Mining collaboration in NSF grants

...with comparison between China & US

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员","code":"B03","conclusionAbstract":"本项目对在纳米孔道限于环境 下水,离子,及生物分子的输运,组装,及其应用进行探索性研究。构筑具有与离 子输运方向平行的(纵向)异质结构的纳米多孔薄膜,合成和制备无机/无机复合 或者有机/无机复合的新颖的纳米异质结构多孔膜材料,并结合化学修饰策略,构 筑具有结构,化学组分,电荷,浸润性等多重非对称元素的复合隔膜,研究其中的 非对称离子输运特性。探索生物大分子、如DNA在孔道受限环境内的组装过程、及 对跨膜离子传输性质的调控。利用石墨烯及其衍生物构筑包含大规模纳米流体网络 的二维层状材料薄膜,并结合化学修饰策略,构筑具有不同电荷极性,不同浸润 性,和不同化学组分的二维纳米通道体系,并使其具有仿生的刺激-响应特性,拓 展二维纳米孔道的应用领域。同样测试其在电解质溶液,包括人工配置的电解质溶 液和部分生物溶液、比如汗液、尿液、模拟组织液等中的能量转换特性。项目执行 期间, 共发表 SCI 论文 30 篇, 包括在J. Am. Chem. Soc. (3 篇), Angew. Chem. Int. Ed. (1 篇), Adv. Mater. (5 篇), Adv. Funct. Mater. (5 篇), ACS Nano (1 篇), Acc. Chem. Res. (1 篇), Chem. Soc. Rev. (1 篇), 等化学, 材料领域的顶级期刊(影响因子均大于 11.0)上 发表学术论文 17 篇。申请中国专利 3 项, PCT 专利 1

项。","dependUintD*:"201049","dependUnit":"中国科学院理社技术研 究所","downloadIterf:""","projectbatractC"、受限子介孔和微孔内的 受限水在生物。地质、科技等领域中起着非常重要的作用。可以这么、说、没有受 限水的研究发生重要。本课题将以均克制备各类尺寸,界面性质的变限载体为基 础、实验、结合理论模拟、研究受限水的分子结构、动力学行为、受限水在受限载 体中的输运和受限水。的相变行为。建立受限水的这些特殊性能与受限载体的基种 性能的相互关系。","projectbatractD*: "The confied water, that is water confined in micro- or mesopores, plays an important.role in various biological, geological,

Important for an Various biological, geological, technological and other processes for example, life is not possible without confined water, which exists mainly in living.organisms.Therefore it is crucial to have a thorough understanding of properties.of confined water. Taking advantage of well-developed processes for the fabrication.of micro- and mesopores in our group, systematic investigation on the molecular.structure, conformation dynamics, phase

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Mapping from name to Acemap-ID: Name (Maria M. Almanzar) -> AuthorID (100000415)

- Large volume of data: **91,458,238** authors in total, took almost **2 min** to traverse, over **8 GB** dump;
- Confusion between duplicate names: more than **10** authors with name 'A. A. A. Mohamed';
- Ambiguity rising from degeneracy: '张三' or 'San Zhang' or 'San ZHANG' or 'Zhang San';
- Multiple Institutions: Geoffrey Hinton worked for Google and the University of Toronto at the same time;
- Typo: 'Keith Ross' (NYU Professor) and 'Keith Rose' (surgeon) and 'Keith Ros' (nobody);

Strategy One: Direct Matching of Name.



Strategy Two: Direct Matching of Name + Affiliation.



Strategy Three: similarity ranking of Name + Affiliation (based on Levenshtein distance).



Strategy Four: similarity ranking of Name + Collaborators (based on Graph Neural Network).



Design of Experiments:

- Use authors from NSF_US as dataset, randomly extract 10% of it as test set;
- Manually create typos at rate **α** in test set (insertions, deletions or substitutions);
- Set a drop rate β of affiliation and collaborators;

	Training Time	Inference Time	Acc*	Acc**
Name	-	0.01 s/item	0.93	0.42
Name + Affiliation	-	0.02 s/item	0.98	0.53
Levenshtein	-	0.42 s/item	0.99	0.89
GNN	2 hours	1.98 s/item	0.97	0.95

* : with α = 0 and β = 0 **: with α = 0.2 and β = 0.8

Deployment:

• We will deploy our algorithms on Acemap server and provide an API for users;

Contribution I: NSF-CN DataBase

Intuition and Contribution:

- Acemap NSF-CN database contains the principal investigator and the grant information;
- We built a table (NSF_CN.grants), using 'grants.projectManager' as foreign key;
- We built a table (NSF_CN.cn_nnsf_participants),

Contribution II : NSF-US Grant Table

Intuition and Contribution:

- Acemap NSF-US database contains the principal investigator and the grant information;
- We built a table (NSF_US.grants) providing detailed information about grants;
- We built a table (NSF_US.participants) providing all investigators in the grants.

Graph Database

- A type of NoSQL database.
- Uses graph structures for semantic queries with nodes, edges, and properties to represent and store data.
- Flexible & Extensible.



JanusGraph

- Deployment
 - Hbase as storage backend.
 - Solr as external index backend.
 - Gremlin as graph traversal language.
- Performance Test
 - 5.75s for finding the US scholar with most collaborations. .



Connect to Gephi



Complex Network Analysis

- Qualitative methods for understanding network characteristics
- Metrics we look at
 - Size
 - Degree distribution, average node degree
 - Diameter
 - Assortativity coefficient: Do connected nodes have similar degrees rich club?
 - Clustering coefficient: Tendency for nodes to cluster together
 - Rich club coefficient: Are well-connected nodes connected?
- Cross-comparison between US, CN and US + CN

Example: US NSF

- Size: |V| = 104524, |E| = 235320
- Average degree: 4.50
- (Pseudo) Diameter: 20
- Assortativity: 0.07
 - \circ Close to 0, not assortative
- Average clustering coefficient: 0.46 (High)

Clustering coefficient distribution



Example: US NSF





Does NOT follow power law

Cross-comparison

Data	Diameter	Assortativity	Average clustering coefficient	Rich club coefficient
US	20	0.07	0.45	< 1
CN	18	0.13	0.56	< 1
CN + US	15	-0.25	0.32	< 1



The Final CN-US collaboration (not coronavirus)

Thanks

Notable Metrics

- Assortativity
 - Two connected nodes imply their similarity.
 - Assortativity coefficient, with regard to a property, measures the overall similarity on this property between two connected nodes?
 - \circ Actually Pearson'r, so falls in [-1, 1]
- Clustering coefficient
 - For each node, the number of edges in its neighborhood / the number of edges if its neighborhood is complete
 - Understood w.r.t a comparable random graph
- Rich club coefficient
 - For degree k, the number of edges in the subgraph formed by nodes with degree >= k / complete graph

Computing the Metrics

- Select a network-analysis framework
 - Strike the right balance between speed and ease of use
 - Contenders: networkx, igraph, graph-tool, SNAP, networkkit
- Networkx
 - The most-feature complete
 - Written in pure Python = extremely slow
 - Benchmarks¹ show that it is 10 times slower than the *slowest* library
- Graph-tool
 - C++ with Python interface = fast (like Numpy)
 - We have to implement the rich club coefficient ourselves
- Why not Gephi
 - Not well-maintained
 - Lack many metrics

1 https://www.timlrx.com/2020/05/10/benchmark-of-popular-graph-network-packages-v2/