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Exact Computation of Graph Edit Distance for Uniform and Non-Uniform Metric Edit Costs

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Overview

- graph edit distance: flexible distance measure for labelled graphs
- supports uniform and non-uniform edit costs
- exact computation is NP-hard
- existing exact algorithms
  - A*-GED (Riesen, Fankhauser, and Bunke 2007)
  - BLP-GED (Lerouge et al. 2016)
  - DF-GED: node-based DFS, designed for non-uniform edit costs (Abu-Aisheh et al. 2015)
  - CSI_GED: edge-based DFS, supports uniform edit costs only (Gouda and Hassaan 2016)
- contributions
  (1) DF-GED^u: speed-up of DF-GED for uniform edit costs
  (2) CSI_GED^{nu}: generalised version of CSI_GED that supports non-uniform edit costs

Two Communities

- Pattern Recognition
- Database Technologies
  - a lot of work o graph edit distance exists
  - publications in venues such as VLDB, ICDE, SIGMOD, TKDE, CIKM
  - main focus: filtering and lower bounds
  - slightly different definitions
  - main difference: restriction on uniform edit costs

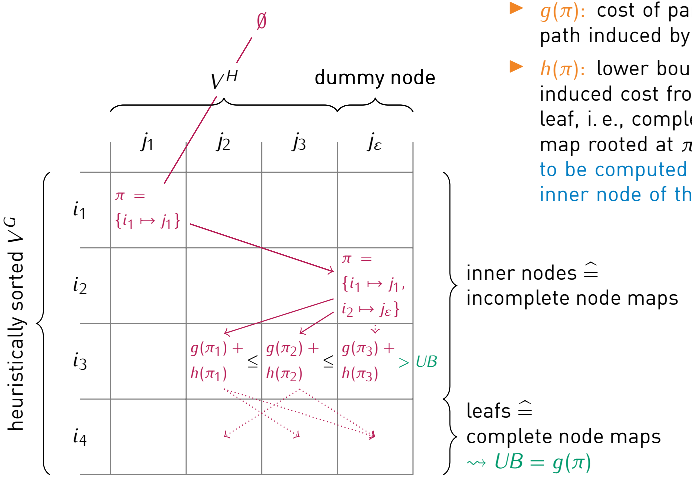
Graph Edit Distance

- labelled undirected graph: 4-tuple $G = (V^G, E^G, \ell_V^G, \ell_E^G)$
- label functions: $\ell_V^G : V^G \to \Sigma_V$ for nodes, $\ell_E^G : E^G \to \Sigma_E$ for edges
- edit path between G and H: sequence of edit operations starting at G and ending at $H' \simeq H$
- edit operations: deleting, inserting, relabelling
- edit costs: $c_V : \Sigma_V \times \Sigma_V \to \mathbb{R}$ for operations on nodes, $c_E : \Sigma_E \times \Sigma_E \to \mathbb{R}$ for operations on edges
- uniform edit costs: $c_V(\alpha, \beta), c_E(\alpha, \beta) = \begin{cases} 1 & \alpha \neq \beta \\ 0 & \alpha = \beta \end{cases}$
- graph edit distance $\lambda(G, H)$: minimum cost of edit path between G and H

Node Maps

- $V^{G+|H|}$: V^G plus $|V^H|$ isolated dummy nodes
- node map: injective partial function $\pi : V^{G+|H|} \rightarrow V^{H+|G|}$ with $V^G \subseteq dom(\pi)$ and $V^H \subseteq img(\pi)$
- edit path induced by node map: let $i \in V^G$, $k \in V^H$, $ij \in E^G$, $kl \in E^H$
  - $\pi(i) = k \rightsquigarrow$ change node label from $\ell_V^G(i)$ to $\ell_V^H(k)$
  - $\pi(i) = k_\varepsilon \rightsquigarrow$ delete node i
  - $\pi^{-1}(k) = i_\varepsilon \rightsquigarrow$ insert node k
  - $\pi(i)\pi(j) = kl \rightsquigarrow$ change edge label from $\ell_E^G(ij)$ to $\ell_E^H(kl)$
  - $\pi(i)\pi(j) \notin E^H \rightsquigarrow$ delete edge ij
  - $\pi^{-1}(k)\pi^{-1}(l) \notin E^G \rightsquigarrow$ insert edge kl
- alternative definition of $\lambda(G, H)$: minimum cost $g(\pi)$ of edit path induced by a node map π

DF-GED: Node-Based DFS



- $g(\pi)$: cost of partial edit path induced by π
- $h(\pi)$: lower bound for induced cost from π to a leaf, i. e., complete node map rooted at π $\rightsquigarrow$ has to be computed at each inner node of the DFS

Our Speed-Up DF-GED^u for Uniform Edit Costs

- $h(\pi)$: defined as $MLA(\overbrace{\ell_V^G(V^{G+|H|-\pi})}^{\text{multiset with unassigned labels from nodes in } V^{G+|H|}} \times \ell_V^H(V^{H+|G|-\pi}), c_V) + MLA(\underbrace{\ell_E^G(E^{G-\pi})}_{\text{multiset with unassigned labels from edges in } E^G} \times \ell_E^H(V^{H-\pi}), c_E)$
- computation for non-uniform edit costs requires cubic time

Lemma

For uniform edit costs, $h(\pi)$ can be computed in linear time.

1. at initialisation, sort node and edge labels
2. compute $MLA(A \times B, c)$ as $\Gamma(A, B) = \max\{|A|, |B|\} - |A \cap B|$

Valid Edge Maps (I)

- $\overrightarrow{E^G}$: one oriented edge (i, j) for each undirected $ij \in E^G$
- $\overleftrightarrow{E^H}$: both (k, l) and (l, k) for each $kl \in E^H$
- edge map: mapping $\phi : \overrightarrow{E^G} \to \overleftrightarrow{E^H} \cup \{e_\varepsilon\}$
- induces relation π_ϕ on $V^G \times V^H$: if $\phi(i, j) = (k, l)$, then $(i, k) \in \pi_\phi$ and $(j, l) \in \pi_\phi$
- valid edge map: ϕ is valid iff π_ϕ is partial injective function

Valid Edge Maps (II)

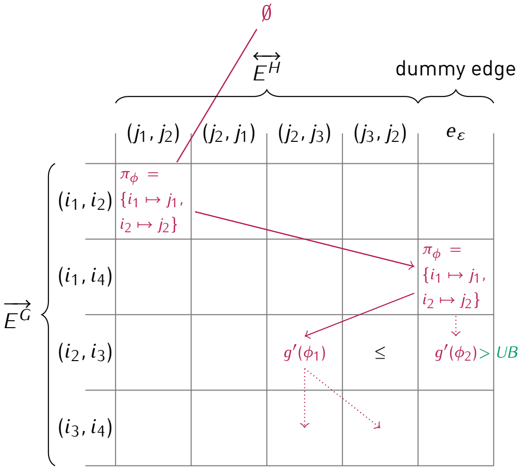
- partial edit path induced by valid edge map: let $i \in V^G$, $k \in V^H$, $(i,j) \in \overrightarrow{E^G}$, $(k,l),(l,k) \in \overleftrightarrow{E^H}$
  - $\phi(i,j) = (l,k) \rightsquigarrow$ change edge label from $\ell_E^G(ij)$ to $\ell_E^H(kl)$
  - $\phi(i,j) = e_\varepsilon \rightsquigarrow$ delete edge ij
  - $\phi^{-1}[\{(k,l),(l,k)\}] = \emptyset \rightsquigarrow$ insert edge kl
  - $\pi_\phi(i) = k \rightsquigarrow$ changed node label from $\ell_V^G(i)$ to $\ell_V^H(k)$

Theorem

$\lambda(G,H) = \min\{g(\phi) + \Gamma(V^{G-\pi_\phi}, V^{H-\pi_\phi}) \mid \phi \text{ is valid edge map}\}$ holds for uniform edit costs, where $g(\phi)$ is the cost of the partial edit path induced by edge map ϕ.

- can compute $\lambda(G,H)$ by traversing space of all valid edge maps

CSI_GED: Edge-Based DFS



- $g(\phi)$: cost of partial edit path induced by ϕ
- $g'(\phi)$: lower bound for induced cost of complete edge map rooted at ϕ

inner nodes $\widehat{=}$ incomplete edge maps

leafs $\widehat{=}$ complete edge maps
$\rightsquigarrow UB = g(\phi) + \Gamma(V^{G-\pi_\phi}, V^{H-\pi_\phi})$

Our Generalisation CSI_GED^{nu}

Theorem

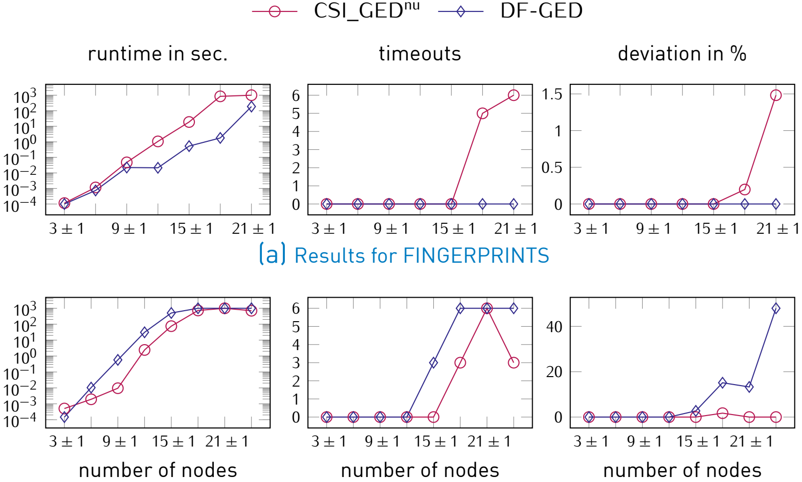
$\lambda(G,H) = \min\{g(\phi) + MLA(\ell_V^G(V^{G+|H|-\pi_\phi}) \times \ell_V^H(V^{H+|G|-\pi_\phi}), c_V) \mid \phi \text{ is valid edge map}\}$ holds for non-uniform metric edit costs.

- can use CSI_GED's DFS framework for non-uniform edit costs
- at leafs, use *MLA* instead of Γ to compute *UB*
- increased complexity at leafs (cubic instead of linear)
- no increased complexity at inner nodes of search tree

Setup

- used the datasets AIDS and FINGERPRINTS (Riesen and Bunke 2008)
- formed groups of size four containing graphs of fixed size and ran all algorithms for all pairs of graphs in one test group
- set time limit of 1000 seconds
- recorded the runtime, the number of timeouts, and the deviation of an algorithm's upper bound after 1000 seconds from the best upper bound

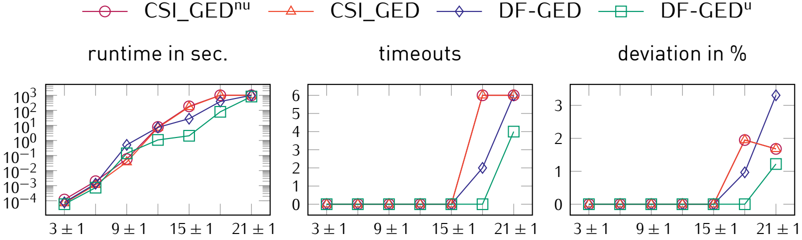
Results for Non-Uniform Metric Edit Costs



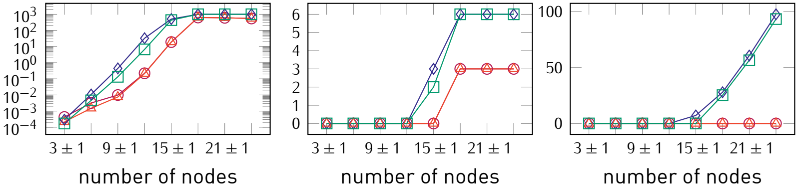
(a) Results for FINGERPRINTS

(b) Results for AIDS

Results for Uniform Edit Costs



(a) Results for FINGERPRINTS



(b) Results for AIDS

Upshot of the Results

- uniform edit costs
  - our speed-up DF-GED^u always outperforms DF-GED
  - CSI_GED and our generalisation CSI_GED^{nu} perform similarly
- general observation: no clear winner between node based and edge based algorithms
- FINGERPRINTS: DF-GED and DF-GED^u perform better
- AIDS: CSI_GED^{nu} and CSI_GED perform better
- CSI_GED and CSI_GED^{nu} are more stable than DF-GED and DF-GED^u: their deviation is small even if DF-GED and DF-GED^u perform better
- no prior knowledge about dataset and both uniform and non-uniform edit costs relevant $\rightsquigarrow$ CSI_GED^{nu} is algorithms of choice

Future Work

- individuate characteristics of datasets, for which the node based/edge based approaches perform better
- develop meta-algorithm based on these characteristics
- combine techniques from both communities in order to come up with significantly faster algorithm

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