Identification of Dynamical Systems using Symbolic Regression

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Abstract. We describe a method for the identification of models for dynamical systems from observational data. The method is based on the concept of symbolic regression and uses genetic programming to evolve a system of ordinary differential equations (ODE). The novelty is that we add a step of gradient-based optimization of the ODE parameters. For this we calculate the sensitivities of the solution to the initial value problem (IVP) using automatic differentiation. The proposed approach is tested on a set of 19 problem instances taken from the literature which includes datasets from simulated systems as well as datasets captured from mechanical systems. We find that gradient-based optimization of parameters improves predictive accuracy of the models. The best results are obtained when we first fit the individual equations to the numeric differences and then subsequently fine-tune the identified parameter values by fitting the IVP solution to the observed variable values.

Keywords: System dynamics, Genetic programming, Symbolic regression

1 Background and Motivation

Modelling, analysis and control of dynamical systems are core topics within the field of system theory focusing on the behavior of systems over time. System dynamics can be modelled using ordinary differential equations (cf. [6]) which define how the state of a system changes based on the current state for infinitesimal time steps.

Genetic programming (GP) is a specific type of evolutionary computation in which computer programs are evolved to solve a given problem. Symbolic regression (SR) is a specific task for which GP has proofed to work well. The goal in SR is to find an expression that describes the functional dependency between a dependent variable and multiple independent variables given a dataset of observed values for all variables. In contrast to other forms of regression analysis it is not necessary to specify the model structure beforehand because the appropriate model structure is identified simultaneously with the numeric parameters.
of the model. SR is therefore especially suited for regression tasks when a para-
metric model for the system or process is not known. Correspondingly, SR could
potentially be used for the identification models for dynamical systems when an
accurate mathematical model of the system doesn’t exist.

We aim to use SR to find the right-hand sides \( f(\cdot) \) of a system of ordinary
differential equations such as:

\[
\begin{align*}
\dot{u}_1 &= f_{\dot{u}_1}(u_1, u_2, \vec{\theta}), \\
\dot{u}_2 &= f_{\dot{u}_2}(u_1, u_2, \vec{\theta})
\end{align*}
\]

We only consider systems without input variables (non-forced systems) and
leave an analysis for forced systems for future work.

1.1 Related Work

The vast literature on symbolic regression is mainly focused on static models in
which predicted values are independent given the input variable values. How-
ever, there are a several articles which explicitly describe GP-based methods
for modelling dynamical systems. A straight-forward approach which can be
implemented efficiently is to approximate the derivatives numerically [5,9,3,14].
Solving the IVP for each of the considered model candidates is more accurate
but also computationally more expensive; this is for instance used in [1].

In almost all methods discussed in prior work the individual equations of the
system are encoded as separate trees and the SR solutions hold multiple trees
[5,9,11]. A notable exception is the approach suggested in [3] in which GP is run
multiple times to produce multiple expressions for the numerically approximated
derivatives of each state variable. Well-fitting expressions are added to a pool of
equations. In the end, the elements from the pool are combined and the best-
fitting ODE system is returned. In this work the IVP is solved only in the model
combination phase.

Identification of correct parameter values is critical especially for ODE sys-
tems. Therefore, several authors have included gradient-based numeric optimiza-
tion of parameter values. In [5], parameters are allowed only for scaling top-level
terms, to allow efficient least-squares optimization of parameter values. In [14]
non-linear parameters are allowed and parameter values are iteratively opti-
mized using the Levenberg-Marquardt algorithm based on gradients determined
through automatic differentiation.

Partitioning is introduced in [11]. The idea is to optimize the individual parts
of the ODE system for each state variable separately, whereby it is assumed that
the values of all other state variables are known. Partitioning reduces computa-
tional effort but does not guarantee that the combined system of equations
models system dynamics correctly.

Recently, neural networks have been used for modelling ODEs [2] whereby
the neural network parameters are optimized using gradients determined via the
adjoint sensitivity method and automatic differentiation. The same idea can be
used to fit numeric parameters of SR models.
2 Methods

We extend the approach described in [5], whereby we allow numeric parameters at any point in the symbolic expressions. We use an iterative gradient-based method (i.e. Levenberg-Marquardt (LM)) for the optimization of parameters and automatic differentiation for efficient calculation of gradients similarly to [14]. We analyse several different algorithm variations, some of which solve the IVP problem in each evaluation step as in [12]. For this we use the state-of-the-art CVODES library for solving ODEs and calculating parameter sensitivities.

We compare algorithms based on the deviation of the IVP solution from the observed data points for the final models. The deviation measure is the sum of normalized mean squared errors:

\[
\text{SNMSE}(Y, \hat{Y}) = \sum_{i=1}^{D} \frac{1}{\text{var}(y_{i,.})} \sum_{j=1}^{N} \frac{1}{N} (y_{i,j} - \hat{y}_{i,j})^2
\]

Where \( Y = \{y_{i,j}\}_{i=1..D,j=1..N} \) is the matrix of \( N \) subsequent and equidistant observations of the \( D \) state variables. Each state variable is measured at the same time points \( (t_{i,j})_{i=1..N} \). The matrix of predicted values variables \( \hat{Y} = \{\hat{y}_{i,j}\}_{i=1..D,j=1..N} \) is calculated by integrating the ODE system using the initial values \( \hat{y}_{i,1} = y_{i,1} \).

2.1 Algorithm description

The system of differential equations is represented as an array of expression trees each one representing the differential equation for one state variable. The evolutionary algorithm initializes each tree randomly whereby all of the state variables are allowed to occur in the expression. In the crossover step, exchange of sub-trees is only allowed between corresponding trees. This implicitly segregates the gene pools for the state variables. For each of the trees within an individual we perform sub-tree crossover with the probability given by the crossover rate parameter. A low crossover rate is helpful to reduce the destructive effect of crossover.

Memetic optimization of numeric parameters has been shown to improve GP performance for SR [13,7]. We found that GP performance is improved significantly even when we execute only a few iterations (3-10) of LM and update the parameter values whenever an individual is evaluated. This ensures that the improved parameter values are inherited and can subsequently be improved even further when we start LM with these values [7]. We propose to use the same approach for parameters of the ODEs with a small modification based on the idea of partitioning. In the first step we use the approximated derivative values as the target. In this step we use partitioning and assume all variable values are known. The parameter values are updated using the optimized values. In the second step we use CVODES to solve the IVP for all state variables simultaneously and

1 https://computation.llnl.gov/projects/sundials/cvodes
to calculate parameter sensitivities. The LM algorithm is used to optimize the
SNMSE (Equation 1) directly. Both steps can be turned on individually and the
number of LM iterations can be set independently.

2.2 Computational experiments

Algorithm configuration Table 1 shows the GP parameter values that have
been used for the experiments.

| Parameter         | Value                                      |
|-------------------|--------------------------------------------|
| Population size   | 300                                        |
| Initialization    | PTC2                                       |
| Parent selection  | proportional (first parent) random (second parent) |
| Crossover         | Subtree crossover                          |
| Mutation          | Replace subtree with random branch         |
|                   | Add $x \sim N(0,1)$ to all numeric parameters |
|                   | Add $x \sim N(0,1)$ to a single numeric parameter. |
|                   | Change a single function symbol.           |
| Crossover rate    | 30% (for each expression)                  |
| Mutation rate     | 5% (for the whole individual)              |
| Offspring selection | offspring must be better than both parents |
| Maximum selection pressure | $100 < \# \text{ evaluated offspring} / \text{population size} \quad$ |
| Replacement       | Generational with a single elite.          |
| Terminal set      | State variables and real-valued parameters |
| Function set      | $+,*,*\sin,*\cos,\ldots$                   |

Table 1. Parameter values for the GP algorithm that have been used for all experiments. The number of generations and the maximum number of evaluated solutions is varied for the experiments.

We compare two groups of different configurations: in the first group we rely solely on the evolutionary algorithm for the identification of parameter values. In the second group we use parameter optimization optimization. Both groups contain three configurations with different fitness functions. In the following we use the identifiers D, I, D+I, $D_{\text{opt}}$, $I_{\text{opt}}$, and $D_{\text{opt}}+I_{\text{opt}}$ for the six algorithm instances. Configuration D uses the SNMSE for the approximated derivatives for fitness assignment as in [5,3,14]; configuration I uses the SNMSE for the solution to the IVP as in [1]; configuration D+I uses the sum of both error measures for fitness evaluation. For the first group we allow maximally 500,000 evaluated solutions and 250 generations; for the second group we only allow 100,000 evaluated solutions and 25 generations. The total number of function evaluations including evaluations required for parameter optimization is similar for all configurations and approximately between 500.000 and 2 million (depending on the dimensionality of the problem).
Problem instances We use 19 problem instances for testing our proposed approach as shown in Table 2 and Table 3. These have been taken from [5,9,10] and include a variety of different systems. The set of problem instances includes simulated systems (Table 2) as well as datasets gathered with motion-tracking from real mechanical systems (Table 3). The simulated datasets have been generated using fourth-order Runge-Kutta integration (RK45). The motion-tracked datasets have been adapted from the original source to have equidistant observations using cubic spline interpolation.

3 Results

Table 4 shows the number of successful runs (from 10 independent runs) for each problem instance and algorithm configuration. A run is considered successful if the IVP solution for the identified ODE system has an SNMSE < 0.01. Some of the instances can be solved easily with all configurations. Overall the configuration I_{opt}+D_{opt} is the most successful. With this configuration we are able to produce solutions for all of the 19 instances with a high probability. The beneficial effect of gradient-based optimization of parameters is evident from the much larger number of successful runs.

Notably, when we fit the expressions to the approximated derivatives using partitioning (configurations D and D_{opt}) the success rate is low. The reason is that IVP solutions might deviate strongly when we use partitioning to fit of the individual equations to the approximated derivatives. To achieve a good fit the causal dependencies must be represented correctly in the ODE system. This is not enforced when we use partitioning.

4 Discussion

The results of our experiments are encouraging and indicate that it is indeed possible to identify ODE models for dynamical systems solely from data using GP and SR. However, there are several aspects that have not yet been fully answered in our experiments and encourage further research.

A fair comparison of algorithm configurations would allow the same runtime for all cases. We have use a similar amount of function evaluations but have so far neglected the computational effort that is required for numerically solving the ODE in each evaluation step. Noise can have a large effect in the numeric approximation of derivatives. We have not yet studied the effect of noisy measurements. Another task for future research is the analysis of forecasting accuracy of the models. So far we have only measured the performance on the training set. Finally, for practical applications, it would be helpful to extend the method to allow input variables (forced systems) as well as latent variables.

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| Instance                  | Expression                                                                 | Initial value | $N$ | $t_{\text{max}}$ |
|---------------------------|------------------------------------------------------------------------------|---------------|-----|-----------------|
| Chemical reaction [5]     | $\dot{y}_1 = -1.4y_1$                                                       | (0.1, 0, 0)   | 100 | 1               |
|                           | $\dot{y}_2 = 1.4y_1 - 4.2y_2$                                               |               |     |                 |
|                           | $\dot{y}_3 = 4.2y_2$                                                        |               |     |                 |
| E-CELL [6]                | $\dot{y}_1 = -10y_1y_3$                                                     | (1.2, 0.0, 1.2)| 40  | 0.4             |
|                           | $\dot{y}_2 = 10y_1y_3 - 17y_2$                                              |               |     |                 |
|                           | $\dot{y}_3 = -10y_1y_3 + 17y_2$                                             |               |     |                 |
| S-System [9]              | $\dot{y}_1 = 15y_3y_5^{0.1} - 10y_1^2$                                      | (0.1, 0.1, 0.1, 0.1) |    |                 |
|                           | $\dot{y}_2 = 10y_1 y_2 - 10y_2^2$                                           | (0.5, 0.5, 0.5, 0.5) | 3 * 30 | 0.3            |
|                           | $\dot{y}_3 = 8y_1^2 y_5^{0.1} - 10y_4^2$                                    | (1.5, 1.5, 1.5, 1.5) |    |                 |
|                           | $\dot{y}_5 = 10y_4^2 - 10y_5^2$                                             |               |     |                 |
| Lotka-Volterra (3 species) [5] | $\dot{y}_1 = y_1(1 - y_1 - y_2 - 10y_3)$                                   | (0.2895, 0.2827, 0.126) | 100 | 100            |
|                           | $\dot{y}_2 = y_2(0.992 - 1.5y_1 - y_2 - y_3)$                               |               |     |                 |
|                           | $\dot{y}_3 = y_3(-1.2 + 5y_1 + 0.5y_2)$                                     |               |     |                 |
| Lotka-Volterra (2 species) [5] | $\dot{y}_1 = y_1(0.04 - 0.0005y_2)$                                       | (20, 20)      | 300 | 300            |
|                           | $\dot{y}_2 = -y_2(0.2 - 0.004y_1)$                                         |               |     |                 |
| Glider [5]                | $\dot{v} = -0.05v^2 - \sin(\theta)$                                       | (1.5, 1)      | 100 | 10             |
|                           | $\dot{\theta} = v - \cos(\theta)/v$                                        |               |     |                 |
| Bacterial respiration [9] | $\dot{x} = (20 - x - xy)/(1 + 0.5x^2)$                                     | (1, 1)        | 100 | 10             |
|                           | $\dot{y} = (10 - xy)/(1 + 0.5x^2)$                                         |               |     |                 |
| Predator-Prey [9]         | $\dot{x} = x(4 - x - y/(1 + x))$                                            | (1.1, 7.36)   | 100 | 10             |
|                           | $\dot{y} = y(x/(1 + x) - 0.075y)$                                           |               |     |                 |
| Bar magnets [9]           | $\dot{\theta}_1 = 0.5 \sin(\theta_1 - \theta_2) - \sin(\theta_1)$        | (0.7, -0.3)   | 100 | 10             |
|                           | $\dot{\theta}_2 = 0.5 \sin(\theta_2 - \theta_1) - \sin(\theta_1)$        |               |     |                 |
| Shear flow [9]            | $\dot{\theta} = \cot(\theta) \cos(\phi)$                                 | (0.7, 0.4)    | 100 | 10             |
|                           | $\dot{\phi} = (\cos(\phi))^2 + 0.1 \sin(\phi)^2 \sin(\phi)$              |               |     |                 |
| Van der Pol Oscillator [9]| $\dot{x} = 10(y - (\frac{1}{3} x^3 - x))$                                   | (2, 0.1)      | 100 | 10             |
|                           | $\dot{y} = -0.1x$                                                          |               |     |                 |

Table 2. The problem instances for which we have generated data using numeric integration.
| Type                        | Name                          | File Name                | Variables | \( N \) |
|-----------------------------|-------------------------------|--------------------------|-----------|-------|
| Simulated Linear oscillator | linear_h_1.txt                |                          | \( x, v \) | 512   |
| Motion-tracked Linear oscillator | real_linear_h_1.txt |                          | \( x, v \) | 879   |
| Simulated Pendulum          | pendulum_h_1.txt              |                          | \( \theta, \omega \) | 502   |
| Motion-tracked Pendulum     | real_pend_h_1.txt             |                          | \( \theta, \omega \) | 568   |
| Simulated Coupled oscillator | double_linear_h_1.txt         |                          | \( x_1, x_2, v_1, v_2 \) | 200   |
| Motion-tracked Coupled oscillator | real_double_linear_h_1.txt   |                          | \( x_1, x_2, v_1, v_2 \) | 150   |
| Simulated Double pendulum   | double_pend_h_1.txt           |                          | \( \theta_1, \theta_2, \omega_1, \omega_2 \) | 1355  |
| Motion-tracked Double pendulum | real_double_pend_h_1.txt^2   |                          | \( \theta_1, \theta_2, \omega_1, \omega_2 \) | 200   |

Table 3. The problem instances for which we used the datasets from [11]. For each system type we use two different datasets, one generated via simulation, the other by motion-tracking the real system.

| Instance                      | \( D \) | \( I \) | \( I+D \) | \( D_{opt} \) | \( I_{opt} \) | \( I_{opt}+D_{opt} \) |
|-------------------------------|---------|--------|---------|-------------|-------------|---------------------|
| ChemicalReaction              | 7       | 4      | 2       | 9           | 10          | 10                  |
| E-CELL                        | 5       | 0      | 4       | 9           | 10          | 10                  |
| S-System                      | 0       | 0      | 0       | 10          | 10          | 10                  |
| Lotka-Volterra (three species)| 0       | 0      | 0       | 0           | 8           |                     |
| Bacterial Respiration         | 5       | 3      | 3       | 10          | 10          | 10                  |
| Bar Magnets                   | 3       | 4      | 5       | 10          | 10          | 10                  |
| Glider                        | 0       | 0      | 0       | 9           | 10          | 10                  |
| Lotka-Volterra                | 0       | 0      | 0       | 1           | 3           | 10                  |
| Predator Prey                 | 0       | 0      | 0       | 3           | 10          | 10                  |
| Shear Flow                    | 0       | 0      | 0       | 7           | 10          | 10                  |
| Van der Pol Oscillator        | 1       | 0      | 1       | 6           | 10          | 10                  |
| Linear Oscillator (motion-tracked) | 0      | 5      | 9       | 1           | 9           | 10                  |
| Linear Oscillator (simulation) | 0       | 0      | 5       | 0           | 10          | 10                  |
| Pendulum (motion-tracked)     | 0       | 0      | 0       | 0           | 10          | 10                  |
| Pendulum (simulated)          | 4       | 9      | 9       | 0           | 10          | 10                  |
| Double Oscillator (motion-tracked) | 0       | 0      | 0       | 0           | 0           | 6                   |
| Double Oscillator (simulated)  | 0       | 0      | 0       | 0           | 0           | 10                  |
| Double Pendulum (motion-tracked) | 0       | 0      | 0       | 0           | 0           | 7                   |
| Double Pendulum (simulated)    | 0       | 0      | 0       | 10          | 0           | 10                  |
| Total                         | 21      | 16     | 29      | 85          | 122         | 171                 |

Table 4. Number of successful runs. A run is successful if the SNMSE for the integrated system is < 0.01. Algorithm configurations: numeric differences (\( D \)), numeric IVP solution (\( I \)), combination of numeric differences and IVP solution (\( I+D \)). The configurations using the subscript \( \text{opt} \) include parameter optimization.
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