Semantic Hierarchies in Knowledge Analysis and Integration

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Information Sciences Group

DIMACS Workshop on Recent Advances in Mathematics and Information Sciences for Analysis and Understanding of Massive and Diverse Sources of Data

May 2007

OUTLINE

- The challenge of semantic information for knowledge systems
- Large computational ontologies
  - Analysis
  - Induction
  - Interoperability
- Order theoretical approaches
  - Ontology anlaysis
  - Concept lattices: Formal Concept Analysis

APPLICATION CHALLENGES

Decision Support: Military, intelligence, disaster response

Intelligence Analysis: Multi-Int integration: IMINT, HUMINT, SIGINT, MASINT, etc.

Biomedicine: Biothreat response

Defense Applications: Defense transformation, situational awareness, global ISR

Bibliometrics: Digital libraries, retrieval and recommendation

Simulation: Interaction with knowledge management/decision support environments

Nonproliferation: "Ubiquitous sensing", information fusion

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KNOWLEDGE SYSTEMS

- Challenge for database integration at the **knowledge** level:

  Connectivity: Wiring everything up, everything *accessible*

  Interoperability: Knowing *what* you have and *where* it is
- Complement *quantitative* statistical techniques with *qualitative* methods:
  - Knowledge representation, natural language processing
  - Search, retrieval, inference
  - Focus on the *meaning* (*semantics*) of information in databases: use, interpretation
- In conjunction with existing capabilities in data mining, machine learning, sensor technology, simulation, etc.
  - **Knowledge-based and data-rich sciences:** Biology, astronomy, earth science
  - **Knowledge-based technologies for national security:** Decision support, intelligence analysis
  - **Knowledge-based technologies supporting the scientific process:** Semantic web, digital libraries, publication process, communities of networked scientists

MULTI-MODAL DATA FUSION

- Qualitative difference:

  Sensors:

  - Physics sensors: nuclear, radiological, chemical
  - Electromagnetic spectrum
  - Acoustic, seismic
  - Images, video

  Information Sources:

  - Geospatial
  - Structured and semi-structured data
  - Relational databases
  - Text, documents
  - Plans, scenarios

- How to bridge?
  - Meta-data
  - Feature extraction from signals, images
  - Feature ontologies and interoperability protocols

LANL KNOWLEDGE AND INFORMATION SYSTEMS SCIENCE

http://www.c3.lanl.gov/knowledge

Semantic Hierarchies for Knowledge Systems

- Representations of *semantic* and *symbolic* information
- Approach from *mathematical systems theory*:
  - Discrete math, combinatorics, information theory
  - Metric geometry approach to order theory (lattices and posets)
- *Hybrid* methodologies combining statistical, numerical, and quantitative with symbolic, logical, and qualitative
- **Ontologies and Conceptual Semantic Systems:** Discrete mathematical approaches
- **Computational Linguistics and Lexical Semantics:** For natural language processing and text extraction
- **Database Analysis:** User-guided knowledge discovery in complex, multi-dimensional data spaces
- **Software Architectures:** Parallel and high performance algorithms

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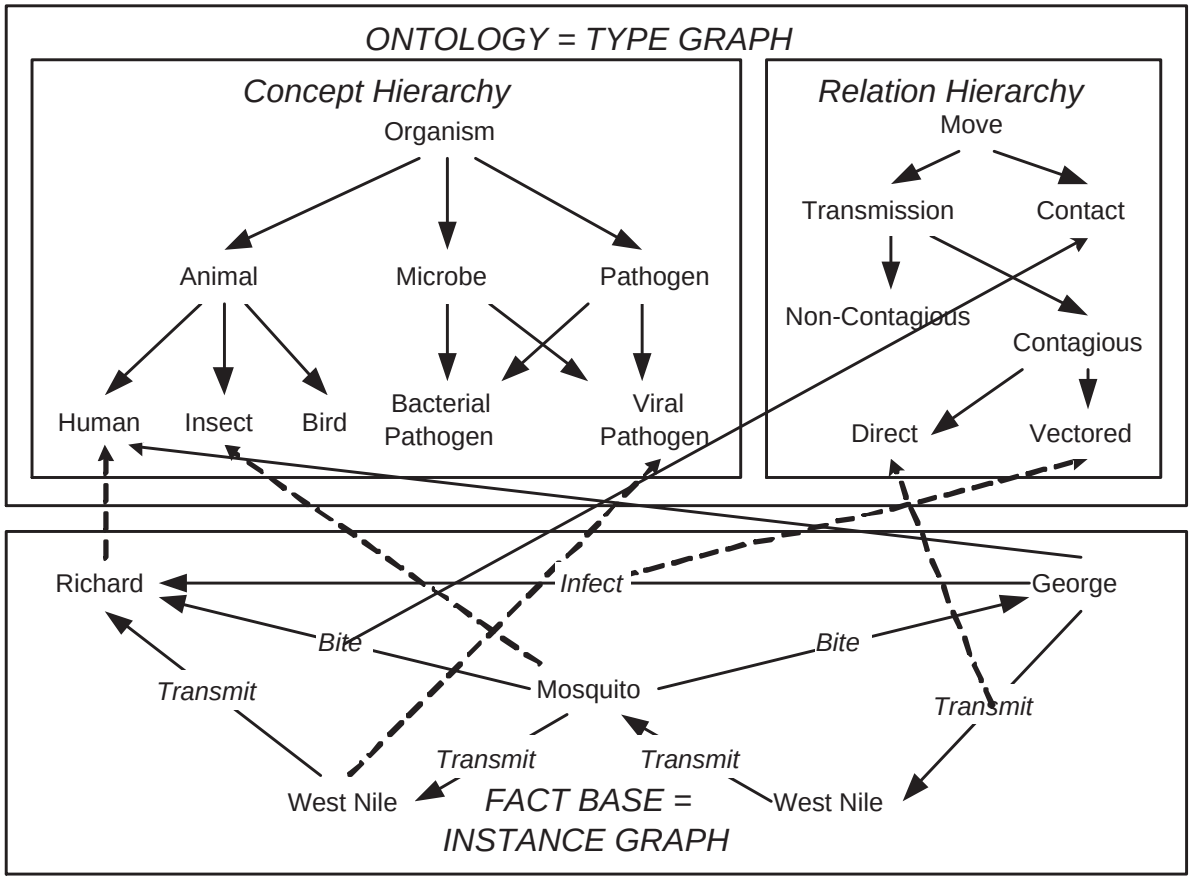
PARADIGM: SEMANTIC NETWORKS

- **Lattice-labeled directed multi-graphs**
- **Increasing size and prominence for databases:** Intelligence analysis, law enforcement, computa-tional biology



- **Challenges:** Typed-link network theory; morphisms of typed graphs; ontology analysis, induction, and interoperability.

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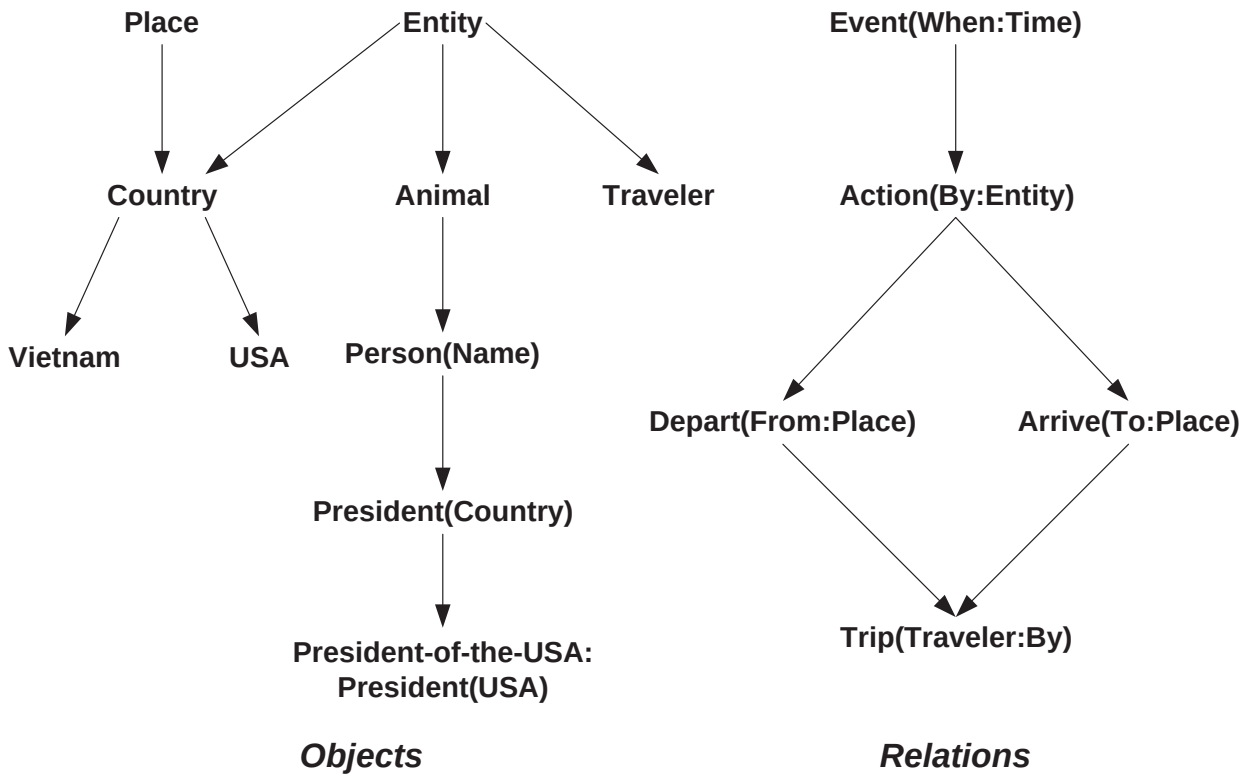
REASONING WITHIN ONTOLOGIES FOR THE SEMANTIC WEB

- Proposed basis for Semantic Web
- Ontological database: interacting hierarchies of objects and relations



- Semantic relations valued on objects
- Description-logic queries

Who was the last president before Clinton to visit Vietnam?

`>>: (Name(By)) ( Trip?`x `( To:Vietman, By:President-of-the-USA ) .and. lub(When(`x`)) <` `1992)`

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BIO-ONTOLOGIES

- Domain-specific concepts, together with *how they're related semantically*
- Crushing need driven by the genomic revolution
- *At least:*
  - **Large** terminological collections (controlled vocabularies, lexicons)
  - Organized in taxonomic, hierarchical relationships
- *Sometimes in addition:* Methods for inference over these structures
- Molecular, anatomy, clinical, epidemiological, etc.:

  Gene Ontology: Molecular function, biological process, cellular location

  Fundamental Model of Anatomy

  Unified Medical Language System: National Library of Medicine, meta-thesaurus

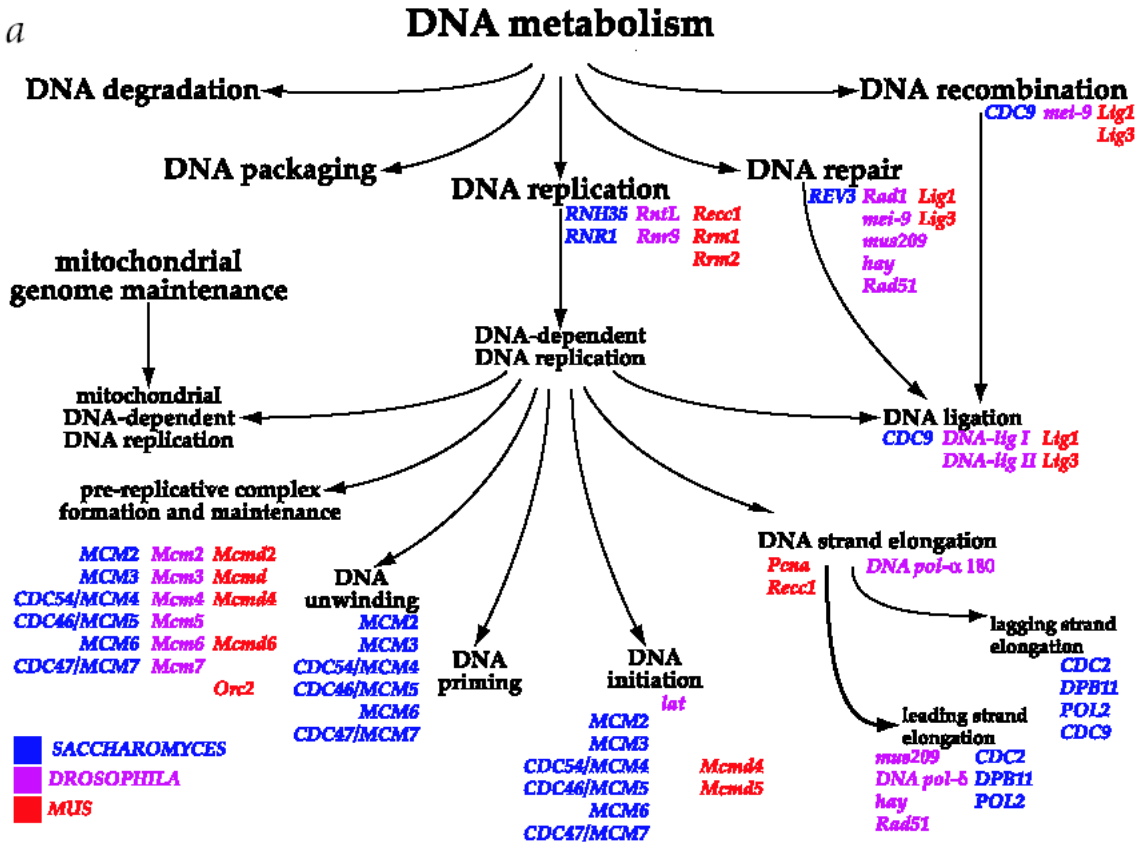
  Open Biology Ontologies

  MEdical Subject Headings (MeSH)

  Enzyme Structures Database: EC numbers

GENE ONTOLOGY (GO): DNA METABOLISM PORTION

- Taxonomic controlled vocabulary
- $\sim 20K$ nodes populated by genes, proteins
- Two orders $\leq_{isa}, \leq_{has}$
- Major community effort: assuming primary position in general bioinformatics



Gene Ontology Consortium (2000): "Gene Ontology: Tool For the Unification of Biology", *Nature Genetics*, 25:25-29

- Tremendous computational resource: large, semantically rich, validated, middle ontology, first (?) in major use

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CATEGORIZATION IN THE GENE ONTOLOLGY

http://www.c3.lanl.gov/posoc

- Develop functional hypotheses about hundreds of genes identified through expression experiments
- Given the Gene Ontology (GO) ...
- And a list of hundreds of genes of interest ...
- "Splatter" them over the GO ...
- Where do they end up?
  - Concentrated?
  - Dispersed
  - Clustered?
  - High or low?
  - Overlapping or distinct?
- POSet Ontology Categorize (POSOC)

C Joslyn, S Mniszewski, A Fulmer, and G Heaton: (2004) "The Gene Ontology Categorizer", *Bioinformatics*, v. **20**:s1, pp. 169-177

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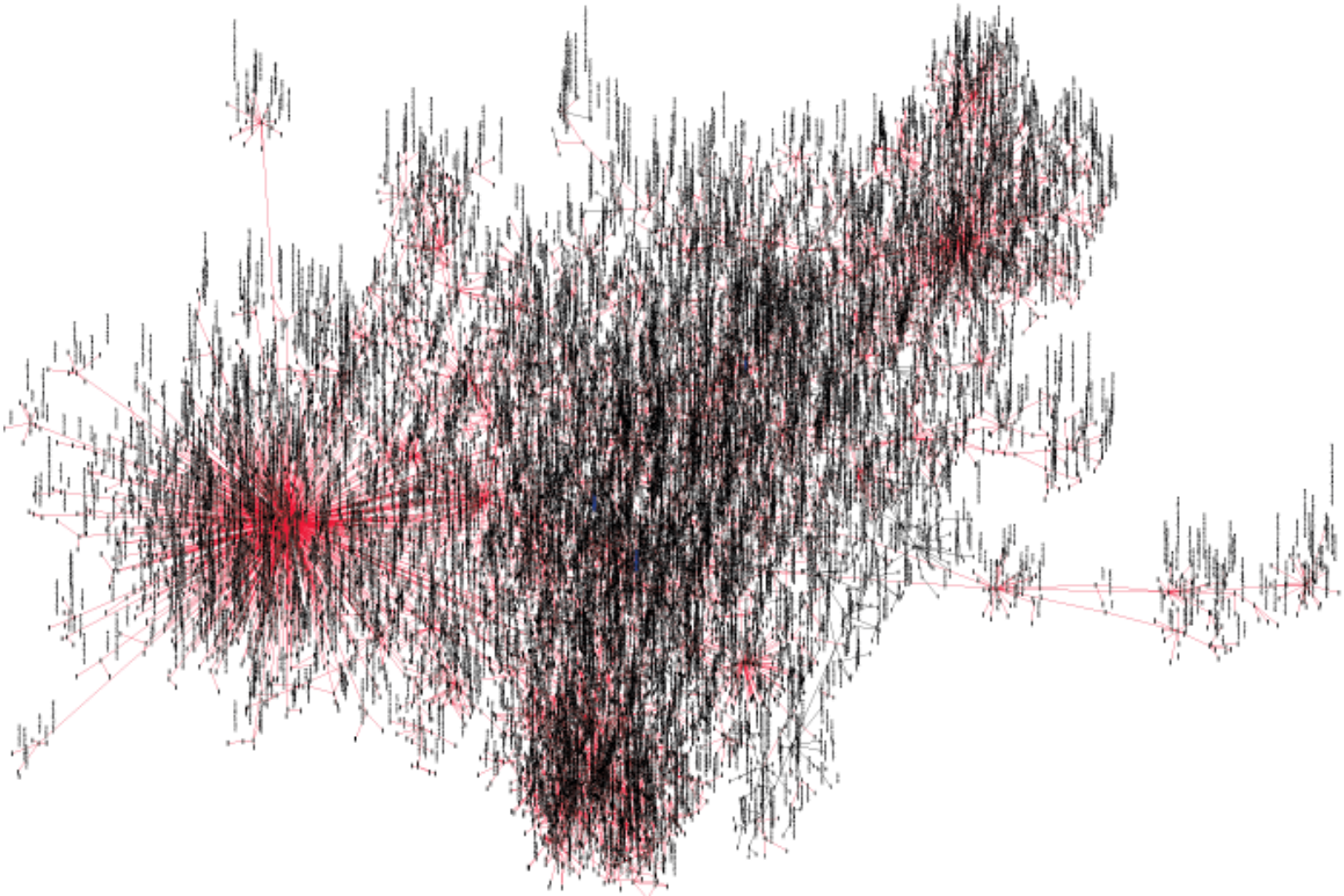
WHOLE GO CA. 2001



Courtesy of Robert Kueffner, NCGR, 2001

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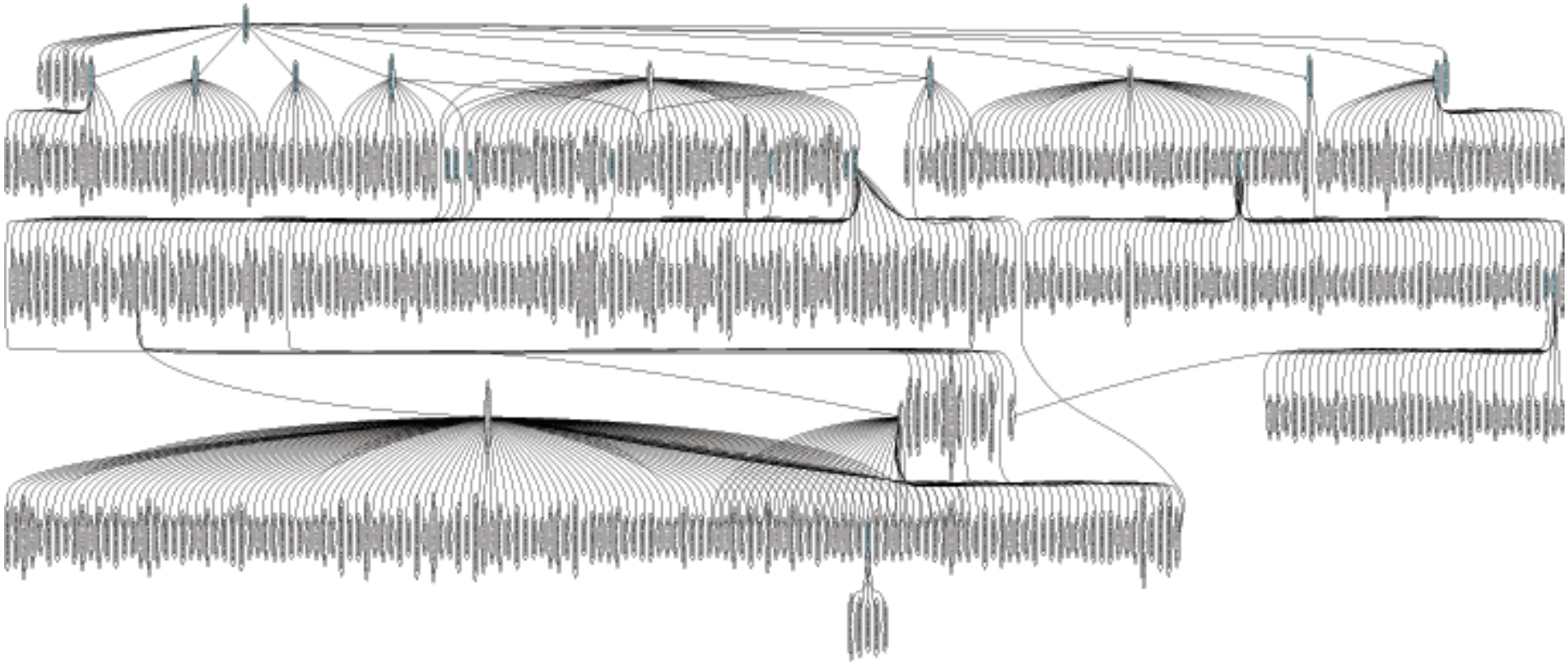
GO PORTION, HIERARCHICAL EYECHART



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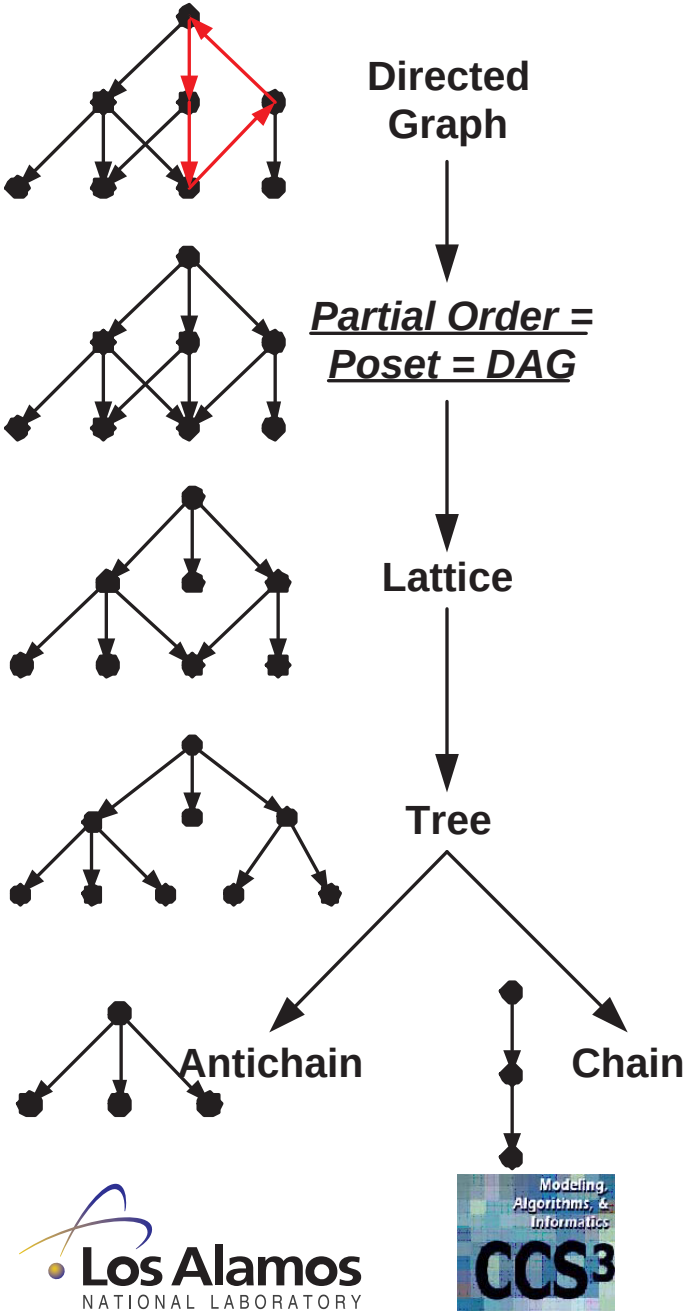
HIERARCHIES AS PARTIALLY ORDERED SETS



- **Partial Order:** Set P; relation $\leq \subseteq P^2$: reflexive, anti-symmetric, transitive
- **Poset:** $\mathcal{P} = \langle P, \leq \rangle$
- Simplest mathematical structures which admit to descriptions in terms of "levels" and "hierarchies"
- More specific than graphs or networks: no cycles, equivalent to Directed Acyclic Graphs (DAGs)
- More general than trees, lattices: single nodes, pairs of nodes can have multiple parents
- Ubiquitous in knowledge systems: constructed, induced, empirical

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BASIC POSET CONCEPTS

Poset: $\mathcal{P} = \langle P, \leq \rangle$

Comparable Nodes: $a \sim b := a \leq b$ or $b \leq a$

Up-Set: $\uparrow a = \{b \geq a\}$, **Down-Set:** $\downarrow a = \{b \leq a\}$

Chain: Collection of comparable nodes: $a_1 \leq a_2 \leq \ldots \leq a_n$

Height: Size maximal chain $\mathcal{H}(\mathcal{P})$

Noncomparable Nodes: $a \not\sim b$

Antichain: Collection of noncomparable nodes: $A \subseteq P, a \not\sim b, a, b \in A$

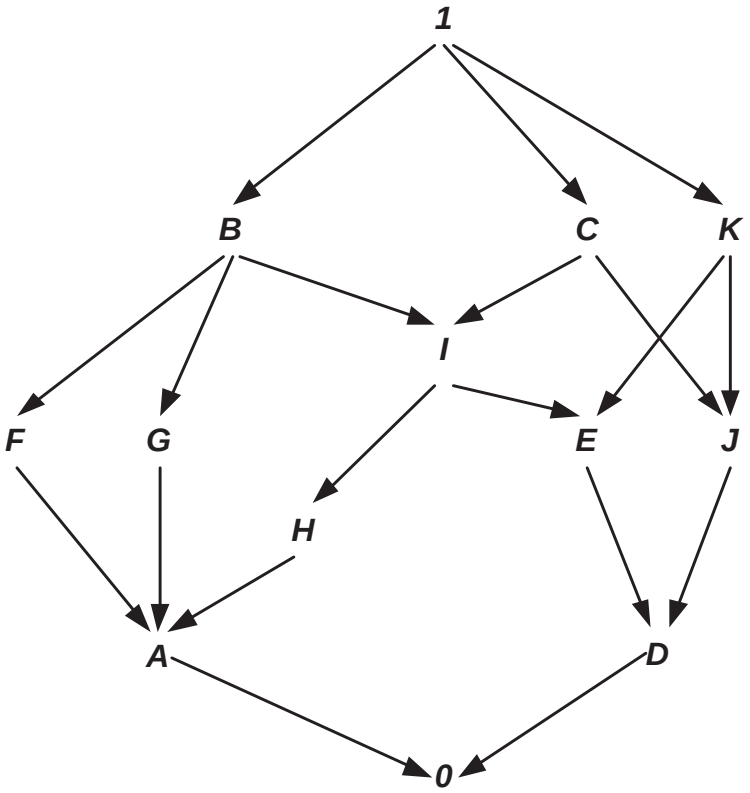
Width: Size maximal antichain $\mathcal{W}(\mathcal{P})$

Interval: $[a, b] := \{c \in P : a \leq c \leq b\}$, a bounded sub-poset of $\mathcal{P}$

Join, Meet: $a \vee b, a \wedge b \subseteq P$

Lattice: Then $a \vee b, a \wedge b \in P$

Bounded: Min $0 \in P$, Max $1 \in P$



. Schröder, BS (2003): *Ordered Sets*, Birkhäuser, Boston

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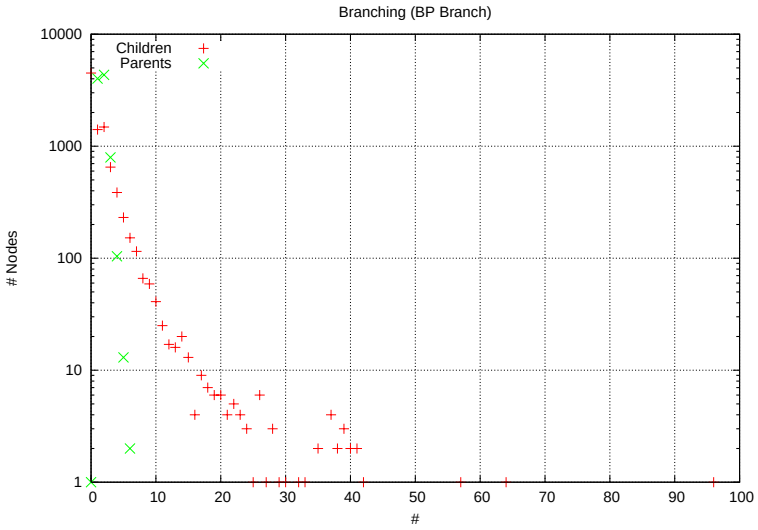
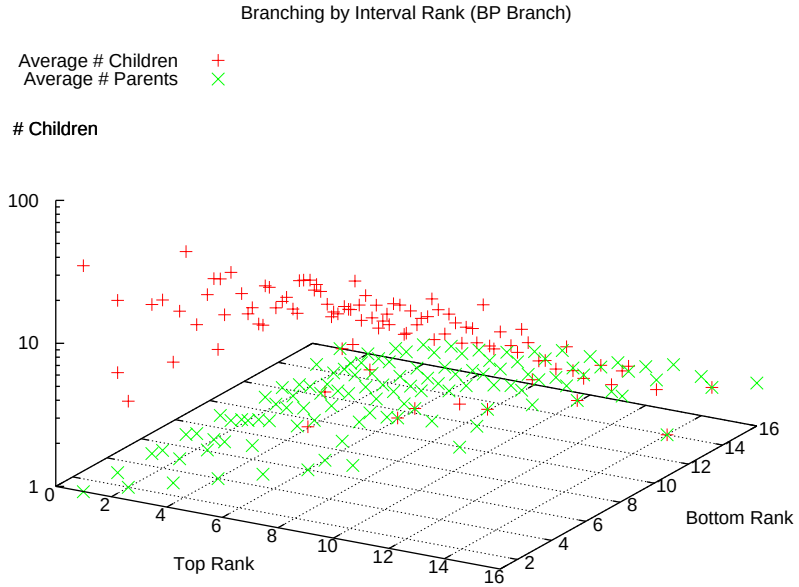
SOME GO QUANTITATIVE MEASURES

	Nodes	Leaves	Interior	Edges	$\mathcal{H}$	$\mathcal{W}$
MF	7.0K	5.6K	1.3K	8.1K	13	$\geq$ 3.5K
BP	7.7K	4.1K	3.6K	11.8K	15	$\geq$ 2.9K
CC	1.3K	0.9K	0.4K	1.7K	13	$\geq$ 0.4K
GO	16.0K	10.6K	5.4K	21.5K	16	$\geq$ 5.9K





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C Joslyn, S Mniszewski, A Fulmer, and G Heaton: (2004) "The Gene Ontology Categorizer", *Bioinformatics*, v. **20**:s1, pp. 169-177

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CHAIN DECOMPOSITION OF INTERVALS

Comparable Nodes: e.g. $D \leq 1 \in P$

Chain Decomposition: Set of all chains connecting them:

$$\begin{aligned}\mathcal{C}(D,1) &= \{C_j\} \\ &= \{D \prec E \prec I \prec B \prec 1, D \prec E \prec I \prec C \prec 1, \\ &\quad D \prec E \prec K \prec 1, D \prec J \prec C \prec 1, \\ &\quad D \prec J \prec K \prec 1\} \subseteq 2^P\end{aligned}$$

Chain Lengths: $h_j := |C_j| - 1$

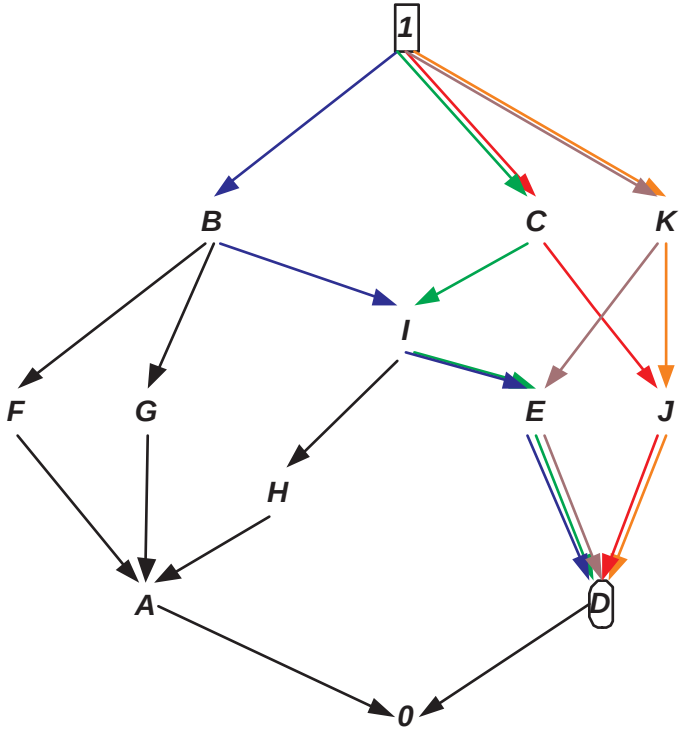
Vectors of Chain Lengths:

$$\vec{h}(a,b) := \left\langle h_j \right\rangle_{j=1}^{M} = \langle 4,4,3,3,3 \rangle$$

Extremes:

$$h_*(a,b) = \min_{h_j \in \vec{h}(a,b)} h_j = 3$$

$$h^*(a,b) = \max_{h_j \in \vec{h}(a,b)} h = 4$$



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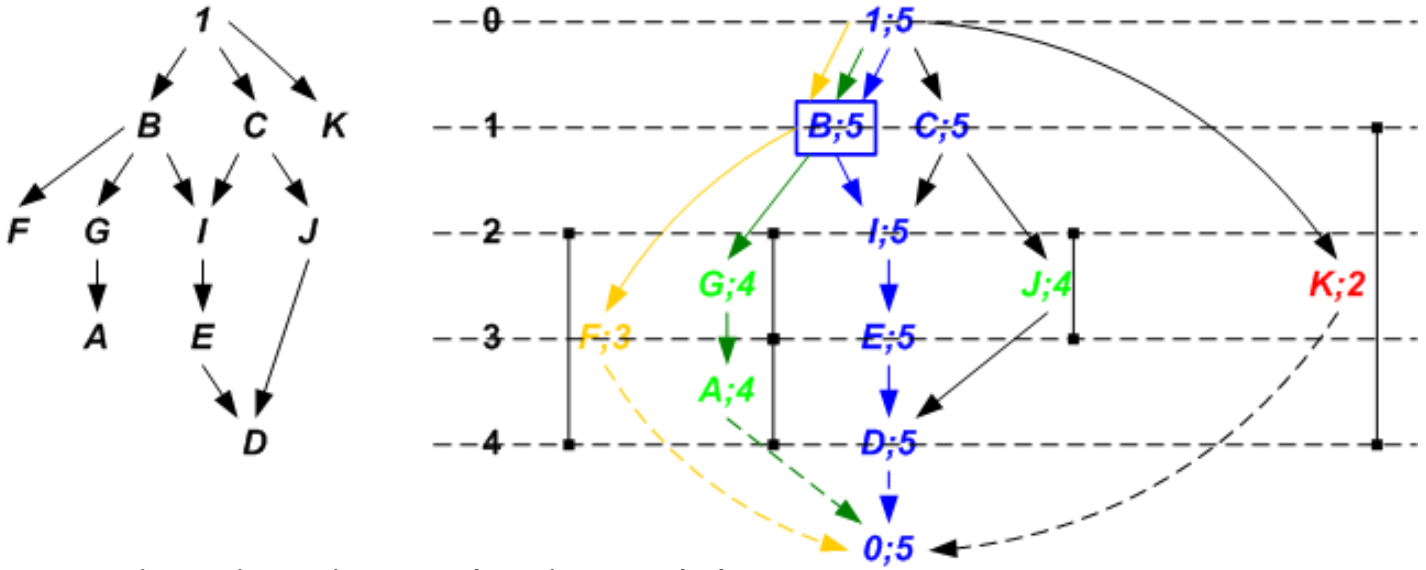
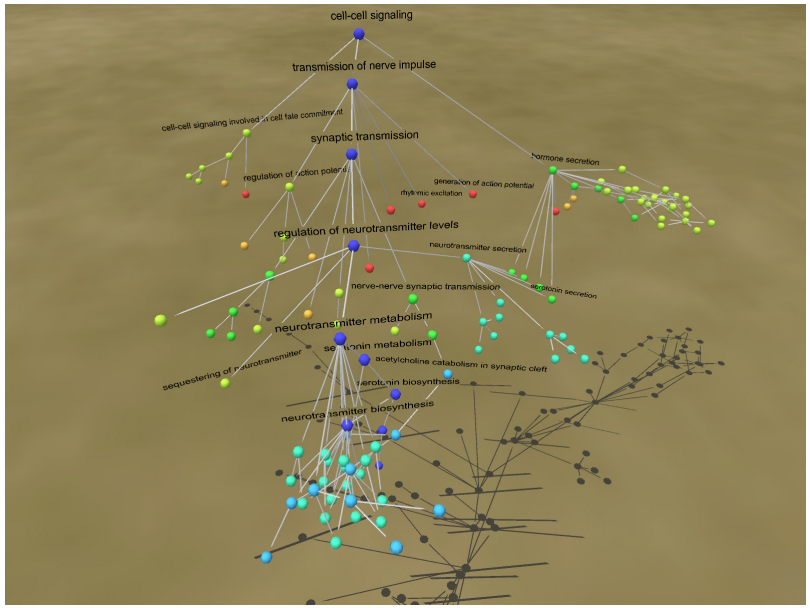
INTERVAL RANK LAYOUT



- Interval valued vertical position (rank)
- Chain decomposition guides horizontal: short maximal chains to outside



CA Joslyn, SM Mniszewski, SA Smith, and PM Weber: (2006) "SpindleViz: A Three Dimensional, Order Theoretical Visualization Environment for the Gene Ontology", *Joint BioLINK and 9th Bio-Ontologies Meeting (JBB 06)*

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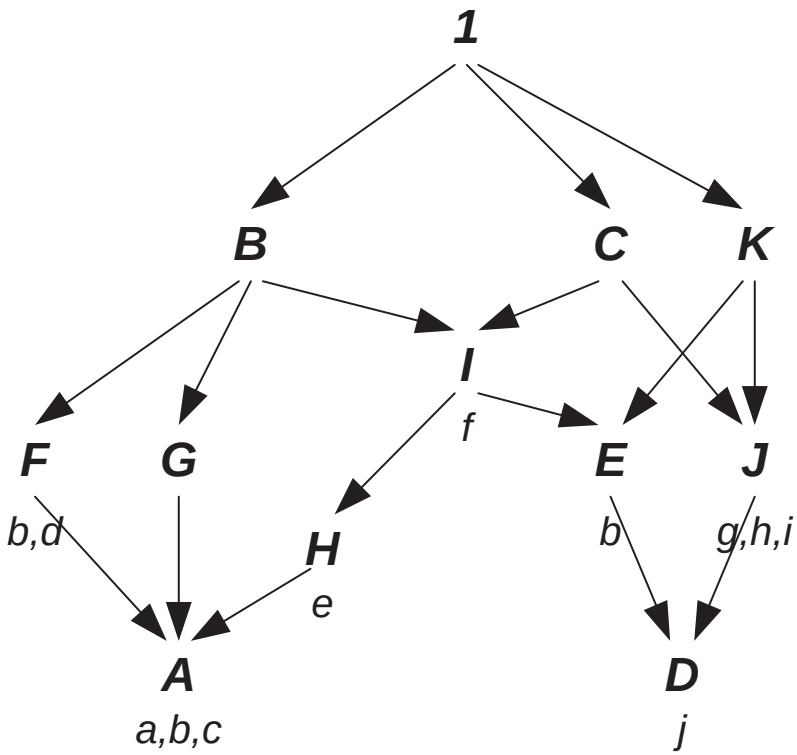
CATEGORIZATION METHOD

- **POSO:** POSet Ontology
  $\mathcal{O} := \langle \mathcal{P}, X, F \rangle, \mathcal{P} = \langle P, \leq \rangle$
  Labels: finite, non-empty set X
  Labeling Function: $F: X \mapsto 2^P$
- Given labels (genes) $c, e, i \ldots$
- What node(s)
  $P = \{A, B, C, \ldots, K\}$ are best to pay attention to?



- Scores to rank-order nodes wrt/gene locations, balancing:
  - **Coverage:** Covering as many genes as possible
  - **Specificity:** But at the "lowest level" possible
- "Cluster" based on non-comparable high score nodes

C Joslyn, S Mniszewski, A Fulmer, and G Heaton: (2004) "The Gene Ontology Categorizer", *Bioinformatics*, v. **20**:s1, pp. 169-177

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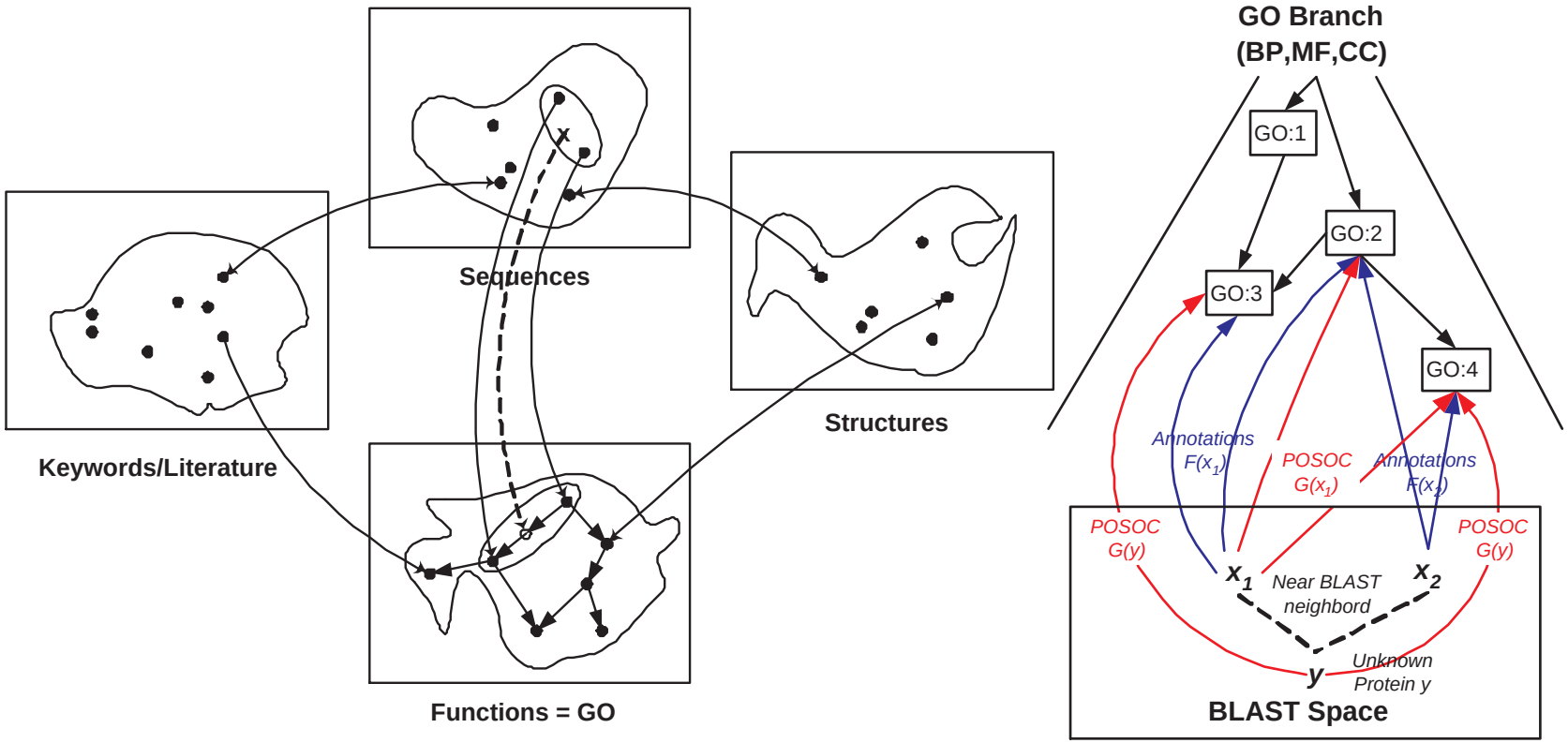
AUTOMATED ONTOLOGICAL PROTEIN FUNCTION ANNOTATION



- Mappings among regions of biological spaces . . .
- . . . into spaces of biological functions
- POSOC annotated BLAST neighborhoods of new proteins
- *How to measure quality of inferred annotations?*

Verspoor, KM; Cohn, JD; Mniszewski, SM; and Joslyn, CA: (2006) "Categorization Approach to Automated Ontological Function Annotation", *Protein Science*, v. **15**, pp. 1544-1549

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HIERARCHICAL EVALUATION METRICS

- Hierarchical measures:

Precision:

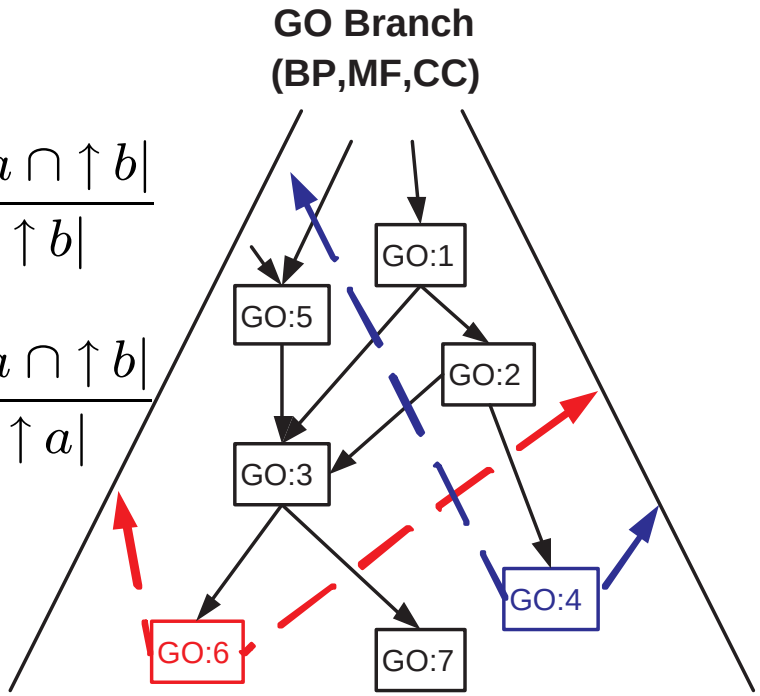
$$HP = \frac{1}{|G(x)|} \sum_{b \in G(x)} \max_{a \in F(x)} \frac{|\uparrow a \cap \uparrow b|}{|\uparrow b|}$$

Recall:

$$HR = \frac{1}{|F(x)|} \sum_{a \in F(x)} \max_{b \in G(x)} \frac{|\uparrow a \cap \uparrow b|}{|\uparrow a|}$$

F-Score:

$$HF = \frac{2(HP)(HR)}{HP + HR}$$



- Example: $F(x) = \{\text{GO:4}\}, G(x) = \{\text{GO:6}\}$
  $\uparrow a = \{\text{GO:1}, \text{GO:2}, \text{GO:4}\}, \uparrow b = \{\text{GO:1}, \text{GO:2}, \text{GO:3}, \text{GO:5}, \text{GO:6}\}$
  $HP = 2/5, HR = 3/5$

S Kiritchenko, S Matwin, and AF Famili: (2005) "Functional Annotation of Genes Using Hierarchical Text Categorization", *Proc. BioLINK SIG on Text Data Mining*

Verspoor, KM; Cohn, JD; Mniszewski, SM; and Joslyn, CA: (2006) "Categorization Approach to Automated Ontological Function Annotation", *Protein Science*, v. **15**, pp. 1544-1549

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SEMANTIC SIMILARITIES

Poset $\mathcal{P} = \langle P, \leq \rangle$, probability distribution $p\colon P \mapsto [0,1], \sum_{a \in P} p(a) = 1$, "cumulative" $\beta(a) := \sum_{b \leq a} p(a)$

Resnik: $\delta(a,b) = \max_{c \in a \vee b} [-\log_2(\beta(c))]$

Lin:

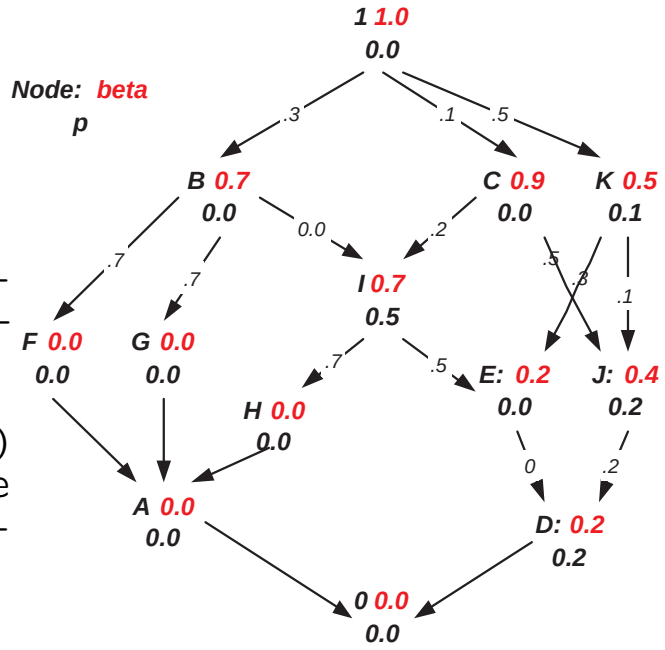
$$\delta(a,b) = \frac{2 \max_{c \in a \vee b} [\log_2(\beta(c))]}{\log_2(\beta(a)) + \log_2(\beta(b))}$$

Jiang and Conrath:

$$\delta(a,b) = 2 \max_{c \in a \vee b} [\log_2(\beta(c))] - \log_2(\beta(a)) - \log_2(\beta(b))$$

Issues:

- General mathematical grounding in poset metrics
- Not *rely* on probabilistic weighting



A Budanitsky and G Hirst: (2006) "Evaluating WordNet-based measures of semantic distance." *Computational Linguistics*, 32(1), 13–47.

Lord, PW; Stevens, Robert; Brass, A; and Goble, C: (2003) "Investigating Semantic Similarity Measures Across the Gene Ontology: the Relationship Between Sequence and Annotation", *Bioinformatics*, v. **10**, pp. 1275-1283

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POSET METRICS

Assume $\langle P, \leq \rangle$ finite, connected, bounded

$$aub := \uparrow a \cap \uparrow b, \quad alb := \downarrow a \cap \downarrow b$$

Isotone Map: $v\colon P \mapsto \mathbb{R}, a \leq b \rightarrow v(a) \leq v(b)$

$$v^+(a,b) := \min_{w \in aub} v(w)$$

$$(aub)_v := \{w \in P : v(w) = v^+(a,b)\}$$

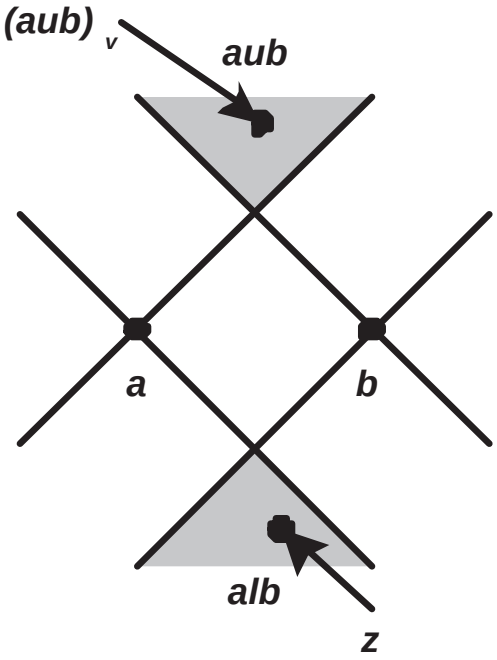
Upper Valuation: $\forall z \in alb$,

$$v(a) + v(b) \geq v^+(a,b) + v(z)$$

Distance: v is an upper valuation iff

$$d(a,b) := 2v^+(a,b) - v(a) - v(b)$$

is a distance (triangle inequality)



	Upper Valuation $z \in alb$	Lower Valuation $z \in aub$
Isotone	$v(a) + v(b) \geq v^+(a,b) + v(z)$ $d(a,b) = 2v^+(a,b) - v(a) - v(b)$	$v(a) + v(b) \leq v^-(a,b) + v(z)$ $d(a,b) = v(a) + v(b) - 2v^-(a,b)$
Antitone	$v(a) + v(b) \leq v^+(a,b) + v(z)$ $d(a,b) = v(a) + v(b) - 2v^+(a,b)$	$v(a) + v(b) \geq v^-(a,b) + v(z)$ $d(a,b) = 2v^-(a,b) - v(a) - v(b)$

Monjardet, B: (1981) "Metrics on Partially Ordered Sets - A Survey" , *Discrete Mathematics*, v. **35**, pp. 173-184

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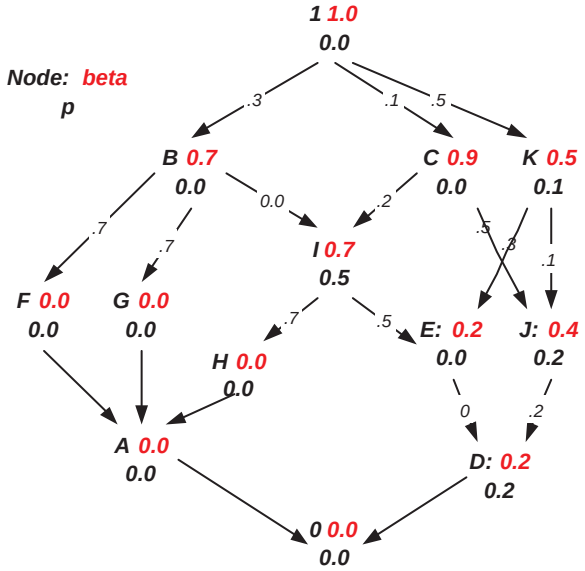
SOME LATTICE METRICS

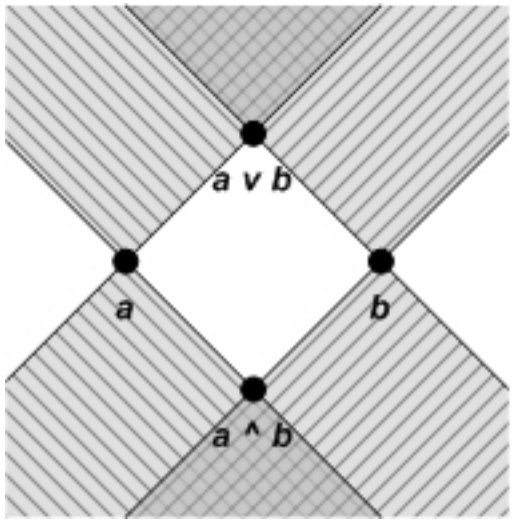
Information Theoretical: Monotone upper valuation

- Let $v(a) = \beta(a)$, "cumulative" probability
- **Proposition:** Jiang and Conrath is a metric, others are not
- $d(a,b) = 2\beta(a \vee b) - \beta(a) - \beta(b)$
- $d(I,J) = 1.53, d(E,J) = 1.64$



Purely Structural: Antitone upper valuation

- $|\uparrow a \cap \uparrow b| = |\uparrow(a \vee b)|$, $|\downarrow a \cap \downarrow b| = |\uparrow(a \wedge b)|$
- Let $v(a) = |\uparrow a|$
- $d(a,b) = |\uparrow a| + |\uparrow b| - 2|\uparrow a \cap \uparrow b|$
- $d(I,J) = 4, d(E,J) = 6$



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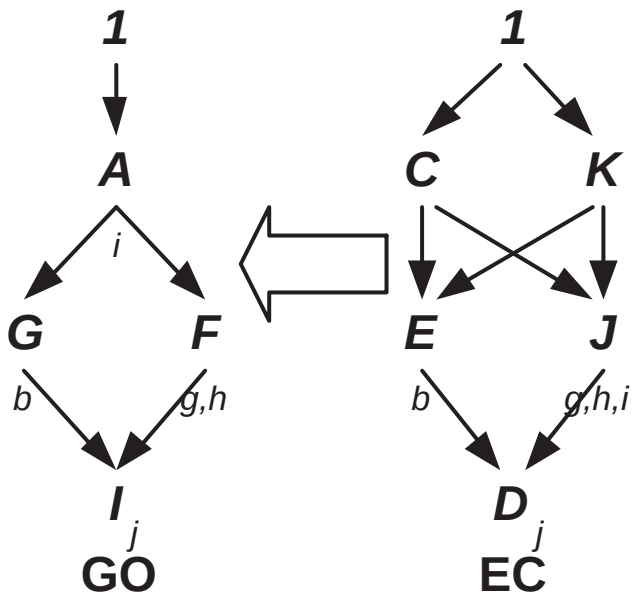
INTEROPERABILITY AND ALIGNMENT

Matching: Measure similarity between two regions of a single ontology

Comparing: Twist one ontology on a given term set into another ordering

Merging: Given two completely distinct ontologies:

- Identify structurally similar regions: intersection
- Create encompassing meta-ontologies: product or union?



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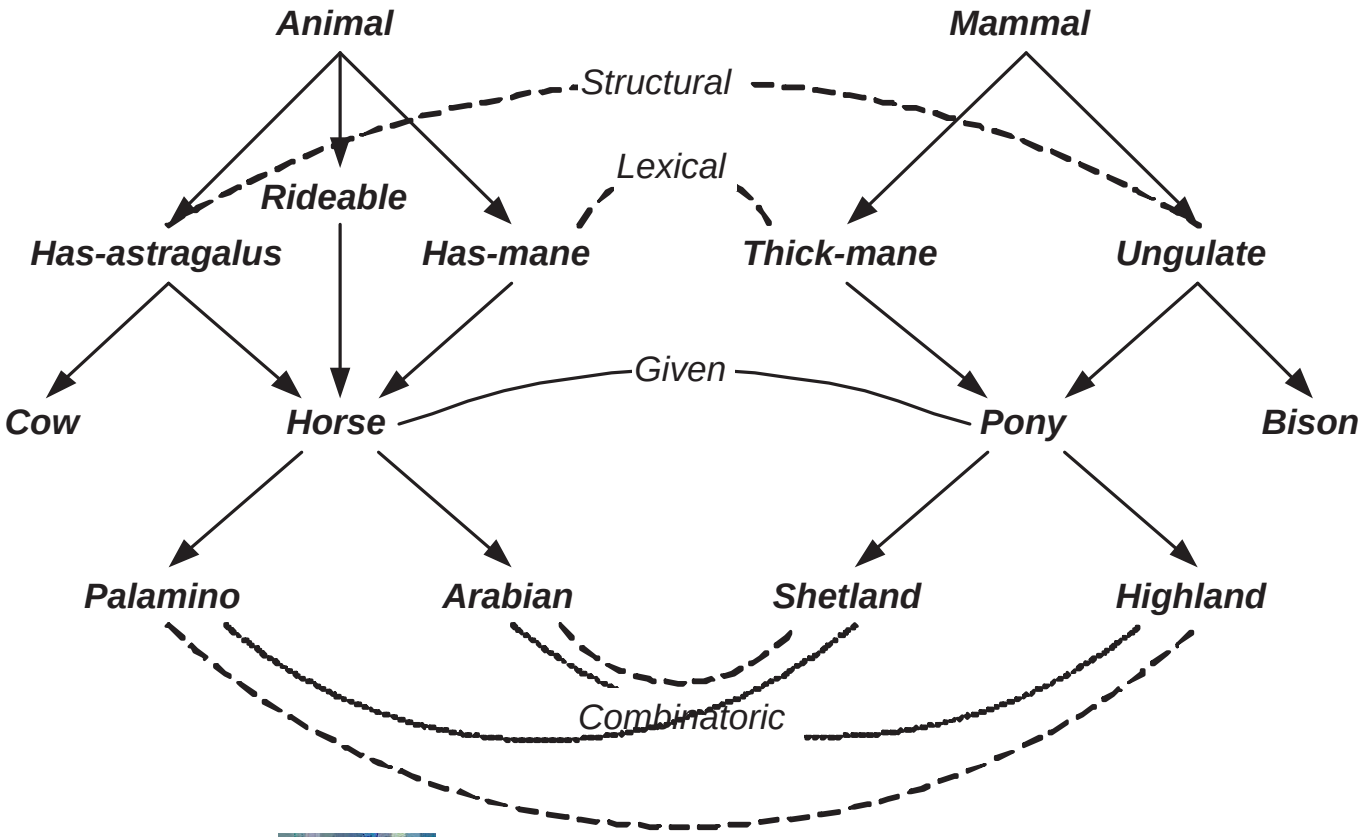
ALIGNMENT METHODS

Ultimate Goal: Construct order morhpisms
Neighborhoods: Around given anchors
Lexical: Matches
Structural: Nodes playing similar structural roles
Combinatoric: Sets of nodes playing similar structural roles
Poset Metrics: Measure candidate alignment, suggest new anchors



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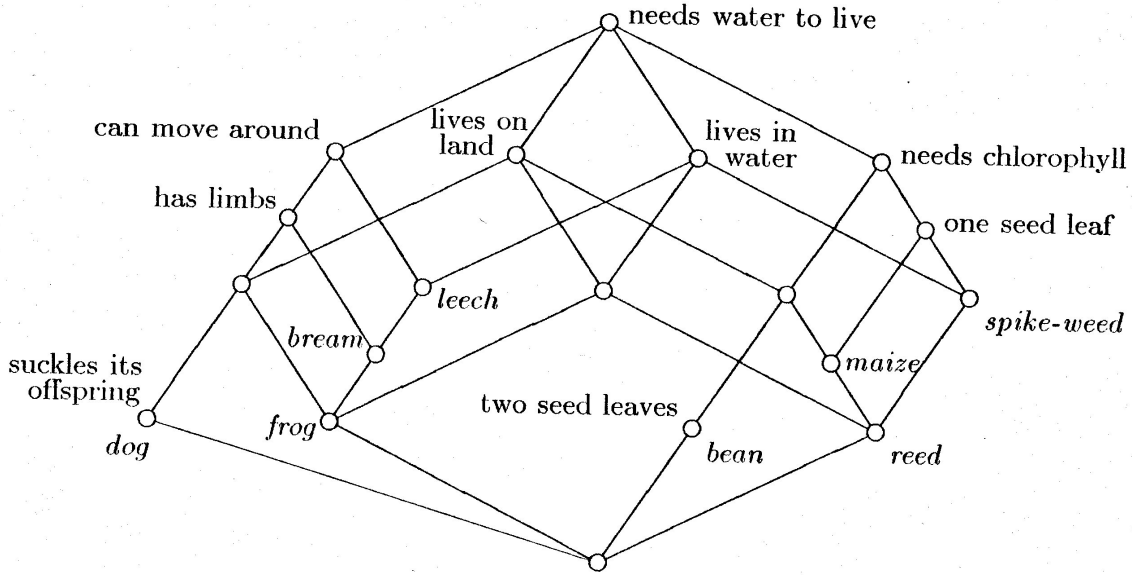
FORMAL CONCEPT ANALYSIS

- Semantic hierarchies from relational data
- Unbiased, graphical, visual representation
- Hypothesis and rule generation and evaluation
- For ontology induction, interoperability

		a	b	c	d	e	f	g	h	i
1	Leech	×	×					×		
2	Bream	×	×					×	×	
3	Frog	×	×	×				×	×	
4	Dog	×		×				×	×	×
5	Spike – weed	×	×		×		×			
6	Reed	×	×	×	×		×			
7	Bean	×		×	×	×				
8	Maize	×		×	×		×			

Figure 1.1 Context of an educational film "Living Beings and Water". The attributes are: a: needs water to live, b: lives in water, c: lives on land, d: needs chlorophyll to produce food, e: two seed leaves, f: one seed leaf, g: can move around, h: has limbs, i: suckles its offspring.



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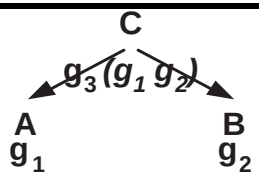
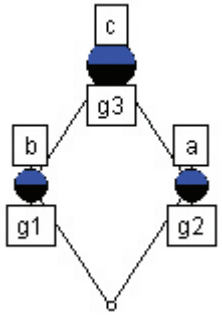
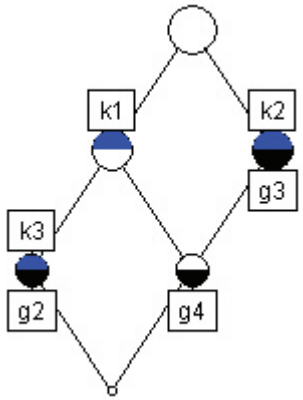
FCA ONTOLOGY MERGER, INDUCTION

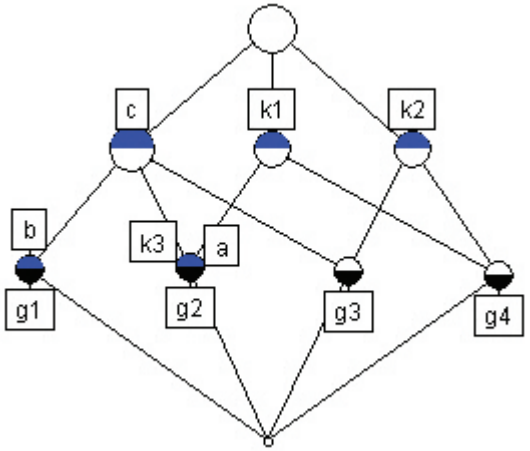
- $\{g_1, g_2, g_3\}$: annotated into an ontology O:



- $\{g_2, g_3, g_4\}$: annotated to keywords $K = \{k_1, k_2, k_3\}$
- *Induce* order on K while *incoporating* order on O
- Amenable to metric treatment of attributes, objects







	a	b	c
g_1		$\surd$	$\surd$
g_2	$\surd$		$\surd$
g_3			$\surd$

	k_1	k_2	k_3
g_2	$\surd$		$\surd$
g_3		$\surd$	
g_4	$\surd$	$\surd$	

	a	b	c	k_1	k_2	k_3
g_1		$\surd$	$\surd$			
g_2	$\surd$		$\surd$	$\surd$		$\surd$
g_3			$\surd$		$\surd$	
g_4				$\surd$	$\surd$	

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