Drug Discovery Main Goals

- Identify a drug’s mechanism of action
- Identify the biological process a drug modulates
- Identify new drugs for specific therapeutic indications

Task Analysis

- **T1: Identify Related Items**
  - Item selection and highlighting
  - Clicking, not hovering, on an item also moves all related items in columns to the top

- **T2: Identify Items that Share a Relationship with a Set of Items**
  - Nesting
  - Recursive Nesting

- **T3: Analyse Network Enrichment**
  - Enrichment Score
    - Judging how specific two items are when compared to a third
  - where $J = \text{Pathways}$
  - $S(i,j) = \text{pair score}$
  - $K_i = \text{clusters}$
  - $J = \text{Pathways}$
  - $k = \text{pair score}$

- **T4: Rank Items**
  - Sorting by interest
  - Sort alpha-numerically

Task Analysis

- **T1: Identify Related Items**
  - Selection-based filters
  - Filter choices when multiple items are selected

- **T3: Analyse Network Enrichment**
  - Enrichment Score
    - Sort by enrichment score

Data Abstraction

- **ConTour**
  - History View
  - Pathway View
  - Compound View
  - Filter View
  - Relationship View

ConTour: Data-Driven Exploration of Multi-Relational Datasets for Drug Discovery
Christian Partl, Alexander Lex, Marc Streit, Hendrik Strobelt, Anne-Mai Wassermann, Hanspeter Pfister and Dieter Schmalstieg

"The multi-relational data exploration problem can be interpreted as a graph exploration problem where each item of each dataset represents a node and the relationships between the items are the edges."
• T4: Rank Items
  - Task Analysis
  - Enrichment Score
  - Sort by enrichment score
  - Sorting by interest
  - Sort alpha-numerically

• T5: Filter Items
  - Task Analysis
  - Depends on tasks 1 and 2
  - Navigation
    - Local Filter: filter within a specific column
    - Global Filter: remove items that are not connected to the source column
  - Simple Nesting
  - Recursive Nesting
  - Selection-based filters

• T6: View items in detail
  - Task Analysis
  - Pathway View
    - Total # of compounds that interact with pathway
    - Total # of compounds that interact with pathway
  - Compound View
    - Hue: Elements
  - Linked Views
    - Highlighting
    - Hover

Implementation Details

source code: https://github.com/Caleydo/

ConTour

Algorithm Design

Relationship View

Approximately 100 numerical values shown here
Conclusions

System ConTour

What: Data Multi-relational databases; node-link graph; clusters (derived)
Why: Tasks Discovery; drill down; highlight relationships
How: Multiple Views Relationship view; pathway view; compound view; history and filters
How: Facet Side-by-side linked views, containing tabular data, bar plots, glyphs
How: Selection & Highlighting Linked highlighting across facets; automatic sorting
How: Filtering Drag and drop (nesting); user control (navigation)
How: Ranking & Sorting Enrichment score; highlight; user control (navigation)
How: Encode Simple marks with manipulation of hue and saturation (pathway view)
Scale: Dozens of columns; upper limit on HD display appears to about 20. Thousands of data items. Up to 8 simultaneous views for compounds; only 1 for pathways

Concluding Thoughts

• Seems like a very good tool for use on structured datasets
• When there are indirect (inferred) relationships, it would be good to highlight this with some uncertainty
• What about incomplete relationships?

Case Studies

• Seems like a very good tool for use on structured datasets
• When there are indirect (inferred) relationships, it would be good to highlight this with some uncertainty
• What about incomplete relationships?