Distilling Free-Form Natural Laws from Experimental Data

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“Even though it looks like it’s changing erratically, there is always something deeper there that is always constant”
Lipson

Introduction

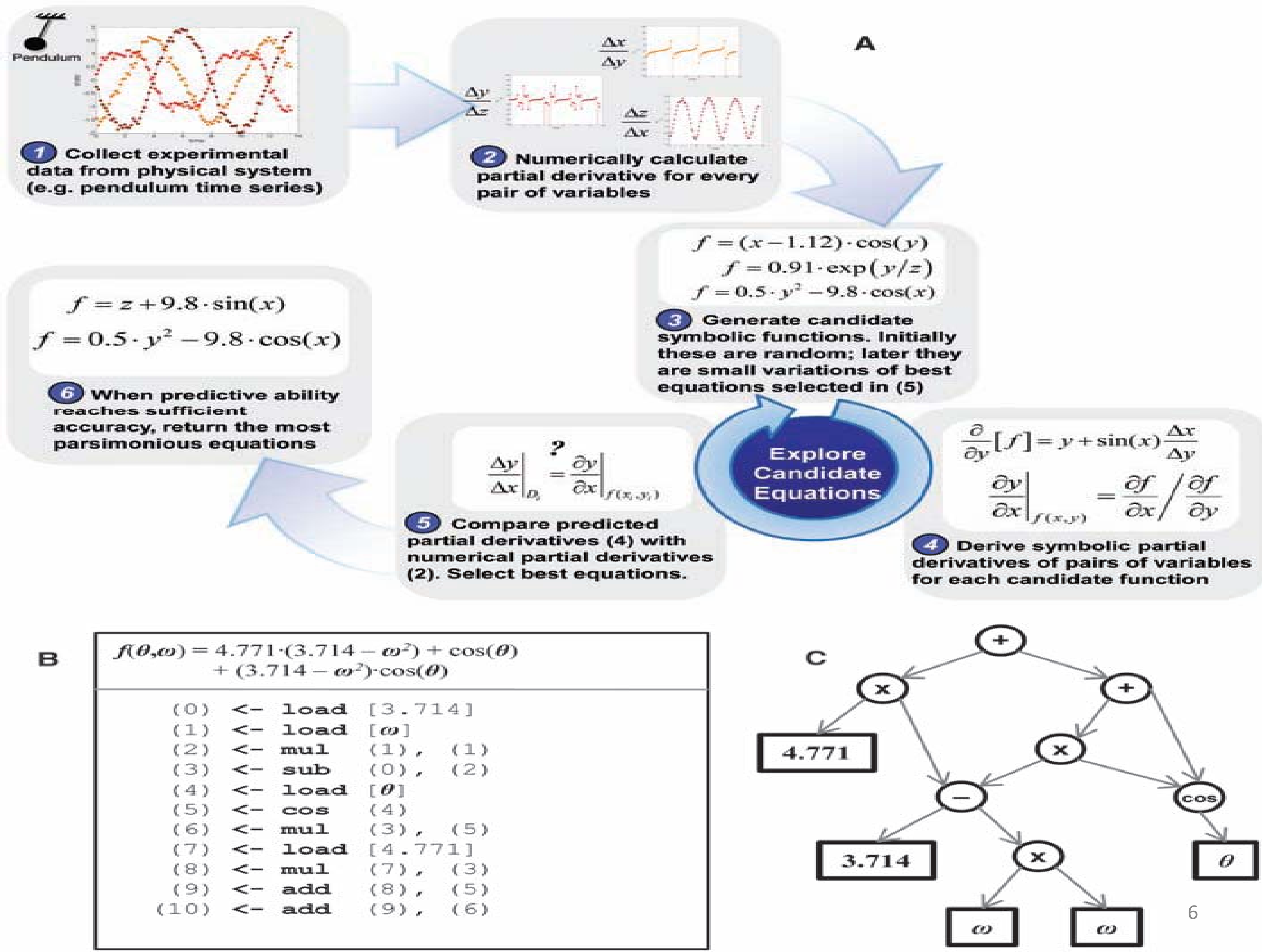
- Scientists for centuries have attempted to identify natural laws that underpin physical phenomena in nature
- Resistance to automation, despite occurrence of increased computer power
- Key to this is finding algorithms correlate correctly to observed data
- The paper proposes a principle for identification of the nontrivial

Goals

- To find natural relations where they exist
- Identify linked factors within a dataset
- Use unconstrained analytical expression that explain symbolically precise relations
- With the ultimate goal of uncovering an “alphabet” to describe the system

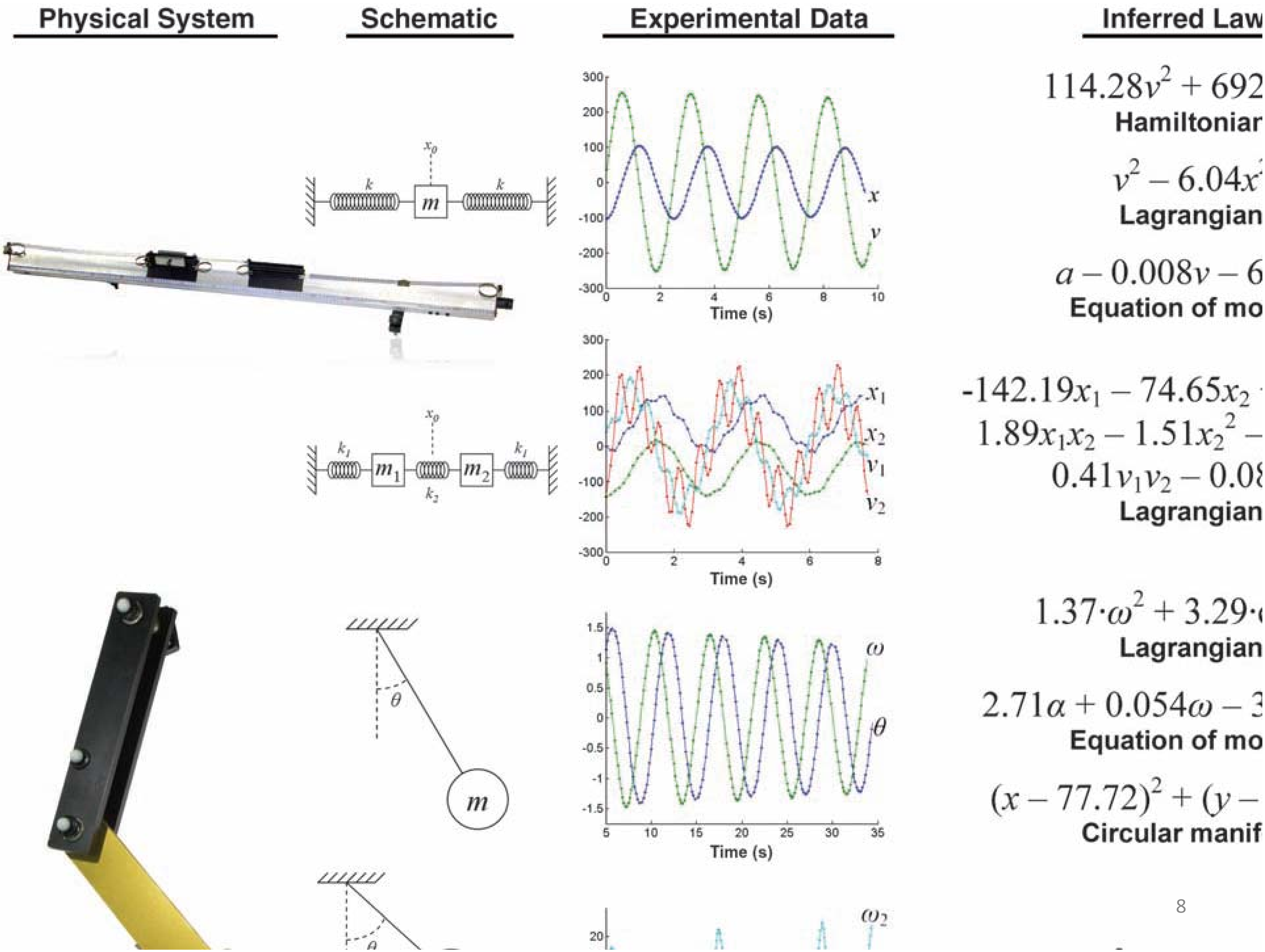
Experiment Setup

- Their process begins by taking the derivatives of every variable observed with respect to every other
- This is mathematical way of measuring how one quantity changes as another changes
- The program creates equations at random using various constants and variables from the data


A
Pendulum
1 Collect experimental data from physical system (e.g. pendulum time series)
2 Numerically calculate partial derivative for every pair of variables
3 Generate candidate symbolic functions. Initially these are random; later they are small variations of best equations selected in (5)
$f = (x - 1.12) \cdot \cos(y)$
$f = 0.91 \cdot \exp(y/z)$
$f = 0.5 \cdot y^2 - 9.8 \cdot \cos(x)$
Explore Candidate Equations
4 Derive symbolic partial derivatives of pairs of variables for each candidate function
$\frac{\partial}{\partial y}[f] = y + \sin(x)\frac{\Delta x}{\Delta y}$
$\left.\frac{\partial y}{\partial x}\right|_{f(x,y)} = \frac{\partial f}{\partial x} \Big/ \frac{\partial f}{\partial y}$
5 Compare predicted partial derivatives (4) with numerical partial derivatives (2). Select best equations.
6 When predictive ability reaches sufficient accuracy, return the most parsimonious equations
$f = z + 9.8 \cdot \sin(x)$
$f = 0.5 \cdot y^2 - 9.8 \cdot \cos(x)$
B
$f(\theta,\omega) = 4.771 \cdot (3.714 - \omega^2) + \cos(\theta) + (3.714 - \omega^2) \cdot \cos(\theta)$
(0) <- load [3.714]
(1) <- load [ω]
(2) <- mul (1), (1)
(3) <- sub (0), (2)
(4) <- load [θ]
(5) <- cos (4)
(6) <- mul (3), (5)
(7) <- load [4.771]
(8) <- mul (7), (3)
(9) <- add (8), (5)
(10) <- add (9), (6)
C
4.771
3.714
cos
θ
ω
ω

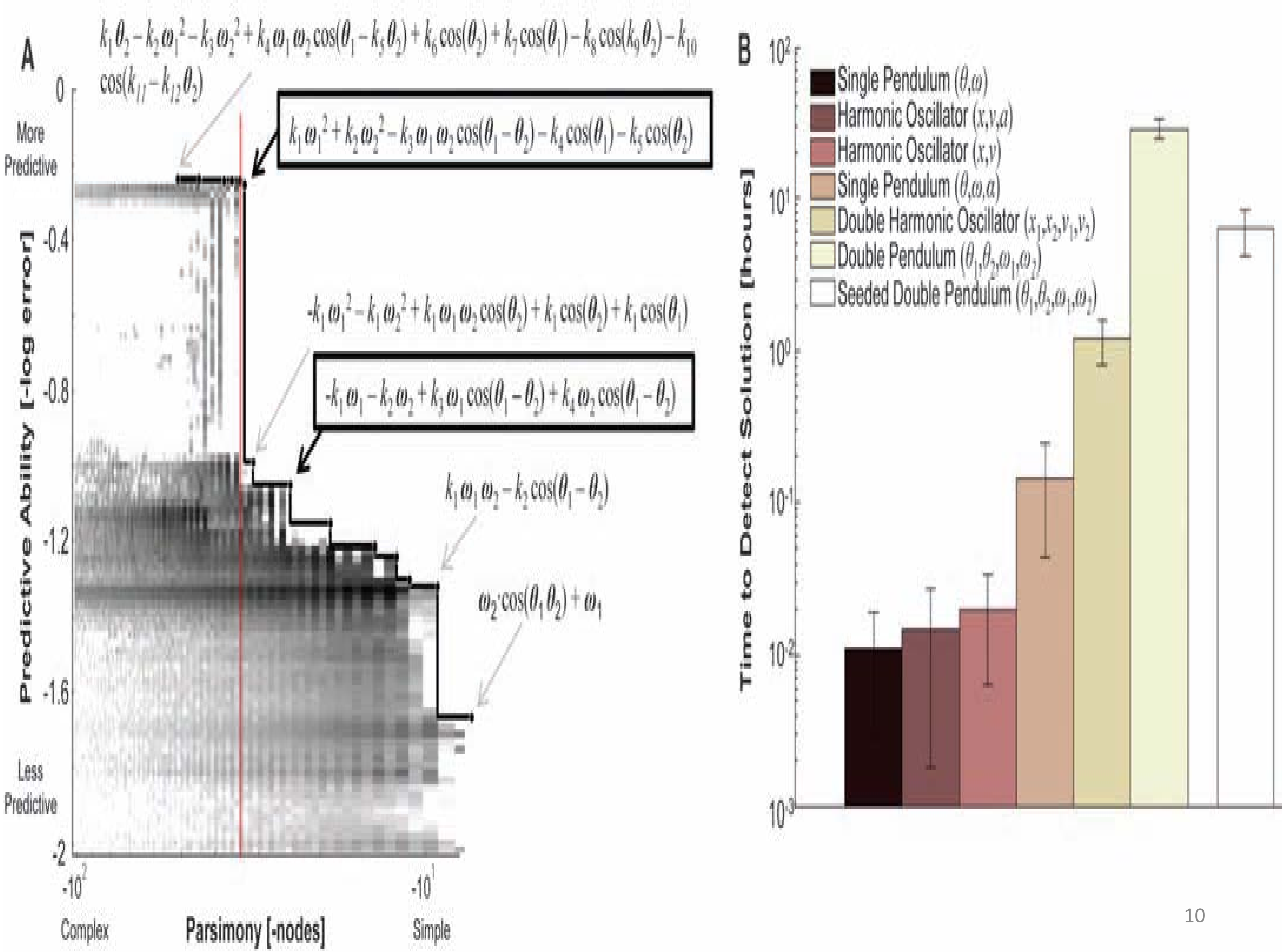
Outcome

- Initially the output failed to explain the data
- But some failures were slightly less wrong than others
- A genetic algorithm the program modified the most promising failures and tested the again chose the best and repeated
- This was repeated until a set of equations evolved to describe the system


Physical System
Schematic
Experimental Data
Inferred Law
114.28v² + 692
Hamiltoniar
v² – 6.04x
Lagrangian
a – 0.008v – 6
Equation of mo
-142.19x₁ – 74.65x₂
1.89x₁x₂ – 1.51x₂² –
0.41v₁v₂ – 0.0
Lagrangian
1.37·ω² + 3.29·
Lagrangian
2.71α + 0.054ω – 3
Equation of mo
(x – 77.72)² + (y –
Circular manif
Time (s)
x
v
x₁
x₂
v₁
v₂
ω
θ
ω₂
k
k₁
k₂
x₀
m
m₁
m₂

Conclusion

- The program evolves these laws without any prior knowledge of physics, kinematics or geometry
- But time consuming
- On a parallel computer with 32 processors, simple linear motion could be analyzed in few minutes, but the complex double pendulum required 30 to 40 hours
- Could be applied to more complex systems such as biology to cosmology



A
$k_1\theta_2 - k_2\omega_1^2 - k_3\omega_2^2 + k_4\omega_1\omega_2\cos(\theta_1 - k_5\theta_2) + k_6\cos(\theta_2) + k_7\cos(\theta_1) - k_8\cos(k_9\theta_2) - k_{10}\cos(k_{11} - k_{12}\theta_2)$
$k_1\omega_1^2 + k_2\omega_2^2 - k_3\omega_1\omega_2\cos(\theta_1 - \theta_2) - k_4\cos(\theta_1) - k_5\cos(\theta_2)$
$-k_1\omega_1^2 - k_1\omega_2^2 + k_1\omega_1\omega_2\cos(\theta_2) + k_1\cos(\theta_2) + k_1\cos(\theta_1)$
$-k_1\omega_1 - k_2\omega_2 + k_3\omega_1\cos(\theta_1 - \theta_2) + k_4\omega_2\cos(\theta_1 - \theta_2)$
$k_1\omega_1\omega_2 - k_2\cos(\theta_1 - \theta_2)$
$\omega_2 \cdot \cos(\theta_1 \theta_2) + \omega_1$
More Predictive
Less Predictive
Predictive Ability [-log error]
0
-0.4
-0.8
-1.2
-1.6
-2
-10^2
-10^1
Complex
Parsimony [-nodes]
Simple
B
Time to Detect Solution [hours]
10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
Single Pendulum (θ,ω)
Harmonic Oscillator (x,v,a)
Harmonic Oscillator (x,v)
Single Pendulum (θ,ω,a)
Double Harmonic Oscillator (x_1,x_2,v_1,v_2)
Double Pendulum $(\theta_1,\theta_2,\omega_1,\omega_2)$
Seeded Double Pendulum $(\theta_1,\theta_2,\omega_1,\omega_2)$

- By "bootstrapping" or seeding the complex pendulum problem with terms from equation for the simple pendulum cut the processing time to 7 or 8 hours.