

Comparing heuristics for graph edit distance computation

D. B. Blumenthal^{1, 2, ✉}, N. Boria³, J. Gamper¹, S. Bougleux³, L. Brun³

¹Free University of Bozen-Bolzano, Faculty of Computer Science, Bolzano, Italy

²Technical University of Munich, Chair of Experimental Bioinformatics, Freising, Germany

³Normandie Université, UNICAEN, ENSICAEN, CNRS, GREYC, Caen, France

✉ david.blumenthal@wzw.tum.de, david.blumenthal@inf.unibz.it

<https://github.com/dbblumenthal/gedlib>

GRAPH EDIT DISTANCE (DEFINITION)

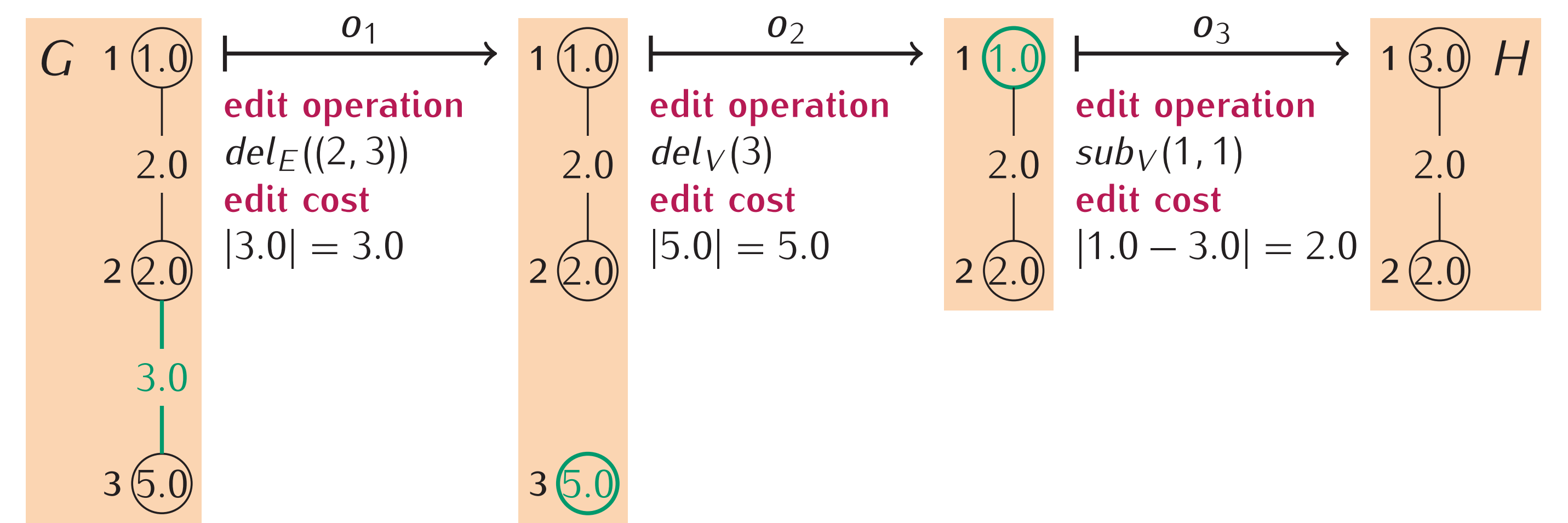
- **GED**(G, H) := $\min\{c(P) \mid P \text{ edit path between } G \text{ and } H\}$
- **labeled graphs**: $G = (V^G, E^G, \ell_V^G, \ell_E^G)$ and $H = (V^H, E^H, \ell_V^H, \ell_E^H)$
- **labeling functions**: $\ell_V^G : V^G \rightarrow \Sigma_V$ and $\ell_E^G : E^G \rightarrow \Sigma_E$
- **node and edge label spaces**: Σ_V and Σ_E
- **edit path**: edit operation sequence $P = (o_1, \dots, o_r)$ transforms G into H
- **edit operations and edit costs** ($i \in V^G, k \in V^H, (i, j) \in V^G, (k, l) \in E^H$):

node edit op.	edit cost	edge edit op.	edit cost
$sub_V(i, k)$	$c_V(\ell_V^G(i), \ell_V^H(k))$	$sub_E((i, j), (k, l))$	$c_E(\ell_E^G(i, j), \ell_E^H(k, l))$
$del_V(i)$	$c_V(\ell_V^G(i), \epsilon)$	$del_E((i, j))$	$c_E(\ell_E^G(i, j), \epsilon)$
$ins_V(k)$	$c_V(\epsilon, \ell_V^H(k))$	$ins_E((k, l))$	$c_E(\epsilon, \ell_E^H(k, l))$

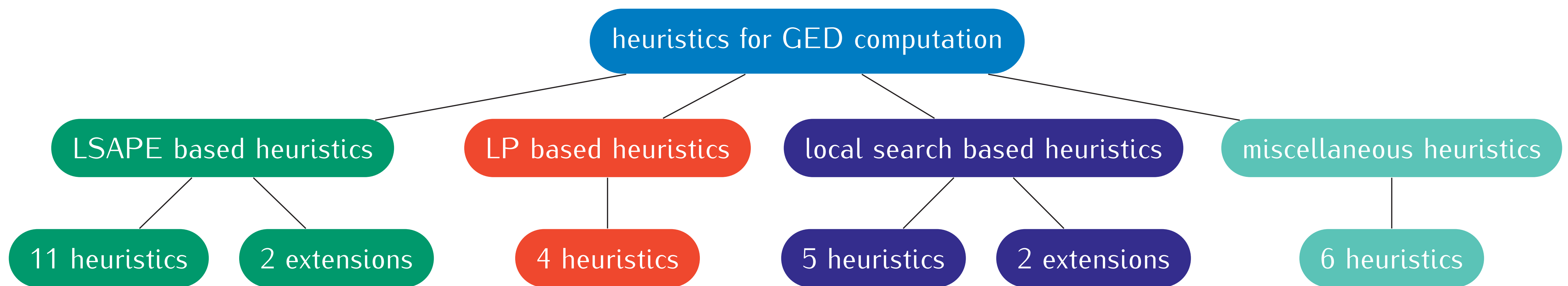
- **edit path cost**: $c(P) = \sum_{i=1}^r c(o_i)$

GRAPH EDIT DISTANCE (EXAMPLE)

- **node and edge label spaces**: $\Sigma_V = \Sigma_E = \mathbb{R}_{\geq 0}$
- **sub. costs**: $c_V(\alpha, \beta) = c_E(\alpha, \beta) = |\alpha - \beta|$
- **del. and ins. costs**: $c_V(\alpha, \epsilon) = c_V(\epsilon, \alpha) = c_E(\alpha, \epsilon) = c_E(\epsilon, \alpha) = |\alpha|$
- **edit path cost**: $c(P) = c(o_1) + c(o_2) + c(o_3) = 3.0 + 5.0 + 2.0 = 10.0$



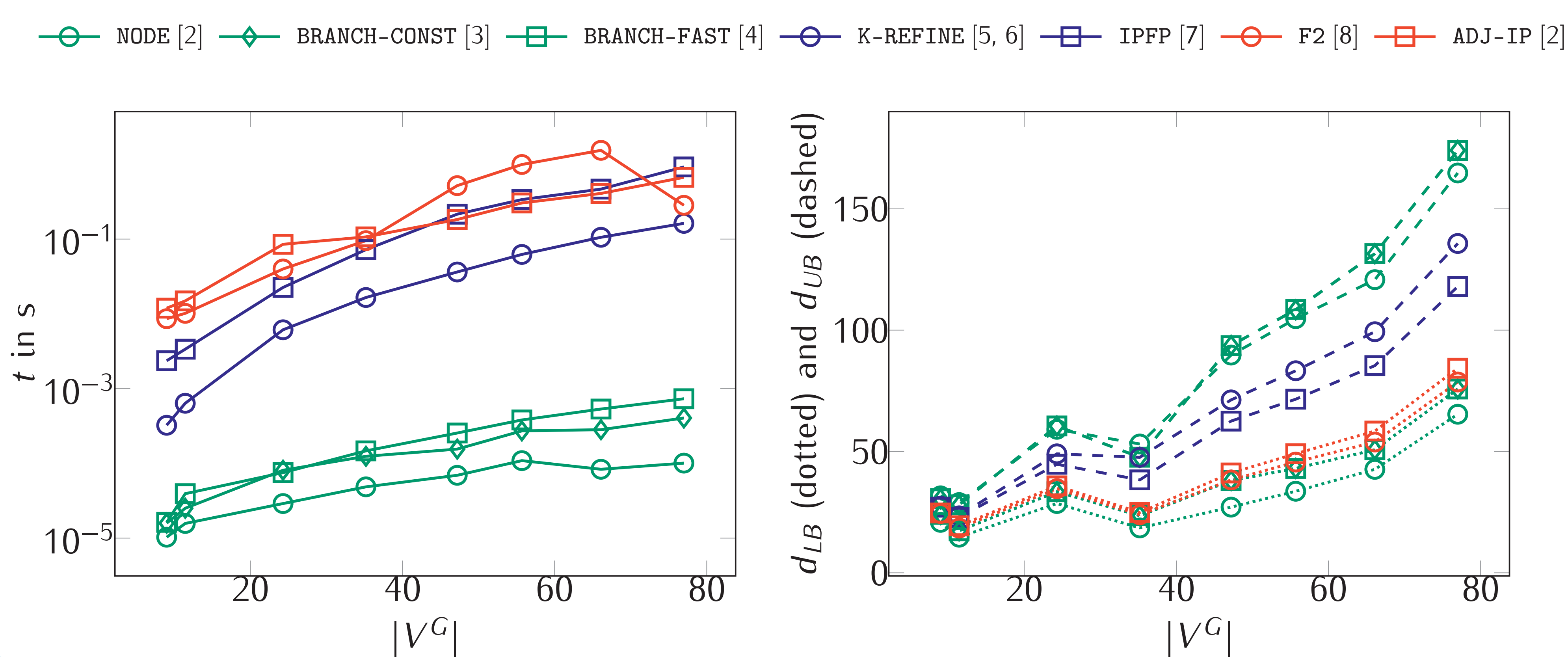
SUGGESTED TAXONOMY AND COMPARED HEURISTICS



EXPERIMENTAL SETUP

- **datasets**: 6 widely used benchmark datasets from IAM Graph Database Repository [1]
- **implementation**: to ensure comparability, all heuristics were re-implemented in C++
- **metrics**: runtime t , lower and upper bounds d_{LB} and d_{UB} , and classification coefficients c_{LB} and c_{UB}

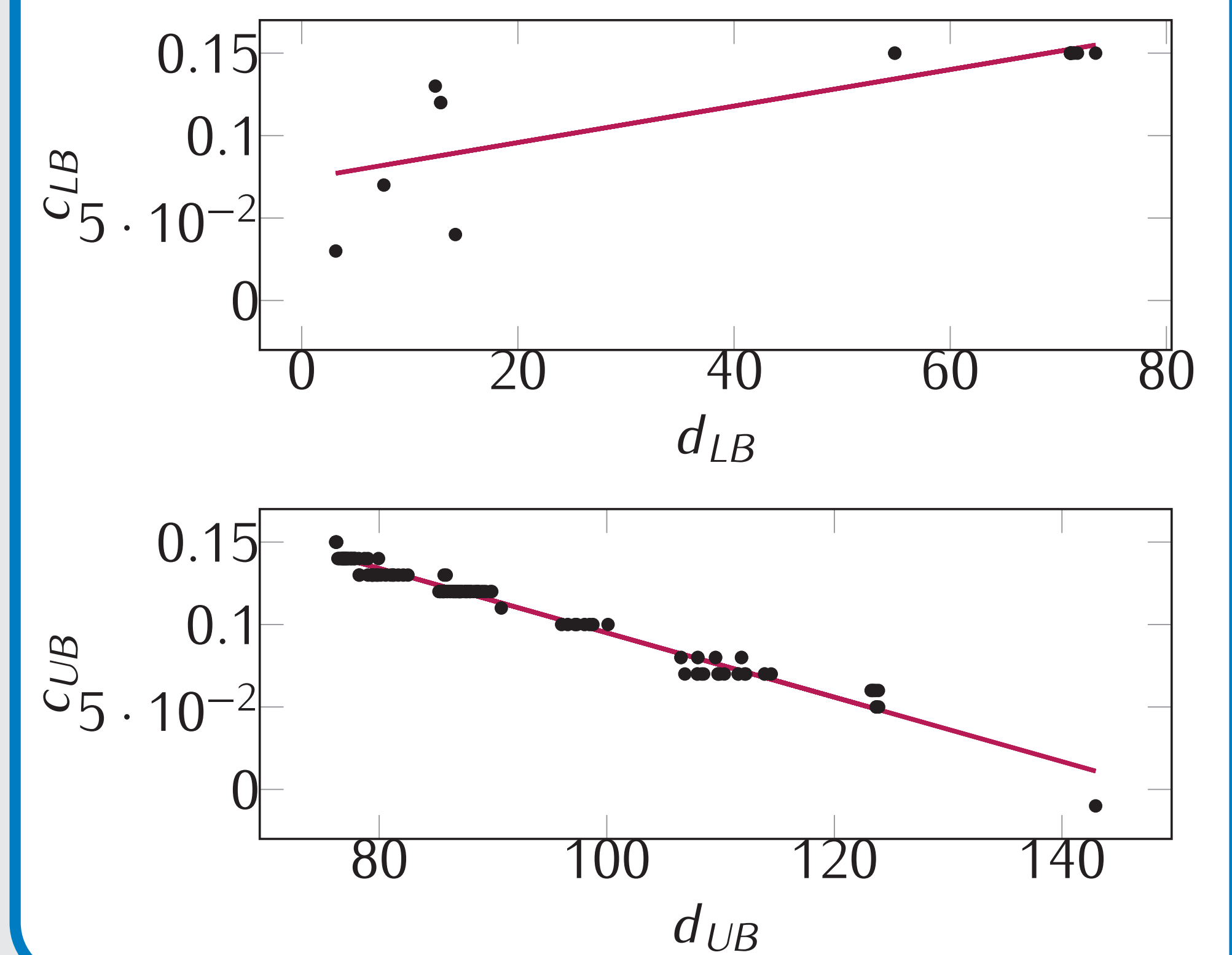
RUNTIMES AND BOUNDS OF GLOBALLY BEST HEURISTICS



MAIN INSIGHTS

- **tightness of lower bound critical**: use **LP based heuristic** F2 [8] or ADJ-IP [2]
- **tightness of upper bound critical**: use **local search based heuristic** IPFP [7] or K-REFINE [5, 6]
- **runtime critical**: use **LSAPE based heuristic** NODE [2], BRANCH-CONST [3], or BRANCH-FAST [4]
- **stability w. r. t. graph size**: ordering of heuristics w. r. t. tightness is independent of graph size
- **confirmed hypothesis**: tight bounds exhibit better classification coefficients than loose bounds
- **gap between best lower and upper bounds**: only grows moderately with increasing graph size

BOUNDS VS. CLASSIF. COEFF.



REFERENCES

- [1] K. Riesen and H. Bunke, "IAM graph database repository for graph based pattern recognition and machine learning," in *S+SSPR*, 2008, pp. 287–297.
- [2] D. Justice and A. Hero, "A binary linear programming formulation of the graph edit distance," *TPAMI*, vol. 28, no. 8, pp. 1200–1214, 2006.
- [3] W. Zheng, L. Zou, *et al.*, "Efficient graph similarity search over large graph databases," *TKDE*, vol. 27, no. 4, pp. 964–978, 2015.
- [4] D. B. Blumenthal and J. Gamper, "Improved lower bounds for graph edit distance," *TKDE*, vol. 30, no. 3, pp. 503–516, 2018.
- [5] Z. Zeng, A. K. H. Tung, *et al.*, "Comparing stars: On approximating graph edit distance," *PVLDB*, vol. 2, no. 1, pp. 25–36, 2009.
- [6] N. Boria, D. B. Blumenthal, *et al.*, "Improved local search for graph edit distance," 2019. arXiv: 1907.02929 [cs.DS].
- [7] S. Bougleux, B. Gaüzère, *et al.*, "Graph edit distance as a quadratic program," in *ICPR*, 2016, pp. 1701–1706.
- [8] J. Lerouge, Z. Abu-Aisheh, *et al.*, "New binary linear programming formulation to compute the graph edit distance," *PR*, vol. 72, pp. 254–265, 2017.