

A Graph Database Repository and Performance Evaluation Metrics for Graph Edit Distance

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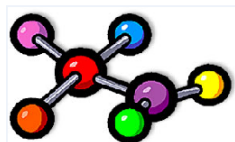
May 14, 2015



"Real-world graphs are everywhere" but how to compare them?



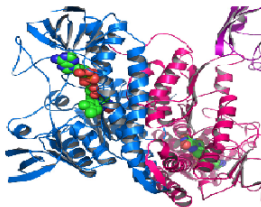
Social Networks



Chemical Bounds

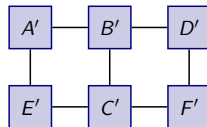
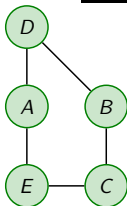


Characters

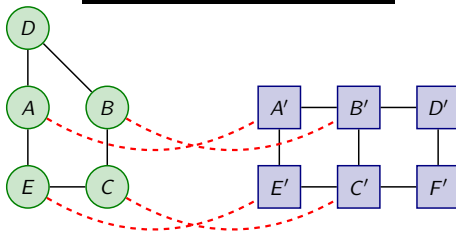


Protein Structures

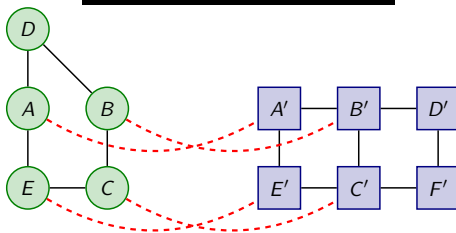
Inexact Graph Matching



Inexact Graph Matching



Inexact Graph Matching



Two Types

Exact
Approaches

Exponential
Complexity

Approximate
Approaches

Polynomial
Complexity

Raised Questions

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- **Q1: How to evaluate error tolerant graph comparison methods ?**

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 - Precision.

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 - **Memory consumption.**

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- **Q1: How to evaluate error tolerant graph comparison methods ?**
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 - Precision.
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 - **Parameter's sensitivity.**

Raised Questions

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 - Graphs types:
 - ★ Different typologies (dense, sparse, etc.).
 - ★ Different kinds of attributes (nominal, numeric, etc.).

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- **Q2: How to choose graph matching databases?**
 - Graphs size.
 - Graphs types:
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 - ★ Different kinds of attributes (nominal, numeric, etc.).
 - Applications types:
 - ★ Not only databases dedicated to classification (e.g., IAM [Riesen2008]).
 - ★ Other databases dedicated to other applications (e.g., matching quality).

Outline

- 1 Introduction
- 2 Related Works
- 3 Graph Repository
- 4 Performance Evaluation Metrics
- 5 Use Case
- 6 Conclusions and Perspectives

Plan

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Graph Edit Distance

Graph Edit Distance

Let $g_m = (V_m, E_m, \mu_m, \zeta_m)$ be the model graph and $g_t = (V_t, E_t, \mu_t, \zeta_t)$ be the target graph. The graph edit distance between G_1 and G_2 is defined by:

$$d_{plain}(g_m, g_t) = \min_{e_1, \dots, e_k \in \gamma(g_1, g_2)} \sum_{i=1}^k c(e_i)$$



Figure: Graph Edit Distance operations

Related Works

Ref	Problem Type	Graph Type	Database Type	Measure Type	Purpose
Santo2003	Exact GM	Non-attributed	Synthetic	Accuracy and scalability	Matching
CMU DataBase	Error-tolerant GM	Attributed	Real-world	Memory consumption, accuracy and matching quality	Matching
Riesen2008	Error-tolerant GM	Attributed	Real-world	Accuracy and running time	Classification
Conte2007, Foggia2001	Exact GM	Attributed	Synthetic	Accuracy and scalability	Matching
Carletti2013	Exact GM	(Non)attributed	Real-world	Scalability	Matching

Table: Synthesis of graph databases.

CMU Database: <http://vasc.ri.cmu.edu/idb/html/motion>

Conclusions of the state of the art

- Lack of performance comparison measures for error-tolerant GM methods.


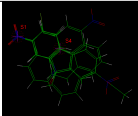
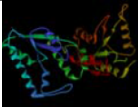
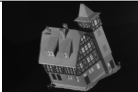
Conclusions of the state of the art

- Lack of performance comparison measures for error-tolerant GM methods.
- None of the repositories was dedicated to assessing the performance of GED.

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Databases

Database	Decomposition	Overview	Purpose
GREC	MIX, 5, 10, 15 and 20 vertices		Classification
MUTA	MIX, 10, 20, ... , 70 vertices		Classification
Protein	MIX, 20, 30 and 40 vertices		Classification
CMU	30 vertices		Matching

Databases

Database	# subsets	Max Graphs Size	# graphs per subset	# comparisons per subset	# optimal solutions
GREC	5 subsets	20	10 graphs	100	441
MUTA	8 subsets	70	10 graphs	100	189
Protein	5 subsets	40	10 graphs	100	47
CMU	1 subset	30	111 graphs	660	128

Table: Overview about the subsets included in the repository.

Repository link: <http://www.rfai.li.univ-tours.fr/PagesPerso/zabuaisheh/GED-benchmark.html>.

Added Low Level Information

- **6 methods:**

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 - ★ Munkres [Riesen2009].
 - ★ Hausdorff [Fischer2013].

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 - Distance between each pair of graphs.

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G1Name	G2Name	Method	Distance	Optimal	Matching
image3.23	image3.25	BS-100	135.178	true	Vertex:0 → 0=37.476/ Vertex:1 → 1=6.519/ Vertex:2 → 2=32.070/ Vertex:4 → 4=34.409/ Vertex:3 → 3=24.703/ Edge:2 ↔ 3 → 2 ↔ 3 =0.0/ Edge:0 ↔ 4 → 0 ↔ 4=0.0

Table: Low level information (taken from the file GREC5.csv)

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- For each graph matching pair:
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Table: Low level information (taken from the file GREC5.csv)

- **Detailed answers:** <http://www.rfai.li.univ-tours.fr/PagesPerso/zabuaisheh/GED-benchmark.html>.

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Performance Evaluation Metrics

- All metrics can be tested under:

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Performance Evaluation Metrics

Performance Evaluation Metrics

- Given the reference answer R :

Performance Evaluation Metrics

- Given the reference answer R :
 - Deviation.

Performance Evaluation Metrics

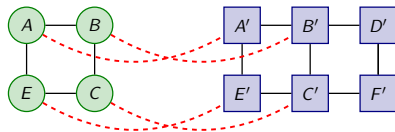
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Performance Evaluation Metrics

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Performance Evaluation Metrics

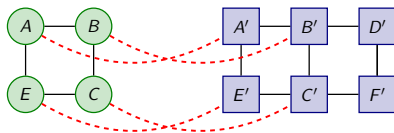
- Reference Distance (RD) = 5
- Reference Matching (RM):



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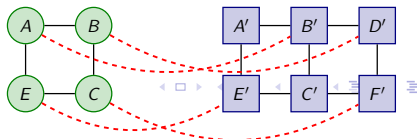
Performance Evaluation Metrics

- Reference Distance (RD) = 5
- Reference Matching (RM):



- Given the reference answer R :
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- Distance found by method (m) = 6.
 - Deviation = 20%.
- Matching found by method (m):
 - Matching Dissimilarity = 75%.



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 - **Mean running time in milliseconds.**

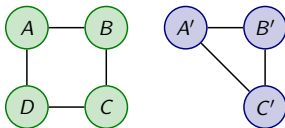
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 - Mean number of explored nodes.
 - Mean running time in milliseconds.
 - **Running time-Deviation plot:**

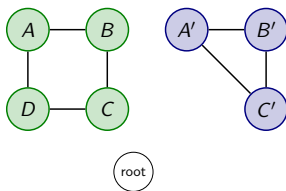
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 - Number of Time-Out and Out-Of-Memory cases.
 - Mean number of explored nodes.
 - Mean running time in milliseconds.
 - Running time-Deviation plot:
 - ★ Projection on a two-dimensional space (\mathbb{R}^2).

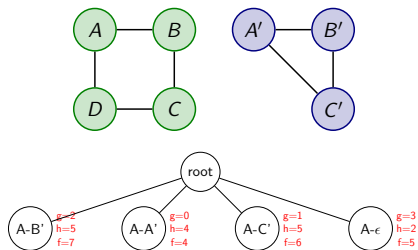
Performance Evaluation Metrics - Example



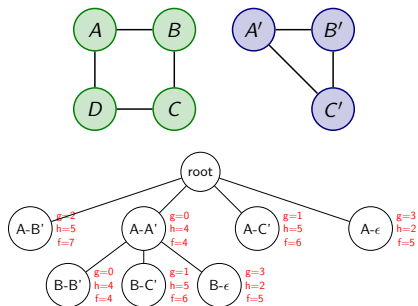
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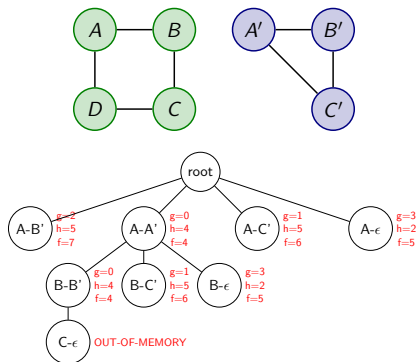
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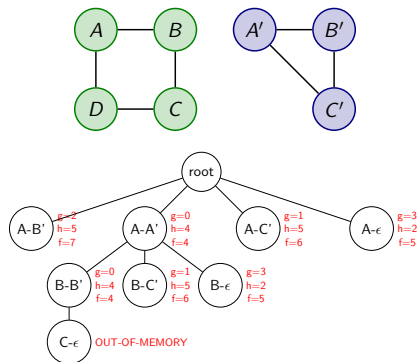
Performance Evaluation Metrics - Example



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Performance Evaluation Metrics - Example



- Out-of-memory.
- Unfeasible solution.
- # of explored nodes = 3.

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Use Case

■ Compared Methods:

Use Case

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Use Case

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■ Constraints:

- $C_T = 300$ seconds.

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■ Constraints:

- $C_T = 300$ seconds.
- $C_M = 1024$ MB.

Results - Comparing with Reference Answers

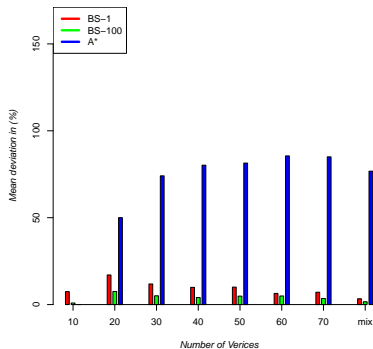


Figure: Deviation

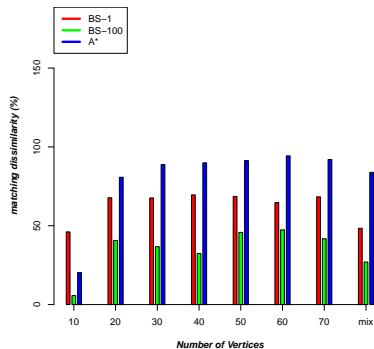


Figure: Matching Dissimilarity

The closer to 0, the better

Results - General Information

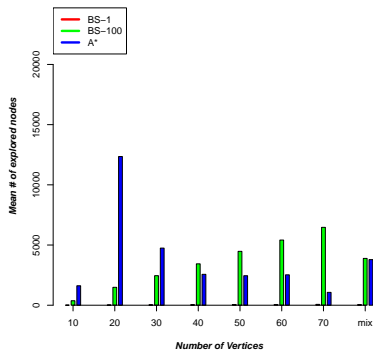


Figure: No of Explored Nodes

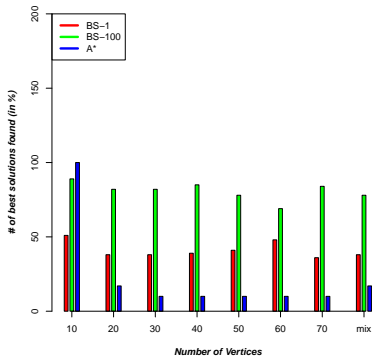


Figure: No of Best Found Solutions

Results - General Information

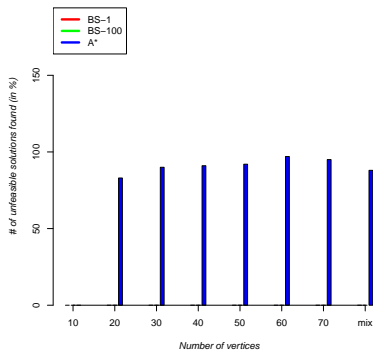


Figure: No of Unfeasible Solutions

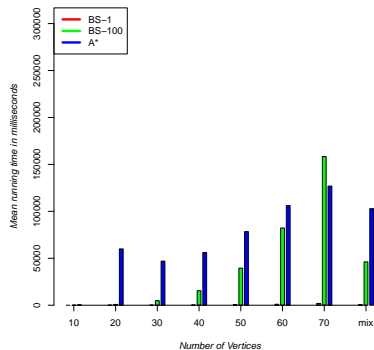


Figure: Running Time

Results - General Information

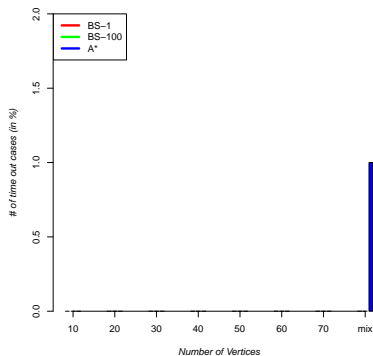


Figure: No of Time-Outs

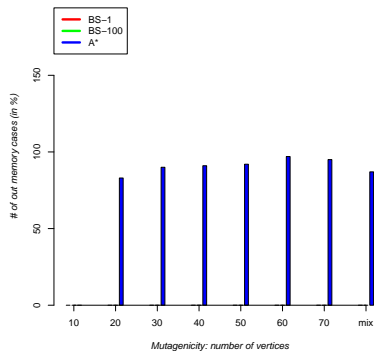
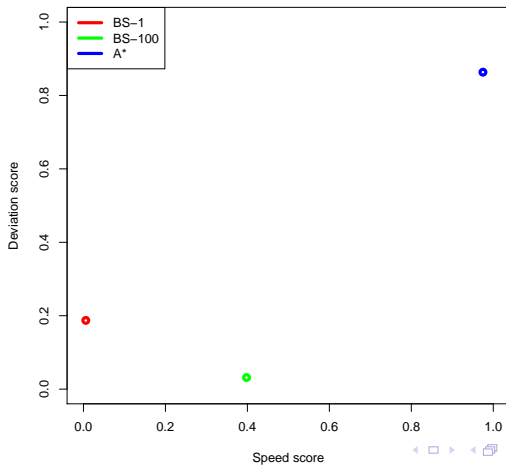


Figure: No of Memory-Outs

Results - Plot



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- **Additional low level annotation:**
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 - 6 methods (3 exact and 3 approximate).
 - Four databases (GREC, Mutagenicity, Protein and CMU).
 - **Scalability:** database decomposition.

Second Contribution

- **Performance evaluation metrics:**

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 - ★ Deviation.

Second Contribution

- **Performance evaluation metrics:**
 - Under time and memory constraints.
 - **Metrics:**
 - ★ Deviation.
 - ★ **Speed.**

Second Contribution

■ Performance evaluation metrics:

- Under time and memory constraints.
- **Metrics:**
 - ★ Deviation.
 - ★ Speed.
 - ★ Matching Dissimilarity.

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 - ★ Deviation-Running time plot.

Second Contribution

■ Performance evaluation metrics:

- Under time and memory constraints.
- **Metrics:**
 - ★ Deviation.
 - ★ Speed.
 - ★ Matching Dissimilarity.
 - ★ Deviation-Running time plot.
 - ★ **Number of optimal solutions.**

Perspectives

- Integrating better answers in the database (if found).

Perspectives

- Integrating better answers in the database (if found).
- Expanding this repository by integrating other publicly available databases.

