Integrating Text and Graph Data for Biomedical Applications

Biomedical data is multimodal

Different data formats …

Detecting Protein–Protein Interaction Based on Protein Fragment Complementation Assay

Tianwen Wang [1], Ningning Yang [1], Chen Liang [1], Hongjv Xu [1], Yafei An [1], Sha Xiao [1], Mengyuan Zheng [1], Lu Liu [1], Gaozhan Wang [1], Lei Nie [1]

Affiliations + expand

PMID: 32053071 DOI: 10.2174/1389203721666200213102829

Abstract

Proteins are the most critical executive molecules by r genetic materials in any form of life. More frequently, that interacts with other protein(s), which is more evic in the real context of a cell. Identifying the interaction: for the biochemistry investigation of an individual pro picture for the interacting members at the scale of prc mapping). Here, we introduced the currently available the interaction between candidate protein pairs based particular proteins. Emphasis was put on the principle systems are dihydrofolate reductase (DHFR), β-lactam luciferase, β- galactosidase, GAL4, horseradish peroxi fluorescent protein (GFP), and ubiquitin.

Keywords: Protein-protein interaction; enzyme; fluor protein complementation assay; ubiquitin.

Bi-dimensional principal gene feature selection from big gene expression data

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Affiliations + expand

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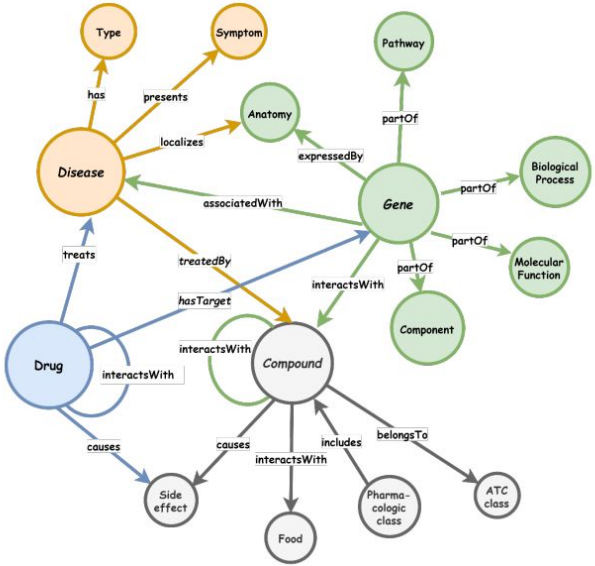
Abstract

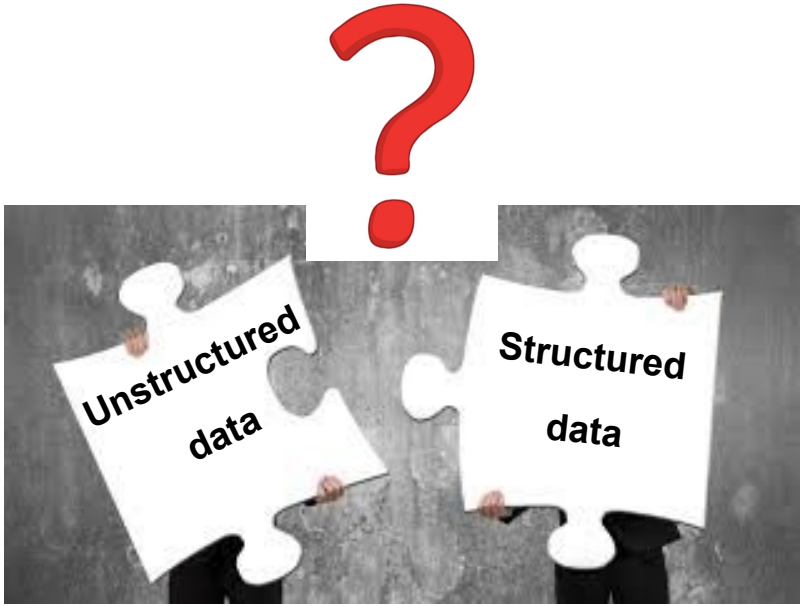
Gene expression sample data, which usually contains massive expression profiles of genes, is commonly used for disease related gene analysis. The selection of relevant genes from huge amount of genes is always a fundamental process in applications of gene expression data. As more and more genes have been detected, the size of gene expression data becomes larger and larger; this challenges the computing efficiency for extracting the relevant and important genes from gene expression data. In this paper, we provide a novel Bi-dimensional Principal Feature Selection (BPFS) method for efficiently extracting critical genes from big gene expression data. It applies the principal component analysis (PCA) method on sample and gene domains successively, aiming at extracting the relevant gene features and reducing redundancies while losing less information. The experimental results on four real-world cancer gene expression datasets show that the proposed BPFS method greatly reduces the data size and achieves a nearly double processing speed compared to the counterpart methods, while maintaining better accuracy and effectiveness.



… require different processing methods

Biomedical data is multimodal

How to integrate and leverage both types of information …



… to derive new biomedical insights?

Team Project Variants

Variant 1

Multimodal Embeddings for Biomedical Concept Alignment

Variant 2

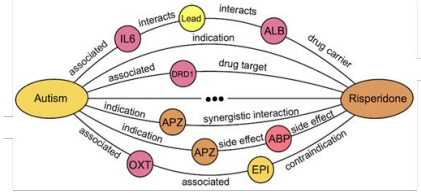
Mapping Biomedical Concepts from Text to KG Triples

Team Project Variants

Variant 1

Multimodal Embeddings for Biomedical Concept Alignment

E.g. Enhance drug discovery through text and graph integration



Review > Chem Biol Interact. 2023 Jan 5:369:110296. doi: 10.1016/j.cbi.2022.110296. Epub 2022 Dec 7.

Neuropharmacological effect of risperidone: From chemistry to medicine

Abstract

As the second-oldest atypical antipsychotic, risperidone has a long history of off-label usage for treating behavioural and psychological signs and symptoms of dementia (BPSD), such as agitation, aggressiveness, and psychosis. Risperidone has been shown in several trials to have a statistically significant benefit when used in a therapeutic context. Several lines of evidence suggest a possible role of risperidone via the antagonistic effect of Dopamine D2 and 5HT-receptor in different neurological diseases like cognitive dysfunction of schizophrenia, neuroinflammation, Huntington's disease, and sleep cycle management. Therefore, the pharmacological interactions of risperidone in all these diseases were investigated. Some reports on the use of risperidone in the treatment of dopaminergic psychosis have been slightly conflicting. However, more research is needed to evaluate the role of risperidone in the treatment of these neurological diseases.

Keywords: Dopaminergic psychosis; Neuroinflammation; Neurological diseases; Neuropharmacological treatment; Risperidone.

Can risperidone be used for traumatic brain injury?

Variant 2

Mapping Biomedical Concepts from Text to KG Triples

E.g. Mapping gene-disease relations from text to links in the graph

***BRCA1* Gene in Breast Cancer**

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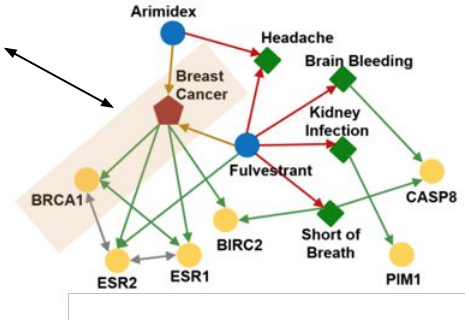
The *BRCA1* gene was identified and cloned in 1994 based on its linkage to early onset breast cancer and breast-ovarian cancer syndromes in women. While inherited mutations of BRCA1 are responsible for about 40–45% of hereditary breast cancers, these mutations account for only 2-3% of all breast cancers, since the *BRCA1* gene is rarely mutated in sporadic breast cancers. However, BRCA1 expression is frequently reduced or absent in sporadic cancers, suggesting a much wider role in mammary carcinogenesis. Since BRCA1 was cloned in 1994, its molecular function has been the subject of intense investigation. These studies have revealed multiple functions of the BRCA1 that may contribute to its tumor suppressor activity, including roles in: cell cycle progression, several highly specialized DNA repair processes, DNA damage-responsive cell cycle checkpoints, regulation of a set of specific transcriptional pathways, and apoptosis. Many of these functions are linked to protein:protein interactions involving different portions of the 1,863 amino acid (aa) BRCA1 protein. BRCA1 functions in cell cycle progression and the DNA damage response appear to be regulated by distinct and specific phosphorylation events, but the molecular pathways activated by these phosphorylations are only beginning to be unraveled. In addition, the reason that BRCA1 mutation carriers develop specific tumor types (breast and ovarian cancers in women and possibly prostate cancers in men) is not clearly understood. Elucidation of the precise molecular functions of the *BRCA1* gene product will greatly enhance our understanding of the pathogenesis of hereditary as well as sporadic mammary carcinogenesis. J. Cell. Physiol. 196: 19–41, 2003.



V1: Multimodal Embeddings for Biomedical Concept Alignment

Goal: Analyze whether richer multimodal representations of biomedical concepts improve performance in downstream tasks

Tasks

- ➔ Data collection
  - ◆ Text data from PubMed (e.g., biomedical paper abstracts)
- ➔ Entity embedding generation
  - ◆ Generate representations of the same entity (e.g., disease) from both unstructured (e.g., w/ pre-trained language models) and structured data (e.g., w/ knowledge graph embeddings)
- ➔ Alignment function design
  - ◆ Explore methods to combine the representations of identical concepts across structured and unstructured data sources
- ➔ Evaluation on biomedical tasks
  - ◆ Use the unified representations in downstream applications (e.g., disease diagnosis, treatment recommendations)

V2: Mapping Biomedical Concepts from Text to KG Triples

Goal: Construct a mapping function which translates relationships between concepts described in the biomedical literature into corresponding triples in a knowledge graph

Tasks

- ➔ Data collection
  - ◆ Text data from PubMed (e.g., biomedical paper abstracts)
- ➔ Entity embedding generation
  - ◆ Generate representations of the same entity (e.g., disease) from both unstructured (e.g., w/ pre-trained language models) and structured data (e.g., w/ knowledge graph embeddings)
- ➔ Mapping function design
  - ◆ Investigate methods for developing a mapping function that, given the representation of the three elements in a triple, can identify the source in the literature
- ➔ Evaluation using biomedical databases

Requirements

- ➔ Duration: 6 months
- ➔ Number of participants: max 6-8
  - ◆ **Applying as a group** is possible and recommended!
- ➔ Prerequisites:
  - ◆ One of Machine Learning, Knowledge Graphs, Data Mining AND
  - ◆ One of Text Analytics, Advanced Methods in Text Analytics AND
  - ◆ **Strong programming skills in Python** (knowledge of HuggingFace Transformer/ PyTorch is a plus)
- ➔ Interest in knowledge representation learning and NLP
- ➔ Biomedical knowledge is not required
- ➔ Applicable: Business Informatics and MMDS
- ➔ Instructors: Andreea Iana, Rita Torres de Sousa