Polynomialization of Ordinary Differential Equations given by Straight-line programs

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Polynomialization example

Initial Value Problem (IVP):

$$\begin{cases} y' = y^{-1} \\ y(0) = \sqrt{2} \end{cases}$$

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Polynomial IVP:

$$\begin{cases} y(0) &= \sqrt{2} \\ z(0) &= \sqrt{2}^{-1} \\ y' &= z \\ z' &= -z^3 \end{cases}$$

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use only ring instructions ≈.5 CPU cycles

Polynomialization examples

Pendulum, mass m, length l:

$$-\frac{g}{l}\sin(\theta) = \theta'' \iff \begin{cases} \theta' &= u, \\ u' &= -\frac{g}{l}\sin(\theta). \end{cases}$$

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≈2 CPU cycles; easier to compute !

Polynomialization

A **polynomialization** of $(E): y' = \Phi(y)$ is a set of functions $w := w(y)$ such that:

$$(\tilde{E}): \begin{pmatrix} y \\ w \end{pmatrix}' = \Pi\left(\begin{pmatrix} y \\ w \end{pmatrix}\right), \Pi \in \mathbb{K}[y_1, \ldots, y_n, w_1, \ldots, w_m]^{n+m}.$$

Polynomializing

Previous work:

- The canonical form of a system of differentialy algebraic equations. APPELROTH, 1902
- Computability with polynomial differential equations. GRAÇA *et al.* 2008.
- Compiling elementary mathematical functions into finite chemical reaction networks via a polynomialization algorithm for ODEs. HEMERY *et al.* 2021.

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Motivations for polynomializing:

- HPC, Numerical integration: Trigonometric functions not available on hardware!
- First step for more complicated problems:
  - Quadratization, BYCHKOV *et al.* 2023, CAI *et al.* 2024, HEMERY *et al.* 2020
  - Computability, BOURNEZ *et al.* 2007.

Straight-Line Program (SLP)

An **SLP Γ** over Σ, is defined by:

- a finite set of variables $\mathcal{V} \subset \mathbb{N}$
- sequence of instructions $\Gamma_1, \ldots, \Gamma_{|\Gamma|}$ of the form:

$$\Gamma_i \equiv X_i := \mathrm{op}_i(X_{i,1}, \ldots, X_{i,|\mathrm{op}_i|}),$$

where $\mathrm{op}_i \in \Sigma$, and $X_i, X_{i,1}, \ldots, X_{i,|\mathrm{op}_i|} \in \mathcal{V}$.

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Fixed Instruction sets:
$\Sigma_{\mathrm{ring}} := \{+, -, \times, \mathrm{fma}, \mathrm{fms}, \mathrm{fnma}, \mathrm{fnms}\}$
$\Sigma_{\mathrm{div}} := \{/, (\cdot)^{-1}\}$
$\Sigma_{\mathrm{special}} := \{\text{Special functions applications}\}$
$\Sigma := \Sigma_{\mathrm{ring}} \cup \Sigma_{\mathrm{div}} \cup \Sigma_{\mathrm{special}}$

Special function
Function solution of a polynomial ODE

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Function solution of a polynomial ODE

Execution Cost $\kappa : \Sigma \to \mathbb{N}$ (in cycles)
$\kappa(*) := .5, * \in \Sigma_{\mathrm{ring}}$
$\kappa(/) = \kappa(\cdot^{-1}) := 8,$
$\kappa(\sigma) \geqslant 16, \sigma \in \Sigma_{\mathrm{special}}.$

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The **cost of execution** of the SLP is:

$$\kappa(\Gamma) := \sum_{i=1}^{l} \kappa(\mathrm{op}_i).$$

The number of instructions Σ_{kind} in Γ is $|\Gamma|_{\mathbf{kind}}$.

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Polynomialization theorem

Theorem (Differential algebra folklore)
Let Γ be any SLP over $\Sigma = \Sigma_{\text{ring}} \cup \Sigma_{\text{div}} \cup \Sigma_{\text{special}}$ then the ODE $y' = \Gamma(y)$ is polynomializable.

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Running example:

IVP

$$(E): \begin{cases} y(0) = y_0 \\ z(0) = z_0 \\ y' = 5\frac{y}{z} + z \\ z' = \cos(y) \end{cases}$$

can be polynomialized.

SLP Γ

Input I_1, I_2
Output O_1, O_2
$X_1 := I_1 / I_2$
$O_1 := \text{fma}(5, X_1, I_2)$
$O_2 := \cos(I_1)$

$\xrightarrow{?}$

IVP SLPs Π polynomial, Φ

$$(\bar{E}): \begin{cases} (y,z,w)(0) = \Phi(y_0, z_0) \\ (y,z,w)' = \Pi(y,z,w) \end{cases}$$

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From Γ, how to obtain Π, Φ such that $(E) \iff (\bar{E})$?

Our contribution: the algorithm

Assumption: For each instruction $\sigma \in \Sigma_{\text{special}}$, there exist $\mu_\sigma \in \mathbb{N}$ and Q_σ SLP such that:

$$(\sigma(t), s_2(t), \ldots, s_{\mu_\sigma}(t))' = Q_\sigma(\sigma(t), s_2(t), \ldots, s_{\mu_\sigma}(t), t)$$

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Algorithm:

Γ

Input $I_1, \ldots, I_n$
Output $O_1, \ldots, O_n$

for $i = 1, \ldots, |\Gamma|$:
$X_i := \text{op}_i(X_{i,1}, \ldots, X_{i,|\text{op}_i|})$

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Algorithm:

Γ	Π
Input $I_1, \ldots, I_n$	Input $i_1, \bar{i_1}, \ldots, i_n, \bar{i_n}, i_{n+1}, \ldots, i_{n+\theta}$, $\theta := \sum_i \mu_{\text{op}_i}$
Output $O_1, \ldots, O_n$	Ouptut $o_1, \bar{o_1}, \ldots, o_n, \bar{o_n}, o_{n+1}, \ldots, o_{n+\theta}$
for $i = 1, \ldots, \lvert\Gamma\rvert$:	Assume all $x_{i,j}$ and $\bar{x_{i,j}}$ were computed
$X_i := \text{op}_i(X_{i,1}, \ldots, X_{i,\lvert\text{op}_i\rvert})$	Lift($X_i := \text{op}_i(X_{i,1}, \ldots, X_{i,\lvert\text{op}_i\rvert})$)
	ensures $x_i, \bar{x}_i$ are computed.

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Input $I_1, \ldots, I_n$ Output $O_1, \ldots, O_n$	Input $i_1, \bar{i_1}, \ldots, i_n, \bar{i_n}, i_{n+1}, \ldots, i_{n+\theta}$, $\theta := \sum_i \mu_{\text{op}_i}$ Ouptut $o_1, \bar{o_1}, \ldots, o_n, \bar{o_n}, o_{n+1}, \ldots, o_{n+\theta}$	Same as Γ input Same as Π input
for $i = 1, \ldots, \lvert\Gamma\rvert$: $X_i := \text{op}_i(X_{i,1}, \ldots, X_{i,\lvert\text{op}_i\rvert})$	Assume all $x_{i,j}$ and $\overline{x_{i,j}}$ were computed $\text{Lift}(X_i := \text{op}_i(X_{i,1}, \ldots, X_{i,\lvert\text{op}_i\rvert}))$ ensures $x_i, \bar{x}_i$ are computed.	Copy Γ instruction, if special, division or inversion, output value.

Running example

SLP Γ
Input I_1, I_2
Output O_1, O_2

$X_1 := I_1 / I_2$

$O_1 := \mathrm{fma}(5, X_1, I_2)$

$O_2 := \cos(I_1)$

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SLP Π
Input $i_1, \overline{i_1}, i_2, \overline{i_2}, i_3, i_4, i_5$
Output $o_1, \overline{o_1}, o_2, \overline{o_2}, o_3, o_4, o_5$

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$x_1 := i_1 \times i_3 \quad (= i_1 / i_2)$
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$o_3 := i_3 \times \overline{i_2} \quad (= \overline{i_2} / i_2)$
$o_3 := \mathrm{nmul}(i_3, o_3) \quad (= -\overline{i_2} / i_2^2)$
$\overline{x_1} := \mathrm{fma}(i_1, o_3, \overline{x_1}) \quad (= \overline{i_1} / i_2 - i_1 \overline{i_2} / i_2^2)$

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Input I_1, I_2
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Input I_1, I_2
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$o_3 := \mathrm{nmul}(i_3, o_3) \quad (= -\overline{i_2} / i_2^2)$
$\overline{x_1} := \mathrm{fma}(i_1, o_3, \overline{x_1}) \quad (= \overline{i_1} / i_2 - i_1 \overline{i_2} / i_2^2)$

$o_1 := \mathrm{fma}(5, x_1, i_2) \quad (= 5 x_1 + i_2)$
$\overline{o_1} := \mathrm{fma}(5, \overline{x_1}, \overline{i_2}) \quad (= 5 \overline{x_1} + \overline{i_2})$

$o_2 := i_4 \quad (= \cos(i_1))$
$o_5 := \overline{i_1} \times i_4 \quad (= \overline{i_1} \cos(i_1))$
$o_4 := \mathrm{nmul}(\overline{i_1}, i_5) \quad (= -\overline{i_1} \sin(i_1))$
$\overline{o_2} := o_4 \quad (= \cos(i_1))$

SLP Φ
Input I_1, I_2
Output $I_1, O_1, I_2, O_2, i_3, i_4, i_5$

$i_3 := 1 / i_2$
$X_1 := i_1 \times i_3$

$O_1 := \mathrm{fma}(5, X_1, I_2)$

Running example

SLP Γ
Input I_1, I_2
Output O_1, O_2

$X_1 := I_1 / I_2$

$O_1 := \mathrm{fma}(5, X_1, I_2)$

$O_2 := \cos(I_1)$

SLP Π
Input $i_1, \overline{i_1}, i_2, \overline{i_2}, i_3, i_4, i_5$
Output $o_1, \overline{o_1}, o_2, \overline{o_2}, o_3, o_4, o_5$

$x_1 := i_1 \times i_3 \quad (= i_1 / i_2)$
$\overline{x_1} := \overline{i_1} \times i_3 \quad (= \overline{i_1} / i_2)$
$o_3 := i_3 \times \overline{i_2} \quad (= \overline{i_2} / i_2)$
$o_3 := \mathrm{nmul}(i_3, o_3) \quad (= -\overline{i_2} / i_2^2)$
$\overline{x_1} := \mathrm{fma}(i_1, o_3, \overline{x_1}) \quad (= \overline{i_1} / i_2 - i_1 \overline{i_2} / i_2^2)$

$o_1 := \mathrm{fma}(5, x_1, i_2) \quad (= 5 x_1 + i_2)$
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$o_2 := i_4 \quad (= \cos(i_1))$
$o_5 := \overline{i_1} \times i_4 \quad (= \overline{i_1} \cos(i_1))$
$o_4 := \mathrm{nmul}(\overline{i_1}, i_5) \quad (= -\overline{i_1} \sin(i_1))$
$\overline{o_2} := o_4 \quad (= \cos(i_1))$

SLP Φ
Input I_1, I_2
Output $I_1, O_1, I_2, O_2, i_3, i_4, i_5$

$i_3 := 1 / i_2$
$X_1 := i_1 \times i_3$

$O_1 := \mathrm{fma}(5, X_1, I_2)$

$i_4 := \cos(i_1)$
$O_2 := I_4$
$i_5 := \sin(i_1)$

Our contribution: theoritical result

Instruction set	Lift number of instructions
Σ_{ring}	3
Σ_{div}	5
Σ_{special}	$\lvert Q_\sigma \rvert + \mu_\sigma + 2$

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Theorem

Let $\Gamma\colon \mathbb{K}^n \to \mathbb{K}^n$ be an SLP over Σ. Then we compute both Π, Φ SLPs in time $O(|\Gamma| + n)$ such that:

$$\begin{cases} y' = \Gamma(y) \\ y(0) = y_0 \end{cases} \iff \begin{cases} (y,w)' = \Pi(y,w) \\ (y,w)(0) = \Phi(y_0) \end{cases}$$

Moreover Π is polynomial and:

$$|\Pi| \leqslant 3|\Gamma|_{\text{ring}} + 5\,|\Gamma|_{\text{div}} + \sum_{1 \leqslant k \leqslant l} (|Q_{\text{op}_k}| + \mu_{\text{op}_k} + 2)$$

Optimizations

Simplify Π:

- Γ represents a polynomial ODE, $\bar{i}$ are output of Γ.
- Apply usual SLP simplification techniques: common subexpression elimination, use fma when possible

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For the running example we obtain the final SLP:

$$
\begin{array}{l}
\Pi \\
\text{Input} \quad i_1, i_2, i_3, i_4, i_5 \\
\text{Output} \quad o_1, o_2, o_3, o_4, o_5
\end{array}
$$

$$
\begin{array}{llll}
\Pi_1 \equiv x_1 := i_1 \times i_3 & & \Pi_4 \equiv o_1 := \mathrm{fma}(5, x_1, i_2) & \\
\Pi_2 \equiv o_3 := \mathrm{nmul}(i_3, i_3) & & \Pi_5 \equiv o_4 := \mathrm{nmul}(o_1, i_5) & \\
\Pi_3 \equiv o_3 := o_3 \times i_4 & & \Pi_6 \equiv o_5 := o_1 \times i_4 & \text{Cost} \approx 3 \text{ cycles}
\end{array}
$$

Our contribution: Practical result

Implementation within the JustInLine (JIL) open-source C++ library:
git clone https://git.renater.fr/anonscm/git/jil/jil.git

```cpp
#include <jil/ode/slp_ode_polynomialize.hpp>
#include <jil/slp/slp_recorder.hpp>

using namespace jil;

template <typename T>
void ode1 (T* out, const T* in) {
  out[0] = 5 * in[0] / in[1] + in[1];
  out[1] = cos (in[0]);
}

int
main (int argc, char** argv) {
  domain tp = r32_domain;
  slp q = as_slp (2, 2, tp, ode1);
  jout << "Original SLP = " << q << "\n";
  slp p = ode_polynomialize (q);
  jout << "Polynomialization = " << p << "\n";
}
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```

```
Original SLP = input    0, 0
input   1, 1
mul     2, 0, 5
div     3, 2, 1
add     4, 1, 3
cos     2, 0
output  0, 4
output  1, 2
data    5, 5.000000e+00

Polynomialization = input       0, 0
input   1, 1
input   2, 2
input   3, 3
input   4, 4
mul     5, 0, 10
fma     6, 2, 5, 1
mul     7, 2, 3
nmul    7, 2, 7
nmul    8, 4, 6
mul     9, 6, 8
output  0, 6
output  1, 3
output  2, 7
output  3, 8
output  4, 9
data    10, 5.000000e+00
```

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input   1, 1
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div     3, 2, 1
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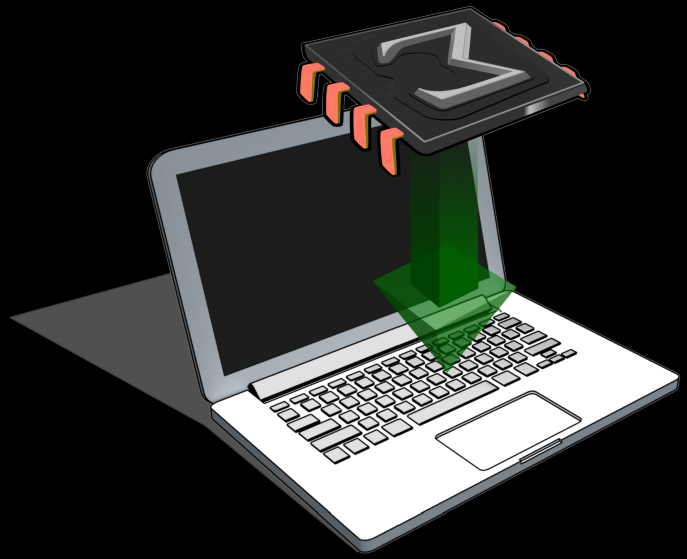
cos     2, 0
output  0, 4
output  1, 2
data    5, 5.000000e+00

Polynomialization = input       0, 0
input   1, 1
input   2, 2
input   3, 3
input   4, 4
mul     5, 0, 10
fma     6, 2, 5, 1
mul     7, 2, 3
nmul    7, 2, 7
nmul    8, 4, 6
mul     9, 6, 8
output  0, 6
output  1, 3
output  2, 7
output  3, 8
output  4, 9
data    10, 5.000000e+00
```

a gcc -O3 -mavx2 later…

	Pratical costs
Gen	253 cycles
Poly	12 cycles

Thank you!



http://www.TeXmacs.org