the variation in output variables.
- If two consecutive runs (e.g., 100 vs. 1000) have very similar variation, choose the lower number of runs (i.e., 100).

Sensitivity analysis challenges

- Large parameter space, leading to huge computational cost.
  - Imagine 10 input variables with 10 possible values each.
    - 10^{10} = 10,000,000,000 = 10 billion runs.
    - What if the variables are continuous.
  - Need ways to reduce computational time, especially for large-scale ABMs.
  - Stochastic simulation needs more runs.
- What is an ideal step-size?
  - What if a small change leads to a chaotic behavior but sensitivity analysis cannot capture it?

Wrap-up and questions

1. Non-terminating simulations
2. Model parameter value estimation
3. Model sensitivity



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