Integral Equation Modelling and Deep Learning

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Thèse débutée en Octobre 2022

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8 Mars 2023

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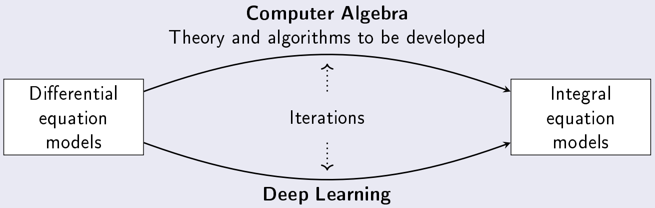

Goals

Algorithm for integral elimination and integration of integro-differential equations.

Application

Parameter estimation with Input/Output integral equations.

Modelling

Differential equation modelling

A type of modelling that describes the evolution of a system (physical, biological, etc.) over time/space.

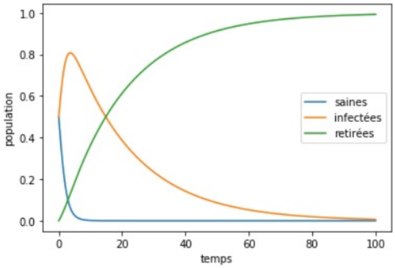

Figure – Epidemic modelling (SIR model)

$$\begin{cases} \dot{R}(t) = cI(t) \\ \dot{S}(t) = -bI(t)S(t) \\ \dot{I}(t) = bI(t)S(t) - cI(t) \end{cases}$$

- Models often have parameters (i.e numerical constants) whose values are unknown
- Experimental curves

Eliminate to estimate

An example of **linear** differential system

$$\begin{cases} \dot{x}(t) = y(t) \\ \dot{y}(t) = \theta x(t) \end{cases}$$

- known quantity : $y(t)$
- unknown quantity : $x(t)$
- parameter : θ

To estimate the value of θ :

1 - **Elimination** : obtain the Input/Output equation : $\ddot{y}(t) = \theta y(t)$ which does not contain unknowns quantities

2 - **Estimation** : estimate the parameters using the previous equation and the experimental datas (e.g : least squares)

Differential elimination and parameter estimation

$$\begin{cases} \dot{x}(t) = y(t) \\ \dot{y}(t) = \theta x(t) \end{cases}$$

$x(t)$ unknown

Differential Elimination

↓

$$\ddot{y}(t) = \theta y(t)$$

Parameter Estimation

↓

$$\hat{\theta} = 3$$

1 - Differential elimination :

$$\dot{x}(t) \xrightarrow{(1)} y(t)$$

$$\theta x(t) \xrightarrow{(2)} \dot{y}(t)$$

with θ(1) et (2)' : $\ddot{y}(t) = \theta y(t)$

2 - Parameter estimation :

$\ddot{y}$ is estimated numerically

$$\begin{cases} \ddot{y}(t_0) - \theta y(t_0) = 0 \\ \ddot{y}(t_1) - \theta y(t_1) = 0 \\ \vdots \\ \ddot{y}(t_n) - \theta y(t_n) = 0 \end{cases}$$

The same idea with integrals, why ?

- Reduce the noise : the numerical computation of the derivatives in the I/O equation amplifies the measurement error

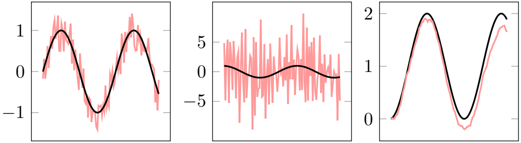

Figure – **A signal (without smoothing), its derivative and its integral In red, the noisy measurement.**

- Reduce the size of I/O equations : they seem shorter, without considering the initial conditions
- Integral equations encode the initial conditions. e^{-t} is coded by $u(t) = 1 - \int_0^t u(\tau)d\tau$ (simply $u = 1 - \int u$)

Two approaches to obtain the I/O integral equation

$$\begin{cases} \dot{x} = y \\ \dot{y} = \theta x^2 \end{cases}$$

x unknown

Differential Elimination

BLAD library [Bou04]

$\longrightarrow$ $4\theta\dot{y}y^2 = \ddot{y}^2$

Integration

(10 steps by hand)

Integrate [BLL+16]

Algorithm

Integral Elimination

(3 steps by hand)

$$y - y_0 = \theta x_0^2 t + 2\theta x_0 \int(\int y) + 2\theta \int(\int y(\int y))$$

Reference works

Differential algebra

- Theory initiated by Ritt[Rit50] et Kolchin[Kol73]
- Algorithmic developed in [BLOP09]
- BLAD (C implementation) [BKL+14]

I/O equations and parameter estimation

- Work by Fliess [Fli89] and many other works

Integration of differential fractions

- Integrate [BLL+16] algorithm
- Doesn't work with all the differential fractions
  Example : $4\theta\dot{y}y^2 = \ddot{y}^2$

Overview

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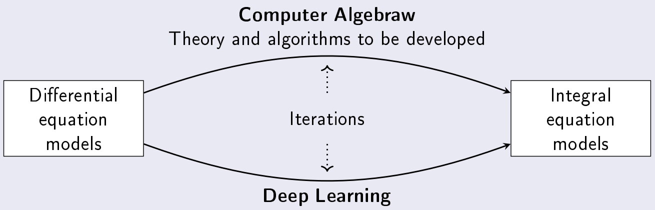
An hybrid approach



Why Deep Learning ? (1/2)

I/O integral equations live in complex algebraic structures

$$-\frac{y}{\theta}+\frac{y_0}{\theta}+x_0^2\int e^{2t}-2x_0\int\left(e^{2t}\int e^{-t}y\right)+2\int\left(e^{2t}\int\left(e^{-t}y\int e^{-t}y\right)\right)=0$$

Which mathematical structures should we consider ?

- Deep Learning allow the manipulation of simple and flexible data structures (e.g trees)
  $\rightarrow$ Allows you to experiment quickly

Why Deep Learning ? (2/2)

- Lample et Charton 2019
  - Symbolic integration with deep learning
    $cos(x) + 1 \xrightarrow{\int} sin(x) + x$
  - Sequential Model : Transformer
  - The integration is seen as a text traduction
  - 95% of accuracy

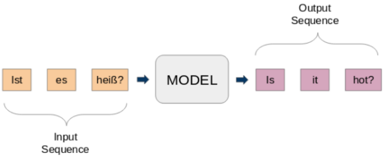


Figure – Input and output of a sequence-to-sequence model (Seq2Seq)

Partial techniques for integral elimination...

$$\begin{cases} x(t) = x_0 + \int y(t) \\ y(t) = y_0 + \theta \int x^2(t) \end{cases}$$

$$x(t) \xrightarrow{(1)} x_0 + \int y(t)$$

$$\int x^2(t) \xrightarrow{(2)} \frac{1}{\theta}(y(t) - y_0)$$

Critical pair between $\int (1)^2$ et (2) :

$$-\theta x_0^2 \int 1 - 2\theta x_0 \int \left(\int y\right) - 2\theta \int \left(\int \left(y \int y\right)\right) - y_0 + y = 0$$

...with a lot of problems

How to eliminate $\int x$ in the second rule ?

$$\begin{cases} x = x_0 + \int x + \int y \\ y = y_0 + \theta \int x^2 \end{cases}$$

$$\int x^2 \xrightarrow{(1)} \frac{y - y_0}{\theta}$$

$$x \xrightarrow{(2)} x_0 + \int y + \int x$$

We introduce $u = 1 - \int u$ (which encodes e^{-t}), and we multiply with (2) :

$$ux = x_0 + \int uy$$

All that remains is to square it.

The solution found contains exponentials

$$-\frac{y}{\theta} + \frac{y_0}{\theta} + x_0^2 \int e^{2t} - 2x_0 \int \left(e^{2t} \int e^{-t} y\right) + 2 \int \left(e^{2t} \int \left(e^{-t} y \int e^{-t} y\right)\right) = 0$$

- Could we avoid the exponentials ?
- Estimation can be hard when the parameters are inside an exponential

Towards an integral elimination prototype

- Arround 20 systems treated by hands with the two approaches
  - Integral elimination
  - Integration of the I/O differential equation
- Useful lemmas obtained by synthesizing the work on these systems

With one of those lemma we can integrate $-\frac{\dot{y}}{\theta} + x_0 + \int y + \frac{1}{\theta^2}\int \dot{y}^2$

We obtain an I/O equation containing :

- nested integrals
- exponentials with θ and y

$$\theta \int \left(e^{\frac{y}{\theta}} \int y e^{-\frac{y}{\theta}} \right) - y + y_0 + \dot{y_0} \int e^{\frac{y-y_0}{\theta}} = 0$$

Deep Learning and integration of integro-differential equations

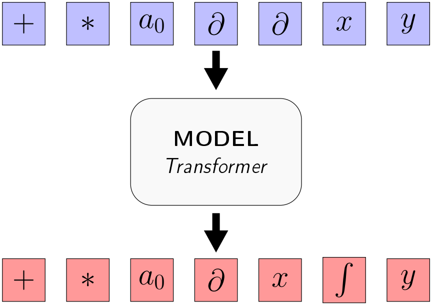


Figure – **Integration of $a_0\ddot{x}(t) + y(t)$ by deep learning.**

Method :

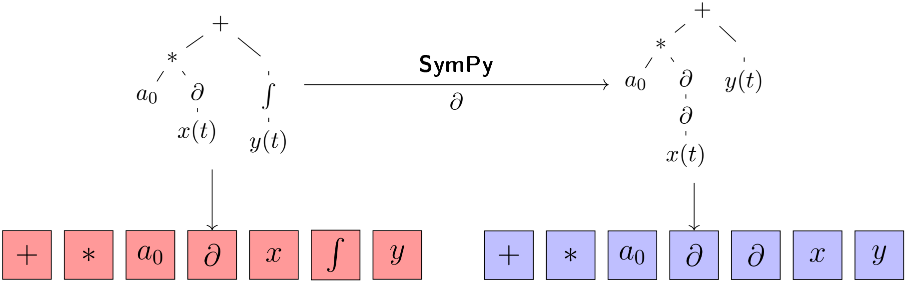
1 - Generation of pairs (f', f)

2 - Train the model

3 - Evaluation of the model accuracy

Dataset generation

$$f : a_0\dot{x}(t) + \int y(t) \xrightarrow{\text{Differentiation}} f' : a_0\ddot{x}(t) + y(t)$$



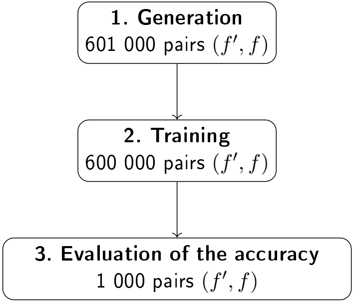
f : Model output

f' : Model input

Experiment parameters

Data

- $+, -, *, \div, \partial, \int$
- $x(t),\ y(t)$
- a_0
- $\sim$ 50 hours of training
- Model size : 2 GO



$$\text{accuracy} = \frac{\text{number of correct integrals}}{\text{number of equations in the test dataset}}$$

Figure – **Learning process and accuracy measurement**

Experiment results (1/2)

Table – **Accuracy of the model versus the accuracy of Maple.**

	Accuracy	Comments
Maple	75.8%	We use int(f,t). Could be enhanced ($+5\%$?) with integration by parts, but it is difficult to automate.
Transformer	96%	Our adapted version of [LC19].

Transformer

Maple		**success**	**fail**	**total**
	success	73%	3%	76%
	fail	23%	1%	24%
	total	96%	4%	

Experiment results (2/2)

Table – **Functions that the model can integrate, but not Maple.**

Equation f'	Solution f
$\frac{1}{\int x} - \frac{tx}{(\int x)^2}$	$\frac{t}{\int x}$
$\frac{(-a_0 x - 1)\int xy + \ddot{y}(t + a_0 \int x) + a_0 xy \int x + xyt - a_0 \dot{y} x - \dot{y}}{(t + a_0 \int x)^2}$	$\frac{\dot{y} + \int xy}{t + a_0 \int x}$

Table – **Functions that Maple can integrate, but not the model.**

Equation f'	Solution f
$x^2 + xy - t^2 \dot{x}^2 + t\dot{x}y + t\dot{y}x - t^2 \ddot{x}x$	$tx^2 + txy - t^2 x\dot{x}$
$\dot{x}y + \dot{y}x - y^2 x - y^2 x \int x - \dot{y}(\int xy)(\int x) - xy \int xy - 2y\dot{y} \int x + a_0 ty \int x + \frac{1}{2} a_0 t^2 \dot{y} \int x + \frac{1}{2} a_0 t^2 xy$	$-y(\int xy)(\int x) - y^2 \int x + \frac{1}{2} a_0 t^2 y \int x + xy$

Conclusion

Goal

Algorithm for integral elimination

Future work

- Prototype (partial) based on an elimination rules system
- Integrate, with deep learning, integro-differential equation containing $\exp$, $\ln$,...
- Adapt deep learning methods to systems of equations.

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Annexes

ES connais-tu des chercheurs en calcul formel français ?

Oui, il y a plusieurs chercheurs français renommés dans le domaine du calcul formel. En voici quelques-uns :

1. Bruno Salvy : Chercheur au CNRS et à l'École Polytechnique, il est connu pour ses travaux sur les algorithmes de calcul formel, en particulier pour la résolution de systèmes d'équations algébriques et la théorie de la complexité.
2. Bernard Mourrain : Chercheur à l'Inria et à l'Université Côte d'Azur, il est spécialisé dans la géométrie algorithmique et la modélisation géométrique, avec des applications en conception assistée par ordinateur, en imagerie médicale et en robotique.
3. François Boulier : Professeur à l'Université de Lorraine, il travaille sur les systèmes d'équations différentielles et les méthodes numériques pour la résolution de problèmes en physique et en ingénierie.
4. Marc Mezzarobba : Chercheur à l'Inria, il est spécialisé dans les algorithmes de calcul formel pour les nombres réels et les fonctions transcendantales, avec des applications en analyse numérique et en physique mathématique.
5. Éric Schost : Professeur à l'Université de Waterloo au Canada, mais originaire de France, il est connu pour ses travaux sur la théorie de Galois effective, la factorisation de polynômes et les algorithmes de calcul formel en caractéristique positive.

Il y a bien sûr de nombreux autres chercheurs français travaillant dans ce domaine passionnant et en constante évolution.

Annexes

$$\begin{cases} \dot{x} = y + x^2 \\ \dot{y} = \theta x \end{cases}$$

$\dot{x} \xrightarrow{(1)} y + x^2$

$x \xrightarrow{(2)} \frac{\dot{y}}{\theta}$

$\dot{x} \xrightarrow{(3)} y + \frac{\dot{y}^2}{\theta^2}$ ((1) et (2))

Avec $\int$ (3) et (1) :

$$\underbrace{\dot{y}}_{A} = \dot{y}_0 + \int \underbrace{\theta y}_{F} + \underbrace{\frac{1}{\theta}\dot{y}}_{G} \underbrace{\dot{y}}_{A}$$

Lemma

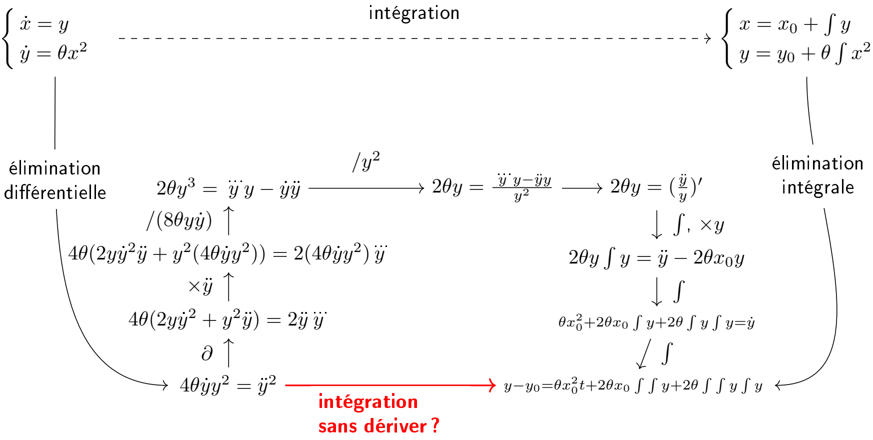
Having : $A = A_0 + \int (A \cdot G + F)$, then by introducing $v = v_0 - \int vG$ and using the product of two integral equations we have :

$$Av = A_0 v_0 + \int vF$$

$\dot{y}v = \dot{y}_0 v_0 + \int \theta v y$

$\theta \int e^{\frac{y}{\theta}} \int y e^{-\frac{y}{\theta}} - y + y_0 + \dot{y_0} \int e^{\frac{y - y_0}{\theta}}$

Annexes



$\begin{cases} \dot{x} = y \\ \dot{y} = \theta x^2 \end{cases}$
intégration
$\begin{cases} x = x_0 + \int y \\ y = y_0 + \theta \int x^2 \end{cases}$
élimination différentielle
élimination intégrale
$2\theta y^3 = \dddot{y}\, y - \dot{y}\ddot{y}$
$/y^2$
$2\theta y = \frac{\dddot{y}\, y - \ddot{y} y}{y^2}$
$2\theta y = (\frac{\ddot{y}}{y})'$
$/(8\theta y\dot{y})$
$4\theta(2y\dot{y}^2\ddot{y} + y^2(4\theta\dot{y}y^2)) = 2(4\theta\dot{y}y^2)\,\dddot{y}$
$\times\ddot{y}$
$4\theta(2y\dot{y}^2 + y^2\ddot{y}) = 2\ddot{y}\,\dddot{y}$
∂
$4\theta\dot{y}y^2 = \ddot{y}^2$
$\int, \times y$
$2\theta y \int y = \ddot{y} - 2\theta x_0 y$
$\int$
$\theta x_0^2 + 2\theta x_0 \int y + 2\theta \int y \int y = \dot{y}$
$\int$
$y - y_0 = \theta x_0^2 t + 2\theta x_0 \int\int y + 2\theta \int\int y \int y$
intégration sans dériver ?

Annexes

$$\begin{cases} \dot{x} = \frac{1}{y+\theta} \\ \dot{y} = x \\ y \text{ connue} \end{cases}$$

Valeurs recherchées :

$$\begin{cases} \theta = 3 \\ y_0 = 1 \\ \dot{y}_0 = 1 \end{cases}$$

Équation	Bruitée	Filtrée
$y - y_0 - \dot{y}_0 t - \int\int \frac{1}{y+\theta}$	$\nabla C(\theta)$: $\theta = 0.048$ $\nabla C(\theta, y_0, \dot{y}_0)$: $\theta = 2.032$, $y_0 = 1.106$, $\dot{y}_0$=0.903	$\nabla C(\theta)$: $\theta = 3.495$ $\nabla C(\theta, y_0, \dot{y}_0)$: $\theta = 2.06143$, $y_0 = 1.0627$, $\dot{y}_0$=0.911
$y - y_0 - \int \sqrt{\dot{y}_0^2 - 2ln(\frac{y+\theta}{y_0+\theta})}$	$\nabla C(\theta)$: $\theta = 0.0345$ $\nabla C(\theta, y_0, \dot{y}_0)$: $\theta = 2.72677$, $y_0 = 1.01819$, $\dot{y}_0$=0.9816	$\nabla C(\theta)$: $\theta = 3.417$ $\nabla C(\theta, y_0, \dot{y}_0)$: $\theta = 2.4859$, $y_0 = 1.0320$, $\dot{y}_0$=0.95885
$\dot{y}^2 - \dot{y}_0^2 - 2ln(\frac{y+\theta}{y_0+\theta})$	$\nabla C(\theta)$:KO $\nabla C(\theta)$: KO	$\nabla C(\theta)$: $\theta = -0.193$ $\nabla C(\theta, y_0, \dot{y}_0)$: $\theta = -0.6417$, $y_0 = 1.1345$, $\dot{y}_0$=0.535
$\ddot{y} - \frac{1}{y+\theta}$	$\nabla C(\theta)$: KO	$\nabla C(\theta)$: $\theta = 2.2007$
$\ddot{y}y + \theta\ddot{y} - 1$	$\nabla C(\theta)$: $\theta = -5.338$ moindres carrés : $\theta = -5.338$	$\nabla C(\theta)$: $\theta = -5.497$ moindres carrés : $\theta = -5.497$