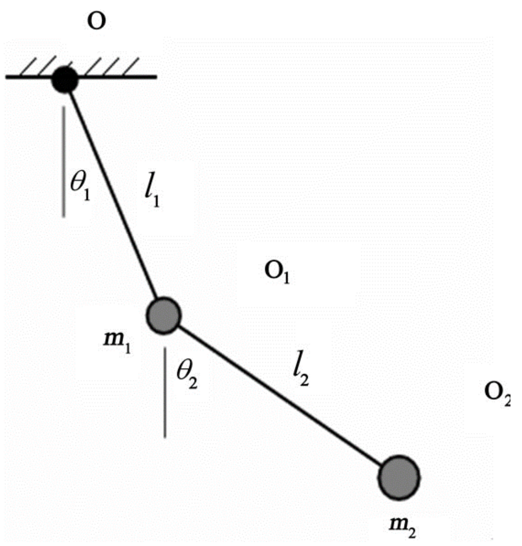
Identification of Dynamical Systems using Symbolic Regression

Gabriel Kronberger, Lukas Kammerer, Michael Kommenda

EuroCAST 2019

SymReg
JOSEF RESSEL CENTER FOR
SYMBOLIC REGRESSION

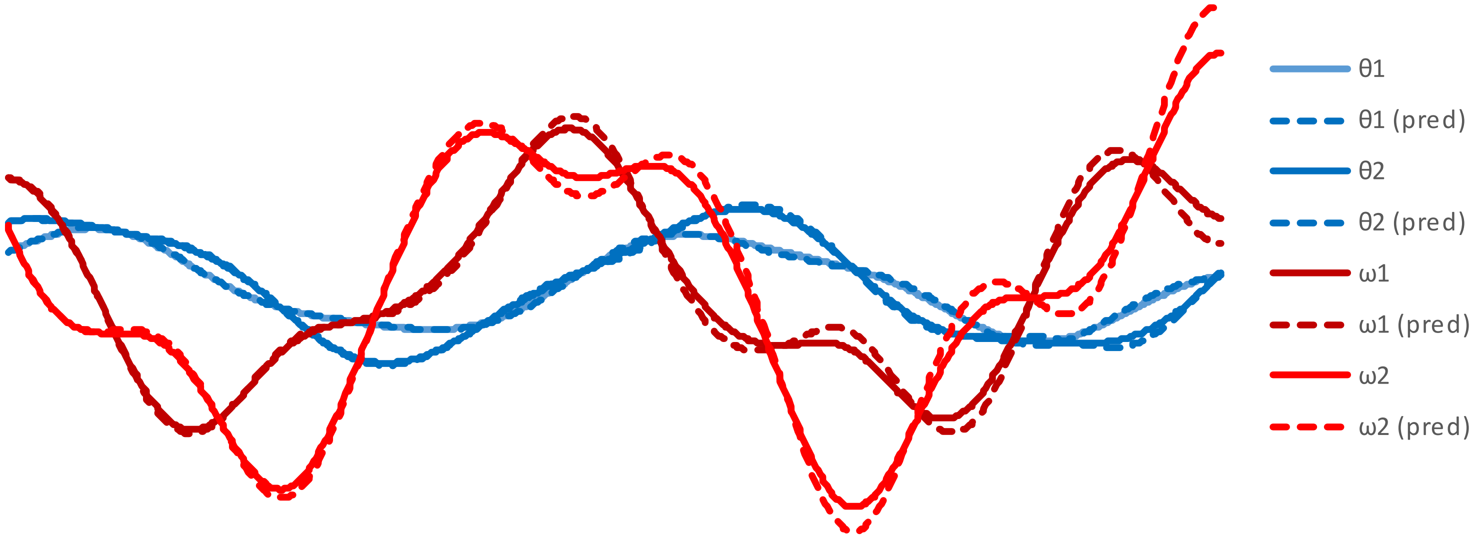


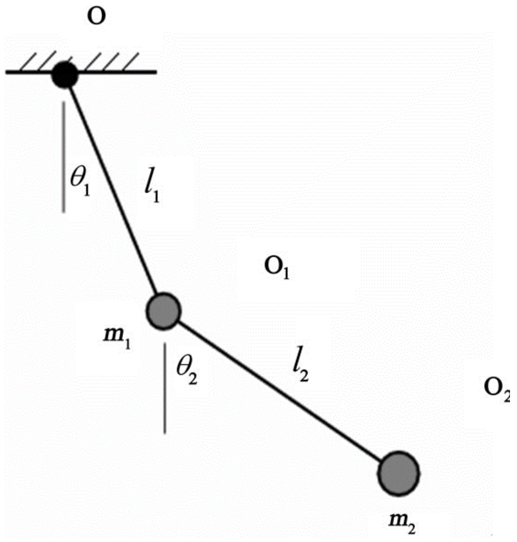
$$\dot{\theta}_1 = f_{\theta_1}(\theta_1, \theta_2, \omega_1, \omega_2, \phi)$$

$$\dot{\theta}_2 = f_{\theta_2}(\theta_1, \theta_2, \omega_1, \omega_2, \phi)$$

$$\dot{\omega}_1 = f_{\omega_1}(\theta_1, \theta_2, \omega_1, \omega_2, \phi)$$

$$\dot{\omega}_2 = f_{\omega_2}(\theta_1, \theta_2, \omega_1, \omega_2, \phi)$$





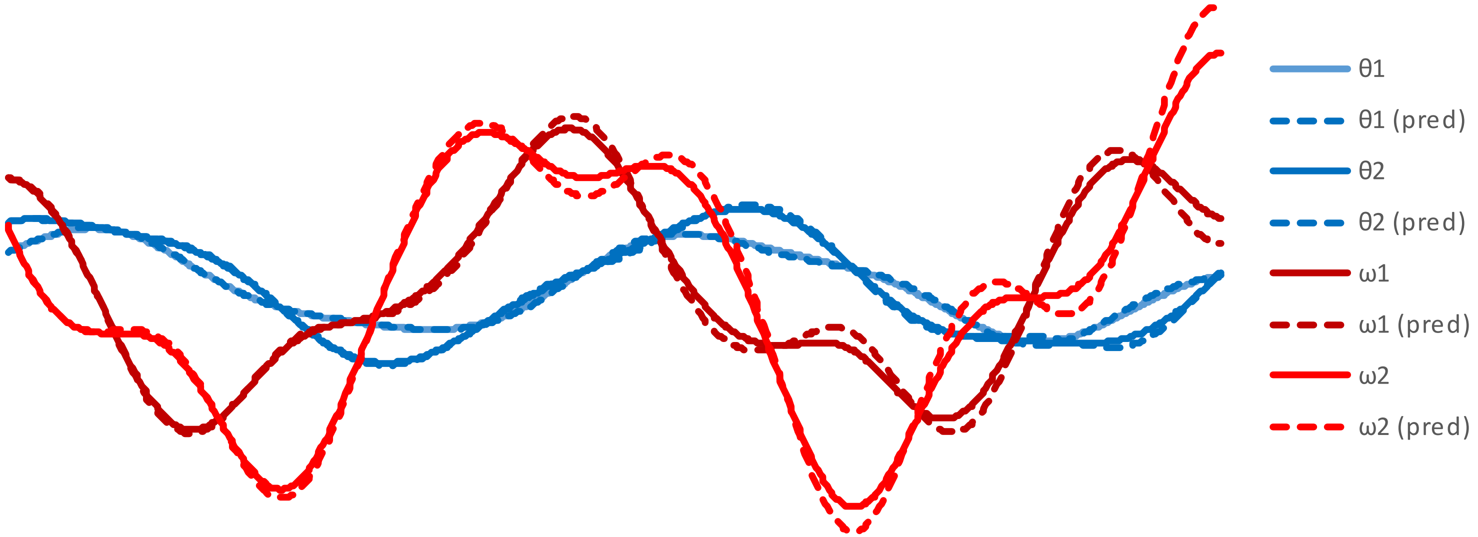
$$\dot{\theta}_1 = \boxed{f_{\theta_1}(\theta_1, \theta_2, \omega_1, \omega_2, \phi)}$$

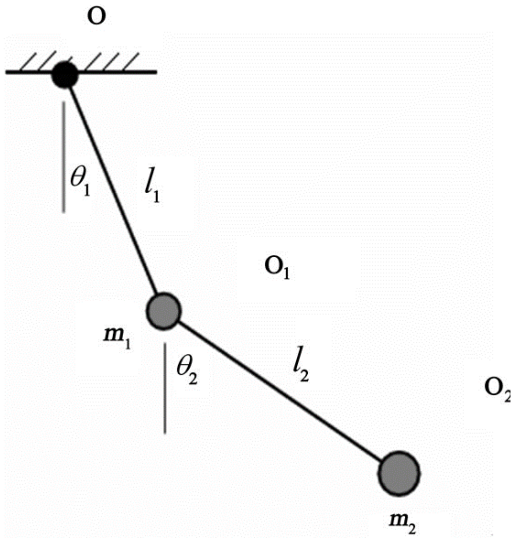
$$\dot{\theta}_2 = \boxed{f_{\theta_2}(\theta_1, \theta_2, \omega_1, \omega_2, \phi)}$$

$$\dot{\omega}_1 = \boxed{f_{\omega_1}(\theta_1, \theta_2, \omega_1, \omega_2, \phi)}$$

$$\dot{\omega}_2 = \boxed{f_{\omega_2}(\theta_1, \theta_2, \omega_1, \omega_2, \phi)}$$

GP / SymReg

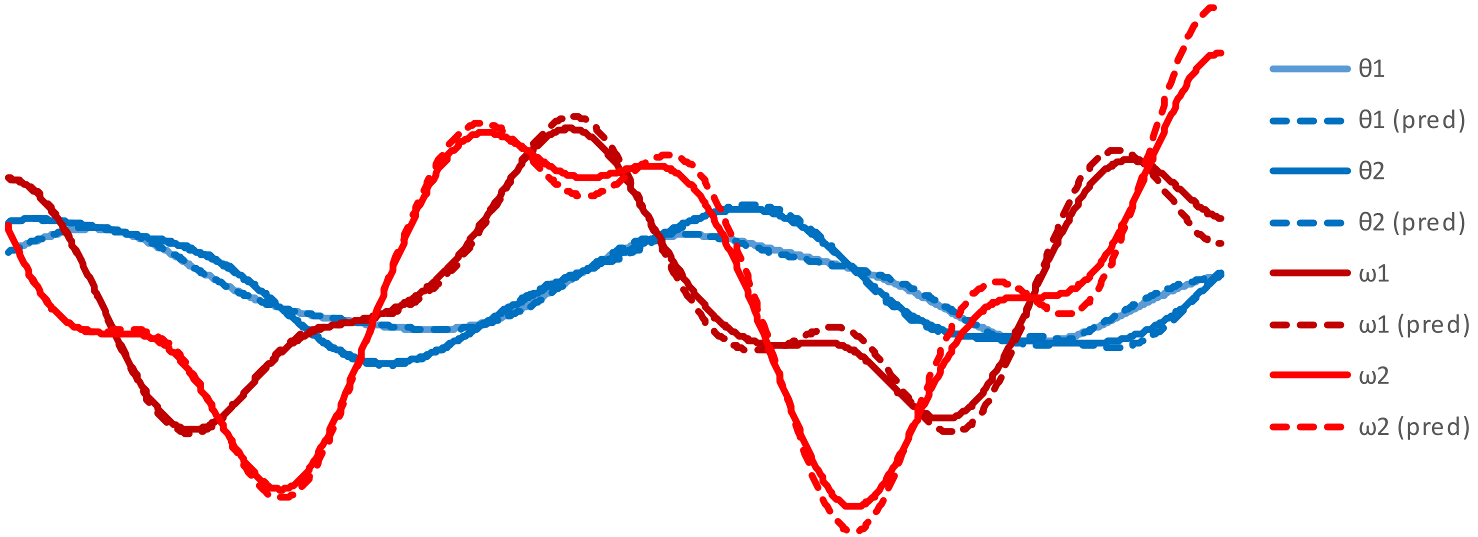




$$\dot{\theta}_1 = f_{\theta_1}(\theta_1, \theta_2, \omega_1, \omega_2, \phi)$$
$$\dot{\theta}_2 = f_{\theta_2}(\theta_1, \theta_2, \omega_1, \omega_2, \phi)$$
$$\dot{\omega}_1 = f_{\omega_1}(\theta_1, \theta_2, \omega_1, \omega_2, \phi)$$
$$\dot{\omega}_2 = f_{\omega_2}(\theta_1, \theta_2, \omega_1, \omega_2, \phi)$$

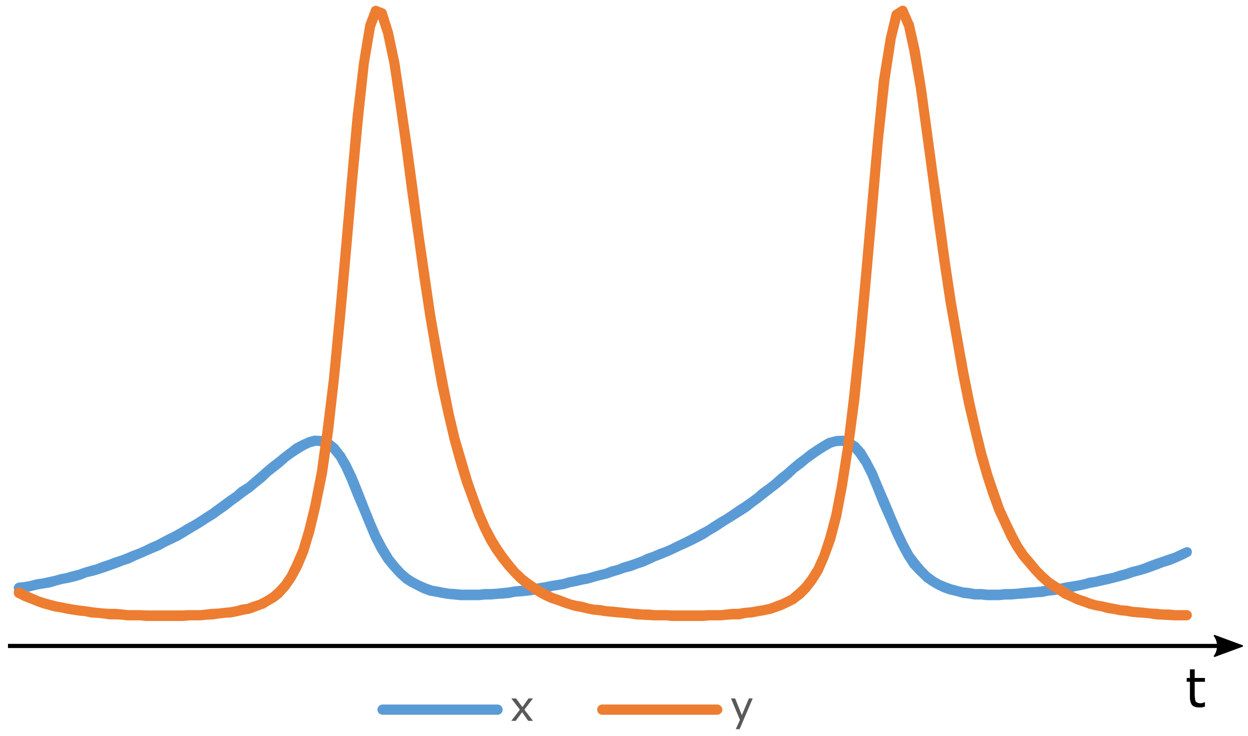
GP / SymReg

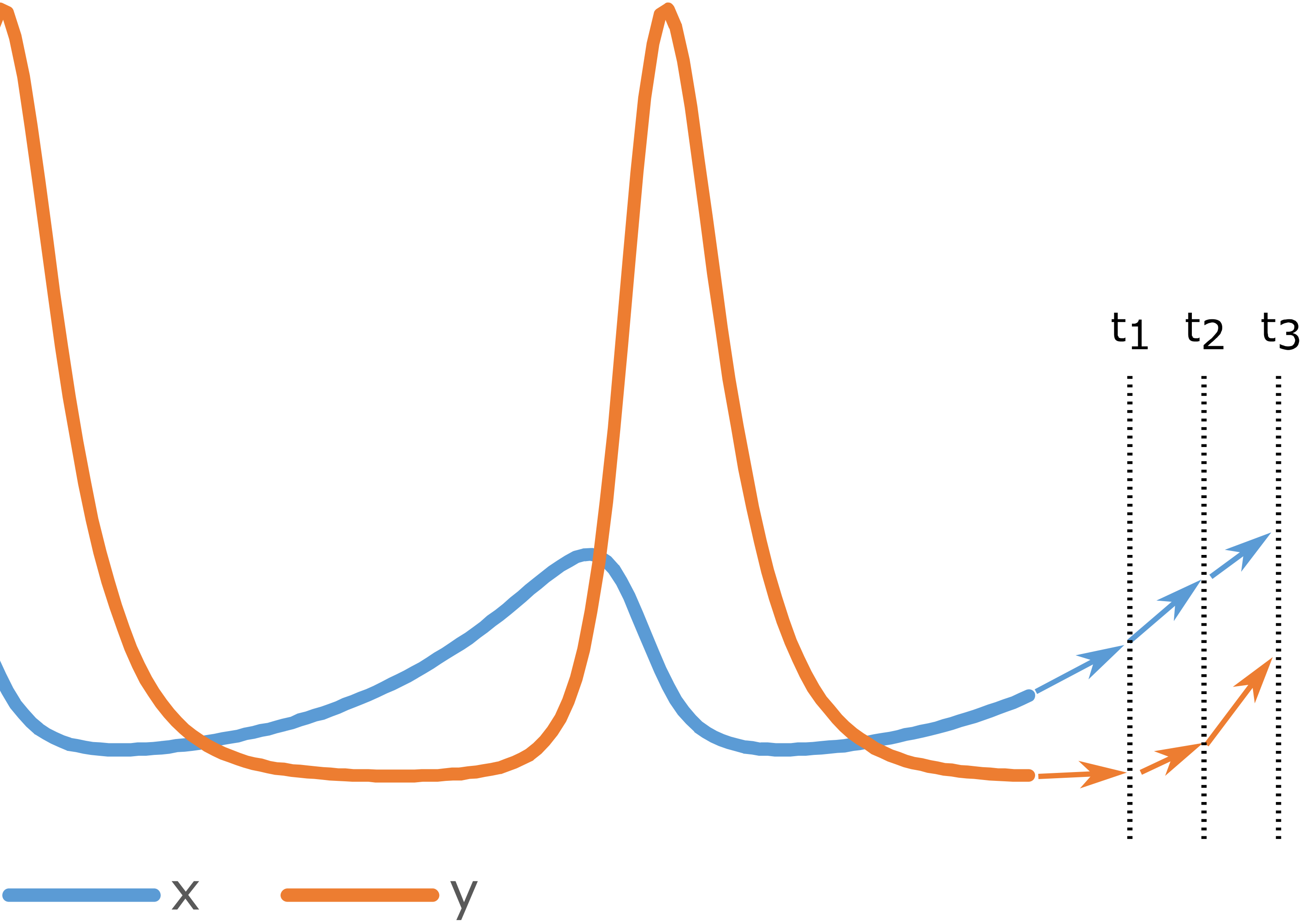
Non-linear least squares optimization



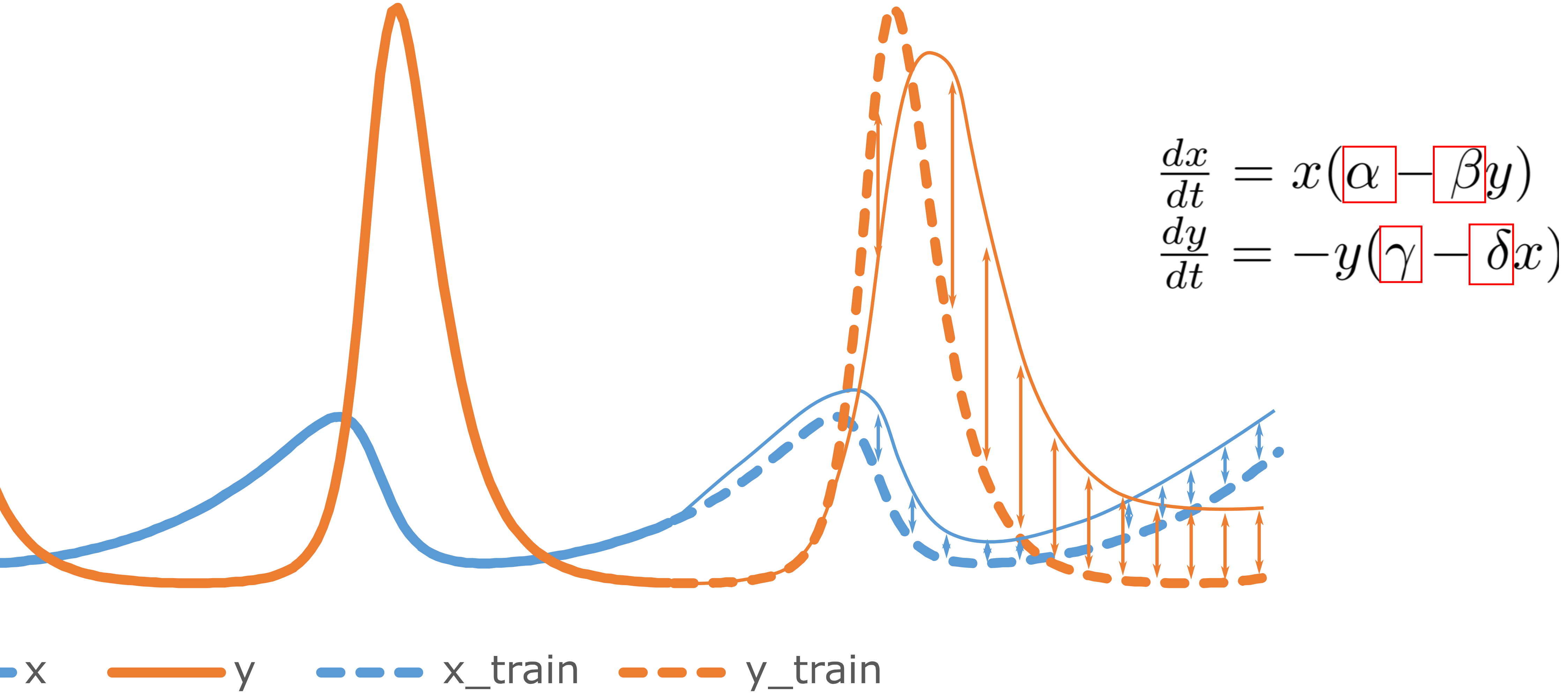
Lotka-Volterra Predator-Prey Model:

$$\frac{dx}{dt} = x(\alpha - \beta y)$$
$$\frac{dy}{dt} = -y(\gamma - \delta x)$$

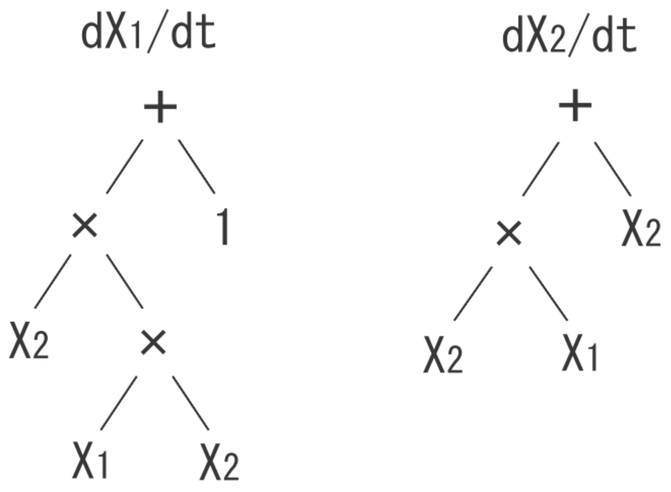




$$\frac{dx}{dt} = x(\alpha - \beta y)$$
$$\frac{dy}{dt} = -y(\gamma - \delta x)$$


$\frac{dx}{dt} = x(\boxed{\alpha} - \boxed{\beta}y)$
$\frac{dy}{dt} = -y(\boxed{\gamma} - \boxed{\delta}x)$
x
y
x_train
y_train

Individual:

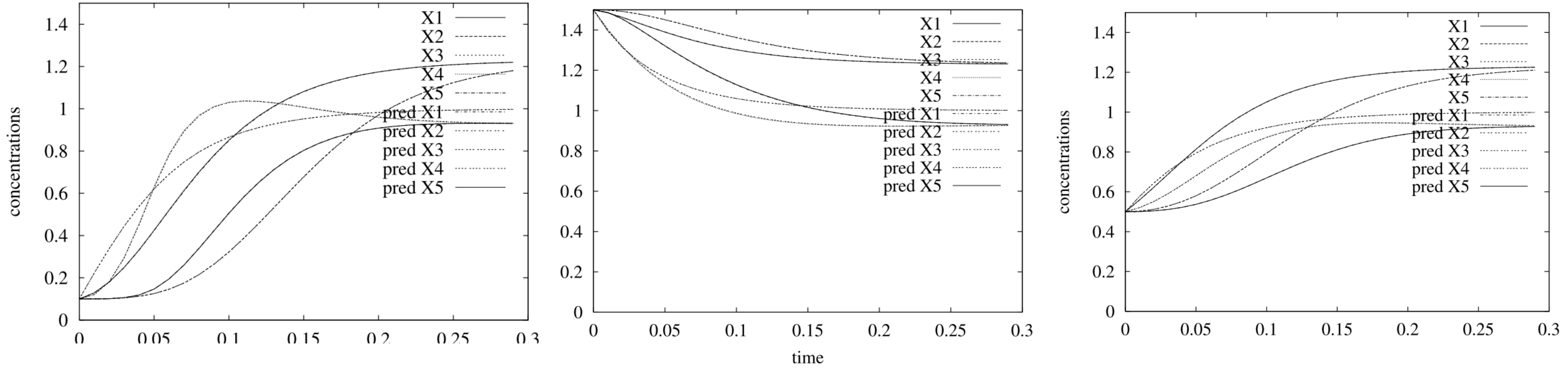


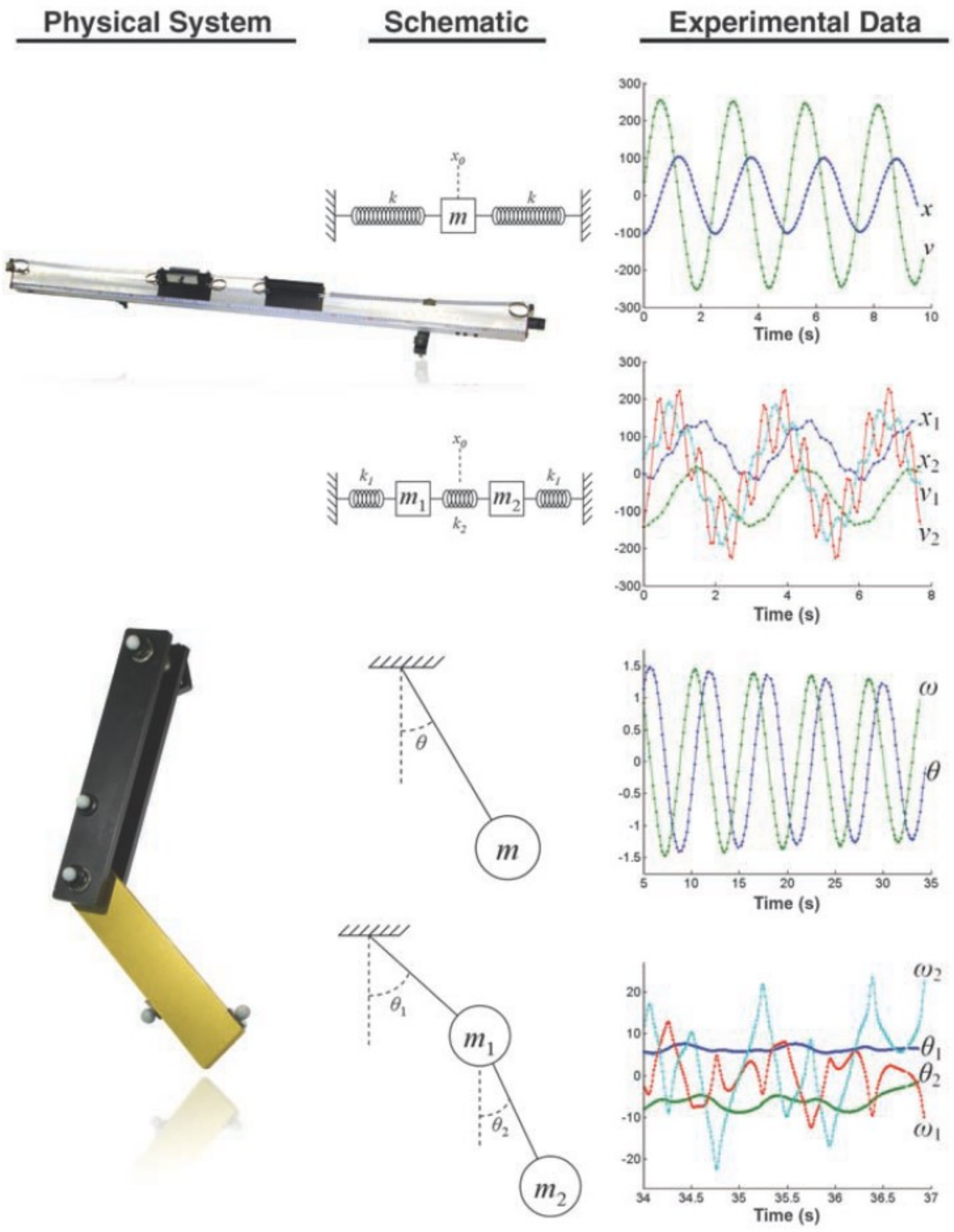
Linear least squares:

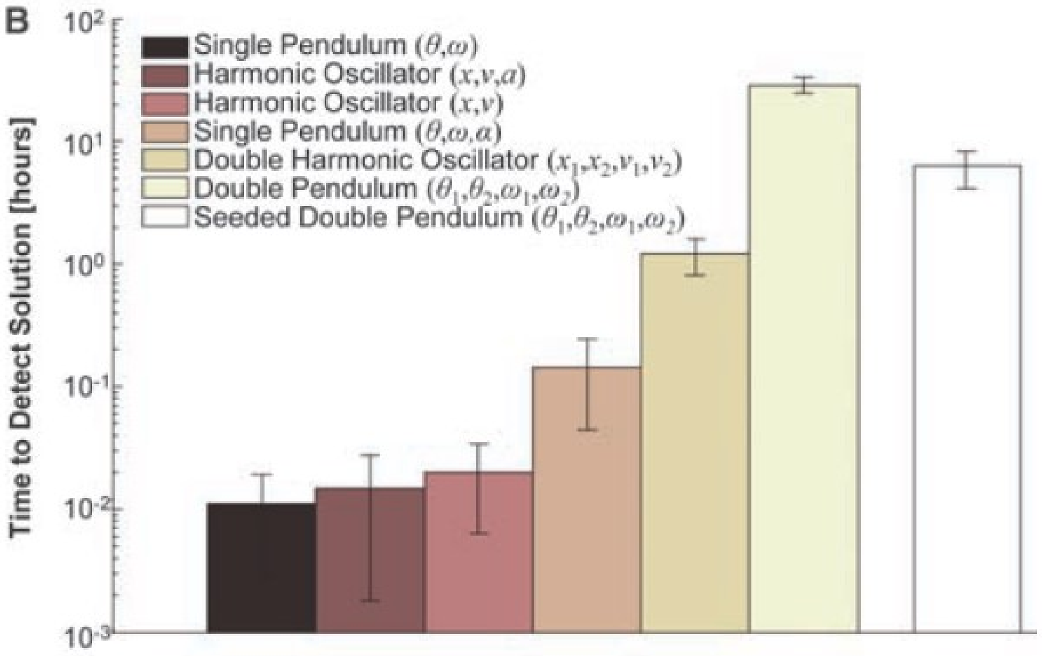
$$\chi^2 = \sum_{i=1}^{N}\left(y(i) - \sum_{k=1}^{M} a_k F_k(x_1(i), \ldots, x_L(i))\right)^2$$

H. Iba, *Inference of Differential Equation Models by Genetic Programming, Information Sciences*, Volume 178, Issue 23, 2008, Pages 4453-4468

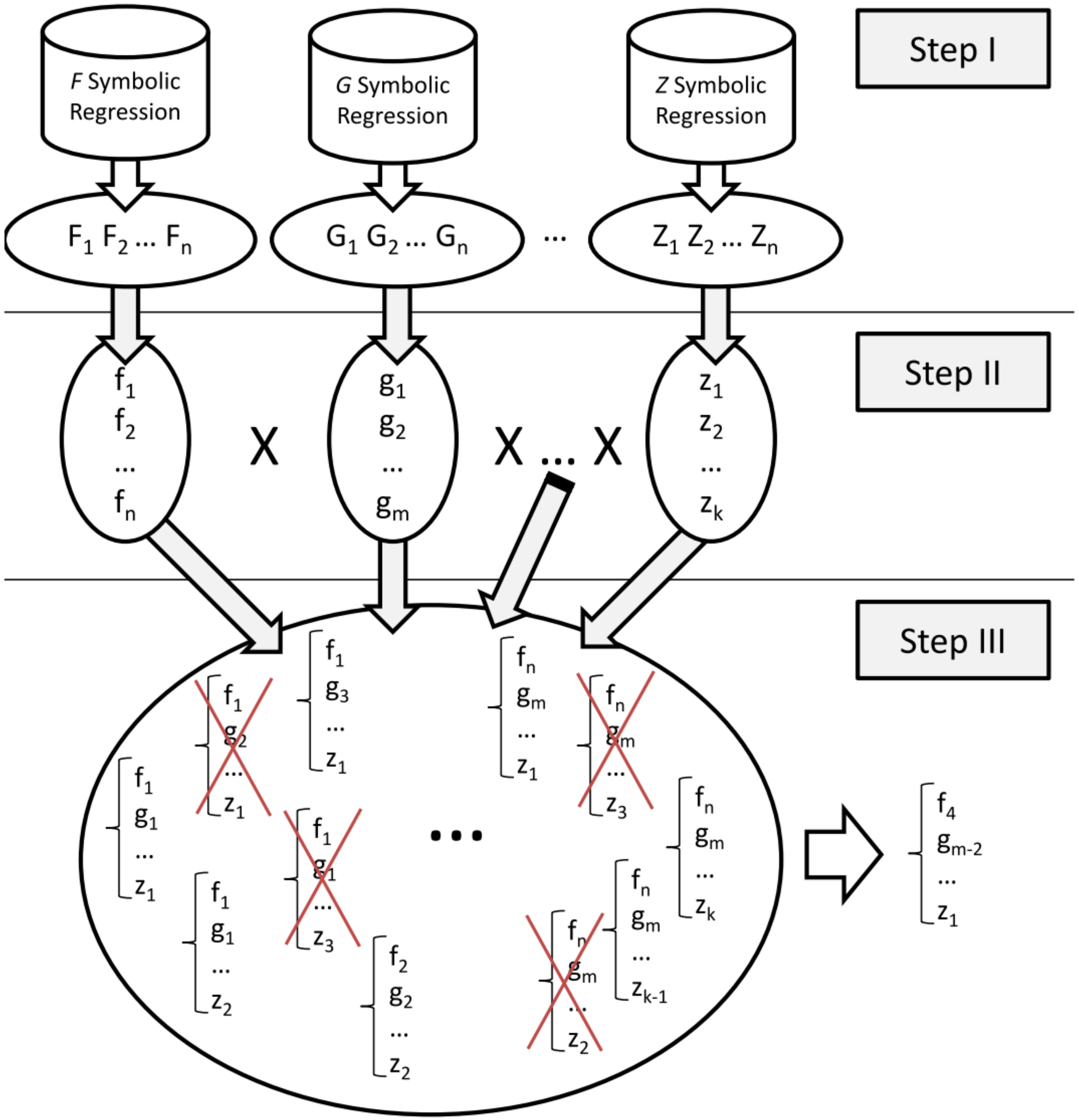
Example:



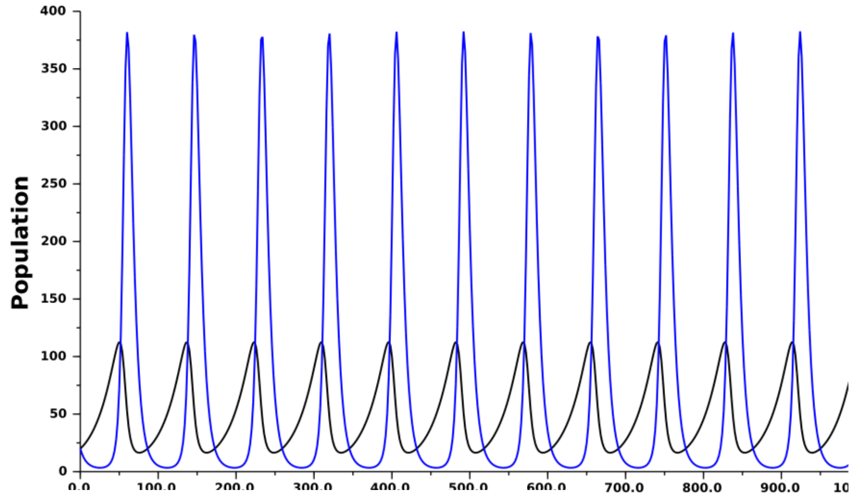


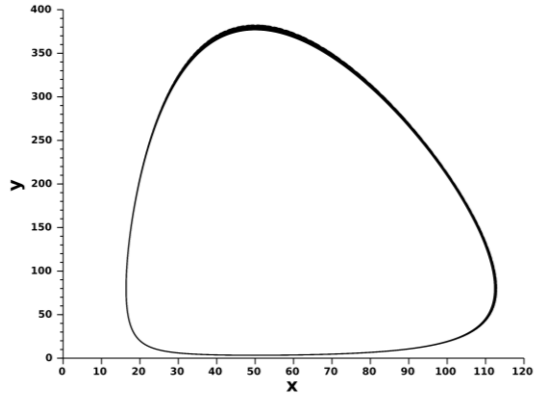


M. Schmidt, H. Lipson:
Distilling Free-Form Natural Laws from Experimental Data
Science Vol. 324, **2009**, pp. 81 – 85



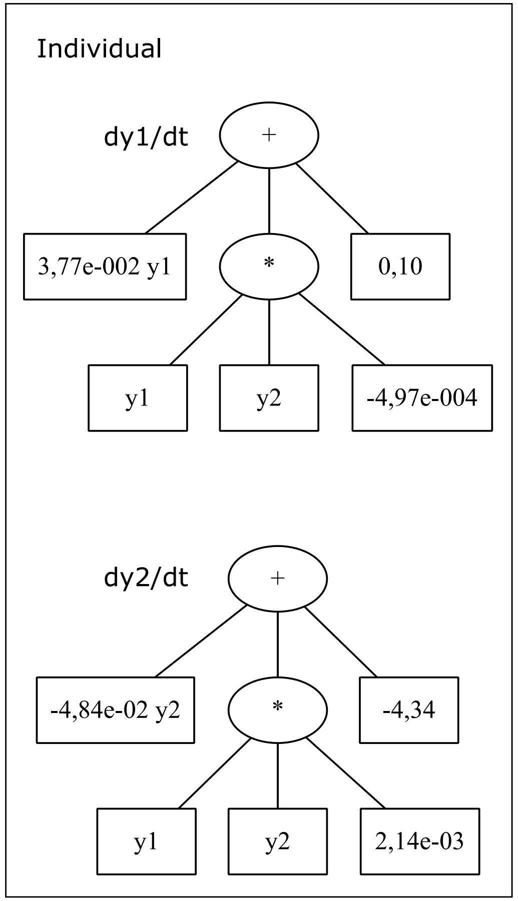
Lotka-Volterra:

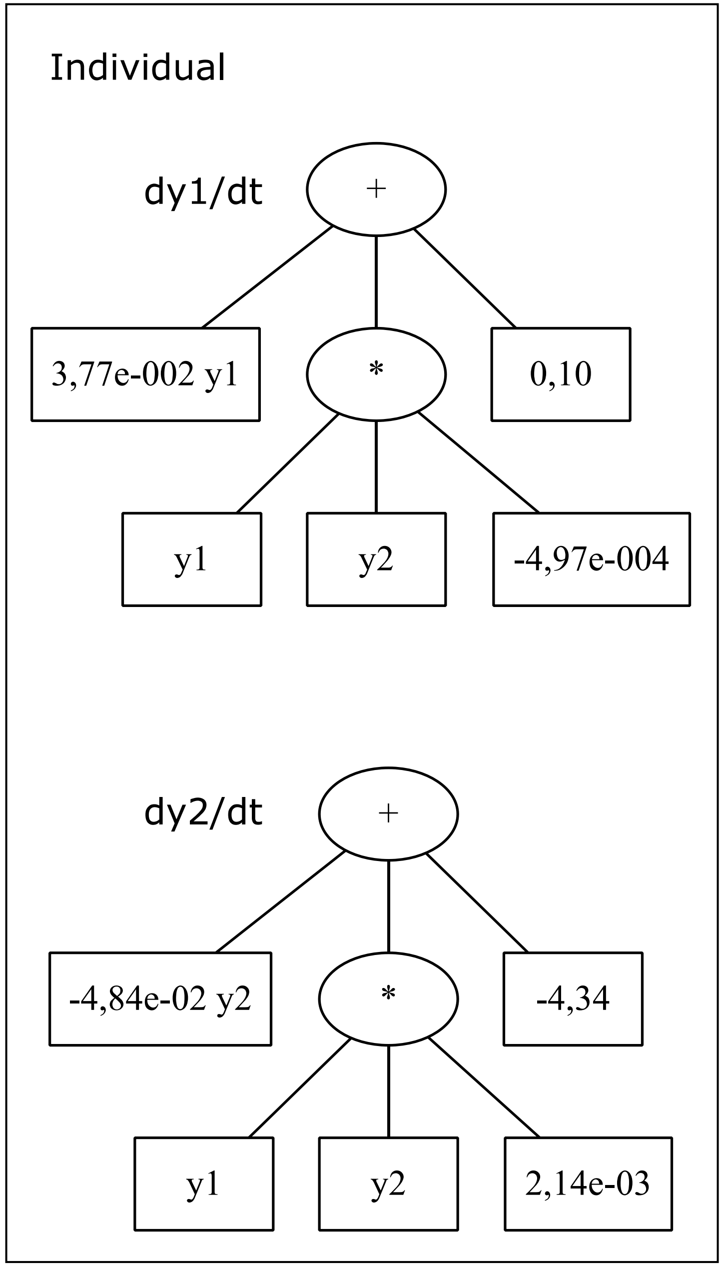


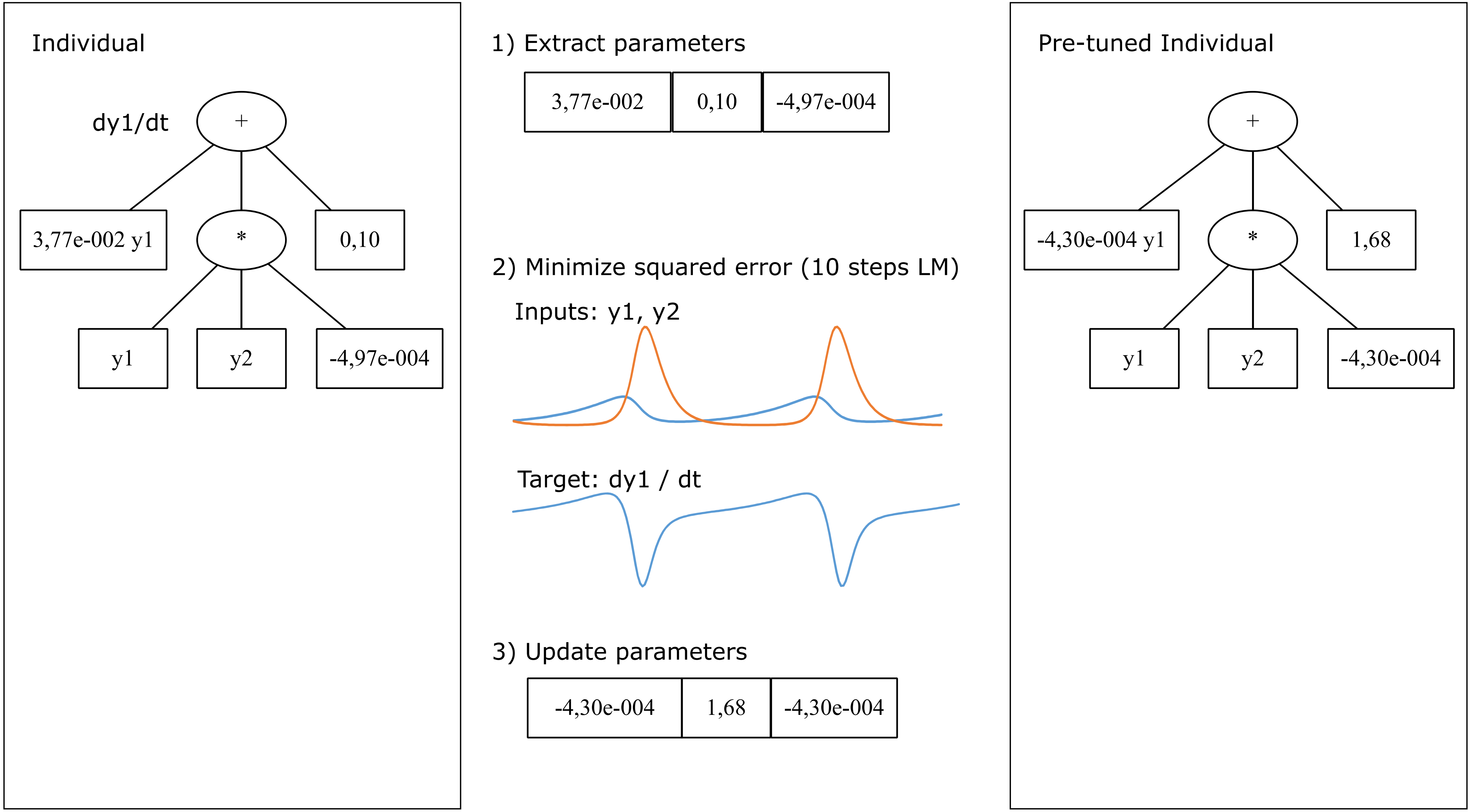


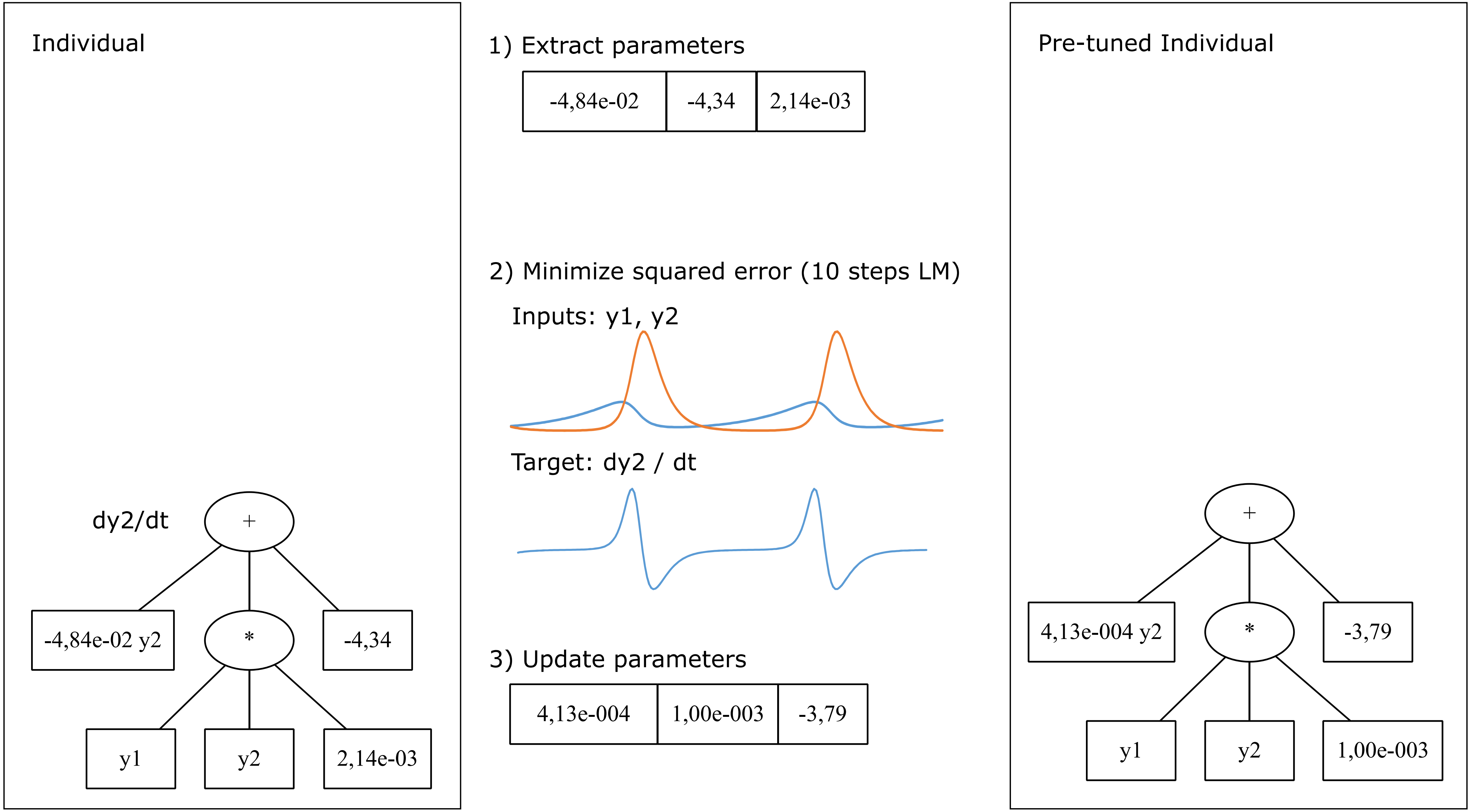
S. Gaucel, M. Keijzer, E. Lutton, A. Tonda:
Learning Dynamical Systems Using Standard Symbolic Regression
EvoStar 2014

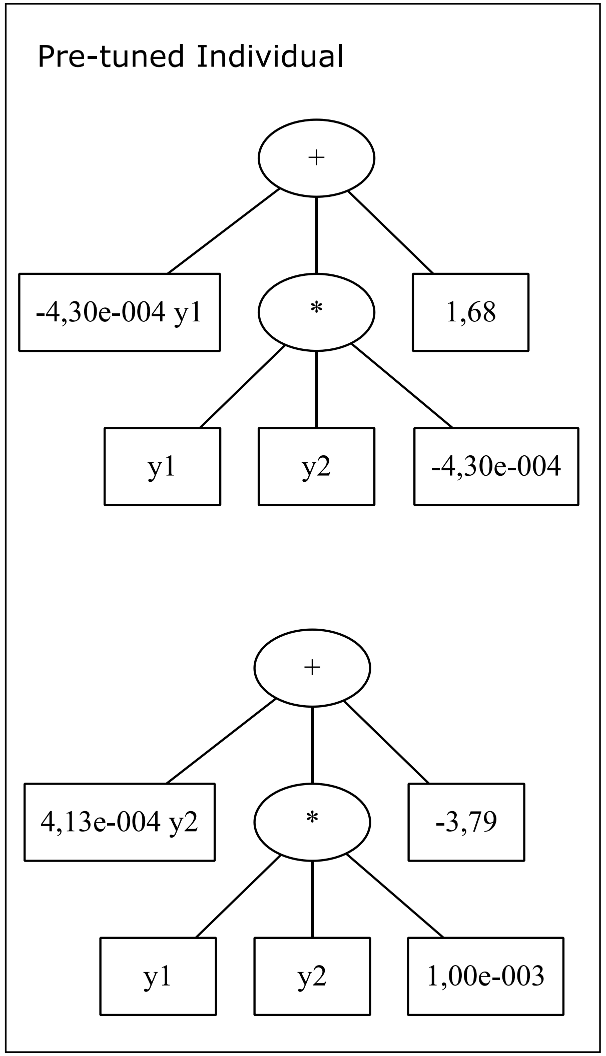
```
Evolutionary Algorithm (maxGenerations, popSize, maxSelectionPressure)
        g = 0;
        pop_g = CreateRandomPopulation(popSize);
        do {
          g++;
          pop_g = Ø;
          candidates = 0;
          do {
            parent_1 = SelectFitnessProportional(pop_g-1);
            parent_2 = SelectRandom(pop_g-1);
            child = Crossover(parent_1, parent_2);

            Mutate(child);
            Optimize(child); // pre-tuning, solve numerically and optimize

            candidates++;
            if (Fitness(child) >= Max(Fitness(parent_1), Fitness(parent_2)))
              pop_g = pop_g ∪ { child };
          } while ( |pop_g| < |pop_g-1| );
          s = candidates / popSize;
        } while (g < maxGenerations && s < maxSelectionPressure);
```




Individual
dy1/dt
+
3,77e-002 y1
*
0,10
y1
y2
-4,97e-004
dy2/dt
+
-4,84e-02 y2
*
-4,34
y1
y2
2,14e-03


Individual
dy1/dt
+
3,77e-002 y1
*
0,10
y1
y2
-4,97e-004
1) Extract parameters
3,77e-002
0,10
-4,97e-004
2) Minimize squared error (10 steps LM)
Inputs: y1, y2
Target: dy1 / dt
3) Update parameters
-4,30e-004
1,68
-4,30e-004
Pre-tuned Individual
+
-4,30e-004 y1
*
1,68
y1
y2
-4,30e-004


Individual
dy2/dt
+
-4,84e-02 y2
*
-4,34
y1
y2
2,14e-03
1) Extract parameters
-4,84e-02
-4,34
2,14e-03
2) Minimize squared error (10 steps LM)
Inputs: y1, y2
Target: dy2 / dt
3) Update parameters
4,13e-004
1,00e-003
-3,79
Pre-tuned Individual
+
4,13e-004 y2
*
-3,79
y1
y2
1,00e-003



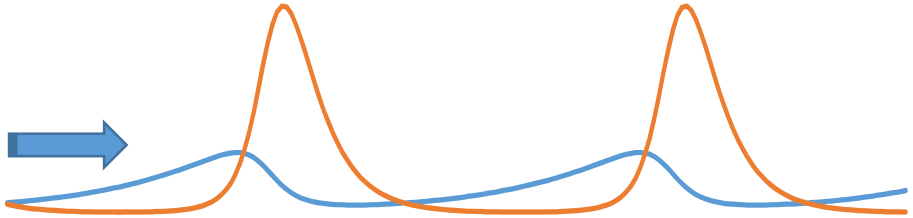
1) Extract parameters

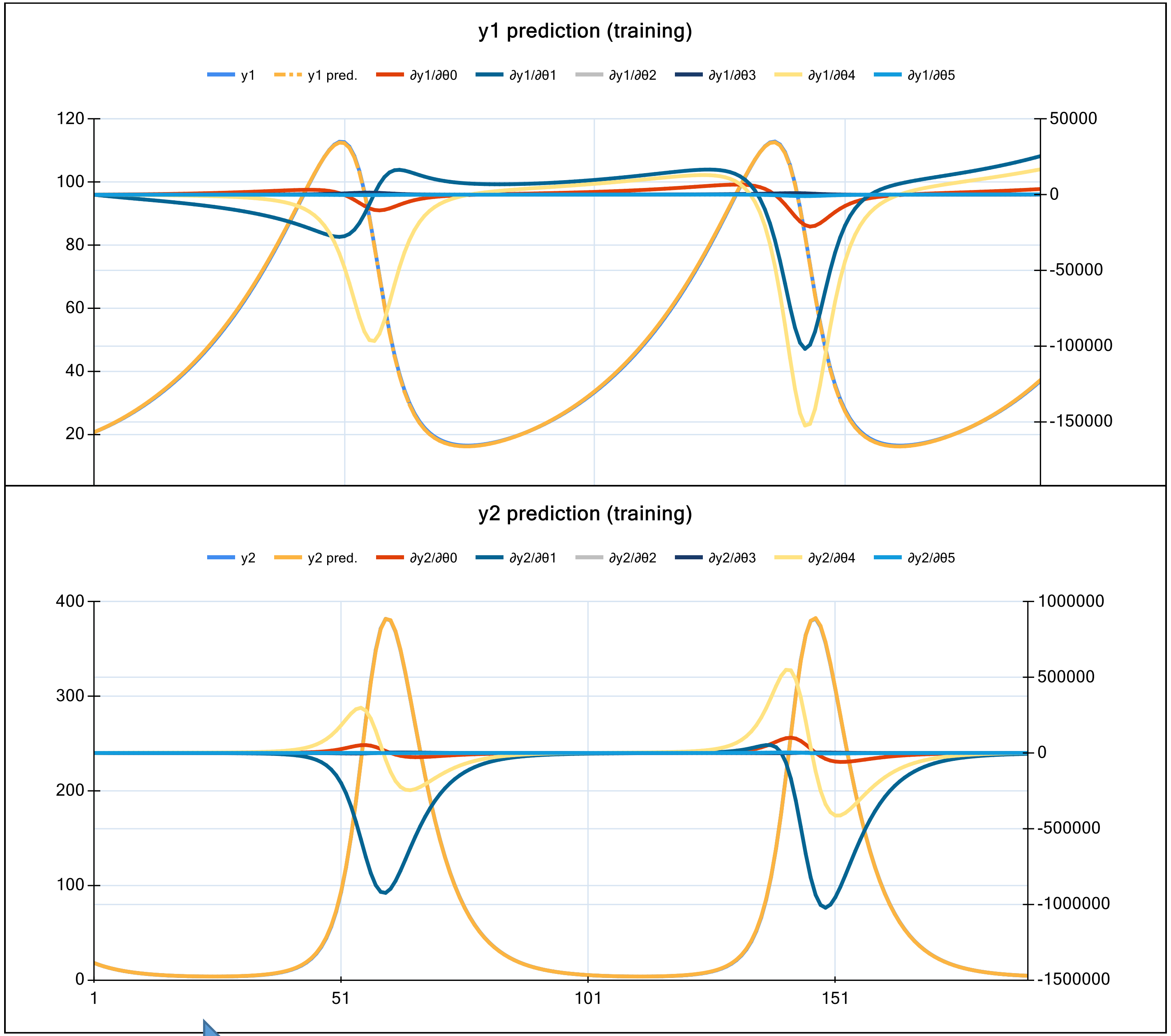
-4,30e-004	1,68	-4,30e-004	4,13e-004	1,00e-003	-3,79

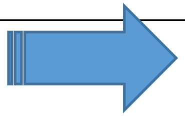
2) Minimize integrated squared error (10 steps LM)

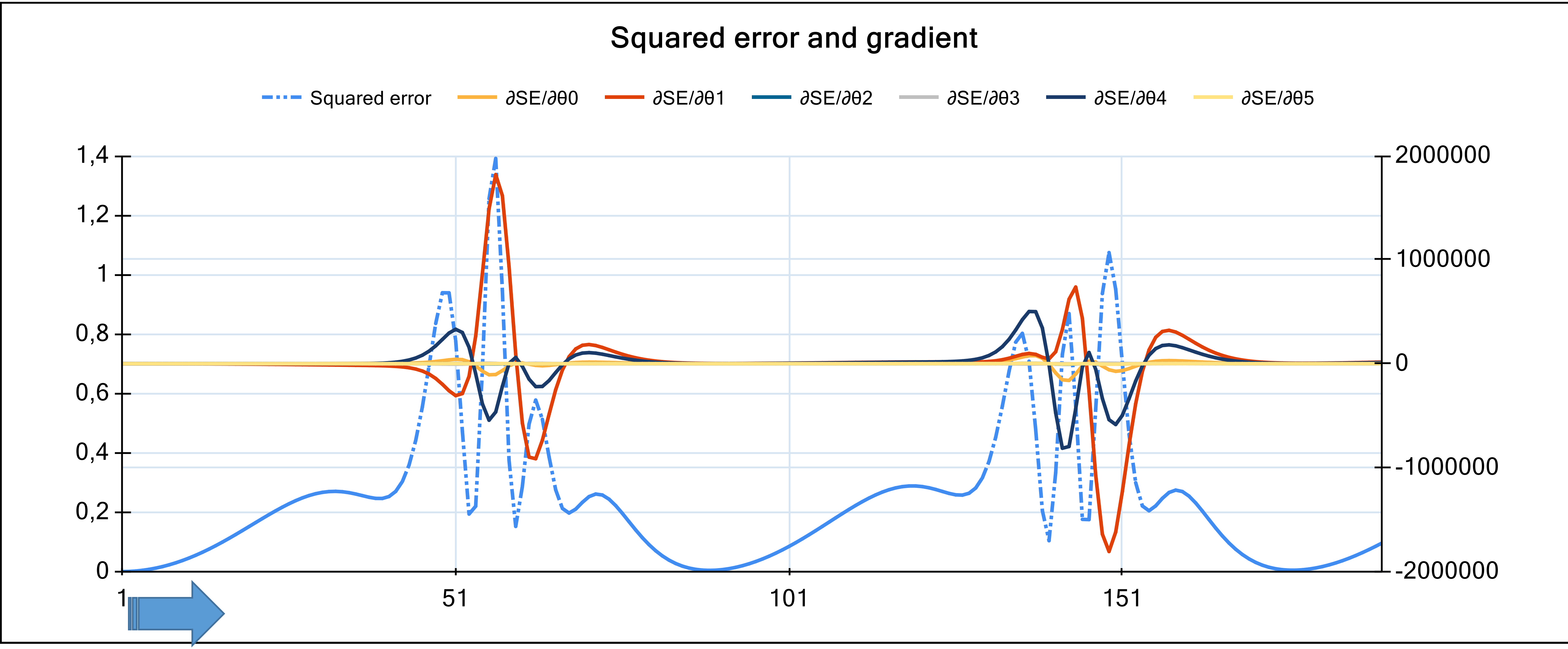
Inputs: none

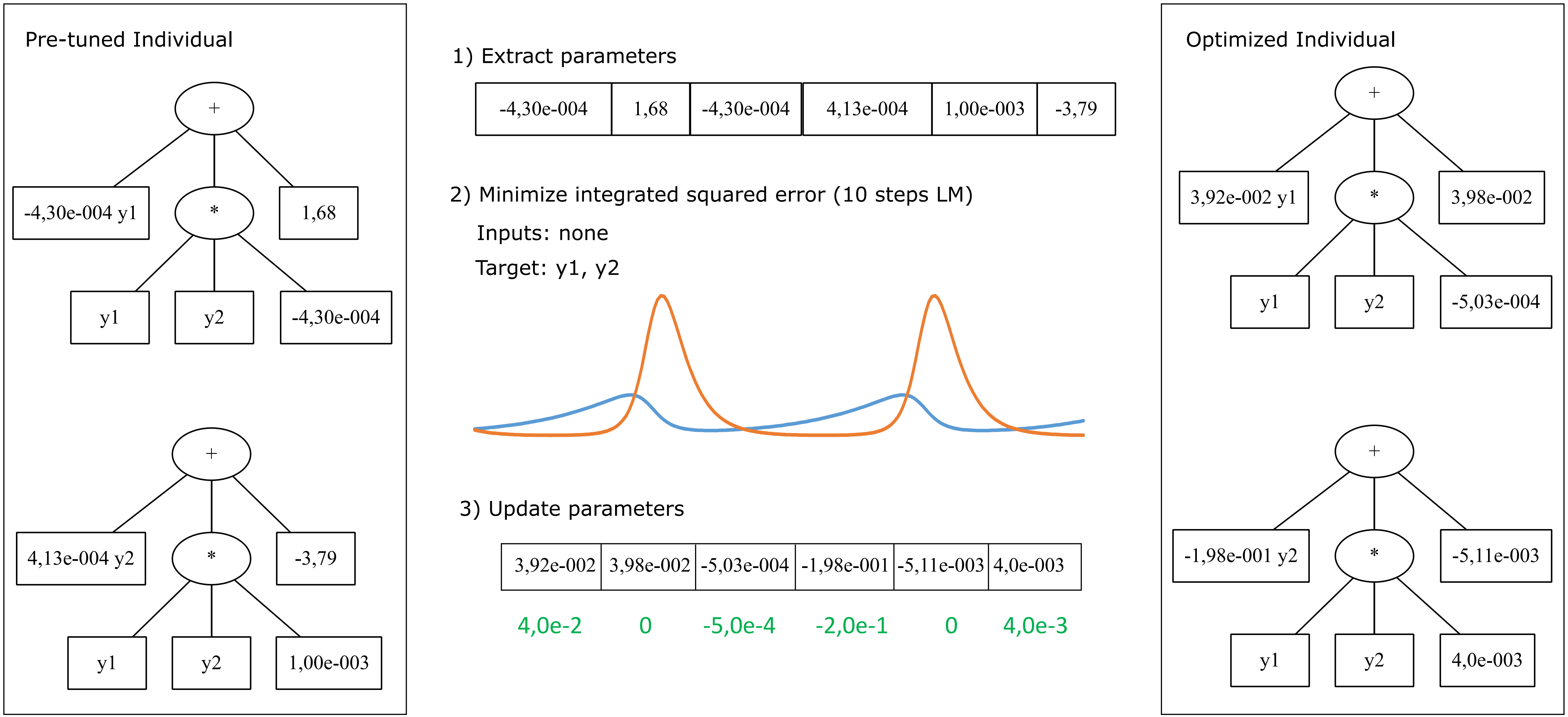
Target: y1, y2




y1 prediction (training)
y1
y1 pred.
∂y1/∂θ0
∂y1/∂θ1
∂y1/∂θ2
∂y1/∂θ3
∂y1/∂θ4
∂y1/∂θ5
120
100
80
60
40
20
50000
0
-50000
-100000
-150000
y2 prediction (training)
y2
y2 pred.
∂y2/∂θ0
∂y2/∂θ1
∂y2/∂θ2
∂y2/∂θ3
∂y2/∂θ4
∂y2/∂θ5
400
300
200
100
0
1000000
500000
0
-500000
-1000000
-1500000
1
51
101
151

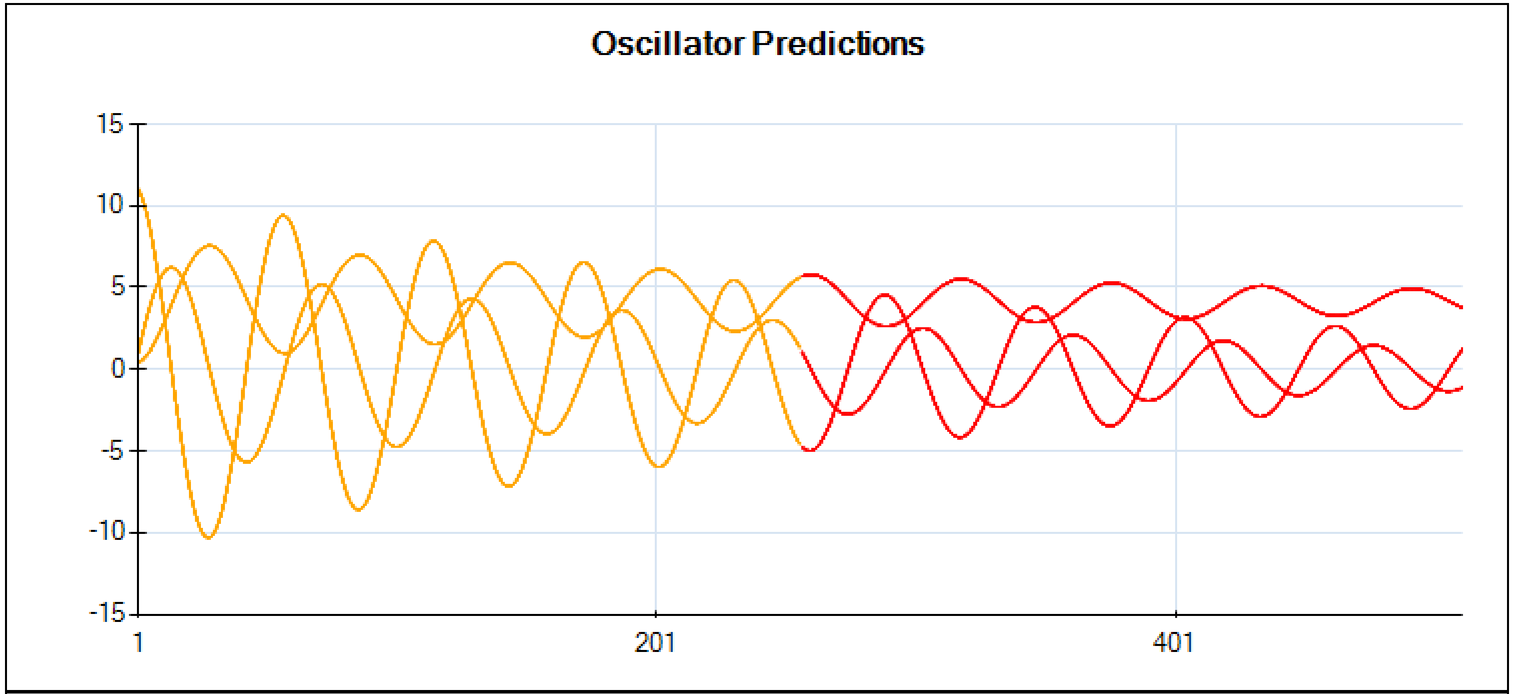


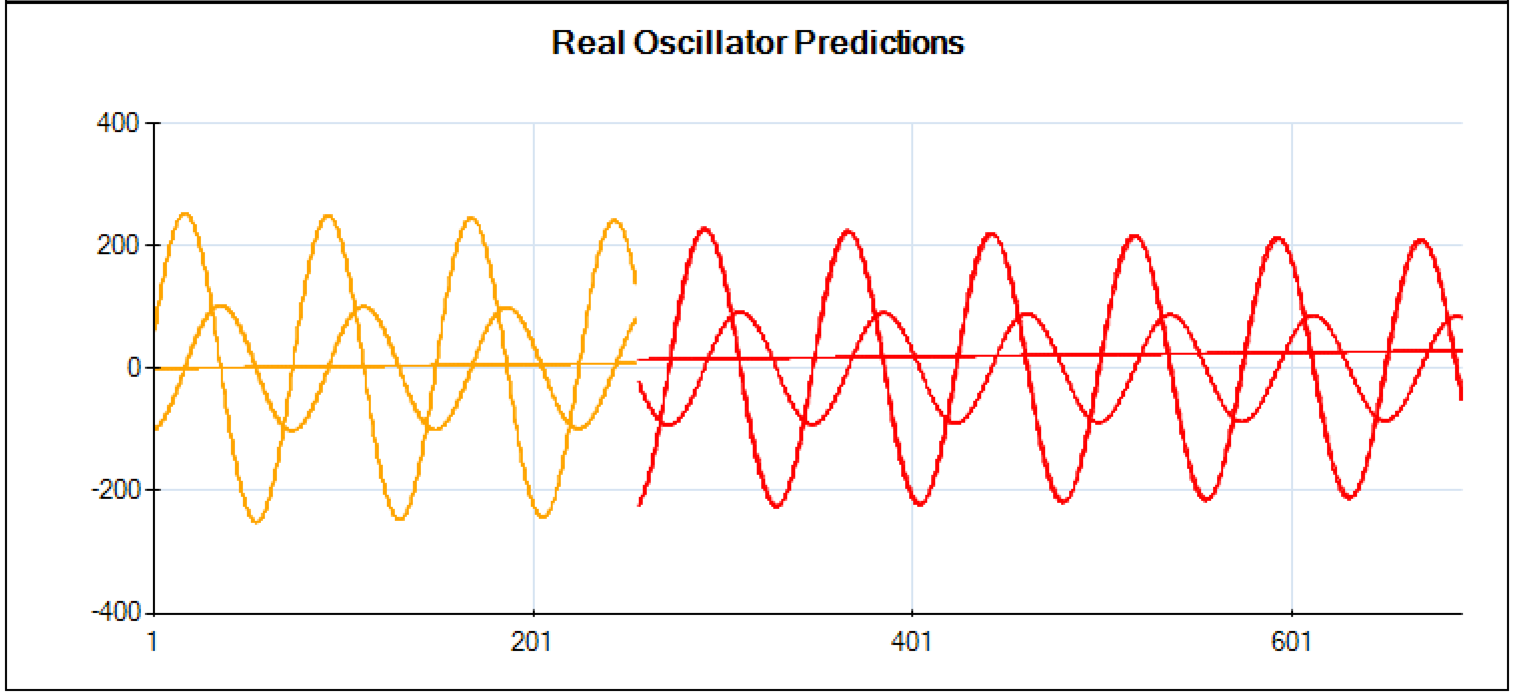

Squared error and gradient
Squared error
∂SE/∂θ0
∂SE/∂θ1
∂SE/∂θ2
∂SE/∂θ3
∂SE/∂θ4
∂SE/∂θ5
1,4
1,2
1
0,8
0,6
0,4
0,2
0
2000000
1000000
0
-1000000
-2000000
1
51
101
151

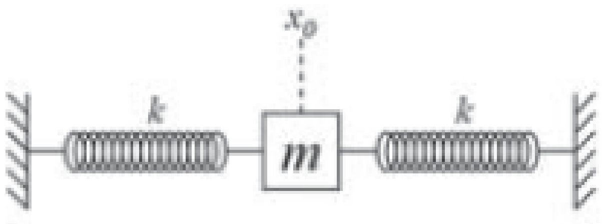


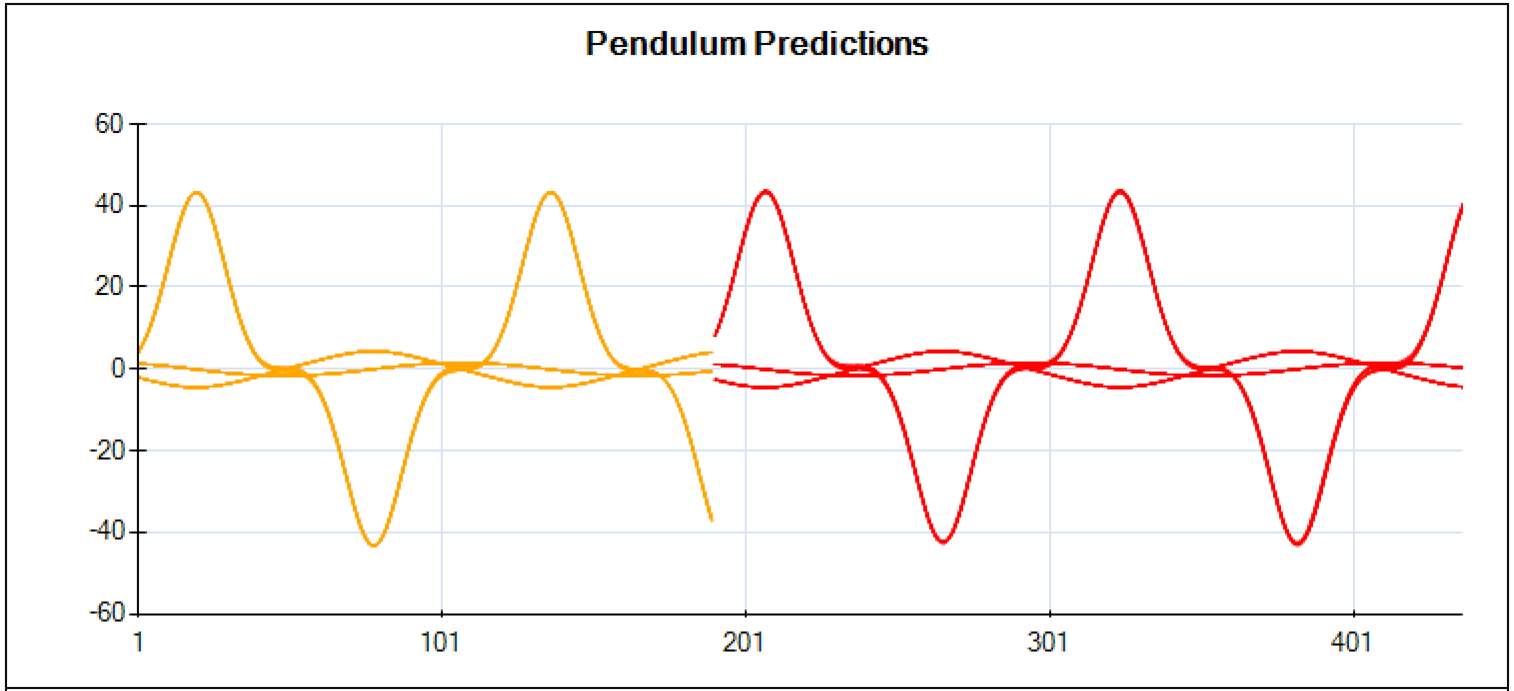
Pre-tuned Individual
+
-4,30e-004 y1
*
1,68
y1
y2
-4,30e-004
+
4,13e-004 y2
*
-3,79
y1
y2
1,00e-003
1) Extract parameters
-4,30e-004
1,68
-4,30e-004
4,13e-004
1,00e-003
-3,79
2) Minimize integrated squared error (10 steps LM)
Inputs: none
Target: y1, y2
3) Update parameters
3,92e-002
3,98e-002
-5,03e-004
-1,98e-001
-5,11e-003
4,0e-003
4,0e-2
0
-5,0e-4
-2,0e-1
0
4,0e-3
Optimized Individual
+
3,92e-002 y1
*
3,98e-002
y1
y2
-5,03e-004
+
-1,98e-001 y2
*
-5,11e-003
y1
y2
4,0e-003

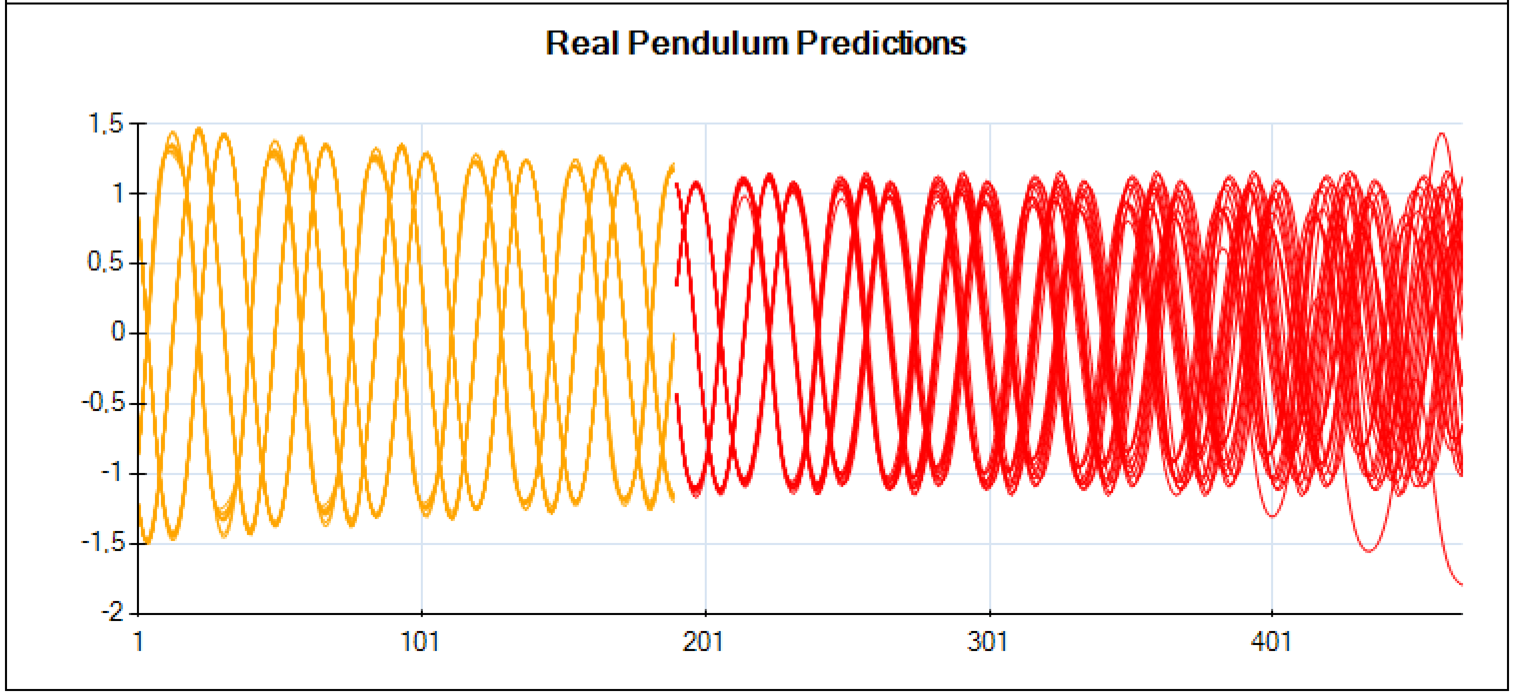
Prior results (without AutoDiff)						Our results (with AutoDiff)					
						Avg. MSE (10 runs)		Avg. NMSE (10 runs)			
Reference	Instance	D	Error	Measure	Avg. Runtime	training	test	training	test	Avg. Runtime	
Iba et al. 2008	Example 1 - Chemical	y1	0	MSE		1,16E-10	NA	6,94E-07	NA	92,4 min	
		y2	2,08E-11	MSE		1,53E-12	NA	8,77E-08	NA		
		y3	1,80E-11	MSE		7,20E-10	NA	1,75E-06	NA		
	Example 2 - Lotka-Volterra (3)	3	4,78E-11	MSE							
	Example 3 - E-CELL	3	2,50E-03	Avg. MSE (10 runs)		6,58E-05	NA	1,27E-03	NA	26,5 min	
	Example 4 - S-System	5	4,50E-06	Avg. MSE (10 runs)		1,71E-05	NA	1,73E-04	NA	4,1 hours	
Gaucel et al. 2014	Lotka-Volterra (2)	2	100%	success rate	15 - 20 min	7,21E-02	2,93E+00	3,64E-05	4,87E-04	23,5 min	
Schmidt et al. 2009	Circle	2			5 min	2,48E-31	1,21E-30	1,15E-31	5,36E-31	37,4 min	
	Oscillator	3			10 min	8,46E-07	5,73E-07	5,54E-08	1,79E-07	2,5 hours	
	Oscillator (real)	3			10 min	1,67E+00	5,62E+00	1,65E-04	2,90E-04	2,0 hours	
	Pendulum (theta, omega, a)	3			15 min	4,15E-02	1,81E-01	2,16E-04	4,78E-04	5,5 hours	
	Pendulum (real)	3			15 min	7,73E-04	7,63E-02	8,79E-04	1,56E-01	3,7 hours	
	Double Oscillator	4			not specified	4,05E-03	1,66E-02	1,58E-02	3,88E-02	22,1 hours	
	Double Oscillator (real)	4			1 - 2 hours	4,81E+02	1,66E+03	3,99E-02	1,82E-01	15,0 hours	
	Double Pendulum	4			not specified	1,34E-05	5,38E-03	9,23E-04	9,22E+00	14,7 hours	
	Double Pendulum (real)	4			1 - 2 days	2,55E-01	3,41E+257	7,34E-03	2,43E+257	3,1 hours	*100 training*
						1,00E+01	9,99E+283	2,22E-01	2,08E+284	12,7 hours	*400 training*
					32 cores					*1 core*	

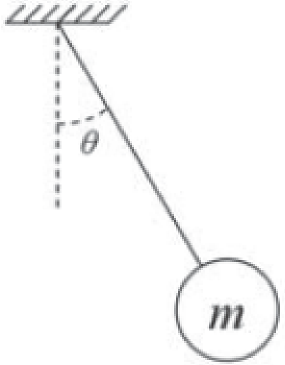

Oscillator Predictions
15
10
5
0
-5
-10
-15
1
201
401

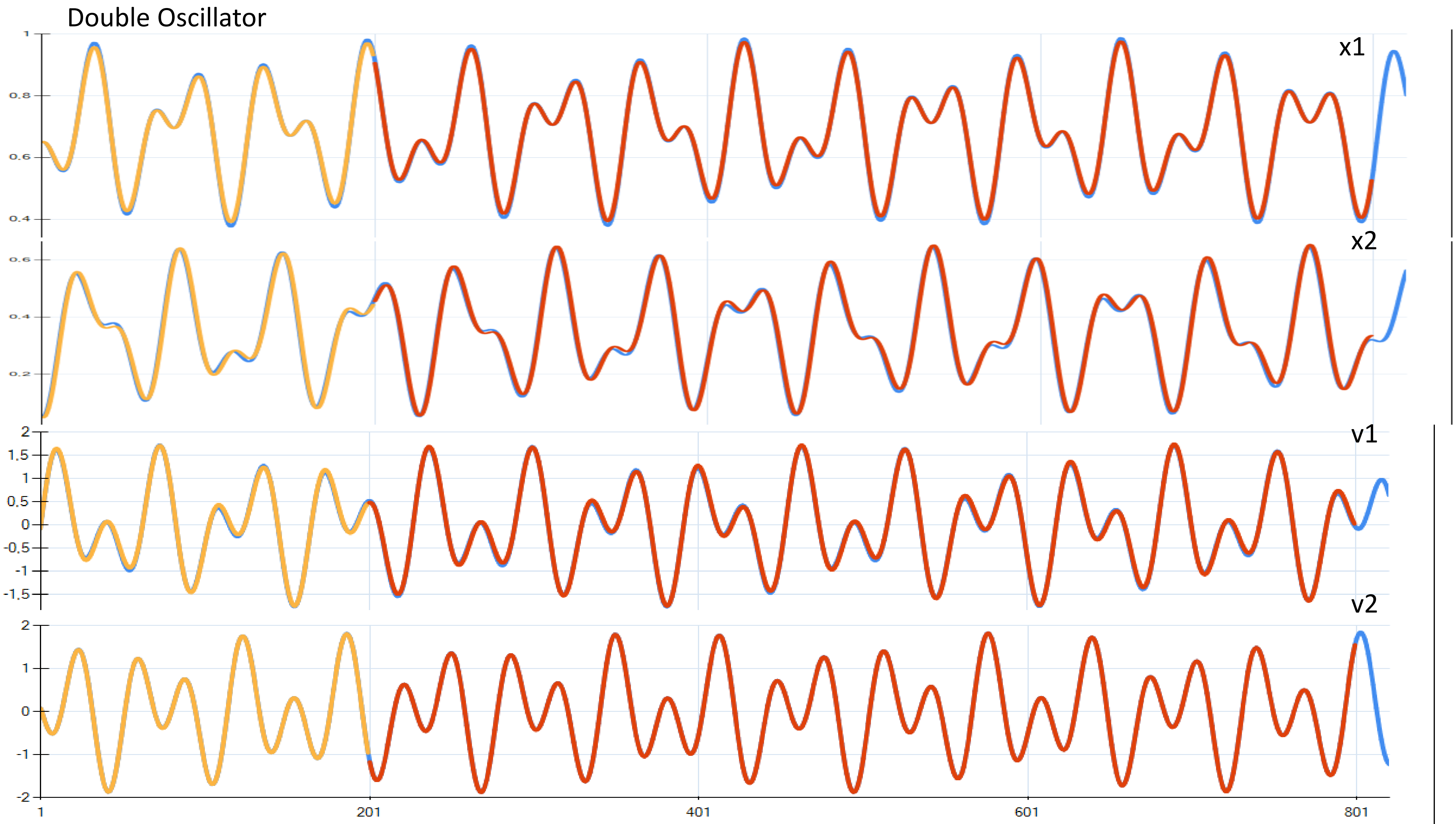

Real Oscillator Predictions
400
200
0
-200
-400
1
201
401
601


x_0
k
m
k

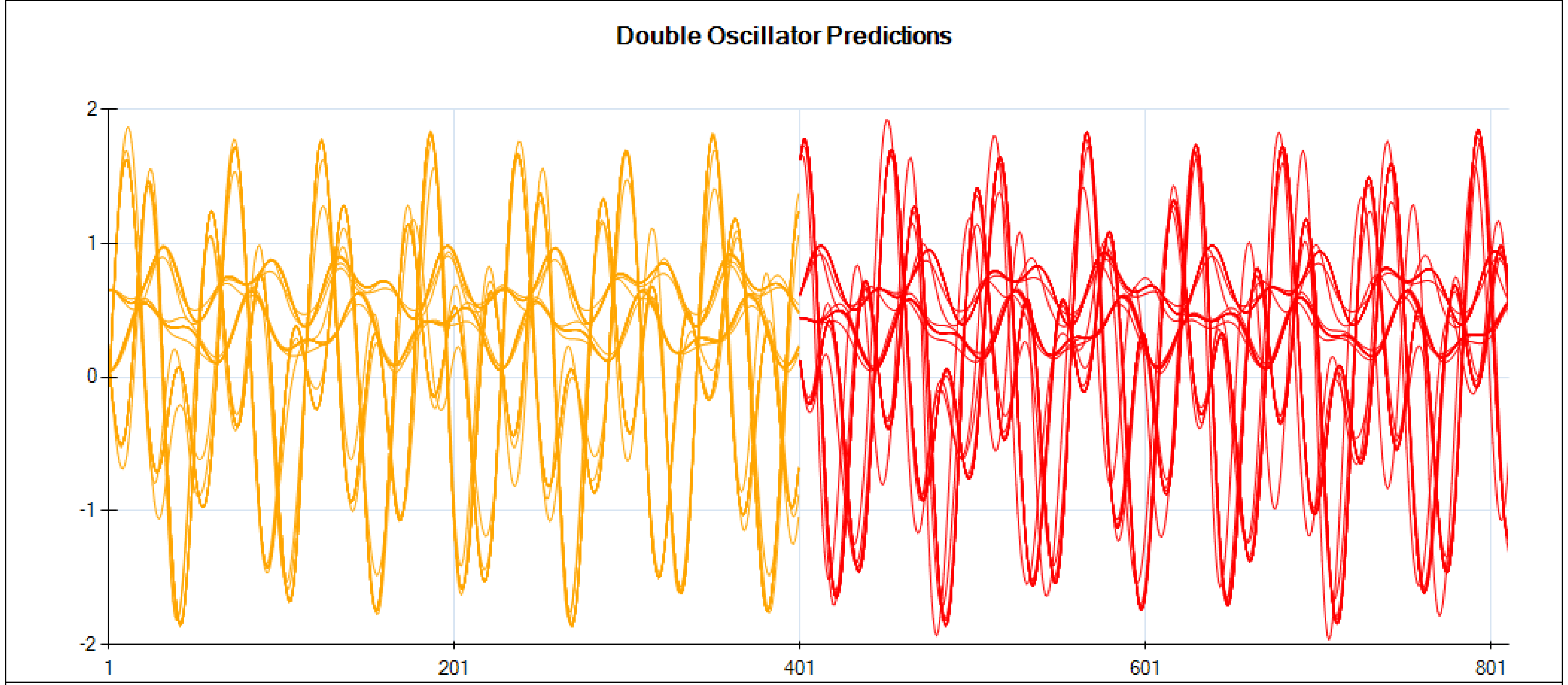

Pendulum Predictions
60
40
20
0
-20
-40
-60
1
101
201
301
401

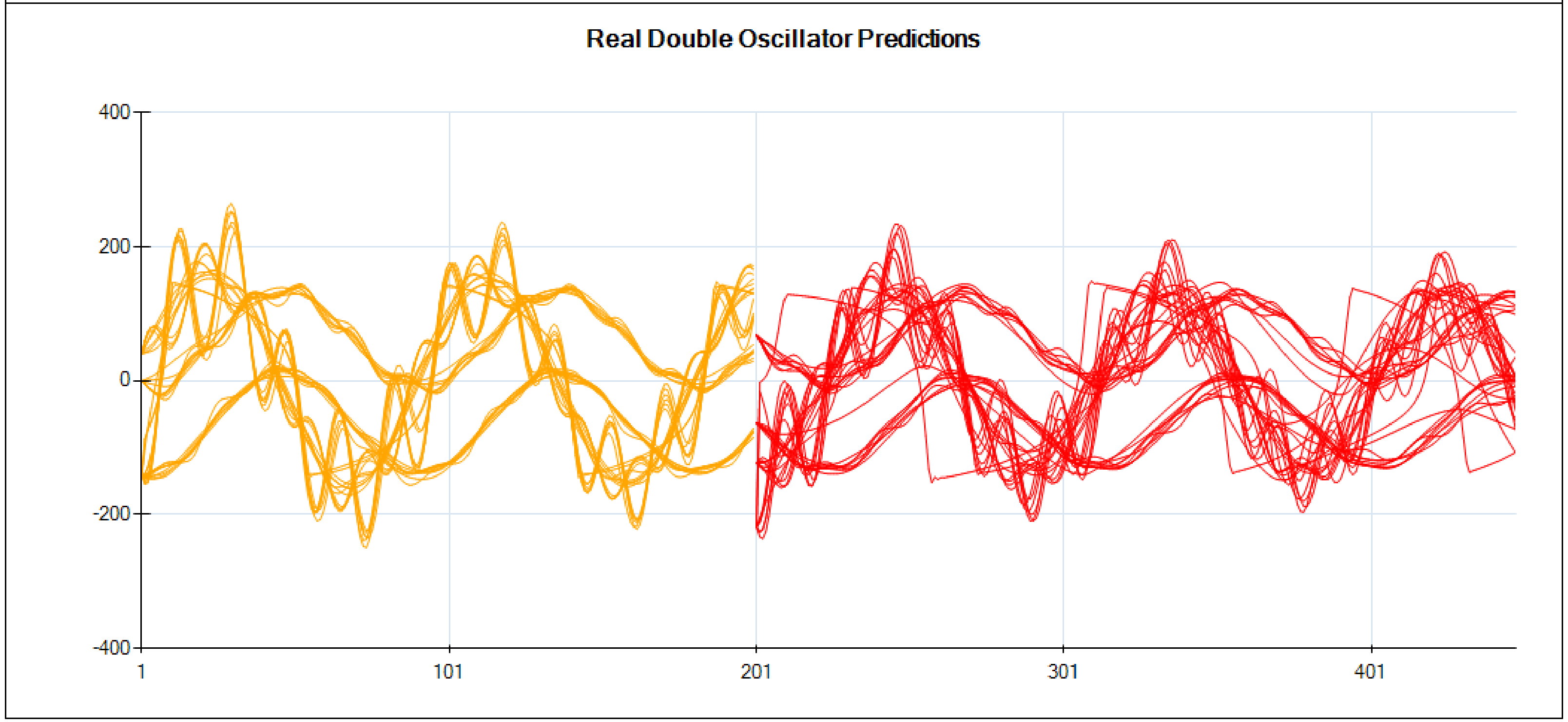

Real Pendulum Predictions
1,5
1
0,5
0
-0,5
-1
-1,5
-2
1
101
201
301
401

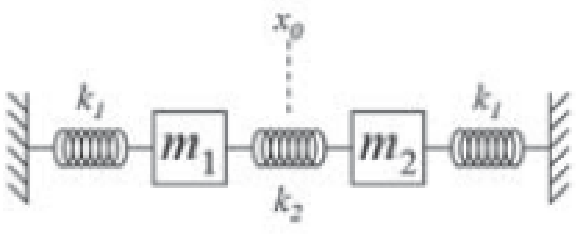

θ
m

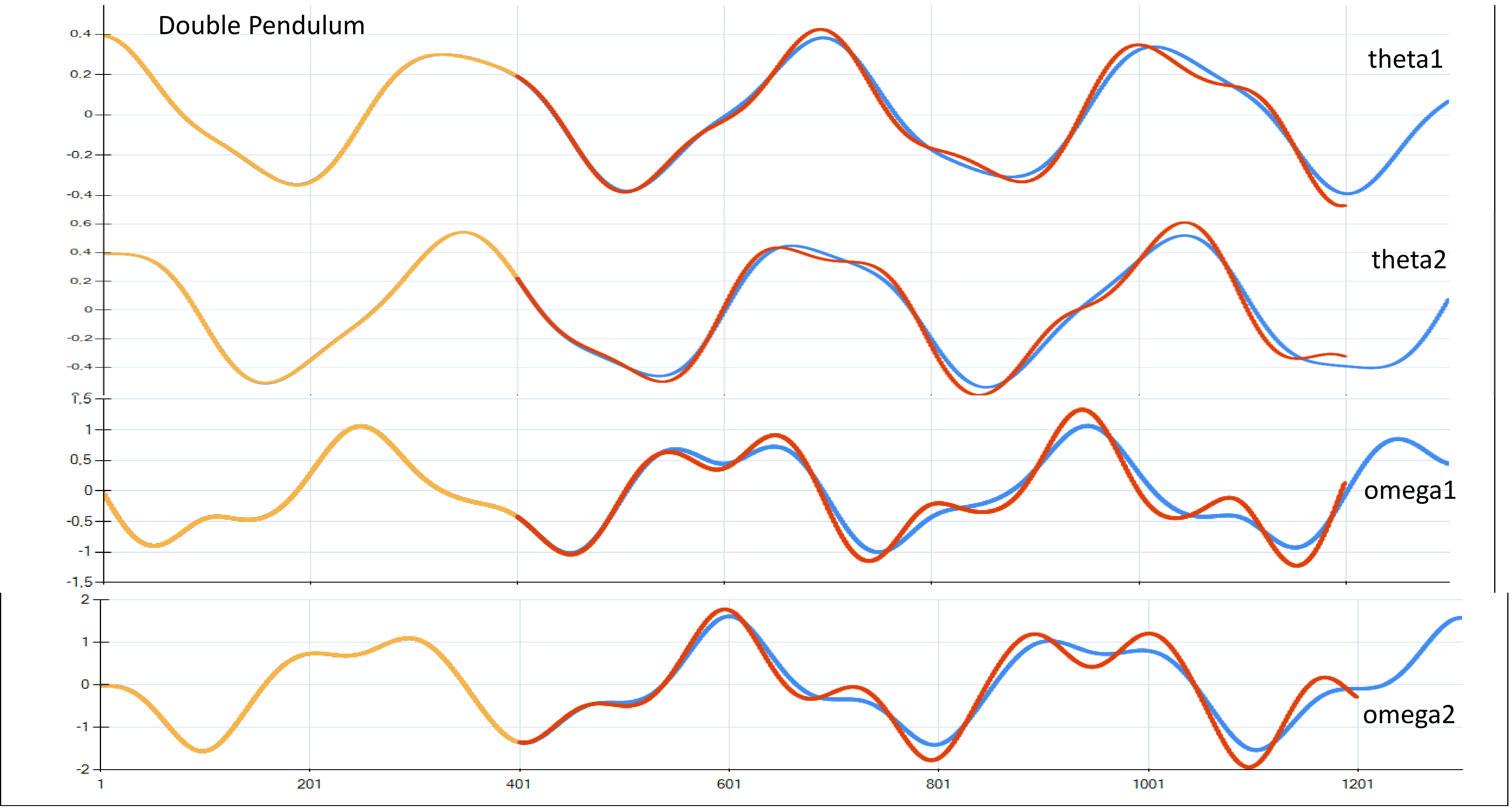


Double Oscillator
x1
x2
v1
v2
1
0.8
0.6
0.4
0.6
0.4
0.2
2
1,5
1
0,5
0
-0,5
-1
-1,5
2
1
0
-1
-2
1
201
401
601
801

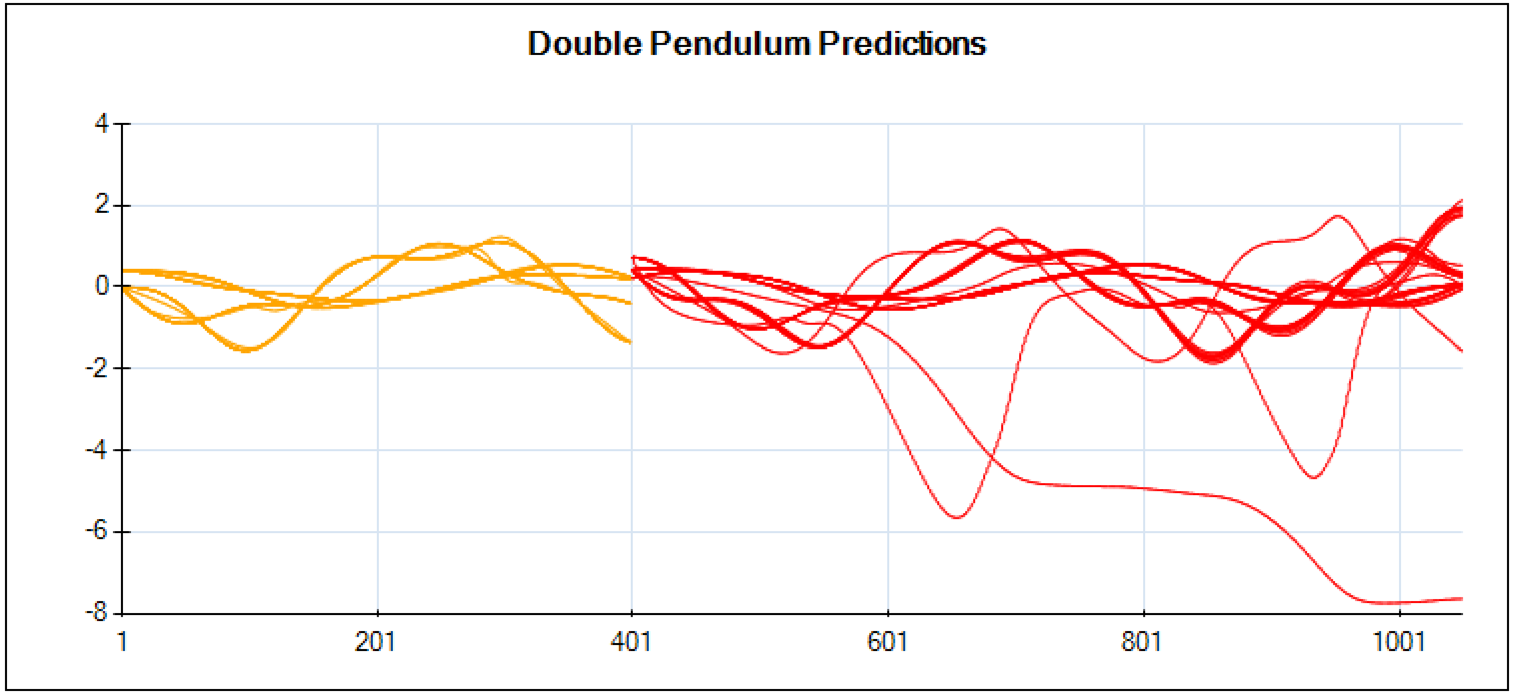

Double Oscillator Predictions
2
1
0
-1
-2
1
201
401
601
801

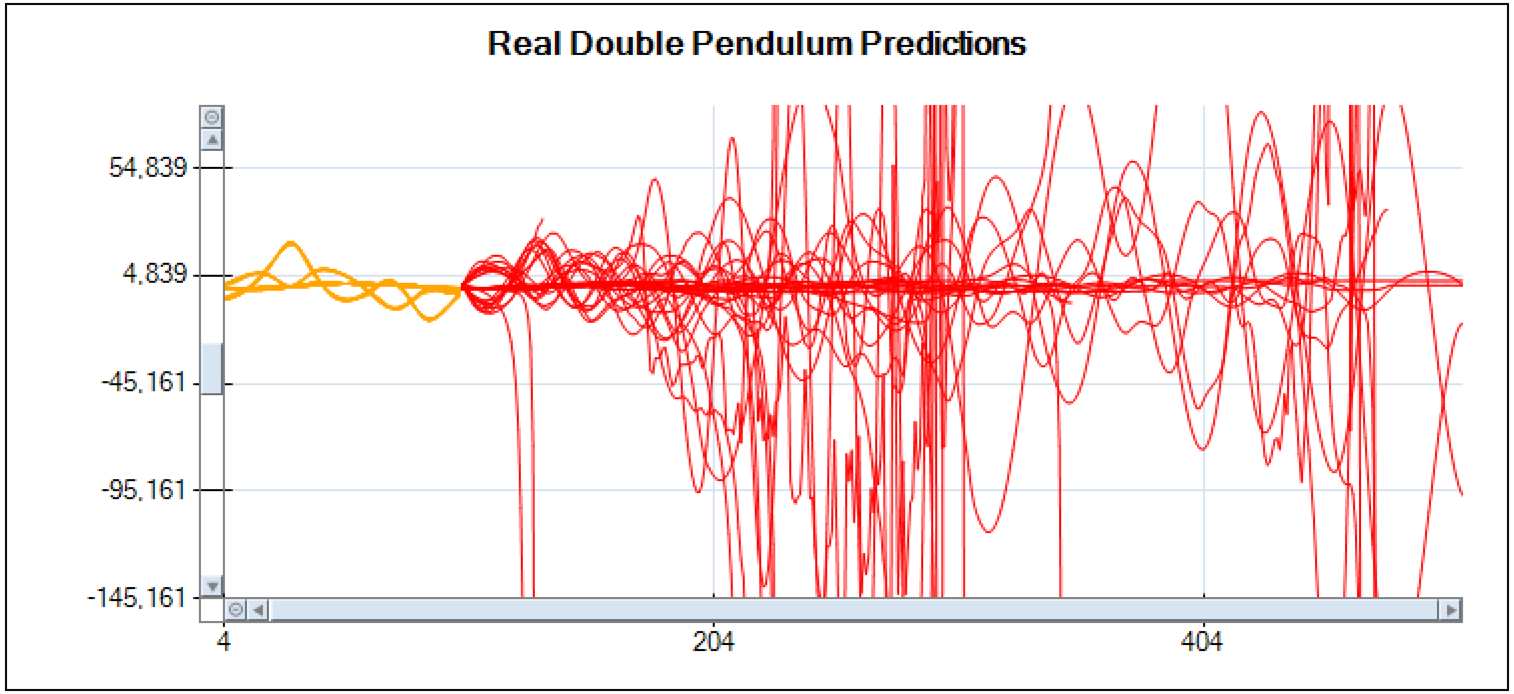

Real Double Oscillator Predictions
400
200
0
-200
-400
1
101
201
301
401

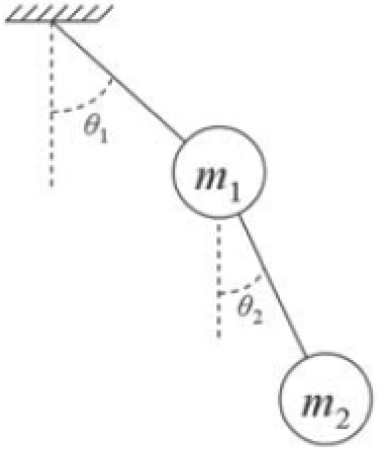

x_0
k_1
m_1
k_2
m_2
k_1

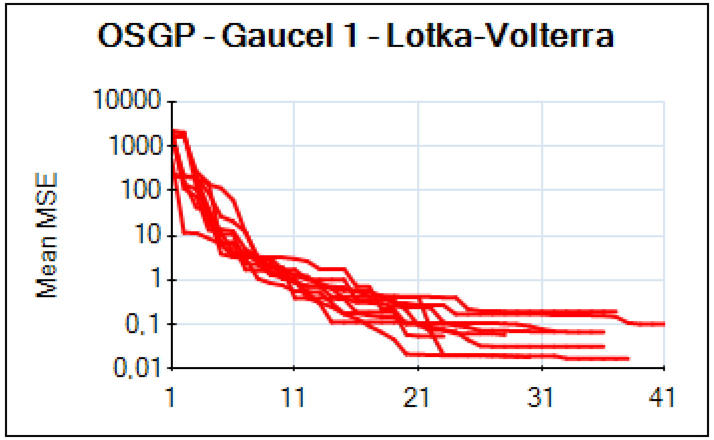


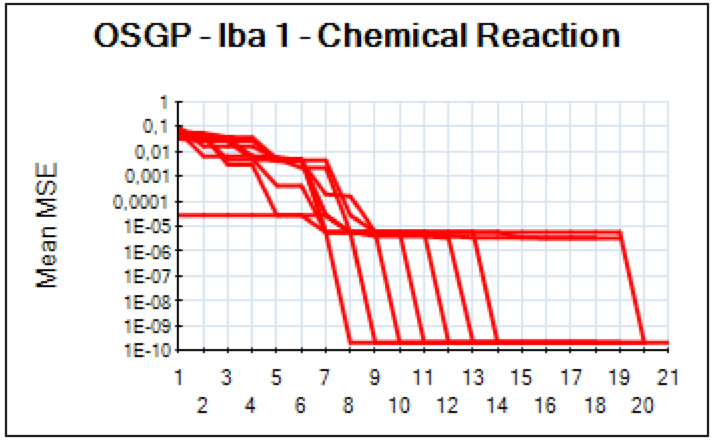
Double Pendulum
theta1
theta2
omega1
omega2
0,4
0,2
0
-0,2
-0,4
0,6
0,4
0,2
0
-0,2
-0,4
1,5
1
0,5
0
-0,5
-1
-1,5
2
1
0
-1
-2
1
201
401
601
801
1001
1201

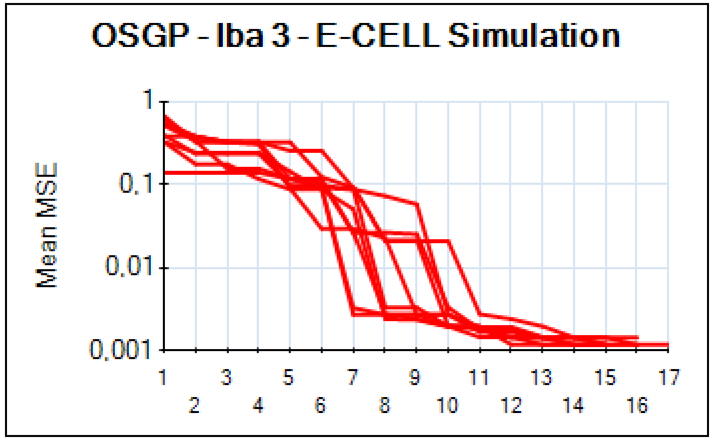

Double Pendulum Predictions
4
2
0
-2
-4
-6
-8
1
201
401
601
801
1001

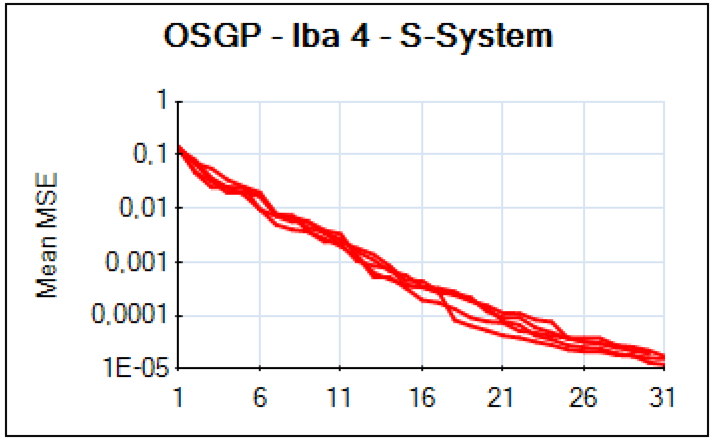

Real Double Pendulum Predictions
54,839
4,839
-45,161
-95,161
-145,161
4
204
404

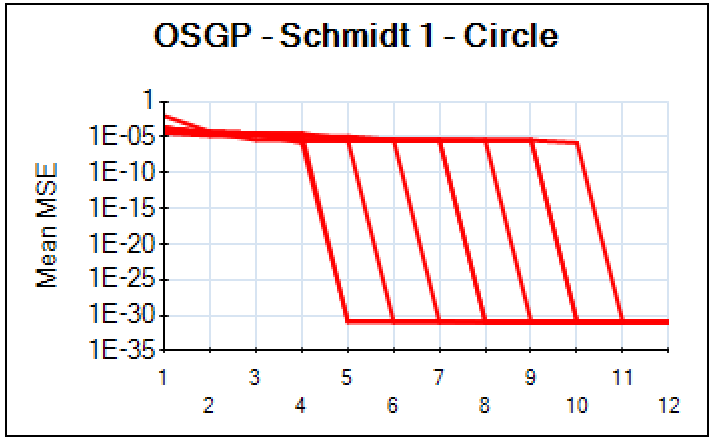

θ_1
m_1
θ_2
m_2

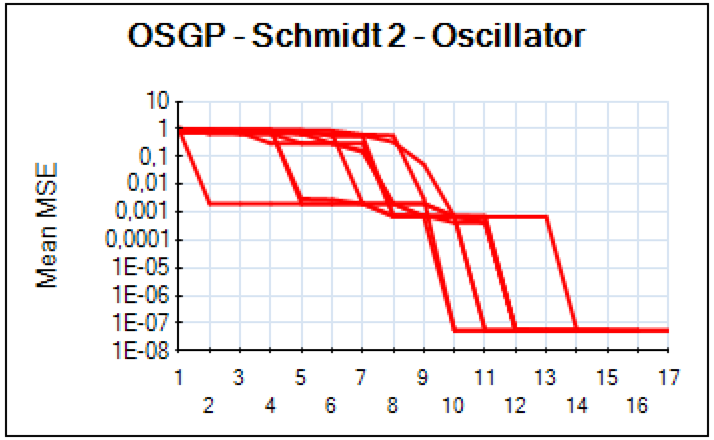

OSGP - Gaucel 1 - Lotka-Volterra
Mean MSE
10000
1000
100
10
1
0,1
0,01
1
11
21
31
41

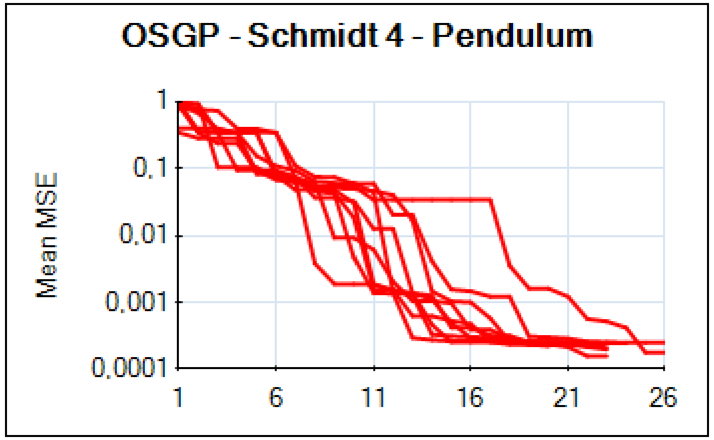

OSGP - Iba 1 - Chemical Reaction
Mean MSE
1
0,1
0,01
0,001
0,0001
1E-05
1E-06
1E-07
1E-08
1E-09
1E-10
1 3 5 7 9 11 13 15 17 19 21
2 4 6 8 10 12 14 16 18 20

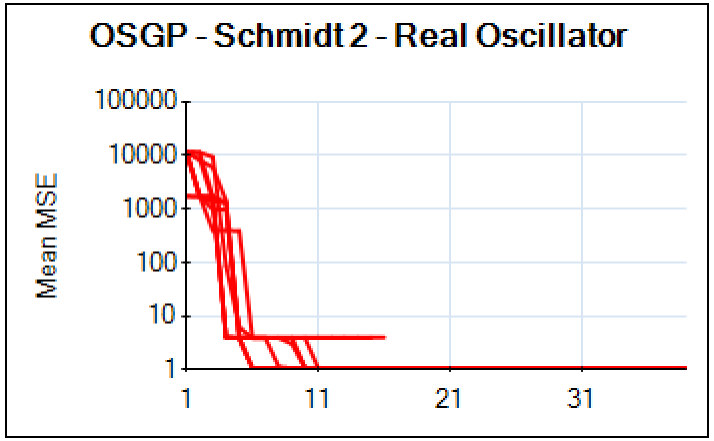

OSGP - Iba 3 - E-CELL Simulation
Mean MSE
1
0,1
0,01
0,001
1 3 5 7 9 11 13 15 17
2 4 6 8 10 12 14 16

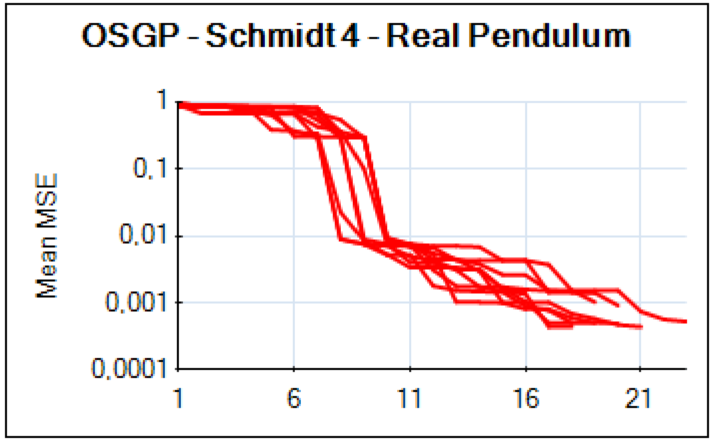

OSGP - Iba 4 - S-System
Mean MSE
1
0,1
0,01
0,001
0,0001
1E-05
1
6
11
16
21
26
31

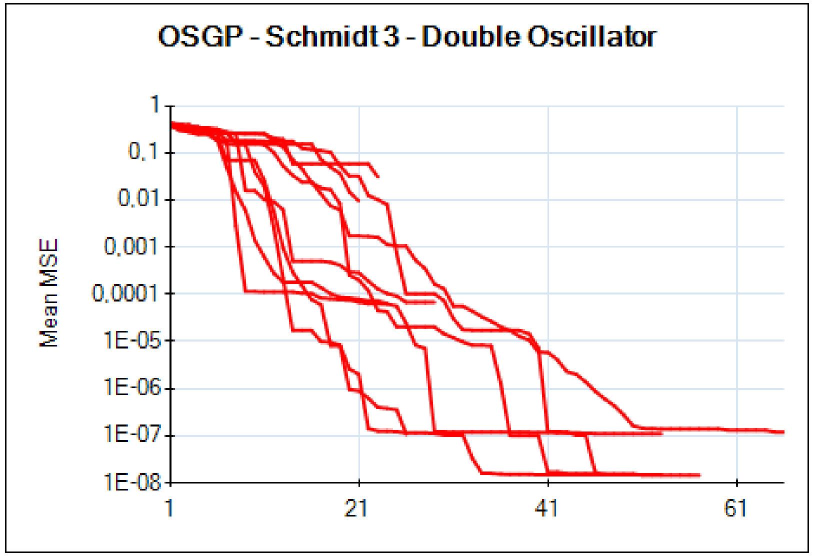

OSGP - Schmidt 1 - Circle
Mean MSE
1
1E-05
1E-10
1E-15
1E-20
1E-25
1E-30
1E-35
1 2 3 4 5 6 7 8 9 10 11 12

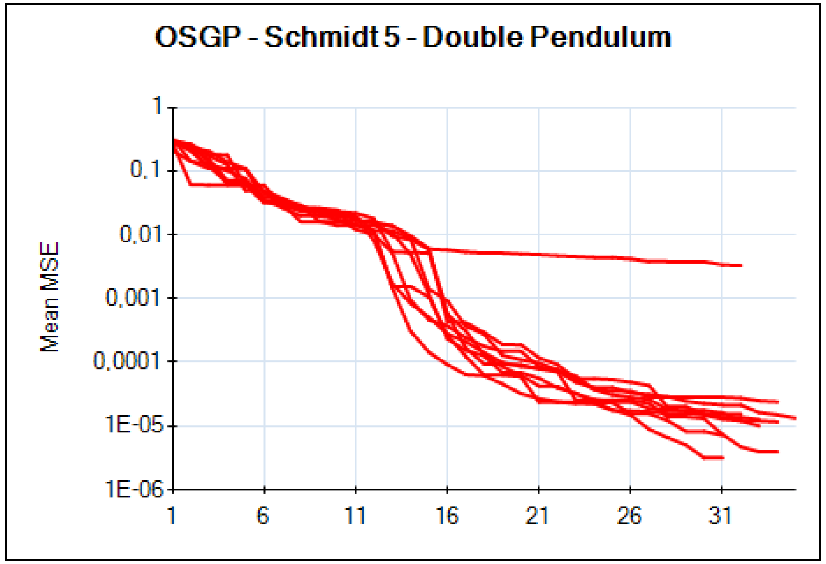

OSGP - Schmidt 2 - Oscillator
Mean MSE
10
1
0,1
0,01
0,001
0,0001
1E-05
1E-06
1E-07
1E-08
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

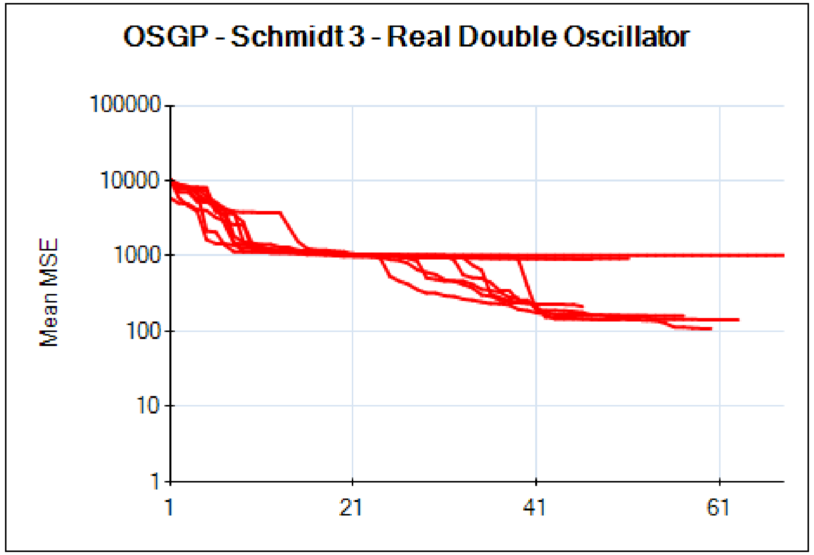

OSGP - Schmidt 4 - Pendulum
Mean MSE
1
0,1
0,01
0,001
0,0001
1 6 11 16 21 26

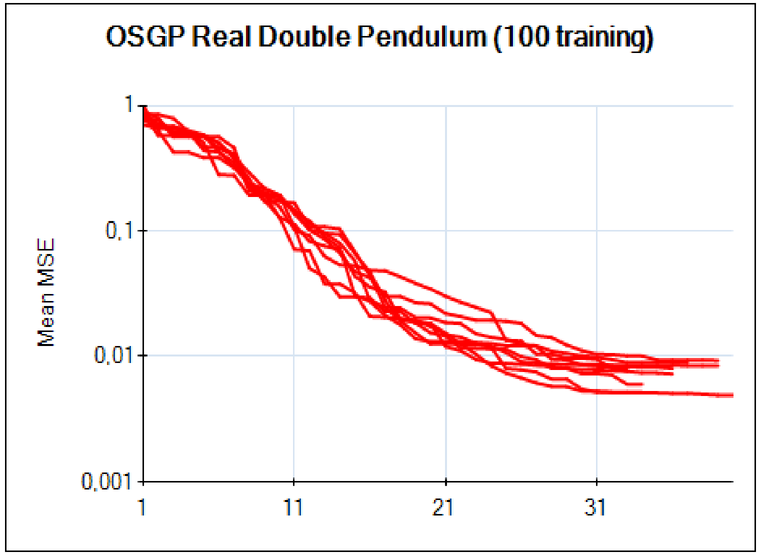

OSGP - Schmidt 2 - Real Oscillator
Mean MSE
100000
10000
1000
100
10
1
1 11 21 31

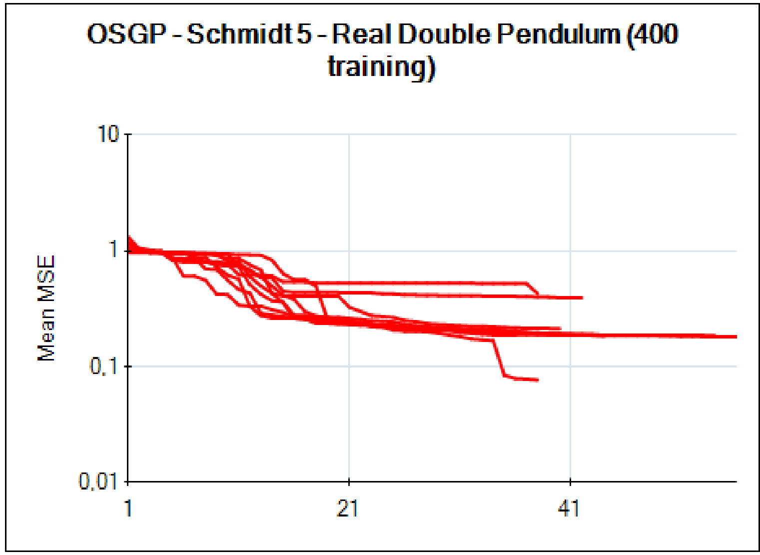

OSGP - Schmidt 4 - Real Pendulum
Mean MSE
1
0,1
0,01
0,001
0,0001
1 6 11 16 21


OSGP - Schmidt 3 - Double Oscillator
Mean MSE
1
0,1
0,01
0,001
0,0001
1E-05
1E-06
1E-07
1E-08
1
21
41
61


OSGP - Schmidt 5 - Double Pendulum
Mean MSE
1
0,1
0,01
0,001
0,0001
1E-05
1E-06
1
6
11
16
21
26
31


OSGP - Schmidt 3 - Real Double Oscillator
Mean MSE
100000
10000
1000
100
10
1
1
21
41
61


OSGP Real Double Pendulum (100 training)
Mean MSE
1
0,1
0,01
0,001
1
11
21
31


OSGP - Schmidt 5 - Real Double Pendulum (400 training)
Mean MSE
10
1
0,1
0,01
1
21
41

Identification of Dynamical Systems using Symbolic Regression

Gabriel Kronberger, Lukas Kammerer, Michael Kommenda

EuroCAST 2019

SymReg
JOSEF RESSEL CENTER FOR
SYMBOLIC REGRESSION