A Case of Identity Crisis

Preserving Identifiability in Linear Compartment Models

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Plan of Attack

Outline of my talk:

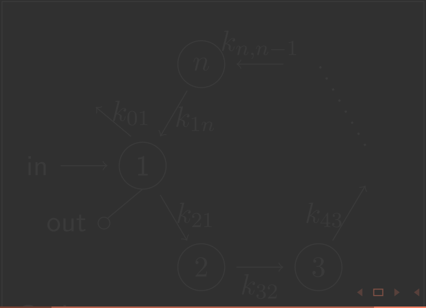
- Set Up:
  1. Linear Compartment Model
  2. Input-Output Equation
  3. Identifiability
- Results
  1. Removing the Leak
  2. Moving the Ouput
  3. New Models
     - Fin/ Nemo Models
     - Wing/ Tweety Bird Models

It's a Set Up: Part 1

Linear Compartment Models

Components of a mode:

- Compartments
- Input
- Output
- Edges (Parameters, $k_{ij}s$)
- Leaks (Optional) (Special kind of parameter, k_{0j})



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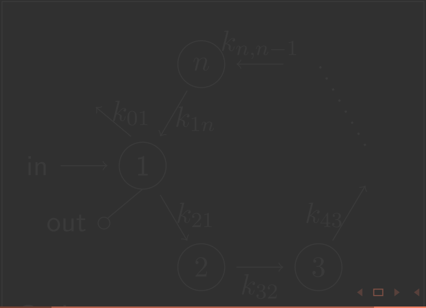

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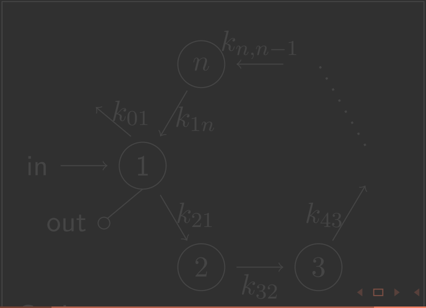

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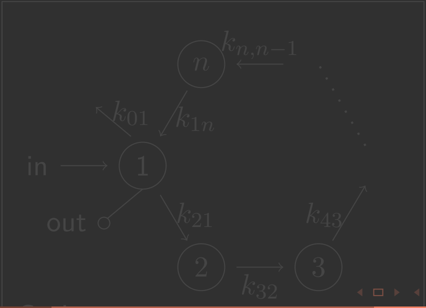

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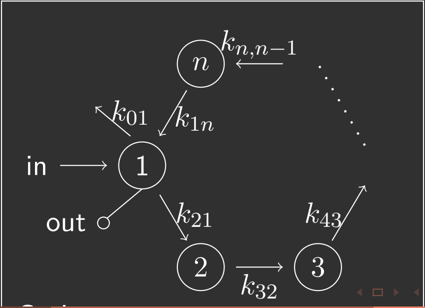

It's still a Set-Up

Input-Output Equation

- Equation which holds along any solution any solution of the ODE, involving only *input* and *output* variables
- General Equation: $\det(\partial I - A)y_i = \sum_{j \in In}(-1)^{i+j}\det(\partial I - A_{ji})u_j$
- Trick lies in computing the determinants
- Gives us *coefficients*
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It's totally a Set-Up

Coefficient Map

- Goes from the parameters to coefficients of *input-output equation*
- Example:

$$c : \mathbb{R}^5 \mapsto \mathbb{R}^5$$

$$(k_{01}, k_{21}, k_{12}, k_{23}, k_{32}) \mapsto$$
$$(k_{21} + k_{32}, k_{32}k_{01}, k_{12}k_{32} + k_{01}k_{21}, k_{12} + k_{21}, k_{01}k_{12}k_{21}k_{23}, k_{32}) \quad (1)$$

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OMG we get it-it's a set-up!

Identifiability

- Only know 2 things: input and output data
- Given the coefficient values, can we figure out what the parameters are?
- For example: Given $(k_{21}+k_{32}, k_{32}k_{01}, k_{12}k_{32}+k_{01}k_{21}, k_{12}+k_{21}, k_{01}k_{12}k_{21}k_{23}, k_{32})$ Can we figure out $(k_{01}, k_{21}, k_{12}, k_{23}, k_{32})$?

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Key tools for identifiability:

- A model is identifiable iff the Jacobian Matrix of the coefficient map has *full rank*
- Full rank means:
  1. Given n parameters...
  2. There exists a $n \times n$ submatrix of the Jacobian matrix...
  3. such that the determinant of the submatrix is nonzero.
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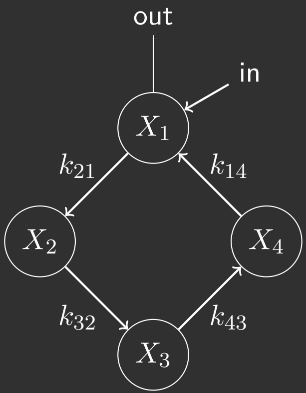

$$X_1'(t) = -k_{21}x_1 + k_{14}x_4$$
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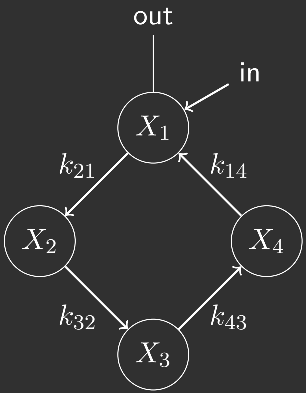

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Example Part 2

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A matrix can be built from those ODEs:

$$
A = \begin{bmatrix} -k_{21} & 0 & 0 & k_{14} \\ k_{21} & -k_{32} & 0 & 0 \\ 0 & k_{32} & -k_{43} & 0 \\ 0 & 0 & k_{43} & -k_{14} \end{bmatrix}
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Example Part 3

- The input-out equation for this model is:

$$\det(\partial I - A)y_1 = \det(\partial I - A)_{11}u_1$$

- The $(\partial I - A)$ matrix is:

$$(\partial I - A) = \begin{bmatrix} \frac{d}{dt} + k_{21} & 0 & 0 & -k_{14} \\ -k_{21} & \frac{d}{dt} + k_{32} & 0 & 0 \\ 0 & -k_{32} & \frac{d}{dt} + k_{43} & 0 \\ 0 & 0 & -k_{43} & \frac{d}{dt} + k_{14} \end{bmatrix}$$

Example Part 4

1. From the input-output equation, derive a *coefficient map*

$$(k_{21}, ..., k_{1n}) \longmapsto (c_1, c_2, ...)$$

2. Take the Jacobian matrix of the coefficient map
3. ***If the Jacobian matrix is full rank, then the model is identifiable***
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Pause...

Any questions about the Set-Up?

Results: Finding identity

Three main results:

- Removing the Leak
- Moving the output in cycle models
- New Models

A Brief Digression

A note on elementary symmetric polynomials

- Essential for proving the results
- Given a set $X = \{x_1, ..., x_n\}$
- The m^{th} elementary symmetric polynomial is:

$$e_m = \sum_{j_1 < j_2 < \cdots < j_m} x_{j_1} ... x_{j_m}$$

- Easier with an example

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It's elementary, my dear Watson

Say $X = \{x_1, x_2, x_3\}$. The Elementary symmetric polynomials on X are:

- $e_0 = 1$
- $e_1 = x_1 + x_2 + x_3$
- $e_2 = x_1x_2 + x_1x_3 + x_2x_3$
- $e_3 = x_1x_2x_3$

IMPORTANT PROPERTY

$$\frac{\partial e_m}{\partial x_i} = \sum_{j_2 < \ldots < j_m} x_{j_2} \ldots x_{j_m} =: e_{m-1}\{\hat{x}_i\}$$

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Given an identifiable model with a leak, does removing the leak preserve identifiability?

YES! for certain models (cycle, catenary, mammillary)

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Basic Proof

Theorem

Let $\tilde{M}$ be a catenary, cycle, or mammillary model that has at least one input and exactly one leak. If $\tilde{M}$ is generically locally identifiable from the coefficient map, then so is the model M obtained from $\tilde{M}$ by removing the leak.

Proof.

Proposition 4.7 from Gross, Harrington, Meshkat, and Shiu (2019) states catenary, cycle, and mammillary models, with no leaks, are locally identifiable from the coefficient map. Then, by Theorem 4.3 from Gross et. al., adding a leak preserves identifiability. Thus, both M and $\tilde{M}$ are generically locally identifiable. □

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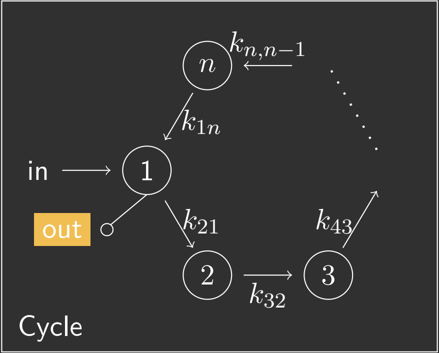
Moving the Output

The Question:

In a cycle model, does removing the output preserve identifiability?

For example:

- Output is located in compartment 1...



Moving the Output

The Question:

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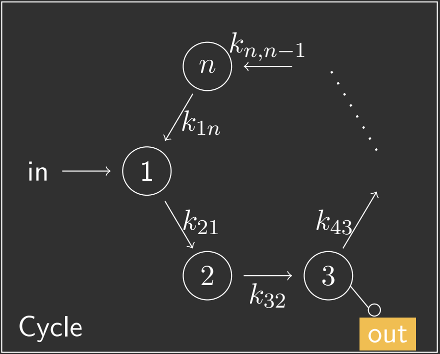
- ... moved to compartment 3



Solution to output distribution

Key takeaways: Let p be the output compartment.

- Input-ouput equation:
  - $\left(\frac{d}{dt}^{n}(e_0) + \frac{d}{dt}^{n-1} e_1 + \cdots + \frac{d}{dt} e_{n-1}\right) y_n =$ $\left(\prod_{i=p+1}^{n+1} k_{i,i-1}\left(\frac{d}{dt}^{p-2} e_0^* + \frac{d}{dt}^{p-3} e_1^* + ... + e_{p-2}^*)\right)\right) u_1$
- Coefficient Map:
  - $$c : \mathbb{R}^n \to \mathbb{R}^{n+p-2}$$

    where

    $$(k_{21}, ..., k_{1n}) \longmapsto (e_1, ..., e_{n-1}, \prod_{i=p+1}^{n+1} k_{i,i-1} e_0^*, ..., \prod_{i=p+1}^{n+1} k_{i,i-1} e_{p-2}^*)$$

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Solution to output distribution pt. 2

Selected submatrix of the Jacobian:

$$J = \begin{bmatrix} 1 & 1 & \dots & 1 & \dots & 1 \\ e_1\{\hat{k}_{21}\} & e_1\{\hat{k}_{32}\} & \dots & e_1\{\hat{k}_{p+1,p}\} & \dots & e_1\{\hat{k}_{1n}\} \\ \vdots & & \ddots & & & \vdots \\ e_{n-2}\{\hat{k}_{21}\} & e_{n-2}\{\hat{k}_{32}\} & \dots & e_{n-2}\{\hat{k}_{p+1,p}\} & \dots & e_{n-2}\hat{k}_{1n}\} \\ 0 & 0 & \dots & \tilde{e}_{n-p+1}\{\hat{k}_{p+1,p}\} & \dots & \tilde{e}_{n-p+1}\{\hat{k}_{1n}\} \end{bmatrix}$$

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- Since determinant is nonzero, model is generically locally identifiable!

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Introducing, New Models!

A new "family" of models

- Fin Model
- Nemo Model
- Wing Model
- Tweety Bird Model

Nemo models derived from Fin models
Tweety Bird models derived from Wing Models

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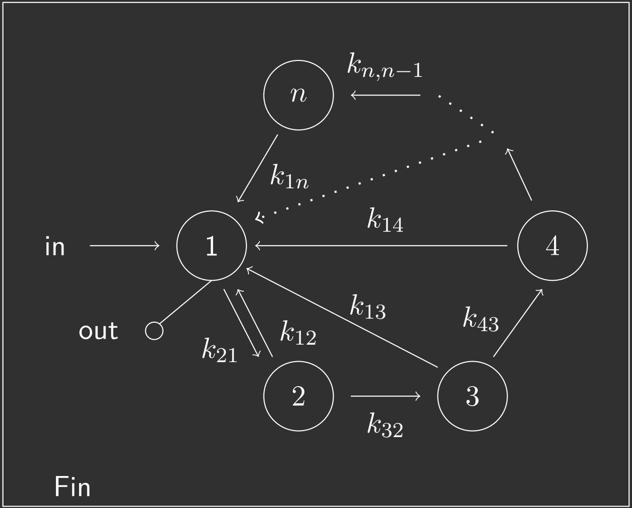
Fin and Nemo Models



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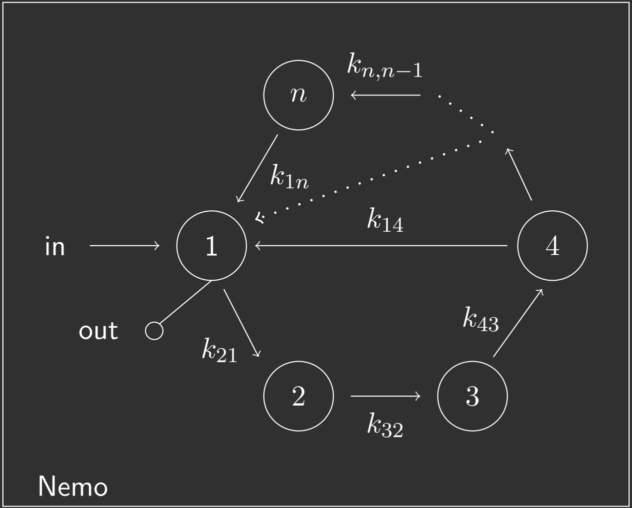

Finding Nemo: an existential crisis

How to find Nemo:

By showing Fin models are identifiable, we can show Nemo models are identifiable.

Finding Nemo: The Lucky Fin

For a Fin Model:

- Input-Output Equation

  ... Too long for this slide...

- Coefficient Map

$$c : \mathbb{R}^{2n-2} \to \mathbb{R}^{2n-1}$$

such that

$$(k_{12}, ..., k_{1n}, k_{21}, ..., k_{n,n-1}) \longmapsto$$

$$(e'_1, ..., e'_{n-1}, e^*_1, e^*_2 + \sum_{i=2}^{2} P_i e^i_{2-i}, ..., e^*_j + \sum_{i=2}^{j} P_i e^i_{j-i}, ..., e^*_n + \sum_{i=2}^{n} P_i e^i_{n-i})$$

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Finding Nemo: The Lucky Fin

For a Fin Model:

- Input-Output Equation
  ... Too long for this slide...
- Coefficient Map

$$c : \mathbb{R}^{2n-2} \to \mathbb{R}^{2n-1}$$

such that

$$(k_{12}, ..., k_{1n}, k_{21}, ..., k_{n,n-1}) \longmapsto$$
$$(e'_1, ..., e'_{n-1}, e^*_1, e^*_2 + \sum_{i=2}^{2} P_i e^i_{2-i}, ..., e^*_j + \sum_{i=2}^{j} P_i e^i_{j-i}, ..., e^*_n + \sum_{i=2}^{n} P_i e^i_{n-i})$$

Finding Nemo: The Lucky Fin, Chapter 2

Selected Submatrix of the coefficient map Jacobian:

- New proof approach
- Break into "block" matrix

$$\tilde{J}(c) = \begin{bmatrix} W & X \\ Y & Z \end{bmatrix}$$

- Only need to show W and Z have nonzero determinants

Finding Nemo: The Lucky Fin, Chapter 2

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Finding Nemo: The Lucky Fin, Chapter 2, pt. 2

$$W = \begin{bmatrix} e^*_{n-1}\{\hat{k}_{21}\} + \beta_2^n & e^*_{n-1}\{\hat{k}_{32}\} + \beta_3^n & \dots & e^*_{n-1} + \alpha_2^{n-3} + \beta_{n-1}^n \\ 0 & e'_1\{\hat{k}_{32}\} & \dots & e'_1\{\hat{k}_{n,n-1}\} \\ \vdots & & & \\ 0 & e'_{n-2}\{\hat{k}_{32}\} & \dots & e'_{n-2}\{\hat{k}_{n,n-1}\} \end{bmatrix}$$

$$\det(W) \neq 0$$

The Lucky Fin, Chapter 2, pt. 2, scene 2

$$Z = \begin{bmatrix} 1 & 0 & 0 & \dots & & 0 \\ e_1^*\{\hat{k}_{1n}\} & \gamma_2^2 & 0 & \dots & & 0 \\ \sigma_3 & \gamma_3^2 & \gamma_3^3 & \dots & & 0 \\ \vdots & & & & & \vdots \\ \sigma_j & \dots & & \gamma_j^j & \dots & 0 \\ \vdots & & & & & \vdots \\ \sigma_{n-1} & \gamma_{n-1}^2 & \dots & \gamma_{n-1}^j & \dots & \gamma_{n-1}^{n-1} \end{bmatrix}$$

$$\det(Z) \neq 0$$

Thus, $\det\left(\tilde{J}\right) \neq 0$, and the model is generically locally identifiable

Finding Nemo: Just keep swimming

Technique:

- When you remove those edges...
- Coefficient map slightly changes
- The W submatrix is essentially unchanged
- Only Z has to be really addressed
  - Remove the column corresponding to the removed parameter
  - Remove the row corresponding to the same parameter

While Z is smaller, it still has a nonzero determinant

Finding Nemo: Just keep swimming

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Nemo Found!

A little more explanation

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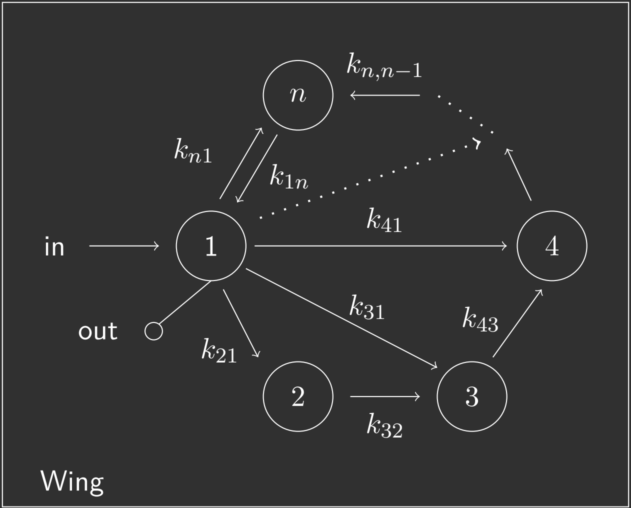
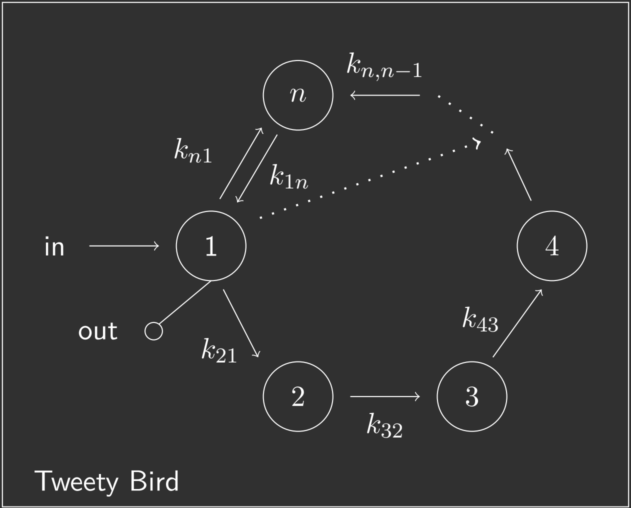
Wing and Tweety-Bird models



Wing and Tweety Bird Models



Finding Tweety Bird

Technique:

- Same idea as Fin/Nemo model
- Coefficients are different...
- But the proof is similar enough
- Both models are identifiable

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Acknowledgments

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The End