

## Hypothesis management in support of the e-scientific method

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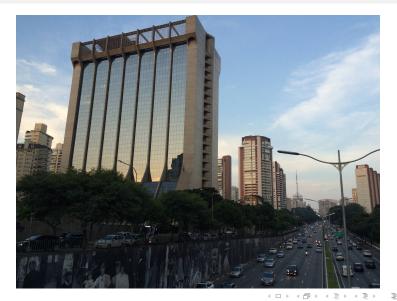
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1 / 49

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### IBM: São Paulo's Building in Vila Mariana



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#### The e-Scientific Method

"Originally, there was just experimental science, and then there was theoretical science, with Kepler's Laws, Newton's Laws of Motion, Maxwell's equations, and so on. Then, for many problems, the theoretical models grew too complicated to solve analytically, and people had to start simulating. These simulations have carried us through much of the last half of the last century. At this point, these simulations are generating a whole lot of data, along with a huge increase in data from the experimental sciences." — Jim Gray, 2007

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• Scientific research is based on the central idea of a hypothesis , meant to be established or refuted.



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 Hypothesis management can be, therefore, closely related to the management of probabilistic data.



• ...A 'crucial experiment' allegedly establishes the truth of one of a set of competing theories (Routledge Encyc. of Philosophy).

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#### **Research Vision** (1)

- Use Case

#### Probabilistic DB Construction Pipeline

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#### From Hypotheses to Data

#### Law of free fall

"If a body falls from rest, then its velocity at any point is proportional to the time it has been falling."

(i)

(iii)

а -g $v = -g t + v_0$  $s = -(g/2) t^2 + v_0 t + s_0$ (ii)

FALL	t	v	5
	0	0	5000
	1	-32	4984
	2	-64	4936
	3	-96	4856
	4	-128	4744

(iv)

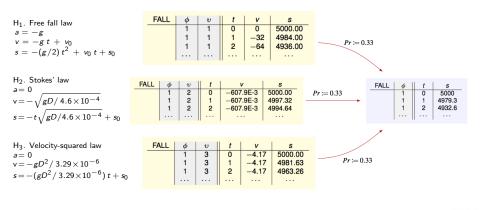
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## Rival Hypotheses: a Probability Distribution

Rival hypotheses supposed to explain the same phenomenon.



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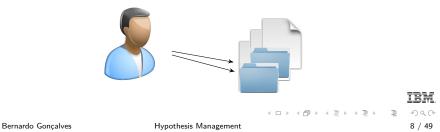
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## Concrete Use Scenario in Computational Science

#### Example 1.

Bob is a computational scientist who is playing with a number of **models and different parameter settings** to see which one gives a best fit to his observation samples.

Each run constitutes a specific model instantiation that is associated with a unique file ('big table'). In the end of the day his resulting datasets are spread over many files and folders.



#### Beyond Files: a Big Table Database

• User's **default** choice: struggle with the files to find relevant data.

#### "There is life beyond files." (Jim Gray)

FALL	tid	t	g	v <sub>0</sub>	<i>s</i> <sub>0</sub>	а	v	5
	1	0	32	0	5000	-32	0	5000
	1	1	32	0	5000	-32	-32	4984
	1	2	32	0	5000	-32	-64	4936
						•••		
	2	0	32.2	0	5000	-32.2	0	5000
	2	1	32.2	0	5000	-32.2	-32.2	4983.9
	2	2	32.2	0	5000	-32.2	-64.4	4935.6

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#### Do Better: a Hypothesis Database

$$a = -g$$
  

$$v = -g t + v_0$$
  

$$s = -(g/2) t^2 + v_0 t + s_0$$

FALL	tid	t	g	V <sub>0</sub>	<i>s</i> 0	a	v	5
-	1	0	32	0	5000	-32	0	5000
	1	1	32	0	5000	-32	-32	4984
	1	2	32	0	5000	-32	-64	4936
	2	0	<mark>32.2</mark>	0	5000	<mark>-32.2</mark>	0	5000
	2	1	32.2	0	5000	-32.2	-32.2	4983.9
	2	2	32.2	0	5000	-32.2	-64.4	4935.6

- Predictive structure: strong correlations from the math models (!).
- Project-level **standardization**: pick a favorite MathML editor to report and manage model equations declaratively.

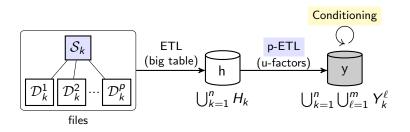
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## Design-by-Synthesis Pipeline



- Technical challenges:
  - 1 **Encoding** : math equations  $\rightarrow$  structural eqs.  $\rightarrow$  functional deps.;
  - 2 Causal reasoning : inferring the causal ordering and u-factors;
  - ③ Probabilistic DB synthesis: normalization based on the u-factors;
  - **Gonditioning**: probability distribution update in face of evidence.

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#### 1 Research Vision

- Hypothesis Management
- Use Case

#### 2 Probabilistic DB Construction Pipeline

- Hypothesis Encoding
- Probabilistic DB Synthesis
- Prototype System

#### 3 Conclusions

- Takeaways
- Future Work
- Appendix

3

## Given set $\mathcal{E}$ of equations over set $\mathcal{V}$ of variables... (1)

Law of free fall:

 $\Sigma = \{$  $\mathcal{H} = \{$  $\phi$  $\rightarrow g$ , g = 32, $v_0 = 0$ .  $\phi$  $\rightarrow$   $v_0$ , h-encode  $s_0 = 5000$ ,  $\phi$  $\rightarrow$   $s_0$ , a = -g,  $g v \rightarrow a$ ,  $\mathbf{v} = -g t + \mathbf{v}_0,$  $g v_0 t v \rightarrow v$ ,  $s = -(g/2)t^2 + v_0 t + s_0$  $g v_0 s_0 t v \rightarrow s \}.$ 

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13 / 49

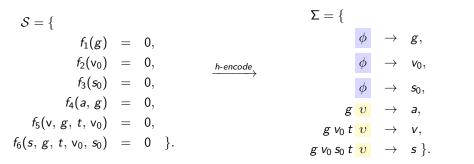
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#### Encoding

## Given set $\mathcal{E}$ of equations over set $\mathcal{V}$ of variables... (2)

I aw of free fall:



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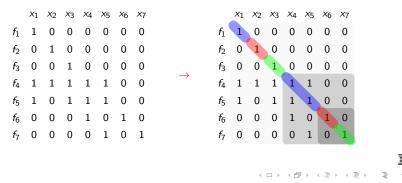
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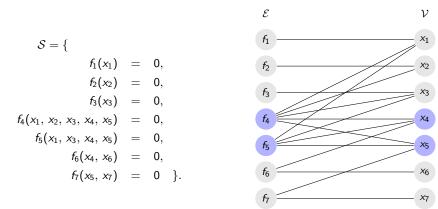
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# Causal Ordering Algorithm (Al Literature)

- Identify 'minimal substructures' at step k;
- 2 Reduce the matrix by eliminating them;
- 3 Call step k+1 recursively.



#### Equivalent to Finding a Biclique $K_{m,n}$ in a Bipartite Graph

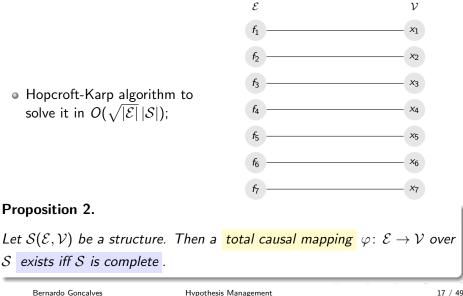


#### Theorem 1.

Let  $S(\mathcal{E}, \mathcal{V})$  be a complete structure. The extraction of its causal ordering by COA(S) tries to solve an NP-Hard problem.

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## Easier: Complete Matching in a Bipartite Graph



#### Provably Correct Approach to Hypothesis Encoding

$$C_{\varphi} = \{ (x_a, x_b) | \text{ there exists } f \in \mathcal{E} \text{ such that } \varphi(f) = x_b \\ \text{ and } x_a \in Vars(f) \}$$

#### Proposition 1.

Let  $S(\mathcal{E}, \mathcal{V})$  be a structure, and  $\varphi_1 \colon \mathcal{E} \to \mathcal{V}$  and  $\varphi_2 \colon \mathcal{E} \to \mathcal{V}$  be any two total causal mappings over S. Then  $C_{\varphi_1}^+ = C_{\varphi_2}^+$ .

## Causal Ordering: Sub-Quadratic Complexity on $|\mathcal{S}|$

#### Corollary 1.

Let  $S(\mathcal{E}, \mathcal{V})$  be a complete structure. Then a total causal mapping  $\varphi \colon \mathcal{E} \to \mathcal{V}$  over S can be found by TCM(S) in time that is bounded by  $O(\sqrt{|\mathcal{E}|} |S|)$ .



Artificial Intelligence Volume 238, September 2016, Pages 154-165



#### A note on the complexity of the causal ordering problem

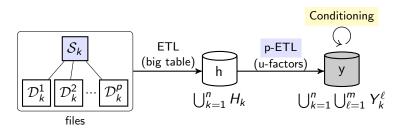
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## Coming Back from Detail



- Technical challenges:
  - **I Encoding** : math equations  $\rightarrow$  structural eqs.  $\rightarrow$  functional deps.;
  - 2 Causal reasoning : inferring the causal ordering and u-factors;
  - ③ Probabilistic DB synthesis: normalization based on the u-factors;
  - 4 Conditioning: probability distribution update in face of evidence.

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#### Bob's Big Table (before our help)

$H_3$	tid	$ \phi$	v	t	<i>x</i> 0	Ь	p	<i>y</i> 0	d	r	x	У
	1	1	3	0	30	.5	.02	4	.75	.02	30	4
	1	1	3		30	.5	.02	4	.75	.02		
	2	1	3	0	30	.5	.018	4	.75	.023	30	4
	2	1	3		30	.5	.018	4	.75	.023		
	3	1	3	0	30	.4	.02	4	.8	.02	30	4
	3	1	3		30	.4	.02	4	.8	.02		
	4	1	3	0	30	.4	.018	4	.8	.023	30	4
	4	1	3		30	.4	.018	4	.8	.023		
	5	1	3	0	30	.397	.02	4	.786	.02	30	4
	5	1	3		30	.397	.02	4	.786	.02		
	6	1	3	0	30	.397	.018	4	.786	.023	30	4
	6	1	3	5	30	.397	.018	4	.786	.023	50.1	62.9
	6	1	3	10	30	.397	.018	4	.786	.023	13.8	8.65
	6	1	3	15	30	.397	.018	4	.786	.023	79.3	8.23
	6	1	3	20	30	.397	.018	4	.786	.023	12.6	30.7
	6	1	3		30	.397	.018	4	.786	.023		

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#### Synthesized Tables: Ready for Predictive Analysis

			x <sub>1</sub> x <sub>1</sub>	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	v 1 2 3				
Y <sup>1</sup> <sub>3</sub> V ×	$( \mapsto D )$ $( :_2 \mapsto 1 )$	∲ <u>×</u> 0 1 30	$\begin{array}{c c} \mathbf{Y}_3^2 & \boldsymbol{V} \mapsto \\ & \mathbf{X}_3 \mapsto \\ & \mathbf{X}_3 \mapsto \\ & \mathbf{X}_3 \mapsto \end{array}$	$\begin{array}{c c} 1 & 1 & . \\ 2 & 1 & . \end{array}$	b 5 4 97	Y	$\begin{array}{c c} V \mapsto \\ x_4 \mapsto \\ x_4 \mapsto \end{array}$	1 1	.020
۲ <sup>4</sup>	$V_1 \mapsto D_1$	$V_2 \mapsto D_2$	$V_3 \mapsto D_3$	$V_4 \mapsto D_4$	$ \phi$	v	t	y y	x
	$x_1\mapsto 3$	$x_2\mapsto 1$	$x_3\mapsto 1$	$x_4\mapsto 1$	1	3	1900	4	30
3	$x_1\mapsto 3$	$x_2\mapsto 1$	$x_3\mapsto 1$	$x_4\mapsto 1$	1	3			
					1	3			
3	$x_1\mapsto 3$	$x_2\mapsto 1$	$x_3\mapsto 3$	$x_4\mapsto 2$	1	3	1900	4	30
:	$x_1\mapsto 3$	$x_2\mapsto 1$	$x_3\mapsto 3$	$x_4\mapsto 2$	1	3	1901	4.12	41.5
2	$x_1\mapsto 3$	$x_2\mapsto 1$	$x_3\mapsto 3$	$x_4\mapsto 2$	1	3	1902	5.78	56.7
2	$x_1 \mapsto 3$	$x_2\mapsto 1$	$x_3\mapsto 3$	$x_4\mapsto 2$	1	3	1903	11.7	72.8
2	$x_1\mapsto 3$	$x_2\mapsto 1$	$x_3\mapsto 3$	$x_4\mapsto 2$	1	3	1904	31.1	75.9
2	$x_1 \mapsto 3$	$x_2\mapsto 1$	$x_3\mapsto 3$	$x_4\mapsto 2$	1	3			

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#### Querying Rival Predictions with Probabilities

$Y_3^4$	$V_1 \mapsto D_1$	$V_2 \mapsto D_2$	$V_3 \mapsto D_3$	$V_4 \mapsto D_4$	$\phi$	v	t	y	x
	$x_1\mapsto 3$	$x_2\mapsto 1$	$x_3\mapsto 1$	$x_4\mapsto 1$	2	3	1900	4	30
	$ x_1 \mapsto 3 $	$x_2 \mapsto 1$	$x_3\mapsto 3$	$\begin{matrix} \\ x_4 \mapsto 2 \end{matrix}$	2	3	1904		75.92

W	$V \mapsto D$	Pr
	$x_1 \mapsto 2$	.33
	$x_1 \mapsto 3$	.33
	$x_1 \mapsto 3$	.33
	$x_2\mapsto 1$	1
	$x_3\mapsto 1$	.33
	$x_3 \mapsto 2$	.33
	$x_3 \mapsto 3$	.33
	$x_4\mapsto 1$	.5
	$x_4 \mapsto 2$	.5

Operation conf();

$$\theta = \{ x_1 \mapsto 3, x_2 \mapsto 1, x_3 \mapsto 3, x_4 \mapsto 2 \},$$
  

$$Pr = .33 * 1 * .33 * .5 \approx .055$$

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#### Prototype System

# Prototype System (1)



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## Prototype System (2)

Phenomenon data definition
Phenomenon id
2
Research
Population dynamics •
Description
Lynx population in Hudson's Bay, Canada, from 1900 to 1920.
A
Upload dataset (CSV format) Choose File Lynx, Hare.csv
Loading observations
70%
Observable
Year
Lynx

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## Prototype System (3)

Hyphotesis data definition		
Hypothesis id		
3		
Name		
Lotka-Volterra model		
Upload structure (XML format)		
Choose File Lotka_Volterra.xml		
	esis structure: 100%	
		-
Phenomenon		
Lynx population in Hudson's Bay, Car	nada, from 1900 to 1920.	
Map symbols		
Variable	Observable	
t	Year	
x	Lynx	
Hypothesis trial datasets (MAT format) Choose Files 10 files		

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## Prototype System (4)

pothesis							
Lotka-Volterra i	nodel						•
nenomenon							
Lynx population	n in Hudson's Bay	/, Canada, fro	m 1900 to	1920.			٠
mulation trial							•
D							•
	1						
Key 1 Key 2							
« 1	2 3 4	5 6 7	8 9	10	20	*	
t	1	у			x		
1904.0	31.10839	20070696		75.91	9696193	2191	
1904.1	34.18958	28779035		74.48	37810531	5043	
1904.2	37.43564	90187431		72.66	57515697	7604	
1904.3	40.80083	12965646		70.47	0587438	5644	
1904.4	44.22626	96820135		67.92	3025178	0413	
1904.5	47.64177	55935588		65.06	54992050	2872	
1904.6	50.96913	09633260		61.94	9374370	0121	

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## Prototype System (5)

enomenon			
ynx population in Hu	idson's Bay, Canada, I	rom 1900 to 1920.	
Observations Predi	ctions		
	K 1 :	23 >>	
	Year	Lynx	Hare
	$\checkmark$	<b>~</b>	● ×
	1900	30	4
	1901	47.2	6.1
	1902	70.2	9.8
	1903	77.4	35.2
	1904	36.3	59.4
	1905	20.6	41.7
	1906	18.1	19
	1907	21.4	13

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## Prototype System (6)

omenon				
ix populatio	n in Huo	ison's Bay, (	anada, from 1900 to 1920.	
servations	Predict	tions		
« 1	2	3 4	6 7 8 9 10	20 »
upsilon	tid	Year	Lynx	conf
aponon	eiu	rear	Lynx	com
3	2	1904	65.060410460081	0.183505
3	6	1904	75.919696193219	0.179993
3	4	1904	77.459735769215	0.175992
3	1	1904	89.592307430943	0.131452
3	5	1904	88.321831841064	0.127000
3	3	1904	90.083803232660	0.124023
1	1	1904	16.487212706992	0.047211
2	2	1904	77.822475573932	0.017372
2	1	1904	79.812581025093	0.013234
1	2	1904	18.221188003898	0.000220

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#### Takeaways

We have seen:

- The automatic construction of a probabilistic DB (out of math equations and datasets) to support the analysis of crucial exps.
- This is hypothesis management (as data management and analytics) in support of the e-scientific method .

(Papers: PVLDB'14, IEEE Computing in Science & Eng.'15, Artif. Intell.'16)

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31 / 49

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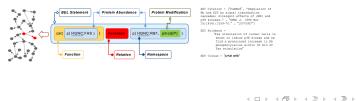
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## Future Work: in the field of Bioinformatics

- Recommendation of crucial experiments;
  - Find 'rival' (structurally similar) math models from a repository;
  - ${\scriptstyle \circ}$  Example: BioModels (EMBL-EBI), with 1.6K+ models stored.

#### Future Work: in the field of Bioinformatics

- Recommendation of crucial experiments;
  - Find 'rival' (structurally similar) math models from a repository;
  - Example: BioModels (EMBL-EBI), with 1.6K+ models stored.
- Refutation attempts (sense of Karl Popper);
  - Look for negative claims in the literature.
  - Example: Causal Biological Networks, with 120+ models stored (each has hundreds of hypothetical claims).



Conclusions Future Work

# Thank you.

#### Acknowledgements





Conselho Nacional de Desenvolvimente Científico e Tecnológico Fundação Carlos Chagas Filho de Amparo à Pesquisa do Estado do Rio de Janeiro

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### Questions?

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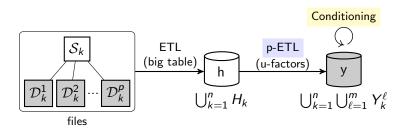
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#### Appendix

#### Design-by-Synthesis Pipeline



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  - **Conditioning**: probability distribution update in face of evidence. 4

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## The Folding $\Sigma^{\ensuremath{\varphi}\ensuremath{\rightarrow}}$ of $\Sigma$

Acyclic pseudo-transitive reasoning

#### $\label{eq:algorithm 1} \textbf{Algorithm 1} \ \textbf{Folding of an fd set}.$

1: **procedure** FOLDING( $\Sigma$ : fd set) **Require:**  $\Sigma$  given encodes complete structure S **Ensure:** Returns fd set  $\Sigma^{\oplus}$ , the folding of  $\Sigma$ 2:  $\Sigma^{\oplus} \leftarrow \emptyset$ 3: **for all**  $\langle X, A \rangle \in \Sigma$  **do** 

4: 
$$Z \leftarrow AFolding(\Sigma, A)$$

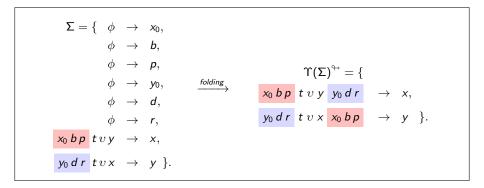
5: 
$$\Sigma^{\Upsilon} \leftarrow \Sigma^{\Upsilon} \cup \langle Z, A \rangle$$

6: return  $\Sigma^{\to}$ 

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## The Folding $\Sigma^{\ensuremath{\gamma}\ensuremath{\rightarrow}}$ of $\Sigma$

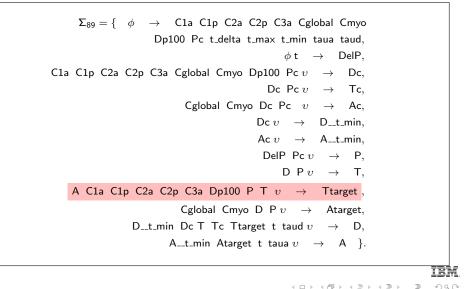
Acyclic pseudo-transitive reasoning



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#### FD set $\Sigma_{89}$ (a real Physiology Model that "fits the screen")



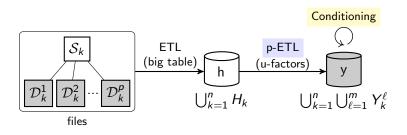
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## Its Folding $\Sigma_{89}^{\hookrightarrow}$

$$\begin{split} \Upsilon(\Sigma_{89})^{\leftrightarrow} &= \{ \begin{array}{ccc} \text{C1a } \text{C2a } \phi \ \upsilon & \rightarrow & \text{A\_t\_min } \text{Ac } \text{D\_t\_min } \text{Dc } \text{Tc}, \\ & \text{C1a } \text{DelP } \phi \ \upsilon & \rightarrow & \text{P}, \\ \end{array} \\ \hline \\ \textbf{C1a } \text{C2a } \text{DelP } \phi \ \textbf{t} \ \upsilon \ \textbf{T} & \rightarrow & \text{A } \text{Atarget } \text{D } \text{Ttarget} \end{array} \}. \end{split}$$

#### Appendix

#### Design-by-Synthesis Pipeline



- Technical challenges: •
  - **Encoding**: math equations  $\rightarrow$  structural eqs.  $\rightarrow$  functional deps.; 1
  - **Causal reasoning**: inferring the causal ordering and u-factors; 2
  - **Probabilistic DB synthesis:** normalization based on the u-factors; 3
  - **Conditioning**: probability distribution update in face of evidence. 4

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Hypothesis Management



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#### Defining the Theoretical U-factor

$$Y_0 := \pi_{\phi, v} ( ext{repair-key}_{\phi}(H_0)).$$

$\phi$		$Y_0$	$V\mapsto D$	$\phi$	v	١	N	$V\mapsto D$	Pr
 1	1		$x_1\mapsto 1$	1	1			$x_1\mapsto 1$	.33
1	2		$\begin{array}{c} x_1\mapsto 1\\ x_1\mapsto 2\end{array}$	1	2			$x_1 \mapsto 2$	.33
1 1 1	3		$x_1 \mapsto 3$	1	3			$x_1 \mapsto 3$	.33

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#### U-factor Learning

Discovery of contingent functional dependencies

- 'Input' relation of the Lotka-Volterra hypothesis. Observe:
  - Multiplicity of parameter values;
  - Correlations between parameter values.

$H_3^1$	tid	$\phi$	<i>x</i> 0	Ь	р	<i>y</i> 0	d	r
	1	1	30	.5	.020	4	.75	.020
	2	1	30	.5	.018	4	.75	.023
	3	1	30	.4	.020	4	.8	.020
	4	1	30	.4	.018	4	.8	.023
	5	1	30	.397	.020	4	.786	.020
	6	1	30	.397	.018	4	.786	.023

$$\Omega = \{ \begin{array}{ccc} \phi \ x_0 & \to & y_0, \\ \phi \ b & \to & d, \\ \phi \ p & \to & r \end{array} \}.$$
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#### **U**-factorization

Defining the Empirical U-factors

$$Y_k^i := \pi_{\phi A G} \left( \mathsf{repair-key}_{\phi @ \mathit{count}} \left( \gamma_{\phi, A, G, \mathit{count}(*)}(H_k) \right) \right).$$

$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Y <sub>3</sub> <sup>2</sup>	$V \mapsto$ $x_3 \mapsto$ $x_3 \mapsto$ $x_3 \mapsto$	$ \begin{array}{c c} D & \phi \\  & 1 & 1 \\  & 2 & 1 \\  & 3 & 1 \end{array} $	b .5 .4 .39	<i>p</i> .5 .8 7.786
	-	W	<i>V</i> ↔	D	Pr 
$\begin{array}{c c c c c c c c c c c c c c c c c c c $			$\begin{array}{c} x_2 \mapsto \\ x_3 \mapsto \\ x_3 \mapsto \\ x_3 \mapsto \end{array}$	1 2	1 .33 .33 .33
			$x_4 \mapsto x_4 \mapsto$	1	.5 .5

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#### **Design-Theoretic Properties**

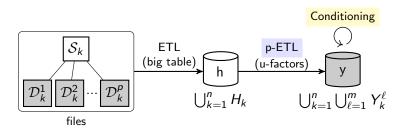
- Desirable properties for probability update are ensured;
  - Claim-centered decomposition.
    - Theorem 6: **BCNF** w.r.t. causal dependencies.
  - **Correctness** of uncertainty decomposition.
    - Theorem 7: Lossless join w.r.t. causal dependencies.

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#### Appendix

### Design-by-Synthesis Pipeline



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#### Systematic Application of Bayesian Inference

- User selection of the **observation** sample;
- ② System selection of the competing prediction samples;
- 3 Bayesian inference ;
- ④ Probability distribution update;

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#### Bayes' Rule

• Normal density **likelihood** function:

$$f(y \mid \mu_k) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(y-\mu_k)^2}$$
(1)

Bayes ' rule:

$$p(\mu_k | y_1, ..., y_n) = \frac{\prod_{j=1}^n f(y_j | \mu_{kj}) p(\mu_k)}{\sum_{i=1}^m \prod_{j=1}^n f(y_j | \mu_{ij}) p(\mu_i)}$$
(2)

----

where  $y_1, \ldots, y_n$  is the observation sample,  $\mu_k$  is prediction k and  $\sigma$  is the standard deviation parameter.

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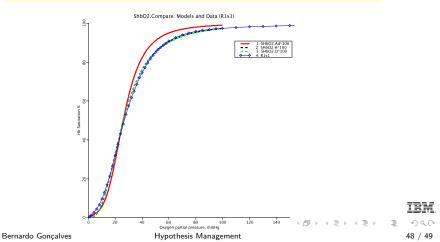
47 / 49

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#### Probability Update in Face of Evidence

STUDY	$\phi$	v	pO2	SHbO2	Prior	Posterior
	1	32	100	9.72764121981342E-1	.333	.335441
	1	28	100	9.74346796798538E-1	.333	.335398
	1	31	100	9.90781330988763E-1	.333	.329161



#### Viewpoint: Why Hypothesis Management?



"Numerical simulations and 'big data' are essential in modern science, but they do not alone yield understanding. Building a massive database to feed simulations without corrective loops between hypotheses and experimental tests seems, at best, a waste of time and money." Nature 513, Sept 2014.

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49 / 49

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