Graph Database on Medical Research Data for Integrated Life Science Research

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Abstract: Indonesia has experienced an increasing surge of published scientific articles in recent years. In medical science, published articles greatly vary from both pre-clinical and clinical studies, where each study possesses a different methodological approach and hypothetical premise. However, some articles do not include rigorous documentation to make it reproducible. Moreover, the lack of centralized database further impedes researcher from reanalysing previous findings and integrating them with the new study. This paper delineates such an issue by constructing a graph database to centralize and integrate clinical research data. The database is constructed using Neo4j and cypher querying language and populated with 5,000 medical records generated by the synthea program. We address the viabilities of our proposed data curation method by simulating data of different sizes. Our database was able to answer queries requiring complex relationships while minimizing the amount of database hits. We conclude that graph databases are quite performant for solving data integration and centralization issues faced by life science research institutes.

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1 INTRODUCTION

Scientific publications in Indonesia have undergone manifold increases within the past decades. As reported by Maula, Fuad and Utarini (2018), numbers of published articles on dengue-related subjects increased 13 times in 2017, as compared to 2007. Such an increase was also followed by *h-index* improvement, resulting in Indonesia being placed as the 5th most scientifically productive ASEAN country in investigating dengue-related topics (Maula, Fuad, and Utarini, 2018). Another bibliometric analysis investigated by Sarwar and Hassan (2015) also enlisted Indonesia within 11 of the most scientifically productive Islamic countries. However, these articles often did not provide a robustly elaboration of the methodological procedure or provide the obtained data for reanalysis; these two factors contribute to reproducibility and credibility in scientific publication (Pashler and Wagenmakers, 2012; Stark, 2018; Resnik and Shamoo, 2016). Besides enabling preprint access (Oakden-Rayner, Beam and Palmer, 2018) and thorough documentation on methodology, data availability is also a crucial component for reproducibility in science (Peng, 2015). Therefore, we proposed utilizing graph databases to integrate research findings in life science-related fields.

1.1 Graph Database

Data management systems should appropriately consider interoperability and scalability, which enable data storing, indexing and retrieving. Databases aggregate integrated objects in a structure defined by its metadata. The presence of metadata implies a self-defined property of the database, whereas in a relational database management system (RDBMS), such a definition is included within its particular schema (Berg, Seymour and Goel, 2012). During the development of RDBMS, the need to quickly retrieve the data through a syntactically and logically feasible manner, therefore inducing the conceptual design of SQL, a structured querying language is emerging.

However, with data being stored in a multi-tabular layout, the relational database (RDB) faced massive disadvantages in handling highly-connected data. Hence the development of a schema-less database initiated by NoSQL (Berg, Seymour, and Goel, 2012; Fabregat et al., 2018), with a graph database being

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one of its variants (Oussous et al., 2015).

A graph database is more performant in storing data with intricate relationships (e.g.., protein interactions or chemical reaction pathways), as compared to its RDB counterparts (Fabregat et al., 2018). Neo4j is a graph database platform developed in Java and compliant towards an ACID system (Atomicity, Consistency, Isolation, Durability) (Oussous et al., 2015). As a native graph database, Neo4j stores data as explicitly defined relationships in a schema-less management system. Therefore, Neo4j treats database querying as a graph traversing process. This redeeming feature of the graph database, in general, enables higher performance and flexibility in storing the data. Neo4j employs cypher as a querying language to define patterns on traversing the relationship graph. Furthermore, the ASCII-Art syntax of cypher enables a more intuitive querying process. Such uniquely written language and ACID-compliant platforms could become a two-fold advantages to use Neo4j in delivering a graph database management system.

1.2 Medical Informatics

Information in the life science-related fields often possesses an intelligible relationship of a causative nature. Such information may present a connection between one entity to another. Interractome, reactome and connectome are common examples we see (Figure 3) that may be found in currently emerging basic science research. In the translational research paradigm, some interests highlighted the importance of genetic and proteomic interaction networks. Meanwhile, in clinical settings, we may also want to consider patient, doctor and institution as separate-yet-related entities. Therefore, the nature of the data in medicine actually closely resembles entity-relationship data. We will undoubtedly consider applying a graph database as an alternative to RDB for use in storing life science-related research data.

2 METHOD

This study utilized a machine with Intel Core i7-7700HQ, 8GB of DDR4 RAM and a 5400 RPM spinning hard disk. We employed Neo4j as a platform to create a graph database with Cypher as the querying language. Data used in this study are generated from a synthea program, producing 5,000 to 50,000 medical records in json-based FHIR (Fast Healthcare Interoperability Resources), whichwas directly converted into *.csv format. As shown in Figure 1, we treated each entity as a vertex and underlying relationship as an edge connecting two

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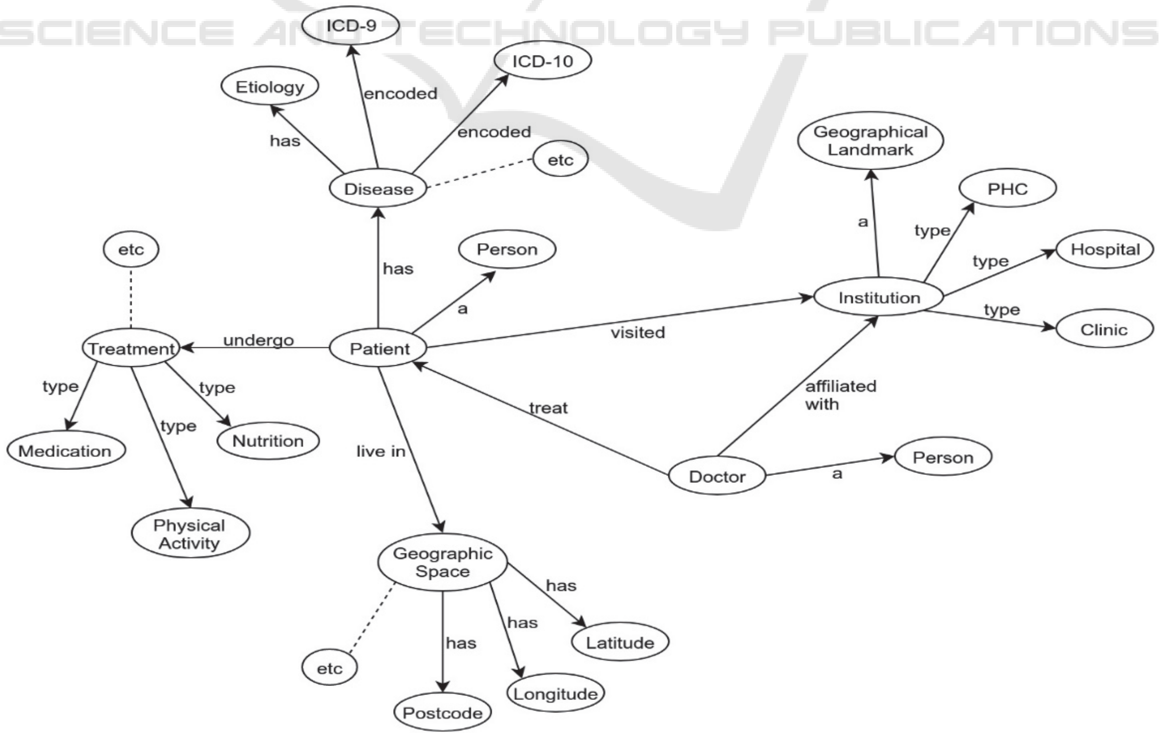

Figure 1: Schematic representation on graph database for medical records.

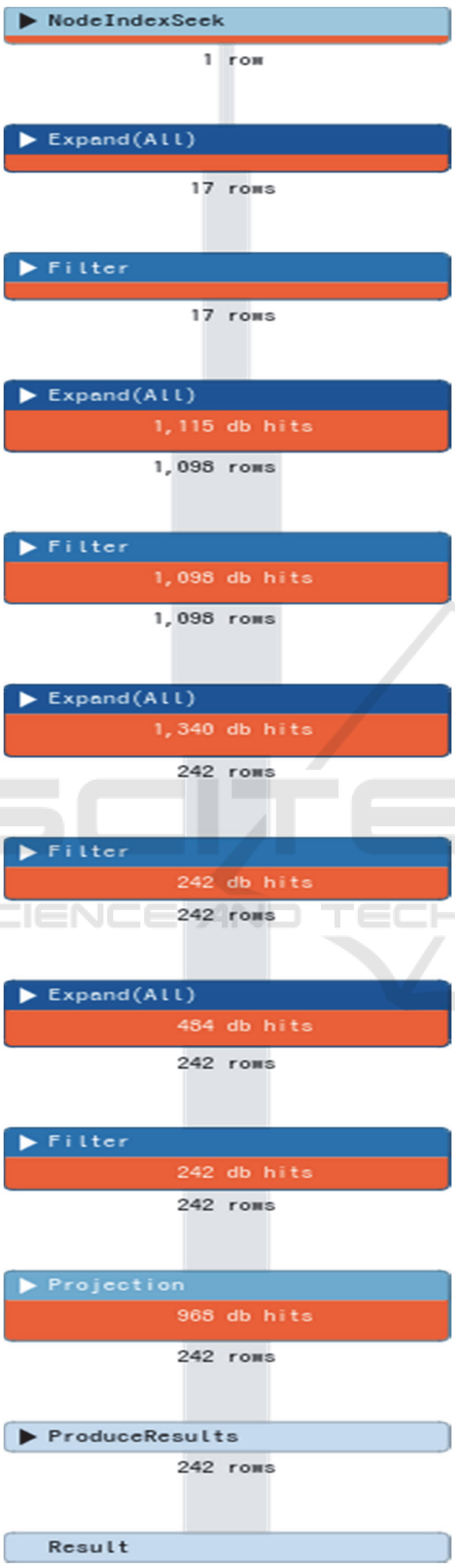

Figure 2: Database hits on the first query.

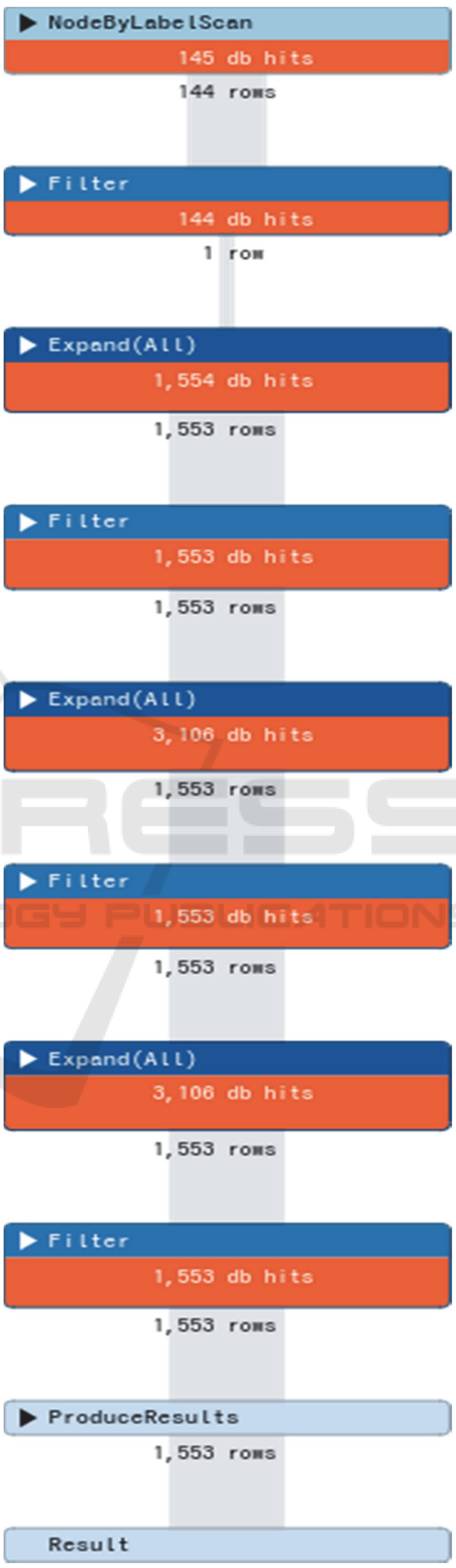

Figure 3: Database hits on the second query.

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vertices. We first designed constraints for unique input and indices for redundant vertices. To prevent random access memory (RAM) bottleneck, we enabled periodic commit for each of the 500 inputs, which was especially beneficial when dealing with numerous entries. Afterwards, we loaded a *.csv file generated by synthea as a query object and set the entity and relationship.

To measure the performance of our proposed database, we created a log containing time consumption and a number of created objects, which included nodes, relationships, graph property and graph labels. Said database model took data of various sizes as input: 5,000, 10,000, 20,000 and 50,000. Considering exponential increment in our data, we applied power transformation according to the Tukey ladder of power to normalize the data. The Anderson-Darling test was then employed to challenge normality assumption. We computed correlation estimates between time and created objects based on *p*-value obtained from a normality test. Kendall's tau estimates the correlation when any of imputed variable has $p < 0.05$; Pearson's is used in other cases. Data was fitted into a generalized linear model (GLM) with the Gaussian link function. The simulation process involved two different queries on all datasets.

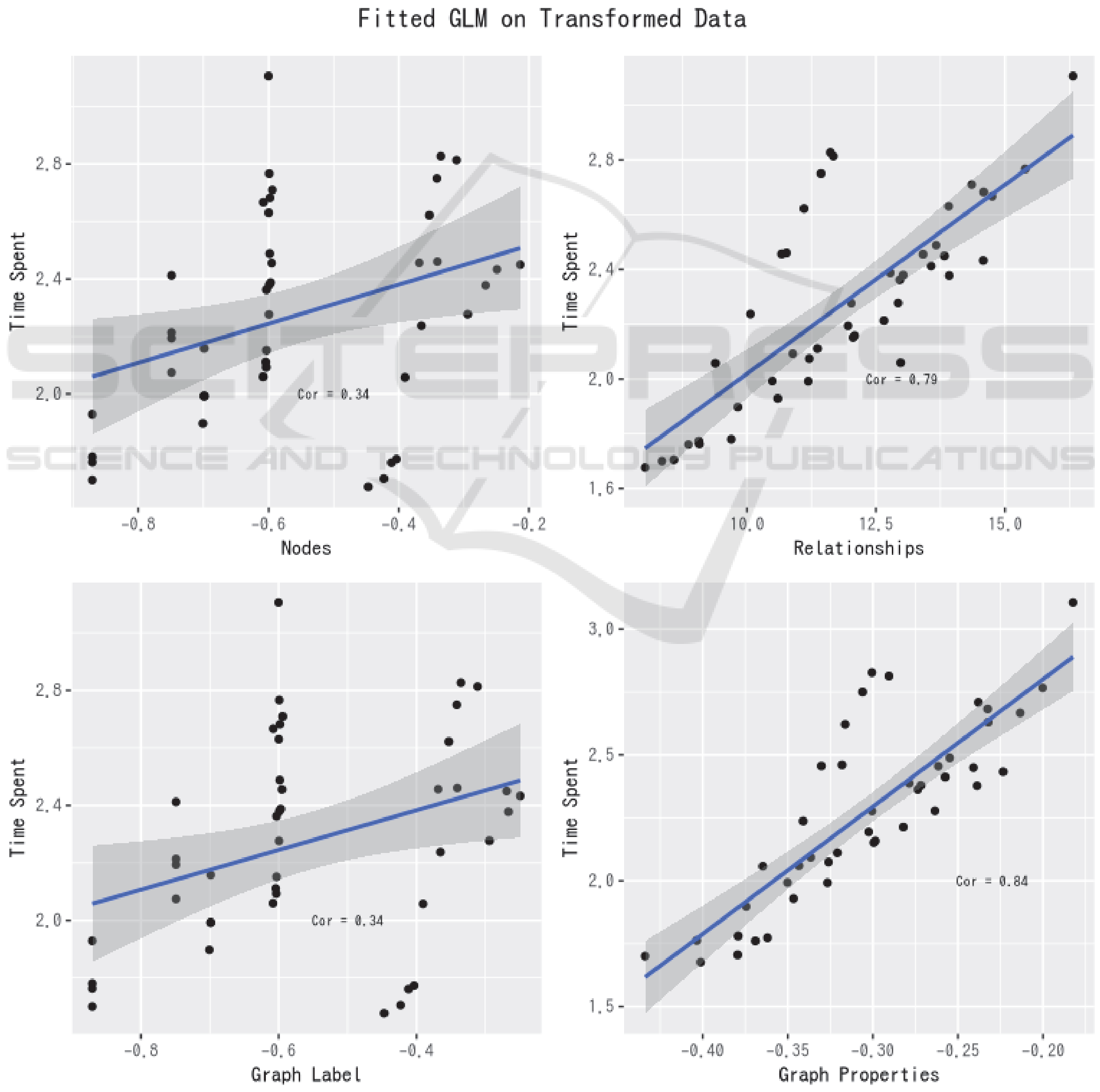

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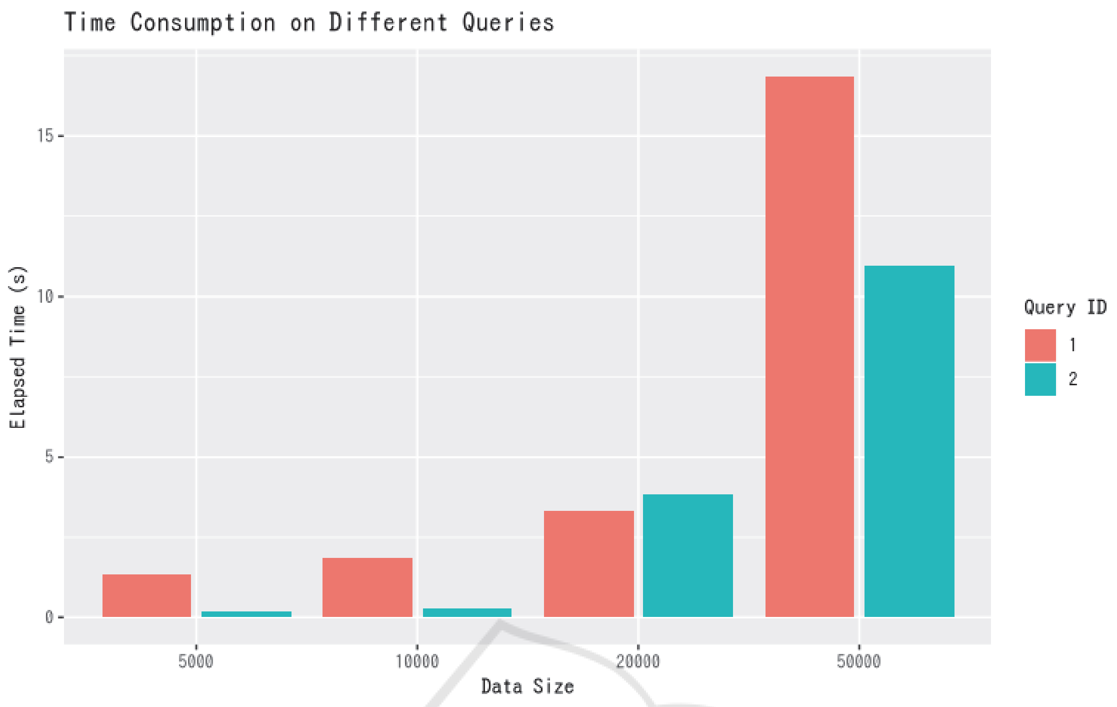
Figure 4: Queries on different datasets. Top: Data size and elapsed time. Bottom: Database hits and elapsed time.



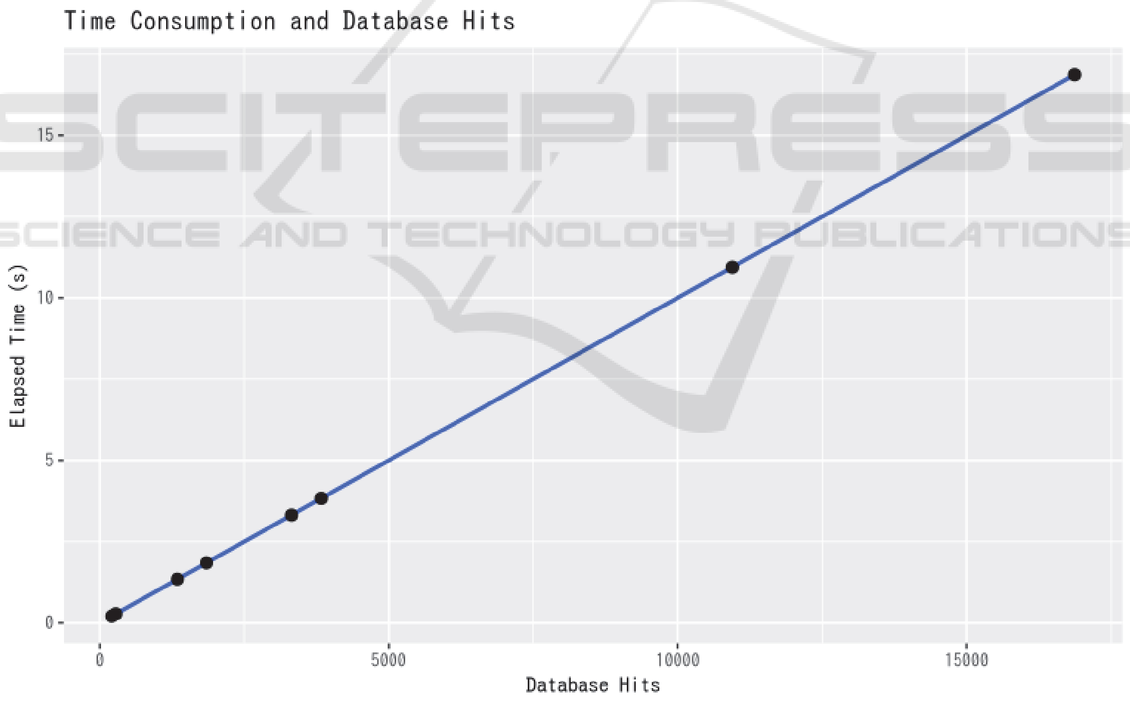


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Figure 5: Data transformation and correlation.

Database hits (db-hits) and time measured the efficacy in handling such queries. Results on simulation presented in bar plot to demonstrate database scalability. Queries are written in cypher and are presented as follows:

```
// List diagnoses in Massachusetts
match (p:Patient) -[:ATTENDED_AN]->
    (e:Encounter) <-[:PROVIDED_AN]-
    (o:Organization) -[:LOCATED_IN]-> (g
:GeoLoc)
match (d:Diagnoses) <-[r:HAS_DIAGNOSES]
- (e:Encounter)
```

```
return p.Name as Patient,
    d.Name as Diagnoses,
    o.Name as Institution,
    g.Name as City,
    r.Date as Date
;
// List patients with hypertension
match (p:Patient) -[:ATTENDED_AN]-> (e:
Encounter)
match (:Diagnoses {Name:'Hypertension'}
) <-[:HAS_DIAGNOSES]-
    (e) <-[:PROVIDED_AN]- (o:Organizati
on)
return p, e, o
;
```

3 RESULT

The constructed database was able to return answers to queries requiring complex relationships. Our previous queries assume data with complex relationships, where each returned a network of patient, institution and the encounter. Figure and depicted profile of database hit from both queries. Depicted in the figure is the representation of query scalability on data with different sizes. Fitted GLM is presented as Figure 4, which shows that relationship and graph property have the most implication on data input runtime (ρ = 0.79, ρ = 0.84).

4 DISCUSSION

Our study demonstrates the graph database as a potential platform to store life science research data. Previous studies emphasized graph database credibility in storing interconnected data, where a graph database pattern query on such data may outperform RDB (Medhi and Baruah, 2017; Fabregat et al., 2018; Mathew and Kumar, 2014). However, in other cases requiring analytical query, RDB outperformed the graph database; in their study, Hölsch, Schmidt and Grossniklaus (2017) argued that Neo4j became less performant due to a less advanced disk and buffer management, compared to RDB. We therefore conclude that a graph database is quite performant for integrating medical health records generated for 5,000 subjects using a synthea program.

Our simulation demonstrated the viability of storing and querying a large dataset. On exponentially increasing data size, time consumption on particular queries also increased exponentially, as demonstrated in Figure 5. However, it appears to us that further optimization should be of essence, considering that query runtime increases from 20,000 to 50,000 dataset. In preparing the database, the log captured objects, thus causing an immense burden during data input. Said objects include relationship and graph property, where previously mentioned graph database stores an object explicitly instead of implying the relationship. This feature aids graph database to answer queries for complex relationships. As such, longer time spent in creating an object within the database will not be an issue. During data preparation, we observed a longer time duration in bigger dataset. It seems Neo4j may perform better when using smaller data, so we suggest dividing data into smaller chunks to improve data input performance.

5 CONCLUSIONS

As a concluding remark, the graph database is quite performant to integrate medical health record generated for 5,000 to 50,000 subjects using synthea.

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