Structural Identifiability via the Web App: A Maple Cloud Toolbox

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Introduction

1. Structural parameter identifiability describes whether a parameter value can be recovered from data before performing experiments.
2. A parameter is can be *locally* (finitely many values) or *globally* (uniquely) identifiable.
3. If neither is the case, we say that a parameter is unidentifiable and we seek *identifiable combinations* (functions of parameters that are globally identifiable).
4. Some parameters may be identifiable from more than one experiment. Finding the bound on the maximal amount of experiments is crucial.

Motivating Examples

- **A simple two-parameter model**

$$\begin{cases} x' = A^2, \\ x(0) = B, \\ y = x \end{cases} \Rightarrow \begin{cases} \text{Globally: } B = y(0), \\ \text{Locally: } A = \pm\sqrt{y(1) - y(0)} \end{cases} \tag{1}$$

- **Unidentifiable case**

$$\begin{cases} x' = 0, \\ y_1 = x,\ y_2 = Cx + D \end{cases} \Rightarrow \begin{cases} \text{Globally: } x(0) = y(0) \\ \text{Unidentifiable: } C, D \end{cases} \tag{2}$$

- The latter case is mitigated by performing *2 experiments:*

$$\begin{cases} x_1' = 0,\ x_2' = 0 \\ y_{11} = x_1,\ y_{12} = Cx_1 + D \\ y_{21} = x_2,\ y_{22} = Cx_2 + D \end{cases} \Rightarrow \begin{cases} \text{Globally: } C, D \end{cases} \tag{3}$$

Web Based Identifiability Toolbox [4]

- All-in-one solution available at `https://maple.cloud/app/6509768948056064/`
- Implements algorithms for individual parameters' global identifiability [3].
- Capable of finding *single-* and *multi-*experiment identifiable combinations of parameters according [5, 6].
- We will refer to these identifiability types as SE and ME, respectively.

Input Format

- Both individual parameter identifiability and identifiable combinations algorithms accept the same input format:

$$\boldsymbol{\Sigma} := \begin{cases} \mathbf{x}' = \mathbf{f}(\mathbf{x}, \mu, \mathbf{u}), \\ \mathbf{y} = \mathbf{g}(\mathbf{x}, \mu, \mathbf{u}). \end{cases}$$

  $\mathbf{f} = (f_1, \ldots, f_n)$ and $\mathbf{g} = (g_1, \ldots, g_n)$ are tuples of rational functions with coefficients in $\mathbb{C}$. Here $\mathbf{x}, \mu, \mathbf{y}, \mathbf{u}$ are states, parameters, outputs, and inputs, respectively.
- Individual parameter results are guaranteed with user-fixed probability of correctness (0.99 by default)
- The combination-wise result is deterministic.
- Lengthy symbolic computing can be sped up via individual parameter *bypass*: if all parameters are globally identifiable we treat them as trivial identifiable combinations

Table: Timings

- Timing of built-in ODE examples

Name	SIAN	ME	SE
`Biohydrogenation`	3.8	160.9	160.9
`Treatment`	2.7	1.5	1.5
`Tumor`	6.8	0.0	0.0
`Chemical Reaction Network`	6.0	0.0	0.0^{8}
`Chemical Reaction Network` (without bypass)	5.0	390.2	390.2

Table 1:CPU Times with bypass for some of the built-in examples

Screenshot

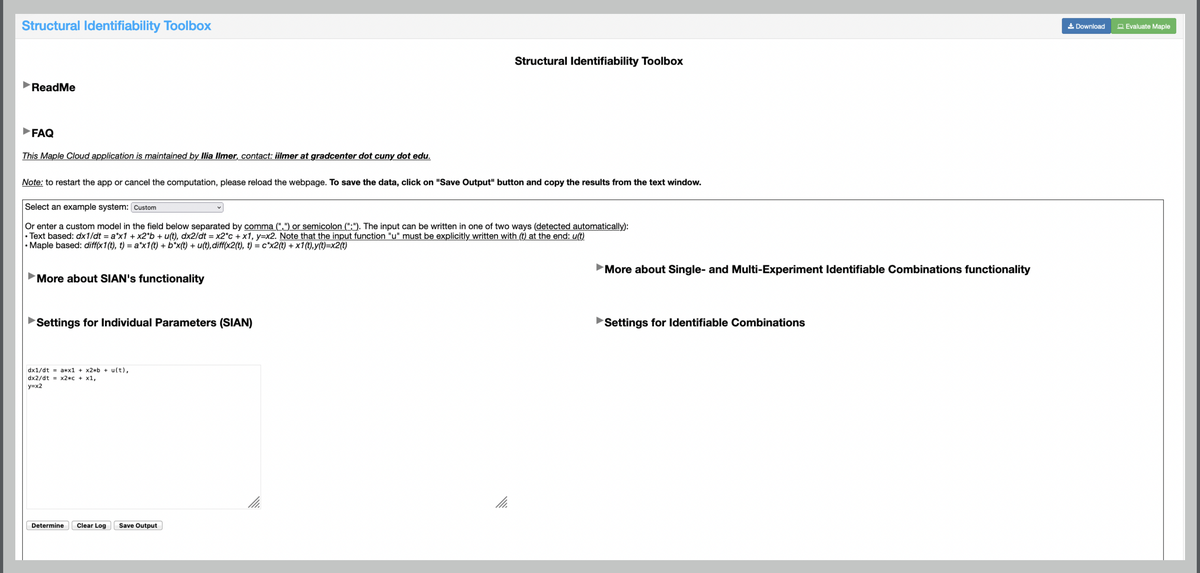

Figure 1:Screenshot of the web-application.

Final Remarks

Our program provides:

- Fast identifiability analysis without requiring any installations.
- Low overhead of individual parameter identifiability can accelerate finding identifiable combination.

Some future work includes:

- Computing characteristic sets via `DifferentialAlgebra` ([1]) is still an overhead.
- We are investigating differential Thomas decomposition for single- and multi-experiment identifiability problems [2].

References

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