#### **Scientific Data Mining**

Distilling Free-Form Natural Laws from Experimental Data

Hod Lipson, Cornell University



















Lipson & Pollack, Nature 406, 2000









## Adapting in simulation



## Adapting in reality



## **Simulation & Reality**







## **Morphological Estimation**



## **Emergent Self-Model**



With Josh Bongard and Victor Zykov, Science 2006

## **Damage Recovery**



With Josh Bongard and Victor Zykov, Science 2006





#### **System Identification**





Photo: Floris van Breugel

1 1

Photo: Floris van Breugel

SPA Links

# Static ID: Damage Diagnosis





With Wilkins Aquino

#### **Discrete Dynamics Inference**



Bongard J. C, Lipson H., (2005) "Active Coevolutionary Learning of Deterministic Finite Automata", Journal of Machine Learning research (JMLR), Vol. 6 No. 10, pp. 1651-1678

# **Circuit Building Blocks**



## Symbolic Regression

What function describes this data?





John Koza, 1992

## **Encoding Equations**

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



John Koza, 1992



**Models:** Expression trees Subject to mutation and selection

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

**Experiments:** Data-points Subject to mutation and selection





#### **Solution Accuracy**



## **Solution Complexity**





1	2	3	4	5	6	7	8	9	10
11	12	13	14	15	16	17	18	19	20
21	22	23	24	25	26	27	28	29	30
31	32	33	34	35	36	37	38	39	40
41	42	43	44	45	46	47	48	49	50
51	52	53	54	55	56	57	58	59	60
61	62	63	64	65	66	67	68	69	70
71	72	73	74	75	76	77	78	79	80
81	82	83	84	85	86	87	88	89	90
91	92	93	94	95	96	97	98	99	100

#### **Semi-empirical mass formula**

Modeling the binding energy of an atomic nucleus

Inferred Formula:  

$$E_B = 14.83 - 13.43A + 12.39A^{0.64} + \frac{0.39Z^2}{A^{0.26}} + \frac{17.29(N-Z)^2}{A} \longrightarrow \mathbb{R}^2 = 0.99944$$

#### Weizsäcker's Formula:

$$E_{B} = a_{V}A - a_{S}A^{2/3} - a_{C}\frac{Z(Z-1)}{A^{1/3}} - a_{A}\frac{(A-2Z)^{2}}{A} + \delta(A,Z) \longrightarrow \mathbb{R}^{2} = 0.999915$$
  
$$\delta(A,Z) = \begin{cases} +\delta_{0} & Z, N \text{ even} \\ 0 & A \text{ odd} \\ -\delta_{0} & Z, N \text{ odd} \end{cases} \delta_{0} = \frac{a_{P}}{A^{1/2}}$$


## Systems of Differential Equations

• Regress on derivative

State Variables

Derivatives

<u>time</u>	<u>x</u> 1	<u>X</u> 2	•••	$\underline{dx_{1}}/\underline{dt}  \underline{x_{2}}/\underline{dt}  \dots$
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



**Original Equations** 

**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 #3-60 ...





Symbolic Regression Inferred *Time-Delay* Model:

$$\frac{dK}{dt} = a_K + \frac{b_K + c_K S}{K}$$
$$\frac{dS}{dt} = a_S + \frac{b_S + c_S K}{S}$$

Biologist's Inferred Model: Gurol Suel, et. al., Science 2007

$$\frac{dK}{dt} = \alpha_k + \frac{\beta_K K^n}{k_0^n + K^n} - \frac{\delta_K K}{1 + K / \Gamma_K + S / \Gamma_S} - \lambda_K K$$
$$\frac{dS}{dt} = \alpha_S + \frac{\beta_S}{1 + (K / k_1)^p} - \frac{\delta_k S}{1 + K / \Gamma_K + S / \Gamma_S} - \lambda_S S$$

## Withheld Test Set #1 Fit

$$\frac{dG_t}{dt} = \frac{1582.0 + 17.3214 \cdot S_{t-51}}{G_{t-18}} - 16.7423$$
$$\frac{dS_t}{dt} = \frac{114.922 + 0.3019 \cdot G_{t-25}}{S_{t-15}} - 3.05$$



## Withheld Test Set #2 Fit

$$\frac{dG_t}{dt} = \frac{3526.92 - 21.312 \cdot S_{t-54}}{G_{t-17}} - 10.1355$$
$$\frac{dS_t}{dt} = \frac{132.271 - 0.0178 \cdot G_{t-57}}{S_{t-18}} - 2.9693$$



## Withheld Test Set #3 Fit

$$\frac{dG_t}{dt} = \frac{5057.1 - 39.7452 \cdot S_{t-46}}{G_{t-21}} - 6.4406$$
$$\frac{dS_t}{dt} = \frac{295.426 - 0.2965 \cdot G_{t-54}}{S_{t-20}} - 3.871$$





# Looking For Invariants

# **Data Mining**









## 42

## 42+x-x

## 42+1/(1000+x<sup>2</sup>)



			Calculate nartial derivatives Numerically
x	У	•••	
0.1	2.3		
0.2	4.5		$\delta x \qquad \delta y$
0.3	9.7		$-$ , $\frac{\cdot}{\circ}$ ,
0.4	5.1		$\partial y \qquad \partial x$
0.5	3.3		·
0.6	1.0		
	•••	•••	



## **Experiments**



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

 $x^3 + x - y^2 - 1.5 = 0$ 

 $x^2 + y^2 + z^2 - 1 = 0$ 





$$H = 114.28 * \left(\frac{dx}{dt}\right)^2 + 692.322 * x^2$$
$$L = 61.591 * \left(\frac{dx}{dt}\right)^2 - 369.495 * x^2$$
.

• 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**











### С

#### Detected Invariance:

 $L_{1}^{2}(m_{1}+m_{2})\omega_{1}^{2}+m_{2}L_{2}^{2}\omega_{2}^{2}+m_{2}L_{1}L_{2}\omega_{1}\omega_{2}\cos(\theta_{1}-\theta_{2})-19.6L_{1}(m_{1}+m_{2})\cos\theta_{1}-19.6m_{2}L_{2}\cos\theta_{2}$ 





eq	9 Untitled - Eureqa 💶 🗖						- = X			
File	Edit Contr	ol Options	Tools View	Help						
	Enter Data	Smooth	Data $f(x)$	Pick Modeling	Task	Start Search	Solu	tion Statistics		
	A	В	С	D	E	F	G	Н	I.	J_
desc	some variable	some other variable	confidence in y							
var	x	у	w							
1	-3.00	-1.62	1.00					1		
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					1		
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							
,72	_1 74	.0 9R	0 55							





Eureqa







							Kraft		Moment
	Bauteil	Formel	nı	n <sub>2</sub>	n <sub>3</sub>				
Cw	Rohr	$C_W = n_1 \left(\beta + \gamma\right)^{n_2} \cdot \left(\tau + \frac{n_3 \tau \cdot \beta}{n_4 - \beta}\right)^{n_5}$	1,3034	0,9145	-0,168	x	-		
	Nocken	$C_W = n_1 \left(\tau \cdot \gamma + n_2  \tau^3 \cdot \beta^3  \gamma + n_3  \tau \cdot \beta \cdot \gamma \right)^{n_4}$	2,149	-0,1871	-0,523				
~	Rohr	$C_L = \tau \left(\gamma + n_1 \beta\right)^{n_2}$	1,729	0,5269					
ն	Nocken	$C_L = exp((\tau \cdot \gamma)^{n_1} - \beta^{\beta})$	0,237					Non-	
~	Rohr	$C_N = n_1 \ \tau \ \beta \ \gamma + n_2 \ \tau \ \beta^2 \ \gamma$	2,233	-1,789					
ч	Nocken	$C_{N}=\beta+n_{1}\ \beta\ \gamma+n_{2}\ \tau\ \beta\ \gamma-\tau\ \beta^{2}\ \gamma+n_{3}\ \beta^{2}\ \gamma$	0,486	1,2526	-0,388		-		
	Rohr	$C_{T}=n_{1}t\pm n_{2}b^{4}$	0,903	0,268		Y			
CT	Nocken	$C_{T} = n_{1} \exp\left(\frac{n_{2} \tau + n_{2} \beta}{1 + n_{4} \gamma}\right)$	0,910	0,2223	0,47 37			X 🕨	No.
	Bauteil	Formel	ոլ	nz	n <sub>3</sub>	z			
Bw	Rohr	$B_W = \exp(n_1 \mid \beta \mid \gamma + n_2) \cdot \tau^{n_x} \cdot \gamma^{n_x}$	3,5363	-1,4796	0,9551)			nungstaktoren tur	
	Nocken	$B_W = n_1 \left(\gamma - \tau\right)^{(n_2 \tau^{n_3})}$	0,6354	0,5072	0,26126			die Rundnocken in der EN 13480-3	
	Rohr	$B_L = \tau \cdot exp((n_1/\gamma)^{n_2} + n_1 \cdot (\beta \cdot \gamma)^{n_3})$	1,6629	-0,07132	-2,645	-0,7284		Kapitel11 für Memb-	
•	Nocken	$B_L = n_1 \cdot exp(n_2 \ \tau \ \gamma + n_3 \ \tau \ \beta^{n_4} + n_5 \ \beta)$	1,0141	0,02131	-0,1538	-0,7421	-0,04504	Table 3: Proposal	
	Rohr	$B_N = n_1 \cdot exp(n_2 \ \beta) \ \cdot \ (n_3 \ \tau \ \gamma)^{(n_4 exp(n_4/\beta))}$	5,2163	0,16729	0,01469	0,7907	0,10408	for new stress	
B <sub>N</sub>	Nocken	$B_{N} = n_{1} \exp \left( \frac{n_{2'} \tau \beta + n_{3'} \tau / \gamma}{(\beta \cdot \tau + (n_{4} / \gamma)^{n_{4}})} \right)$	1,0523	1,7175	-7,1793	7,8903	1,4792	Intensification factor formulars for circular attachments in the EN 13480-3	
	Rohr	$B_T = n_1 \cdot \tau \cdot exp\left(\frac{n_2}{\gamma \cdot \beta^{\tau} \cdot (\tau \cdot \beta^2 - 1) - \beta \cdot \gamma \cdot (1 + n_3 \cdot \tau \cdot \beta)}\right)$	1,0646	2,008	0,02014			clause 11 for memb- rane stresses.	
Вт	Nocken	$B_{T} = n_{I} \left( \frac{\beta \cdot \gamma^{(n_{J}) \beta}}{\exp(n_{3} \tau)} \right)^{(1/(\gamma + n_{s} \beta)' \tau)}$	0,9369	2,594	2,0855	2,4033			

Von Thomas Hermanowski, Dr. Andreas Rick, Dr. Jochen Weber



# Scalability

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

## **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 (4 <sup>th</sup> order)			

# Alphabet



# **Time to Regress**



## **STOCHASTIC MODELS**
### 10% Noise



#### 30% Noise





### 70% Noise







## **Regressing Stochastic elements**

Add a "noise" building block

-1









#### Likelihood Fitness

# Find a model that maximizes the probability of seeing this data



# **Sample the Timespan**





#### **Short Time Gaps in Experimental Data:**



Long Time Gaps in Experimental Data:



# **Concluding Remarks**

Chris Anders

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

Wired 16.07

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

# The New York Eimes

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

## The end of insight

I am worried that we have enjoyed a brief window in human history where we could actually understand things, but that period may be coming to an end.

-- Steve Strogatz







 $k_{1}/k_{1} = 1$   $k_{2}/k_{1} = m_{2}L_{2}^{2}/(m_{1}L_{1}^{2} + m_{2}L_{1}^{2})$   $k_{3}/k_{1} = 2.00055m_{2}L_{2}/(m_{1}L_{1} + m_{2}L_{1})$   $k_{4}/k_{1} = 19.6/L_{1}$   $k_{5}/k_{1} = 19.6 \cdot m_{2}L_{2}/(m_{2}L_{1}^{2} + m_{1}L_{1}^{2})$   $L_{1}^{2}(m_{1} + m_{2})\omega_{1}^{2} + m_{2}L_{2}^{2}\omega_{2}^{2} + 2 \cdot m_{2}L_{1}L_{2}\omega_{1}\omega_{2}\cos\left(\theta_{1} - \theta_{2}\right)$   $-19.6 \cdot L_{1}(m_{1} + m_{2})\cos\theta_{1} - 19.6m_{2}L_{2}\cos\theta_{2}$