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Moliere: Automatic Biomedical Hypothesis Generation

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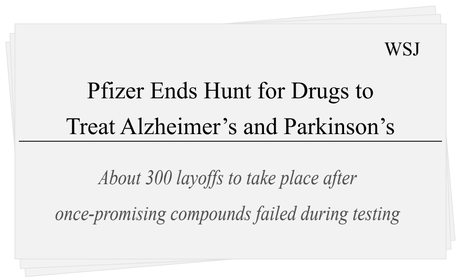
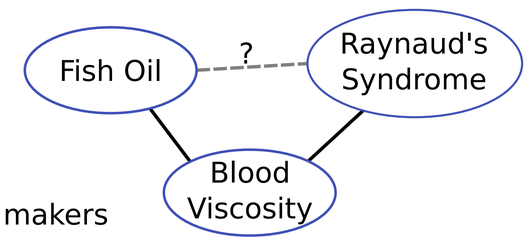
Problem

- Medical research needs early investment
- 2-4k bio papers published daily
- Missed connections lead to missed treatment options, costing lives



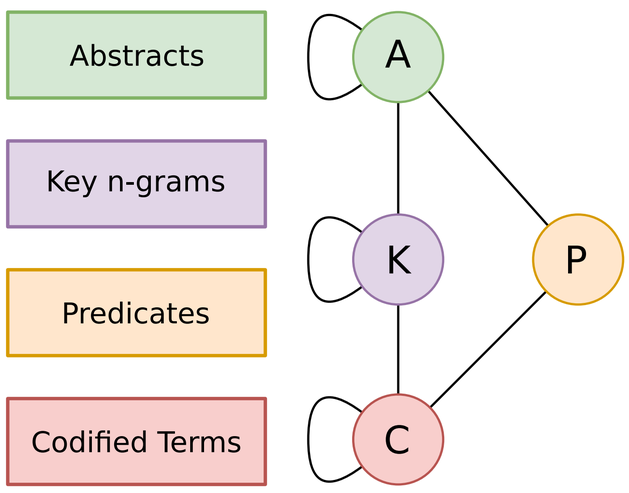
Hypothesis Generation

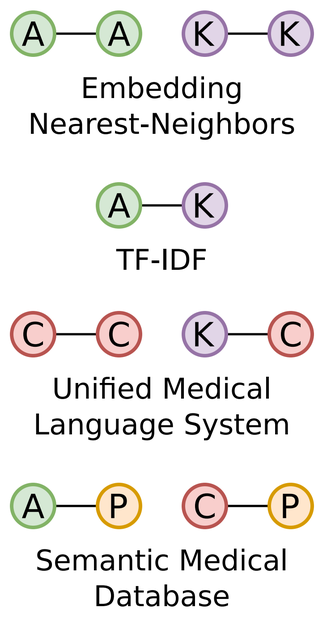
- Understand all available research
- Identify missed implicit connections
- Provide early information to decision makers



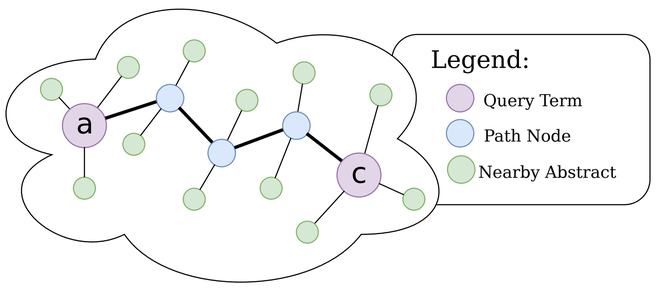
Generating Hypotheses Automatically

- Construct network with NLM sources

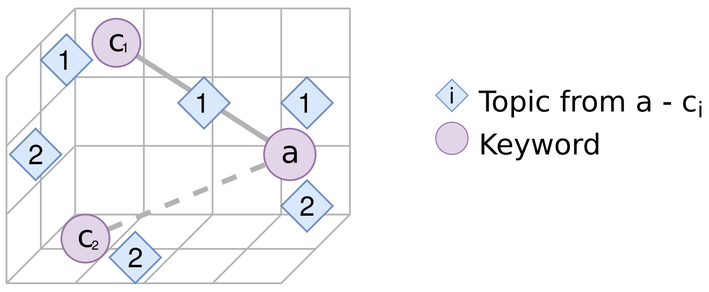




- Describe potential connections through shortest-paths

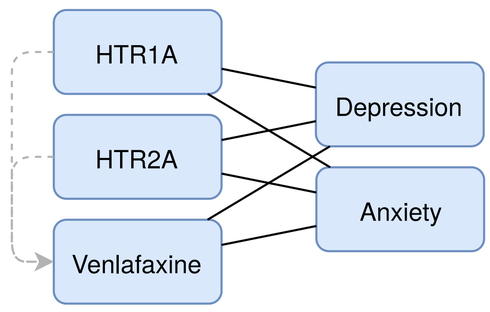


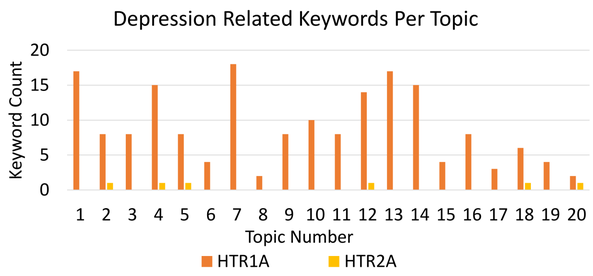
- Generate topic model from cloud and apply metrics



HTR[12]A & Venlafaxine

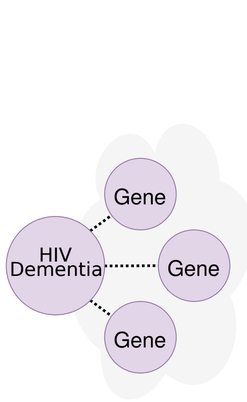
- Initial validation example
- Rediscover exsiting HRT1A connection
- Detect lack of HTR2A connection
- Uses pre-2010 data





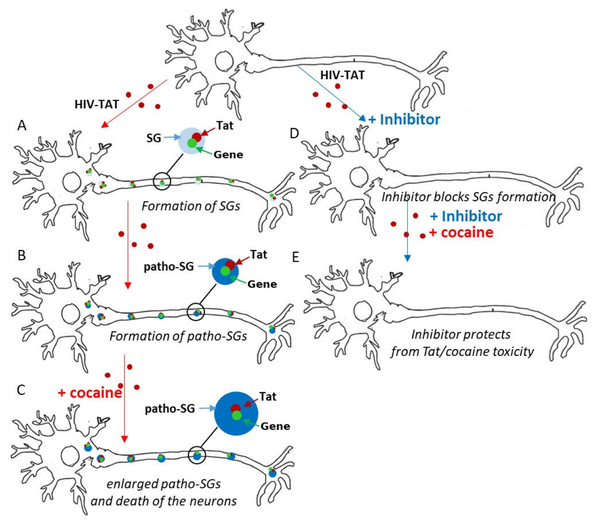
Discovering New Treatments

- 25-33% of HIV+ patients develop HIV-Associated Dementia
- Apply MOLIERE to identify treatment options
- Rank all human genes & create candidate set
- Discover treatment option via lab experiments



ranking

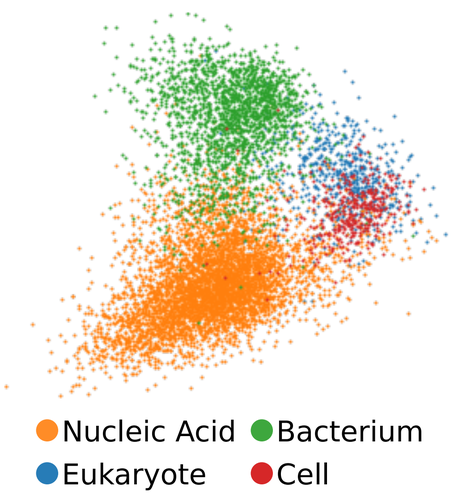
lab experiments



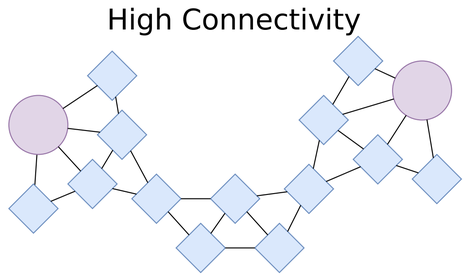
Ranking Hypotheses

- Quantify connections through heuristics
- Derived via embeddings & topic network

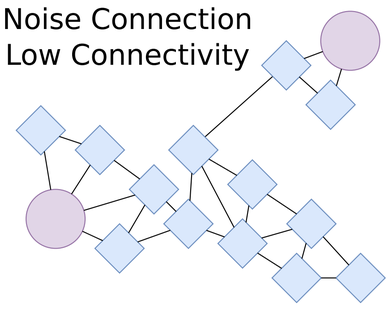
- Example Metrics:
  - Distance between terms
  - Distance to topic centroids
  - Correlation w.r.t. topic model
  - Betweenness of topic network
  - Topic network clustering coef.
  - Polynomial combination



Published Connection
High Connectivity

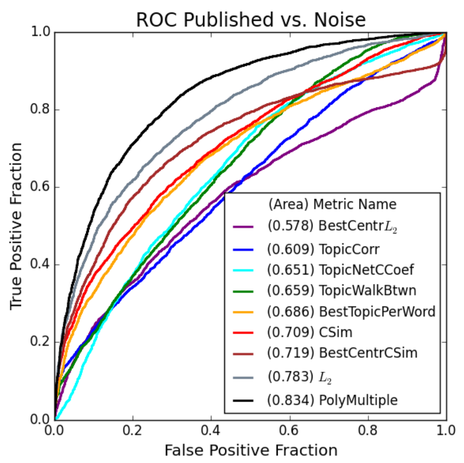


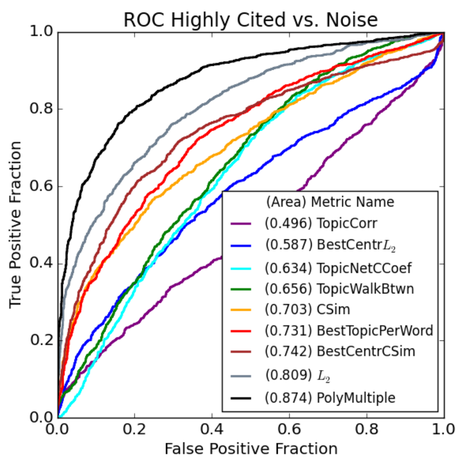
Noise Connection
Low Connectivity



Large-Scale Validation

- Evaluate system without expert input
- Holdout experiment with historical data
- Evaluate thousands of potential hypotheses
- Rank via above metrics





See more here

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