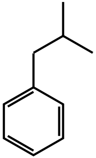
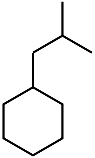
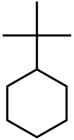
Measuring Change and Similarity of Graphs

Martin Grohe

Which of these graphs are most similar?

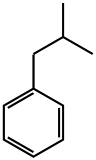




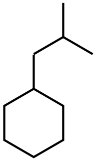


Which of these graphs are most similar ...

...when it comes to designing synthetic fuels?



Iso-Butylbenzene



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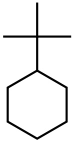

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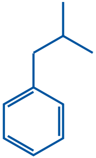

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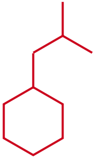

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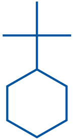

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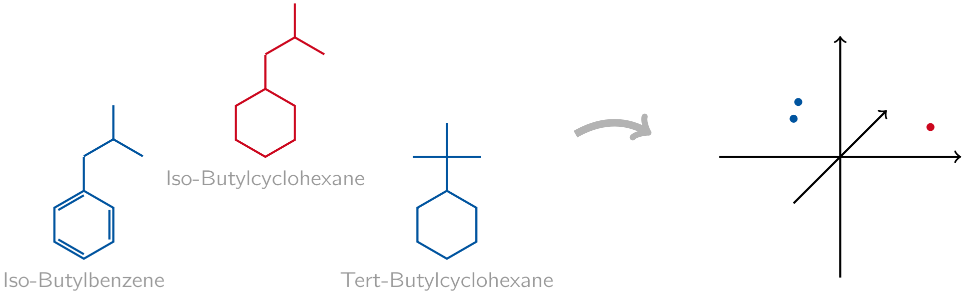

Schweidtmann, Rittig, König, G., Mitsos, Dahmen, *Energy and Fuels 2021*

Machine Learning on Graphs

- machine learning is based on the promise that similar objects should have similar properties
- what "similar" means depends on the properties we are interested in

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- could be measured by difference quotients

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distance between G and $\widetilde{G}$

class of all graphs

A graph metric is an isomorphism-invariant mapping $\delta : \mathscr{G} \times \mathscr{G} \to \mathbb{R}_{\geq 0}$ such that for all graphs G, H, I:

(i) $G \cong H \implies \delta(G, H) = 0$;

(ii) $\delta(G, H) = \delta(H, G)$;

(iii) $\delta(G, I) \leq \delta(G, H) + \delta(H, I)$.

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It would be more precise to speak of a graph pseudo metric, and only of a metric if the converse of (i) holds as well (but we don't).

Measuring Similarity

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Similarity measures can be derived from metrics by applying an anti-monotone function, for example,

$$\sigma(G,H) := \exp\bigl(-c\cdot\delta(G,H)\bigr)$$

for a graph metric δ and a constant $c>0$.

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Graph Edit Distance

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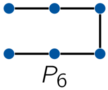
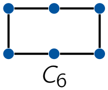
Examples





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   Then $\delta_{\mathrm{ed}}(P_n, C_n) = 1$.

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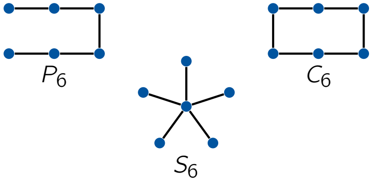

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   Then $\delta_{\mathrm{ed}}(P_n, C_n) = 1$.
2. S_n := star with $n-1$ tips.
   Then $\delta_{\mathrm{ed}}(S_n, C_n) = 2n-5$ and $\delta_{\mathrm{ed}}(S_n, P_n) = 2n-6$.

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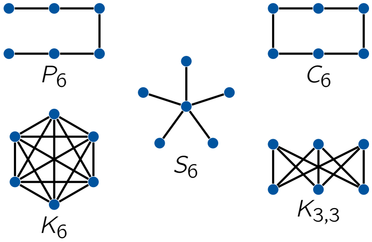

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3. K_n := complete graph on n vertices; $K_{\ell,m}$ complete bipartite graph with parts of size ℓ, m.
   Then $\delta_{\mathrm{ed}}(C_n, K_n) = \frac{n(n-3)}{2}$ and $\delta_{\mathrm{ed}}(K_n, K_{\frac{n}{2},\frac{n}{2}}) = \frac{n}{2}(\frac{n}{2}-1)$ if n is even.

Entrywise Norms

For a matrix $A = (A_{ij}) \in \mathbb{R}^{n \times n}$ and $p \geq 2$ we let

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Observation

$$\delta_{\mathrm{ed}}(G,H) = \frac{1}{2} \min_{\pi \in S_n} \left\| A_G^{\pi} - A_H \right\|_{(1)}$$

where

- *$A_G, A_H \in \{0,1\}^{n \times n}$ are the adjacency matrices of G, H;*
- *S_n is the set of all permutations of $[n]$;*
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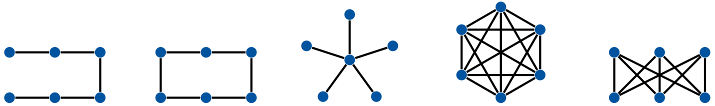

P_6 C_6 S_6 K_6 $K_{3,3}$

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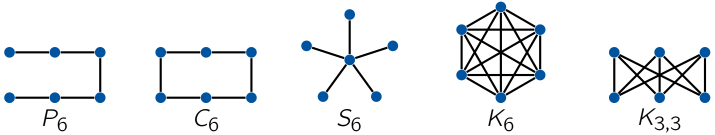

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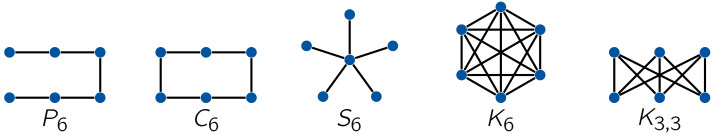

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Observation (Gervens, G. 2022)

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Remark

Another interesting graph metric is derived from the spectral norm:

$$\delta_{\mathrm{sp}}(G, H) := \min_{\pi \in S_n} \left\|A_G^\pi - A_H\right\|_2.$$

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$$\delta_\square(G,H) := \min_{\pi \in S_n} \max_{S,T \subseteq [n]} \Big| e_G(S,T) - e_H\big(\pi(S), \pi(T)\big) \Big|.$$

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Theorem (Lovász (?))

For random graphs $G, H \sim \mathcal{G}(n, \frac{1}{2})$, with high probability it holds that

$$\delta_\square(G,H) = O(n^{3/2}) \quad \textit{and} \quad \delta_{\mathrm{ed}}(G,H) = \Omega(n^2).$$

Cut Norm

For a matrix $A = (A_{ij}) \in \mathbb{R}^{n \times n}$ we let

$$\|A\|_{\square} := \max_{S,T \subseteq [n]} \left| \sum_{i \in S, j \in T} A(i,j) \right|.$$

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Observation

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Local Edit Distance via Matrix Norms

Cut Norm

For a matrix $A = (A_{ij}) \in \mathbb{R}^{n \times n}$ we let

$$\|A\|_\square := \max_{S,T \subseteq [n]} \left| \sum_{i \in S, j \in T} A(i,j) \right|.$$

Observation

$$\delta_\square(G,H) = \min_{\pi \in S_n} \left\| A_G^\pi - A_H \right\|_\square.$$

Theorem (Nikiforov 2009)

$$\frac{1}{n}\delta_\square(G,H) \leq \delta_{\mathrm{sp}}(G,H) \leq 2\sqrt{\delta_\square(G,H)}.$$

Observation

The metrics scale differently. Denoting the edgeless graph with n vertices by L_n, for all metrics δ considered so far we have

$$\delta(L_n, K_n) = \max\{\delta(G, H) \mid |G| = |H| = n\}.$$

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Furthermore,

$$2\delta_{\mathrm{ed}}(L_n, K_n) = \delta_{\square}(G, H) = n(n-1) \sim n^2,$$
$$\delta_{\mathrm{led}}(L_n, K_n) = \delta_{\mathrm{sp}}(G, H) = n - 1 \sim n.$$

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Normalised Metrics

$$\widehat{\delta_{\mathrm{ed}}}(G,H) := \frac{2}{n^2}\delta_{\mathrm{ed}}(G,H), \qquad \widehat{\delta_{\square}}(G,H) := \frac{1}{n^2}\delta(G,H),$$
$$\widehat{\delta_{\mathrm{led}}}(G,H) := \frac{1}{n}\delta_{\mathrm{ed}}(G,H), \qquad \widehat{\delta_{\mathrm{sp}}}(G,H) := \frac{1}{n}\delta_{\mathrm{sp}}(G,H).$$

Example

$$\widehat{\delta_{\mathrm{ed}}}(S_n, C_n) = \frac{2(2n-5)}{n^2} \xrightarrow[n\to\infty]{} 0 \qquad \text{and} \qquad \widehat{\delta_{\mathrm{led}}}(S_n, C_n) = \frac{n-3}{n} \xrightarrow[n\to\infty]{} 1.$$

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Corollary

For random graphs $G, H \sim \mathscr{G}(n, \frac{1}{2})$, with high probability it holds that

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Relations Between the Normalised Metrics

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Corollary

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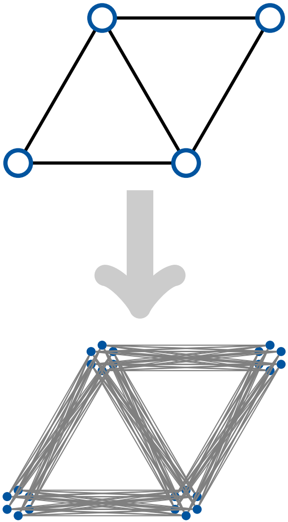

Comparing Graphs of Distinct Sizes

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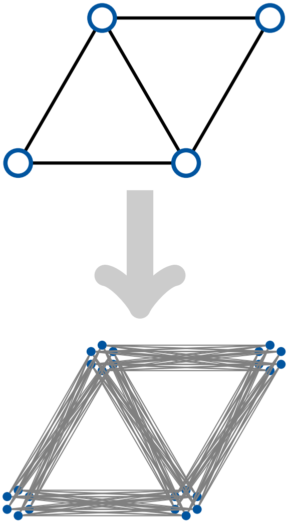


Blow-up Distance

For every normalised metric $\widetilde{\delta}$ and graphs G, H of order $m := |G|, n := |H|$ we define

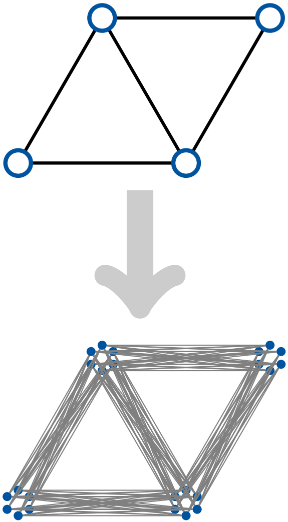
$$\delta^{\text{💣}}(G,H) := \lim_{\ell \to \infty} \widetilde{\delta}(G^{\text{💣}n\ell}, H^{\text{💣}m\ell}).$$

Comparing Graphs of Distinct Sizes

The Blow-up Construction

$G^{\text{💣}k}$ obtained from G by

- replacing each node by a set of k nodes;
- replacing each edge by a complete bipartite graph.



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Remark

There is an alternative way of defining the blow-up distances through an optimal transport formulation.

Observation

Let δ be one of the metrics considered so far.

1. *For all graphs G and $k \geq 1$ we have $\delta^{\text{💣}}(G, G^{\text{💣}k}) = 0$.*

Properties of the Blow-up Distances

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1. *For all graphs G and $k \geq 1$ we have $\delta^{💣}(G, G^{💣k}) = 0$.*
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Furthermore, there are example of graphs where the inequality is strict.

Theorem (Borgs et al. 2008, Pikhurko 2010)

For all graphs G, H of the same order we have

$$\delta^{\bullet}_{\mathrm{ed}}(G,H) \geq \frac{1}{3}\widehat{\delta_{\mathrm{ed}}}(G,H) \qquad \textit{and} \qquad \delta^{\bullet}_{\square}(G,H) \geq \left(\frac{\widehat{\delta_{\square}}(G,H)}{32}\right)^{67}.$$

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$$\delta_\eta(G, H) := \|\eta(G) - \eta(H)\|_{\mathbb{H}} = \sqrt{\left\langle \eta(G) - \eta(H), \eta(G) - \eta(H) \right\rangle_{\mathbb{H}}}.$$

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$\eta : \mathcal{G} \to \mathbb{R}^k$ mapping G to the k largest eigenvalues of its adjacency matrix A_G in decreasing order.

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Idea

Define vector embedding in such a way that the geometry of the latent space has a semantic meaning on the space of graphs.

Example (Subgraph Embeddings)

For graphs $F_1, \ldots, F_k$, we define a vector embedding $\mathsf{sub}_{F_1,\ldots,F_k} : \mathscr{G} \to \mathbb{R}^k$ by

$$\mathsf{Sub}_{F_1,\ldots,F_k}(G) := \big(\mathsf{sub}(F_1, G), \ldots, \mathsf{sub}(F_k, G)\big),$$

where $\mathsf{sub}(F, G)$ is the number of subgraphs of G isomorphic to F.

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Example (Logic Embeddings)

For formulas $\varphi_1, \dots, \varphi_k$ of some logic on graphs (say, first-order logic), we define a vector embedding $\mathbf{mod}_{\varphi_1,\dots,\varphi_k} : \mathcal{G} \to \mathbb{R}^k$ by

$$\mathsf{Mod}_{\varphi_1,\dots,\varphi_k}(G) := (b_1, \dots, b_k),$$

where $b_i = 1$ if $G \models \varphi_i$ and $b_i = 0$ otherwise.

A graph kernel is a function $\kappa : \mathcal{G} \times \mathcal{G} \to \mathbb{R}$ such that

- $\kappa(G, H) = \kappa(H, G)$ for all graphs G, H;
- for all graphs $G_1, \ldots, G_n$, the $(n \times n)$-matrix K with entries $K_{ij} := \kappa(G_i, G_j)$ is positive semi-definite.

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Theorem (Folklore)

Let κ be a graph kernel. Then there is a vector embedding $\eta : \mathscr{G} \to \mathbb{H}$ such that

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Example

Weisfeiler-Leman kernels (Shervashidze et al., 2009) are efficiently computable without ever explicitly computing the vector embedding into the infinite dimensional latent space.

Counting Homomorphisms

A homomorphism between graphs is a mapping between the vertices that preserves adjacency.

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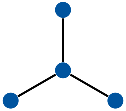
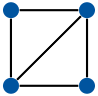
Example





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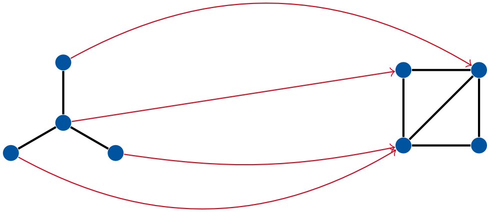

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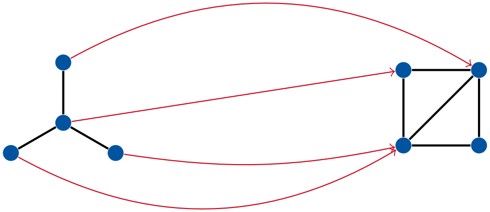

For all graphs F, G of orders $k := |F|, n := |G|$:

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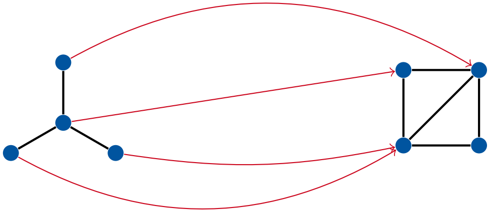

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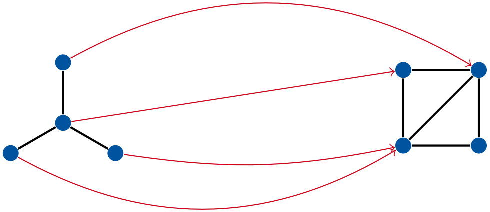

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where h is mapping from $V(F)$ to $V(G)$ chosen uniformly at random.

For every class $\mathscr{F}$ of graphs, we define a vector embedding $\mathsf{Hd}_{\mathscr{F}} : \mathscr{G} \to \mathbb{R}^{\mathscr{F}}$ by

$$\mathsf{Hd}_{\mathscr{F}}(G) := \big(\mathsf{hd}(F, G)\big)_{F \in \mathscr{F}}.$$

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It gives us the (normalised) graph metric

$$\delta_{\mathscr{F}}(G,H) = \sqrt{\sum_{k \in \mathbb{N}} \frac{1}{2^k |\mathscr{F}_k|} \sum_{F \in \mathscr{F}_k} \big(\mathrm{hd}(F,G) - \mathrm{hd}(F,H)\big)^2},$$

where $\mathscr{F}_k$ is the set of graphs of order k in $\mathscr{F}$.

Operational View

Two graphs are similar if they can easily be transformed into each other.

Examples

edit distance, all distances based on matrix norms

Advantage:

gives an alignment between graphs

Two Sides of Similarity

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Question: How do these relate?

Comparing the Topologies (Definitions)

Let δ, δ' be graph metrics. We say that δ is coarser than δ' (we write $\delta \sqsubseteq \delta'$) if for all $\epsilon > 0$ there is an $\epsilon' > 0$ such that

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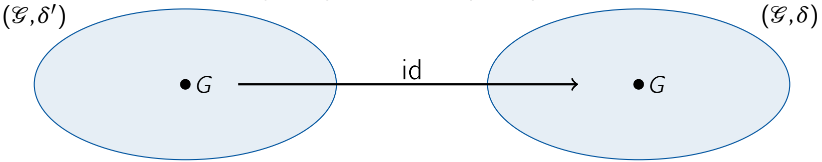

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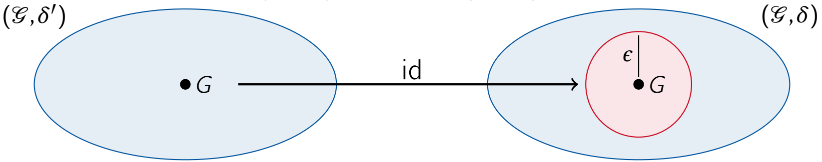

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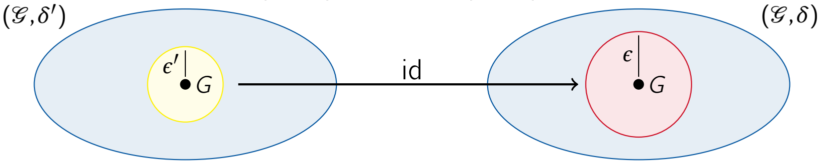

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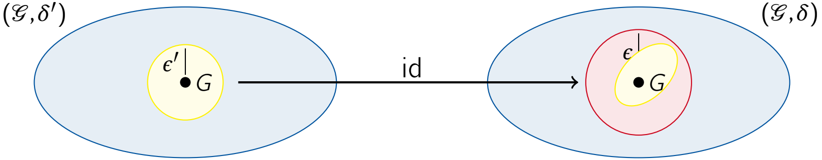

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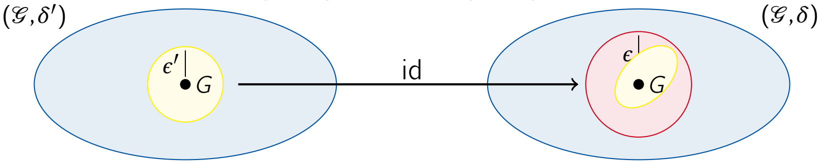

Moreover, δ and δ' are topologically equivalent (we write $\delta' \equiv \delta$) if $\delta \sqsubseteq \delta'$ and $\delta' \sqsubseteq \delta$, and δ is strictly coarser than δ' (we write $\delta \sqsubset \delta'$) if $\delta \sqsubseteq \delta'$ and $\delta' \not\sqsubseteq \delta$.

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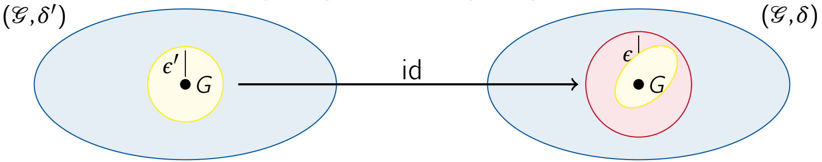

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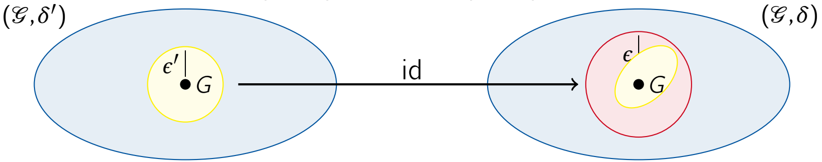

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Moreover, $\delta \equiv \delta'$ if and only if δ and δ' define the same topology on $\mathscr{G}$.

Comparing the Topologies (Results)

Graph Metrics Based on Matrix Norms

$$\delta^{\Bomb}_{\square} \equiv \delta^{\Bomb}_{\mathrm{sp}} \sqsubset \delta^{\Bomb}_{\mathrm{ed}} \sqsubset \delta^{\Bomb}_{\mathrm{led}}.$$

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Theorem (Borgs et al. 2008)

$$\delta^{\faBomb}_{\square} \equiv \delta_{\mathscr{G}}.$$

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Computing δ_{ed},δ_{led},δ_{sp} is NP-complete even if both input graphs are trees.

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Remarks

- Various other hardness results are known. In particular, the distances are also hard to approximate.

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Remarks

- Various other hardness results are known. In particular, the distances are also hard to approximate.
- The problem of computing the distances is closely related to the notoriously hard quadratic assignment problem from combinatorial optimisation.

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Theorem

δ^*_{ed}, δ^*_{led}, δ^*_{sp} *can be computed in polynomial time.*

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Theorem (Böker 2021, Grebík and Rocha 2022)

$$\delta_{\mathrm{sp}}^{*} \quad \equiv \quad \delta_{\square}^{*} \quad \equiv \quad \delta_{\mathscr{T}}\,.$$

Learned Embeddings

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Theorem (Böker et al. 2023)

1. *Let δ be a bounded graph metric computed by a GNN. Then $\delta \sqsubseteq \delta_{\mathscr{T}}$.*
2. *For every n there is a graph metric $\delta^{(n)}$ computed by a GNN such that $\delta^{(n)} \equiv \delta_{\mathscr{T}}$ on graphs of order at most n.*

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Concluding Remarks

- Matrix norms and homomorphism counts give principled ways to define graph metrics, and there are deep and interesting connections between them.
- There are other natural ways of defining graph metrics, most notably by viewing graphs as finite metric spaces and using notions from discrete geometry (e.g. Gromov-Wasserstein metric).

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- The normalisation we chose is tailored towards dense graphs. Under our normalised metrics, all sparse graphs are close to the empty graph.

  There is no fully developed theory for sparse graphs.

Further Reading

Most of the material of this talk is covered in the following article.

Grohe, M. (2024). Some Thoughts on Graph Similarity.
arXiv:2411.10182