Finding exact linear reductions of dynamical models

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March 30, 2023

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Some things are smaller than they appear

Exact reduction: a toy example

Setup

Consider a dynamical system in three variables x_1, x_2, x_3:

$$\begin{cases} \dot{x}_1 = x_2^2 + 4x_2x_3 + 4x_3^2 & , \\ \dot{x}_2 = 4x_3 - 2x_1, \\ \dot{x}_3 = x_1 + x_2. \end{cases}$$

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Reduction

For $y := x_2 + 2x_3$:

$$\dot{y} = \dot{x}_2 + 2\dot{x}_3 = 4x_3 + 2x_2 = 2(x_2 + 2x_3) = 2y.$$

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Thus, x_1 and y themselves form a reduced dynamical system:

$$\begin{cases} \dot{y} = 2y, \\ \dot{x}_1 = y^2. \end{cases}$$

Exact reduction: more than one

Reduction to dimension 2 from before:

$$\begin{cases} \dot{x}_1 = x_2^2 + 4x_2x_3 + 4x_3^2, \\ \dot{x}_2 = 4x_3 - 2x_1, \\ \dot{x}_3 = x_1 + x_2. \end{cases} \longrightarrow \begin{cases} \dot{y} = 2y, \\ \dot{x}_1 = y^2. \end{cases}$$

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In general, an infinite number of linear reductions is possible.

Exact reduction: formal statement

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We had $y = x_2 + 2x_3$, or, equivalently,

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Example

Any linear first integral is a linear reduction with $\dot{\mathbf{y}} = 0$

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Output (many reductions): a sequence of linear transformations

$$\mathbf{y}_1 = \mathbf{x}L_1, \ \ldots, \ \mathbf{y}_\ell = \mathbf{x}L_\ell$$

where each $\mathbf{y}_i = \mathbf{x}L_i$ is a reduction, $0 < m_1 < \ldots < m_\ell < n$, and $L_{i-1} = L_i A_i$ for some A_i.

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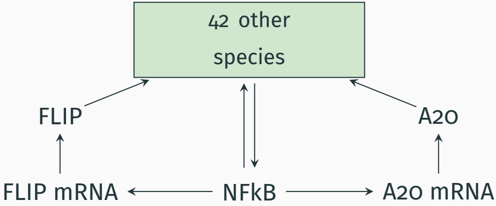
Such sequence is called a chain of reductions and has finite length

Real-world example

Model of cell death, *Schlieman et al. (2011)*



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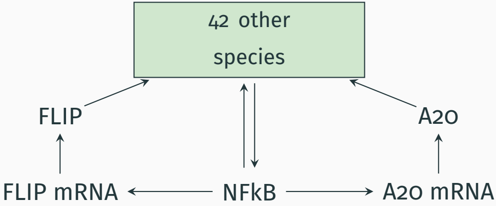

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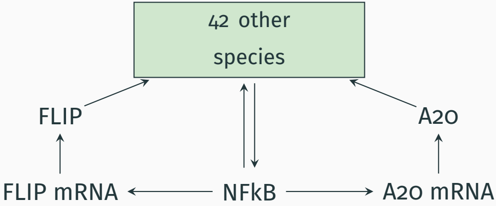

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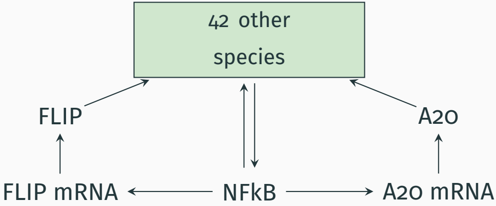

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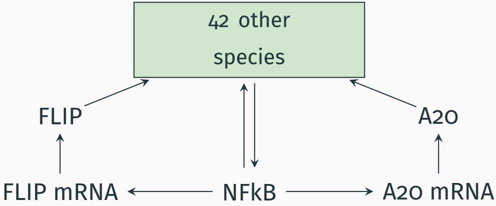

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$$\begin{cases} y_1 = \frac{k_6}{k_1}[A20] - \frac{k_5}{k_3}[FLIP], \\ y_2 = k_6[A20\ mRNA] - k_5[FLIP\ mRNA] \end{cases}$$

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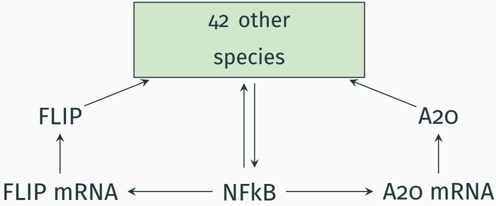

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Plus 16 other reductions (!)

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Focus on finding a single reduction subject to some constraints
$\longrightarrow$ won't autonomously find reductions from our examples

Our results

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We present an algorithm that finds a chain of exact linear reductions without restriction on the coefficients.

The chain will have the maximal possible length.

Real-world example #2

Reaction network

(enzyme deactivation)

$$\begin{array}{ccccc} E + S & \rightleftharpoons & ES & \rightleftharpoons & E + P \\ & & \downarrow & & \\ & & E^* + S & & \end{array}$$

$$E \rightleftharpoons E^*$$

Real-world example #2

Reaction network
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Corresponding ODE system:

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3. And zoom in: $y = E + ES - E^*$ ($\dot{y} = -2y$)

Algorithm outline: existing tools

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Proposition

For linear forms $y_1, \ldots, y_m$ in $\mathbf{x}$, the following are equivalent:

- $\dot{y}_1, \ldots, \dot{y}_m$ are polynomials in $y_1, \ldots, y_m$;
- the linear span of $y_1, ..., y_m$ is invariant under M_λ for every $1 \leq i \leq m$, $\lambda \in \Lambda$.

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$V = \langle e_1, e_2 \rangle$ is invariant.

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$V = \langle e_1, e_2 \rangle$ is invariant.

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Long story short. The problem is reduced to

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- but the input is sparse
- and the output is usually *very simple*

The implementation

Package ExactODEReduction.jl, in the Julia language

`https://github.com/x3042/ExactODEReduction.jl`

Running on models from BioModels repository:

Models info		Reductions		Runtime
Dimension	# Models	# Total	# Non-equivalent	Average
2 - 9	44	4.02	1.39	0.6 s
10 - 19	**41**	**8.15**	**2.61**	**0.21 s**
20 - 29	46	9.65	2.13	0.44 s
30 - 39	17	19.41	2.71	1.74 s
40 - 59	25	29.08	6.08	4.58 s
60 - 79	20	37.25	6.95	34.57 s
80 - 99	11	42.91	7.09	96.38 s
100 - 133	4	89.0	21.5	202.52 s

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And now software demo

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2. Exact reductions as a way to verify the accuracy of numerical simulations
3. Exact reductions for other types of structured dynamical systems, such as, e.g., *graph-based models*

Thank you !

..and my supervisors