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 Output
  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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- Equation which holds along any solution any solution of the ODE, involving only input and output variables

- General Equation:
  \[ \det(\partial I - A)y_i = \sum_{j \in I_n} (-1)^{i+j} \det(\partial I - A_{ji})u_j \]

- Trick lies in computing the determinants

- Gives us coefficients

- Derive a coefficient map
It’s still a Set-Up

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It’s totally a Set-Up

Coefficient Map

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

\[
c : \mathbb{R}^5 \rightarrow \mathbb{R}^5
\]

\[
(k_{01}, k_{21}, k_{12}, k_{23}, k_{32}) \mapsto (k_{21} + k_{32}, k_{32}k_{01}, k_{12}k_{32} + k_{01}k_{21}, k_{12} + k_{21}, k_{01}k_{12}k_{21}k_{23}, k_{32})
\]  (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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Can we figure out $$(k_{01}, k_{21}, k_{12}, k_{23}, k_{32})$$?
At this point it’s obviously a set-up

Key tools for identifiability:

- A model is identifiable iff the Jacobian Matrix of the coefficient map has \textit{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.
- We need only one to be nonzero.
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Example Part 1

\[ X'_1(t) = -k_{21}x_1 + k_{14}x_4 \]
\[ X'_2(t) = -k_{32}x_2 + k_{21}x_1 \]
\[ X'_3(t) = -k_{43}x_3 + k_{32}x_2 \]
\[ X'_4(t) = -k_{14}x_4 + k_{43}x_3 \]
Example Part 1

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Example Part 2

\[
X'_1(t) = -k_{21}x_1 + k_{14}x_4 \\
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\]

A matrix can be built from those ODEs:

\[
A = \begin{bmatrix}
-k_{21} & 0 & 0 & k_{14} \\
 k_{21} & -k_{32} & 0 & 0 \\
 0 & k_{32} & -k_{43} & 0 \\
 0 & 0 & k_{43} & -k_{14}
\end{bmatrix}
\]
Example Part 2

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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:
  \[
  (\partial I - A) = \begin{bmatrix}
  \frac{d}{dt} + k_{21} & 0 & 0 & -k_{14} \\
  -k_{21} & \frac{d}{dt} + k_{32} & 0 & 0 \\
  0 & -k_{32} & \frac{d}{dt} + k_{43} & 0 \\
  0 & 0 & -k_{43} & \frac{d}{dt} + k_{14}
  \end{bmatrix}
  \]
1. From the input-output equation, derive a coefficient map

\[
(k_{21}, \ldots, k_{1n}) \mapsto (c_1, c_2, \ldots)
\]

2. Take the Jacobian matrix of the coefficient map

3. If the Jacobian matrix is full rank, then the model is identifiable

4. The example I showed was identifiable
Example Part 4

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

\[(k_{21}, \ldots, k_{1n}) \rightarrow (c_1, c_2, \ldots)\]

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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From the input-output equation, derive a coefficient map

\[(k_{21}, ..., k_{1n}) \mapsto (c_1, c_2, \ldots)\]

1. Take the Jacobian matrix of the coefficient map
2. *If the Jacobian matrix is full rank, then the model is identifiable*
3. The example I showed was identifiable
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 $X = \{x_1, \ldots, x_n\}$
- The $m^{th}$ elementary symmetric polynomial is:
  
  $$e_m = \sum_{j_1 < j_2 < \cdots < j_m} x_{j_1} \cdots x_{j_m}$$

- Easier with an example

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- Easier with an example
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**

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

Elementary symmetric polynomials are linearly independent.
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\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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Elementary symmetric polynomials are linearly independent
Removing the Leak

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

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

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Removing the Leak

Given an identifiable model with a leak, does removing the leak preserve identifiability?
YES! for certain models (cycle, catenary, mammillary)
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. □
Basic Proof

Theorem

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

For example:
- Output is located in compartment 1...
The Question:

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

- ... moved to compartment 3
Key takeaways: Let $p$ be the output compartment.

- **Input-output equation:**
  \[
  \left( \frac{d}{dt} n^1(e_0) + \frac{d}{dt} n^{-1} e_1 + \cdots + \frac{d}{dt} e_{n-1} \right) y_n = \\
  \left( \prod_{i=p+1}^{n+1} k_{i,i-1} \left( \frac{d}{dt} p^{-2} e_0^* + \frac{d}{dt} p^{-3} e_1^* + \cdots + e_{p-2}^* \right) \right) u_1
  \]

- **Coefficient Map:**
  \[
  c : \mathbb{R}^n \rightarrow \mathbb{R}^{n+p-2}
  \]
  where
  \[
  (k_{21}, \ldots, k_{1n}) \mapsto (e_1, \ldots, e_{n-1}, \prod_{i=p+1}^{n+1} k_{i,i-1} e_0^*, \ldots, \prod_{i=p+1}^{n+1} k_{i,i-1} e_{p-2}^*)
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Key takeaways: Let $p$ be the output compartment.

- **Input-output equation:**
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  \]
Selected submatrix of the Jacobian:

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

- Determinant is nonzero

- Since determinant is nonzero, model is generically locally identifiable!
Selected submatrix of the Jacobian:

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\hat{e}_1\{\hat{k}_2\} & \hat{e}_1\{\hat{k}_3\} & \cdots & \hat{e}_1\{\hat{k}_{p+1}\} & \cdots & \hat{e}_1\{\hat{k}_n\} \\
\vdots & \vdots & \ddots & \vdots & \cdots & \vdots \\
\hat{e}_{n-2}\{\hat{k}_2\} & \hat{e}_{n-2}\{\hat{k}_3\} & \cdots & \hat{e}_{n-2}\{\hat{k}_{p+1}\} & \cdots & \hat{e}_{n-2}\{\hat{k}_n\} \\
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Solution to output distribution pt. 2

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- Determinant is nonzero
- Since determinant is nonzero, model is generically locally identifiable!
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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Nemo models derived from Fin models
Tweety Bird models derived from Wing Models

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A Case of Identity Crisis

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The diagram represents a network of models labeled Fin and Nemo. The nodes are labeled as 1 to 4, with directed edges indicating the flow between them. The edges are labeled with parameters such as $k_{n,n-1}$, $k_{1n}$, $k_{14}$, $k_{21}$, $k_{43}$, and $k_{32}$. The network appears to illustrate a case of identity crisis, possibly indicating transitions or interactions between different states or models.
Finding Nemo: an existential crisis

How to find Nemo:

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

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Finding Nemo: The Lucky Fin

For a Fin Model:

- **Input-Output Equation**
  
  ... Too long for this slide...

- **Coefficient Map**

  \[
  c : \mathbb{R}^{2n-2} \rightarrow \mathbb{R}^{2n-1}
  \]

  such that

  \[
  (k_{12}, \ldots, k_{1n}, k_{21}, \ldots, k_{n,n-1}) \rightarrow \left( e'_1, \ldots, e'_{n-1}, e^*_1, e^*_2 + \sum_{i=2}^{2} P_ie^*_i, \ldots, e^*_j + \sum_{i=2}^{j} P_ie^*_i, \ldots, e^*_n + \sum_{i=2}^{n} P_ie^*_i \right)
  \]
Finding Nemo: The Lucky Fin

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\]

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Finding Nemo: The Lucky Fin

For a Fin Model:

- Input-Output Equation
  ... Too long for this slide...
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such that

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(k_{12}, \ldots, k_{1n}, k_{21}, \ldots, k_{n,n-1}) \longrightarrow \\
(e'_1, \ldots, e'_{n-1}, e^*_1, e^*_2 + \sum_{i=2}^{2} P_i e^*_{2-i}, \ldots, e^*_j + \sum_{i=2}^{j} P_i e^*_{j-i}, \ldots, e^*_n + \sum_{i=2}^{n} P_i e^*_{n-i})
\]
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
Selected Submatrix of the coefficient map Jacobian:

- New proof approach
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\[ \tilde{J}(c) = \begin{bmatrix} W & X \\ Y & Z \end{bmatrix} \]

- Only need to show $W$ and $Z$ have nonzero determinants
Finding Nemo: The Lucky Fin, Chapter 2, pt. 2

\[ W = \begin{bmatrix}
  e_{n-1}^* \{k_{21}\} + \beta_n^2 & e_{n-1}^* \{k_{32}\} + \beta_3^n & \ldots & e_{n-1}^* + \alpha_{2-3}^n + \beta_{n-1}^n \\
  0 & e_{1}^* \{k_{32}\} & \ldots & e_{1}^* \{k_{n,n-1}\} \\
  \vdots & \vdots & \ddots & \vdots \\
  0 & e_{n-2}^* \{k_{32}\} & \ldots & e_{n-2}^* \{k_{n,n-1}\}
\] 

\[ \det(W) \neq 0 \]
\[ Z = \begin{bmatrix}
1 & 0 & 0 & \ldots & 0 \\
\sigma_3 & \gamma_2 & 0 & \ldots & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
\sigma_j & \vdots & \gamma_j & \ldots & 0 \\
\sigma_{n-1} & \gamma_{n-1} & \ldots & \gamma_j & \ldots & \gamma_{n-1}
\end{bmatrix} \]

\[ \det(Z) \neq 0 \]

Thus, \( \det(\tilde{J}) \neq 0 \), 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
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While $Z$ is smaller, it still has a nonzero determinant
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Nemo Found!

A little more explanation

\[
Z = \begin{bmatrix}
1 & 0 & 0 & \ldots & 0 \\
\mathbb{e}_1^* \left\{ \hat{k}_{1n} \right\} & \gamma_2 & 0 & \ldots & 0 \\
\sigma_3 & \gamma_3^2 & \gamma_3 & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\sigma_j & \ldots & \gamma_j & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\sigma_{n-1} & \gamma_{n-1}^2 & \gamma_j & \ldots & \gamma_{n-1}
\end{bmatrix}
\]
Wing and Tweety-Bird models

A Case of Identity Crisis

(S. Gerberding, USD)
Wing and Tweety Bird Models

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Finding Tweety Bird

Technique:

- Same idea as Fin/Nemo model
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A Case of Identity Crisis July 22, 2019
Finding Tweety Bird

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The End