Title: The Robotic Scientist: Mining experimental data for scientific laws, from cognitive robotics to computational biology

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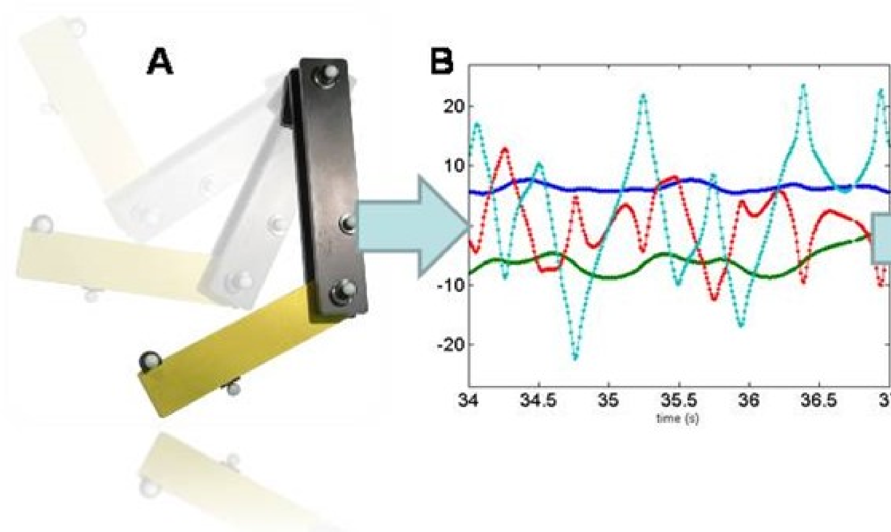
URL: http://pirsa.org/09020048

Abstract: For centuries, scientists have attempted to identify analytical laws that underlie physical phenomena in nature. Despite todayâ€™s computing power, the process of finding natural laws and their corresponding equations has resisted automation. A key challenge to finding analytic relations automatically â€“ that is, building an autonomous robot - is defining algorithmically what makes a correlation in observed data important and insightful. Scientists are gradually uncovering an â€˜alphabetâ€™ that can be used to describe the simplest to most complex physical systems â€“ and by seeking dynamical invariants, researchers go from finding simple predictive models to discovering deeper natural laws. Dr. Lipson will demonstrate the process on a variety of mechanical, biological, and robotic systems.

The robotic Scientist

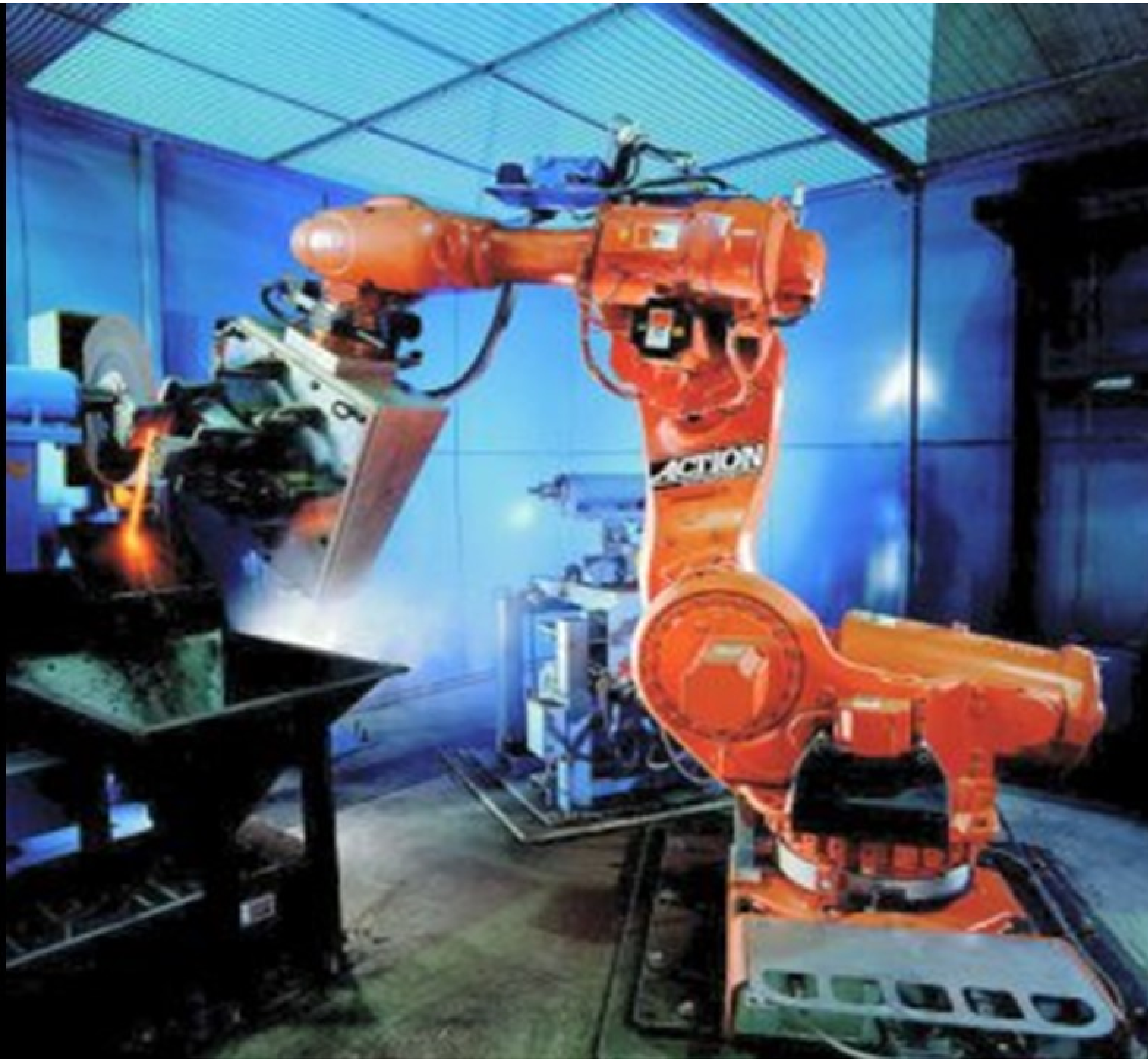
Hod Lipson, Cornell University

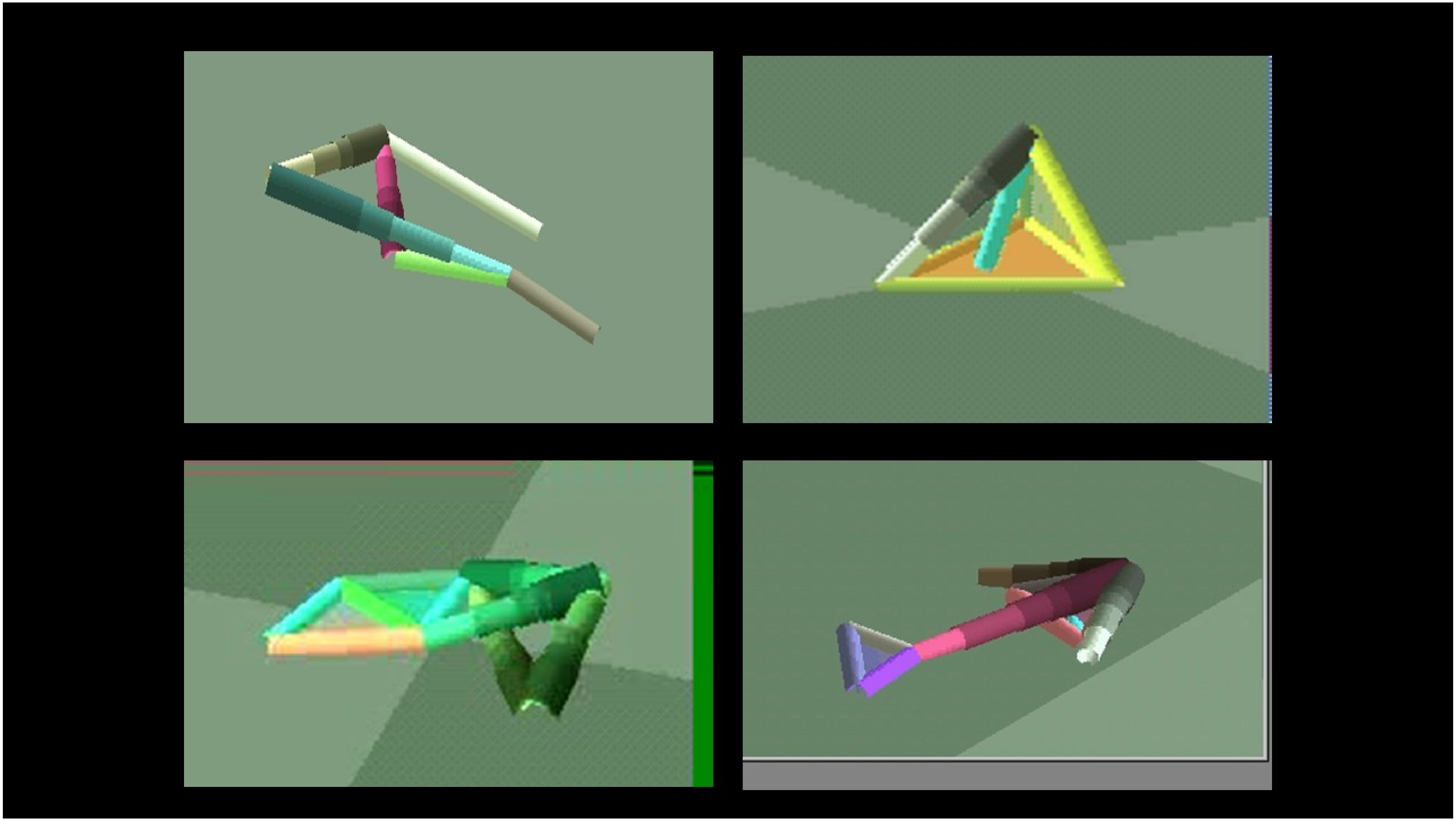


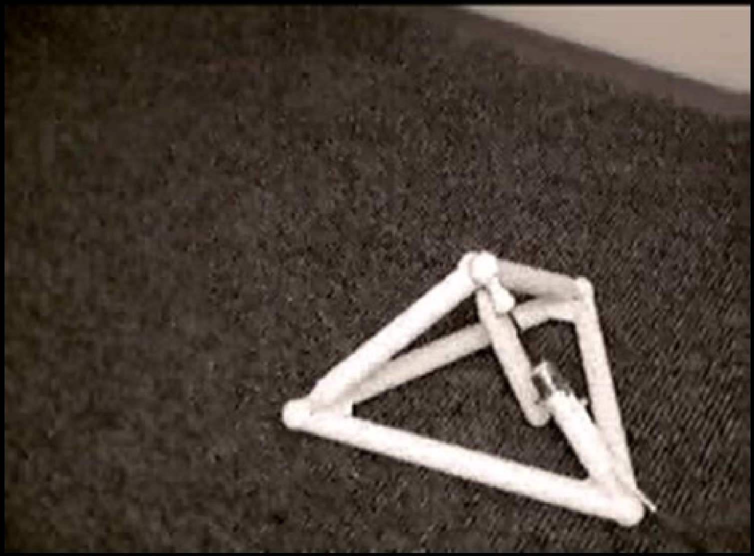
C

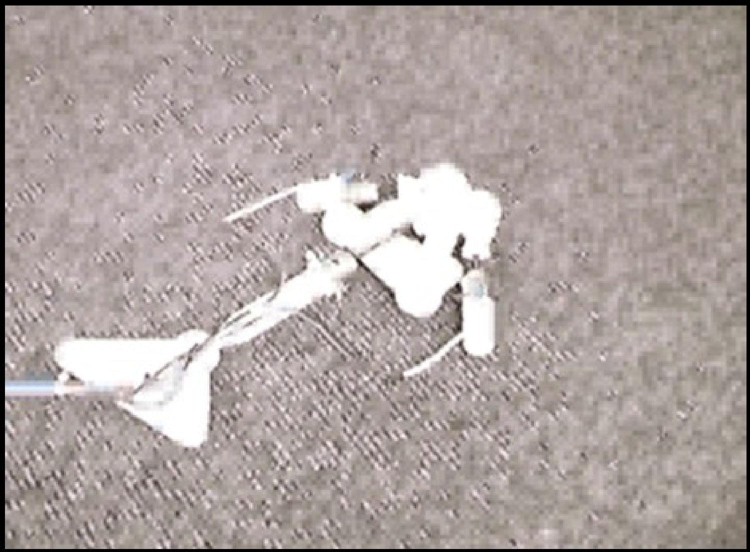
Detected Invariance:

$$L_1^{\,2}(m_1+m_2)\boldsymbol{\omega_1}^2 + m_2L_2^{\,2}\boldsymbol{\omega_2}^2 + m_2L_1L_2\boldsymbol{\omega_1}\boldsymbol{\omega_2}\cos(\boldsymbol{\theta_1}-\boldsymbol{\theta_2}) - 19.6L_1(m_1+m_2)\cos\boldsymbol{\theta_1} - 19.6m_2L_2\cos\boldsymbol{\theta_2}$$

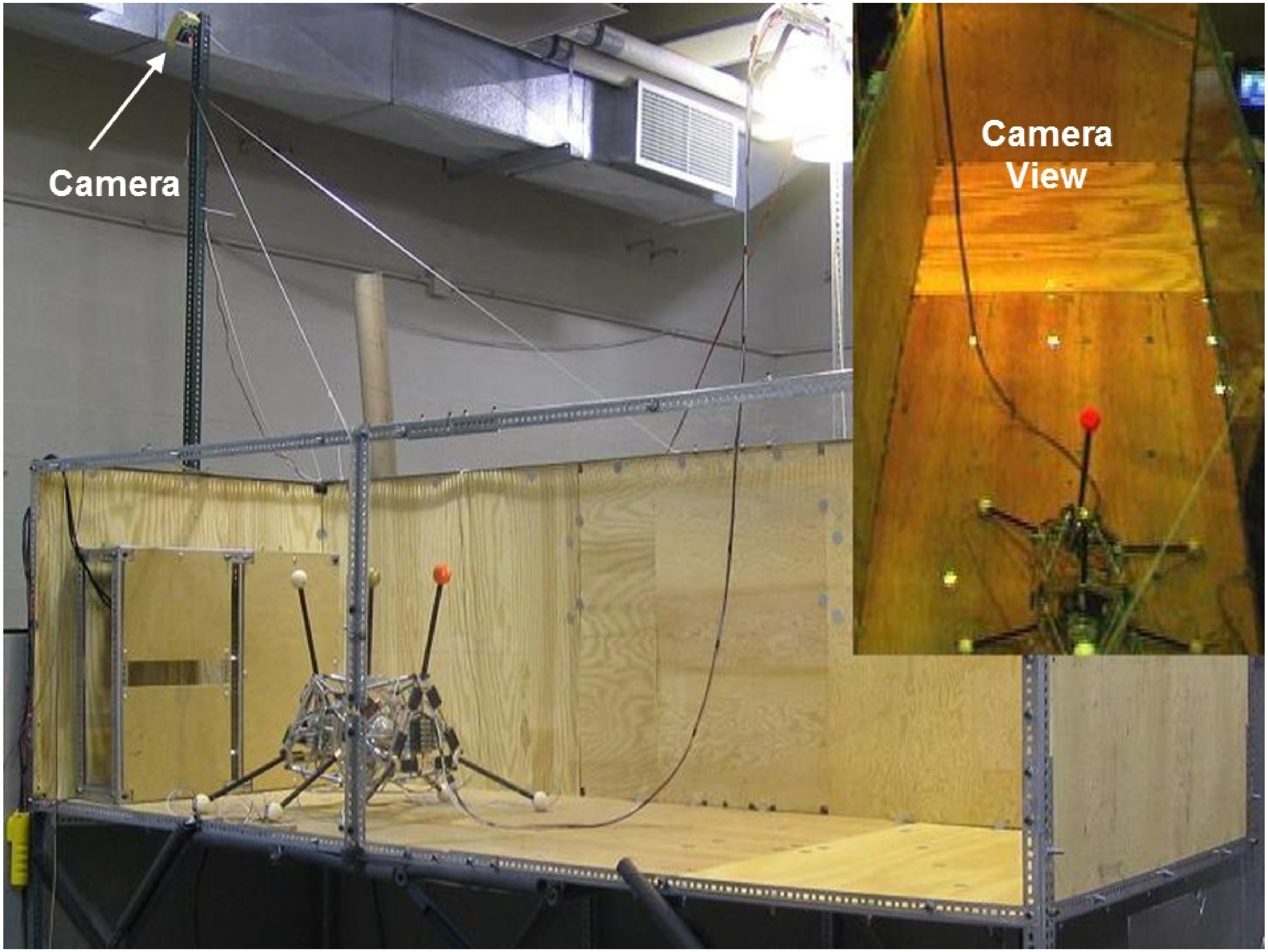

ACTION

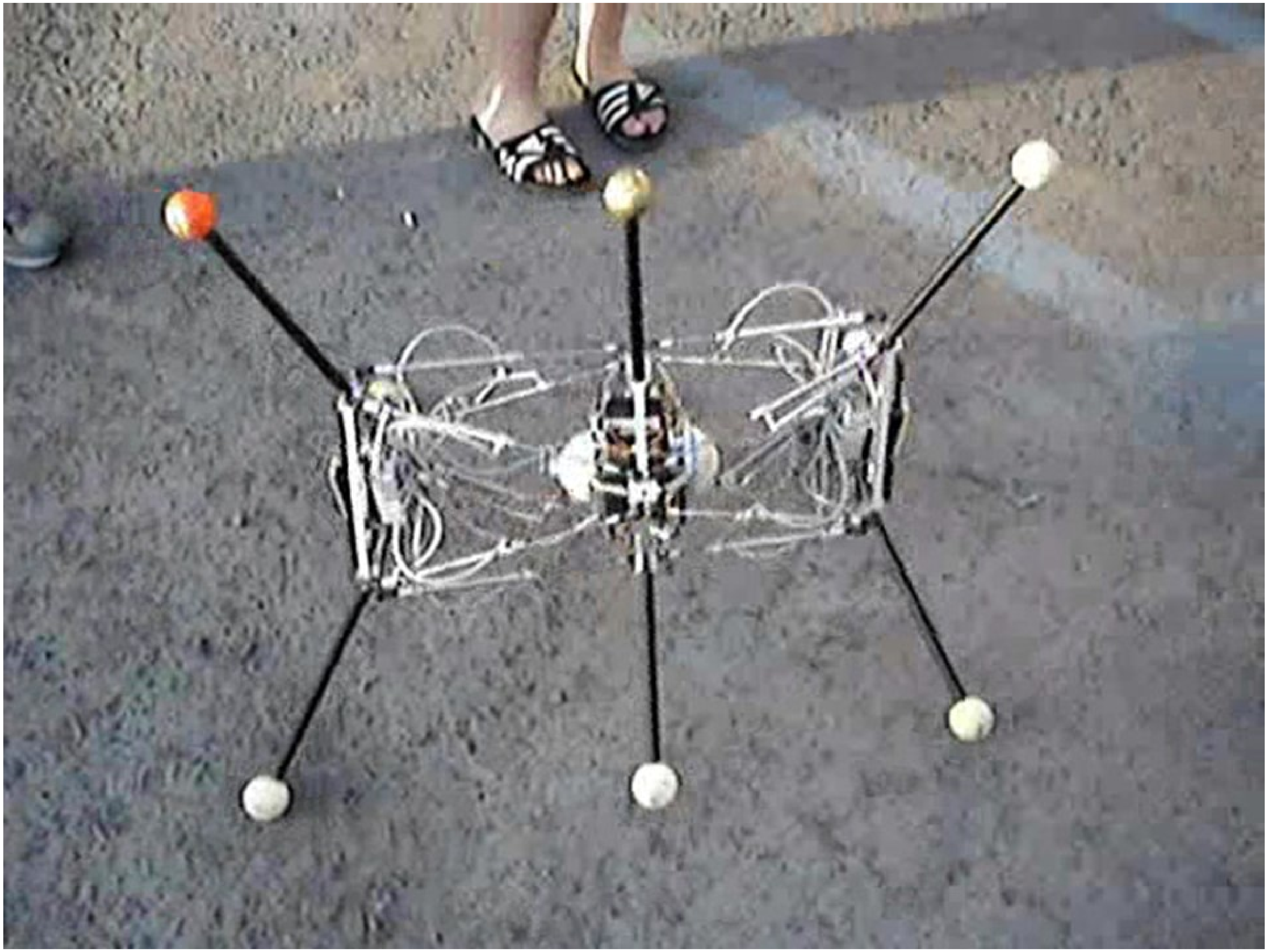




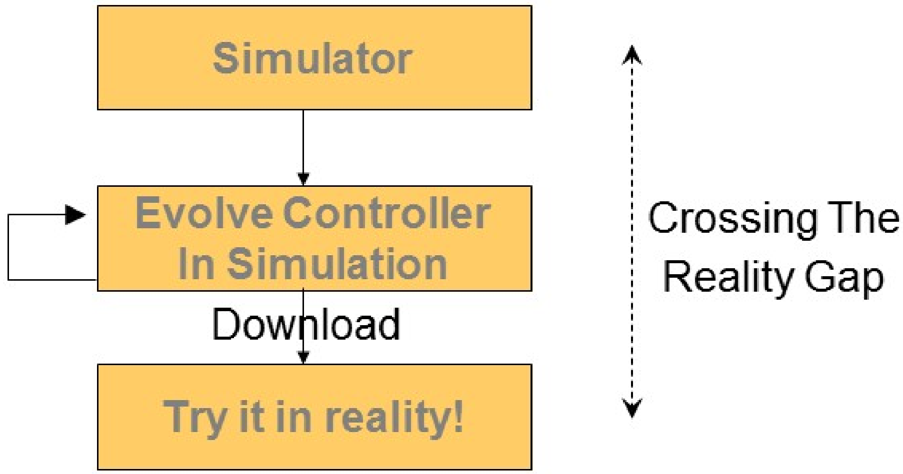


Lipson & Pollack, Nature 406, 2000


Camera
Camera
View

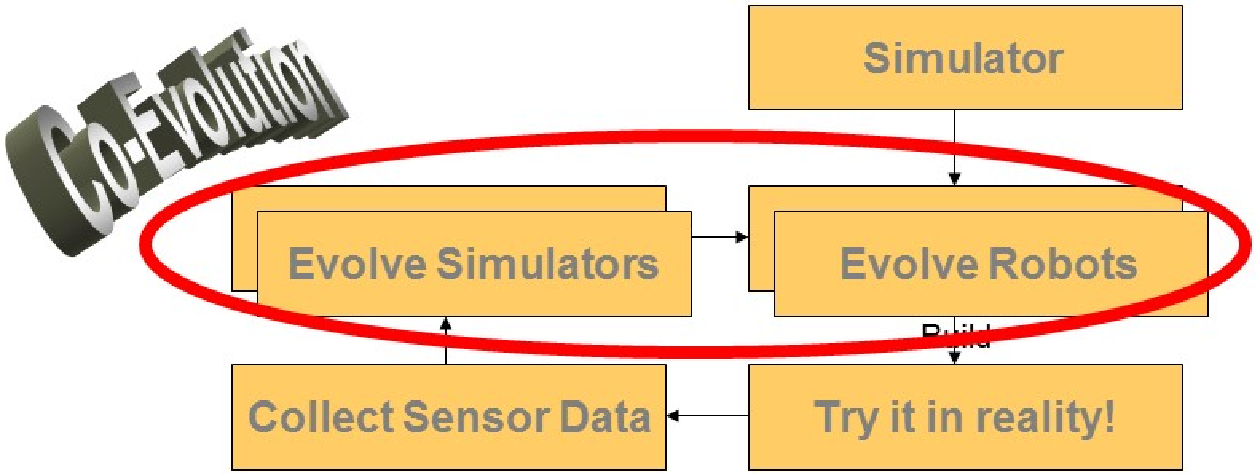


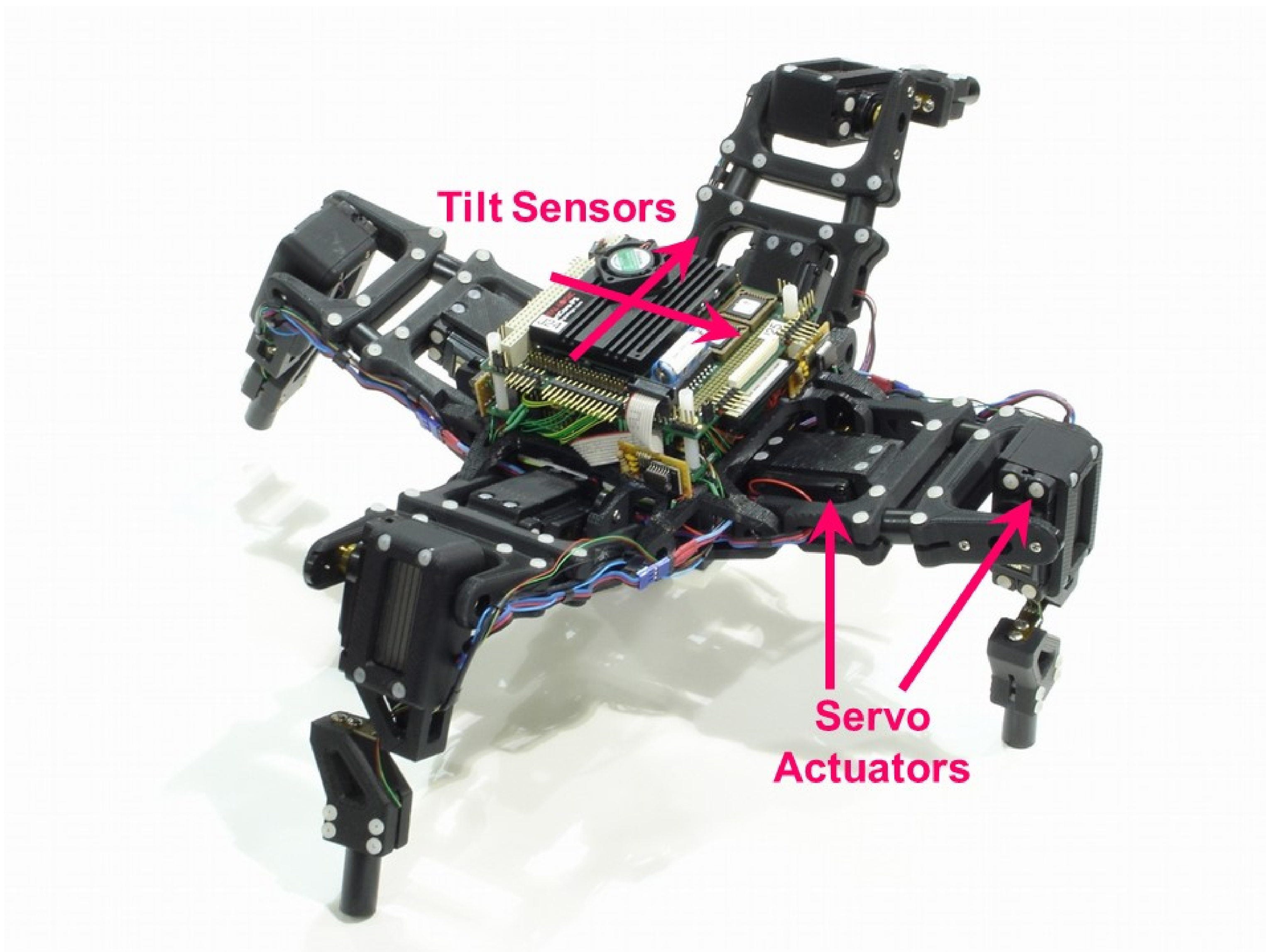
Adapting in simulation

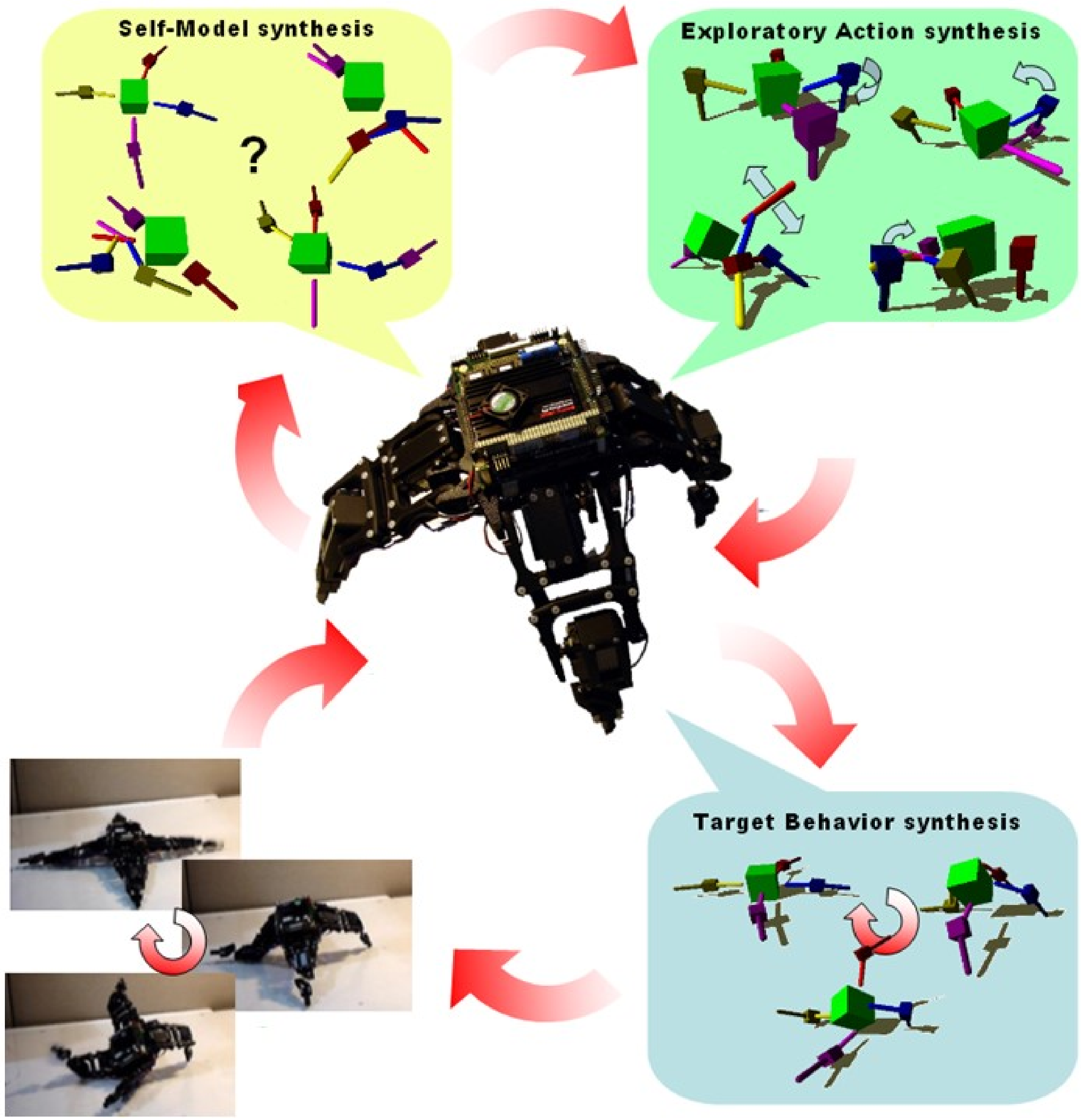


Adapting in reality

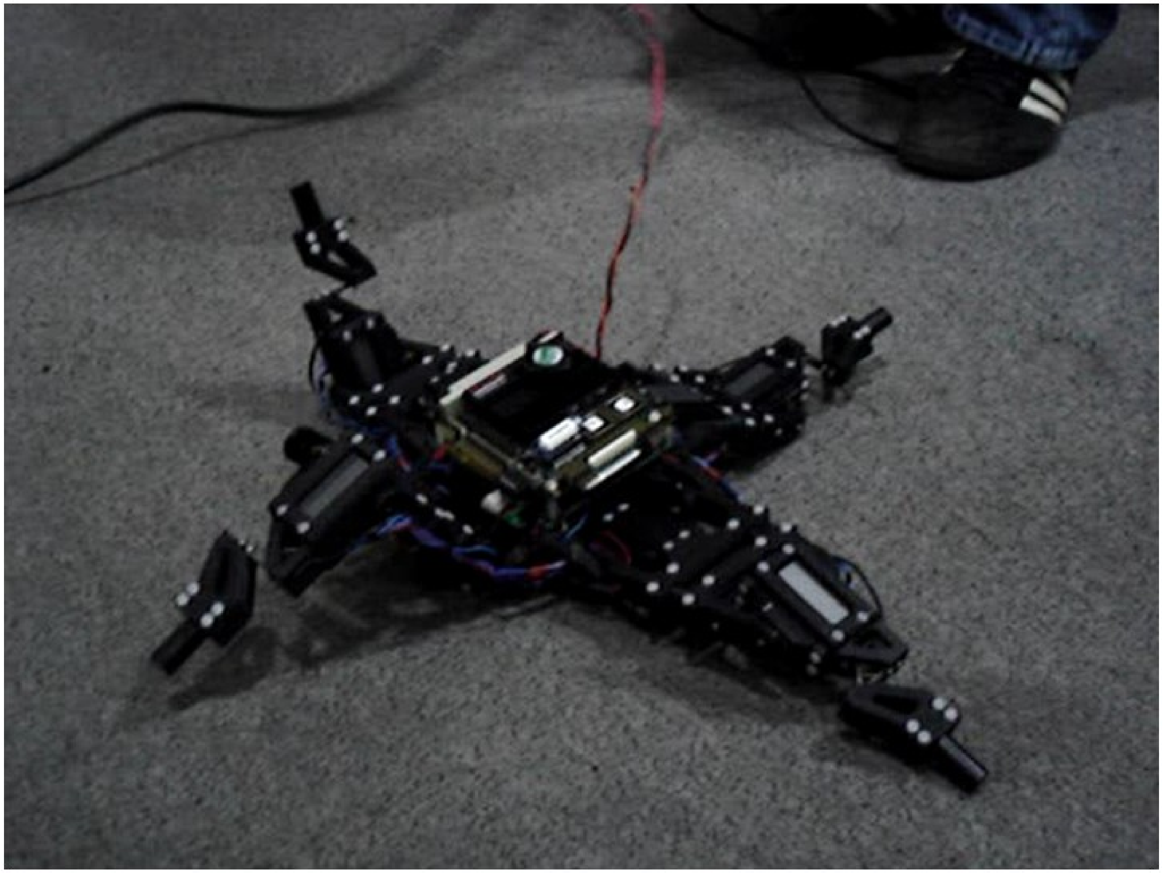
Simulation & Reality



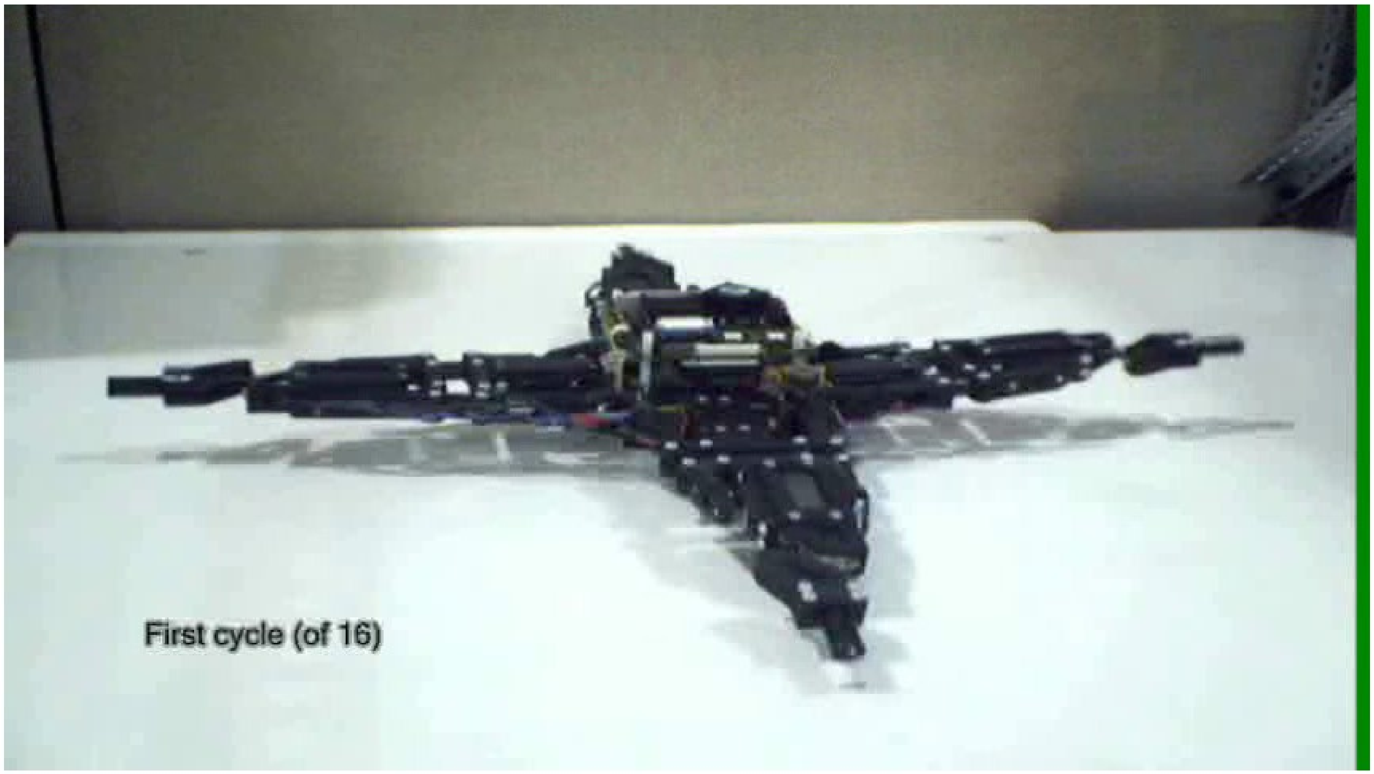

Tilt Sensors
Servo
Actuators


Self-Model synthesis
?
Exploratory Action synthesis
Target Behavior synthesis

Morphological Estimation

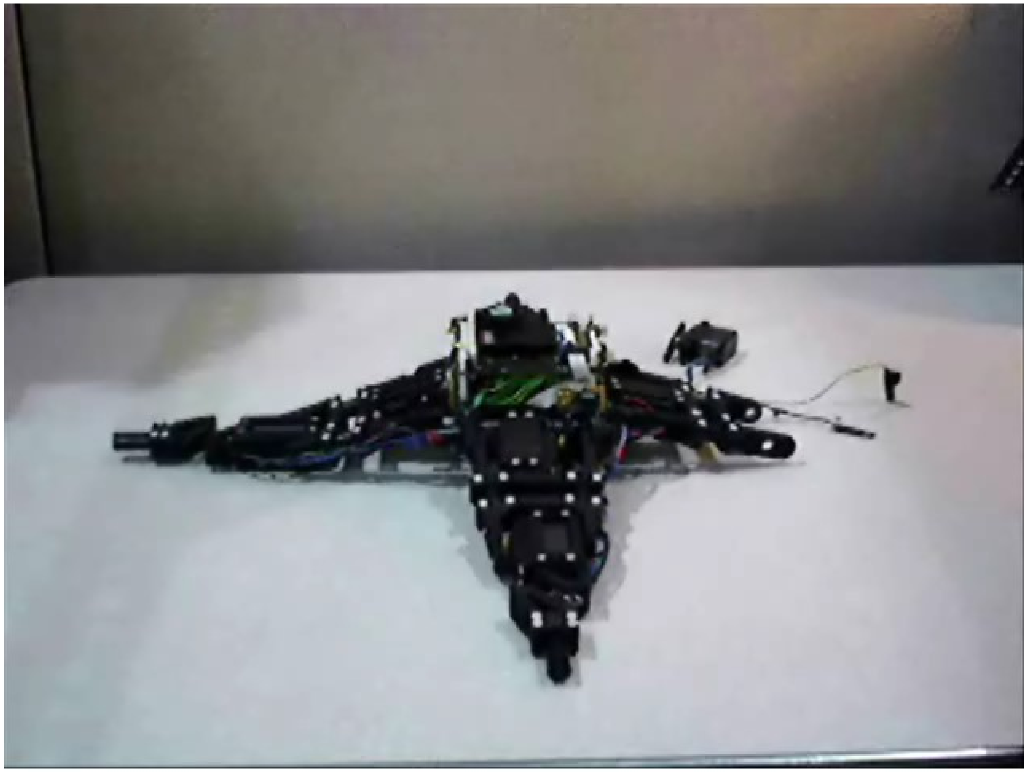


Emergent Self-Model

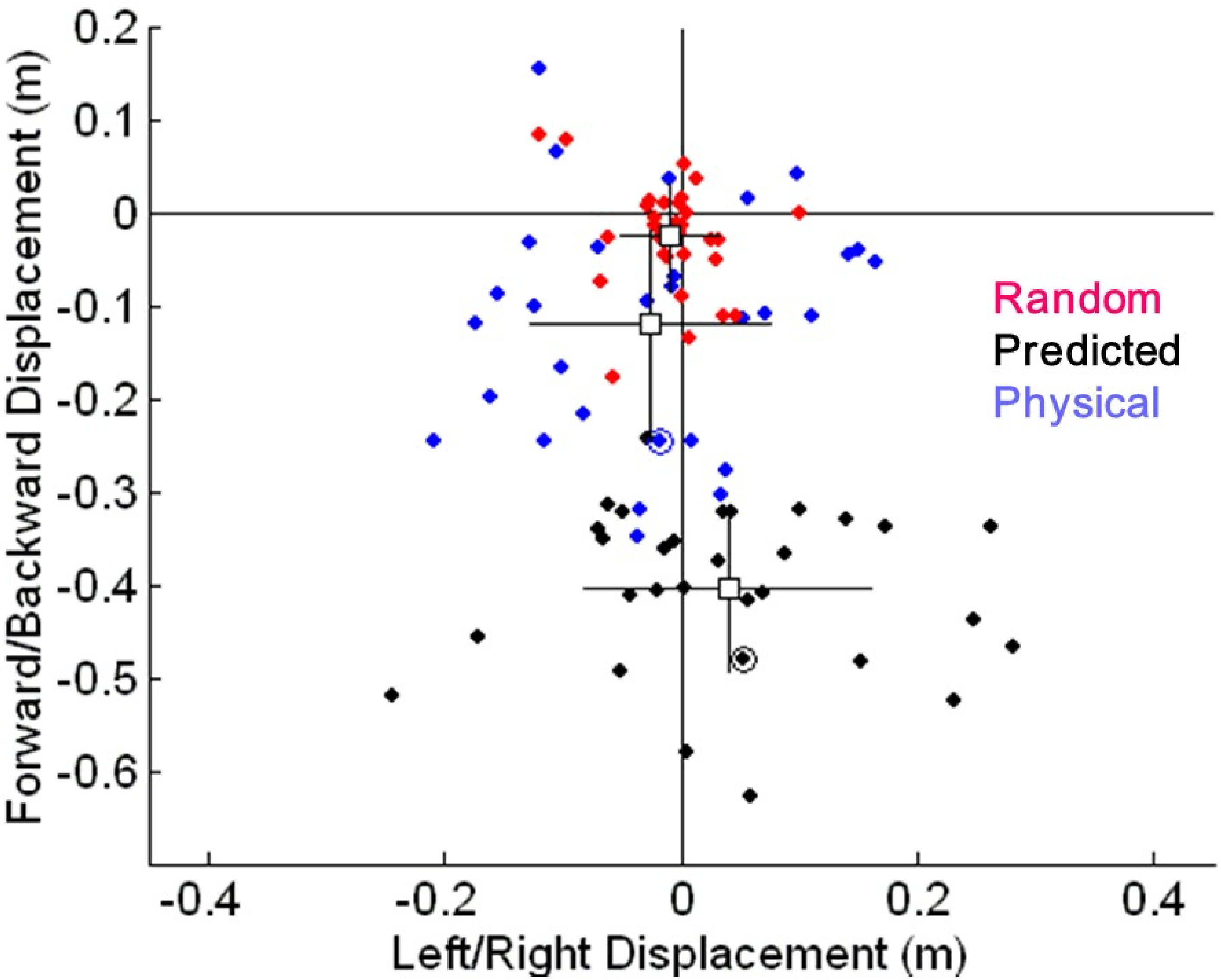


With Josh Bongard and Victor Zykov, Science 2006

Damage Recovery

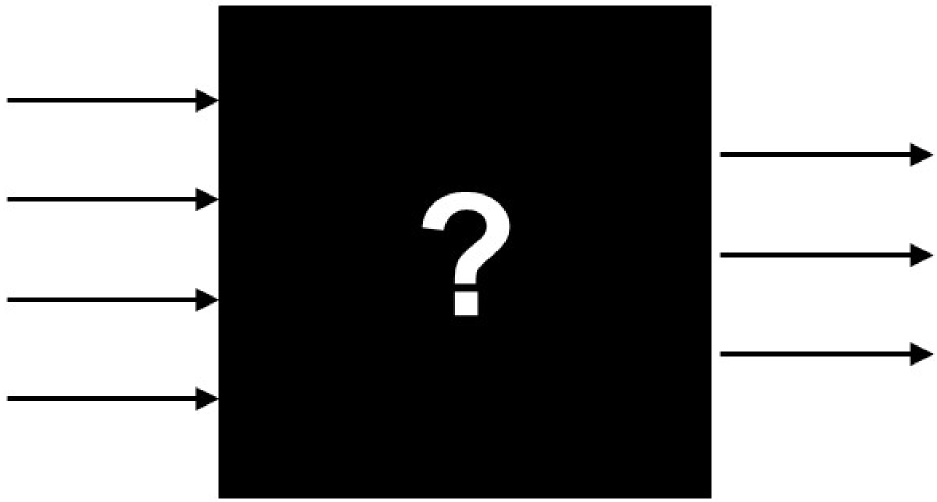


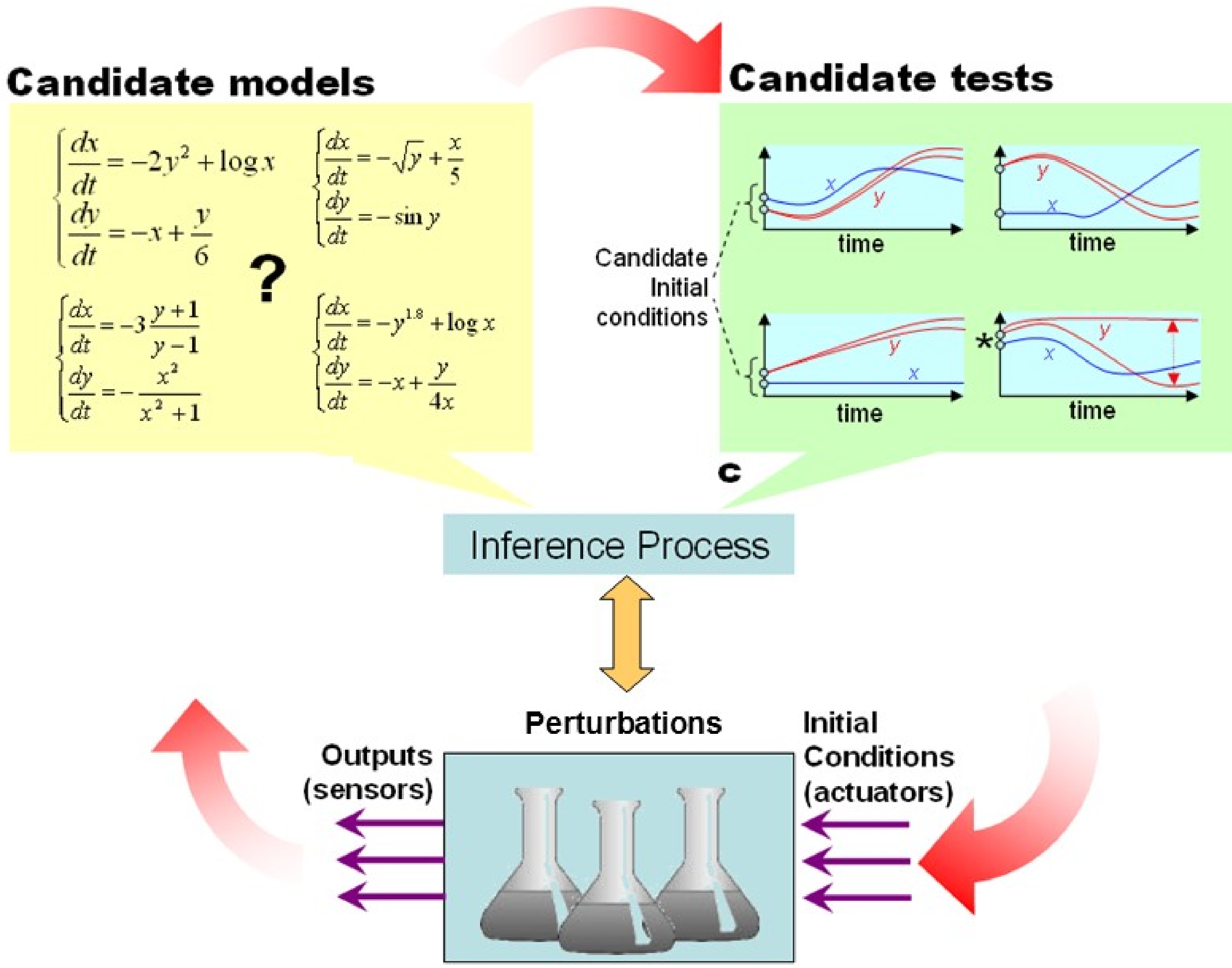
With Josh Bongard and Victor Zykov, Science 2006



0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
Forward/Backward Displacement (m)
-0.4
-0.2
0
0.2
0.4
Left/Right Displacement (m)
Random
Predicted
Physical

System Identification



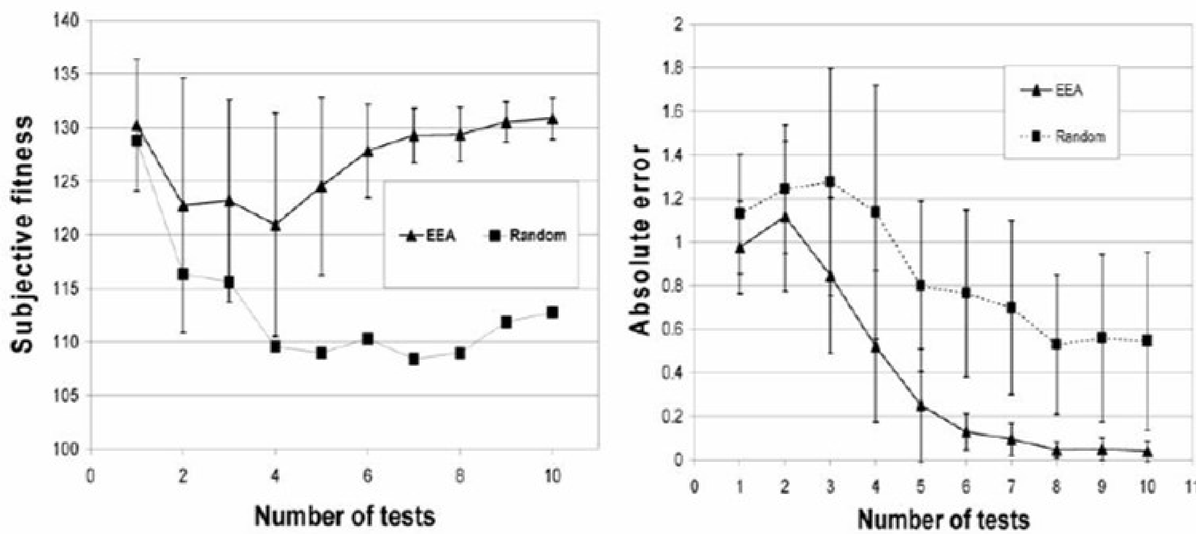


Candidate models
$\frac{dx}{dt} = -2y^2 + \log x$
$\frac{dy}{dt} = -x + \frac{y}{6}$
$\frac{dx}{dt} = -\sqrt{y} + \frac{x}{5}$
$\frac{dy}{dt} = -\sin y$
?
$\frac{dx}{dt} = -3\frac{y+1}{y-1}$
$\frac{dy}{dt} = -\frac{x^2}{x^2+1}$
$\frac{dx}{dt} = -y^{1.8} + \log x$
$\frac{dy}{dt} = -x + \frac{y}{4x}$
Candidate tests
Candidate Initial conditions
x
y
time
c
Inference Process
Perturbations
Outputs (sensors)
Initial Conditions (actuators)


Photo: Floris van Breugel


Photo: Floris van Breugel

Static ID: Damage Diagnosis

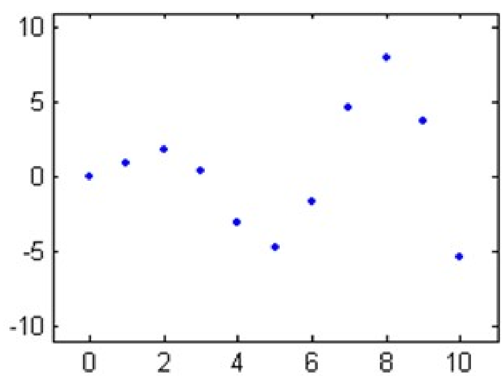


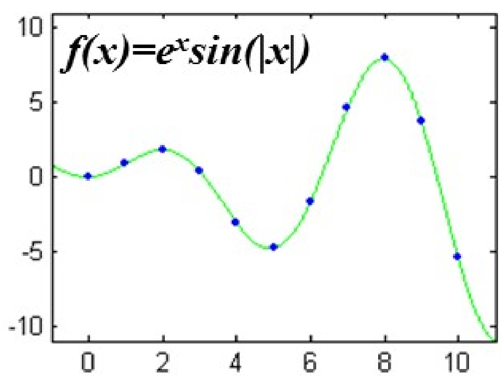
(a) (b)

With Wilkins Aquino

Symbolic Regression

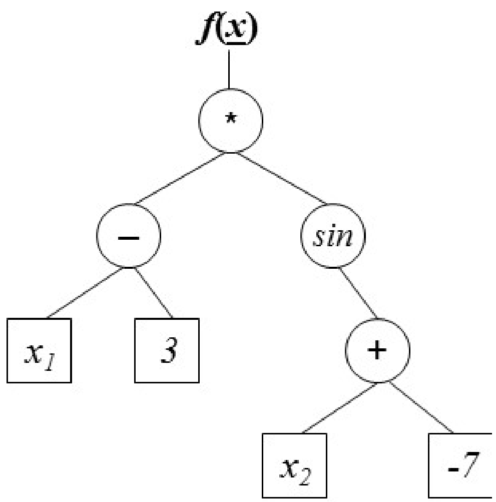
What function describes this data?

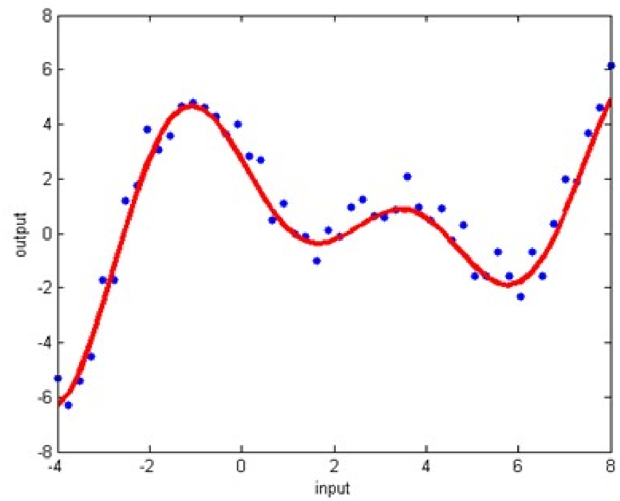




Encoding Equations

Building Blocks: + - * / sin cos exp log … etc





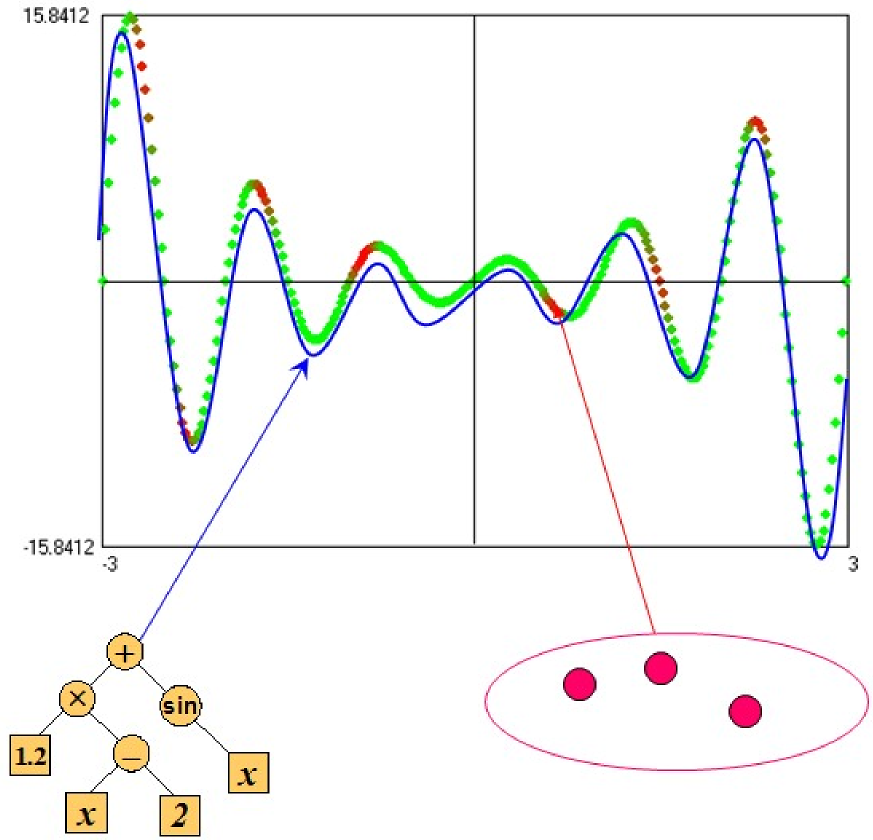
sin(x_2)

x_1*sin(x_2)

(x_1 – 3)*sin(x_2)

(x_1 – 3)*sin(-7 + x_2)

Run…



Models: Expression trees
Subject to mutation and selection

`{const,+,-,*,/,sin,cos,exp,log,abs}`

Experiments: Data-points
Subject to mutation and selection

Michael D. Schmidt, Hod Lipson (2006)

Systems of D.E.'s

- Regress on derivative

State Variables				*Derivatives*		
time	**x_1**	**x_2**	**…**	**dx_1/dt**	**x_2/dt**	**…**
0	3.4	-1.7	…	-2.0	8.0	…
0.1	3.2	-0.9	…	-1.0	8.0	…
0.2	3.1	-0.1	…	-4.0	1.3	…
0.3	2.7	1.2	…	-5.7	1.9	…
…	…	…	…	…	…	…

Inferring Biological Networks

$$\frac{dS_1}{dt} = \underbrace{2.5}_{J_0} - \underbrace{100\left(\frac{S_1 * A_3}{1+13.6769 * A_3^4}\right)}_{-v_1}$$

$$\frac{dS_2}{dt} = \underbrace{200\left(\frac{S_1 * A_3}{1+13.6769 * A_3^4}\right)}_{2*v_1} - \underbrace{6*S_2*N_1}_{-v_2} - \underbrace{12*S_2*N_1}_{-v_6}$$

$$\frac{dS_3}{dt} = \underbrace{6*S_2*N_1}_{v_2} + \underbrace{16*S_3*A_2}_{v_3}$$

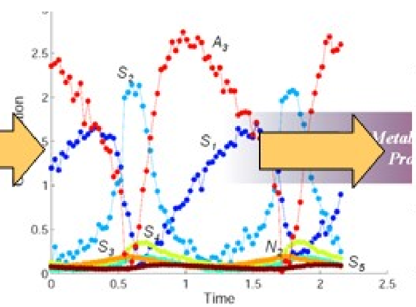
$$\frac{dS_4}{dt} = \underbrace{16*A_2*S_3}_{v_3} - \underbrace{100*N_2*S_4}_{-v_4}$$

$$\frac{dN_2}{dt} = \underbrace{6*S_2*N_1}_{v_2} - \underbrace{100*N_2*S_4}_{-v_4}$$

$$\frac{dA_3}{dt} = \underbrace{-200\left(\frac{S_1 * A_3}{1+13.6769 A_3^4}\right)}_{-2*v_1} + \underbrace{32*A_2*S_3}_{2v_3} - \underbrace{1.28*A_3}_{-v_5}$$

$$\frac{dS_5}{dt} = \underbrace{-1.3*S_5}_{\varphi J}$$

Original Equations



$$\frac{dS_1}{dt} = \underbrace{2.42114}_{J_0} - \underbrace{99.2721\left(\frac{S_1 * A_3}{1+13.5956 * A_3^4}\right)}_{-v_1}$$

$$\frac{dS_2}{dt} = \underbrace{199.935\left(\frac{S_1 * A_3}{1+13.6734 * A_3^4}\right)}_{2*v_1} - \underbrace{5.99475*S_2*N_1}_{-v_2} - \underbrace{11.9895*S_2*N_1}_{-v_6}$$

$$\frac{dS_3}{dt} = \underbrace{5.99857*S_2*N_1}_{v_2} + \underbrace{15.99606*S_3*A_2}_{v_3} \underbrace{-0.01286*S_3}_{extraneous}$$

$$\frac{dS_4}{dt} = \underbrace{15.997*A_2*S_3}_{v_3} - \underbrace{100.015*N_2*S_4}_{-v_4}$$

$$\frac{dN_2}{dt} = \underbrace{5.99857*S_2*N_1}_{v_2} - \underbrace{99.9963*N_2*S_4}_{-v_4}$$

$$\frac{dA_3}{dt} = \underbrace{-197.781\left(\frac{S_1 * A_3}{1+13.2633 A_3^4}\right)}_{-2*v_1} + \underbrace{31.9682*A_2*S_3}_{2v_3} - \underbrace{1.29659*A_3}_{-v_5}$$

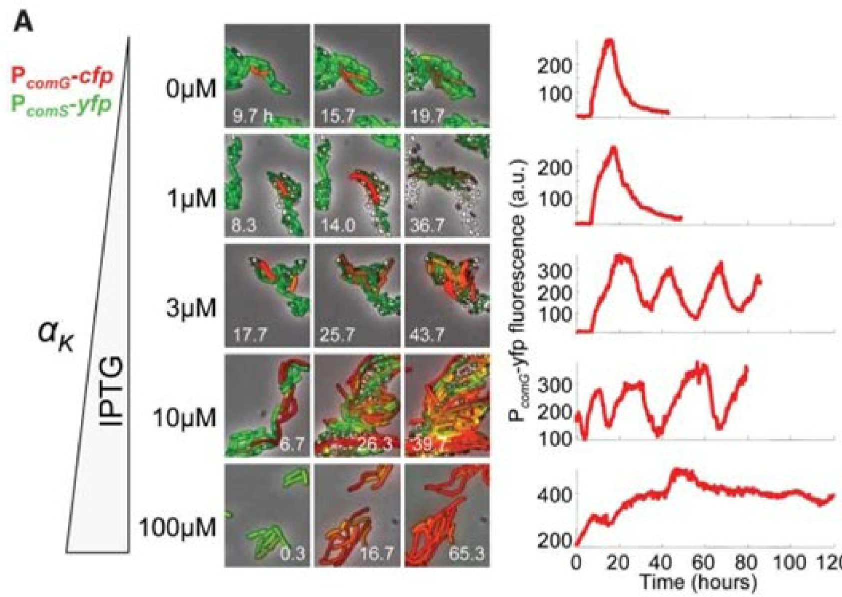
$$\frac{dS_5}{dt} = \underbrace{-1.29626*S_5}_{\varphi J}$$

Inferred Equations

With Michael Schmidt, John Wikswo (Vanderbilt), Jerry Jenkins (CFDRC)

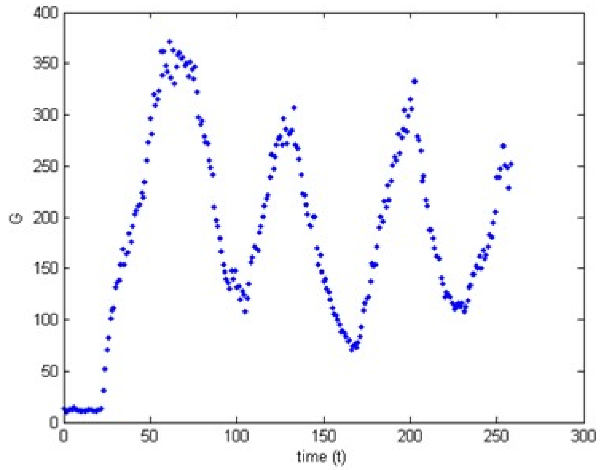
Wet Data, Unknown System

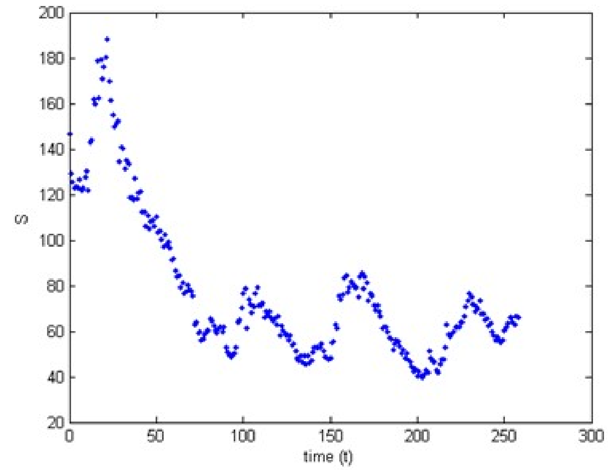
Bacillus Bacteria



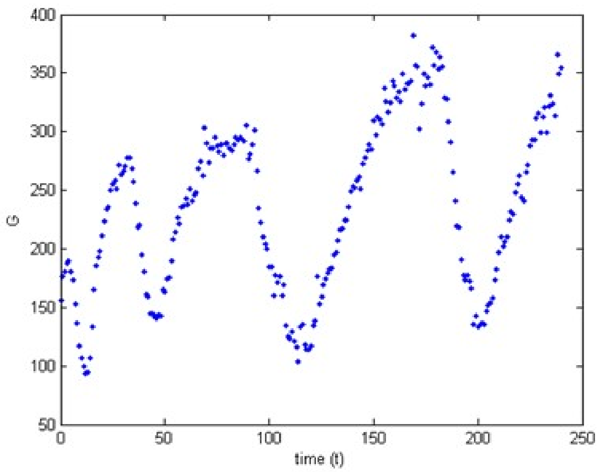
With Michael Schmidt (Cornell) and Gurol Suel (UT Southwestern)

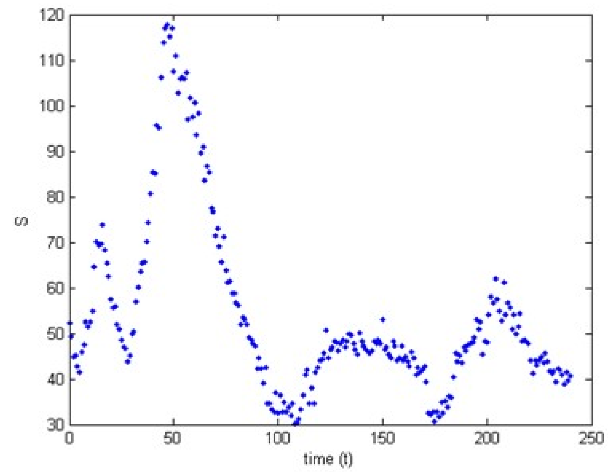
Cell #1





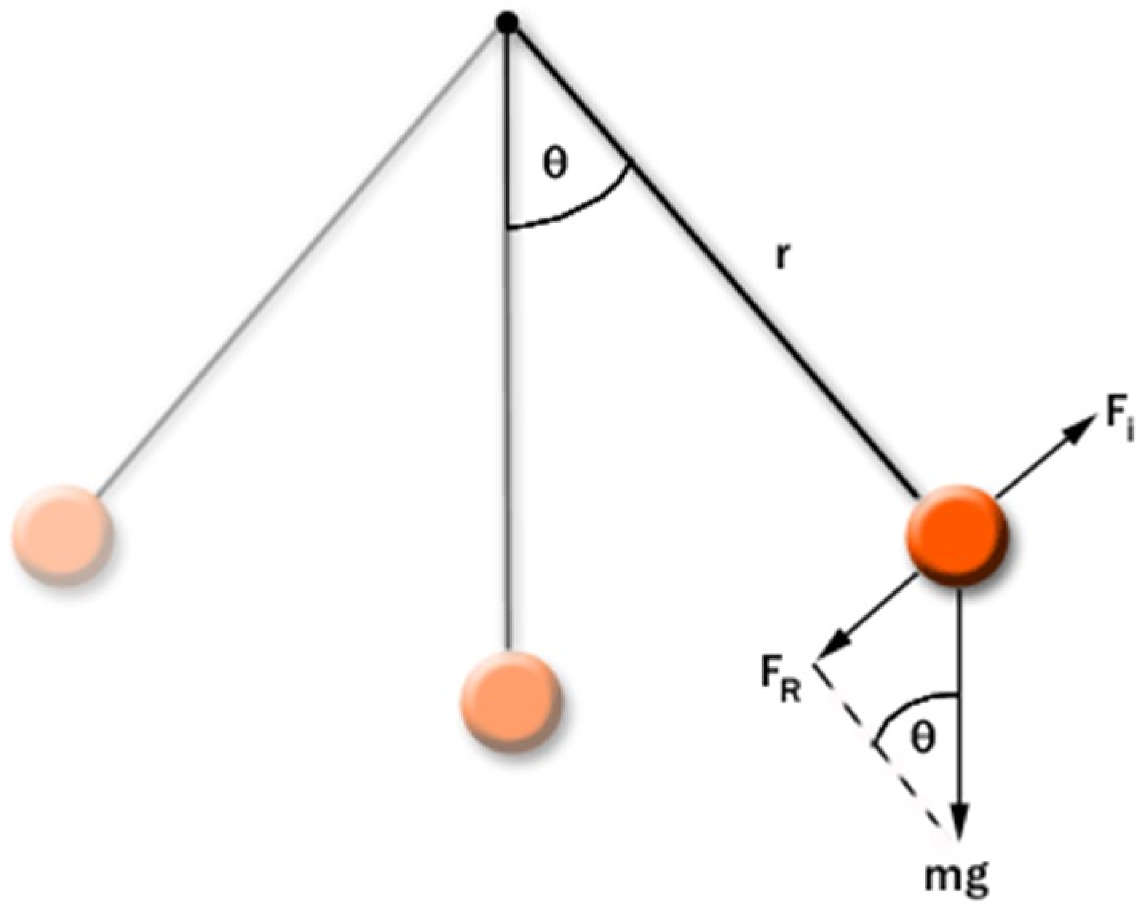
Cell #2





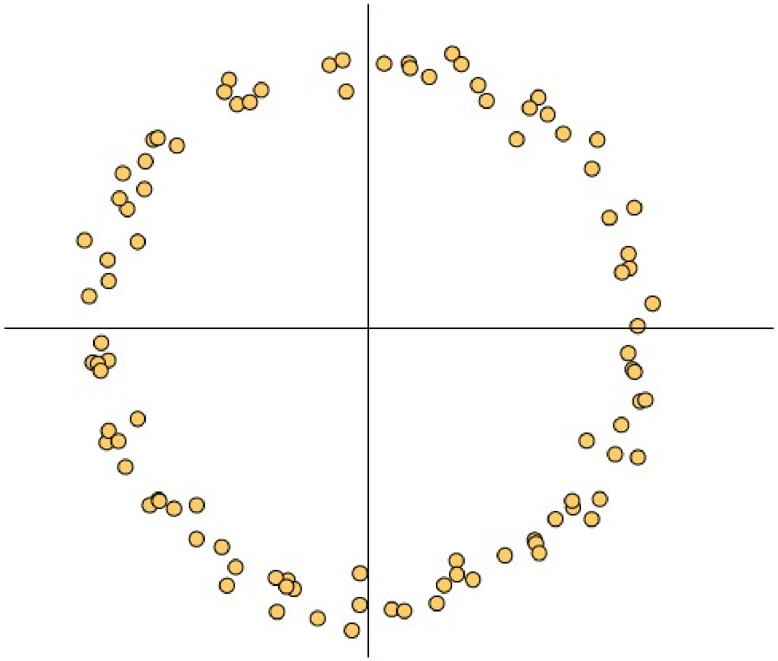
Cell #3-60 …

Looking For Invariants


θ
r
F_i
F_R
θ
mg

Implicit Equations

Mining for invariants in data



$$x^2+y^2-1 \approx 0$$

From Data:

x	y	…
0.1	2.3	
0.2	4.5	
0.3	9.7	
0.4	5.1	
0.5	3.3	
0.6	1.0	
…	…	…

Calculate partial derivatives Numerically:

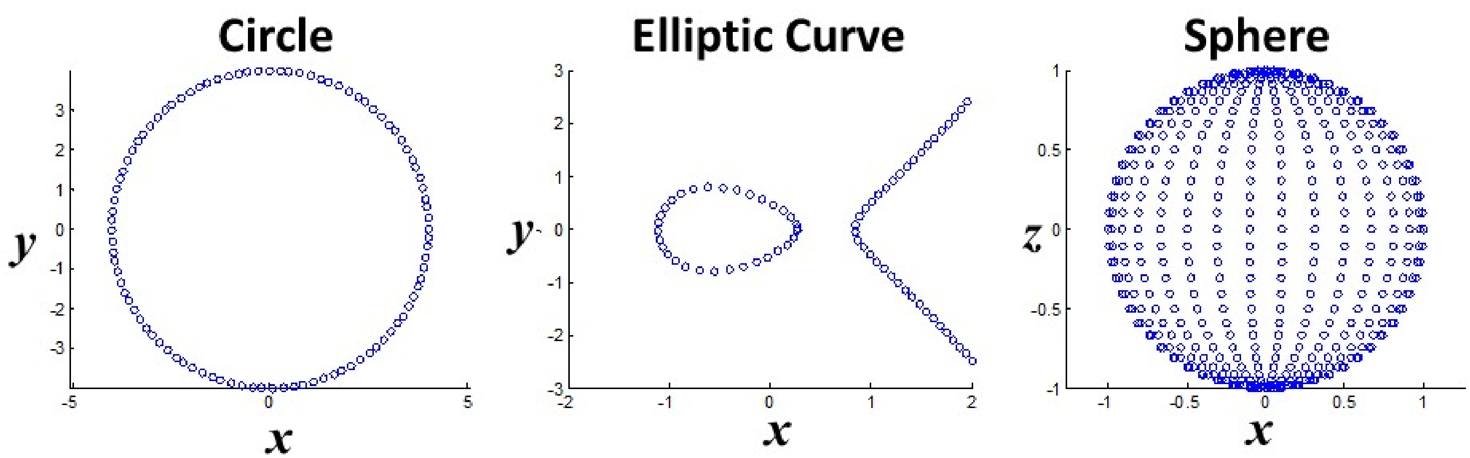
$$\longrightarrow \quad \frac{\delta x}{\delta y}, \quad \frac{\delta y}{\delta x}, \quad \cdots$$

From Equation:

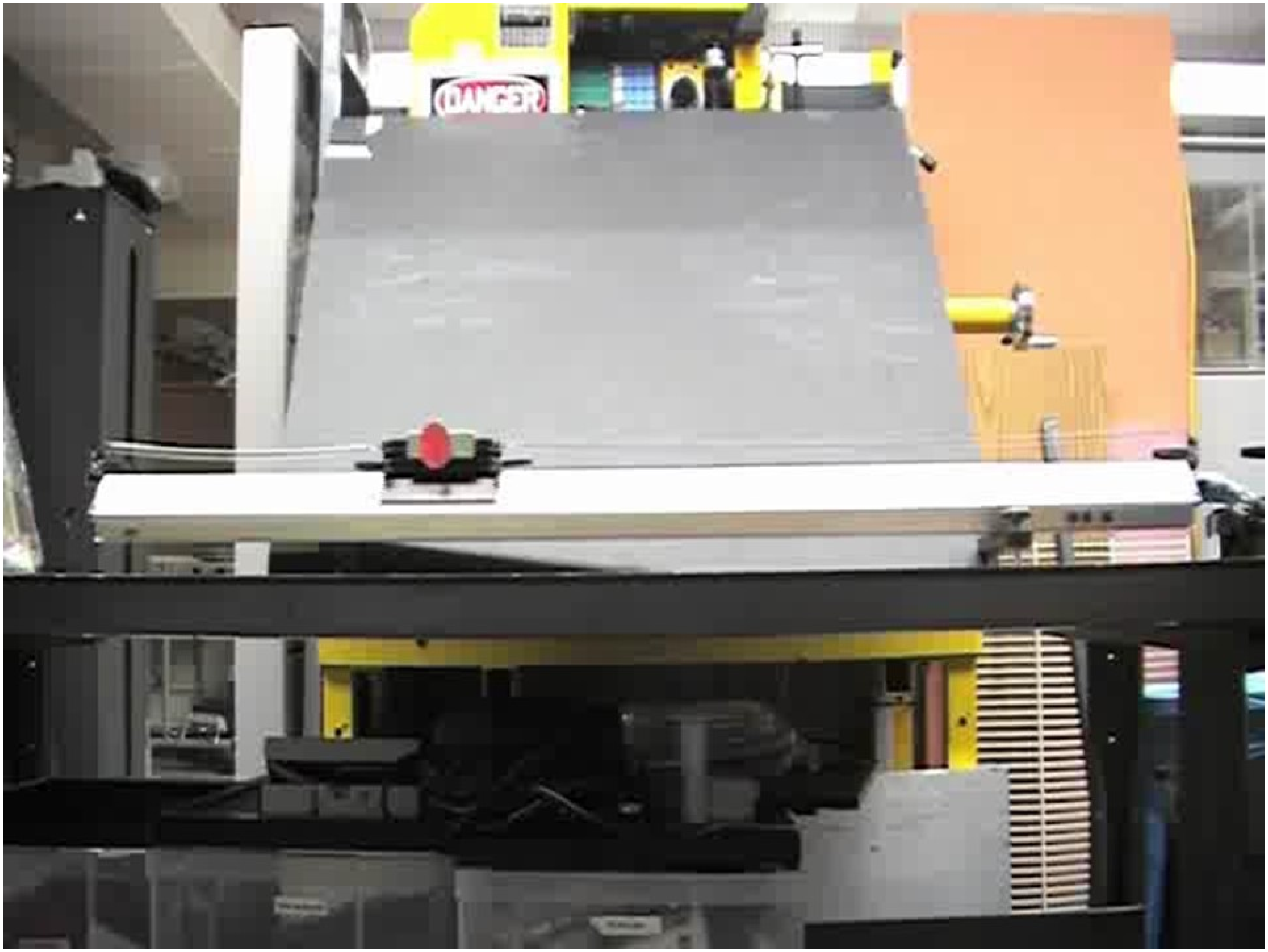
Calculate predicted partial derivatives Symbolically:

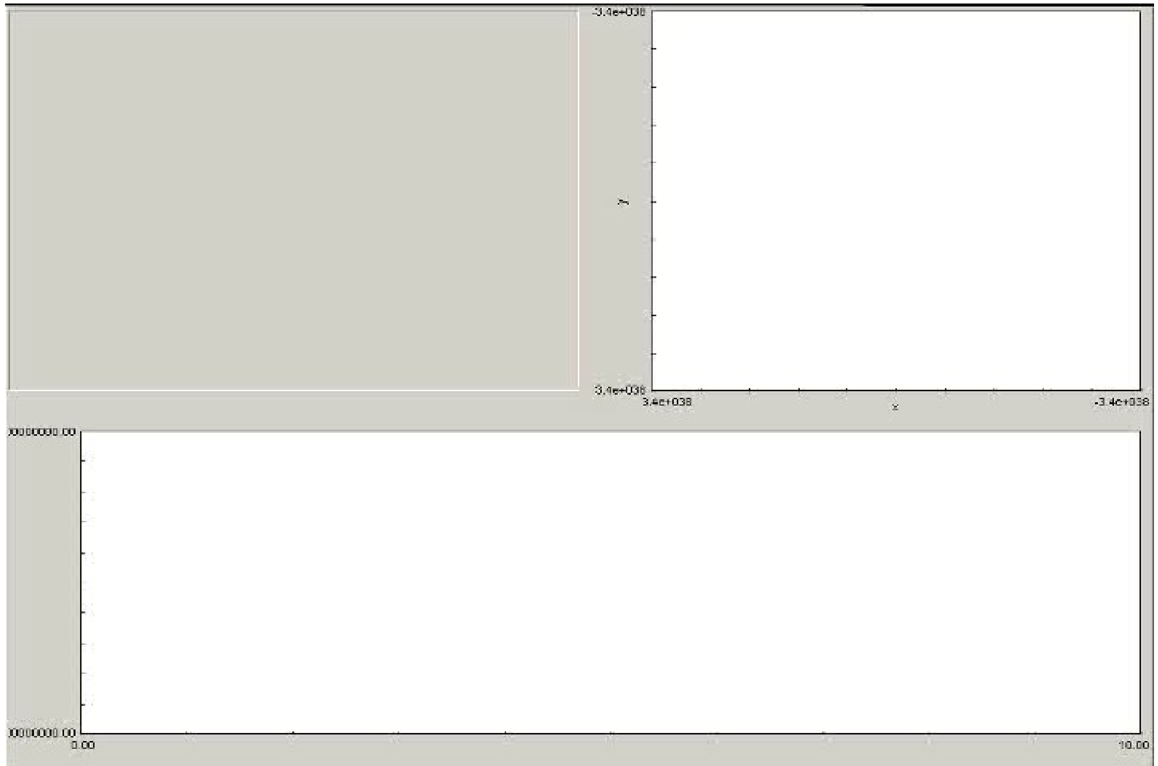
$$\frac{\delta f}{\delta x} \Big/ \frac{\delta f}{\delta y} \longrightarrow \quad \frac{\delta x'}{\delta y'}, \quad \frac{\delta y'}{\delta x'}, \quad \cdots$$

Experiments



$x^2 + y^2 - 16 = 0$ $\qquad$ $x^3 + x - y^2 - 1.5 = 0$ $\qquad$ $x^2 + y^2 + z^2 - 1 = 0$

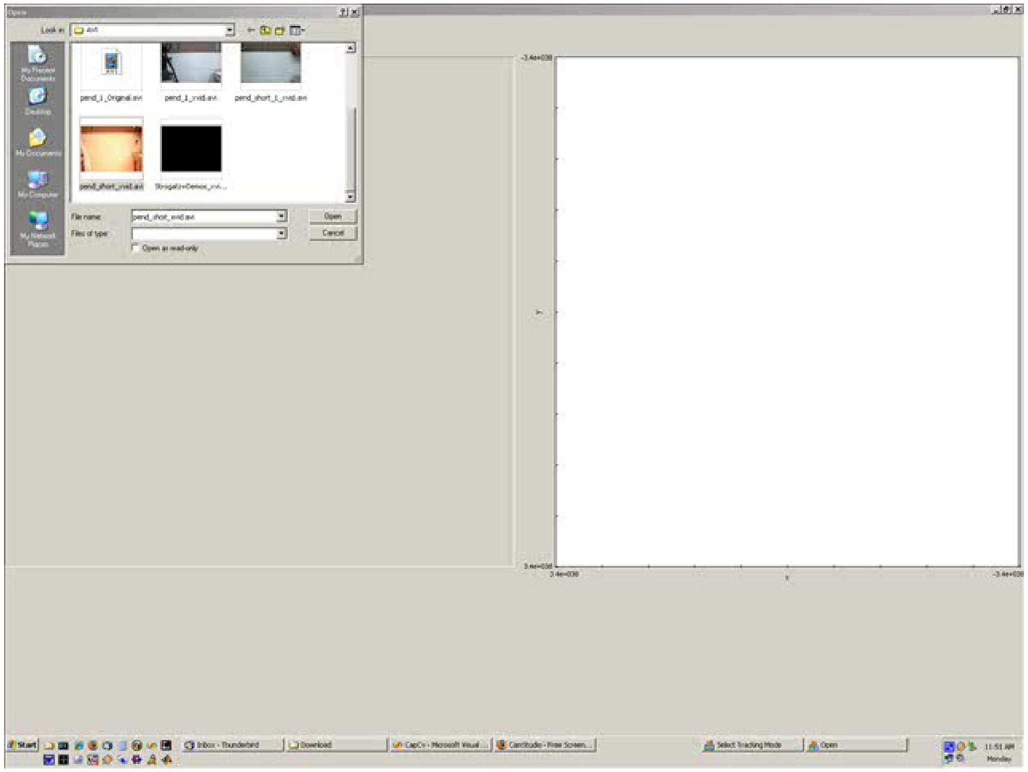

DANGER



$$H = 114.28 * \left(\frac{dx}{dt}\right)^2 + 692.322 * x^2$$

$$L = 61.591 * \left(\frac{dx}{dt}\right)^2 - 369.495 * x^2$$

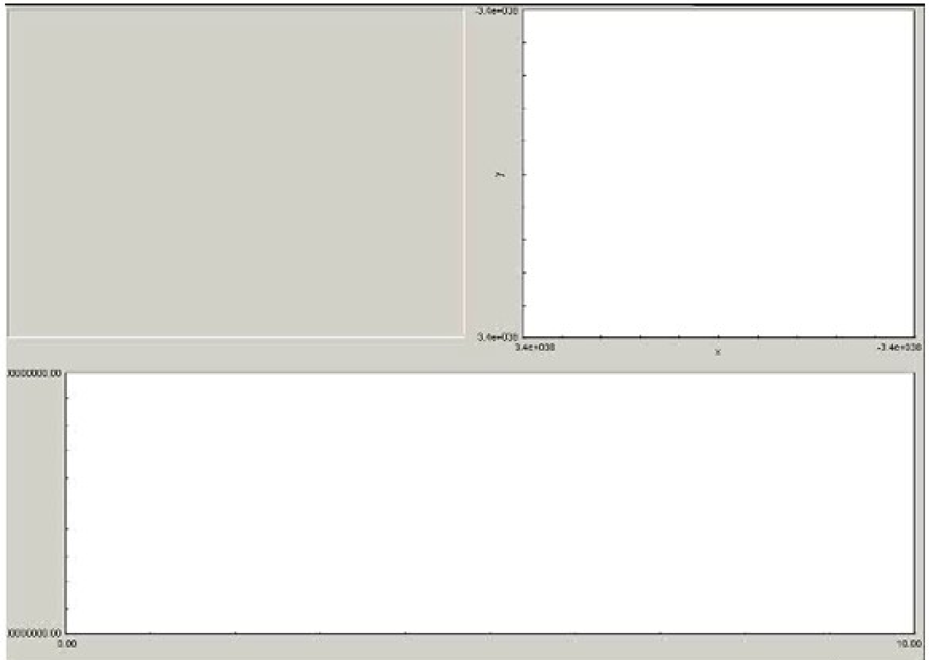
• Coefficients may have different scales and offsets each run



$$\mathbf{H} = \left(\frac{d\theta}{dt}\right)^2 + 2.42847 * \cos(\theta)$$

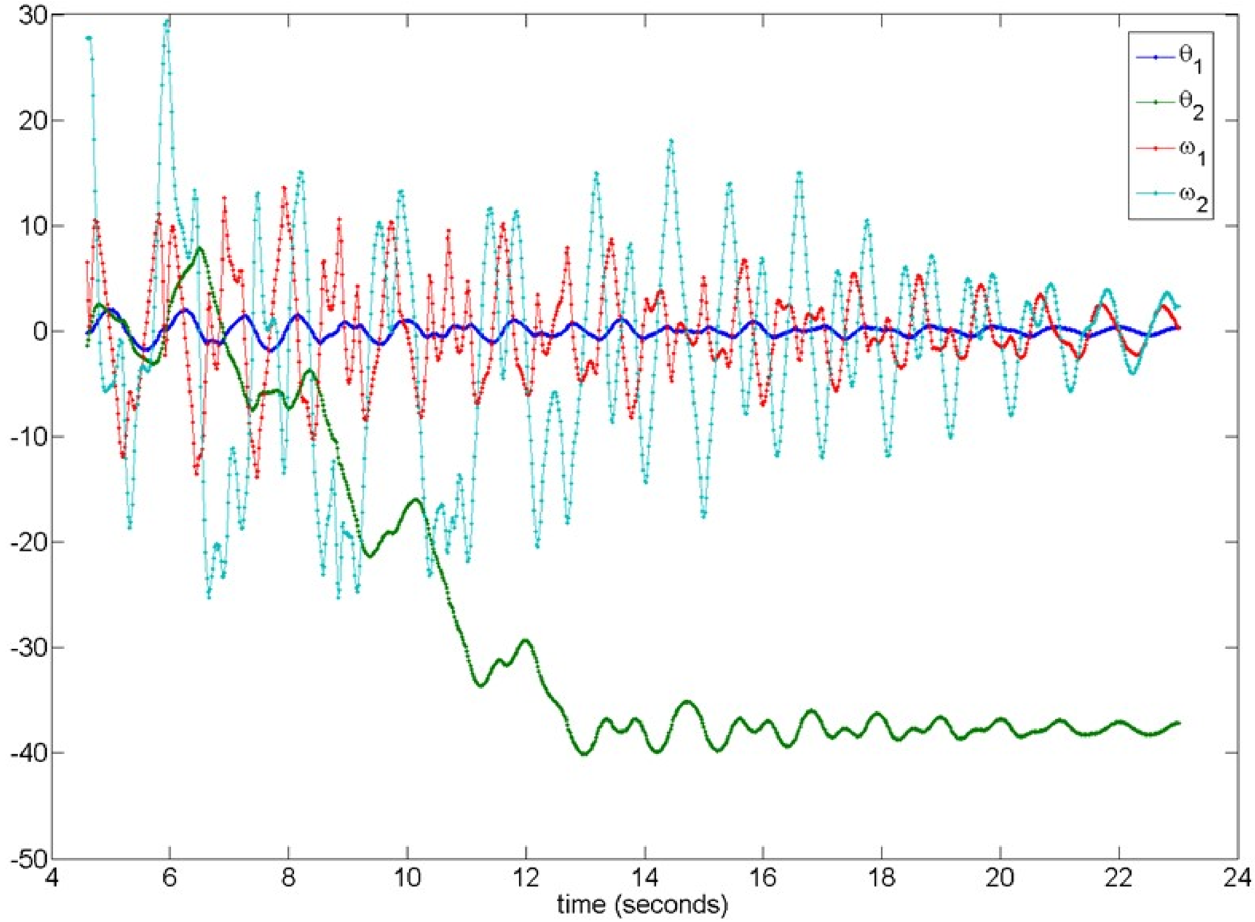
$$\mathbf{L} = 3.52768 * \left(\frac{d\theta}{dt}\right)^2 - 9.43429 * \cos(\theta)$$

Double Linear Oscillator



$$H = -14.691 * x_1^2 - 15.551 * x_2^2 - 21.676 * x_1 x_2 + 8.3808 * \left(\frac{dx_2}{dt}\right)^2 + 2.6046 * \left(\frac{dx_1}{dt}\right)^2$$

would be plus for Lagrangian



30
20
10
0
-10
-20
-30
-40
-50
4
6
8
10
12
14
16
18
20
22
24
time (seconds)
θ1
θ2
ω1
ω2

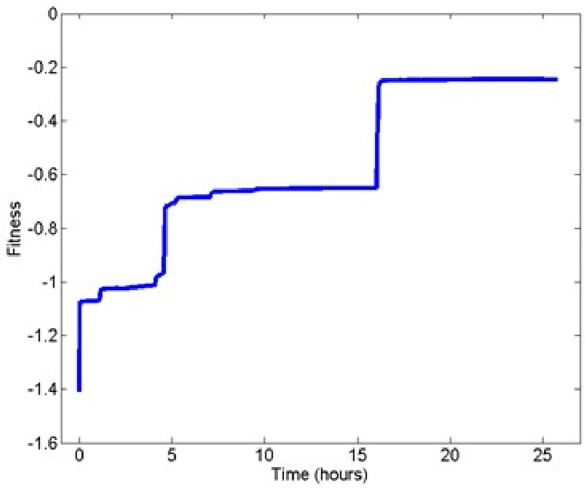
Solution found for the real double pendulum:

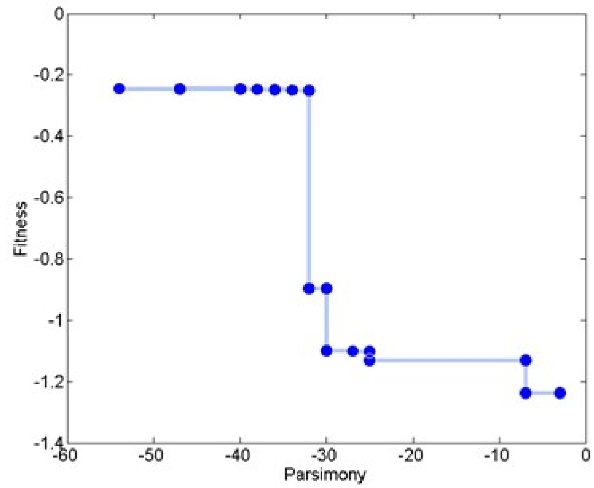
$$L = 4344822 \cdot \omega_1^2 - 204496973 \cdot \cos(\theta_2) + 1396004 \cdot \omega_2^2 - 538760938 \cdot \cos(\theta_1) - 3581621 \cdot w1 \cdot w2 \cdot \cos(\theta_1 - 1.0001 \cdot \theta_2)$$

$$L = \omega_1^2 + 0.3213 \cdot \omega_2^2 + 0.8243 \cdot \omega_1 \cdot \omega_2 \cdot \cos(\theta_1 - \theta_2) + 124.0007 \cdot \cos(\theta_1) + 47.0668 \cdot \cos(\theta_2)$$

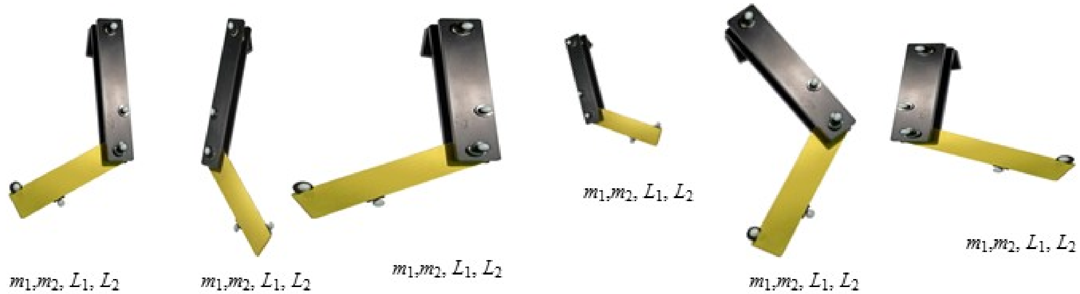
$$L = \omega_1^2 + \alpha \cdot \omega_2^2 + \beta \cdot \omega_1 \cdot \omega_2 \cdot \cos(\theta_1 - \theta_2) + \gamma \cdot \cos(\theta_1) + \lambda \cdot \cos(\theta_2)$$

$$\alpha = 0.3213$$
$$\beta = 0.8243$$
$$\gamma = 124.0007$$
$$\lambda = 47.0668$$





$$k_1\omega_1^2 + k_2\omega_2^2 + k_3\omega_1\omega_2\cos(\theta_1-\theta_2) - k_4\cos\theta_1 - k_5\cos\theta_2$$



$k_1/k_1 = 1$

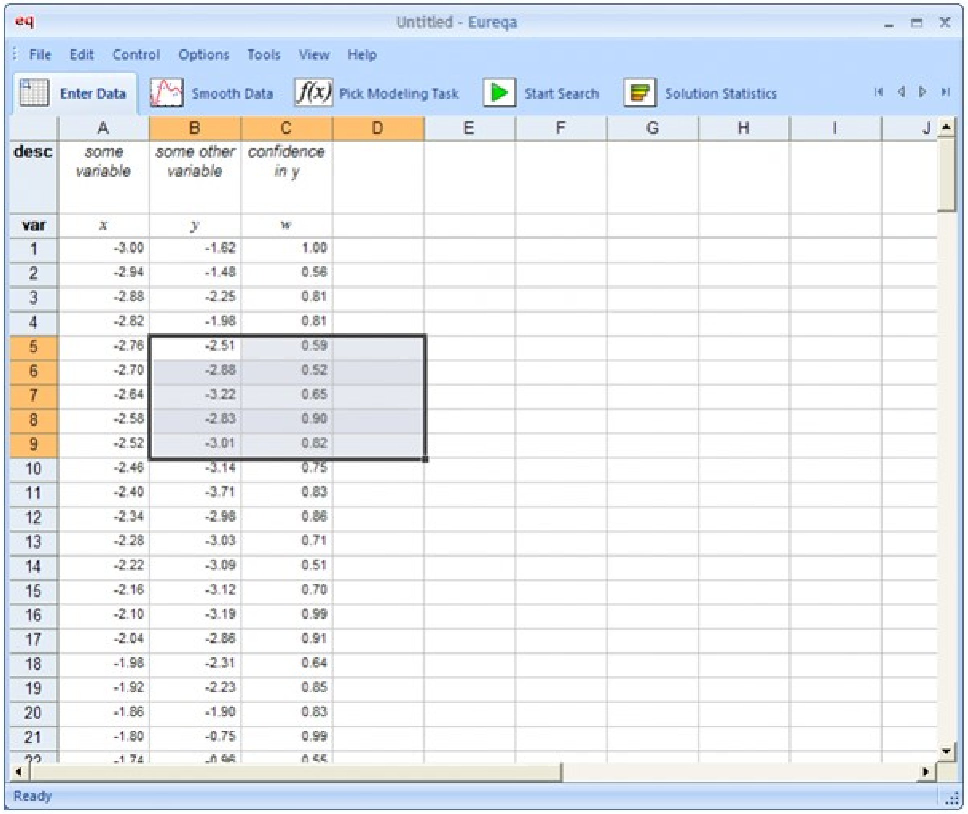
$k_2/k_1 = m_2L_2{}^2/(m_1L_1{}^2 + m_2L_1{}^2)$

$k_3/k_1 = 2.00055m_2L_2/(m_1L_1 + m_2L_1)$

$k_4/k_1 = 19.6/L_1$

$k_5/k_1 = 19.6\cdot m_2L_2/(m_2L_1{}^2 + m_1L_1{}^2)$

$$L_1^2(m_1+m_2)\omega_1^2 + m_2L_2^2\omega_2^2 + 2\cdot m_2L_1L_2\omega_1\omega_2\cos(\theta_1-\theta_2)$$
$$-19.6\cdot L_1(m_1+m_2)\cos\theta_1 - 19.6m_2L_2\cos\theta_2$$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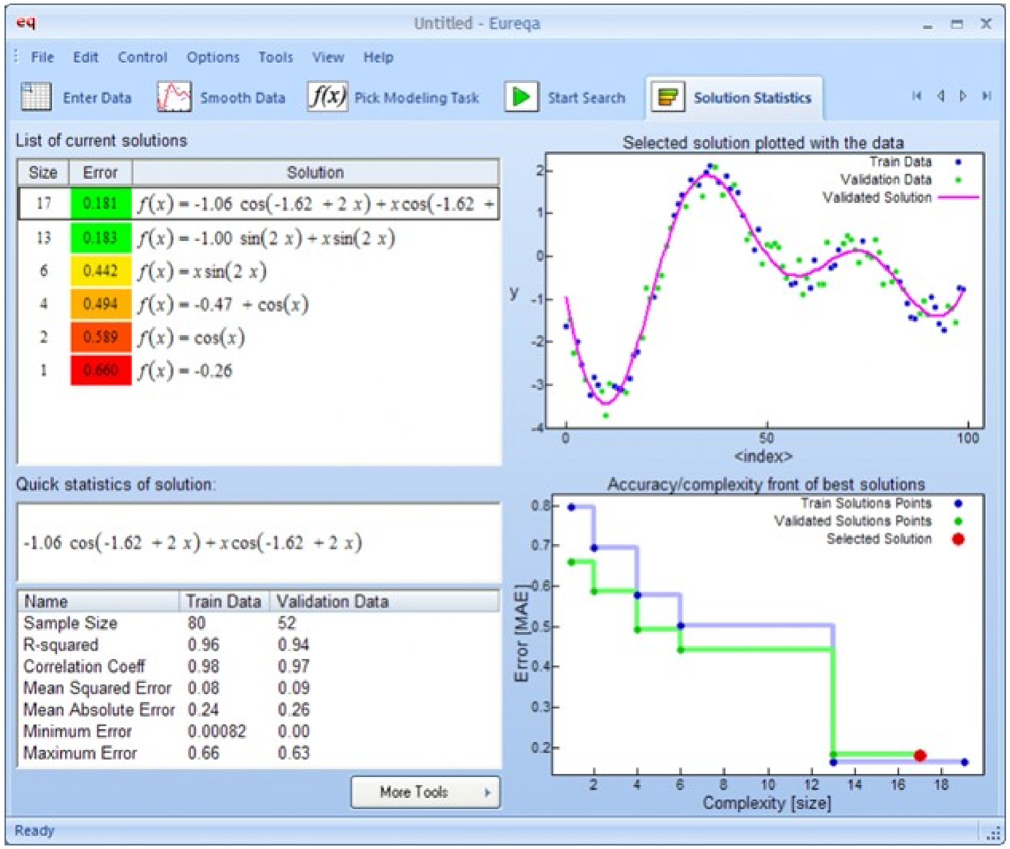
Enter Data
Smooth Data
Pick Modeling Task
Start Search
Solution Statistics
A B C D E F G H I J
desc | some variable | some other variable | confidence in y
var | x | y | w
1 -3.00 -1.62 1.00
2 -2.94 -1.48 0.56
3 -2.88 -2.25 0.81
4 -2.82 -1.98 0.81
5 -2.76 -2.51 0.59
6 -2.70 -2.88 0.52
7 -2.64 -3.22 0.65
8 -2.58 -2.83 0.90
9 -2.52 -3.01 0.82
10 -2.46 -3.14 0.75
11 -2.40 -3.71 0.83
12 -2.34 -2.98 0.86
13 -2.28 -3.03 0.71
14 -2.22 -3.09 0.51
15 -2.16 -3.12 0.70
16 -2.10 -3.19 0.99
17 -2.04 -2.86 0.91
18 -1.98 -2.31 0.64
19 -1.92 -2.23 0.85
20 -1.86 -1.90 0.83
21 -1.80 -0.75 0.99
Ready

Eureqa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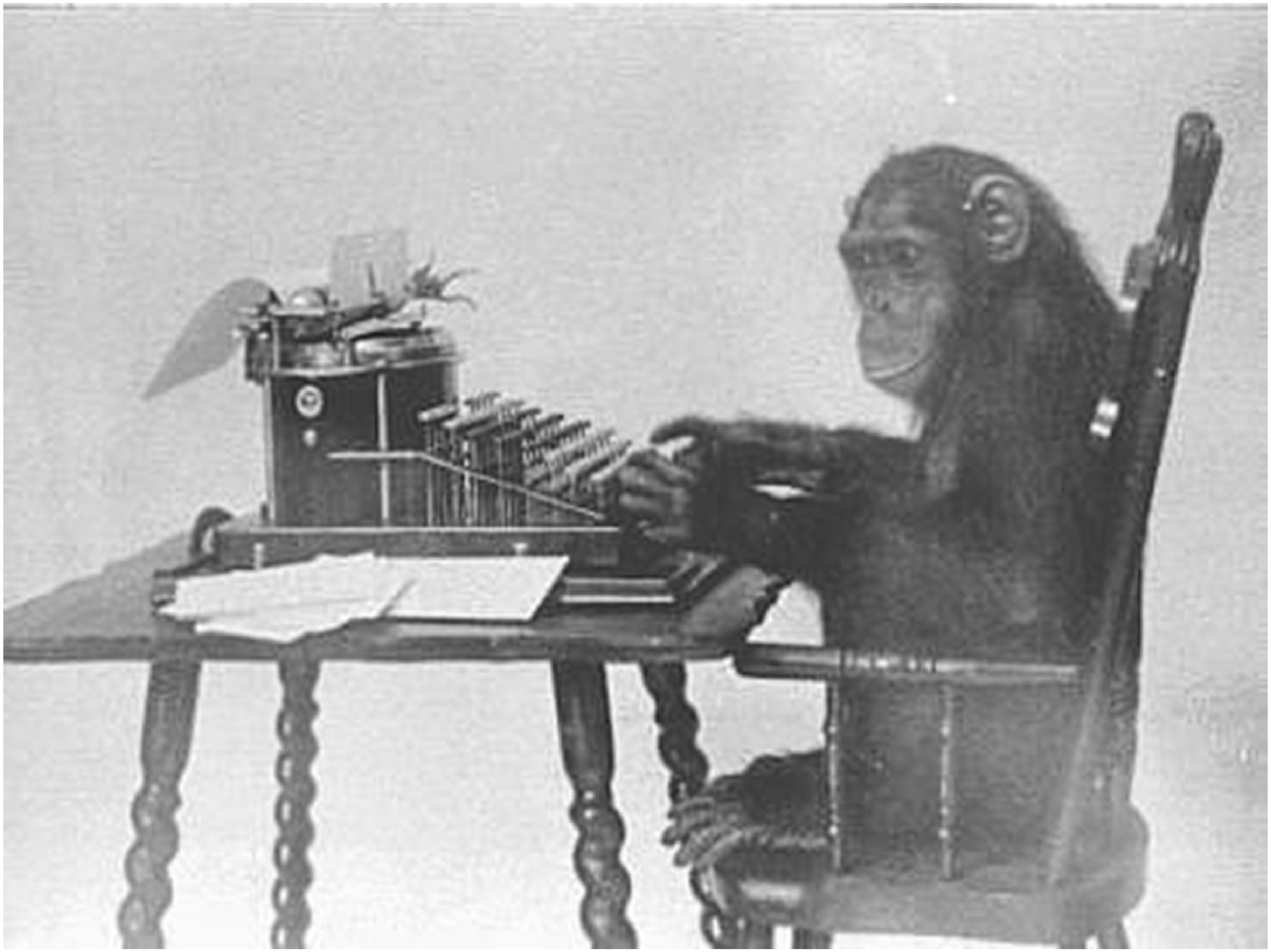
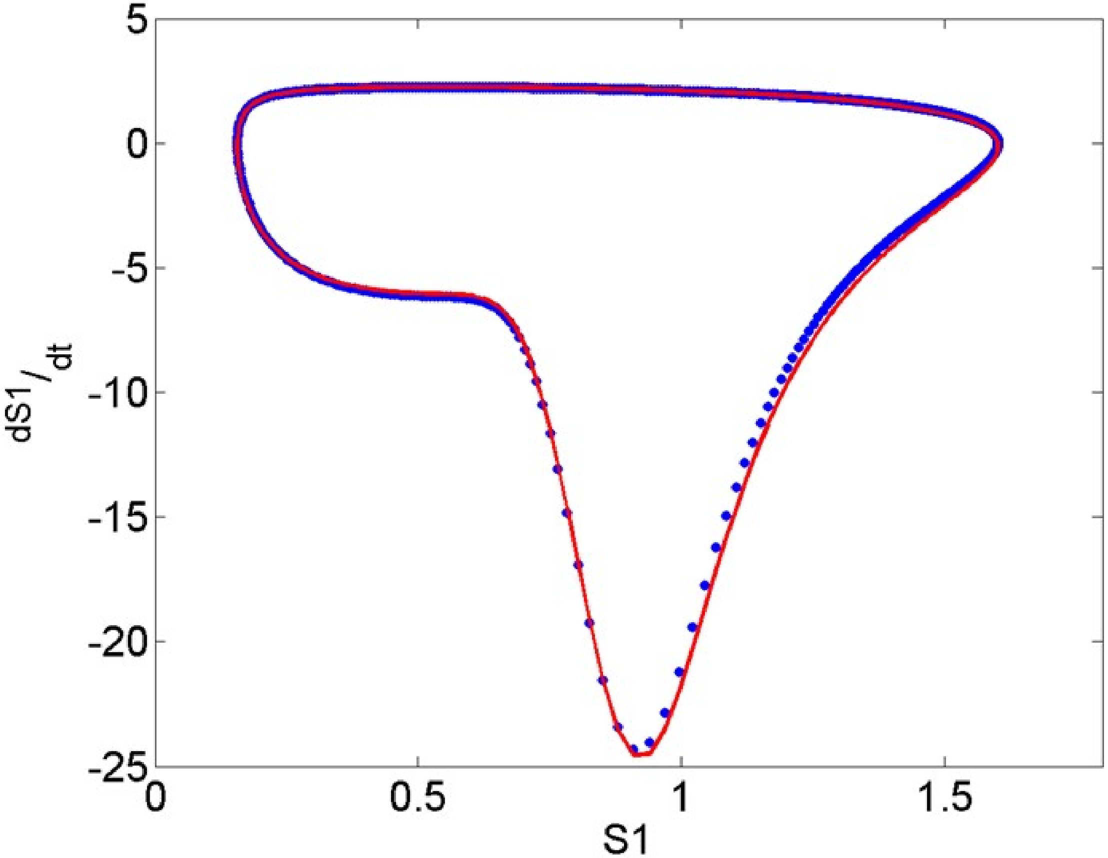
File Edit Control Options Tools View Help
Enter Data
Smooth Data
Pick Modeling Task
Start Search
Solution Statistics
List of current solutions
Size Error Solution
17 0.181 f(x) = -1.06 cos(-1.62 + 2 x) + x cos(-1.62 +
13 0.183 f(x) = -1.00 sin(2 x) + x sin(2 x)
6 0.442 f(x) = x sin(2 x)
4 0.494 f(x) = -0.47 + cos(x)
2 0.589 f(x) = cos(x)
1 0.660 f(x) = -0.26
Quick statistics of solution:
-1.06 cos(-1.62 + 2 x) + x cos(-1.62 + 2 x)
Name Train Data Validation Data
Sample Size 80 52
R-squared 0.96 0.94
Correlation Coeff 0.98 0.97
Mean Squared Error 0.08 0.09
Mean Absolute Error 0.24 0.26
Minimum Error 0.00082 0.00
Maximum Error 0.66 0.63
More Tools
Selected solution plotted with the data
Train Data
Validation Data
Validated Solution
y
<index>
Accuracy/complexity front of best solutions
Train Solutions Points
Validated Solutions Points
Selected Solution
Error [MAE]
Complexity [size]
Ready

Eureqa

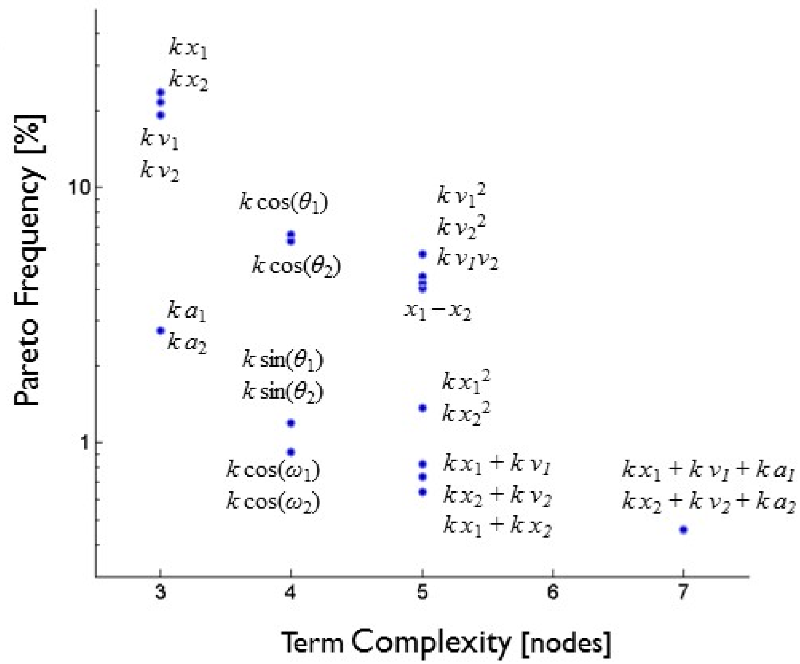


$$2.53075122833252 - \frac{42.3825454711914 \cdot S_1}{5.432642911755188 \cdot {A_3}^3 + \frac{0.429036676883698}{A_3}}$$



Alphabet

Term	Complexity	Frequency	Systems
$k x_2$	1	23.578	4
$k x_1$	1	21.6514	4
$k v_2$	1	21.5596	4
$k v_1$	1	19.1743	4
$k \cos(\theta_2)$	2	6.51376	2
$k \cos(\theta_1)$	2	6.14679	2
$k v_2^2$	3	5.50459	4
$k v_1^2$	3	4.49541	4
$(x_1 - x_2)$	3	4.22018	2
$k v_1 v_2$	3	4.0367	2
$k a_2$	1	2.75229	2
$k a_1$	1	2.75229	2
$k x_2^2$	3	1.37615	2
$k \sin(\theta_2)$	2	1.19266	2
$k \sin(\theta_1)$	2	1.19266	2
$k \cos(\theta_1)$	2	0.917431	2
$k \cos(\theta_2)$	2	0.917431	2
$k x_1^2$	3	0.825688	2
$k x_1^2$	3	0.825688	2
$k x_1 + k v_1$	3	0.733945	3
$k x_2 + k v_2$	3	0.733945	3
$k x_1 + k x_2$	3	0.642202	2
$k x_1 + k v_1 - k a_1$	5	0.458716	2
$k x_2 + k v_2 - k a_2$	5	0.458716	2



Concluding Remarks

Wired 16.07

Chris Anderson

“Correlation is enough. Faced with massive data, [the Scientific Method] is becoming obsolete. We can stop looking for models.”

The data deluge accelerates our ability to hypothesize, model, and test.

The New York Times

Theoretical physicists are not yet obsolete, but scientists have taken steps toward replacing themselves

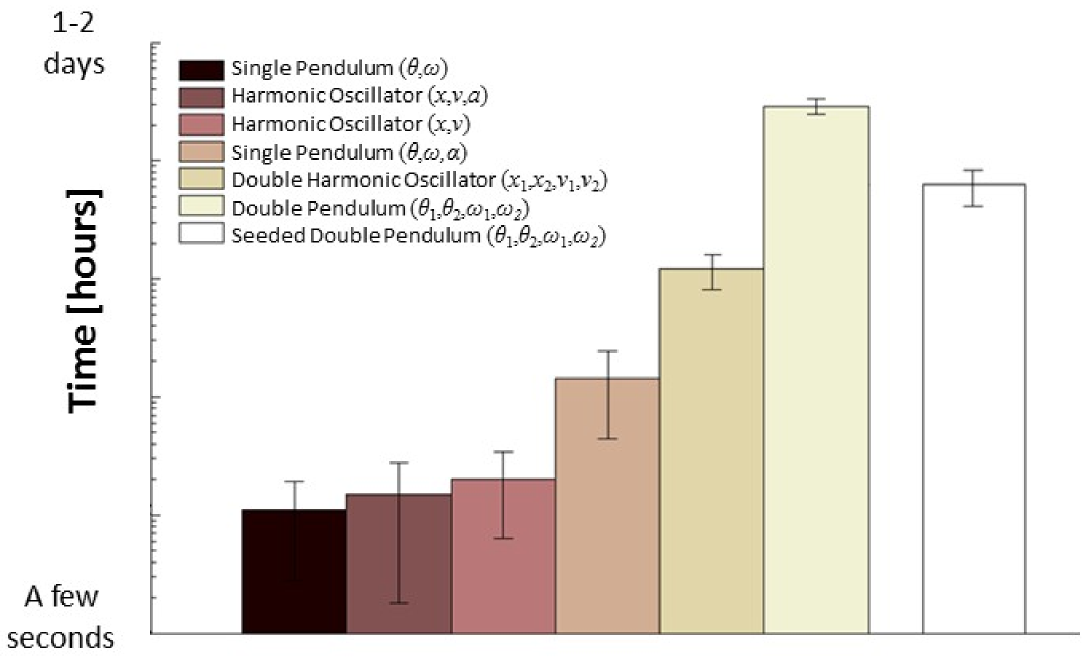
Scalability

- Complexity
- Noise
- Hidden (unobservable) variables
- Justification

Conclusions

- **Cognitive robotics**
  - Generate predictive model of self
- **Interrogating controller**
  - "intelligent" probing to extract invariants
- **Finding conservations**
  - Generate dynamical model of hidden nonlinear systems

Time to Regress



Approximations

Building Blocks	Detected Pendulum Law	Approximation
*, +, −, cos(), sin()	$\omega^2 - 19.6 \cdot \cos(\theta)$	*Exact Solution*
*, +, −, sin()	$\omega^2 - 19.5999 \cdot \sin(-1.57079 + \theta)$	*Trigonometric identity*
*, +, −	$\omega^2 + 9.7108 \cdot \theta^2 - 0.7042 \cdot \theta^4$	*Taylor series expansion (4th order)*