Issues in the visualization and navigation of biomedical knowledge
Outline

◆ Biomedical terminologies as a source of biomedical knowledge
◆ Structural perspective on the Metathesaurus
◆ Visualizing biomedical knowledge
◆ From structure to semantics
  ● Inherit relationships
  ● Path between two concepts
  ● Limitations
Biomedical terminologies
Biomedical knowledge organization

Terminologies

Semantic Spaces

Medical Subject Headings
International Classification of Diseases
SNOMED

[...]

Cyc
WordNet
Digital Anatomist
[...]

Ontologies

UMLS
Biomedical terminologies

◆ Core vocabularies
  ● anatomy (UWDA, Neuronames)
  ● drugs (First DataBank, Micromedex)
  ● medical devices (UMD, SPN)

◆ Several perspectives
  ● clinical terms (SNOMED, CTV3)
  ● information sciences (MeSH, CRISP)
  ● administrative terminologies (ICD-9-CM, CPT-4)
  ● standards (HL7, LOINC)
Biomedical terminologies (cont’d)

- Specialized vocabularies
  - nursing (NIC, NOC, NANDA, Omaha, PCDS)
  - dentistry (CDT)
  - oncology (PDQ)
  - psychiatry (DSM, APA)
  - adverse reactions (COSTART, WHO ART)
  - primary care (ICPC)

- Knowledge bases (AI/Rheum, DXplain, QMR)
UMLS

◆ Two-level structure
  ● Semantic Network
    ■ 134 Semantic Types (STs)
    ■ Relationships among STs
  ● Metathesaurus
    ■ 800,000 concepts
    ■ Inter-concept relationships
  ● Link = categorization
    ■ Often isa
    ■ Rarely is an instance of
Addison’s disease

- Addison's disease is a rare endocrine disorder
- Addison's disease occurs when the adrenal glands do not produce enough of the hormone cortisol
- For this reason, the disease is sometimes called chronic adrenal insufficiency, or hypocortisolism
Structural perspective on the Metathesaurus
Hierarchy

- Hierarchical relationships
  - Taxonomy (isa)
  - Meronomy (part of)
- Partial ordering
  - [Reflexivity]
  - Antisymmetry
  - Transitivity
- Inheritance
- Reasoning

Hierarchy
Principles of subsumption

[Bernauer, AMIA 1994]

Aneuvrysm

isa

Aortic Aneuvrysm

isa

Aortic Aneuvrysm, Thoracic

isa

Thoracoabdominal Aortic Aneuvrysm

aneuvrysm

an. of the aorta

partitive refinement of a concept element

introduction of a specializing criterion

conjunctive coordination

an. of the thoracic aorta

an. of the thoracic aorta and abdominal aorta
Hierarchies in source vocabularies

◆ Structure
  ● Single tree
  ● Polyhierarchical (multiple parents)

◆ Relationships
  ● Usually implicit
  ● May be other than *isa* or *part of*
    - E.g., Thesaurus relationships
AD in medical vocabularies

**Contexts**

**SNOMED**

- Diseases
  - Endocrine Diseases
    - Adrenal Gland Diseases
      - Addison’s Disease

**MeSH**

- Diseases
  - Endocrine Diseases
    - Adrenal Gland Diseases
  - Immunologic Diseases
    - Autoimmune Diseases
  - Addison’s Disease

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AD in UMLS  

Contexts

Endocrine Diseases

Adrenal Gland Diseases

Adrenal Cortex Diseases

Hypoadrenalism

Adrenal Gland Hypofunction

Adrenal cortical hypofunction

Addison’s Disease
AD in UMLS  SNOMED context

Endocrine Diseases

Adrenal Gland Diseases

Addison’s Disease
AD in UMLS  MeSH context

Endocrine Diseases

Adrenal Gland Diseases

Adrenal Gland Hypofunction

Addison’s Disease
AD in UMLS  Read Codes context

- Endocrine Diseases
  - Adrenal Gland Diseases
    - Hypoadrenalism
    - Adrenal Gland Hypofunction
    - Adrenal cortical hypofunction
    - Addison’s Disease
AD in UMLS  AOD Thes. context

- Endocrine Diseases
  - Adrenal Gland Diseases
    - Adrenal Cortex Diseases
      - Adrenal cortical hypofunction
        - Addison’s Disease
Hierarchies in source vocabularies

- Often task-driven rather than based on principles
- Usually suitable for information retrieval
  - Better recall
  - Precision may not be crucial
- Not necessarily suitable for reasoning
- But expected to be consistent structurally
AD in UMLS  Contexts

- Multiple tree structures combined into a graph structure
- Directed acyclic graph (DAG)
Actually, there are some cycles

- Anti-infective Agents
- Disinfectants and Cleansers
- Disinfectants
- Disinfectant soap
- Germicidal soap
Issues with cycles

◆ Theoretical
  ● Violate the antisymmetry property of partial ordering relations

◆ Practical
  ● Loops in graph traversal
  ● Impossible to perform transitive reduction
Cycle due to underspecification

- Specified and underspecified terms
  - May appear at different levels in a source hierarchy
  - Are clustered into the same concept (same meaning)
Other causes

- **Compound terms**
  - Nausea
  - Nausea and Vomiting

- **Metadata**
  - HYDROCELE, Hydrocele

- **Classes and member**
  - Purines, Purine

- **Organizational conventions**
  - Acid + Base ↔ Salt + Water

- **Idiopathic**
  - Wrong relationships
  - Use of non-hierarchical relationships in “hierarchies”

[Bodenreider, AMIA 2001]
Visualizing biomedical knowledge
Visualizing biomedical knowledge

◆ Objectives
  ● Make knowledge navigable by users
  ● Make knowledge available to applications

◆ Common issues
  ● Reduce complexity
  ● Provide consistent views across the domain
  ● Extend views to fit specific needs

- UMLS Semantic Navigator
  umlsks.nlm.nih.gov → Resources → Semantic Navigator
UMLS Semantic Navigator

- Visualize semantic locality
- Features
  - All relationships presented simultaneously
    - Metathesaurus relationships
    - Semantic network relationships
  - Hierarchical relationships presented graphically
  - Dynamic and navigable
  - Transitive reduction
Siblings

Disorders

- Acquired Immunodeficiency Syndrome □
- Acute adrenal insufficiency □
- Addisonian crisis □
- Adrenal Gland Hyperfunction □
- Adrenal insufficiency due to adrenal metastasis □
- Allergic/autoimmune thyroiditis □
- Allergic arthritis □
- Ankylosing Spondylitis □
- Antiphospholipid Syndrome □
- Asthma □
- Autoimmune Disease of the Nervous System □
- Autoimmune hemolytic anemia □
- Autoimmune hemolytic anemia, cholestatic □
- Autoimmune hemolytic anemia, secondary □
- Autoimmune hemolytic anemia, primary □
- Autoimmune hemolytic anemia, congenital □
- Autoimmune lymphoproliferative disorder □
- Autoimmune lymphoproliferative disease □
- Autoimmune lymphoproliferative syndrome □
- Autoimmune lymphoproliferative syndrome, primary □
- Battered Child Syndrome □
- B-cell lymphoma □
- Cystic Fibrosis □
- Congenital hypothyroidism □
- Congenital hypothyroidism, primary □
- Congenital hypothyroidism, secondary □
- Congenital hypothyroidism, transient □
- Congenital hypothyroidism, permanent □
- Congenital hypothyroidism, transient neonatal □
- Congenital hypothyroidism, permanent neonatal □
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UMLS Semantic Navigator Concepts

Other Related Concepts

Disorders

- Addisonian crisis
- Addisons Disease
- Secondary To Adrenal Destruction
- Addisons Disease
- Secondary To Idiopathic Atrophy
- Adrenal cortical hypofunction
- Autoimmune Syndrome Type II, Polyglandular
- ENDO/METAB PROBLEM
- Hypoglycemia
- Hyponatremia
- Tuberculosis
- Tuberculosis of adrenal glands
- Tuberculous Addison's
UMLS Semantic Navigator

Concepts
UMLS Semantic Navigator

Relationships
of **Addison's Disease** (C1)  
*Disease or Syndrome*
to **Adrenal Cortex** (C2)  
*Body Part, Organ, or Organ Component*

**Metathesaurus Relationships**

C1 co-occurs with C2
Frequency = 12  • MEDLINE

**Semantic Network Relationships**

*Disease or Syndrome*  • has_location  *Body Part, Organ, or Organ Component*

Close this window

Interface version: 2.01  UMLS data: UMLS_2000
Visualization Research directions

◆ Selecting relevant co-occurring concepts
  ● Based on the relative frequency
  ● Compared to symbolic relationships

◆ Visualizing the paths between two concepts
  ● Display polyhierarchy
  ● Graph theory algorithms
Object-oriented model  Specifications

◆ Knowledge-oriented
◆ Simple
◆ High-level methods
◆ Independent
  ● From the UMLS relational format
  ● From back-end implementation
◆ Extendable
Design choices

◆ Object-oriented model
  ● Extensible through derivation

◆ Limited number of classes
  ● Not as comprehensive as the UMLS itself

◆ Methods
  ● Accessor methods (properties)
  ● High-level methods
4 major classes

- Class **SemType**
- Class **Concept**
- Semantic Type 1
- Semantic Type 2
- Concept \( \text{Concept}_1 \)
- Concept \( \text{Concept}_2 \)
- Class **SemNet**
- Class **Relationship**

Semantic Network

Metathesaurus
Class **Concept**

◆ **Properties**

- Unique identifier (CUI)
- List of synonymous terms [in a given source/language]
- List of definitions
- List of sources
- Set of related concepts (instances of **Concept**)
- Set of semantic types (instances of **SemType**)
- *Total frequency of co-occurrence in MEDLINE*
Class **Concept**

- **Methods provided for convenience**
  - $\text{anc}1 = \text{par} \cup \text{bro}$

- **Higher-level methods**
  - $\text{sibx}: \text{Extended siblings}$
  - $\text{par}_\text{tr}: \text{Transitive reduction}$

![Diagram showing parent and broader relationships between classes Ca,Cb,Cc]
Architecture

Application

O-O model

Database mediator class

KSS API

Local UMLS database

Knowledge Source Server

UMLS classes

Mediator classes

Back-end
From structure to semantics

1. Inherit relationships
Semantic Network

- Semantic types (134)
  - tree structure
  - 2 major hierarchies
    - Entity
      - Physical Object
      - Conceptual Entity
    - Event
      - Activity
      - Phenomenon or Process
Semantic Network

- Semantic network relationships (54)
  - **hierarchical** (isa = is a kind of)
    - among types
      - Animal isa Organism
      - Enzyme isa Biologically Active Substance
    - among relations
      - treats isa affects
  - **non-hierarchical**
    - Sign or Symptom diagnoses Pathologic Function
    - Pharmacologic Substance treats Pathologic Function
“Biologic Function” hierarchy (isa)

Biologic Function

Physiologic Function
- Organ Function
  - Mental Process
- Organ or Tissue Function
- Cell Function
- Molecular Function
  - Genetic Function

Pathologic Function
- Cell or Molecular Function
  - Mental or Behavioral Dysfunction
- Disease or Syndrome
  - Neoplastic Process
- Experimental Model of Disease
Associative (non-isa) relationships

Diagram showing relationships between biological concepts such as organs, systems, and functions. The diagram includes terms like "organism," "finding," "physiologic function," "pathologic function," "embryonic structure," "anatomical abnormality," "congenital abnormality," "acquired abnormality," "fully formed anatomical structure," "body system," "body part, organ or organ component," "tissue," "cell," "cell component," "body substance," "gene or genome," "body location or region," "body space or junction," "location of," "process of," "evaluation of," "contains," "conceptual part of," "part of," "disrupts," "co-occurs with," "adjacent to."
Role

- A relationship between 2 STs is a possible link between 2 concepts that have been assigned to those STs
  - The relationship may or may not hold at the concept level
  - Other relationships may apply at the concept level
- A child ST inherits properties from its parents (isa relationships)
Applications

◆ To help qualify inter-concept relationships
  ● using the relationships defined between their semantic types in the semantic network

◆ To strengthen the structure of the Metathesaurus
  ● a relationship between 2 concepts should be consistent with the relationships defined between their semantic types in the semantic network

◆ Semantic interpretation
  ● finding semantic relationships between concepts in text
Experiment

- 3764 concepts related to Heart
- 6894 pairs of related concepts
  - A relation can be inferred unambiguously from the Semantic Network (65%)
  - Multiple semantic links possible (22%)
  - Violation of the Semantic Network (13%)
    - Wrong inter-concept relationship
    - Wrong categorization
    - Both

[McCray & al. (in press)]
From structure to semantics

2. Find a path between two concepts
Co-occurrence Overview

- Co-occurrence between MeSH descriptors in MEDLINE citations
- 8 M pairs of co-occurring concepts
- Implicit semantics
- The UMLS provides knowledge for helping make this relationship explicit
  - Corresponding symbolic knowledge (Metathesaurus)
  - Categorization (Semantic Network)
Co-occurrence Example

- Adrenal cortical hypofunction
- Addison's disease (Co-occurrence (frequency = 20))
- Cortisol

Adrenal gland
- Cortex
- Medulla
Co-occurrence Methods

- Based on Metathesaurus relationships
  - Does “Cortisol” belong to the family of “Addison’s disease”?

- Based on Semantic Network relationships
  - What is the relationship between the semantic types of “Cortisol” and “Addison’s disease”?

![Diagram showing co-occurrence between Addison's disease and Cortisol with a frequency of 20]
Family relationships

Diagram showing family relationships with nodes labeled C, S, U, A_1, A_2, and D_1 connected by lines indicating relationships.
Does "Cortisol" belong to the family of "Addison's disease"?
Co-occurrence Results

◆ Family
  - Only 6% of the relationships between co-occurring concepts correspond to symbolic relationships recorded in the Metathesaurus

◆ Semantic types
  - The semantics of the relationship often remains ambiguous
Bioinformatics Overview

◆ Association in LocusLink between a Gene / Gene product and
  ● Phenotype
  ● Molecular function
  ● Biological process
  ● Cellular component

◆ Explicit relationship

◆ Most concepts presents in the UMLS

◆ Is the relationship present in the UMLS?
Bioinformatics Example

Dystrophin

LocusLink association

Cytoskeleton

Gene product

Cellular component
Bioinformatics  Relationships explored

Hierarchical
Associative
Co-occurrence
Bioinformatics Example

Dystrophin

Cytoskeleton

Gene product

Cellular component

UMLS Relationship
(Co-occurrence
Freq=83483)

LocusLink association
Bioinformatics Results

- 70% of LocusLink associations supported by some kind of relationship in the UMLS
- Many UMLS relationships supporting LocusLink associations are co-occurrence relationships
- Variation per domain
  - Phenotype 64%
  - Molecular function 83%
  - Biological process 60%
  - Cellular component 70%
From structure to semantics

3. Limitations
Insufficient

- **Identifying vs. solving problems**
  - **Cycles**
    - Which edge to remove?
    - Underlying issues
  - **Inconsistency between Semantic Network and Metathesaurus relationships**
    - Wrong Metathesaurus relationship
    - Wrong / missing Semantic Network relationship
    - Wrong categorization
Insufficient, but…

- Identifying problems is already important
- Possible uses
  - Retrospectively: To focus the work of human editors of the UMLS
  - Prospectively: Structural constraints could be used as filters integrated to the UMLS editing environment
- Additional clues are sometimes available
  - Redundancy
  - Linguistic features
Structure + redundancy (1)
Structure + linguistic features (2)

Syntactic analysis

Mapping to UML

Semantic rules

Semantic network relationships

Select matching rule

Hemofiltration in digoxin overdose

Hemofiltration

Digoxin overdose

Therapeutic or Preventive Procedure

Ther. or Prev. Procedure

Ther. or Prev. Procedure

Ther. or Prev. Procedure

Ther. or Prev. Procedure

Disease or Syndrome

Disease or Syndrome

Disease or Syndrome

Disease or Syndrome

Disease or Syndrome

Disease or Syndrome

Ther. or Prev. Procedure

Ther. or Prev. Procedure

Ther. or Prev. Procedure

Ther. or Prev. Procedure

Ther. or Prev. Procedure

Semantic interpretation
Conclusions
Conclusions

◆ Good knowledge resources should be structurally sound
◆ Identifying structural abnormalities may help identify semantic problems
◆ Like syntax, structure alone does not ensure that the semantics is correct
◆ Close to approaches based on description logics
A Semantic Space For Kids To Play With®
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